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Determining Detailed Reaction Kinetics for Nitrogen-and Oxygen-Containing Fuels

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DETERMINING DETAILED REACTION KINETICS FOR NITROGEN- AND OXYGEN-CONTAINING FUELS

A Dissertation Presented

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DEDICATION

For my dad, who made me realize I wanted to be a chemical engineer.

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ABSTRACT

DETERMINING DETAILED REACTION KINETICS FOR NITROGEN- AND OXYGEN-CONTAINING FUELS

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With the emergence of new biorenewable transportation fuels, the role of heteroatoms in combustion has increased tremendously. While petroleum-based fuels are primarily hydrocarbons, many biorenewable fuels contain heteroatoms such as oxygen and nitrogen, introducing new challenges associated with toxic emissions. A fundamental understanding of the chemical kinetics of combustion of these heteroatomic fuels is necessary to elucidate the pathways by which these toxic emissions are formed and may be achieved through the development of combustion models. Reaction sets, the core of these combustion models, may be assembled for individual fuels through a balance of employing vetted rate constants from prior publications, quantum chemistry calculations, and rate constant estimations. For accuracy, reaction sets should be tested against experimental combustion studies such as low-pressure flame experiments using molecular-beam mass spectrometry (MBMS) or chemiluminescence and high-pressure shock-tube experiments.

This dissertation presents the development of a new reaction set to describe gas-phase combustion chemistry of fuels containing only hydrogen, carbon, oxygen, and

nitrogen. The foundation of this model was a reaction set to describe combustion of ammonia flames. This reaction set contains only H/N/O chemistry for simplicity. The new reaction set was tested against a pyrolysis shock-tube study, as well as 12 MBMS flame experiments under a variety of conditions, including different mixtures of fuels and oxidizers (NH_3, N_2O, H_2, NO, O_2), fuel equivalence ratios (lean to rich), pressures, and concentrations of diluent gas. Additionally, the base H/N/O mechanism was expanded to include carbon chemistry and was tested against flames of dimethylamine, ethylamine, and a methane/ammonia mixture.

This reaction set was employed to study heterocyclic biofuels including a fuel-rich flame of tetrahydropyran, the monoether analogue to cyclohexane and the basic ring in cellulose. Additionally, the model was used in a study of morpholine, a 6-membered ring with both ether and amine functionalities, testing the model against fuel-rich flame studies using both MBMS and chemiluminescence techniques and high-pressure shock-tube studies for both oxidation and pyrolysis at elevated temperatures and pressures. Lastly, the model was used to study the combustion of hypergolic rocket fuels, specifically monomethyl hydrazine and tetramethylethyldiamine with red fuming nitric acid.

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CHAPTER 1

INTRODUCTION AND BACKGROUND

Combustion is a highly important chemical process by which society is able to obtain the energy necessary to perform everyday tasks in daily life routines such as running automobiles, heating homes, providing electricity to power appliances, and cooking food. The fuels of choice for these processes in the past century have been dominated by fossil fuels, primarily because of their high energy density and portability. Oil has been a particularly attractive fuel source given it is a liquid fuel, which is ideal for storage and use. Due to their extensive use and the fact that they are non-renewable, however, fossil-fuel supplies have been waning and access to oil has become a sensitive matter in world politics and economic stability. As a result, there has been a recent push for the advancement of biofuels and other alternative fuel sources to fossil fuels.

1.1 Biofuels

Like many fashionable ideas, biofuels are just a recycled idea from the past, reinvented for modern times. In 1890, a young inventor named Rudolf Diesel moved to Berlin, Germany, and began work developing a new engine from the foundation of his work on an engine he developed to run on ammonia vapor. This new engine, based on the Carnot Cycle, was first published in 1893 and became what today is known as the Diesel engine [1]. This new engine was presented at the Exposition Universelle in Paris, France, in 1900 and ran not on fossil fuels, but peanut oil [2]. Just a few years later in 1908, the Henry Ford Motor Company began production on what is now probably their most famous car, the Ford Model T. This car was designed to run on gasoline or kerosene, but it also had the ability to run on ethanol with the American farmer in mind so that they

could run the automobile without purchasing fuel [3]. Petroleum-derived fuels dominated transportation fuels and were plentiful and inexpensive at the time, and thus interest in renewable engine fuels dwindled until recently.

In the United States, the primary source of energy consumption switched from renewable timber sources to fossil fuels at the start of the 20th century. Since then, U.S. energy consumption has been dominated by fossil fuels. The US Annual Energy Review estimates that sources of energy consumption may be broken down as 82.9% fossil fuels, 8.8% nuclear power, and 8.2% renewable energy sources. Of the fossil-fuel consumption, 45.0% came from crude oil, 29.8% from natural gas, and 25.2% from coal [4]. Dependence on fossil fuels has its consequences. One such concern is that fossil fuels are limited, non-renewable resources. Another major concern is the environmental impact of using fossil fuels. By burning fossil fuels, CO_2 is emitted, which is well known as a greenhouse gas contributor and is considered a major contributor to global warming [5]. Hydrocarbon fuels have a propensity for soot formation [6], and some fossil fuels are known to contain traces of dangerous pollutants. For example, U.S.-mined coal has been found to have up to a 1.8 ppm concentration of mercury [7].

To address some of the concerns from petroleum-based fuels, several new biorenewable fuels have been put into production. Biofuels that have been in use to date have primarily been alcohols and biodiesel. Biodiesel is vegetable oil esterified with alcohols to lower the viscosity and raise the volatility of vegetable oil to be close to the properties of diesel fuel for use in diesel engines [8]. However, alcohols such as ethanol have been the predominant biofuel of choice, produced through fermentation of sugars from plant resources such as corn and sugar cane, which is then further distilled to

produce ethanol. Ethanol production has dominated US biofuel production primarily because it uses existing technology that has been used for years in the brewing industry [9]. Unfortunately, ethanol production today relies heavily on using food sources as a main feed stock, potentially raising food costs with increased production. Studies question whether ethanol from corn is environmentally beneficial, considering the amount of water needed for ethanol production, forest areas being cleared for crop space, and soil contamination [10].

Biofuels are considered to be more carbon-neutral in many cases, and they can reduce emissions of aromatic hydrocarbons and soot, addressing some of the concerns about traditional fossil fuels. However, carbonyl pollutants like aldehydes may be formed by biofuel combustion [11-13]. Oxygenate functional groups, as seen in biomass-derived fuels, have already proven to lead to potential pollutants [14, 15-25] and have been addressed in relation to alternative transportation fuels such as alcohols, ethers, and esters. Other hazardous emissions may also result from biofuel combustion, varying from fuel to fuel due to chemical structure differences. The effect of particular functional groups in biofuels has been investigated recently due to the increased use of biofuels [14].

Across the wide variety of new biofuels available now, the chemical composition of biofuels can greatly vary. Biomass has a high fraction of fuel-bound oxygen [26-28] and fuel-bound nitrogen in different concentrations and functional forms [29-33]. For example, woody biomass has been found to have 0.6-9.0 wt% nitrogen and 30-50 wt% oxygen [26]. Nitrogen content may be found higher in biomass, bound in proteins, free amino acids, nucleic acids, alkaloids, inorganic compounds, and chlorophyll [31].

Various agricultural biomass fuels were also compared in devolatilization experiments equipped with FTIR and were found to have higher than expected HCN yields [30].

The fuel-nitrogen functions of biofuels are a major source of NO_x emissions [26, 34-35], and are being addressed accordingly. Studies of fuel-nitrogen conversion, mostly in relation to coal combustion, accept that NH_3 and HCN are the major precursors to NO_x production. Mechanisms for their oxidation have been proposed [34, 36-40]. Although it is believed that the pathways for fuel-nitrogen conversion in biomass differ from the pathways in coal (which are predominantly through HCN), amines in proteins of biomass have been found to supply the NO_x precursor NH_3 [41-42]. In a pyrolysis study of several biomass representatives used in co-firing, several oxygen- and nitrogen-containing products were observed by GC-MS, including N_2, HCN, NO, HNCO, N_2O, NO_2, and C_2N_2 [43].

In addition to these pyrolysis studies of the fate of typical nitrogenous structures in biomass, reactions under combustion conditions need further investigation. Combustion models can aid in capturing important features of the conversion of the important small nitrogen compounds under realistic conditions [27, 44] and to understand the detailed reaction sequences in flames of individual nitrogen-containing fuels representative of typical structures.

1.2 Combustion chemistry

A fundamental understanding of combustion chemistry is necessary in order to predict how switching to biofuels could potentially affect combustion, particularly with regard to fuel performance, pollutant formation, and environmental impacts. Starting from the broadest definition, combustion is defined as "any relatively fast exothermic

gas-phase chemical reaction" by Fristrom and Westenberg [45]. From this broad definition, combustion can be further classified into different types of combustion based on their physical characteristics. For example, combustion can be classified by flow as either laminar or turbulent combustion.

Another classification in combustion is based upon fuel equivalence ratio, Φ, which describes the ratio of fuel to oxygen relative to that of a stoichiometric mixture:

$$\Phi = \frac{(\text{moles fuel / moles oxygen})_{\text{actual}}}{(\text{moles fuel / moles oxygen})_{\text{stoichiometric}}} \tag{1.1}$$

A stoichiometric mixture is defined as a mixture with the exact ratio of fuel to oxygen needed such that all fuel is converted into H_2O, CO_2, and N_2. In this case, fuel equivalence ratio is 1. In cases where fuel equivalence ratio is less than 1, combustion is described as fuel-lean. In cases where fuel equivalence ratio is greater than 1, combustion is described as fuel-rich.

Combustion chemistry behaves differently as fuel equivalence ratio changes from fuel-lean to fuel-rich. The following is a discussion on the chemistry of combustion under these different conditions.

1.2.1 Combustion chemistry in the fuel-lean limit

At fuel-lean conditions, there is more oxygen than needed for complete conversion of fuel to H_2O, CO_2 and N_2 products. Often in practical conditions, engines are run under very lean conditions to reduce emissions of soot and carbon monoxides. In other cases, pockets of lean combustion may be found in engines where uneven mixing is involved. Lastly, even in premixed systems, combustion occurs under the most lean conditions, determining the chemistry of ignition. In these cases where there is an

abundance of oxygen present and often the mixtures are at low temperatures, combustion is dominated by QOOH chemistry until a radical pool is established to maintain combustion.

The first step in QOOH chemistry, which is outlined in Fig. 1 and described in [46], is the breaking of a bond in the fuel molecule. Energy from an external source such as a spark from a spark plug allows a dissociation reaction to occur, homolytically cleaving a bond to leave two radical species. For example, a fuel such as ethanol could, with enough energy, thermally dissociate to form an ethanol radical and an H-atom radical. Once the initial radical is formed, O_2 can attach to the fuel radical species, R, and form a new R-O-O· radical species shown as RO_2.

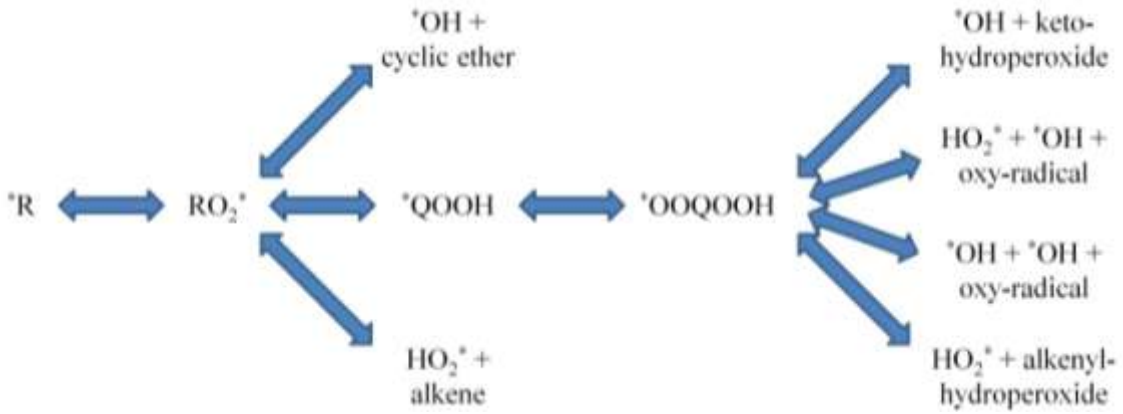

Figure 1. 1: QOOH chemistry: Kinetic routes for O_2 addition chemistry to a fuel radical as described in [46].

Once an RO_2 species is formed, it can undergo several different reactions. The radical at the end of the O_2 group can internally abstract a hydrogen from a position adjacent to the site where the O_2 group is attached and leave as an HO_2. The fuel becomes a π-bonded alkene as a result. A second pathway also involves an internal hydrogen abstraction by the O_2 group from an atom bonded directly to the site where the O_2 group

is attached. In this case, before the HO_2 group can leave, the new radical electron on the fuel attacks the first O-atom, forming a cyclic ether and kicking off a hydroxyl group. A last option is for the O_2 group to abstract a hydrogen atom from anywhere within the structure that it can reach. The O_2 group is transformed into a peroxyl group and the R group from the original fuel structure loses a hydrogen to form a new radical group Q. The new species is thus named QOOH.

If a QOOH group forms, once again an O_2 group can attach to the radical site, forming a new species, ·OOQOOH. Like with RO_2, reactions of ·OOQOOH occur through internal hydrogen abstraction. In this case, the abstraction reactions predominantly proceed to yield one of four different sets of products: OH + a keto-hydroperoxide, HO_2 + an alkenyl-hydroperoxide, OH + OH + an oxy-radical, and HO_2 + OH + an oxy-radical. The result of this type of chemistry is to provide a rich pool of radicals that can propagate combustion chemistry post-ignition.

1.2.2 Combustion chemistry in the fuel-rich limit

For cases where fuel equivalence ratio is greater than 1, combustion is considered to be fuel-rich. In this case, there is an excess in fuel so it is impossible for complete the transformation of products into H_2O, CO_2, and N_2. Burning slightly fuel-rich has its advantages, generally maximizing overall heat release at slightly fuel-rich stoichiometries. However, the richer the mixture, more fuel is consumed and more pollutants such as soot and carbon monoxide form. In the absolute extreme, reaction can occur in the presence of supplied heat but no oxygen, which is called pyrolysis.

In pyrolysis, the fuel is thermally decomposed at an elevated temperature by adding the fuel to a pyrolysis reactor and holding it at a certain temperature until

decomposed into products. This process is used industrially to transform large, complex molecules into smaller molecules [47]. For example, using pyrolysis with cellulosic biomass, a complex structure found in wood and non-food biomass resources, can yield liquid chemical products such as bio-oil, which is a mixture of several products including levoglucosan. Liquid chemicals such as levoglucosan can be upgraded via deoxygenation and form products such as furans, which can be used directly as transportation fuels [48].

In the absence of oxygen, pyrolysis chemistry is dominated by thermal decomposition and unimolecular isomerization reactions. By heating the system, the molecule can gain enough energy to overcome the activation energy need to break bonds in the fuel via simple bond fission resulting in two radicals. Alternatively, pericyclic reactions and hydrogen-shift reactions can occur under pyrolysis conditions to isomerize the fuel in and out of ring structures, break the fuel into smaller components, and introduce radicals in the system to fuel combustion.

1.2.3 Combustion chemistry in conditions between fuel rich and fuel lean limits

While chemistry in the fuel-lean and fuel-rich limits are important for modeling real engines where mixing is heterogeneous and for modeling pyrolysis reactors and ignition chemistry, the majority of reactions in combustion chemistry occur in a regime between these two limits. Upon achieving steady state, a vast radical pool becomes present in a flame, and combustion chemistry becomes dominated by radical chemistry, both via abstraction reactions and β-scission reactions. Here, stoichiometric ($\Phi = 1$) cyclohexane combustion is used as an example of steady-state combustion as seen in Li et al. [49].

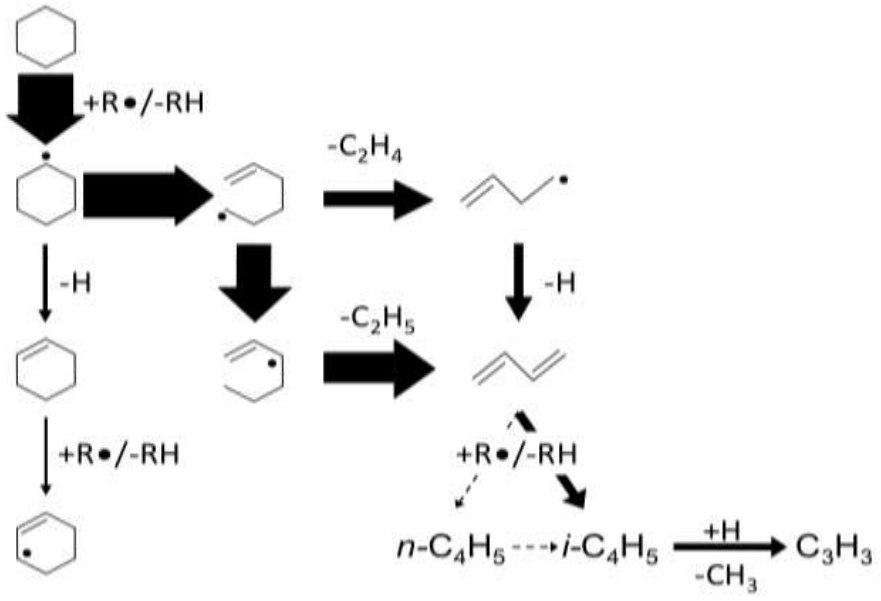

Figure 1. 2: Reaction path diagram for stoichiometric (Φ = 1) cyclohexane combustion from Li et al. [49].

Figure 1.2 is a reaction path diagram for stoichiometric cyclohexane combustion in a laminar premixed flame. A reaction path diagram describes the dominant reaction routes indicated by the thickness of the arrows (i.e. the thicker the arrows, the more likely the path for reaction). In this instance, cyclohexane combustion, like with other fuels, is initiated by abstraction of a hydrogen atom by any of several radical species, R, available in the radical pool. The result is a fuel radical, and in the case of cyclohexane, the result is a cyclohexyl radical. These fuel radicals then predominantly undergo β-scission reactions, where a bond is formed between the radical site and a neighboring atom (in the "α" position), while simultaneously a second bond is broken, two positions away from the radical site (in the "β" position). For cyclohexyl there are two possibilities: β-scission of a C-H bond to form cyclohexene and H-atom or, the more dominant path, β-scission of a

C-C bond, forming a linear 1-hexene radical. This pattern of abstraction reactions and β-scissions continues until small-molecule products are formed.

1.3 Research objectives

In an effort to model combustion chemistry of novel biofuels with heteroatomic functionalities, comprehensive reaction sets are needed that describe the combustion of these fuels under a wide range of conditions extending from fuel-lean to fuel-rich. The broad objectives of this research are to develop and validate sets of elementary, gas-phase chemical reactions for combustion of fuels containing carbon, oxygen, hydrogen, and nitrogen exclusively, emphasizing chemistry of the N-containing fuels, and to infer the chemical mechanisms behind the general sets. "Reaction sets" are defined here as lists of reactions and their stoichiometries and rate constants, necessary thermochemistry, and transport properties. These reaction sets are compilations of data from the literature when available. Where literature data are unavailable, computational quantum chemistry, statistical thermodynamics, and reaction theory are used to predict these properties.

The work in this thesis may be categorized into three specific sub-objectives based on molecular structure. The first objective, small-molecule chemistry, specifically addresses the need for a new reaction set to describe small molecule combustion chemistry for nitrogen-containing compounds. The second objective is a study of heterocyclic compounds, specifically looking at how model biofuels with six-heavy-atom cyclic structures change in combustion chemistry upon addition of heteroatoms, O and N, to the ring. The last objective is to look at hypergolic propellants, which not only are complex nitrogen compounds in themselves, but typically are reacted with red fuming nitric acid (RFNA) instead of O_2 as seen in traditional combustion.

Small-molecule chemistry. The goal of this objective is to form a comprehensive base reaction set to describe combustion of nitrogen compounds and subsequent radical chemistry for two-heavy-atom and smaller species that can be applied to wide ranges of conditions. An accurate reaction set was developed to model:

- H/N/O combustion, including a NH_3/O_2/Ar flame [50], 8 $NH_3/O_2/H_2$/Ar flames [51], a NH_3/NO/Ar flame [52], a N_2O/H_2/Ar flame [53], a $N_2O/H_2/NH_3$/Ar [53], and NH_3 pyrolysis shock-tube experiments [54].
- H/C/N/O flames, including $NH_3/CH_4/O_2$/Ar [55], CH_3NHCH_3/O_2/Ar [56], and $CH_3CH_2NH_2/O_2$/Ar flames [56].

Heterocyclic biofuel chemistry. Adding to the small-molecular kinetics, reaction sets were developed for the six-heavy-atom heterocyclic species tetrahydropyran (THP) and morpholine. These fuels were chosen both for their structural similarities to biomass structures and for a comparative study to previously studied cyclohexane flames [49] as a commentary on the effect of heteroatoms, O and N, on combustion. In this task, accurate reaction sets were developed for:

- THP, as the base ring structure in cellulose.
- Morpholine, as structurally similar to natural rings in biomass.

Hypergolic propellant chemistry. As an additional look into nitrogen-containing compounds, a study was conducted on hypergolic rocket propellants with red fuming nitric acid (RFNA) as the oxidizer. Since the ultimate goal of the propellant study was to model real engines, reaction sets and reduced models for describing combustion were also developed for:

- MMH (monomethyl hydrazine) hypergolic propellant, including reduced-size sets.
- The hypergolic propellant TMEDA (tetramethylethanediamine).

These models were tested against data where possible, and the mechanism of conversion was identified. In addition to intellectual insights, such models will be useful for the modeling community to develop clean and efficient fuels and processes.

1.4 Outline of Dissertation

The goal of this thesis is to describe the combustion kinetics of several different heteroatomic fuels. In Chapter 2, the different types of experiments studied previously in the literature and used this work are described as well as their benefits in elucidating combustion kinetics. In Chapter 3, the methods by which the reaction sets for these heteroatomic fuels were developed is described, including thermodynamics, estimation techniques, and kinetics theory. Chapter 4 describes the different numerical models used to describe each of the different types of experiments and the implementation of the reaction sets in these models for comparison against the experimental data.

The small molecule chemistry work is described in Chapters 5 and 6. Chapter 5 specifically describes the development of a reaction set for combustion of nitrogen-containing compounds in the absence of carbon. The results are compared against a large number of experimental data sets from the literature and the reaction set performance is analyzed through sensitivity analysis. Chapter 6 is an extension of the H/N/O reaction set developed in Chapter 5 to include carbon chemistry. This reaction set is again compared to published experimental data for validation.

The heterocyclic combustion chemistry work is described in Chapters 7, 8, and 9. In Chapter 7, fuel-rich combustion of THP is explored against new premixed MBMS flat flame experimental data using a new reaction set describing THP flame chemistry. Chapter 8 involves a similar study for morpholine using a new combustion chemistry reaction set and comparing to new MBMS experimental data. Chapter 9 extends the morpholine work to data for shock-tube pyrolysis species time-histories and for shock-tube ignition delay times.

The hypergolic rocket propellant chemistry work is described in Chapters 10 and 11. Chapter 10 looks specifically at the combustion of monomethyl hydrazine with red fuming nitric acid. A new set was developed and compared to previously published shock tube species time history data. This set was also reduced for use in computational fluid dynamics (CFD) codes where smaller reaction sets are needed. A second reaction set for TMEDA is presented in Chapter 11, and again data is compared to shock-tube pyrolysis data.

Lastly, Chapter 12 summarizes the work to date and offers a proposal for improvements and future work.

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CHAPTER 2

EXPERIMENTAL METHODS TO ELUCIDATE COMBUSTION CHEMISTRY

Experimental methods have been developed to explore all aspects of flames and reaction sets, determining features such as physical structure, chemical composition, heat release, and kinetics. With a variety of experimental techniques available, one may focus on specific techniques that resolve certain flame characteristics well. For example, to resolve the chemical pathways in a flame for a particular fuel, it is important to place experimental emphasis on velocity, temperature profiles, and species concentration profiles. In many cases, these features are difficult to measure precisely, e.g., when a flame is turbulent [1].

With regard to ignition kinetics, several experimental techniques have been developed, including unstirred batch reactors, continuous-flow well-mixed reactors, laminar flow reactors, and rapid-compression reactors. These techniques can provide intermediate species and temperature changes [2]. However, the rapid dynamics of ignition make it hard to capture concentration profiles in time. Additionally, sampling free radicals and other non-stable intermediates proves to be a difficult challenge with these techniques [3]. Two other combustion experiments, shock-tube experiments and molecular-beam mass spectrometry (MBMS) experiments are particularly useful for determining combustion chemistry.

2.1 Shock tubes

One experimental method to resolve specific kinetic rates is the shock tube. In shock-tube experiments, reactants can be heated nearly instantaneously and products quenched quickly, allowing for data to be recovered at very specific conditions. When

coupled with highly sensitive diagnostic equipment, experimental data such as ignition delay times and species concentration time histories. Under conditions where the reactant gas is diluted to very low concentrations, the amount of sequential reactions is reduced so that a few specific reactions can be isolated for experiment such that specific rate constants may be measured [4].

In general, a shock tube consists of two sections: the driver section and the driven section. These two sections are separated by a diaphragm that is either rated to burst at a specific pressure or is burst mechanically. The fuel mixture is usually highly diluted and contained in the driven section at low pressure. In the driver section, an inert gas is contained at very high pressures. When the driver section reaches the bursting pressure of the diaphragm, the high-pressure gases are released into the driven section, causing a shock wave to run through the driven section, reflect off the end, and bounce back towards the driver section. This reflection instantaneously heats the driven section, and the gas behind the reflected shock is considered at rest [3]. Laser diagnostics and pressure transducers are used to measure concentration profiles and ignition-time delays as a function of time from the incident shock. A diagram of a shock tube is displayed in Fig. 2.1.

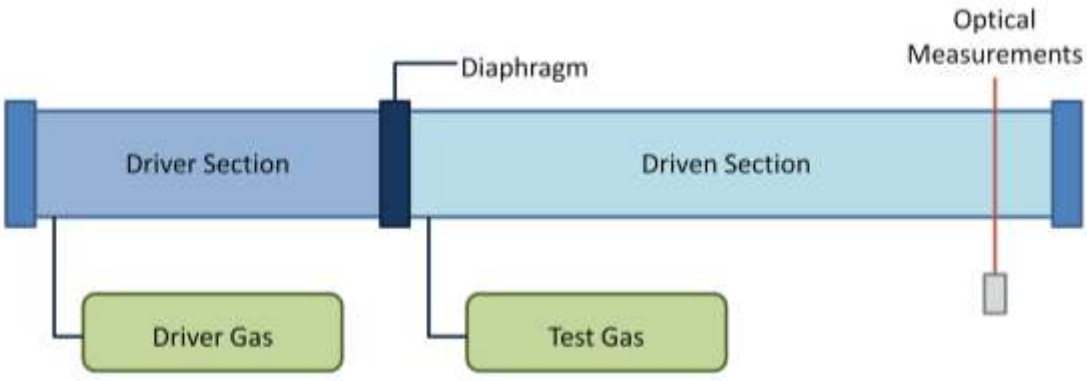

Figure 2. 1: Schematic of shock-tube/laser-absorption diagnostic setup.

The Stanford high-pressure shock tube, used to generate data modeled in this work, has a stainless-steel driven section 5 m long with a 5 cm inner diameter and a driver section that is 3 m long with an inner diameter of 7.5 cm. Shock-tube driver inserts are used to achieve uniform test conditions at lower temperatures where facility effects at long test times (*dP/dt* and *dT/dt*) are most significant. The incident shock speed, critical to the accurate determination of reflected shock pressure and temperature, is determined using five piezoelectric pressure transducers that are spaced at approximately 30-cm intervals over the last 2 m of the shock tube. Temperatures and pressures in the post-shock region are determined from the incident shock speed at the endwall using standard normal shock relations. Ignition pressure is monitored using a piezoelectric pressure transducer (Kistler Model 603B1) located 1 cm from the end wall. Ignition delay times are determined by extrapolating, back to the baseline pressure, the steep increase in pressure concurrent with ignition. To avoid condensation to the shock tube wall, the driven section is heated to mitigate condensation of fuel on the wall [5].

2.2 Flame-sampling molecular-beam mass spectrometry

One particularly powerful method for exploring combustion chemistry is molecular-beam mass spectrometry (MBMS) sampling of a laminar, premixed, flat flame. Other experiments either require setting a temperature profile or limit detection to a few species, but in MBMS experiments, concentration profiles for molecular, radical, and atomic species and temperatures may be recorded in a free-standing flame from close to the burner out into the post-flame zone. As the name suggests, premixed refers to a mixing of reactants prior to combustion such that a homogenous mixture is fed to the burner. Flat refers to the dimensionality of the flame, though the flame is not perfectly

flat. If attached to a burner, a flame will mimic the geometry of the support to which it is attached [6]. The resulting flame is disc-like in shape and flat near the axis.

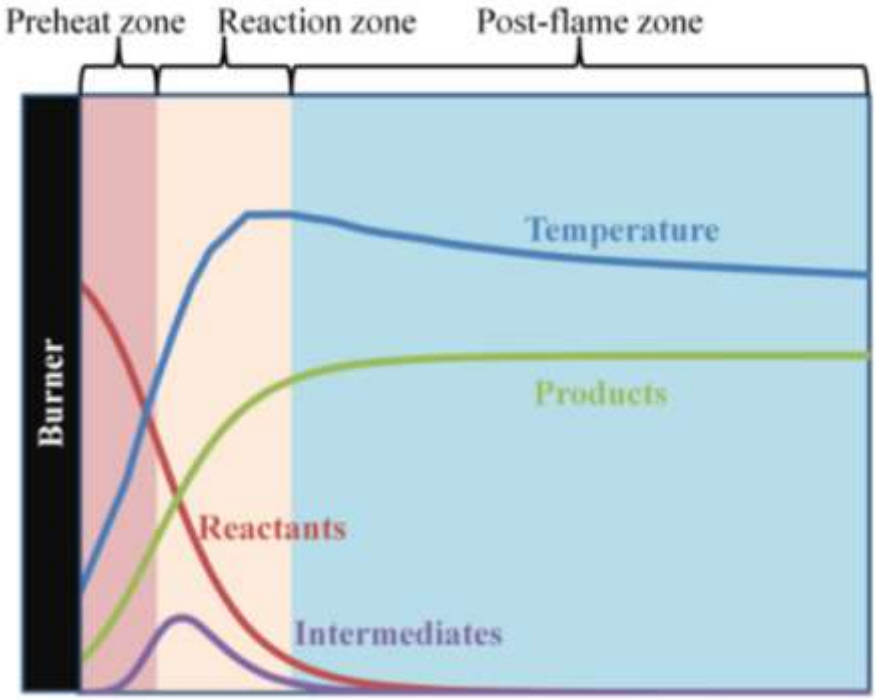

Figure 2. 2: Diagram of a flat flame showing the consumption of reactants, generation of intermediates and products, and evolution of the temperature profile through the preheat, reaction, and post-flame zones.

A laminar, premixed flat flame has a distinct axial structure that is shown in Fig. 2.2. The premixed gases enter the flame from the burner and enter the first zone of the flame, called the pre-heat zone. In this region, the feed gases are rapidly heated via conduction from the flame until combustion temperatures are reached. Here, changes in concentration profiles are mostly due to diffusion. Next, the gases enter the reaction zone. In this region, most reactions occur, releasing heat to sustain combustion. Intermediate species can be observed most prevalently in this region as the fuel is converted into products. Once the fuel is consumed, the product gases enter the post-flame zone. In this region, the exhaust gases are converted to final products, the temperature cools, and

remaining radical species are eliminated via third-body-mediated combination reactions [7].

Figure 2.3 is an example of a MBMS flame apparatus, which has previously been described in depth [7-8]. First, the fuel, oxidizer, and a carrier gas (such as Ar) are premixed using mass flow controllers to meter flow of the gases. When liquid fuels are used, the fuel is vaporized prior to addition to the oxidizer and carrier gas. The premixed fuel mixture is fed to a burner-stabilized flame, typically on a water-cooled, movable McKenna-type burner. The two systems where new data was produced in this work, the Bielefeld University system and the Advanced Light Source (ALS) system, both use McKenna-type burners with 6.34-cm and 6-cm diameters respectively. In this technique, a flame is burned under low-pressure and laminar-velocity conditions, creating a nearly uniform concentration across the burner surface, while expanding the flame significantly in thickness for sampling [7].

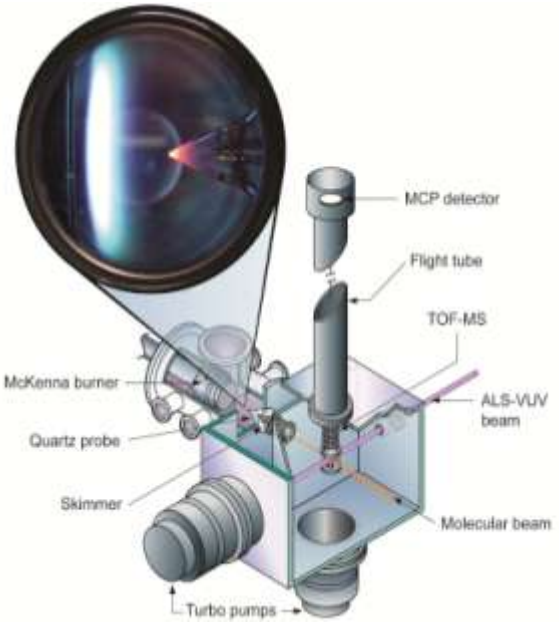

Figure 2. 3: MBMS experimental apparatus at the Advanced Light Source in Berkeley, CA. This particular system uses time-of-flight mass spectrometry and vacuum-ultraviolet radiation [9].

With an established flame, the McKenna burner is moved towards and away from a probe cone to sample along the z-axis of the flame. The probe-cone geometry can have a dramatic effect on probe perturbations if too large a cone angle is used, shifting the reaction zone away from the burner and narrowing the span of the reaction zone [8]. For the Bielefeld University system, experiment uses a quartz cone with a 0.50-mm-diameter orifice at the tip and an angle of 25°. The ALS apparatus uses a quartz cone also, but with a slightly different geometry: 0.40-mm-diameter orifice at the tip and an angle of 40°. The wall thickness of the probes is near 50 μm (PI-MBMS: 100 μm) at the tip. The gas sample is expanded to low pressure (~10^{-4} mbar in the Bielefeld and ALS systems) in the first pumping stage. The center of the gas cloud is then extracted by a skimmer, forming a molecular beam which then enters the ionization region of the mass spectrometer, kept at lower pressure (~10^{-6} mbar in the Bielefeld and ALS systems). The flame can be sampled carefully to minimize probe effects and recombination loss of radicals in the system [4].

The molecular beam is ionized in the ionization chamber with photons or electrons and then analyzed using mass spectrometry [8]. Thus, with this technique, concentration profiles of species along the z-axis of the flame may be resolved within the experimental limits of the techniques described above. MBMS has been used with either photoionization (PI) by vacuum-ultraviolet synchrotron radiation or with election impact (EI) [7, 10]. The ALS system is a PI-MBMS system and uses tunable VUV radiation to ensure high energy resolution. The Bielefeld system has EI-MBMS capabilities, equipped with a reflectron time-of-flight (TOF) mass analyzer for high mass resolution.

Photoionization with the ALS instrument is performed with a continuous photon beam of ~10^{13} photons/s at energies between 8.00 and 17.00 eV; the energy resolution as

about 0.05 eV. Analysis relies on a linear TOF mass spectrometer with a mass resolution of $m/\Delta m$ = 400. In the Bielefeld experiment, the sample is ionized with a pulsed electron beam (~10^9 electrons/pulse) using several different energies to analyze the flame and minimize fragmentation. Mass spectra are obtained with a mass resolution of $m/\Delta m$ = 4000.

The signal measured in the mass spectrometer for a particular ion *i* can be related to the partial pressure of species by:

$$S_i(T) = CP_i(T)\sigma_i(E)D_i\varphi_p(E)F(k,T,P) \tag{2.1}$$

In Eq. 2.1, S_i is the ion signal measured, C is the proportionality constant, and P_i and T are species partial pressure and temperature. Photoionization cross section, represented by $\sigma_i(E)$, is measured at a photon energy of E. The tendency of species to diffuse away from the molecular beam is represented by mass discrimination factor D_i. The ratio of signals of two species can be written as:

$$\frac{S_i(T)}{S_j(T)} = \frac{x_i(T)\sigma_i(E)D_i}{x_j(T)\sigma_j(E)D_j} \tag{2.2}$$

where x_i is the mole fraction of species i. In this equation, a reference species j can be used to calculate the mole fraction of i knowing the cross section and mass discrimination factor. The same equation can also be used to calculate the mass discrimination factor for a particular species with known mass fractions and cross sections. The D_i of CO_2 is often taken as 1.0 and used as reference for the calculation of D_i of other species (Fig. 2.4).

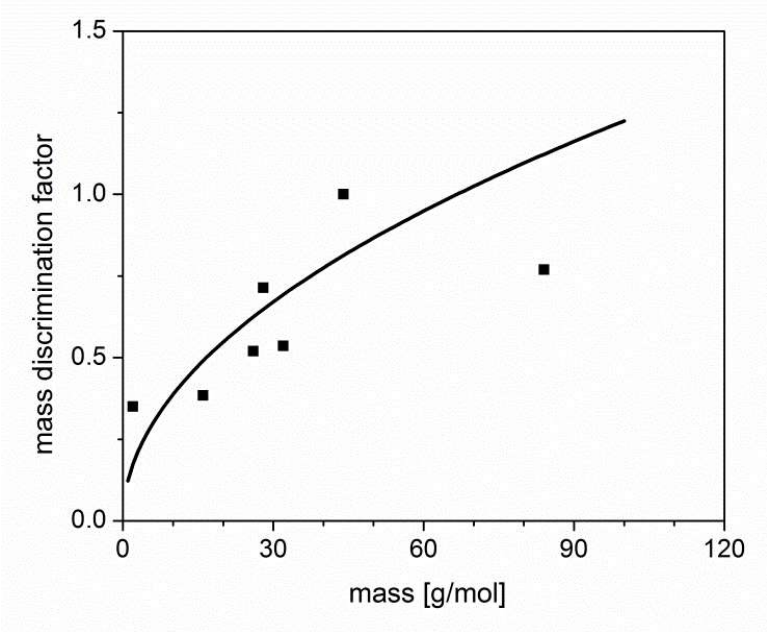

Figure 2. 4: Mass discrimination factor measured as a function of molecular mass with CO_2 as reference species.

The ratio of signals of a particular species at two different temperatures yields

$$\frac{S_i(T)}{S_i(T_0)} = \frac{x_i(T)F(k,T,P)}{x_i(T_0)F(k,T_0,P)} = \frac{x_i(T)}{x_i(T_0)} FKT(T,T_0) \tag{2.3}$$

The instrument function *FKT* can be calculated using the procedure outlined by Cool et al. [11]. The mole-fraction profile of the species for which the inlet mole fraction is known can be found using *FKT*. Along with a carbon-atom balance in the post-flame zone, direct calibration experiments can be performed to compute the mole fractions of CO and CO_2 relative to Ar. H_2 and H_2O profiles can be computed using an H-atom balance. This method is outlined in [12] and was further adapted for nitrogen balances in [13]. Once the main species profiles are calculated, they can be used as reference to calculate the minor species using Eq. 2.2 and further can be converted to mole fraction relative to Ar. Once all the mole fractions are calculated relative to Ar, the definition of

mole fraction can be manipulated to compute x_{Ar} (Eq. 2.4) and thus all the mole fractions. The cross section of the species can be found in the literature or can be estimated.

$$\sum_{i \neq j} \left(\frac{x_j}{x_i} + 1 \right) = \frac{1}{x_i} \tag{2.4}$$

Simultaneous multi-species measurements with optical methods are difficult, especially quantification. Often for radical species, cross section data are unavailable [14]. The error in estimation of main species can be about 5%, and for minor species, it can be easily a factor of 2 depending on the accuracy of the cross section [13].

2.3 Temperature profile determination

In MBMS flame experiments, one of the biggest experimental challenges is temperature resolution. Minimizing or correcting for perturbations is the principal challenge. Thermocouples have been employed successfully to measure the temperatures of a flame. They may perturb the flame physically (thermally), and glass-coated thermocouples may be necessary to prevent catalytic reactions and reduce experimental uncertainties [4]. Alternatively, laser-induced fluorescence, particularly of OH or NO radical, can also be used to measure quite accurately the temperature profile in low-pressure flames. However, LIF techniques are capable of producing very large errors if the entire fluorescence spectrum is not collected [14], and LIF may also have trouble resolving temperatures at ambient or higher pressures [4].

In this work, the temperature profiles used for model calculations are determined from the temperature dependence of the sampling rate through the probe orifice, combined with high-temperature LIF measurements. Using this method, the profiles benefit from the accuracy of LIF measurements away from the burner while still

preserving the probe perturbation effects with the pressure measurements. Assuming a constant pumping speed, the sampling rate can be expressed by the pressure of the first-stage chamber (p_{1st}), as previously described [13]. This dependence is described by

$$\mathrm{p_{1st}} = C\sqrt{\frac{\gamma}{\overline{M}\cdot T}}\left(\frac{2}{\overline{M}\cdot T}\right)^{Z} \tag{2.5}$$

with $Z = \frac{(\gamma+1)}{2(\gamma-1)}$, $\overline{M}$ is the mean molar mass, γ is the adiabaticity coefficient (C_p/C_v), and C is a device-specific constant that is determined by solving Eq. 2.5 with the post-flame gas temperature taken from the LIF measurement.

To determine the adiabaticity coefficient, γ, functions for $C_p(T)$ are derived for each species i observed experimentally, where there were no ambiguities regarding isomer identification using published thermodynamic data such as that used in the fuel model. The thermodynamic database employs the NASA seven-parameter format, which is based on $C_p(T)$ being a simple fourth-order polynomial (Eq. 2.6). The $C_p(T)$ function is then multiplied by the mole fraction for each species, m_i, for each experimental sampling point. The average $C_{p,ave}(T)$ function is then calculated by summing over all species i for each sampling point and normalized by the total mole fraction of all species considered (Eq. 2.7). The result is a function for average C_p at each sample point, from which γ and Z may be calculated. The same logic can be applied to get the mean molar mass, $\overline{M}$.

$$C_{p,i}(T) = a_{1,i} + a_{2,i}\cdot T + a_{3,i}\cdot T^2 + a_{4,i}\cdot T^3 + a_{5,i}\cdot T^4 \tag{2.6}$$

$$C_{p,ave}(T) = \frac{1}{\sum_i m_i}\sum_i m_i C_{p,i}(T) \tag{2.7}$$

The last variable to be determined to solve for temperature as a function of chamber pressure is the device-specific constant, C. To determine C, the post-flame LIF

measurements are averaged in the post-flame zone, where the measurements are most accurate. With an average experimental post-flame temperature, *C* is then calibrated by solving Eq. 2.5 at each of several representative chamber-pressure sampling points, which represent measurements well into the post-flame zone, and is averaged among the representative points. With all variables solved in terms of temperature, Eq. 2.5 can be solved for each data point using an iterative solver. The LIF temperature data is then shifted away from the burner to match the chamber-pressure temperature data because the chamber-pressure temperature profile reflects the actual probe distortion more accurately. An example of determining the temperature profile via LIF and chamber pressure data is presented in Fig. 2.5.

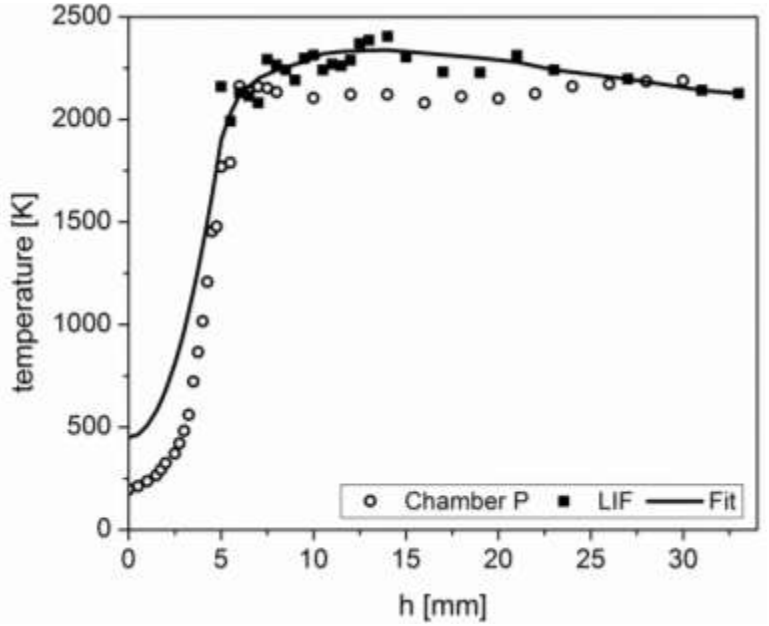

Figure 2. 5: Temperature profile measurements and fit for THP. The open circles represent the temperature profile derived by the chamber pressure measurements. The squares represent the LIF temperature measurements shifted away from the burner 2.4 mm to fit the chamber pressure temperature profile. The line is the smoothed temperature profile set to 450 K at the burner and matching the LIF temperature data.

For CHEMKIN simulations, a smooth temperature profile is required as an input parameter. The LIF data are averaged and smoothed to represent temperatures in the exhaust. For the temperatures prior to the shifted LIF data, the temperature profile was determined by fixing the burner temperature at a slightly elevated temperature due to radiative heating from the flame (on the order of 400-500K) and scaling the chamber-pressure temperature profile such that it reflected the curvature of the measured profile and match the LIF data at the exhaust. An example of a smoothed profile is presented in Fig. 2.5.

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CHAPTER 3

KINETIC THEORY FOR COMBUSTION MODEL DEVELOPMENT

In order to understand the chemistry of combustion, kinetic models have been developed to help explain the physical data from combustion experiments. Perhaps the most difficult task in assembling these kinetic flame models is the development of a reaction set. Not only does one have to be mindful to include all possible chemical reactions, but reaction rates must be available for each individual reaction, as well as thermochemical data for each species included. Quite often thermochemical or kinetics data are not available through prior experimental and computational studies. Several estimation techniques and computational chemistry methods have become available to estimate these parameters.

With advances in computing over the past two decades, computational chemistry has become accessible via programs such as Gaussian 09 [1], which use quantum chemistry to calculate the geometry, vibrational frequencies, and energies of molecules and transition states, from which ideal-gas thermochemistry for each molecule or transition state may be predicted with statistical mechanics [2]. Alternatively, estimation techniques, such as group additivity, have proven to be quick and accurate methods of calculating thermochemistry without the need for expensive computation. Rate constants can also be estimated in a similar manner [3].

3.1 Kinetic models used today

Obtaining an accurate description for combustion of the multitude of different fuels used today has been an ongoing challenge for several decades. As a result, countless reaction sets have been proposed throughout the years and made public through

publication. Several issues have risen as a result of this boom in available reaction sets, including publication of reaction sets that are not comprehensive (i.e., these reaction sets have not been tested under a wide range of conditions for validity) [4]. In such cases, incorrect thermochemistry or reaction rate constants, which may not significantly impact model results for the original work so issues are unnoticed, may be repeated in subsequent models where the issues could become significant.

Several reaction sets have been developed taking an approach where the reaction set is optimized to a series of experimental data sets. One set developed to model natural gas combustion, GRI-Mech 3.0 [5], is a comprehensive mechanism that models methane and hydrogen combustion with inclusion of NO_x chemistry. GRI-Mech was developed by assembling thermochemistry and rate constants for natural gas combustion, assigning error limits for these parameters, and adjusting the parameters within the error limits until matching the data from several representative experimental studies. Another mechanism, USC mech II out of the University of Southern California [6], employs similar methodology for development. The reaction set is a high-temperature combustion model targeted towards combustion of H_2 and C_1-C_4 compounds and was validated against a series of experiments including ignition delay times, flame speeds, flow reactor and shock tube experiments, and flame experiments. Currently, this approach of wide-range validation is only appropriate for fuels with few heavy atoms because reaction sets become exponentially larger with increases in fuel molecule size.

Another approach is to develop very large models capable of predicting the chemistry of real fuels, which are quite large molecules and are often blends of different fuels. For these expansive reaction sets, estimation techniques are heavily employed to

determine reaction rate constants, and these mechanisms are often not widely tested against data for other fuels for validation. Despite the inherent inaccuracies in these practices, these models are the closest to elementary reaction models for real transportation fuels that exist today. An example of this is the gasoline surrogate model developed at Lawrence Livermore National Laboratory [7], which has predictive capabilities for toluene and C_5-C_6 olefins, and has been tested against some experimental data, focusing on ignition delay times. Often for larger fuels, reaction sets available are limited. In cases where new reaction sets must be developed, extensive work has been published in several databases to determine the thermochemistry for combustion intermediates [8-10].

3.2 Estimation techniques

With the emergence of several new biofuels and the increase in computational power to model real fuels with much larger mechanisms than previously developed, there is interest in modeling fuels that have not been studied previously or have limited data available. Assembling new reaction sets for these fuels can be a daunting task considering the huge number of new intermediate species and reactions to be included. Fortunately, there are several different methods for estimating thermochemistry and reaction rate constants for reaction set development. This section is an overview of some of the estimation techniques used in the reaction set development in this work.

3.2.1 Thermochemistry estimations

In the late 1950's, Sidney Benson began developing a method for estimating thermochemistry for molecules based on their molecular geometries which is now known as group additivity [3]. Group additivity is based on the principle that thermochemistry

for a specific molecule can be approximated by an additive sum of contributions for every polyliganded atom. Using experimental measurements as a basis, Benson tabulated contributions to heat capacity, heat of formation, and entropy as functions of different types of atoms and the atoms to which they were bonded. For example, propane would have contributions from two carbon groups that are bonded to three hydrogen atoms and one carbon atom, as well as a contribution from a carbon group that is bonded to two hydrogen atoms and two carbon atoms.

Complications arise as molecular structures become more complicated. The inclusion of ring structures, cis and trans isomers, steric hinderances, etc. are all considered and may be approximated through additive corrections. However, problems still exist when properties for functional groups are missing. This situation often arises because some molecules are unstable and accurate measurement of thermodynamic data is difficult. As a result, data are missing for several types of group contributions, especially for radical species. While hydrocarbon contributions have been catalogued extensively, oxygen and nitrogen contributions are often incomplete, and inorganic groups such as halogens are much less studied. Despite the limitations, the result is a generally accurate approximation to molecular thermodynamics.

3.2.2 Reaction rate constants from estimation

Several different estimation techniques also exist for reaction rate constant estimations. One of the estimation techniques uses principles similar to what was done for the Lawrence Livermore National Laboratory gasoline surrogate model [7] and has analogies to the Benson group additivity priniciples [3].like how thermochemistry can be approximated based on molecular structure, as can rate constants. The rate constant for

breaking a C-H bond via H-abstraction by methyl radical from a secondary carbon in propane will have a similar reaction rate to the breaking of a C-H bond via H-abstraction by methyl radical from a secondary carbon in butane. The main difference between the two rate constants is the difference in the number of hydrogen atoms attached to secondary carbon atoms in both molecules; propane has two hydrogen atoms attached to secondary carbon atoms, while ethane has four. As an estimation, the reaction rate constant for ethane is assumed to be the same as for propane, multiplying the rate constant by its reaction path degeneracy (RPD). In the case of H-abstraction from the secondary carbons in ethane versus propane, the RPD factor is 4 secondary hydrogen atoms divided by 2 secondary hydrogen atoms. As such, the estimated rate constant for H-abstraction from the secondary carbons in ethane is double the rate constant for H-abstraction from the secondary carbon in propane.

Additionally, one may relate the energy of activation for a particular bimolecular reaction based on the co-reactant in the reaction. As the enthalpy of reaction increases (becomes more positive), the energy of activation also increases. This relationship is called the Bell-Evans-Polanyi Relationship [11-13]. As an example, if the kinetics for hydrogen abstraction from a particular molecule is known for a few reaction partners, activation energy for additional abstraction partners can be estimated knowing the enthalpy of reactants.

3.3 Quantum chemistry calculations

Estimation techniques are quite powerful and provide a good first-pass estimation to a reaction set. However, it is often necessary to have a higher degree of accuracy than estimation techniques can provide. A decade ago, quantum chemistry techniques were

not feasible for large systems due to the long computational times needed to calculate molecular structure accurately. Today, advances in computation and availability of supercomputers have made quantum-chemistry calculation much more practical, as has the availability of commercial quantum-chemistry codes such as Gaussian 09 [1]. Limitations still exist with these large calculations, however, as computation time increases exponentially with each heavy atom included in the system or increasing the robustness of the level of theory used. This section is an overview of some of the quantum-chemistry methods used in this work.

3.3.1 Levels of theory

Quantum-chemistry calculations have been used to predict electronic structure and molecular energy for compounds by solving the time-independent Schrödinger Equation:

$$\hat{H}\psi = E\psi \tag{3.1}$$

At the core of these calculations is a model chemistry, defined as any specific combination of the method (the procedure by which the Schrödinger Equation is approximated) and a basis set (the mathematical representation of the molecular orbitals in the molecule) [15-16]. Several different methods exist for model chemistries (often referred to as "levels of theory"), ranging in different techniques and accuracy. One of the simpler models is Hartree-Fock (HF) theory, which solves the Schrödinger Equation with a Hamiltonian that describes kinetic energy, coulombic attraction energy, and coulombic repulsion energy using a Slater-determinant wavefunction [15]. One of the biggest limitations of HF theory is the fact that correlation energy is excluded, neglecting the fact that electron motion is directly correlated to the positions of other electrons in the

molecule [16]. Other methods such as second-order Møller-Plesset (MP2) and fourth-order Møller-Plesset (MP4) theory use perturbation theory to approximate configuration state functions as an approximation to electronic correlation theory [15]. As one would expect, MP4 is generally more accurate than MP2, given the addition of third- and fourth-order terms into the perturbation theory. Even larger methods exist, such as QCISD(T), where a quadratic configuration-interaction method is employed with third-order terms treated with perturbation theory [16] in the effort to approximate a full configuration interaction method, in which the configuration interactions among all electron orbitals is accounted for.

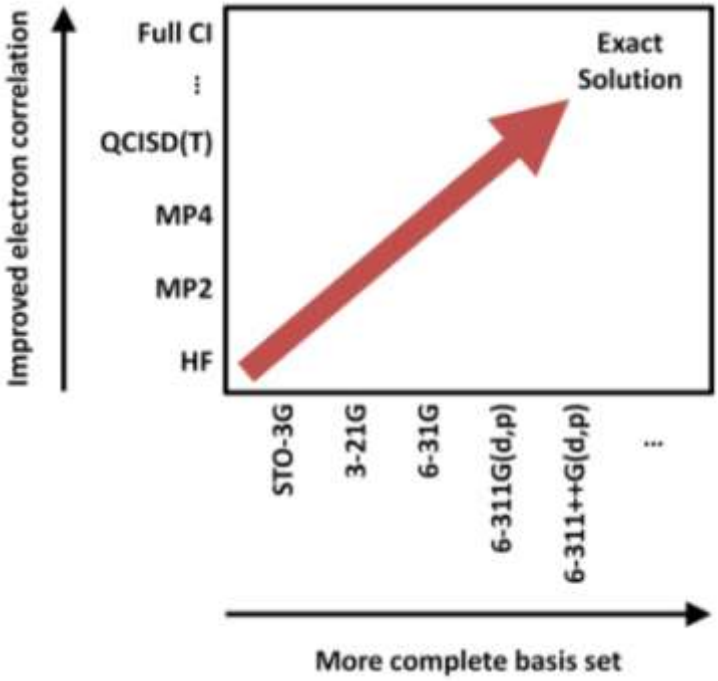

Figure 3.1: Correlation between electronic structure calculation method and basis set with calculation accuracy.

The second part of the model chemistry is the basis set function. Electronic structure methods generally approximate electronic orbitals as linear combinations of the electronic orbital functions. Generally, these basis sets use Gaussian-type orbitals and

require a minimum number of orbitals equal to the number of core and valence electrons in the system. Larger basis sets use large numbers of molecular orbitals. For example, double-zeta basis sets use twice as many molecular orbitals as there are core and valence orbitals, triple-zeta basis sets use three times as many molecular orbitals, and so on [15]. Additionally, polarizability and diffuse functions can be incorporated, accounting for higher angular momentum functions and Rydberg states [15].

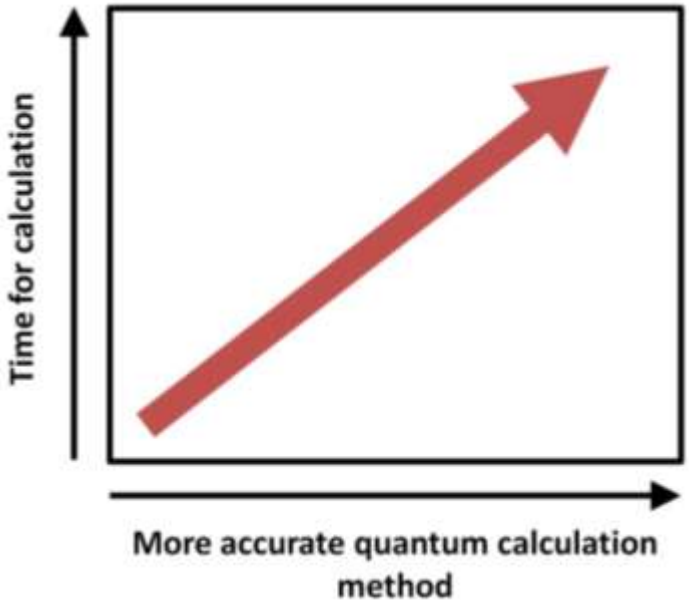

Figure 3.2: Correlation between size and accuracy of a quantum calculation with the time it takes to compute.

As larger methods for calculating electronic structure and larger basis sets are used, as shown in Fig. 3.1, the calculation results become more closely approximate the exact solution to the Schrödinger Equation. However, as illustrated in Fig. 3.2, for the larger quantum chemistry calculation, longer calculation times are required to complete the calculation. Additionally, as the molecule increases in size, increasing the overall number of molecular orbitals to approximate, the calculation time also increases significantly, making high-level calculations for large molecules impractical. To balance

the issues associated with need for accuracy while reducing the amount of computation time, composite methods were developed such as the Complete Basis Set methods (CBS) [17] and the G_n methods (G2, G3, G4, etc.). These methods use different methods and basis sets for calculating molecular geometry and zero point energy, and then they extrapolate to higher levels of theory to determine electronic energy, approximating the accuracy of higher-level calculations while reducing the time for computation significantly [16].

3.3.2 Thermochemistry calculations

With quantum chemistry calculations, molecular structure, electronic energy, and molecular partition functions may all be calculated. Electronic energy can be translated to thermochemistry via atomization methods described in [2]. In short, the heat of formation may be calculated by Eq. 3.2,

$$\Delta_f H_0^\circ = \sum_{\text{atoms}} x\, \Delta_f H_{x,0}^\circ - \sum D_\circ \tag{3.2}$$

where $\Delta_f H_0^\circ$ is the standard heat of formation at 0 K for the molecule, x is the stoichiometric coefficient for atom X in the molecule, $\Delta_f H_{x,0}^\circ$ is the standard heat of formation of atom X at 0 K calculated at the particular level of theory of interest, and $D_\circ$ is the atomization energy of the molecule. For heat of formation at 298 K, Eq. 3.3 may be solved

$$\Delta_f H_{298}^\circ = \Delta_f H_0^\circ + \left(H_{298}^\circ - H_0^\circ\right)_{\text{molecule}} - \sum_{\text{atoms}} x\left(H_{298}^\circ - H_0^\circ\right)_X \tag{3.3}$$

where $\Delta_f H_{298}^\circ$ is the standard heat of formation at 298 K, $\left(H_{298}^\circ - H_0^\circ\right)_{\text{molecule}}$ is the enthalpy correction term for the molecule calculated, and $\left(H_{298}^\circ - H_0^\circ\right)_X$ is the

experimental enthalpy correction term for atom X, which is catalogued for many atoms in [18].

3.3.3 Transition state theory (TST)

Once thermochemistry is available for the reactants and transition states for a reaction of interest, there are classical theories to calculate reaction rate constants. Perhaps the simplest of these is transition-state theory (TST). Canonical transition-state theory operates on the assumption that the reactant is in equilibrium with a transition state, thus allowing calculation of the concentration of the transition state. The overall rate constant is then found from the effective concentration of the transition state, multiplied by a universal frequency factor that represents the frequency of transitions crossing over to products rather than returning to the reactants [19]. The result is the Eyring equation (Eq. 3.4), which provides a high-pressure-limit kinetic rate constant:

$$k_{TST} = \frac{k_b T}{h} exp\left(\frac{\Delta S^{\neq}}{R}\right) exp\left(-\frac{\Delta H^{\neq}}{RT}\right) \tag{3.4}$$

where k_b is the Boltzmann constant, T is temperature, h is Planck's constant, $\Delta H^{\neq}$ is the enthalpy of activation, R is the universal gas constant, and $\Delta S^{\neq}$ is the entropy of activation. Several other versions of transition-state theory have been developed, such as variational TST, quantum TST, variational quantum TST, and non-separable quantum TST [20]. Codes for calculation of rate constants based on these methods are available, such as POLYRATE for variational TST [21].

3.3.4 Unimolecular reaction theory

In order to describe the kinetics of molecular decomposition and isomerization, unimolecular reaction theory was developed. Unimolecular reaction theory is based on

the Lindemann-Christiansen Hypothesis, stating that a unimolecular reaction proceeds as a two-step process as shown in Eq. 3.5.

$$\begin{gathered} A + M \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} A^* + M \\ A^* \overset{k_2}{\rightarrow} Products \end{gathered} \tag{3.5}$$

In the case of Eq. 3.5, A is collisionally activated to an energized form of A with enough energy to react called A^* at a rate of k_1. A^* can then proceed one of two ways; either A* can be collisionally deactivated back to a de-energized A at a rate of k_{-1} or A^* can proceed with reaction to products at a rate of k_2 [19,22].

Based on the reaction scheme of Eq. 3.5, an overall rate constant for unimolecular reaction of A can be described through an overall reaction rate of

$$r_{unimolecular} = k_2[A^*] = \frac{k_1 k_2 [A][M]}{k_{-1}[M] + k_2} \tag{3.6}$$

where brackets denote the molecular concentration of the species [19]. The formalism of Eq. 3.6 suggests a change in kinetics with pressure, given a direct correlation with concentration of 3rd body species *M* with pressure due to the ideal gas law. At the high-pressure limit, $k_{-1}[M] >> k_2$. Thus, in the limit of high pressure, the rate constant may be described as shown in Eq. 3.7.

$$r_{high\ pressure\ limit} = k_\infty[A] = \frac{k_1 k_2}{k_{-1}}[A] \tag{3.7}$$

Likewise, in the low-pressure limit, $k_{-1}[M] << k_2$, leading to a low pressure limit as described in Eq. 3.8.

$$r_{low\ pressure\ limit} = k_o[A][M] = k_1[A][M] \tag{3.8}$$

As shown in Eqs. 3.7-8, a clear dependence on pressure is demonstrated. As pressure decreases, so does the rate constant until the rate constant becomes a linear function of pressure. The transitional regime between high- and low-pressure limits is known as the fall-off region. To describe this transitional regime, many formulations have been developed. The simplest of the treatments is the Lindemann formulation [23], which relates the low- and high-pressure limit rate constants:

$$k = k_\infty \left(\frac{P_r}{1 + P_r}\right)$$
$$P_r = \frac{k_o[M]}{k_\infty} \tag{3.9}$$

More accurate formalisms are available through the Troe formalism [24] and the Tsang and Herron formalism [25].

Several methods have been developed to explore low-pressure kinetics building from the simplified Lindemann-Christiansen Hypothesis. One method is known as Quantum Rice-Ramsperger-Kassel (QRRK), which can be used to estimate rate constants at the low-pressure limit and in falloff, as well as rate constants for chemically activated reactions based on a quantized energy distribution [26-29]. A more robust and accurate method of calculating pressure dependence is Rice-Ramsperger-Kassel-Marcus (RRKM) theory. In RRKM theory as in QRRK theory, a reactant is collisionally activated until it has enough energy to react. The ensemble of energized molecules can then proceed through a transition state in an additional step to that proposed in the Lindemann-Christiansen Hypothesis. Equations to describe the development of RRKM theory for unimolecular rate constant calculations have been described in detail elsewhere [19,22].

One of the key assumptions of RRKM theory is that all collisions are strong collisions, which is often not the case, creating error in this approach. Using state-specific rate constants and equilibrium energy distributions from RRKM theory, the Master Equation approach was developed to calculate unimolecular reactions with both strong and weak collisions [30-31], calculating along a continuum kinetics of chemical activation, deactivation, isomerization, and reaction using time-dependent population densities [19]. Several programs for its calculation have been developed [32-36].

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CHAPTER 4

METHODS FOR MODELING COMBUSTION EXPERIMENTS

The task of modeling a flame or combustion system is quite complicated due to the particular dynamics of a flame. Consider that in combustion, several dynamics must be simultaneously accounted for, including fluid dynamics as fuel flows to the flame and exits in the exhaust. Additionally transport phenomena have to be considered in the context of the thousands of reactions are occurring, generating new species while consuming reactants and intermediates providing a molecule source and sink, and also in terms of convection and diffusion. Lastly, thermodynamic modeling is necessary due to the significant heat and gas generation in combustion systems. A combustion model must include conservation of mass, momentum, and energy and an equation of state [1].

In an effort to model the wide range of physical phenomena for simplified combustion applications, CHEMKIN was developed as a suite of subroutines to be compiled into the models that describe combustion applications of interest [2-5]. An older version has been made widely available as Fortran source code for personal adaptation as CHEMKIN II [2-5], though users must compile their own executables and the program does not feature a GUI. A newer commercial version based on the older CHEMKIN II, ChemkinPro [6], has been developed with a GUI and preset models to describe different combustion applications. Adaptation of the source code for this version is not available, so users are limited to the models available. This package has the ability to model shock tubes, perfectly stirred reactors, diffusion flames, premixed flames, internal combustion engines, and more.

4.1 General structure of CHEMKIN

No matter what type of calculation being run with the CHEMKIN suite, the program itself has the same basic structure. The first piece of the program is the interpreter. Inputs to the interpreter are the chemical kinetic reaction set, which contains a list of types of atoms to be considered, a list of species to be considered, a list of possible reactions and their corresponding rate constants, and the thermodynamic database, which is a tabulation of thermodynamic fits for specific molecules. The interpreter combines the data from the reaction set with the necessary thermodynamic parameters from the thermodynamic database, checks for errors, and outputs a binary-format "linking" file with all the necessary information for the model. The next step in a calculation is, when necessary, assembly of the transport database. The linking file from the interpreter is used to determine which species are relevant to the problem to be solved, and appropriate data are extracted from the transport database. The result is a second linking file containing the transport information for the model.

The last step in a CHEMKIN II calculation is to run the simulation that appropriately describes the chemical kinetic model of interest. Using the gas-phase subroutine library, a driver program is created, linking the appropriate subroutines that describe the physical phenomena in the system of interest. Several driver programs are included in the suite as examples of commonly used reacting-flow models, such as premixed flat flames, perfectly stirred reactors, and basic shock tubes. In the case of ChemkinPro, these driver programs are already preassembled for use. To use these driver codes, inputs for the specifications of the system and the linking files are needed. The

code returns information on concentrations, thermodynamics, pressure, and chemical production rates.

4.1.1 Thermodynamic database

As a key element to a CHEMKIN model, a thermodynamic database is necessary with information included for each of the species to be considered. The thermodynamic database employs the NASA seven-coefficient thermodynamic format to describe constant-pressure heat capacity, enthalpy, and entropy [5]. The thermodynamic properties are fitted over two different overlapping temperature ranges using the formalism:

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \tag{4.1}$$

$$\frac{H^\circ}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \tag{4.2}$$

$$\frac{S^\circ}{RT} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \tag{4.3}$$

In addition to the two seven-parameter fits for thermochemistry, additional information is needed. For each species, requirements are a reference name (no longer than 18 characters), a chemical formula for the molecule of interest, a species phase, the range over which the two thermodynamic fits span, and the point at which the two thermodynamic fits are matched.

4.1.2 Reaction set formalism

Kinetic rate constant data is provided in CHEMKIN models as reaction sets (also commonly referred to as “mechanisms”). These reaction sets have three key pieces: a list of all elements to be considered, a list of all molecular species to be considered, and a database of all chemical reactions to be considered. The most extensive piece of the

reaction set is the reaction database, often totaling hundreds and even thousands of possible reactions. The CHEMKIN program accepts kinetic rate constants in the form of three coefficients corresponding to A, b, and E_a in the modified Arrhenius kinetic rate constant expression:

$$k = A \cdot T^b \cdot exp\left(\frac{-E_a}{R \cdot T}\right) \tag{4.4}$$

Additionally, information may be included in cases where pressure dependence is considered. Using the "LOW" keyword, a second rate constant may be considered in addition to the high-pressure-limit rate constant. If no additional information for fall-off is included, the Lindemann formalism [7] is used to bridge the high- and low-pressure limits. Otherwise, keywords "TROE" or "SRI" may be used with the corresponding parameters to use the TROE formalism [8] or the SRI formalism [9] to describe fall-off. Chaperone efficiencies may also be included to describe collision efficiencies of particular third bodies [2].

4.1.3 Transport database

Transport properties are necessary for several combustion models, especially where diffusion is included. In contrast, transport properties are unimportant in an insulated, perfectly stirred reactor where complete mixing is assumed,. The transport database is an assembly of chemical properties for each species. The first required piece of information is the character name to describe the particular molecule. Next, a coefficient is required to describe the molecular structure. This coefficient is 0 for single atoms, 1 for a linear, 2-D molecule, and 2 for a 3-D, nonlinear molecule. The third piece of information is the Lennard-Jones potential well depth in degrees Kelvin, followed by the Lennard-Jones collision diameter in Angstroms. Next is information on the dipole

moment of the molecule in Debye units, and the polarizability of the molecule in Ångstroms^3. The last required piece of information is the rotational relaxation collision number at 298 K [3].

4.2 Chemical models within CHEMKIN

As stated before, including the newest version of CHEMKIN, the CHEMKIN suite has the ability to model shock tubes, perfectly stirred reactors, diffusion flames, premixed flames, internal combustion engines, and more. Preassembled driver programs and executables exist to model several different reactive-flow phenomena using CHEMKIN II and ChemkinPro,.the gas-phase subroutine library from CHEMKIN II could be used as a basis to compile new models for several different systems of interest. In this dissertation, two different models were primarily used: SENKIN to model perfectly mixed, closed chemical reactors and PREMIX to model laminar, pre-mixed, 1-D flames.

4.2.1 Modeling shock tubes with SENKIN

The SENKIN program [10] was developed particularly to spontaneous ignition problems and may be applied in some cases for modeling shock tubes. This particular program considers several different iterations of the closed homogeneous reactor problem. The first three cases all assume the reactor is adiabatic and consider the system to be at either constant pressure, constant volume, or volume specified as a function of time. SENKIN also can be used to model systems where both the temperature and pressure are held constant or where the pressure is constant and the temperature is a function of time. In each case, the following three equations are solved:

$$\frac{dY_k}{dt} = V\dot{\omega}_k W_k \quad (k = 1, \ldots, K) \tag{4.5}$$

$$c_v \frac{dT}{dt} + p\frac{dv}{dt} + v\sum_{k=1}^{K} e_k \dot{\omega}_k W_k = 0 \qquad (k = 1, \ldots, K) \tag{4.6}$$

$$\rho = \frac{p\bar{W}}{RT} \tag{4.7}$$

where Y_k is the mass fraction of species k, t is time, V is the volume of the system, $\dot{\omega}_k$ is the molar production rate of species k by reaction, W_k is the molecular weight of species k, c_v is the constant-volume heat capacity, T is temperature, p is pressure, v is specific volume, e_k is the internal energy of species k, ρ is the mass desnsity, $\bar{W}$ is the average molecular weight of the mixture, and R is the universal gas constant. In all cases, the terms are for the mixture unless indicated by a subscript k, where k refers to the kth species of K total species. Further details for the SENKIN model may be found in [10].

4.2.2 Modeling flat flames with PREMIX

The PREMIX flame code [4] is used to model flat flames such as flames analyzed by MBMS. This code solves for a one-dimensional, premixed flame using a Newton's method solver and finite differencing for two situations: either a burner-stabilized flame, where either an experimental temperature profile is specified or heat losses are known to be negligible, or an adiabatic, freely propagating flame, where the temperature profile is unknown. In each case, the following four equations are solved for a steady-state flame at constant pressure:

$$\dot{M} = \rho u A \tag{4.8}$$

$$\dot{M}\frac{dT}{dx} - \frac{1}{c_p}\frac{d}{dx}\left(\lambda A\frac{dT}{dx}\right) + \frac{A}{c_p}\sum_{k=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dx} + \frac{A}{c_p}\sum_{k=1}^{K}\dot{\omega}_k \hbar_k W_k = 0 \qquad (4.9)$$

$$\dot{M}\frac{dY_k}{dx} + \frac{d}{dz}(\rho A Y_k V_k) - A\dot{\omega}_k W_k = 0 \quad (k = 1, \ldots, K) \qquad (4.10)$$

$$\rho = \frac{p\overline{W}}{RT} \qquad (4.11)$$

where $\dot{M}$ is the mass flow rate, ρ is the mass density, u is the fluid velocity, A is the cross-sectional area of the stream tube encompassing the flame, taken to be unity and constant by default, T is temperature, c_p is the constant-pressure heat capacity, λ is thermal conductivity, Y is the mass fraction, V is the diffusion velocity, $\dot{\omega}$ is molar rate of production by chemical reaction per unit volume, h is specific enthalpy, W is the molecular weight, p is the pressure, $\overline{W}$ is the average molecular weight of the mixture, and R is the universal gas constant. In all cases, the terms are for the mixture unless indicated by a subscript k, where k refers to the k^{th} species of K total species.

The boundary conditions for this system are different for the burner-stabilized and freely propagating cases. In the case of burner-stabilized premixed flames, the temperature, total flow rate, and mass fractions at the burner are known. At the exhaust boundary, a boundary condition is imposed such that all gradients go to zero, and at the burner surface, a Danckwerts boundary condition is applied. For the freely propagating flame, the mass flow rate must be determined, so an additional boundary condition is needed. In this case, a temperature near the burner is fixed. More details on the model may be found in [4].

4.3 Post-processing CHEMKIN solutions

CHEMKIN model solutions provide a wealth of data for analysis. The first set of output data is the numerical solution of the model itself, providing concentration profiles as functions of time or space, temperature profiles, and when appropriate, ignition delay times. These data can be directly compared to experimental data when available, providing a one-to-one comparison for model validation. Perhaps more insightful for the modeling, however, is reaction path analysis and sensitivity analysis as a secondary evaluations of the model.

4.3.1 Reaction path analysis

In the CHEMKIN model, rates of production are calculable for each species and each reaction. The rate of production provides a measure of the contribution of each reaction to the formation or destruction of a particular species by calculating the molar production of a species per unit volume for each rate constant at each time or distance point in the model. Examination of the rates of production provides insight into which reactions are directly responsible for the evolution of a particular species concentration profile at a particular time or location.

The local rates of production can be further integrated across the entire area of interest or through the entire time of reaction to get an overall metric of species flux via a particular reaction. Normalizing these overall fluxes to a particular species and summing the fluxes for particular kinetic routes, a reaction path diagram can be assembled, highlighting the main kinetic pathways by which the reactants turn into product species. These diagrams are particularly important in discovering the mechanisms for fuel decomposition and pollutant formation.

4.3.2 Sensitivity analysis

A second form of reaction set analysis is sensitivity analysis, a second metric of reaction importance in the overall model. Instead of considering the direct contribution to species formation, sensitivity analysis considers reactions not related to a species of interest by observing the change in concentration of a species by varying rate constants. Specifically, the sensitivity analysis coefficients are calculated as follows [10]:

$$\left.\frac{\partial \ln X_i}{\partial \ln \alpha_j}\right|_{z,t} = \frac{\alpha_j}{X_i} \cdot \left.\frac{\partial X_i}{\partial \alpha_j}\right|_{z,t} \tag{4.12}$$

where X_i is the mole fraction of species i, and α_j is the rate coefficient of reaction j. The derivatives are evaluated locally at a specific time, *t*, and location, *z*. With this method, impact of reactions that do not directly involve species *i* can be assessed in terms of their influence on the concentration profiles of species *i*.

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CHAPTER 5

KINETICS OF AMMONIA: BUILDING AN H/N/O REACTION SET

Nitrogen chemistry plays an important role in combustion due to nitrogen content in coal [1], biofuels [2-3], and NO_x production from combustion with air [4-5]. Combustion with nitrogen-containing fuels and in the presence of air presents the potential of environmental impacts by pollutants such as amines, cyanides, and NO_x [6-12] are formed. For these reasons, a solid understanding of nitrogen chemistry under combustion conditions is critical. While nitrogen combustion chemistry has been previously studied extensively in the context of NO_x [13-14] and fuel-nitrogen conversion [15], current reaction sets to model nitrogen chemistry still need improvement.

To address these issues, a new reaction set was developed to describe combustion chemistry, focusing on systems containing only hydrogen, nitrogen, and oxygen for simplicity. This chapter first describes several relevant reaction sets and experimental studies that are available in the literature as well as and the ability of these models to predict a wide range of experimental data in comparison to the new H/N/O reaction set.

5.1 Previous H/N/O flame and shock tube studies

Several different experimental studies have been conducted in the past to elucidate the chemistry of nitrogen-containing compounds, several of which were conducted using MBMS flame studies.

Bian et al. [16] conducted an NH_3/O_2 flame experiment to understand fuel-nitrogen combustion better. The feed-mixture composition was fuel-lean: 48% NH_3, 51% O_2, and 1% Ar (Φ=0.70). The experiment again used a 5-cm-diameter Spalding-Botha

style burner, and it was conducted at a flow velocity of 60.8 cm/s and a pressure of 35 Torr (0.046 atm). Several mole fraction profiles were determined, including NH_3, O_2, Ar, N_2, H_2O, NO, N_2O, OH, H_2, NH_2, HNO, NH, O, and H. The study reported detection of NNH, but this assignment was questioned in the commentary following the conference presentation, which suggested it was an ionization fragment of N_2H_2 rather than a flame species.

In another MBMS study from the same group, Vandooren et al. [17] applied MBMS to a fuel-rich flame of 46.1% NH_3, 47.2% NO, and 6.7% Ar flame (fuel-equivalence ratio Φ=1.46) in hopes of a better understanding NH_2 + NO kinetics. The experiment used a 5-cm-diameter Spalding-Botha style burner and was conducted at a flow velocity of 60.0 cm/s and a pressure of 54 Torr (0.071 atm). In this experiment, the authors were able to obtain mole fraction profiles for major species NH_3, N_2, NO, Ar, H_2O, and H_2. Profiles for intermediate species H, N_2O and NH_2 were also sampled.

Duynslaegher et al. conducted a study on eight different flames of mixtures of NH_3, H_2, O_2, and Ar [18]. In this study, all the flames were heavily diluted with Ar (43-48% Ar) and were conducted at low pressures of 50-120 mbar (0.049-0.118 atm). The first four flame experiments (Flames I - IV) were all stoichiometric flames where O_2 concentrations were held at 21%. The ratio of NH_3 to H_2 was varied to show the effect of fuel mixture on the flame. Flames III, V, and VI explored the effect of fuel equivalence ratio, keeping the concentrations of NH_3 and H_2 at 22% and 10% respectively, while varying the amount of oxygen in the system from 20% to 24% (Φ = 0.9, 1.0, and 1.1). The last set compared Flame I with Flames VII and VII to explore pressure effects. These flames had different pressures (P = 60, 90, and 120 mbar; i.e., 0.059, 0.088, 0.118 atm)

but constant feed mixtures (25% NH_3, 5% H_2, 21% O_2, and 48% Ar). Mole fraction profiles were sampled for NH_3, NO, N_2, N_2O, H_2, and NH_2.

Another MBMS study was conducted by Sausa et al., examining H_2 mixtures with N_2O as the oxidant [19]. The objective of this study was to understand how ammonia aids the NO to N_2 conversion in flame conditions. In this experiment, a $\Phi \sim 1.1$ H_2/N_2O/~25% Ar flame was compared to the same flame doped with 4% NH_3. These flames were observed using a 6-cm-diameter burner at a pressure of 30 Torr (0.039 atm). Profiles were observed for NO, N_2O, H_2, H_2O, and N_2 for both flames. For the doped flame, NH_3 was also measured.

Lastly, a shock-tube study was also considered. Davidson et al. looked at several different shock-tube species time-history experiments for ammonia pyrolysis [20]. Experiments were conducted from 2200-3300 K and 0.75-1.025 atm. Ammonia concentrations were 1000, 3000, 8000, and 10000 ppm NH_3 in Ar. Species time histories were recorded for NH_2 and NH radicals. For each of the different ammonia mixtures, trend lines were plotted for temperature vs. peak mole fraction of NH_2 and NH, as well as for temperature vs. time of peak mole fraction of NH_2 and NH.

5.2 Performance of previous models

There have been several published modeling studies to describe the combustion chemistry of ammonia over the last few decades. The most prominent early review of nitrogen combustion chemistry is the widely cited 1989 paper of Miller and Bowman [15]. As in the present work, Miller and Bowman conducted an extensive study of the then-current status of nitrogen kinetics, exploring the different routes for NO_x production and testing their detailed mechanism against several sets of experimental data to cover a

wide range of conditions. The study relied heavily on sensitivity analysis of rates of production to determine key reaction routes and propose the mechanism by which fuel nitrogen may be converted into NO_x and N_2. The resulting mechanism has been updated steadily by Miller since the 1980s, and he has shared it here for comparison purposes. This newer mechanism will be henceforth referred to as the "Miller mechanism" [21].

Further advancements in nitrogen kinetic modeling were achieved with the 1999 release of GRI-Mech 3.0 [22]. The goal of GRI-Mech 3.0 was to describe the combustion of natural gas and is widely used today still for that purpose, including NO_x chemistry was included to describe the chemistry of air-based combustion and NOx formation. Its central idea was to refine parameters within their uncertainties by comparison to a set of experimentally measured target characteristics.

The 2000 review of Dean and Bozzelli in [23] sought to build upon the work of Miller and Bowman [15] as well as other studies to provide an updated table of rate constants for nitrogen kinetics. Perhaps the most significant improvement in the text was the inclusion of pressure (third-body) dependences via Quantum-RRK theory.

Glarborg and his co-workers have made many recent contributions to nitrogen kinetic modeling. Several extensive and improved H/C/N/O reaction sets have been published through these collaborations, including modeling of an ammonia/ methane/oxygen flame [24]. That reaction set has been further improved through a joint experimental and modeling study on ethyl amine and dimethyl amine flames with O_2 [25]. Additionally, in collaboration with Steven Klippenstein at Argonne National Laboratory, the Glarborg reaction set was used as a base set for improving the description of NNH's role in NO_x production [26].

Nitrogen kinetic modeling has also been driven by the need to describe propellant combustion. One of the earlier advances in nitrogen-containing propellant kinetic modeling was the development of a database to provide kinetic rate constants for propellant combustion [27]. In this work, Tsang and Herron catalogued reaction rate coefficients for several different nitrogen-species reactions by fitting to experimental data and employing RRKM theory for pressure dependence. This database has been used heavily for constructing several other propellant mechanisms, including the monomethyl hydrazine/ red fuming nitric acid reaction set of Anderson et al. [28]. Additional propellant models have been published, including a monomethyl hydrazine pyrolysis reaction set by Sun et al. [29] and a dicyanamide reaction set by Catoire et al. [30].

In this study, an improved set and several of the existing reaction sets were used to model the different H/N/O flames of Bian et al. [16], Sausa et al. [19], Vandooren et al. [17], and Duynslaegher et al. [18]. Simulations were run using the Chemkin PREMIX program [31] using ChemkinPro [32]. The literature-model results were compared without any adjustment of the model to the experimental data such that there is a direct comparison to the experimental data. Models selected for comparison were the ARL mechanism [28], the reaction set from Catorie et al. [30], GRI Mech 3.0 [22], the most recent Glarborg reaction set [25], the updated Glarborg mechanism from Klippenstein et al. [26], and the updated Miller mechanism [21]. The reaction sets of Tsang and Herron [27], Dean and Bozzelli [23], and Sun [29] were not sufficiently complete to use across such a wide range of data and thus were not included for comparison.

Agreement of the predictions with the reported data is subject to uncertainties in the data and in the modeling. The sampling probe perturbs experimental temperature in

magnitude and position, and the temperature used for modeling may not capture this perturbation sufficiently well. Reported positions of the experimental mole fractions are slightly shifted by fluid-mechanics and temperature effects, but the principal source of uncertainty is expected to be the magnitude calibration. Direct MBMS calibration should give mole fractions within 25%, while ionization cross-sections are expected to give calibrations within a factor of two [33].

5.2.1 Existing models compared to fuel-lean NH_3/O_2 flame of Bian et al.

The ammonia/oxygen flame of Bian et al. [16] had the most extensive listing of mole fraction profiles among the literature experimental studies. Figure 5.1 shows the mole fraction profiles for the seven main species sampled experimentally: NH_3, O_2, N_2, H_2O, H_2, Ar, and NO. The reported experimental temperature profile was used for all predictions.

Performance of the existing models varies among the different species. In general. NH_3, O_2, and Ar profile predictions are reasonable, subject to the question of experimental uncertainties, while N_2 and H_2O appear overpredicted and H_2 and NO appear underpredicted. The authors do not indicate what the calibration uncertainties are, but a factor of two or less would be expected. Note that the post-flame convergence of most profiles suggests that deviation from the data may be due to temperature uncertainty, which could cause a different post-flame equilibrium level. The ARL set performs best, but the Catoire reaction set, Glarborg reaction set, and Klippenstein reaction set all perform similarly to it. The main differences arise in the H_2 and NO profiles; all four reaction sets underpredict H_2 to varying degrees, while NO predictions for the ARL mechanism are comparable to the Glarborg reaction set and slightly better

than the Catoire reaction set. The Klippenstein reaction set predicts NO quite well. The Miller mechanism is also off, though not much more than the other four reaction sets. The largest deviations involve the older GRI-Mech 3.0.

For the seven intermediate species profiles (Fig. 5.2), model predictions vary much more than for the main species profiles. While it did not appear to give the best predictions for the main species, the Miller mechanism predicts the intermediate species best overall, with near perfect agreement for N_2O and NH_2. It also performs best for the H, O, HNO, and OH predictions, although no model has excellent agreement with those experimental data. GRI-Mech 3.0 is the least satisfactory set for predicting the intermediate species, having the worst predictions for every intermediate species profile except HNO.

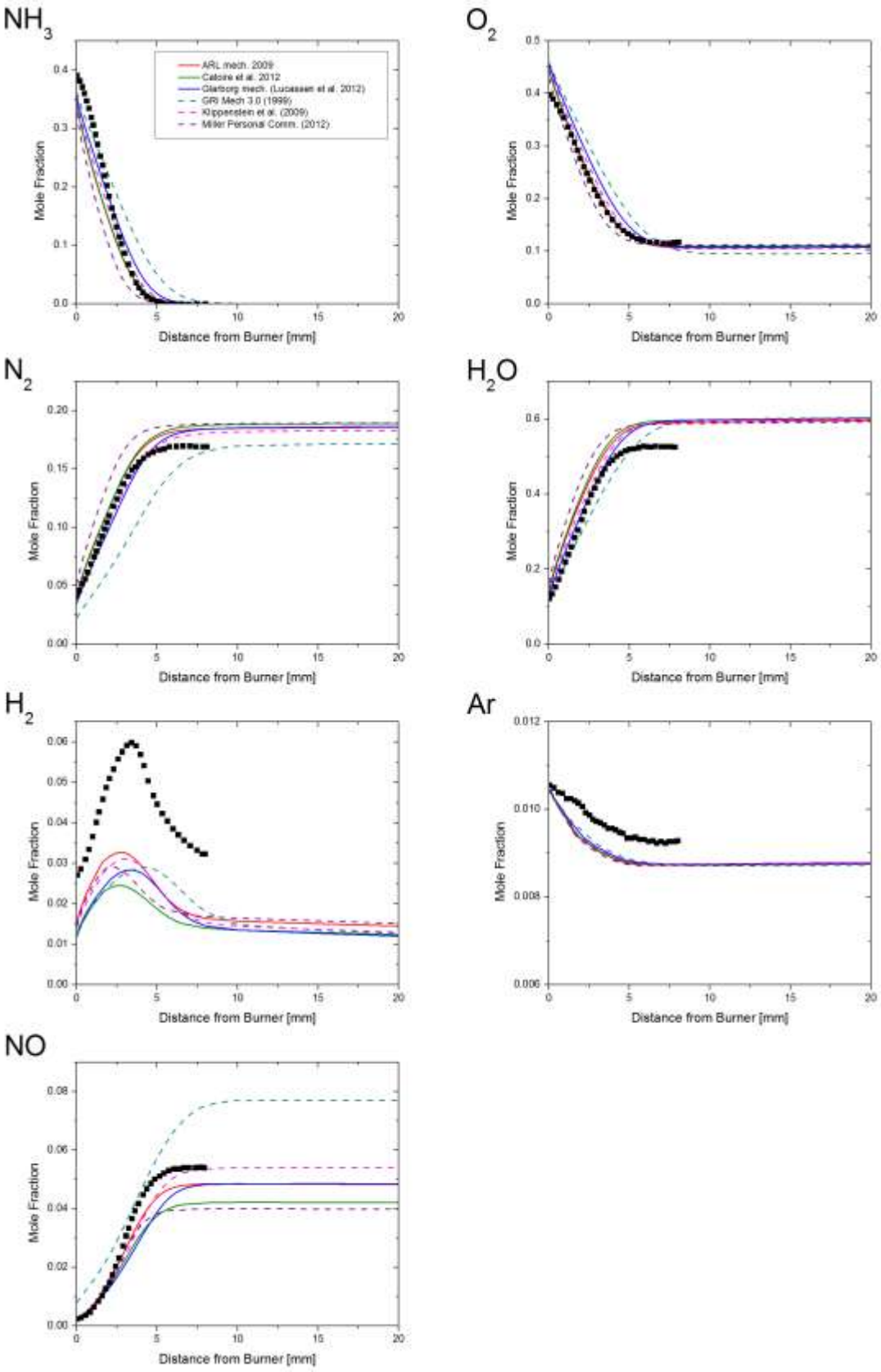

Figure 5.1: Comparison of previous models to data from Bian et al. (main species).

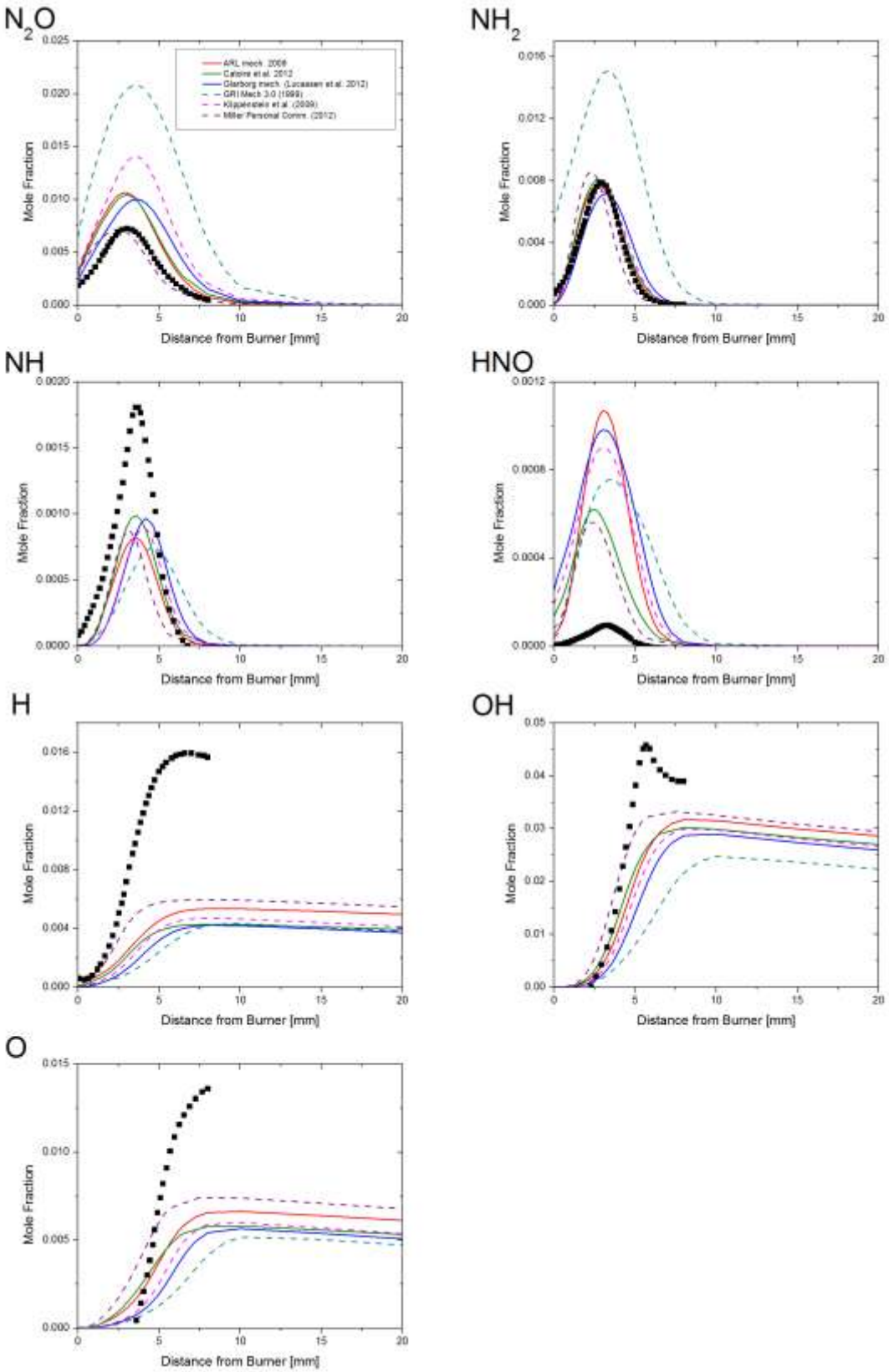

Figure 5.2: Comparison of previous models to data from Bian et al. (intermediate species).

5.2.2 Existing models compared to NH_3/NO flame of Vandooren et al.

The study by Vandooren et al. [17] was conducted on an NH_3/NO/Ar flame and provided mole fraction profiles for nine different species (see Fig. 5.3). In comparing the results of the models, the degree to which they matched the experimental data was quite consistent. The ARL and Miller mechanisms produced quite similar results while also providing the best agreement to the data overall. The only significant differences between the two were the results for H-atom and N_2O. The Miller mechanism had a better H prediction, though still quite a bit lower than the experimental data, and also a better N_2O prediction, which was in excellent agreement with the data.

The Glarborg and Catoire reaction sets gave the overall next best agreement, closely followed by the model results of the Klippenstein reaction set. Although generally slow in comparison to the other models, the Klippenstein reaction set did predict the NH_2 profile best. The GRI-Mech 3.0 results gave the poorest predictions in comparison to the experimental data because reactions of NH_3 + NO (the only oxidizer) were not present.

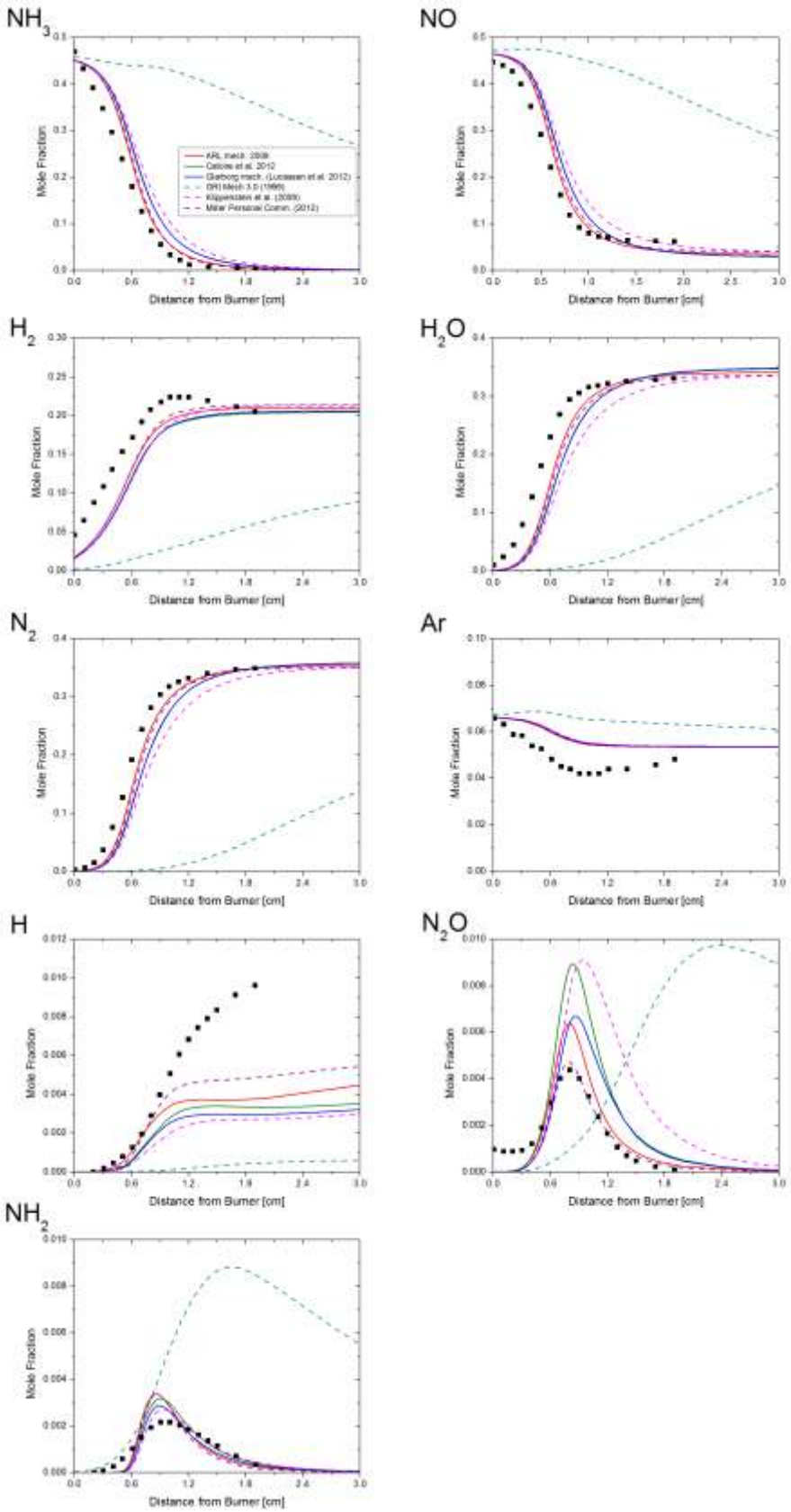

Figure 5.3: Comparison of previous models to data from Vandooren et al..

5.2.3 Existing models compared to $H_2/N_2O(/NH_3)$ flames of Sausa et al.

The Sausa et al. study [19] was a series of two different H_2/N_2O/Ar flames. The first flame was fed with ammonia but the second was doped with 4% ammonia. The undoped flame (see Fig. 5.4) had mole fraction profiles for N_2O, H_2, N_2, NO, and H_2O. Overall, the models match the experimental data well. GRI-Mech 3.0, the Klippenstien reaction set and the ARL mechanism are somewhat slow in N_2O decomposition rate and in N_2 and H_2O formation. The main modeling issues for the undoped flame involve NO predictions. Each of the models greatly overpredicts the NO concentration profiles. The Catoire reaction set performs the best, but it still is high by about 0.02 mole fraction.

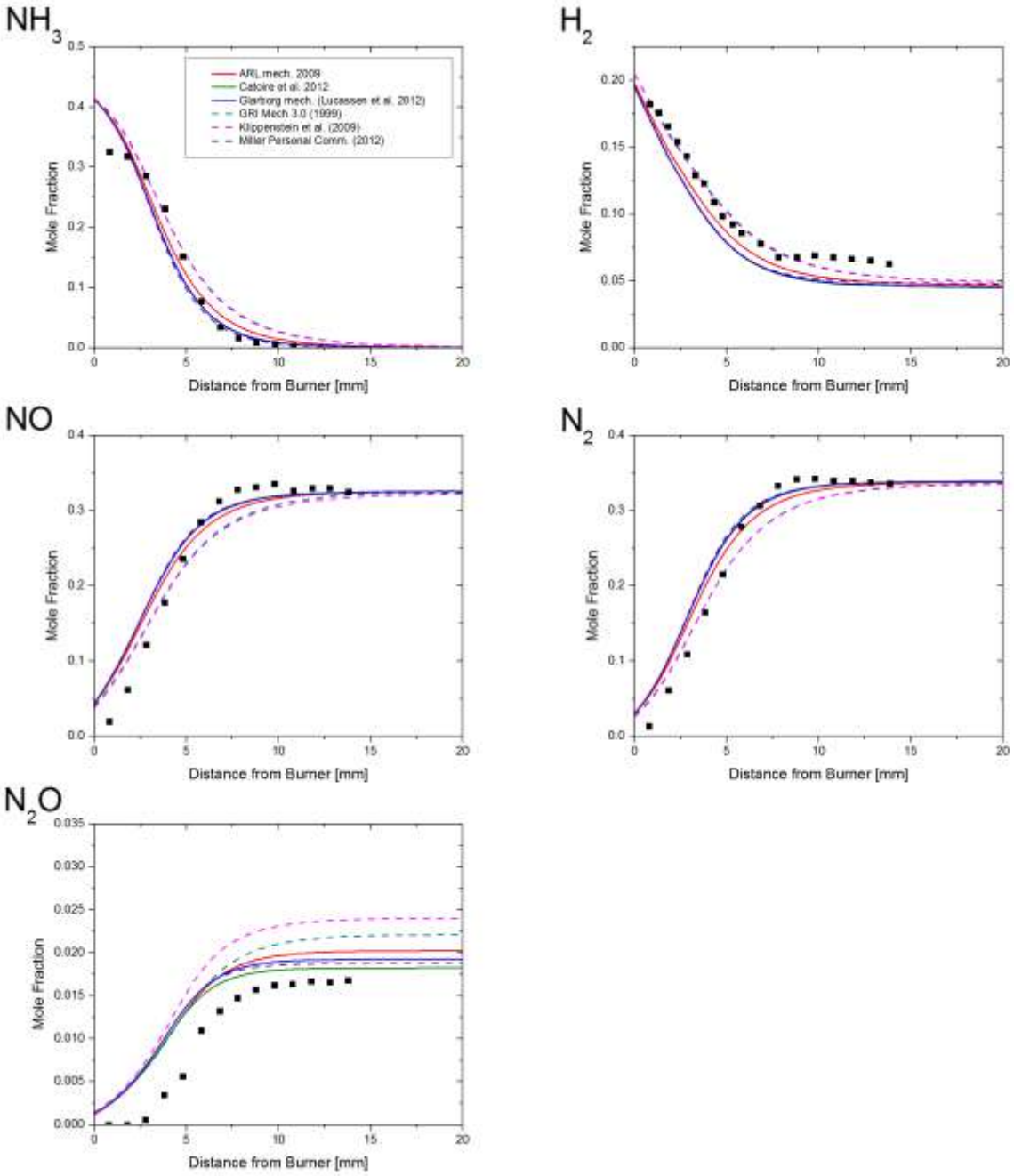

Figure 5.4: Comparison of previous models to data from undoped experiment of Sausa et al.

The undoped flame (see Fig. 5.5) had mole fraction profiles for N_2O, H_2, N_2, NO, and H_2O, as well as NH_3. With the addition of ammonia, overall model performance declines significantly for all models with the exception of the Miller mechanism. The

N_2O and NH_3 profiles are greatly overpredicted by all but the Miller mechanism. H_2O and N_2 formation is too slow across the board for the other reaction sets as well. Despite the generally good agreement of the Miller mechanism, it overpredicts the NO profile by about a factor of two. The NO profile is overpredicted by all the other reaction sets, but not as much.

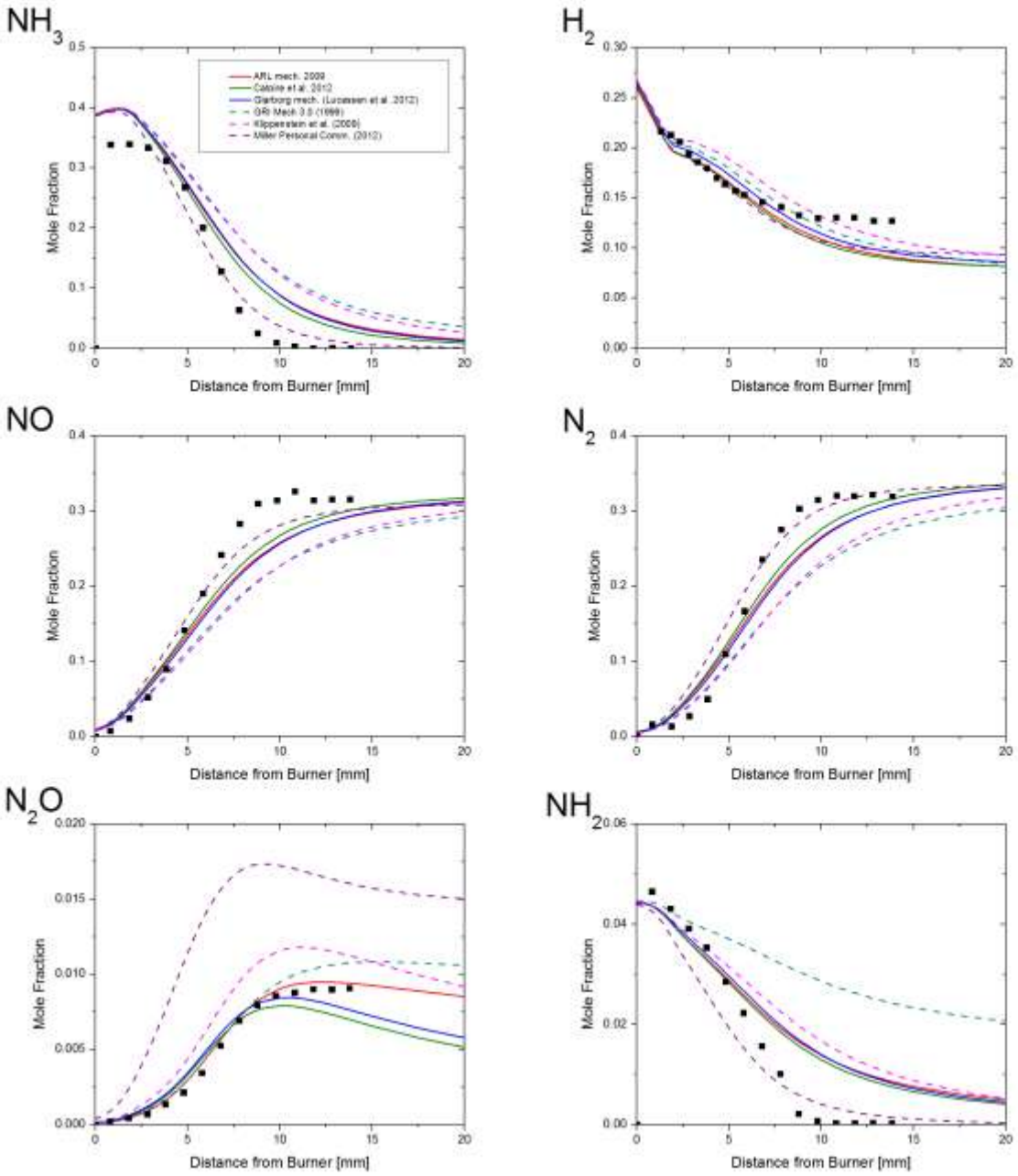

Figure 5.5: Comparison of previous models to data from NH_3-doped experiment of Sausa et al.

5.2.4 Existing models compared to H_2/NH_3 flames of Duynslaegher et al.

Duynslaegher et al. [18] examined several different $H_2/NH_3/O_2/Ar$ flames varying in feed composition, stoichiometry, and pressure.

The first four flames, Flame I (Fig. 5.6), Flame II (Fig. 5.7), Flame III (Fig. 5.8), and Flame IV (Fig. 5.9), are stoichiometric but vary the feed ratio of H_2 and NH_3. The feed concentration of H_2 increases with each flame, with the lowest concentration of H_2 in Flame I and the largest concentration of H_2 in Flame IV. Ammonia profiles for Flames I-IV are modeled well in general, improving as the ratio of H_2 to NH_3 increases. Overall, the GRI-Mech 3.0 model results are unsatisfactorily slow. The same trend is also valid for N_2. H_2 is predicted well for all four flames with the exception of GRI-Mech 3.0, capturing the bump in the experimental data between 5 and 10 mm from the burner. N_2O is generally underpredicted, and NH_2 is generally overpredicted by all models with the exception of GRI-Mech 3.0 by a factor of 2. GRI-Mech 3.0 overpredicts both N_2O and NH_2 with a broadened peak width. The last set of mole fractions, those for NO, are significantly underpredicted by all models. Although the ARL set generally does the best, the predictions are off by several mole percent.

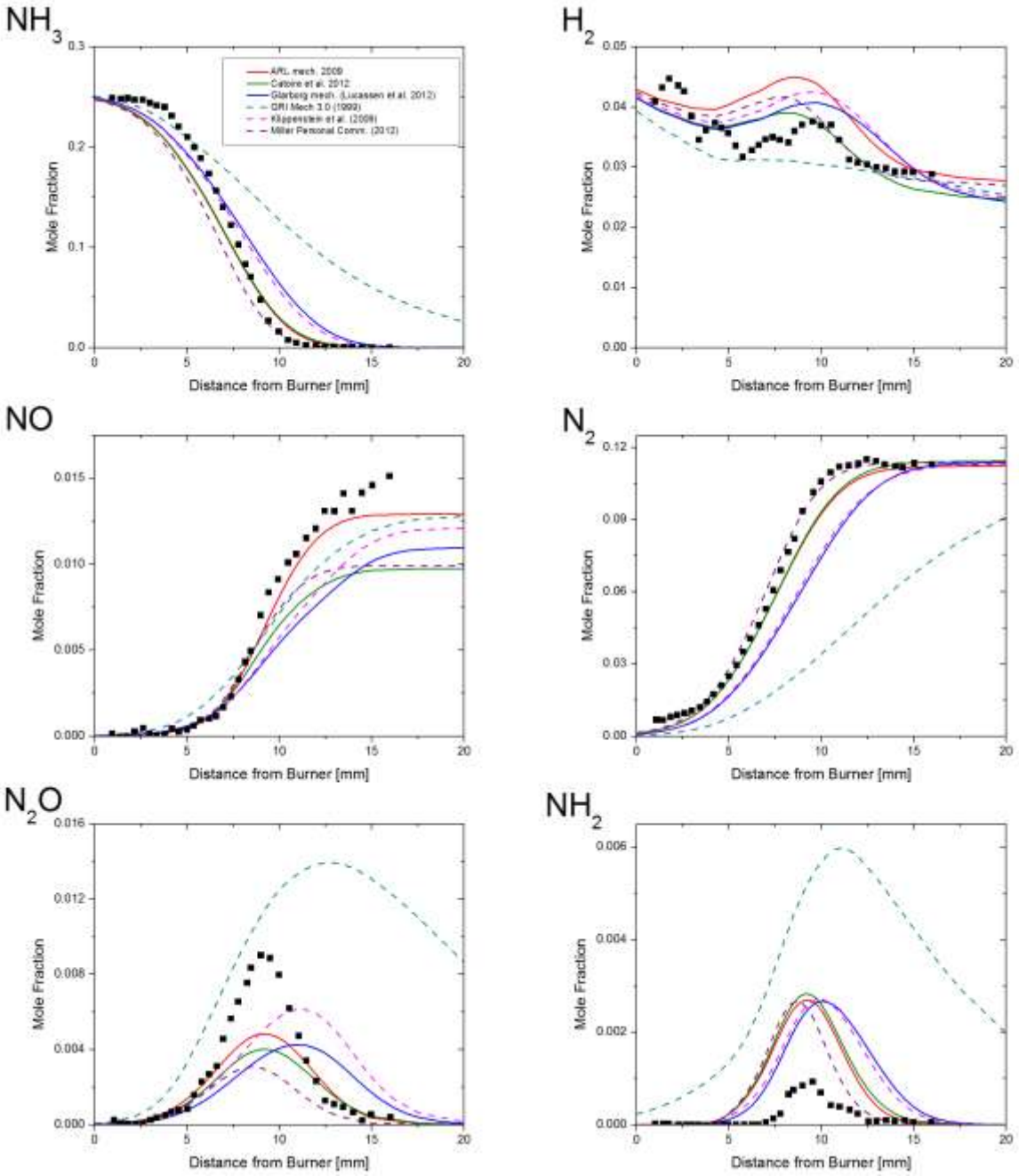

Figure 5.6: Comparison of previous models to data from Flame I of Duynslaegher et al.

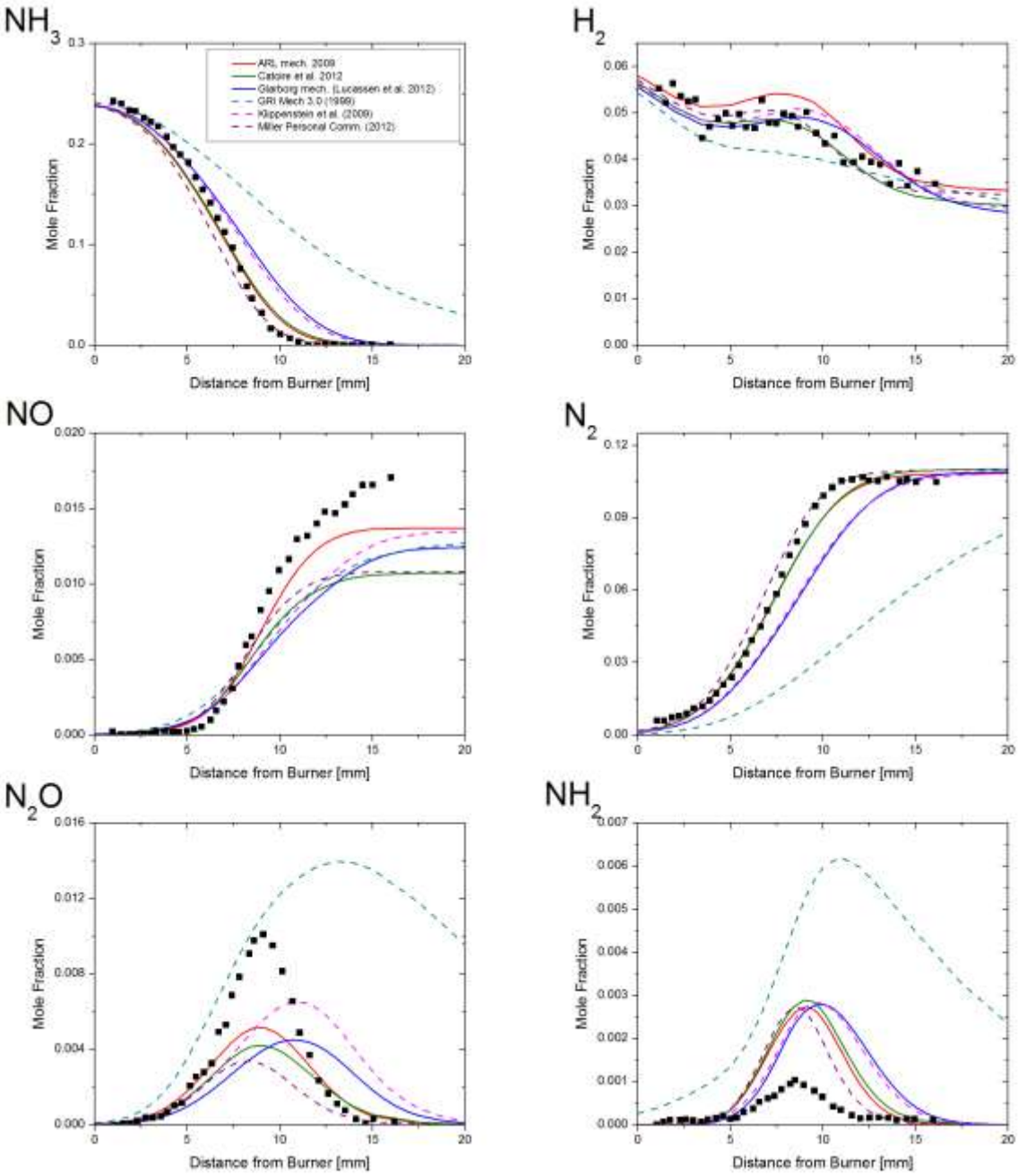

Figure 5.7: Comparison of previous models to data from Flame II of Duynslaegher et al.

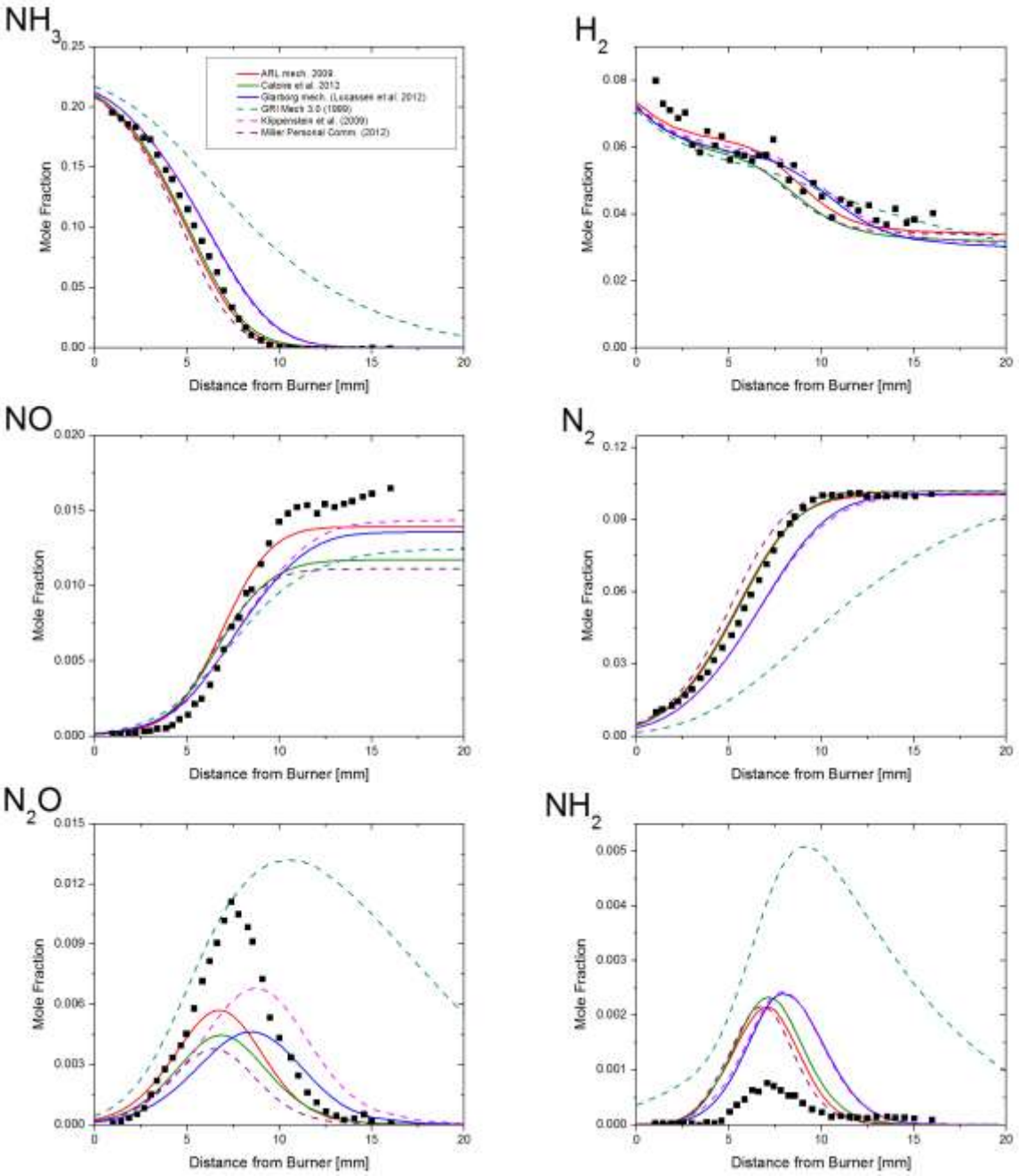

Figure 5.8: Comparison of previous models to data from Flame III of Duynslaegher et al.

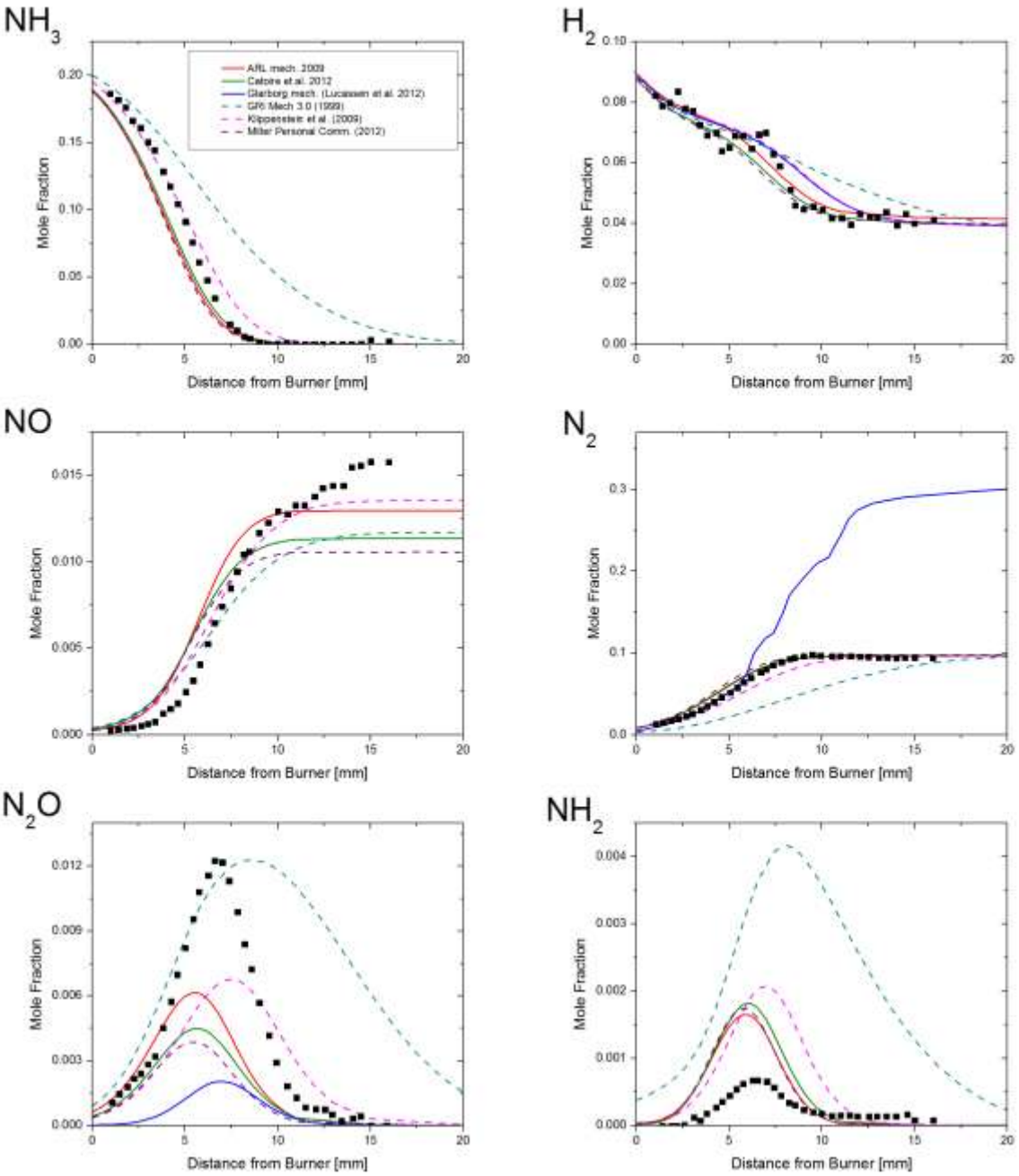

Figure 5.9: Comparison of previous models to data from Flame IV of Duynslaegher et al.

The second set of Duynslaegher flames compares effects of fuel equivalence ratio with a stoichiometric Flame III (Fig. 5.8), a slightly fuel-lean ($\Phi = 0.9$) Flame V (Fig. 5.10), and a slightly fuel-rich ($\Phi = 1.1$) Flame VI (Fig. 5.11). The mole-fraction

predictions for the stoichiometric and lean flames are quite similar to each other with the exception of NO profiles. The disagreement for all models with the experimental data for NO in the lean flame is even worse than for the stoichiometric flame. For the fuel-rich flame, the experimental data profiles are broadened in comparison to the stoichiometric and fuel-lean flames. The models are unable to capture the broadening and, as a result, fare worse in agreement in comparison to the fuel-lean and stoichiometric flames. The NO profile is predicted somewhat better in comparison to the other flames. however, and it is most closely modeled by the ARL set.

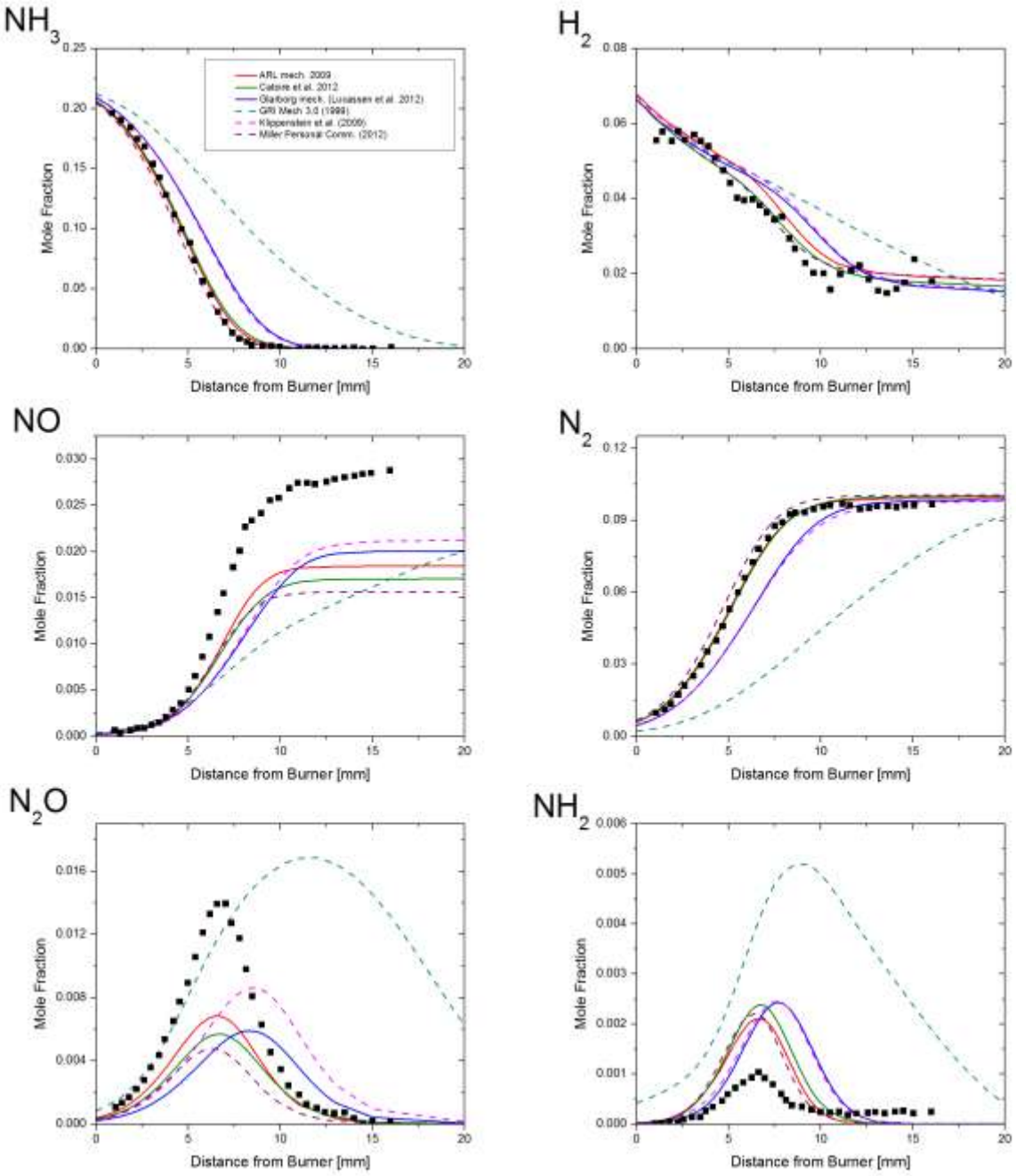

Figure 5.10: Comparison of previous models to data from fuel-lean Flame V of Duynslaegher et al.

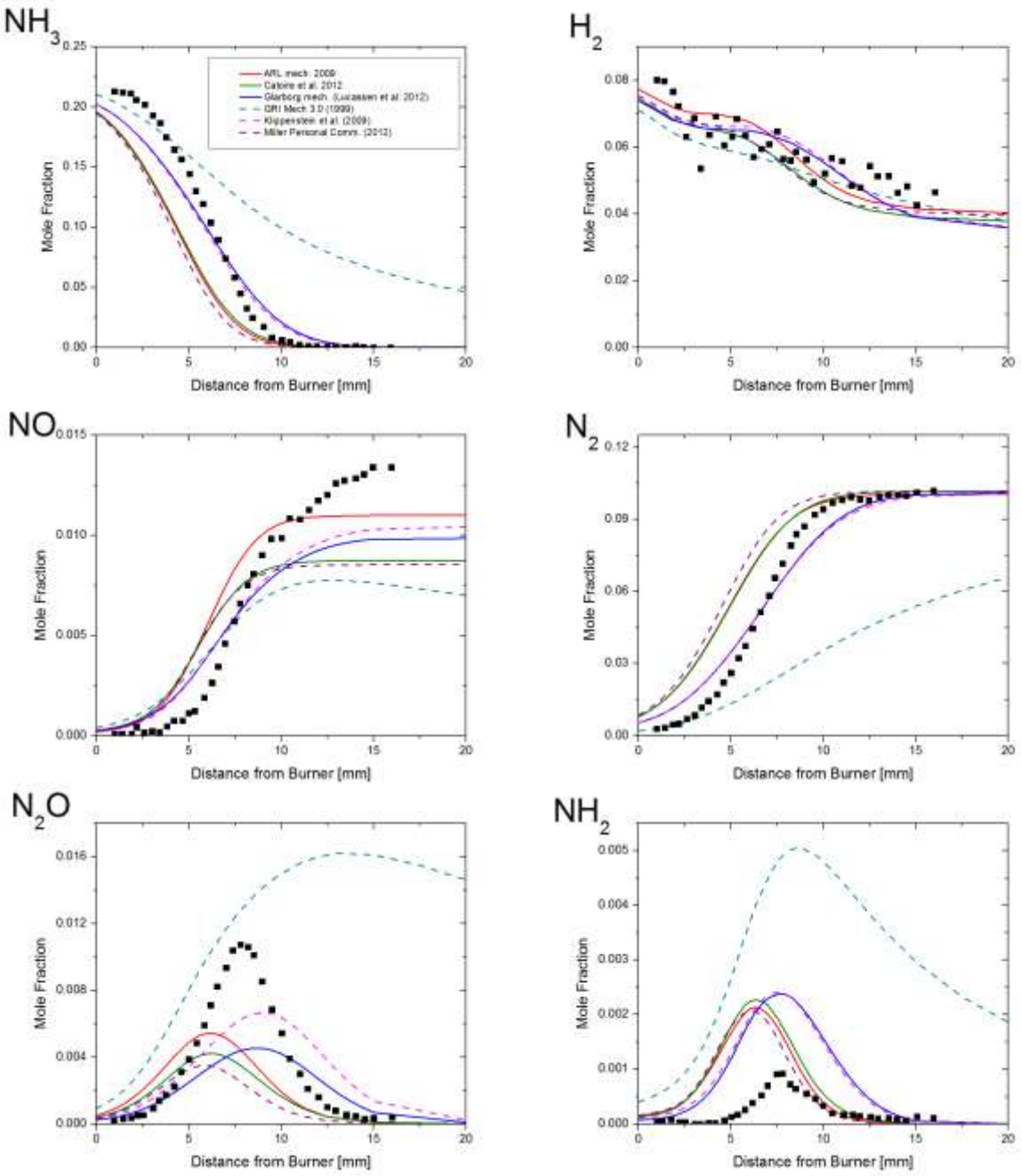

Figure 5.11: Comparison of previous models to data from fuel-rich Flame VI of Duynslaegher et al.

The last experimental set explores the effect of pressure, increasing pressure from 60 mbar for Flame I (Fig. 5.6) to 90 mbar for Flame VII (Fig. 5.12) and 120 mbar for Flame VIII (Fig. 5.13). For Flame VIII, the double peak in NH_2 seems unphysical, but the

comparison is still presented. Going from low pressure (60 mbar) to the mid-range pressure (90 mbar), modeling results are similar. Most significantly, the NO profile predictions are in better agreement with the experimental data (best described by ARL mechanism), although with a wide scatter among all model profiles. At the highest pressure, the disagreement between the models and the experimental data becomes much more significant.

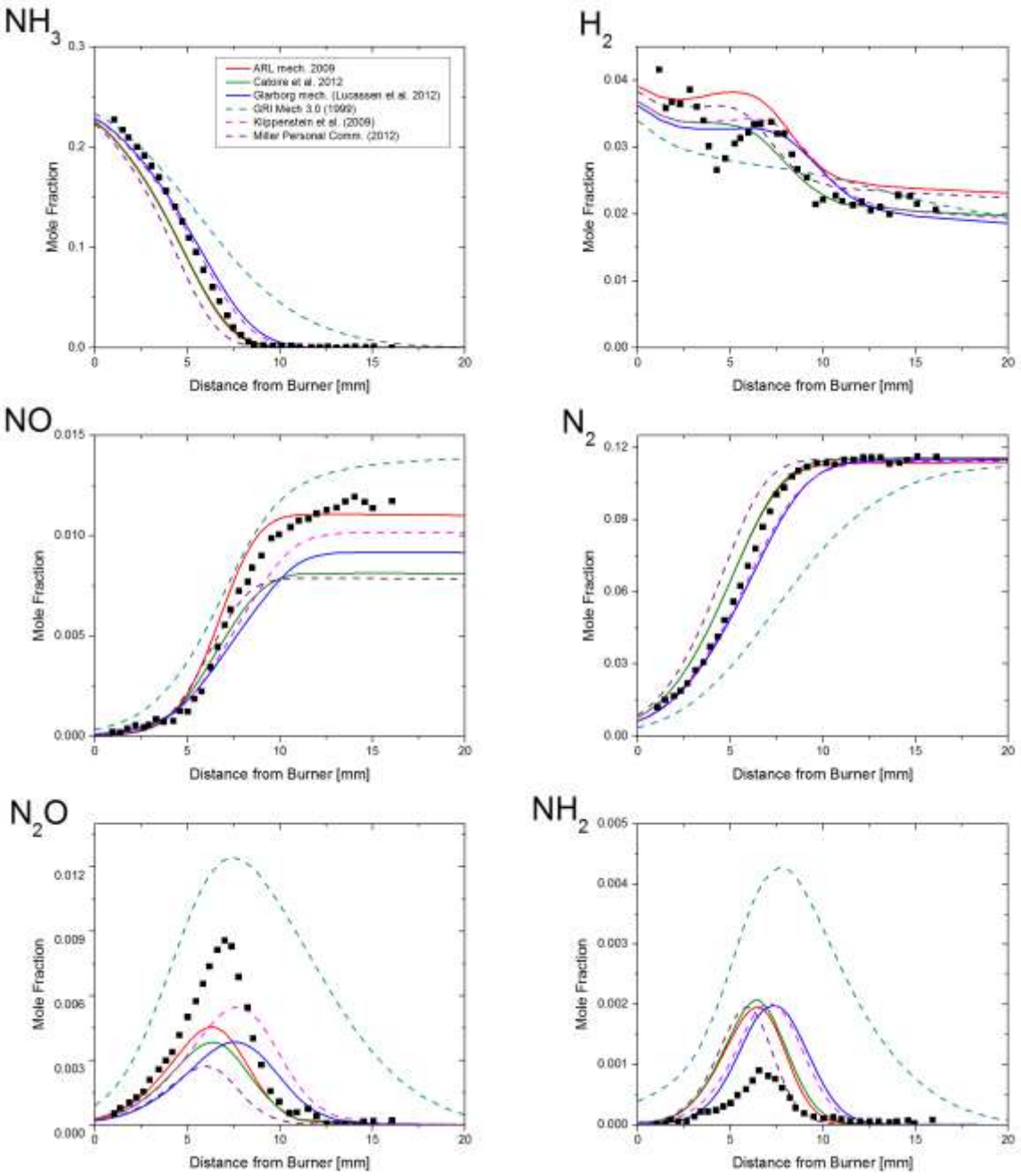

Figure 5.12: Comparison of previous models to data from 90-mbar Flame VII of Duynslaegher et al.

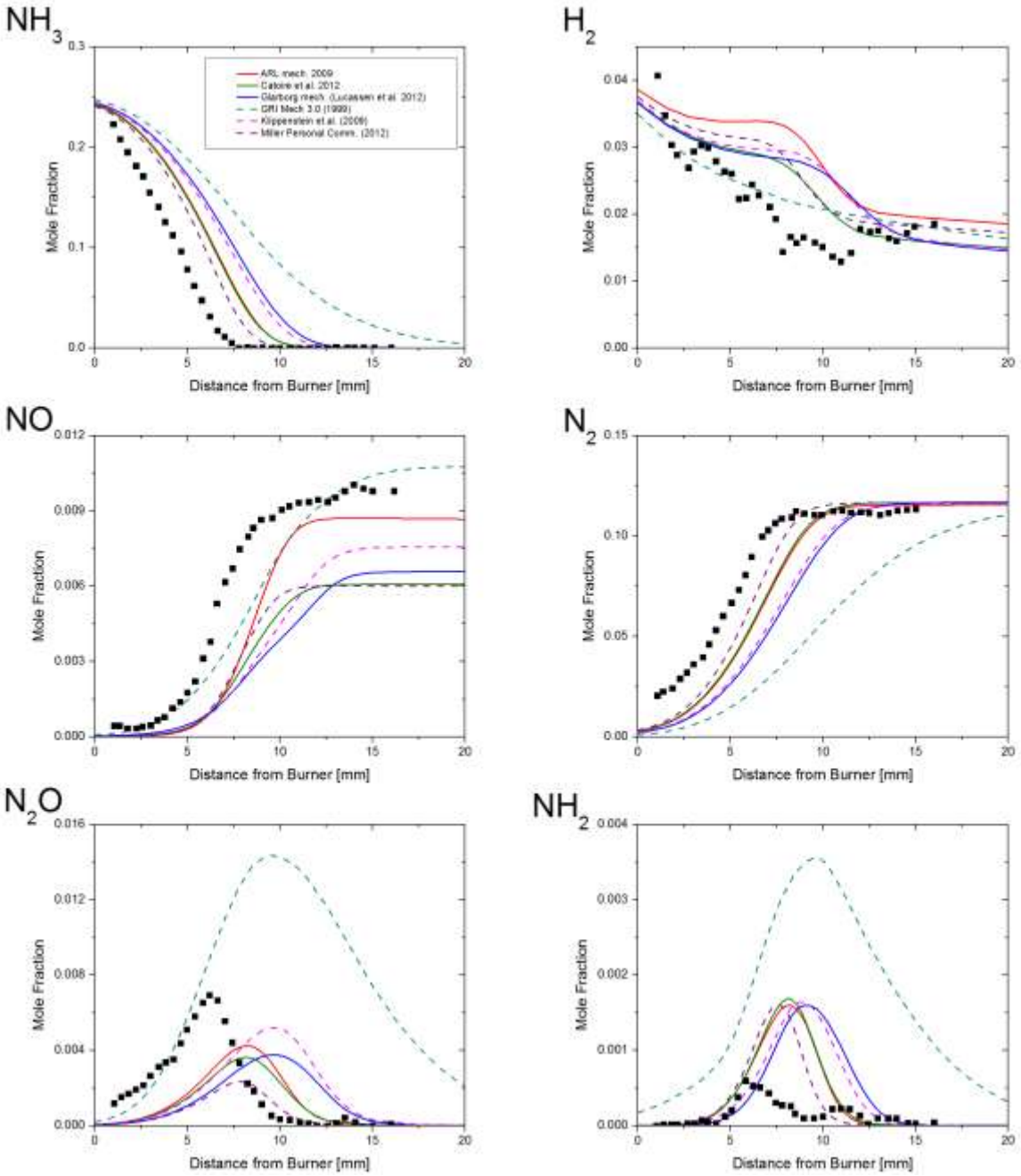

Figure 5.13: Comparison of previous models to data from 120-mbar Flame VIII of Duynslaegher et al.

Overall, agreement between experimental data from the selected H/N/O flames and the models is fair but reveals many issues to be resolved. Many of the models often are unable to predict NO profiles, as well as intermediate species such as NH_2 and N_2O.

The Miller mechanism in general does the best job describing the H/N/O flames (especially for N_2O). GRI-Mech 3.0, which was not designed to model nitrogen combustion, does the worst overall.

5.2.5 Global sensitivity analysis to identify key rate constants

In order to identify the key model reactions in these different flames, local sensitivity analysis was performed for all species in each of the models for all 12 flame studies. The top 10 most sensitive reactions for each species were determined for each flame model, using $\partial(\ln x_i)/\partial(\ln k_j)$ as a measure of sensitivity to rate constants. Finally, the absolute values for the sensitivities were summed for each reaction over all flames and over all models with the exception of GRI-Mech 3.0. This overall sensitivity was then ranked from highest to lowest. The top 25 overall most sensitive reactions for modeling H/N/O chemistry are shown in Fig. 5.14.

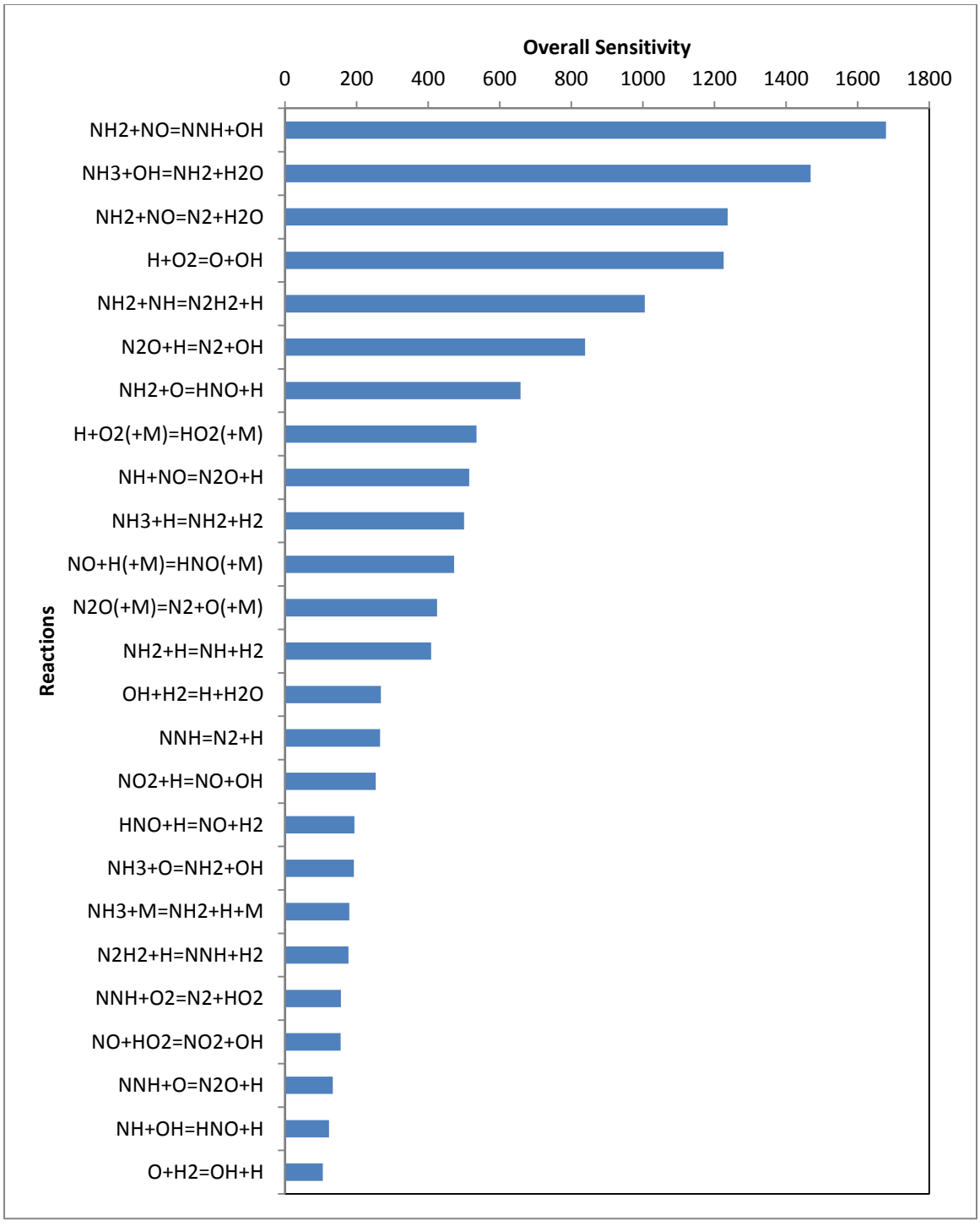

Figure 5.14: Overall sensitivity analysis for all 12 MBMS flame experiments showing the 25 most sensitive reactions.

Sensitivity analysis shows that the most sensitive reaction overall is the NH_2 + NO <=> NNH + OH reaction, followed by NH_3 + OH <=> NH_2 + H_2O, NH_2 + NO <=> N_2 + H_2O, and H + O_2 <=> OH + H. As expected with several ammonia flames studied, NH_3, NH_2, and NH reactions are often among the top 25 most sensitive. Also common are reactions in the hydrogen peroxide part of the mechanism. Lastly, the NNH and N_2O parts of the mechanisms play a large role in the models, appearing 5 and 4 times in the top 25 most sensitive reactions list, respectively.

5.3 Development and testing of the new reaction set

In order to address the discrepancies between the experimental data and the models, a new reaction set for H/N/O combustion has been developed and tested against the same experimental data for validation. The approach of this work was to catalogue the reaction rate constants that were available in several models [21-22,24-26,28,30] as well as several other sources [23,27,29,34]. Additionally, the H_2O_2 chemistry from the acetylene set of Li [35] was incorporated into the reaction set. These reaction rates, including duplicates, were assembled into one master reaction set that is available in Appendix C. The result is the most extensive reaction set H/N/O combustion to date.

Initially, a first-pass selection of rate constants was completed by eliminating rate constants with unphysical behavior. Rate constants with fall-off were preferentially selected over rate constants that neglected it. Starting from the initial set, several iterations of the reaction set were then tested against the experimental data, focusing heavily on rate constants that appeared on the most sensitive reaction list and tailoring the set to the rate constants in models where agreement was superior to other models. Thermochemistry was also assembled for all species in the H/N/O reaction set. There

were few differences between the thermodynamic databases of the models, with the largest updates involving O/H species from [36].

The resulting reaction set has a total of 43 different species and 307 elementary reactions. This new set was used to model all 12 flame experiments [16-19] used to compare the existing models' performance as well as a shock-tube pyrolysis study [20]. Overall, the model performs as well or better than the existing models. The following is a discussion of the new model's performance in context of both the experimental data and the existing models.

5.3.1 Testing the new model against fuel-lean NH_3/O_2 flame of Bian et al.

For the flame of Bian et al. [16], performance of the existing models varied among the different species. For NH_3, as seen in Fig. 5.15, the new model predicts decomposition faster than the experimental data and is in line with the ARL mechanism's predictions. O_2 predictions are quite good. Both N_2 and H_2O are slightly overpredicted, but no more so than by the other models. The Ar profile shows one of the biggest differences, with the new model having much lower concentrations at the burner. Improvements were observed for H_2, where the new model still underpredicts the experimental data but is the closest of all the models, and for NO, which predicts the data remarkably well.

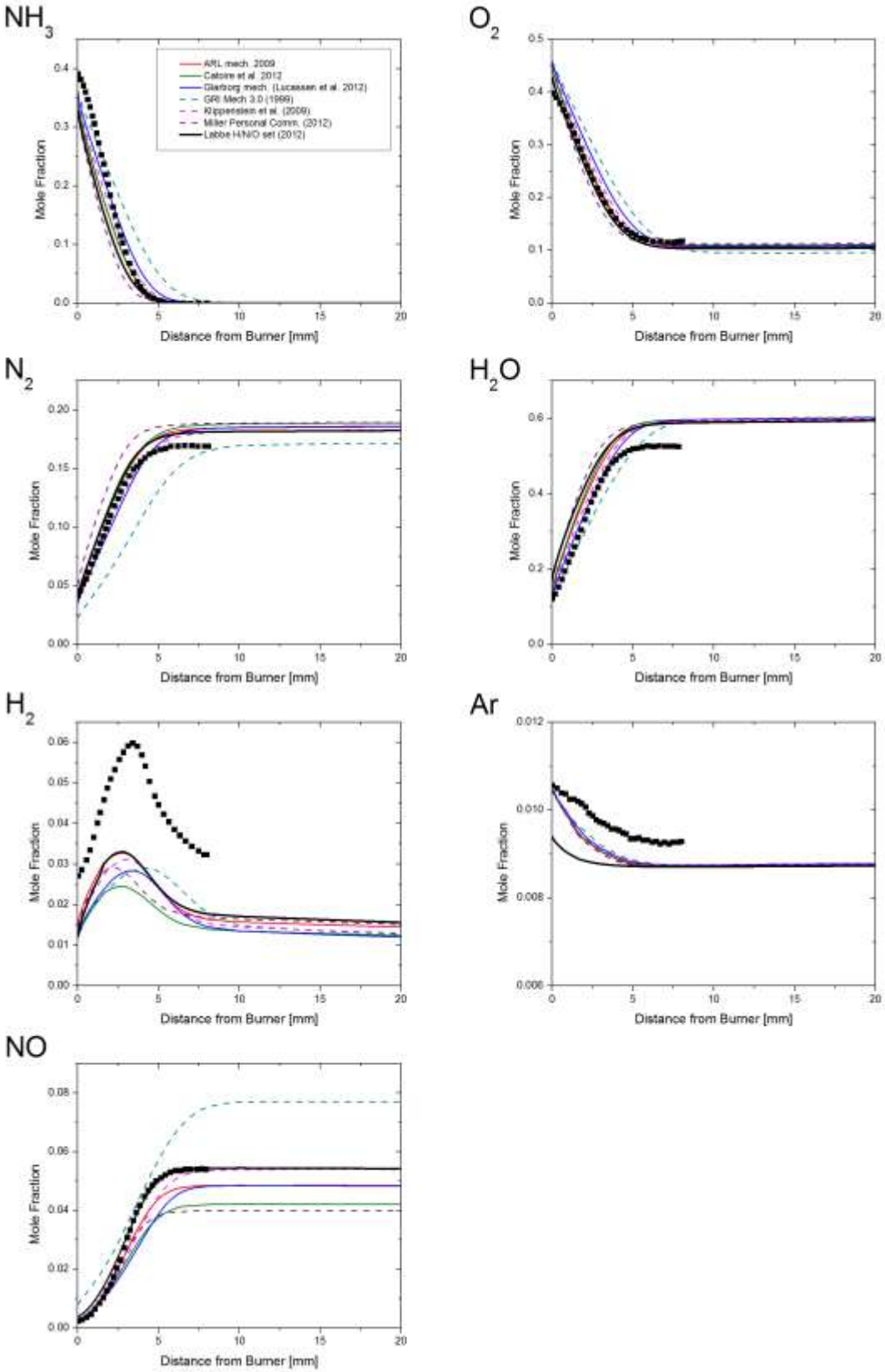

Figure 5. 15: New model results for flame of Bian et al. compared to previous models (main species).

For the intermediate species predictions (Fig. 5.16), the new model gives similar results to the previous models. N_2O and NH_2 are predicted as well as by the Miller mechanism, which had the best agreement of the other models. The NH prediction is somewhat lower than the other models, but still in the same range. HNO is still overpredicted significantly, but it is among the lowest peak predictions of all models. H, O, and OH profiles have slight improvements over the other models, but are still quite low compared to the experimental data.

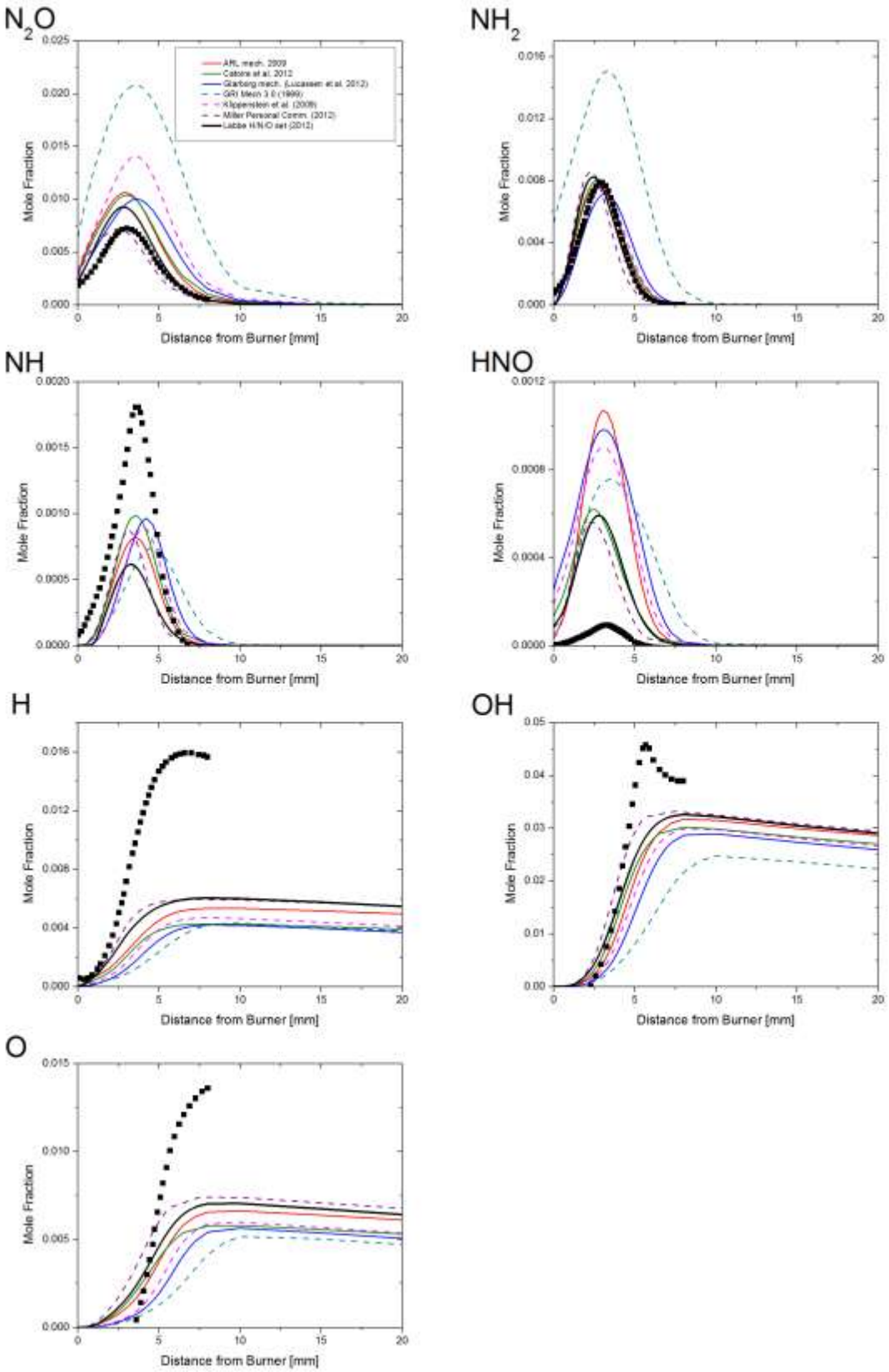

Figure 5. 16: New model results for flame of Bian et al. compared to previous models (intermediate species).

5.3.2 Testing the new model against NH_3/NO flame of Vandooren et al.

For the Vandooren flame [17] (Fig. 5.17), the new mechanism provided quite a few improvements. The NH_3 profile is now quite consistent with the experimental data, as well as the NO profile and the H_2 profile from the burner to 1 cm away from the burner. The H_2O and N_2 profiles are slightly underpredicted, but the general shape of the profile is much more improved compared to the other models. The prediction for H atom is consistent with the Miller mechanism, which was the best of the other models. Ar predictions are in line with the other models. Lastly, N_2O and NH_2 predictions are somewhat high but are within the general accuracy of the other models.

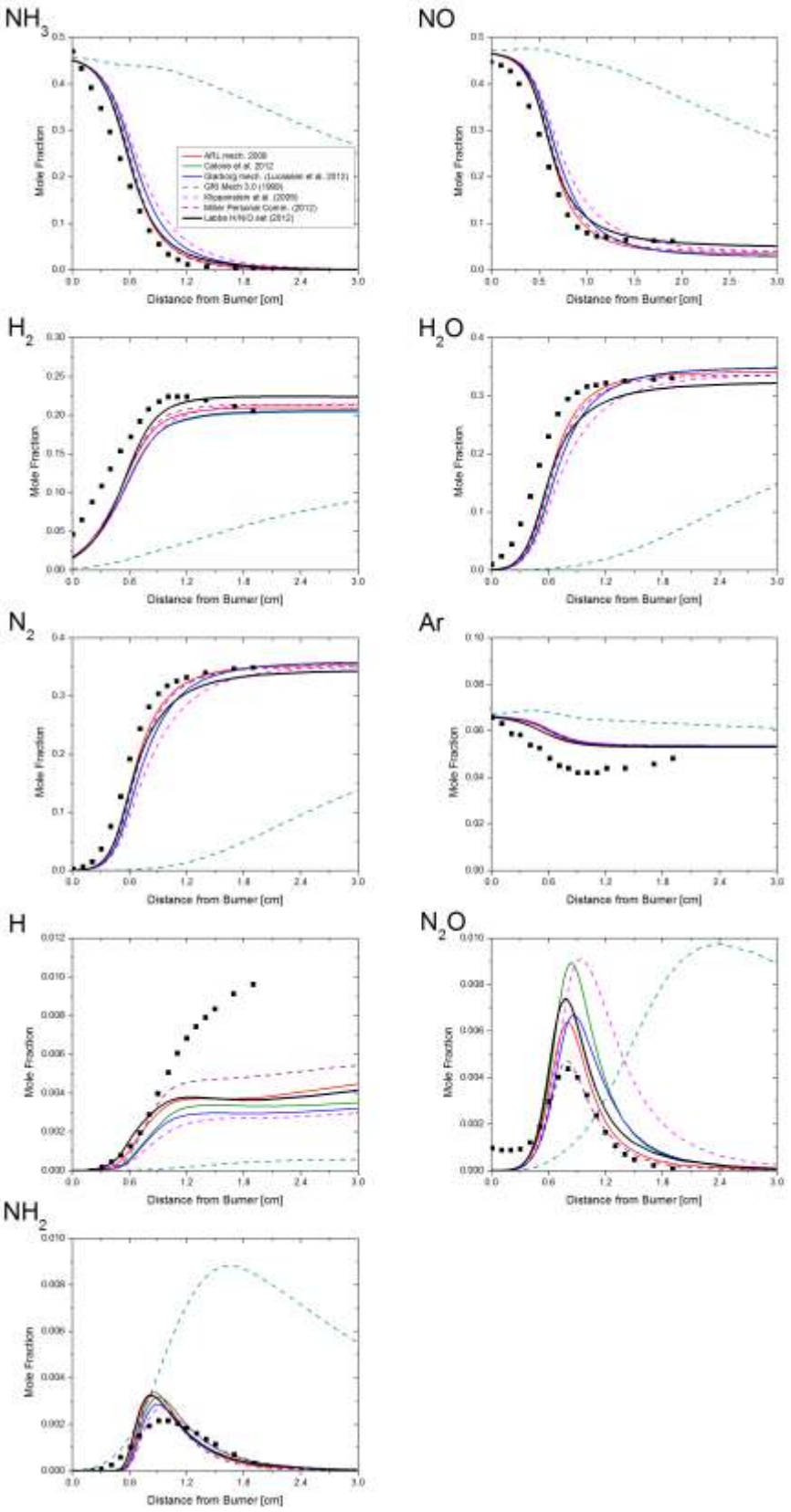

Figure 5.17: New model results for flame of Vandooren et al. compared to previous models.

5.3.3 Testing the new model against $H_2/N_2O(/NH_3)$ flames of Sausa et al.

The flames of Sausa et al. [19] were the furthest in disagreement with the new model. However, in the case of the undoped Sausa flame (no NH_3, Fig. 5.18), the new model is still within the same level of accuracy of the other models presented. The worst prediction by far was that of NO, which was among the highest of the previous model predictions. The same is the case for the NH_3-doped flame predictions (Fig. 5.19), although the NO prediction for the doped flame is much more consistent with the experimental data than it was with the neat flame.

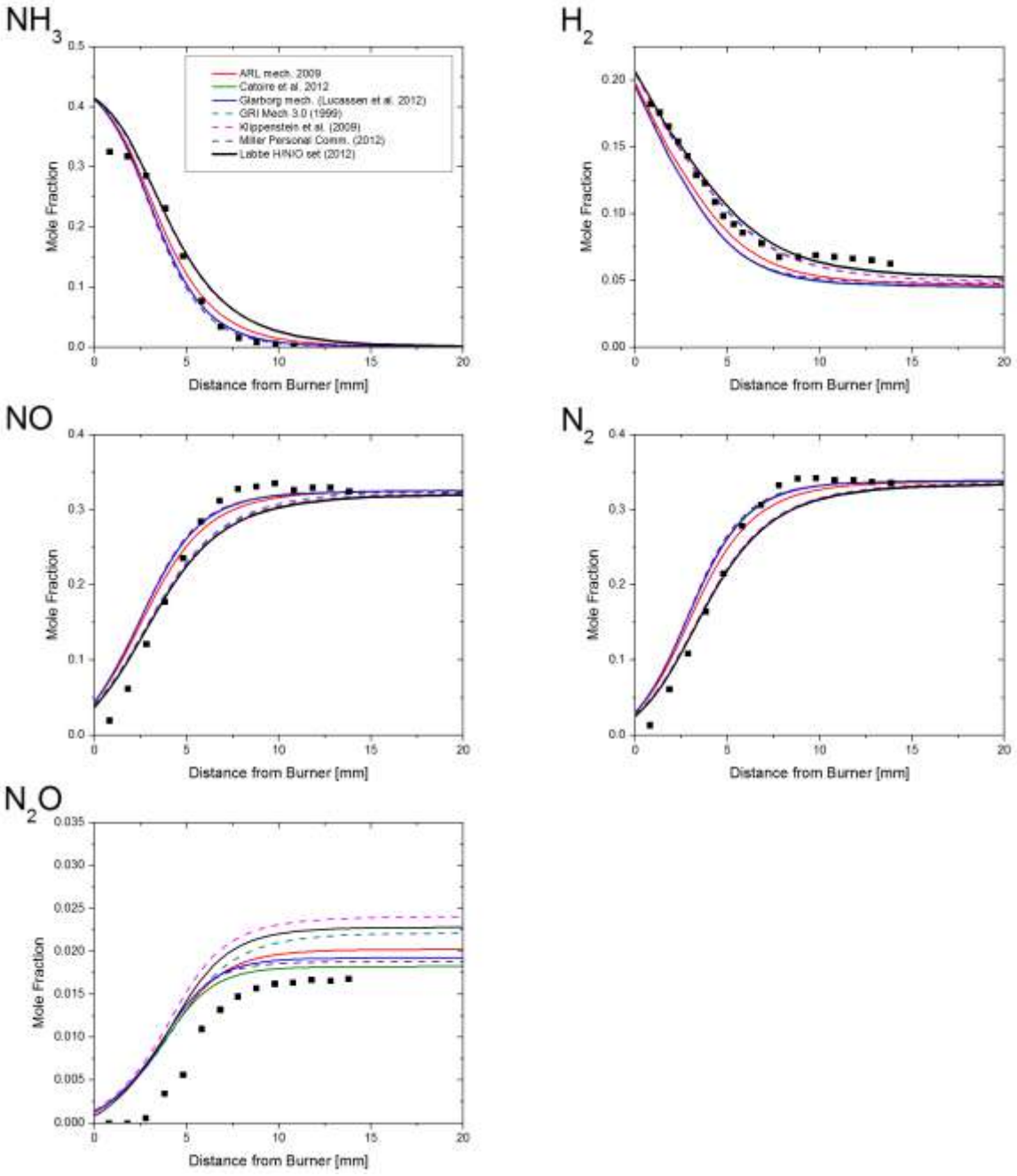

Figure 5.18: New model results for undoped experiment of Sausa et al. compared to previous models.

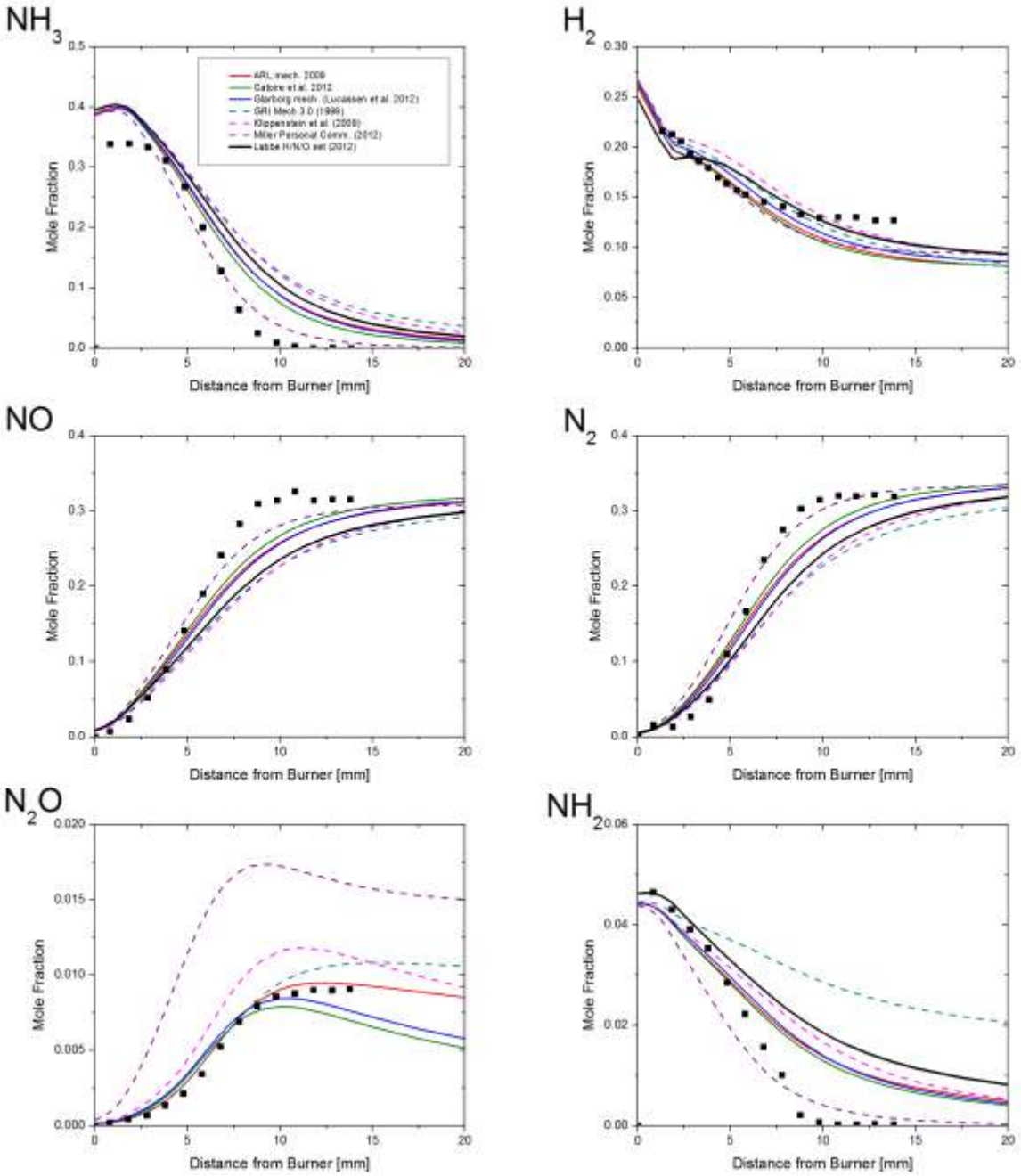

Figure 5.19: New model results for the NH_3-doped experiment of Sausa et al. compared to previous models.

5.3.4 Testing the new model against H_2/NH_3 flames of Duynslaegher et al.

As previously stated, Duynslaegher et al. [18] examined several different $H_2/NH_3/O_2/Ar$ flames varying in feed composition, stoichiometry, and pressure. The first four flames, Flame I (Fig. 5.20), Flame II (Fig. 5.21), Flame III (Fig. 5.22) and Flame IV

(Fig. 5.23) display how a stoichiometric flame of H_2 and NH_3 varies with a change of feed ratio of H_2 and NH_3. The previous models showed a trend of increasing accuracy as the ratio of H_2 to NH_3 increased, which holds true for the new mechanism. Again, NH_3, N_2, and H_2 are predicted quite well with the new mechanism, although the H_2 profile for Flame I is a bit high. N_2O and NH_2 are both within the accuracy of the other models (about a factor of 2). The biggest changes are with the NO profiles, which are significantly improved over the other models for all four flames.

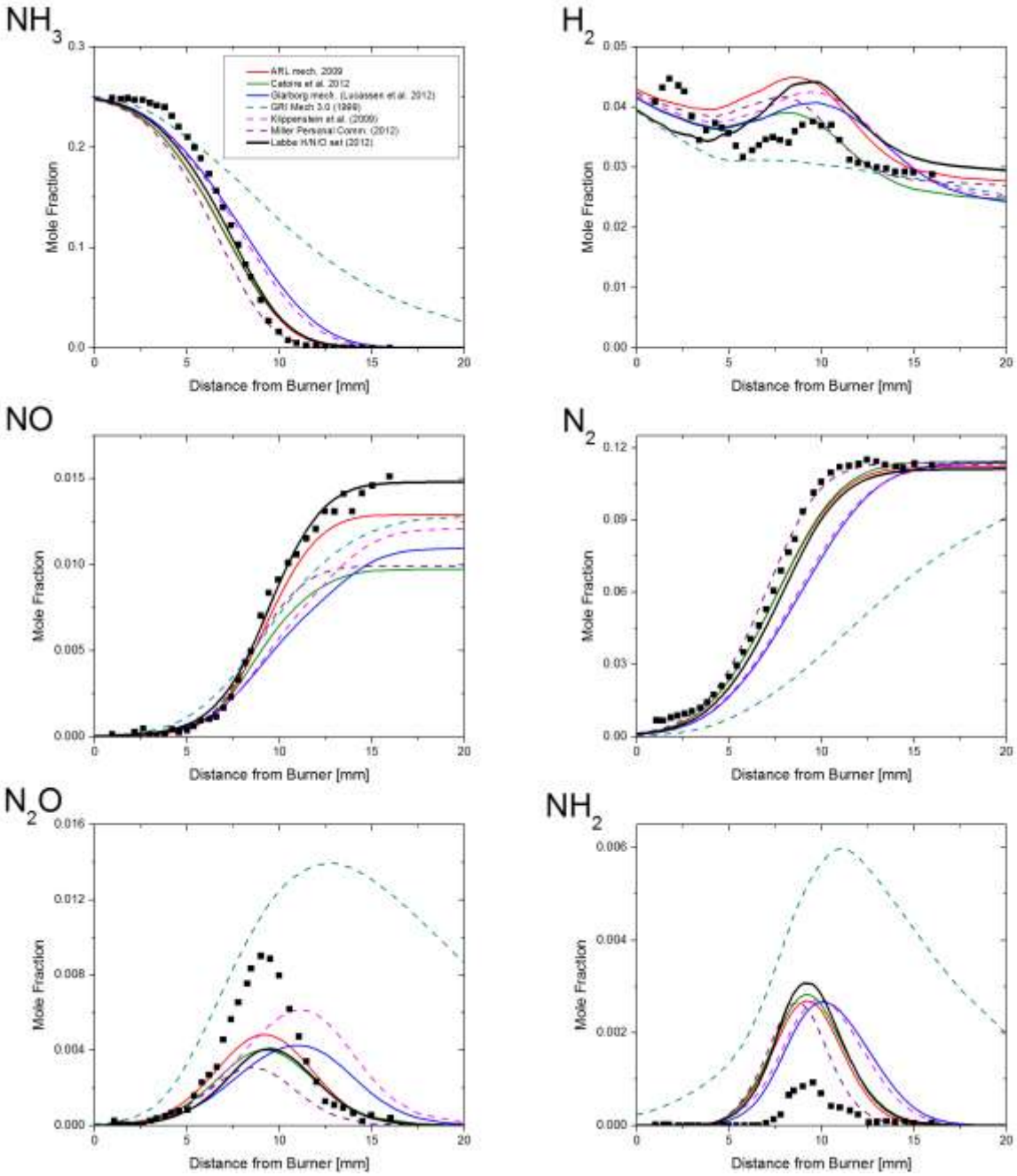

Figure 5.20: New model results for Flame I of Duynslaegher et al. compared to previous models.

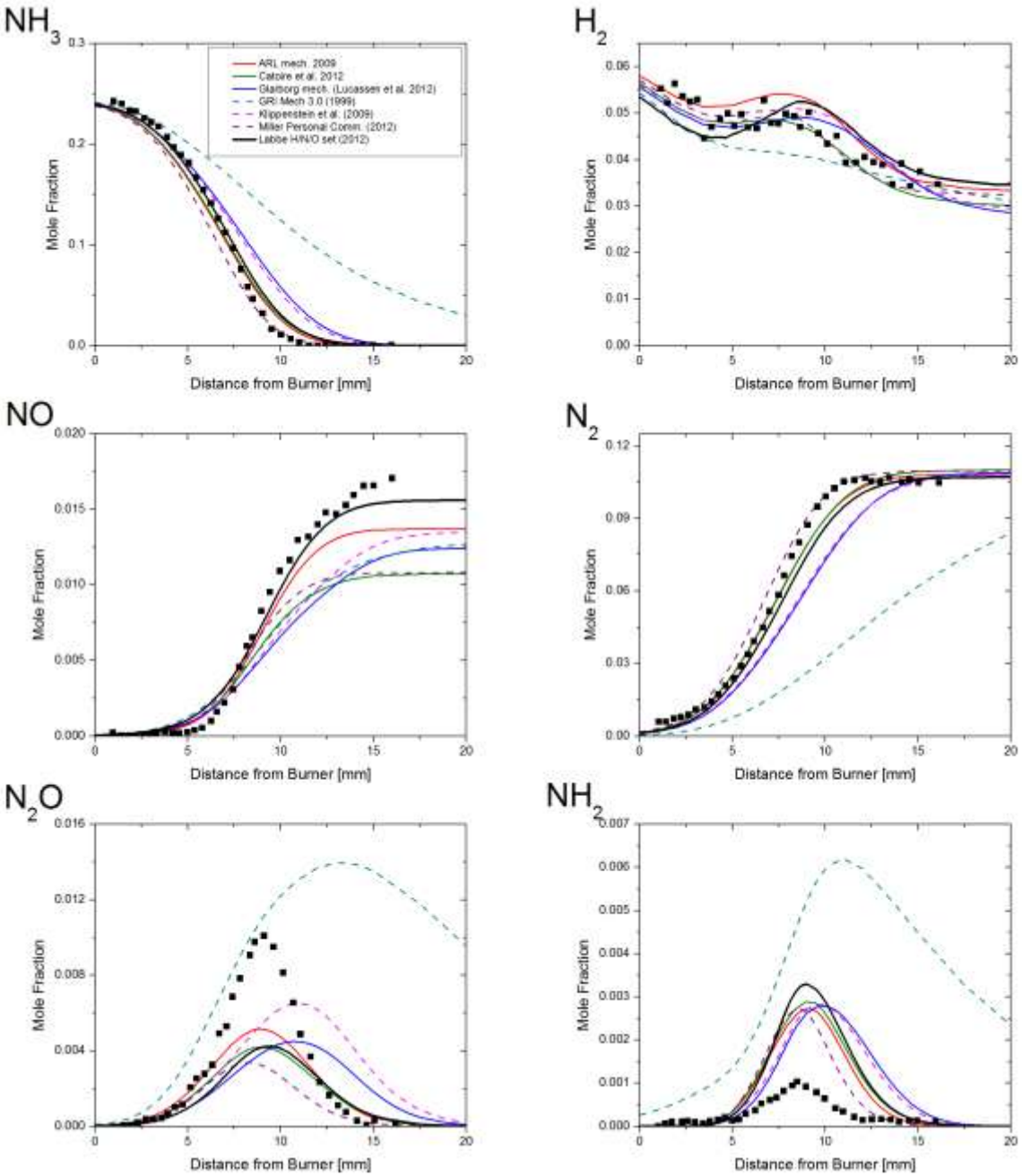

Figure 5.21: New model results for Flame II of Duynslaegher et al. compared to previous models.

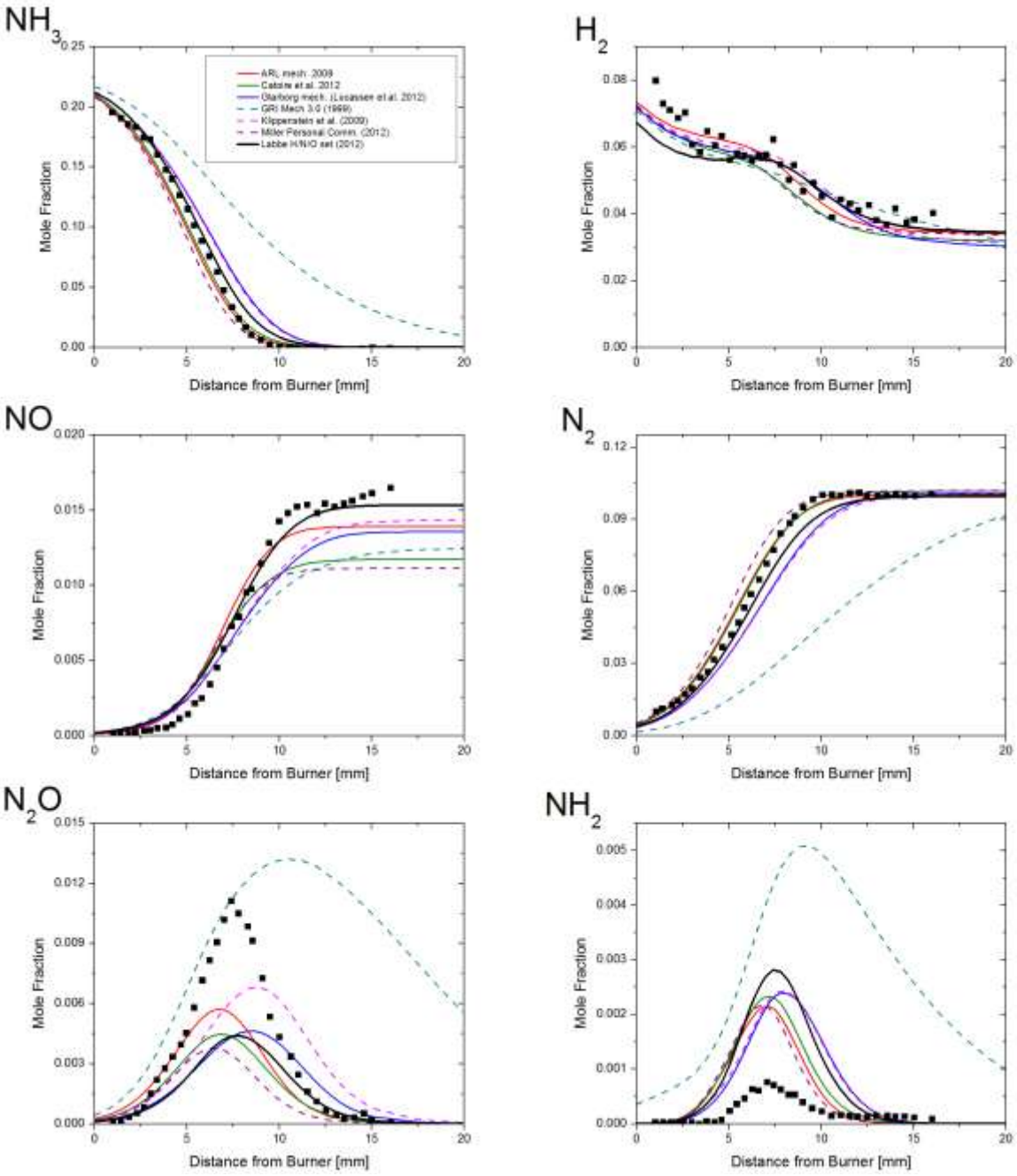

Figure 5.22: New model results for Flame III of Duynslaegher et al. compared to previous models.

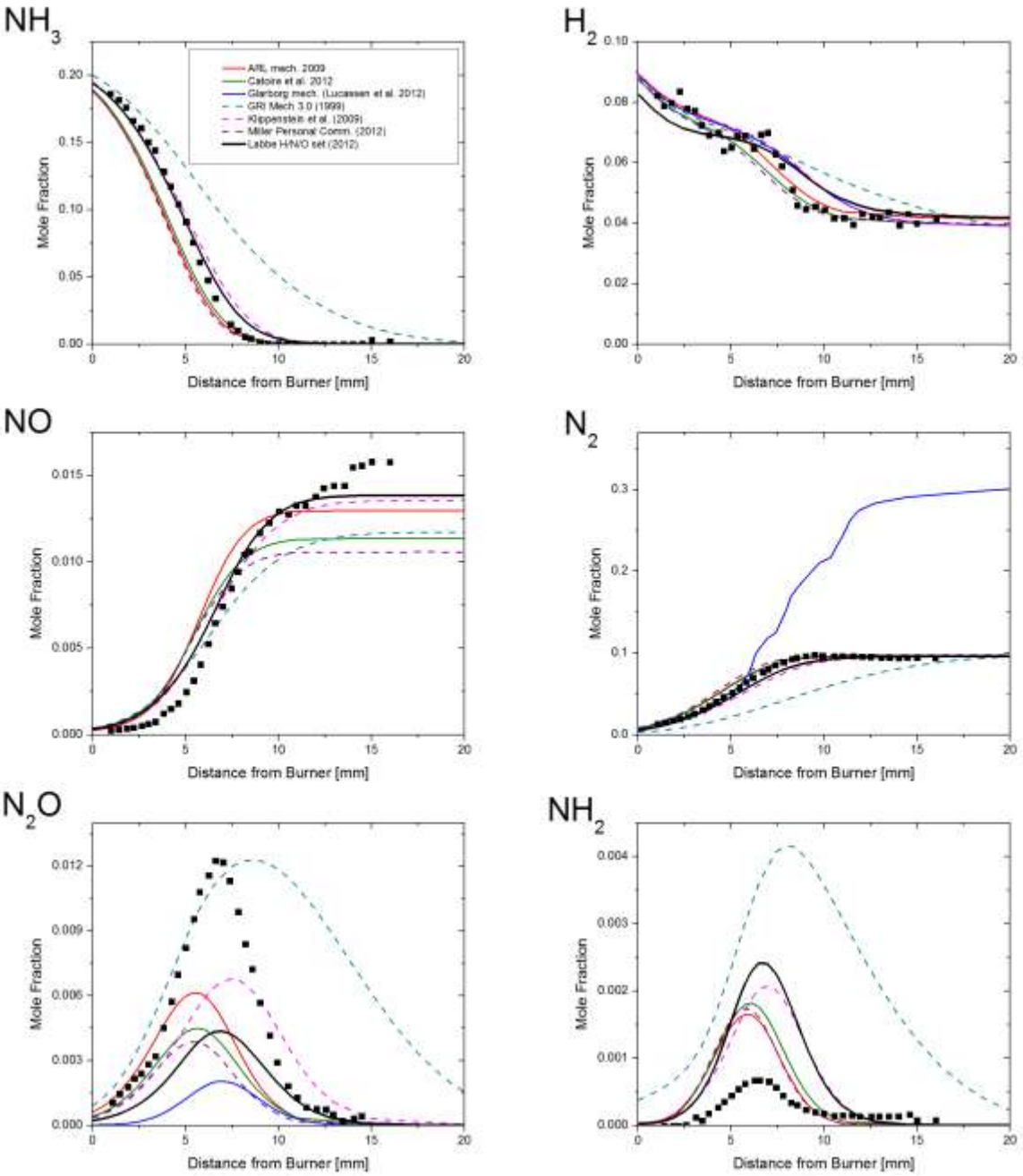

Figure 5. 23: New model results for Flame IV of Duynslaegher et al. compared to previous models.

The fuel-equivalence-ratio study, comparing the stoichiometric Flame III (Fig. 5.22), the slightly fuel-lean (Φ = 0.9) Flame V (Fig. 5.24), and the slightly fuel-rich (Φ = 1.1) Flame VI (Fig. 5.25), again shows similar trends to the previous models. The new

model performs similarly under lean conditions as it did at stoichiometric, again with the exception of NO. The disagreement for the new model with the experimental data for NO is quite large, matching the peak of the Klippenstein set (the best of the other models) though with an improvement in profile shape. For the fuel-rich flame, the experimental data profiles are broadened in comparison to the stoichiometric and fuel-lean flames, and like the other models, the new reaction set was unable to capture the shape broadening, yielding worse agreement in comparison to the fuel-lean and stoichiometric flames. The NO profile is much better in comparison to the other models, and like many of the other models, many of the profiles have shifts towards the burner compared to the data.

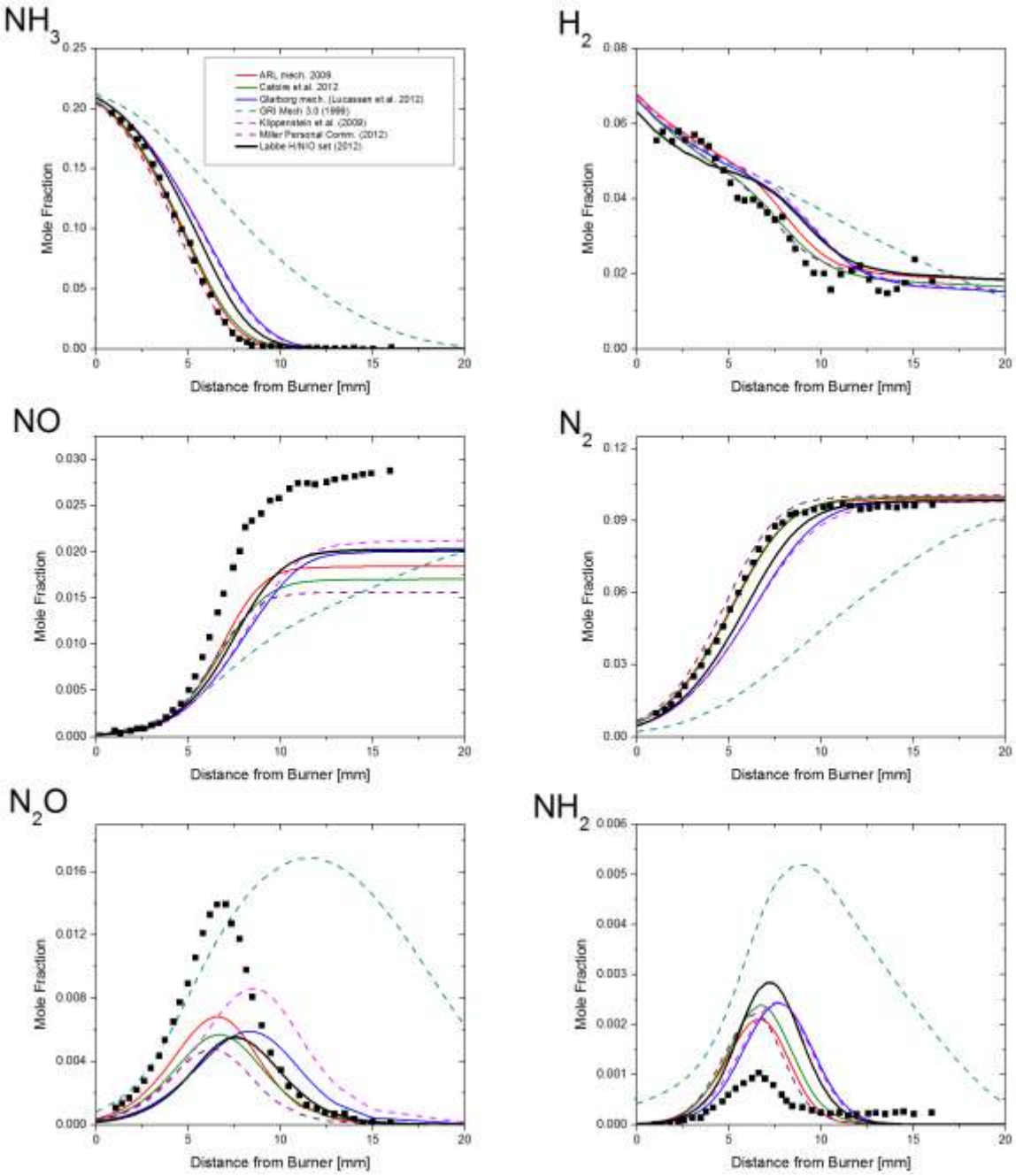

Figure 5.24: New model results for Flame V of Duynslaegher et al. compared to previous models.

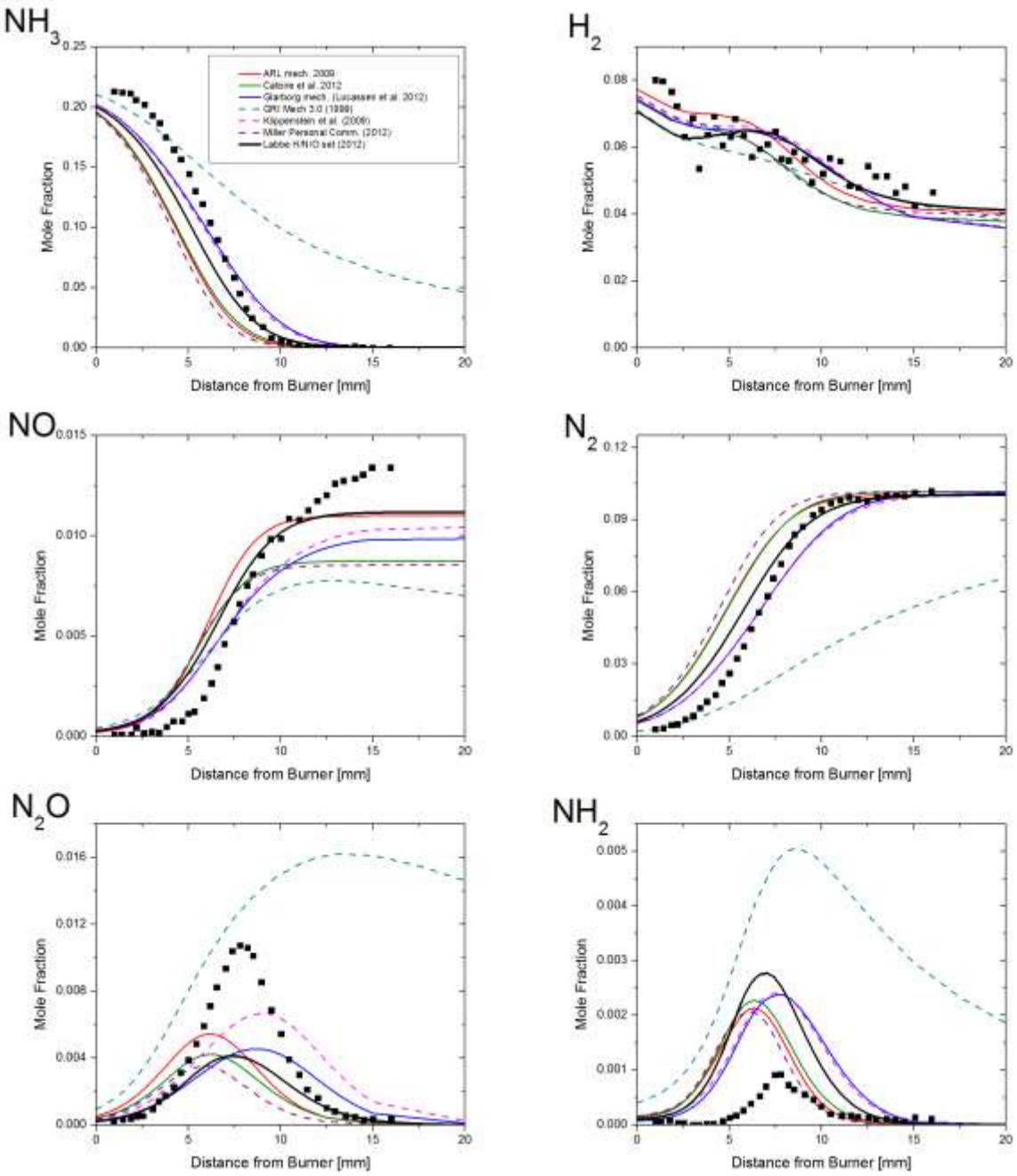

Figure 5.25: New model results for Flame VI of Duynslaegher et al. compared to previous models.

The trend of pressure is examined with Flame I (Fig. 5.20), Flame VII (Fig. 5.26) and Flame VIII (Fig. 5.27). Going from low pressure (60 mbar) to the mid-range pressure (90 mbar), modeling results are similar, still showing good agreement that is overall

consistent with the other models. For Flame VIII, the new model performs quite well, although with an apparent shift in data towards the burner and an unphysical double peak in the experimental NH_2 data. Despite the shift, predictions with the new model are still within good agreement and are consistently among the best predictions compared to the other models.

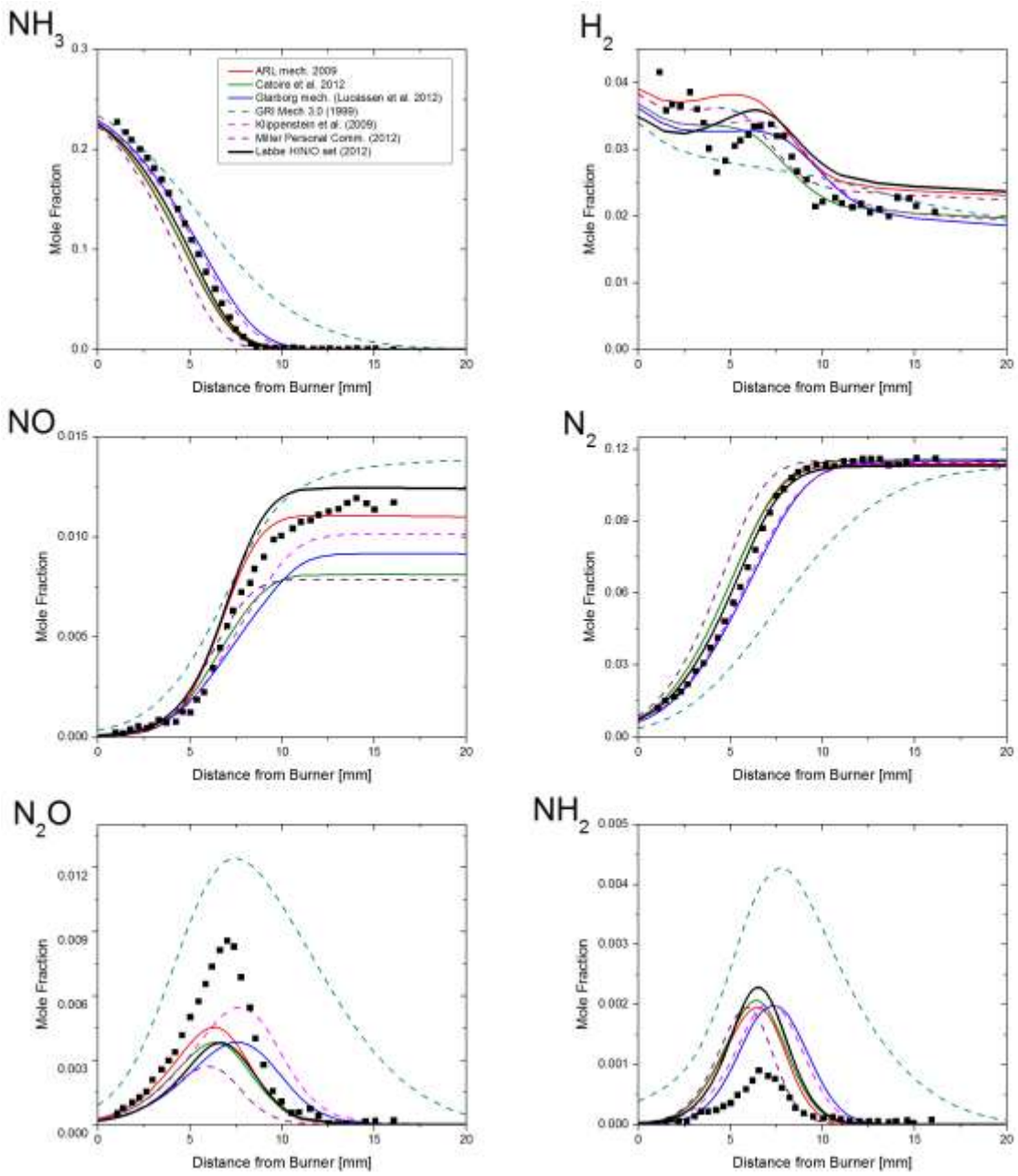

Figure 5.26: New model results for Flame VII of Duynslaegher et al. compared to previous models.

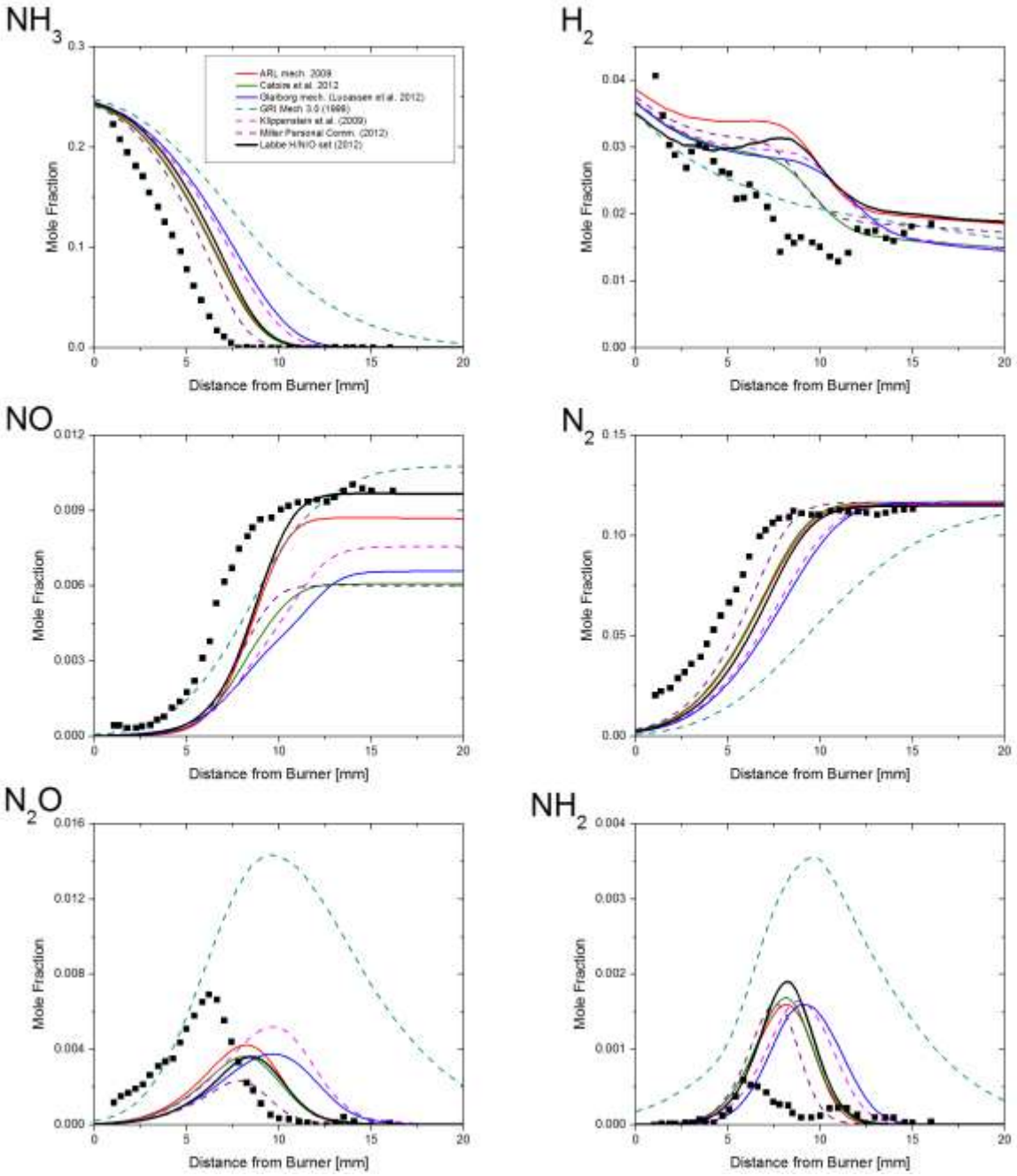

Figure 5.27: New model results for Flame VIII of Duynslaegher et al. compared to previous models.

5.3.5 Testing the new model against shock tube experiments of Davidson et al.

As an additional demonstration of the robustness of the new H/N/O reaction set, the new set was used to model an ammonia shock-tube pyrolysis study [20]. In this study, species time histories were monitored for both NH (see Fig. 5.28) and NH_2 (see Fig.

5.29) at temperatures of about 2300-2800 K and pressures around 1 atm. The experiment was modeled as a zero-dimension adiabatic batch reactor at constant pressure from the Chemkin suite [37] using ChemkinPro [32]. The model results (in red in Figs. 5.28-29) are quite close to the experimental data species time histories, with excellent agreement at about 2300 K and slight underprediction at around 2800 K for both NH and NH_2.

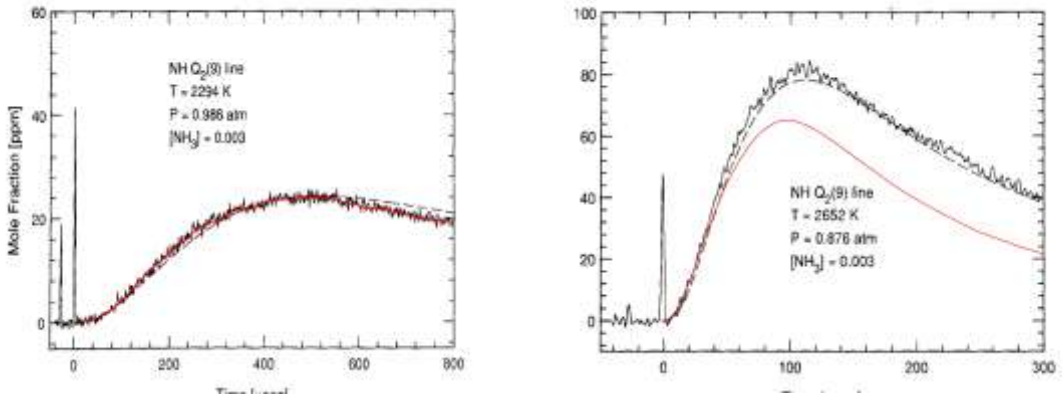

Figure 5.28: Species time histories for NH from Davidson et al. Smooth solid lines (in red) show new H/N/O model results superimposed over Figures 1 & 2 from [20].

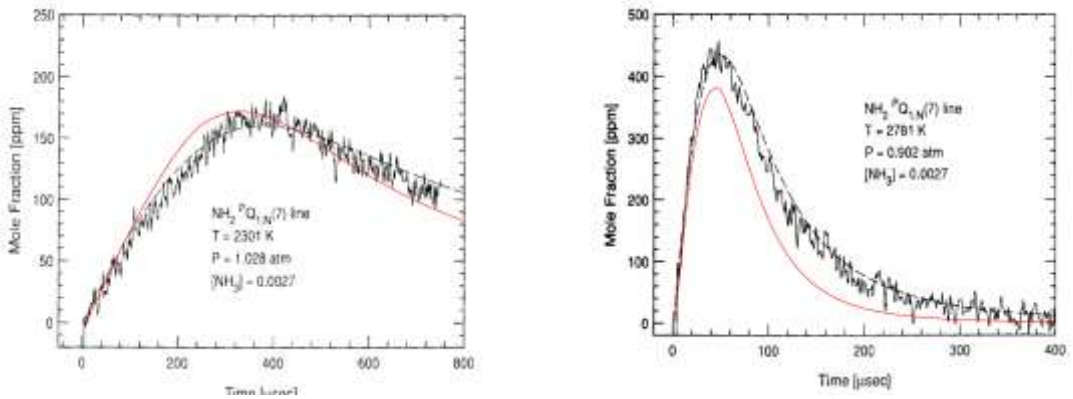

Figure 5.29: Species time histories for NH_2 from Davidson et al. Smooth solid lines (in red) show new H/N/O model results superimposed over Figures 3 & 4 from [20].

Additionally, trends were plotted for the temperature dependence of peak mole fractions of NH and NH_2 (see Fig. 5.30) and for the time to reach peak mole fraction of

NH and NH_2 as a function of temperature (see Fig. 5.31). Again, the new reaction set was able to predict the pyrolysis chemistry quite well. For the peak mole fraction predictions vs. temperature, the model captured the trends quite well (solid lines in red) with the largest discrepancies occurring at temperatures above 3000 K. The temperature trends for the time of peak mole fraction of NH are also predicted quite well (solid lines in red). The largest disagreements between the pyrolysis experimental data and the new model were for trend predictions for the time of peak mole fraction of NH_2 versus temperature, where the peak mole fraction times were slightly longer than observed experimentally.

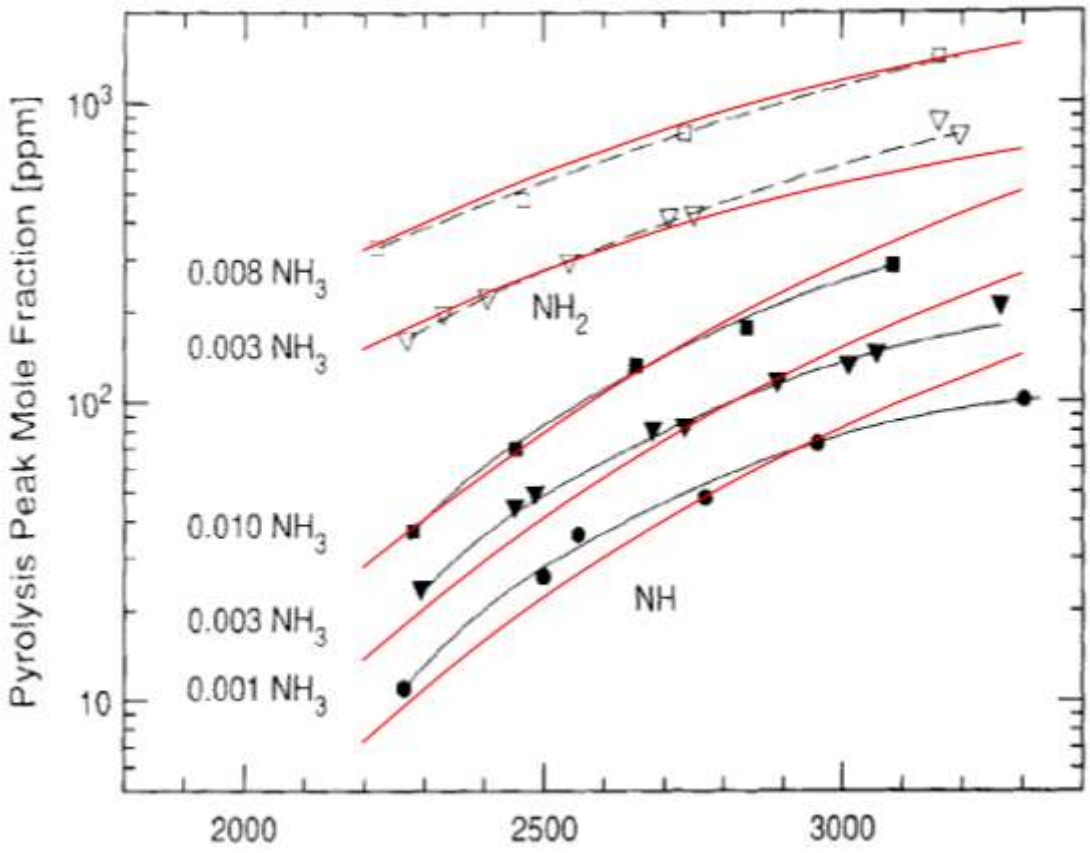

Figure 5.30: Peak mole fractions of NH and NH_2 as a function of temperature. H/N/O model results (solid lines in red) were superimposed over Figure 5 from Davidson et al. [20] for comparison.

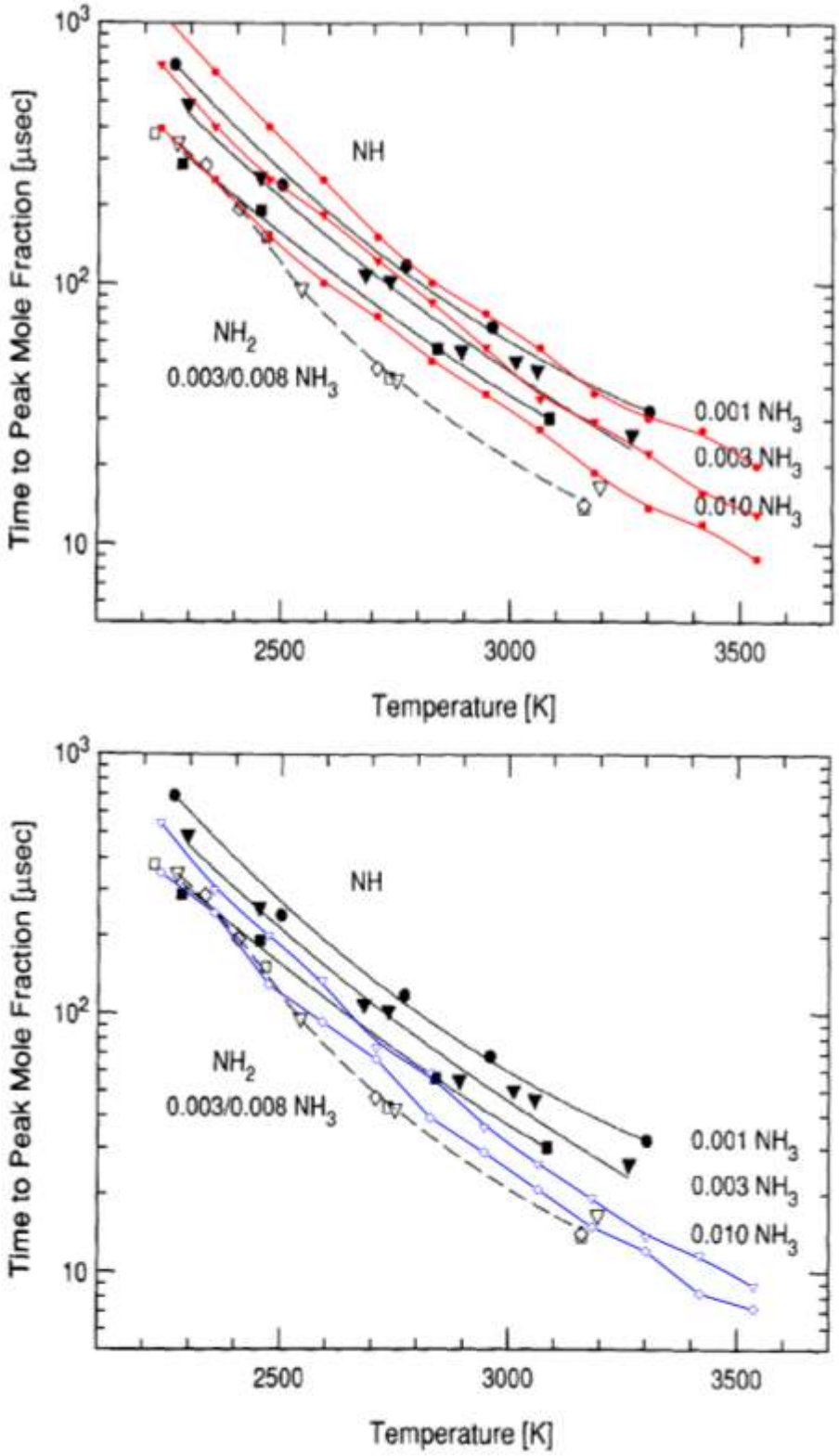

Figure 5.31: Time to reach peak mole fractions of NH and NH_2 as a function of temperature. H/N/O model results (solid lines in red for NH in the top graph, solid lines in blue for NH_2 in the bottom graph) were superimposed over Figure 6 from Davidson et al. [20] for comparison.

5.4 Summary and Conclusions

With continual scrutiny of combustion for pollution control and environmental impact, a fundamental understanding of H/N/O chemistry is crucial for predicting nitrogen-containing pollutant formation as a result of combustion of coal, propellants, and biomass, as well as combustion of any fuel in air. Several experimental studies and modeling efforts have been completed previously, however, there are still discrepancies between the models and the experimental data.

This work, in an effort to better model H/N/O combustion globally over several experimental conditions, created a new H/N/O reaction set, which is currently the largest elementary reaction set for H/N/O combustion available. This model was compiled as an extensive database of available elementary rate constants that was optimized via sensitivity analysis over the currently available H/N/O models. The new reaction set has 43 species and 307 reactions. It was tested over twelve experimental MBMS flame data sets and compared against six different models. Additionally, the new reaction set was compared against a pyrolysis shock tube study. The results showed overall agreement with the experimental data, providing generally model results that were as good as or better than the current models available. Major improvements on N_2 and NO modeling results were achieved, and intermediate radical species were generally predicted within a factor of 2.

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CHAPTER 6

KINETICS OF AMMONIA + HYDROCARBONS: BUILDING AN H/C/N/O REACTION SET

Studying the combustion of fuels with only H, O, and N atoms is desirable for its simplicity. It helps to elucidate key kinetic pathways without the complication of greatly increasing the total number of species and elementary reactions in the overall model. However, real combustion situations involving nitrogen chemistry more often than not include the presence of carbon. In this chapter, the H/N/O combustion reaction set of Chapter 5 is expanded to include hydrocarbon chemistry as well as H/C/N/O chemistry.

6.1 Assembly of a base H/C/N/O reaction set

The expanded reaction set for H/C/N/O combustion was developed with the approach of cataloguing reaction rate constants that were available in several sources. The first main addition to the H/N/O reaction set was the addition of hydrocarbon chemistry. The basis of the hydrocarbon chemistry was the acetylene and cyclohexane sets of Li [1-2]. These sets were tested against flame experiments varying from fuel-lean to fuel-rich. Additionally, ethanol and dimethyl ether chemistry was added, originating from Cool et al. [3].

The second major addition to the H/N/O set was H/C/N/O chemistry added from several sources. Several rate constants came from the review chapter of Dean and Bozzelli [4] in which gas-phase rate constants for nitrogen-containing species were catalogued and pressure dependence was assessed. GRI-Mech 3.0 [5] was also considered because it is widely used in engine models currently. Several reaction sets based in propellant chemistry were also used, including the reaction set for monomethyl

hydrazine with red fuming nitric acid from the Army Research Laboratories [6] and the monomethyl hydrazine pyrolysis mechanism from Sun et al. [7]. The reaction set of Catoire et al. was also sampled [8], which emphasizes hypergolic ionic liquids such as dicyanimide combustion. Lastly, the recent work of Glarborg was included through his work on modeling methane/ammonia flames [9] and ethylamine and dimethylamine flames [10]. These reaction rates, including duplicates, were assembled into one master reaction set.

Upon assembly, a first-pass selection of H/C/N/O rate constants was completed by inspection, eliminating rate constants with non-physical parameters. Rate constants with fall-off were preferentially selected over other rate constants. The reaction set was then tested against experimental data and rate constant selection was further refined through analysis of the model results versus experimental data. Thermochemistry was also assembled for all species in the H/C/N/O reaction set. The hydrocarbon chemistry was not altered. The resulting reaction set has a total of 216 different species and 1854 elementary reactions. The new set may be found in Appendix D. This new set was used to model the three Glarborg flame experiments [9-10] for validation. Overall, the model performs as well as the Glarborg model, though the new model also includes a much larger wealth of H/C/N/O chemistry, making the reaction set more globally applicable to small H/C/N/O fuels. The following is a discussion of the new model's performance in context of both the experimental data and the Glarborg models.

6.2 Comparison of new model to experimental data

6.2.1 Comparison to a stoichiometric $CH_4/NH_3/O_2$ flame

Tian et al. [9] conducted an MBMS flame study on several stoichiometric $CH_4/NH_3/O_2$ flames, varying the ammonia/methane ratio *R* from no ammonia to an equimolar mixture of the two fuels. Their study, motivated by the need for a better understanding of the combustion of fuel nitrogen, aimed to obtain data for intermediate species which is generally lacking in other studies. The study was conducted on a 6 cm McKenna style burner at 40 mbar, and mole fraction profiles were obtained for all main species: CH_4, NH_3, O_2, Ar, H_2, H_2O, CO, CO_2, NO and N_2. Intermediate species C_2H_2, HCN, and NO_2 were also sampled.

For validation purposes in this work, the $R = 0.5$ flame (a stoichiometric flame with a 1:2 ratio of NH_3:CH_4) was modeled as a premixed, 1-D flame using the PREMIX code [11] from ChemkinPro [12] and the experimental temperature profile reported by Tian et al. as well as a perturbed temperature profile used by Tian et al. for modeling [Glarborg, Personal Communication]. Successfully modeling the work with the reaction set published by Tian et al. [9] required, a 4.5mm shift of the temperature profile away from the burner. Glarborg confirmed that this approach was adapted in the modeling although it was inadvertently not reported in the publication [9] (see Fig. 6.1). The shift suggests a possible detachment of the flame from the burner during mole-fraction profile measurement, although Tian [Personal communication, 6 Aug 2010] was unable to detect any hysteresis in the profile measurements. Until further measurements are made, this difference remains an unresolved uncertainty.

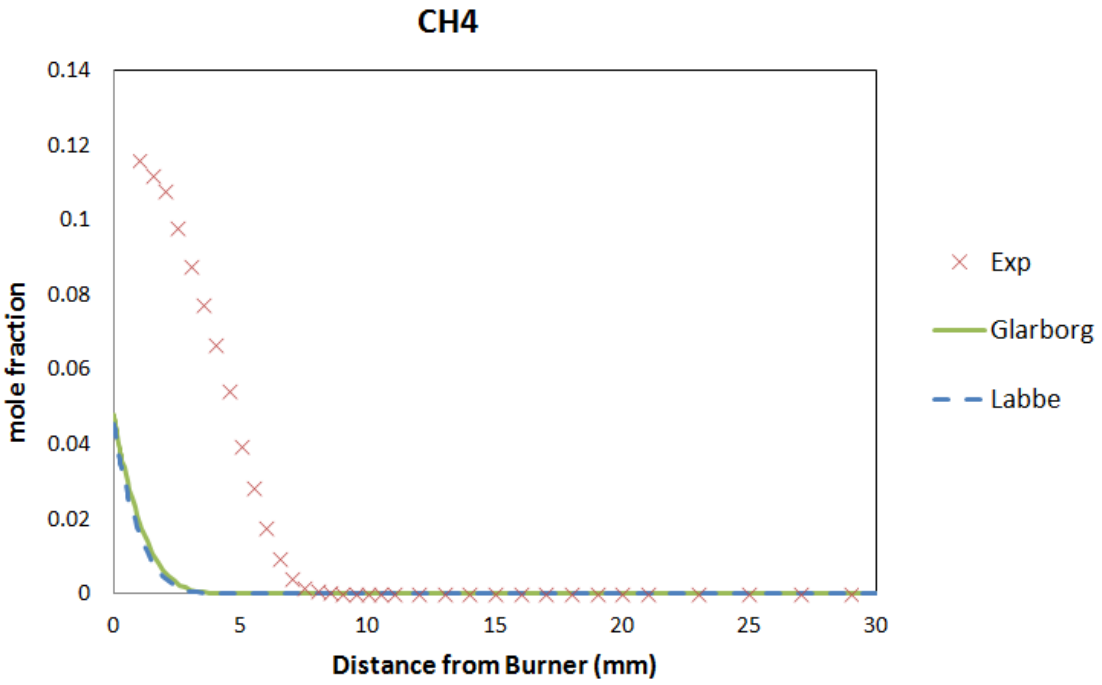


Figure 6.1: Modeling differences in the R = 0.5 flame when using the unperturbed temperature profile reported in [9], shown to be independent of reaction-set differences by comparing predictions with the reaction sets of Glarborg and the present work.

The modeling results are presented in Figs. 6.2 and 6.3 for the R = 0.5 flame with the 4.5-mm shifted temperature profile. Figure 6.2 shows the predicted mole-fraction profiles for the main species using the present reaction set and the set from the paper [9]. Overall, the predictions of the main-species experimental data are in excellent to fair agreement, and CH_4, NH_3, and CO_2 are predicted particularly well. Relative to the experimental data, O_2 is slightly overpredicted at >10 mm from the burner, while H_2O is slightly underpredicted in the same range. Compared to the experimental data, H_2 is underpredicted, as well as CO, but not to the degree by which H_2 is underpredicted. N_2 and NO are both overpredicted. The two models are nearly identical in behavior for all the major species.

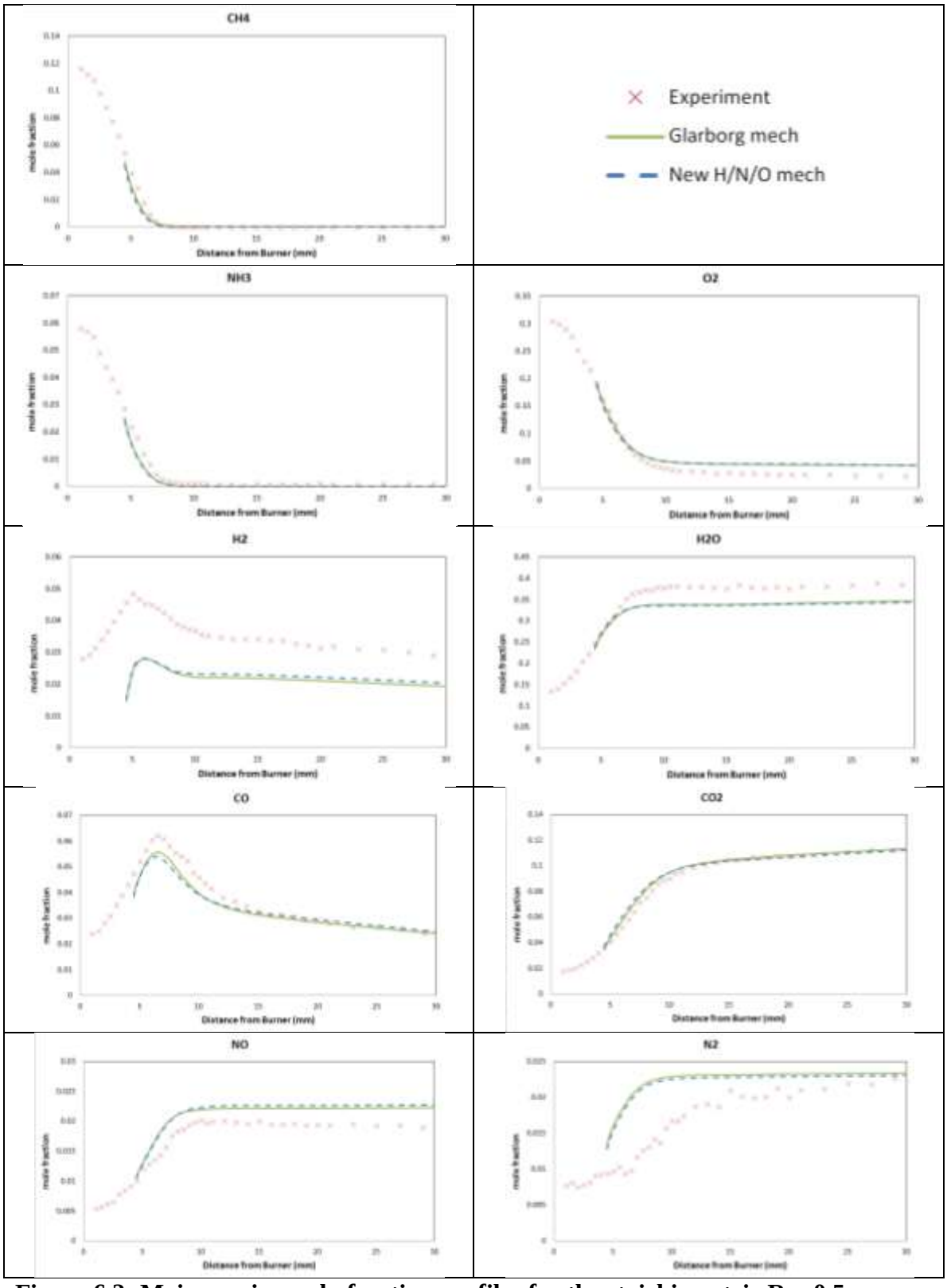


Figure 6.2: Main species mole-fraction profiles for the stoichiometric R = 0.5 $CH_4/NH_3/O_2$ flame of Tian et al. [9] compared to the published model and the current model from this work.

For the intermediate species (see Fig. 6.3), much larger discrepancies arise in the model predictions. The acetylene predictions are quite poor, being low by approximately an order of magnitude for both models. The same applies for the NO_2 predictions, which are much lower than the experimental data. The argon profile is overpredicted quite consistently by about 10 mole percent, again suggesting a possible issue with the experimental data. For HCN, the Glarborg model performs quite well, underpredicting the profile slightly. The new H/C/N/O model does not perform as well, overpredicting the profile by more than a factor of 2.

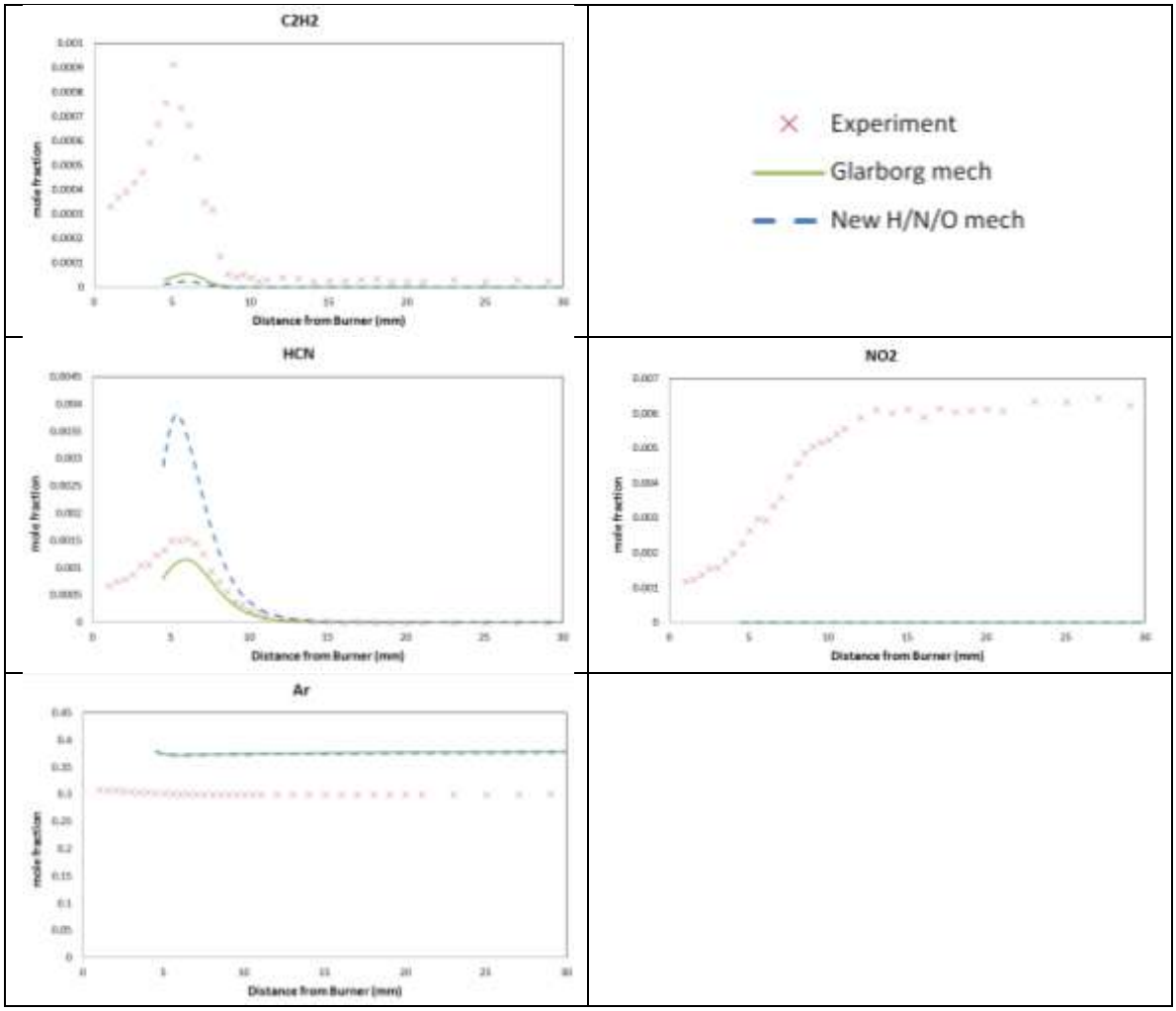


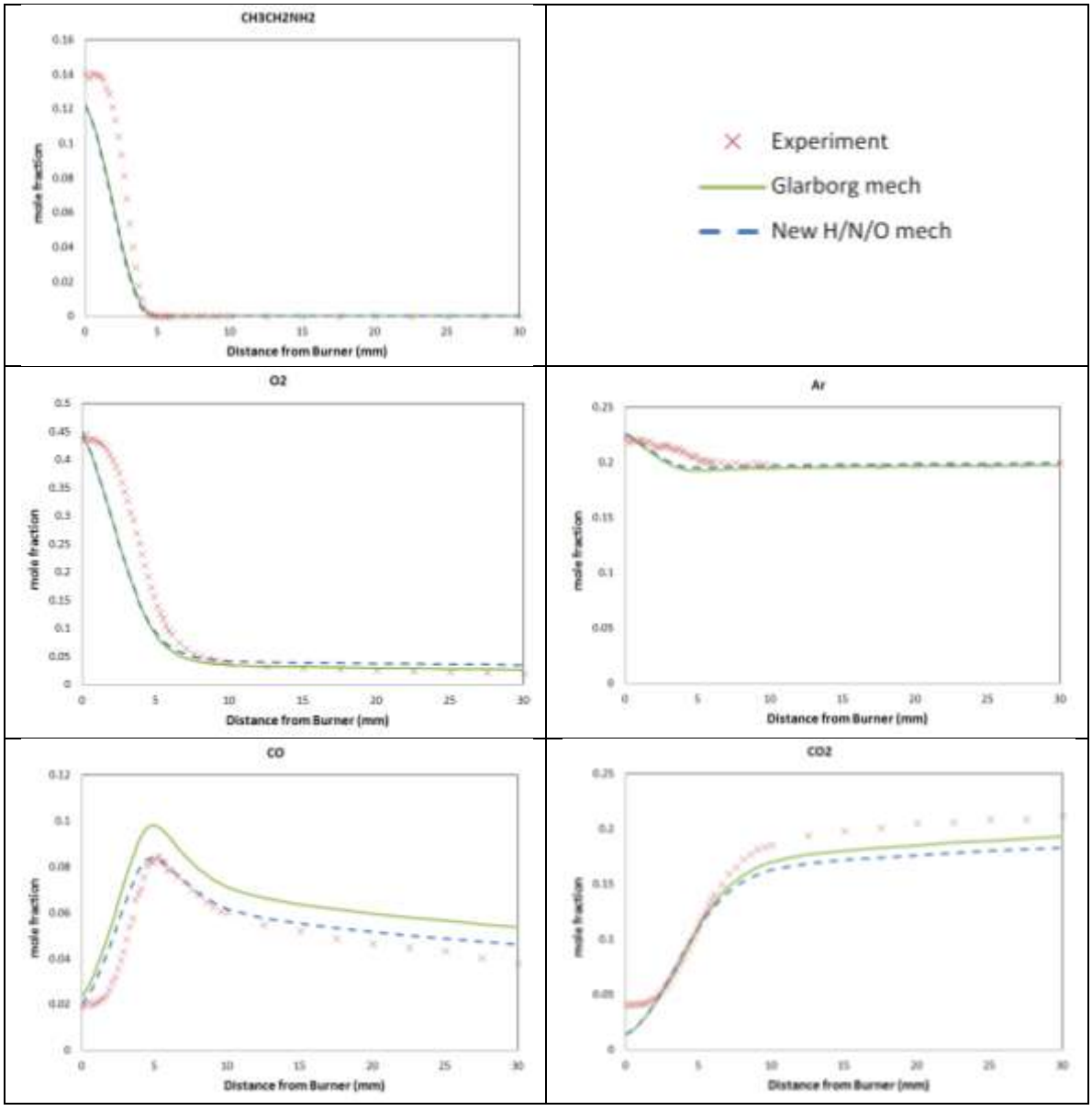
Figure 6.3: Intermediate species mole fraction profiles for the stoichiometric R = 0.5 $CH_4/NH_3/O_2$ flame of Tian et al. [9] compared to the published model and the current model from this work.

6.2.1 Comparison to a stoichiometric ethylamine flame

In a second experimental study aimed at looking at the combustion of nitrogen-containing biofuels derived from biomass, Lucassen et al. [10] studied a series of ethylamine/O_2 and dimethylamine/O_2 flames ranging from slightly fuel-lean ($\Phi = 0.8$) to slightly fuel-lean ($\Phi = 1.3$). The study was conducted on a 6.34-cm-diameter burner at a pressure of 40 mbar for EI measurements and a 6.0-cm-diameter burner also at 40 mbar for PI measurements. A revised version of the Glarborg reaction set from [9] was used to model the experimental data. The stoichiometric ethylamine/O_2 and stoichiometric dimethyl amine flames were selected for validation of the new reaction set and were again modeled using the experimental temperature profiles with the PREMIX code [11] from ChemkinPro [12]. The published reaction set [10] was also remodeled in this work as a check, though no shifts were needed for this series of flames.

For the stoichiometric ethylamine/O_2 flame, mole fraction profiles were recorded for several different main species (presented with modeling results in Fig. 6.4), including ethylamine ($CH_3CH_2NH_2$), O_2, Ar, CO, CO_2, H_2, H_2O, NO, and N_2. The experimental data profiles are quite flat for the first 2 mm or so of the flame, but any data within 1-2 mm of the burner should be discounted due to probe perturbation of the flame. Ethylamine is predicted well, although the slope of the initial decomposition of ethylamine is slightly lower than that of the experimental data for both models, which are indistinguishable. The same can be said for O_2, Ar, H_2O, and N_2, although H_2O is slightly underpredicted. The new reaction set improves CO modeling to near-perfect agreement (the Glarborg reaction set overpredicts CO), but it fares worse for CO_2 prediction, underpredicting the experimental data slightly more than the Glarborg model. The new set also improves the predictions of H_2 relative to the Glarborg model, and NO

predictions, though similar for both models, capture the magnitude but not the exact shape of the NO experimental data.



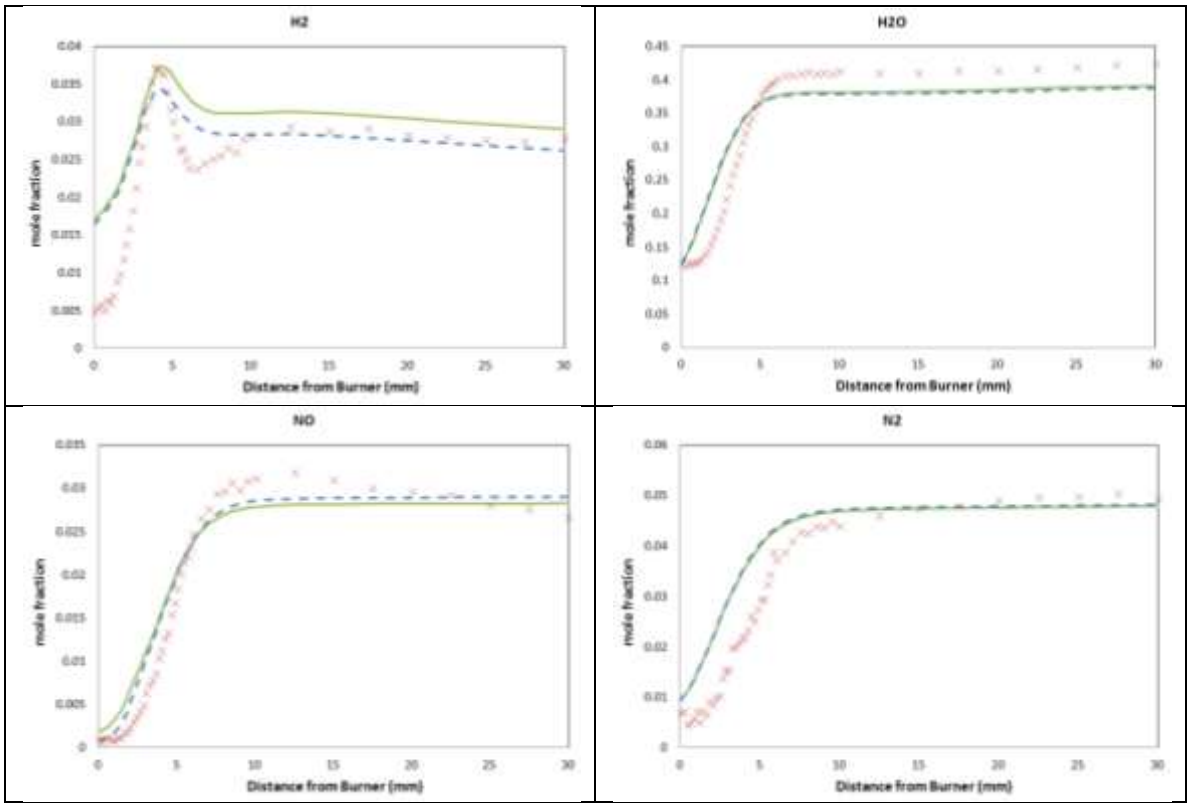
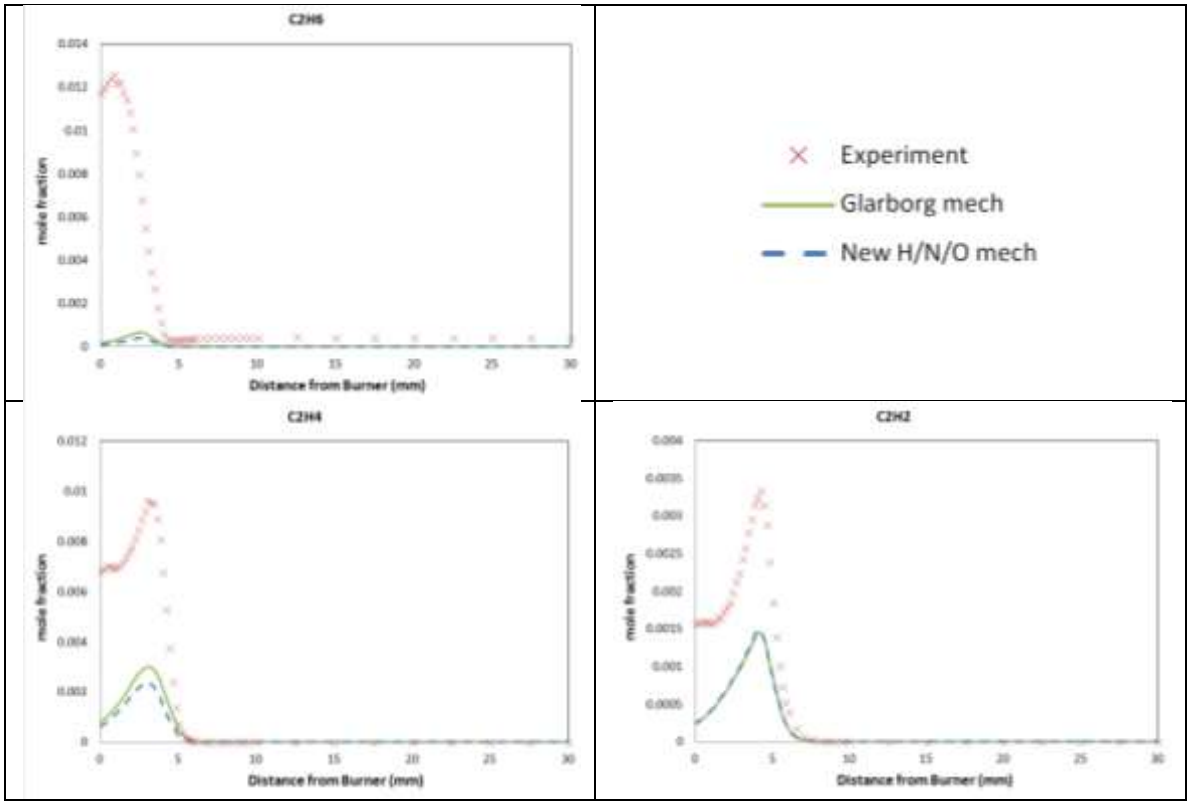


Figure 6.4: Main species mole fraction profiles for the stoichiometric ethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

Several different hydrocarbon intermediate species were detected in the ethylamine flame (Fig. 6.5), including C_2H_6, C_2H_4, C_2H_2, CH_4, CH_3, CH_3OH, CH_2O, CH_2CO, and CH_3CHO. As with the NH_3/CH_4 flames, the largest disagreements with the experimental data and the largest differences between the two models are observed with the intermediate species. C_2 species in general are underpredicted. While ethane is underpredicted by both models by over an order of magnitude, ethylene is closer (about a factor of 3), and acetylene the closest (low by a factor of 2). For all C_2's, the differences between the models are minor. Methane model results are also low (by a factor of 2 for the new set, 1.5 for the Glarborg set), as well as for methyl radical (by a factor of 4 for the new set, 3 for the Glarborg set). The large discrepancies among the hydrocarbon

chemistry suggest that further improvements are needed in the hydrocarbon reaction set. Again, data within 1-2 mm of the burner cannot be used for comparison with the model, which does not capture the probe perturbation.

For the oxygenated species, the Glarborg reaction set models CH_3OH and CH_2O quite well compared to the experimental data. Predictions by the new H/C/N/O set are off by a factor of 2. Both models are low by about a factor of 2 for CH_2CO data, and for CH_3CHO, both models are low by a factor of 4. The differences in the H/C/O chemistry can largely be explained through the differences in the hydrocarbon part of the reaction sets.



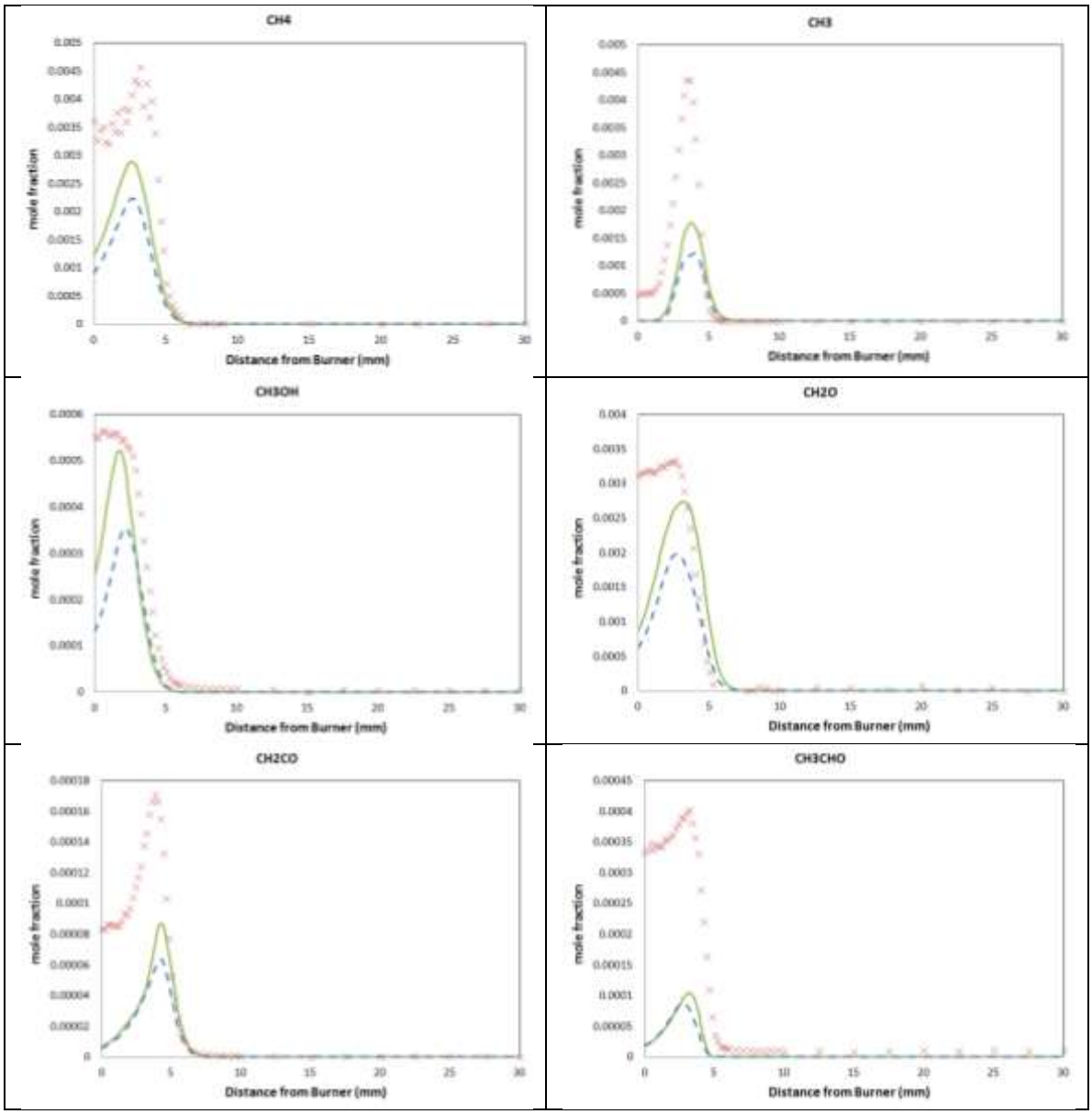
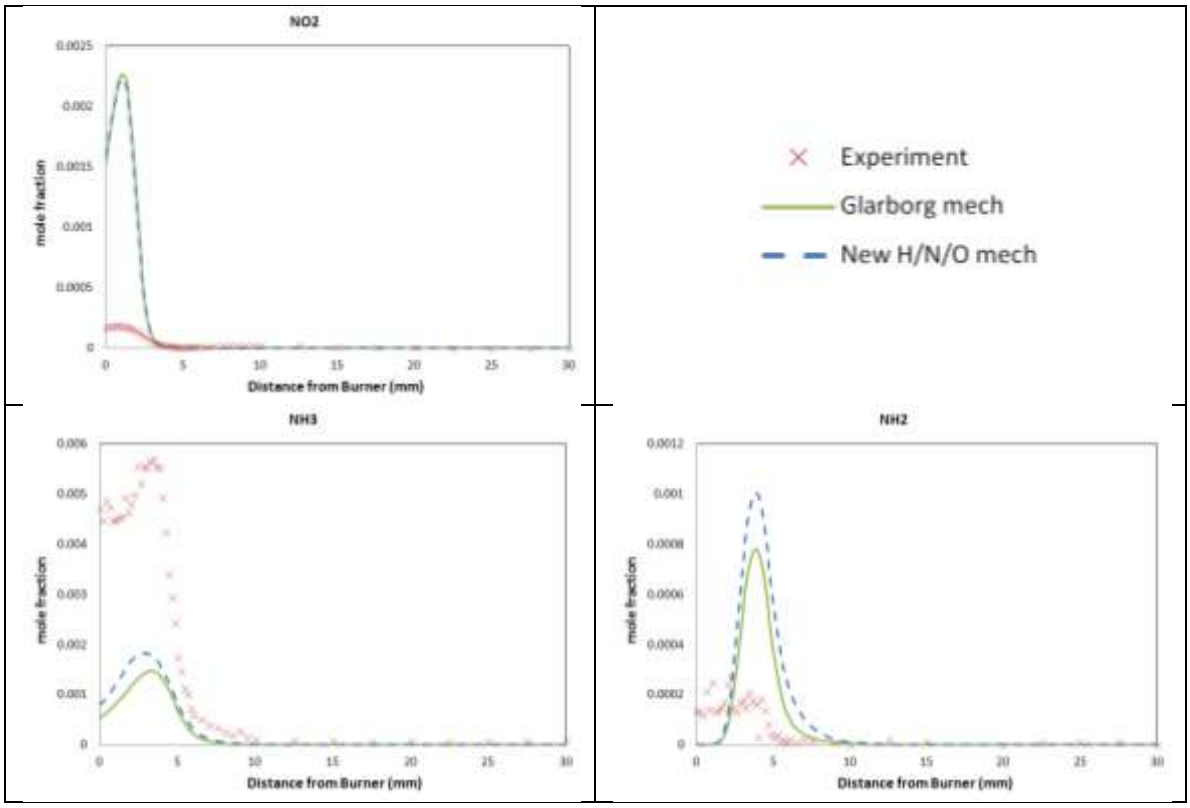


Figure 6.5: Intermediate H/C/O species mole fraction profiles for the stoichiometric ethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

Several nitrogen-containing intermediate species were also identified (see Fig. 6.6), including NO_2, NH_3, NH_2, HCN, H_2CN, CH_2NH, CH_3NH_2, and HNCO. As with the NH_3/CH_4 flame, the NO_2 predictions are quite different than the experimental data, this time overpredicting by a factor of 10. The new model shows slight improvements in the

predictions of HCN and NH_3 compared to the Glarborg model, but still the models underpredict the data. NH_2 is over predicted and the new model fares slightly worse than the Glarborg model. The experimental data suggests relatively high concentrations of H_2CN (~0.25%); however, neither model predicts H_2CN concentrations of any significance. The new model also does not predict significant CH_2NH, though the Glarborg model quite accurately predicts a peak at 0.3% total mole fraction. The Glarborg model also predicts CH_3NH_2 quite well, and the new model is well within a factor of 2. The last nitrogen intermediate, HNCO, is predicted by the new model within a factor of two, improving upon the accuracy of the Glarborg model, which is low by approximately a factor of 4. The model results suggest there should be greater focus applied to the HCN chemistry for better modeling results.



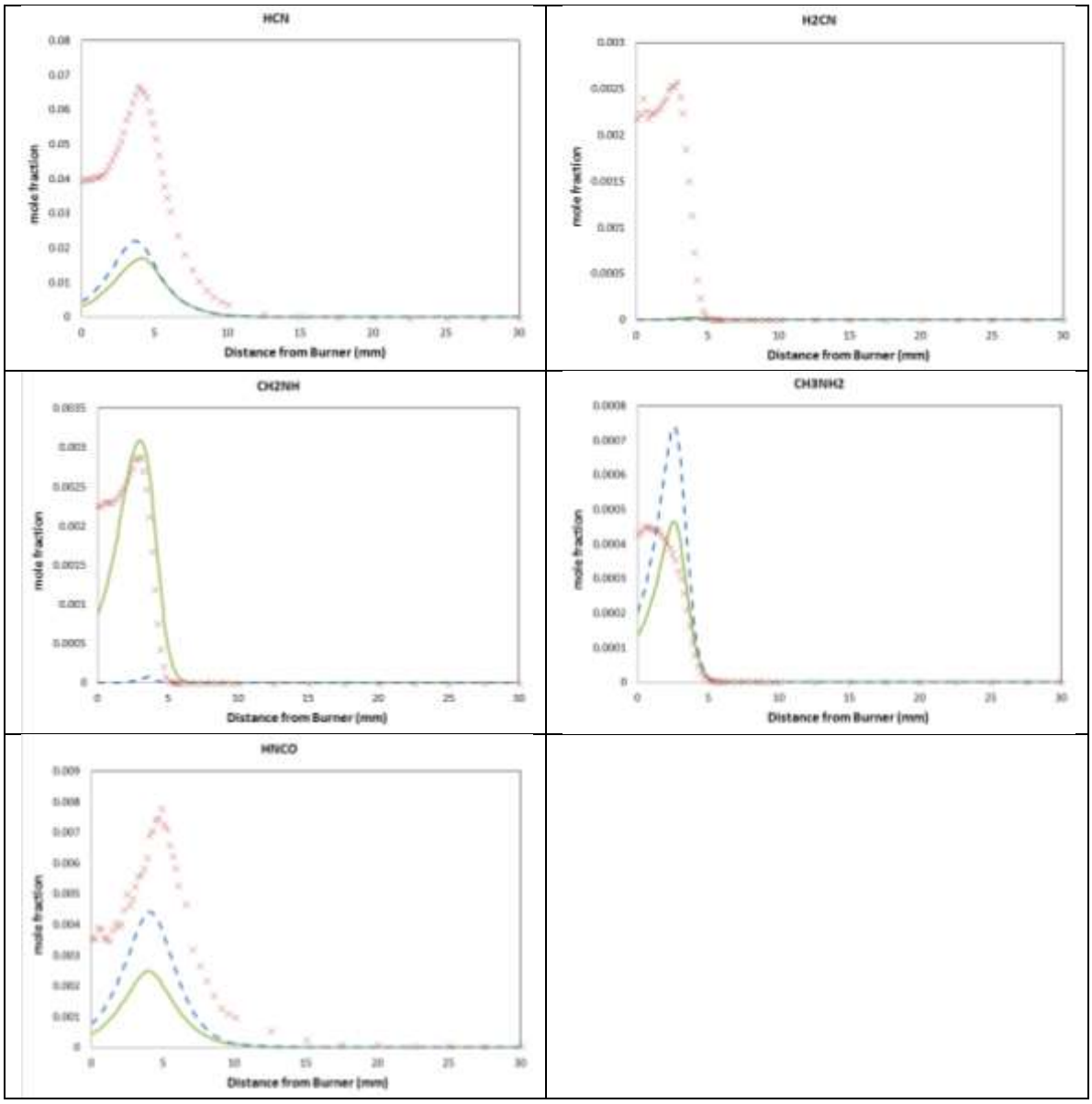


Figure 6.6: Nitrogen-containing intermediate species mole fraction profiles for the stoichiometric ethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

The last intermediate-species data are for the direct decomposition species of ethylamine (see Fig. 6.7). Specific isomers of the different species could not be identified in the experimental analysis, and uncertainty of these profiles is particularly high as a result. To compare to the data, mole fraction profiles for all ethylamine isomers of the same molecular composition were summed. C_2H_6N corresponds to one or more of three

ethylamine radical species. C_2H_5N is one or both of two ethylamine-ene species. C_2H_4N represents five different radicals of the ethylamine-ene species, and C_2H_3N can be a triple-bonded species, $CH_2=C=NH$, or a cyclic C_2H_3N species. In all cases, the two model predictions were indistinguishable from each other. C_2H_6N was predicted within a factor of 3 of the experimental value, C_2H_4N and C_2H_3N were low by about an order of magnitude, and C_2H_5N was only slightly higher than the peak experimental mole fraction.

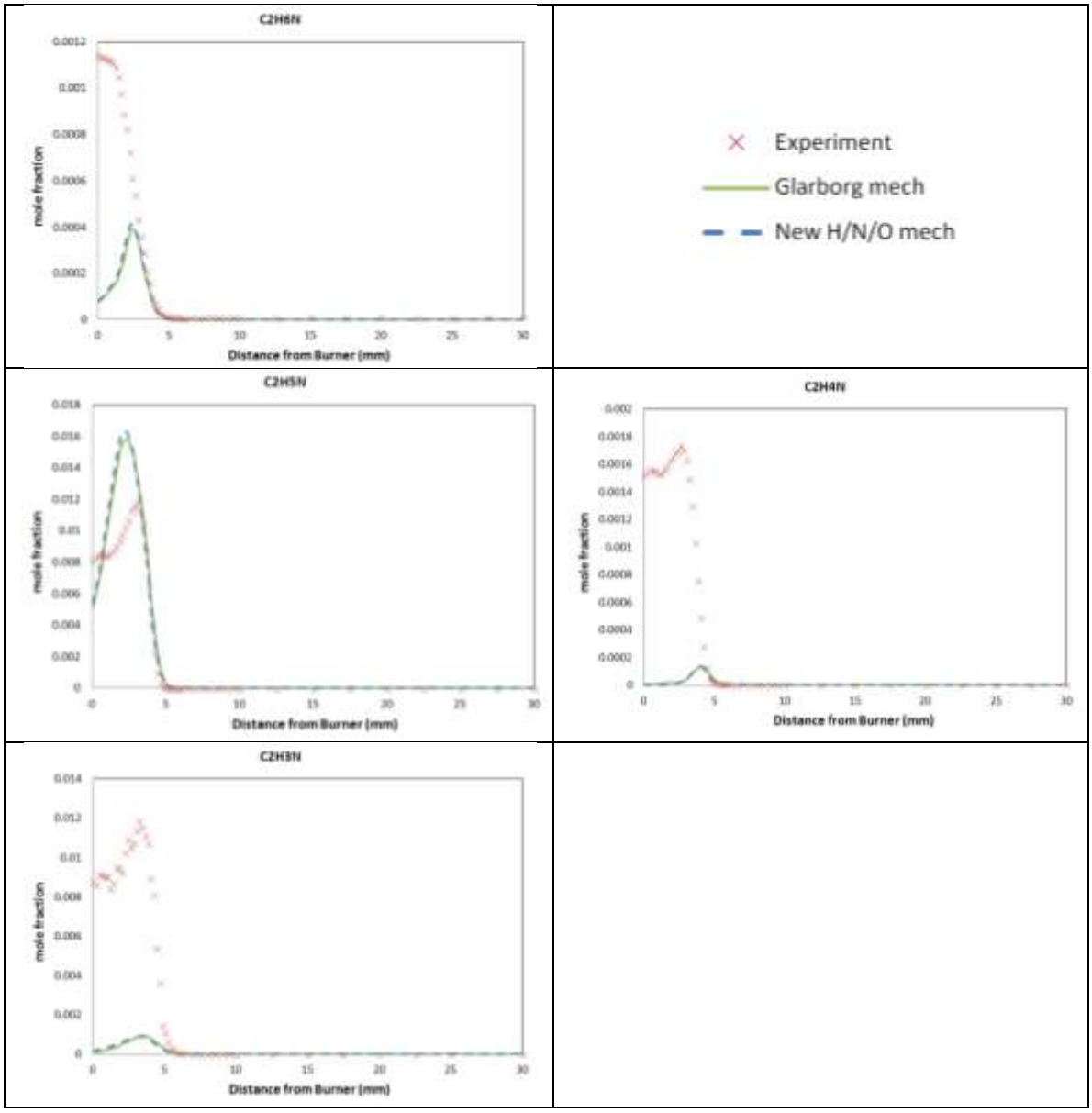
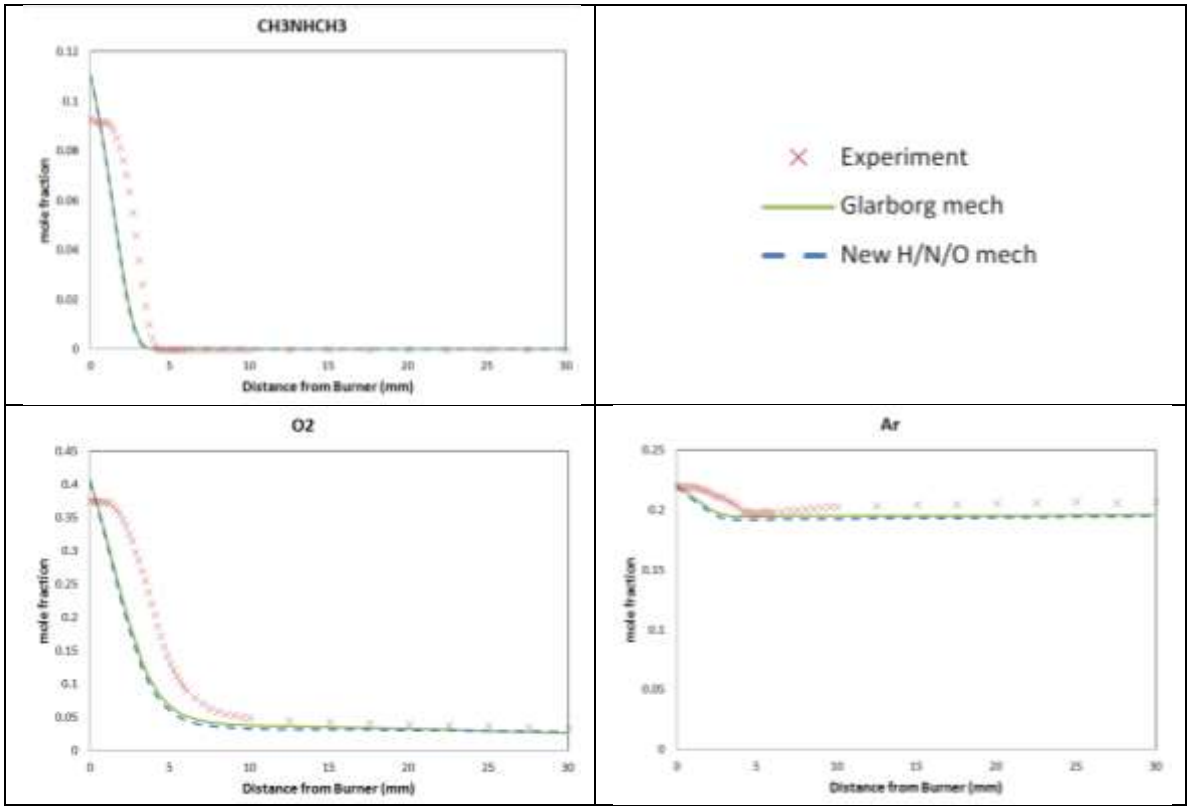


Figure 6.7: Mole fraction profiles for ethylamine decomposition species from the stoichiometric ethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

6.2.1 Comparison to a stoichiometric dimethylamine flame

For the stoichiometric dimethylamine/O_2 flame of Lucassen et al. [10], mole fraction profiles were recorded for main species (presented with modeling results in Fig. 6.8) including dimethylamine (CH_3NHCH_3), O_2, Ar, CO, CO_2, H_2, H_2O, NO, and N_2. The

experimental data profiles are again not meaningful for the first 2 mm of the flame. Dimethylamine is predicted well, although compared to the experimental data, the profile seems slightly shifted towards the burner for both models, which are indistinguishable. The same can be said for O_2, Ar, CO_2, and H_2O, although CO_2 and H_2O are somewhat underpredicted. The new reaction set improves the initial peak height for CO modeling (the Glarborg reaction set underpredicts the CO peak), but neither is able to capture the decay of the CO profile fully beyond 10 mm. The new set also improves the predictions of N_2 over the Glarborg model, and H_2 predictions, though significantly overpredicted for both models, are somewhat higher than the Glarborg model predictions.



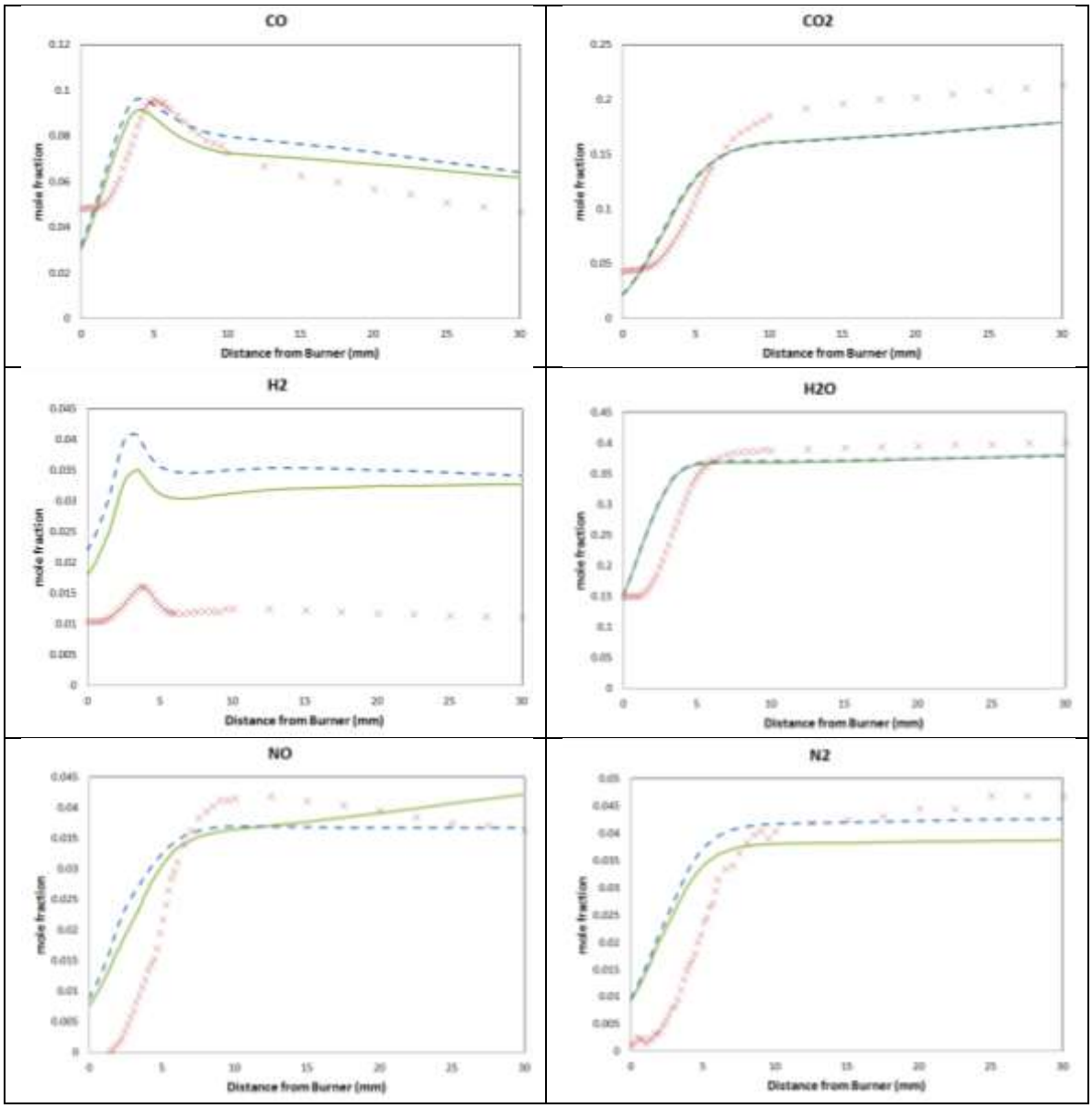
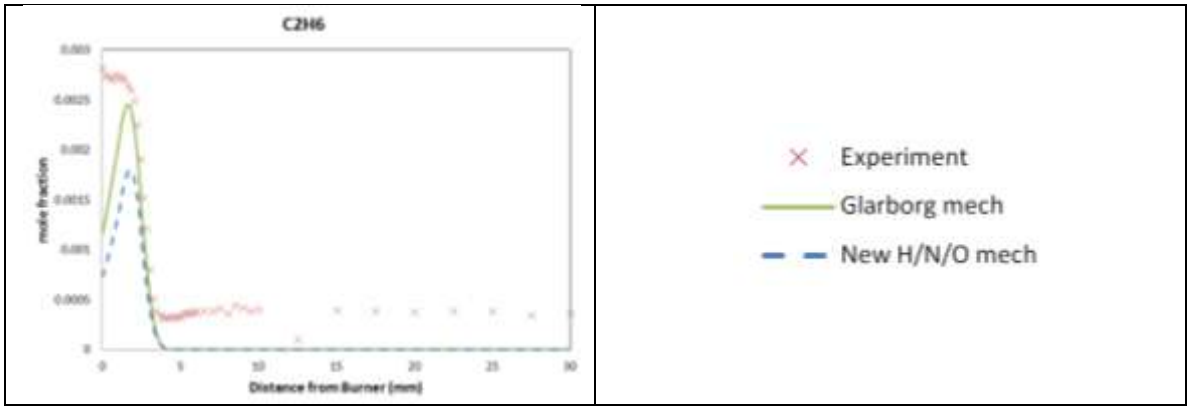


Figure 6.8: Main species mole fraction profiles for the stoichiometric dimethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

Several hydrocarbon intermediate species were detected in the ethylamine flame (Fig. 6.9), including C_2H_6, C_2H_4, C_2H_2, CH_4, CH_3, CH_3OH, CH_2O, CH_2CO, and CH_3CHO. As with the NH_3/CH_4 flames, the largest disagreements with the experimental data and the largest differences between the two models are observed with the

intermediate species. C_2 species in general are underpredicted. Ethane is predicted well by both models (near perfect agreement for the Glarborg model, and well within a factor of 2 for the new model), while the ethylene predictions are worse (about a factor of 3 for the Glarborg set and 6 for the new set), and acetylene is the worst (low by an order of magnitude). This trend is the opposite observed for ethylamine. Methane model results are high (by a factor of 2 for the new set, 1.5 for the Glarborg set), while methyl radical predictions are low (both by a factor of 2). Although much improved over the ethylamine predictions, the discrepancies among the hydrocarbon chemistry still suggest that further improvements are needed in the hydrocarbon reaction set.

Among the oxygenated species, CH_3OH and CH_2O are modeled quite well by the new model compared to the experimental data. The new H/C/N/O set predicts lower CH_3OH than the data by a factor of 3 (compared to an order of magnitude off for the Glarborg model), and CH_2O is nearly perfect for both models. Both models are low by about a factor of 1.5 for CH_2CO and for CH_3CHO. Again, the larger discrepancies between the two models for the H/C/O species may be contributed to the differences in the H/C/O parts of the reaction sets. For the new model, as explained earlier, the H/C/O portion of the reaction set was left largely intact.



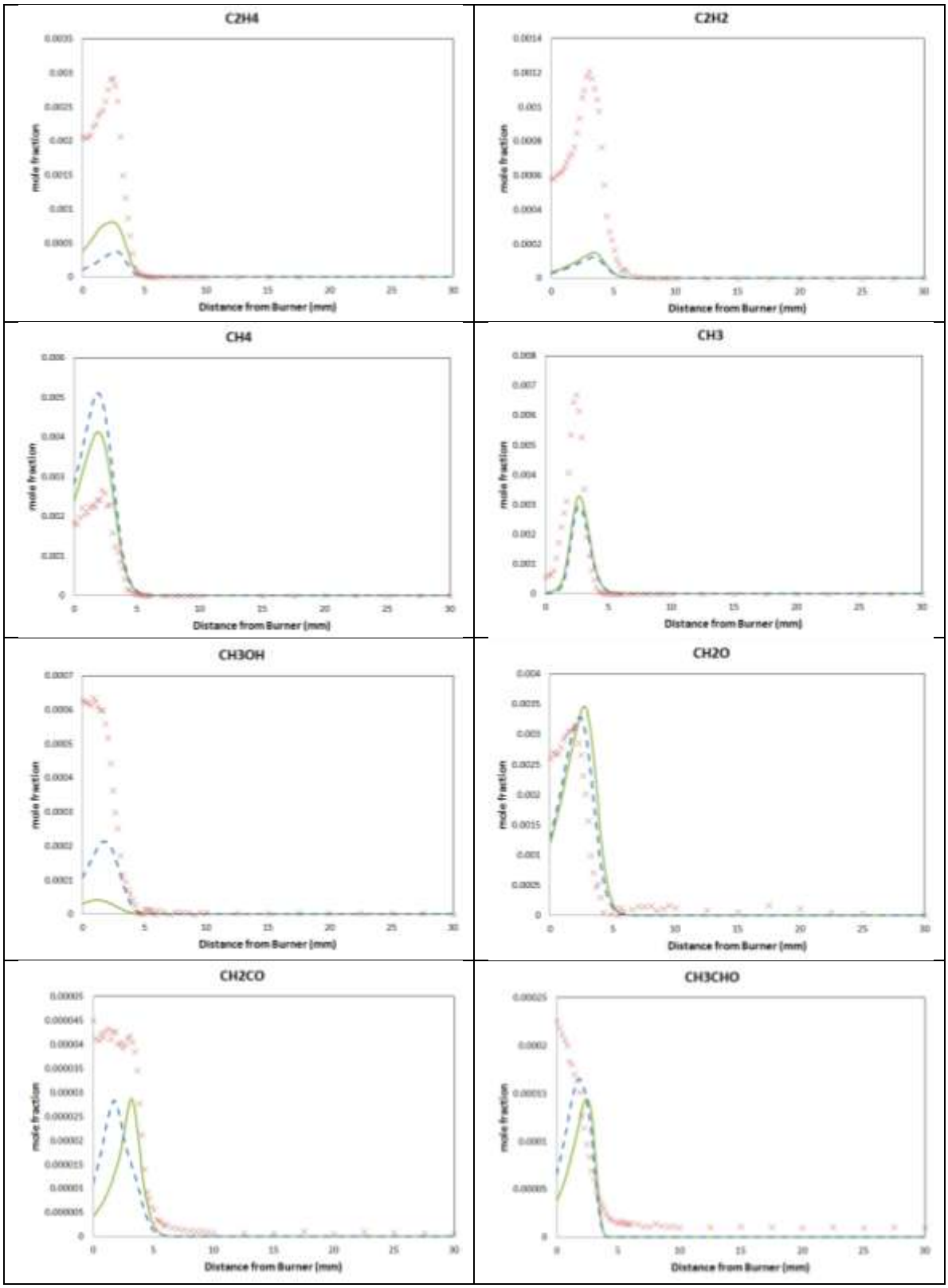
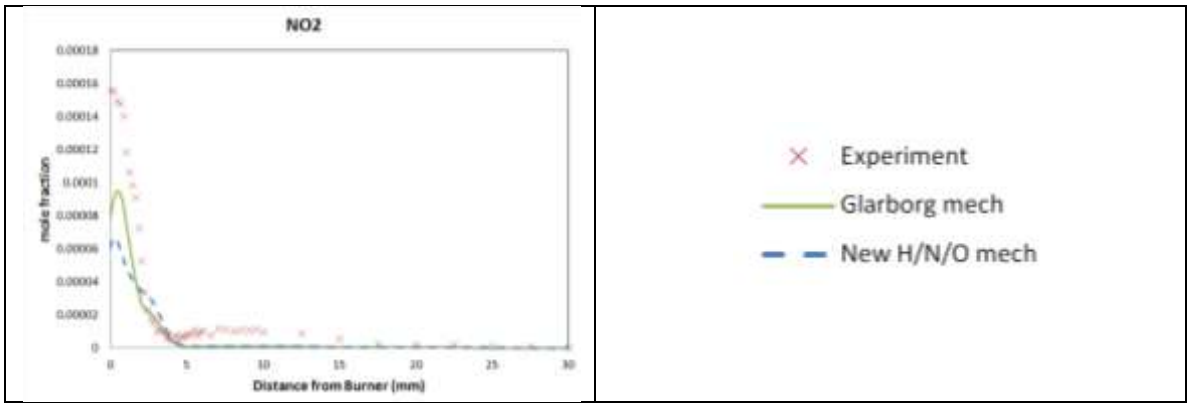


Figure 6.9: Intermediate H/C/O species mole fraction profiles for the stoichiometric dimethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

Several nitrogen-containing intermediate species were also identified (see Fig. 6.10), including NO_2, NH_3, NH_2, HCN, H_2CN, CH_2NH, CH_3NH_2, and HNCO. For this flame, the NO_2 predictions are low by about a factor of 2, although the profile prediction with the new set is not a smooth profile. The new model is able to predict NH_3 nearly perfectly (compared to an underprediction by the Glarborg reaction set of a factor of 5), however, for NH_2, the new model fares less well, overpredicting the data by a factor of 4 while the Glarborg model peak is within the experimental data scatter. The new model shows slight improvements in the predictions of HCN compared to the Glarborg model, but still the models underpredict the data. Neither model predicts H_2CN concentrations of significance, as seen with the ethylamine flame. The new model also does not predict significant CH_2NH, though the Glarborg model overpredicts the peak mole fraction by a factor of 1.5. The Glarborg model predicts CH_3NH_2 quite well, and the new model is well within a factor of 1.5. The nitrogen intermediate, HNCO, is predicted by the new model within a factor of 3, improving upon the accuracy of the Glarborg model, which is low by nearly an order of magnitude. Again the modeling results suggest that the HCN chemistry needs improvement and could benefit from additional scrutiny of the HCN rate constants and from additional experimental data focusing on HCN chemistry.



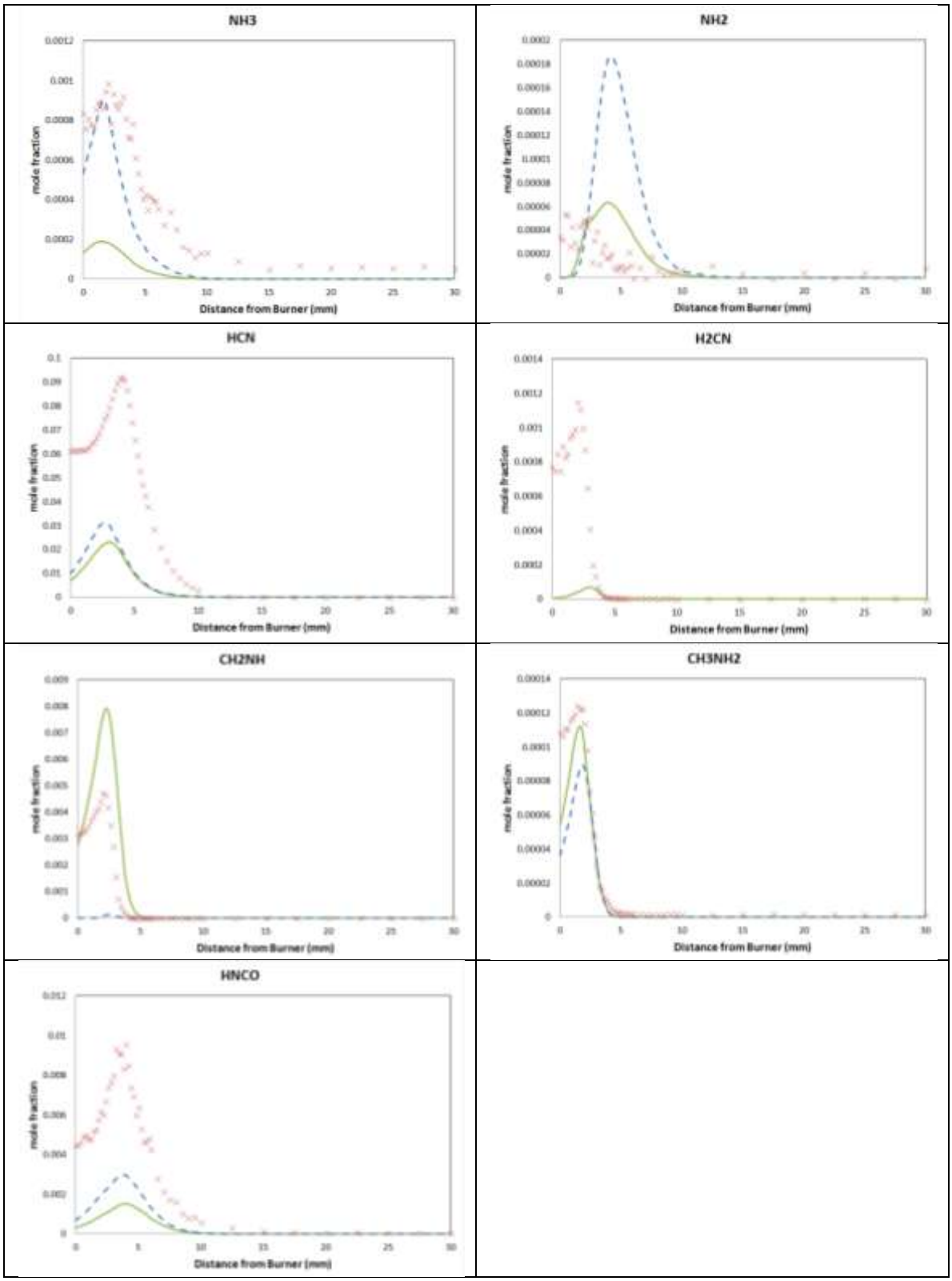


Figure 6.10: Nitrogen-containing intermediate species mole fraction profiles for the stoichiometric dimethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

The last intermediate species data are the direct-decomposition products of dimethylamine (see Fig. 6.11). Specific isomers of the different species could not be identified in the experimental analysis, and uncertainty of these profiles is particularly high as a result. To compare to the data, mole fraction profiles for all dimethylamine isomers of the same molecular composition were summed. C_2H_6N corresponds to two predicted dimethylamine radical species. C_2H_5N can be CH_3-N=CH_2 and/or CH_2=CH-NH_2. C_2H_4N is one or more of five radicals of C_2H_5N, and C_2H_3N can be CH_3CN, formed through secondary reactions, or a cyclic C_2H_3N species.

Again for C_2H_6N, C_2H_5N, and C_2H_4N, the model predictions were indistinguishable from each other. Compared to the data, total C_2H_5N was predicted within a factor of 3, C_2H_6N and C_2H_4N were low by about an order of magnitude, and C_2H_3N was low for both models by over an order of magnitude. It also displayed an unphysical second larger peak closer to the burner for the new model compared to the single peak in the Glarborg model.

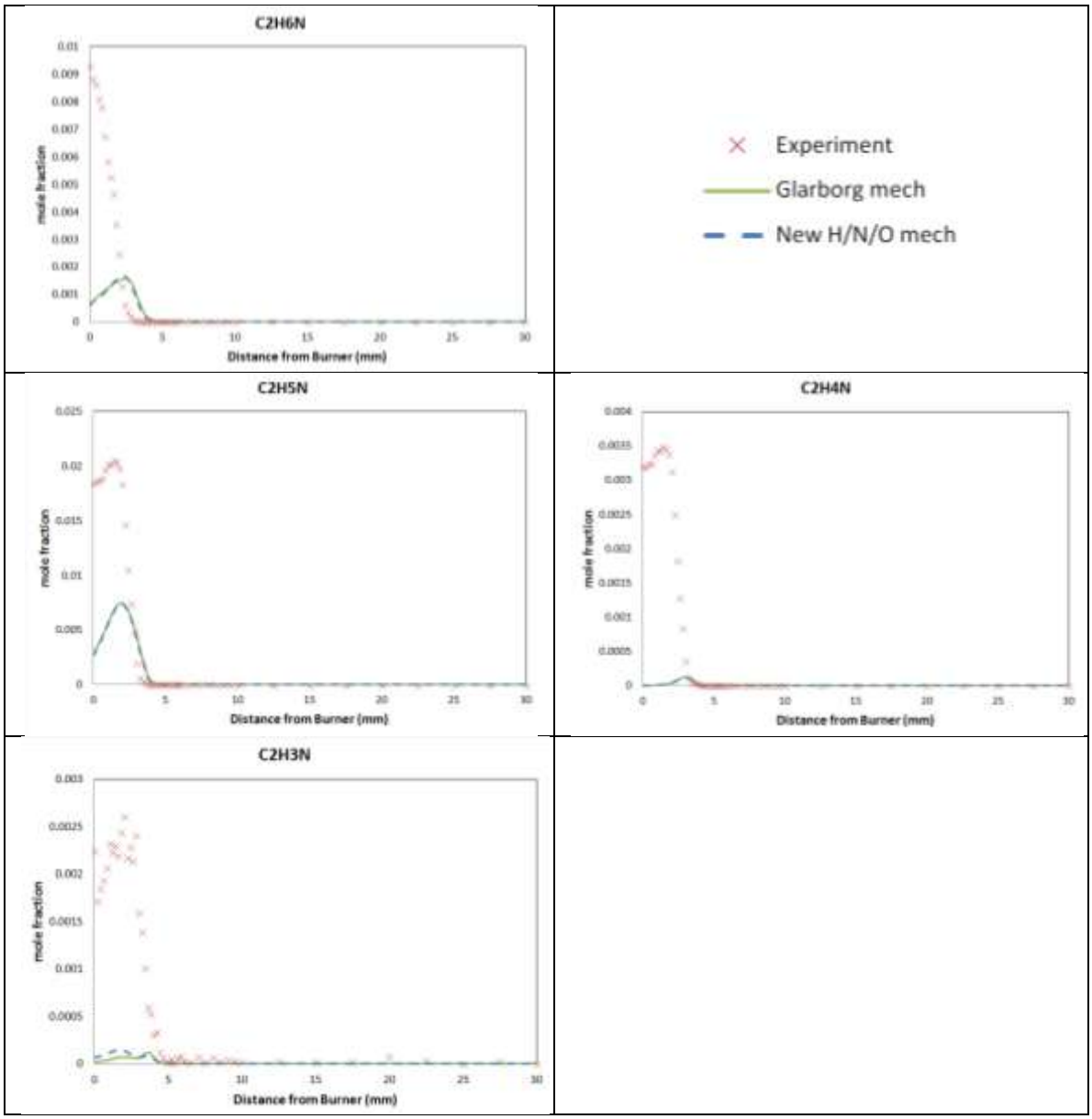


Figure 6.11: Mole fraction profiles for dimethylamine decomposition species from the stoichiometric dimethylamine flame of Lucassen et al. [10] compared to the published model and the current model from this work.

6.3 Summary and Conclusions

The existing H/N/O reaction set described in the previous chapter was expanded to include carbon chemistry. The hydrocarbon chemistry was drawn largely from the reaction sets of [1-3] and was left unchanged as the kinetics had been previously tested. H/C/N/O chemistry was drawn from several sources and compiled into one master

database and reaction set. This new set was tested against three different stoichiometric flames, including an NH_3/CH_4 flame, an ethylamine flame, and a dimethylamine flame.

The overall agreement of the new reaction set versus the experimental data and the model results published in the flame experiment studies was good. The largest issues arose in the predictions of intermediate species, which often were predicted poorly by both models. While some intermediate species were not predicted as well as by the published model, other predictions were improved.

Future work on the new H/C/N/O model is needed on three fronts. First, more reliable experimental data must be obtained for comparison and model validation, as there are many questions with the current studies and a broad enough range of conditions has not been sampled. Secondly, the chemistry in the hydrocarbon part of the set needs further testing and validation. Evidence from the study suggests there are issues in the H/C/O chemistry that could possibly affect the H/C/N/O set. Lastly, with a wider range of data for comparison, the H/C/N/O set should be further refined by the same approach by which the H/N/O model was refined in the previous chapter.

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CHAPTER 7

HETEROATOMIC FUELS: THP AND THE EFFECT OF FUEL OXYGEN ON FLAME CHEMISTRY[1]

Biofuels are of great interest because they come from renewable sources and can reduce emissions of aromatic hydrocarbons and soot relative to combustion of fossil fuels. Tetrahydropyran (THP) is the monoether analog of cyclohexane and is the core structure of many sugars and polysaccharides including glucose, a common feedstock for biogenic fuels that have multiple furan and THP-based isomers [1]. These sugars can be pyrolyzed to produce biofuels and bio-derived industrial chemicals, many of which are substituted furans and pyrans [2-3]. Oxidation of THP has been studied in a jet-stirred reactor as a surrogate fuel for diesel models [4] and in shock-tube experiments to understand autoignition of alkanes [5]. THP has been identified as a functional group in several intermediate species in low-temperature oxidation studies of n-alkanes [6].

In the present work, the combustion chemistry of THP is studied to understand the effect of ether linkages on pollutant formation in cyclic fuels, complementing previous studies of the structurally analogous fuels cyclohexane [7], morpholine (1-oxa-4-aza-cyclohexane) [8], and tetrahydrofuran [9]. Photoionization molecular-beam mass spectrometry (PI-MBMS) was conducted on a fuel-rich, laminar flat flame of THP/O_2/Ar to determine mole-fraction profiles. Based on a newly developed THP reaction set, pathways are identified for fuel decomposition and chemical production of potentially harmful emissions.

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[1] Adapted from N. J. Labbe, V. Seshadri, T. Kasper, N. Hansen, P. Oßwald, P. R. Westmoreland, "Flame chemistry of tetrahydropyran as a model heteroatomic biofuel," *Proc. Combustion Inst.* **34** (online 2012; in print 2013): http://www.sciencedirect.com/science/article/pii/S1540748912003197

7.2 Experiments and Procedures

THP/O_2/25% Ar (Φ=1.75) was burned in a laminar, premixed flat flame at 2.66 kPa (20.0 Torr) and feed mass flux of 0.0443 kg•m^{-2}•s^{-1}. The flame was analyzed using photoionization molecular-beam mass spectrometry (PI-MBMS). Tunable vacuum ultra-violet (VUV) radiation from the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory allowed single-photon ionization with high energy resolution. This experimental arrangement has been described in detail previously [10-14] and here will be described only briefly. The flame was stabilized on a 6.0-cm diameter, stainless-steel, McKenna-type burner. Gas flows were controlled with calibrated mass flow controllers, and liquid THP was metered by a syringe pump, evaporated, and added to the gas stream. Samples were withdrawn through a 0.40-mm-diameter orifice at the tip of a 40° quartz cone; wall thickness is near 50 μm at the tip. Sampled gas was expanded to ~10^{-4} mbar in the first pumping stage and extracted by a skimmer, forming a molecular beam that passes through the mass spectrometer's (MS) ionization region (~10^{-6} mbar).

Photoionization was by a quasi-continuous photon beam of ~10^{13} photons/s at energies between 8.00 and 17.00 eV, resolved to ~0.05 eV by a 3-m Eagle monochromator. Analysis employed a linear time-of-flight mass spectrometer (TOF-MS) with a mass resolution of $m/\Delta m$=400. Ions were detected by a multichannel plate and integrated with a multichannel scaler with a sensitivity of ~10^{-5}. Mass spectra were collected as functions of the distance *h* to the burner ("burner scan") or as functions of the photon energy at a fixed distance ("energy scan"). Spectra were corrected for fragmentation and ^{13}C and ^{18}O contributions. Thirty-one species were identified (see Table 7.1).

Table 7. 1: List of species with their peak mole fractions, peak positions, method of measurement, energy at which the species were measured, and ionization energies.

Species	Formula	Mass (g/mol)	Peak Value	Peak position (mm)	Measurement method	Cross section & IE[a] reference	Cross section (Mb)	Energy (eV)	IE (eV)
hydrogen	H_2	2	1.9E-01	30.6	H Atom balance	[15-16]	9.5	16.65	15.42
methyl	CH_3	15	3.3E-03	4.9	Reference species (C_2H_2)	[17]	12.1	13.2	9.84
methane	CH_4	16	8.6E-03	4.4	Reference species (C_2H_2)	[18]	4.6	13.2	12.61
water	H_2O	18	2.8E-01	7.1	H Atom balance	[19]	15.2	16.65	12.62
acetylene	C_2H_2	26	3.0E-02	5.4	Reference species (H_2O)	[20]	39.1	13.2	11.4
ethylene	C_2H_4	28	4.4E-02	4.4	Reference species (C_2H_2)	[21]	13.3	12.3	10.51
carbon monoxide	CO	28	3.7E-01	16.6	Direct Calibration and C atom balance	[22]	23.9	14.35	14.01
formyl	HCO	29	5.0E-03	3.1	Reference species (C_2H_2)	[23]	8.0	12.3	8.12
formaldehyde	H_2CO	30	1.2E-02	4.4	Reference species (C_2H_2)	[24]	16.4	12.3	10.88
oxygen	O_2	32	5.0E-01	0.9	FKT	[25]	39.1	13.2	12.07
propargyl	C_3H_3	39	7.7E-04	4.9	Reference species (CH_3)	[26]	8.9	10.5	8.67
allene	C_3H_4	40	3.5E-04	4.4	%Contribution using energy scan	[21]	18.9	10.5	9.69
propyne	C_3H_4	40	5.3E-04	4.4	Reference species (CH_3)	[21]	23.1	10.5	10.36
argon	Ar	40	2.1E-01	0.6	FKT	[27]	32.3	16.65	15.76
allyl	C_3H_5	41	6.9E-04	3.9	Reference species (CH_3)	[28]	6.1	10.5	8.18
ketene	CH_2CO	42	7.2E-04	2.4	%Contribution using energy scan	[29]	21.6	10.5	9.62
propylene	C_3H_6	42	2.9E-03	2.4	Reference species (CH_3)	[21]	10.7	10.5	9.73
carbon dioxide	CO_2	44	9.1E-02	16.6	Direct Calibration and C atom balance	[30]	18.6	14.35	13.78
diacetylene	C_4H_2	50	9.6E-04	6.6	Reference species (CH_3)	[20]	23.8	10.5	10.17
vinylacetylene	C_4H_4	52	5.9E-04	4.4	Reference species (CH_3)	[20]	32.5	10.5	9.58
1,3-butadiene	C_4H_6	54	4.0E-03	3.6	Reference species (CH_3)	[20]	17.6	10.5	9.07

1-oxoprop-2-enyl/ butenyl	C_3H_3O/ C_4H_7	55	7.9E-04	3.1	Reference species (CH_3)	Est., [31][a]	10.0	10.5	<8.5[b]
Propenal	C_3H_4O	56	5.0E-03	2.4	Reference species (CH_3)	Est., [32][a]	10.0	10.5	10.11
1-butene/2-butene	C_4H_8	56	3.1E-03	2.4	Reference species (1,3-butadiene)	Est., [33-34][a]	5.0	9.8	9.55/-9.10
furan/1,4-pentadiene /2-butynal/but-3-ynal/ 1,2-butadienal	C_4H_4O/ C_5H_8	68	6.9E-04	2.4	Reference species (CH_3)	Est.	10.0	10.5	8.5[b]
1-pentene/2-butenal	C_4H_6O/ C_5H_{10}	70	1.6E-03	2.9	Reference species (CH_3)	Est.	10.0	10.5	9.25[b]
benzene	C_6H_6	78	7.8E-05	2.6	Reference species (CH_3)	[20]	31.8	10.5	9.25
pent-2-ynal	C_5H_6O	82	6.1E-04	2.4	Reference species (CH_3)	Est.	10.0	10.5	10.2[b]
3,4-dihydropyran /2-pentenal	C_5H_8O	84	4.7E-04	2.6	Reference species (1,3 butadiene)	Est.	10.0	9.8	9.2[b]
THP-yls and their isomeric beta-scission compounds	C_5H_9O	85	1.2E-03	2.4	Reference species (1,3-butadiene)	Est.	10.0	9.8	10.0[b]
tetrahydropyran	$C_5H_{10}O$	86	1.2E-01	0.6	FKT	[29]	8.5	9.8	9.25

"Est." refers to estimation. The cross section was estimated based on similar species. For species for which the exact structure is not known, the IE is left blank. Superscript 'a' denotes that the reference is for the IE. Superscript 'b' denotes the energy where the signal starts for a particular mass (this information is given where no species could be identified conclusively). For the species where identification was not possible, a list of possible species (separated by '/') is given in the species column.

The temperature profile used for model calculations combines laser-induced fluorescence (LIF) data with a profile determined from skimmer-chamber pressure. High temperatures were measured with LIF using the frequency-doubled output of an optical parametric oscillator (Continuum Sunlite EX OPO) near 306 nm to excite the OH A–X(0,0) transition. Total fluorescence is monitored with a solar-blind photomultiplier tube with gain set to produce a linear response over the expected range of signals. Accuracy is estimated to be ±150 K in the postflame and reaction zones but is not adequate in the preheat zone, where the OH concentration is much smaller and its concentration gradient is much steeper [35]. Assuming a constant pumping speed, sampling rate through the probe orifice can be expressed as a function of skimmer-chamber pressure and source temperature. LIF data are shifted 2.4 mm to match the skimmer-chamber-pressure temperature profile. The temperature profile is fixed as 450 K at the inlet, post-flame gas temperature is taken from the LIF measurement, and the shape and position of the profile are from the skimmer-chamber-pressure analysis.

7.3 Model Development and Simulations

A reaction set for THP combustion was developed by analogy to cyclohexane, as shown in Fig. 7.1. A recent modeling study of cyclohexane combustion at low pressure showed that steady-state, laminar combustion of cyclohexane favors hydrogen-abstraction reactions for cyclohexane destruction [7]. Like cyclohexane, THP is a 6-heavy-atom, saturated ring molecule. Unlike cyclohexane, there are three different distinct hydrogen sites on THP: on the carbons directly adjacent to the ether oxygen (the “2” and “6” carbons), the next neighboring two carbons (the “3” and “5” carbons), and

the “4” carbon opposite the oxygen. As a result, there are three distinct routes for THP H-abstraction, each having different reactivities.

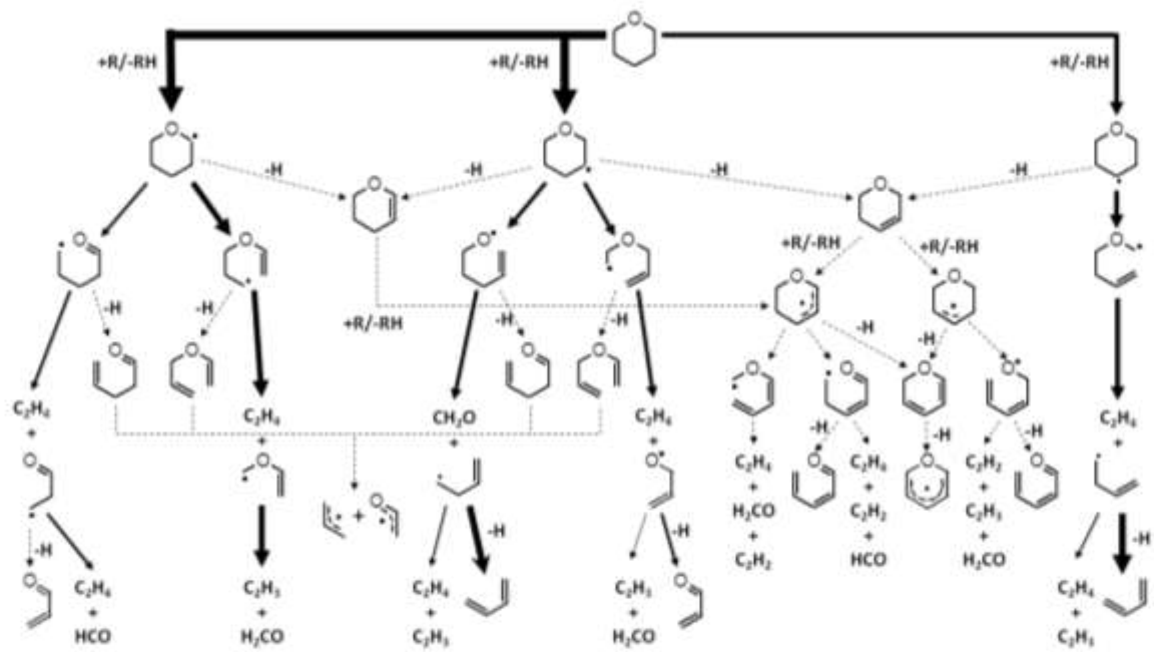

Figure 7.1: Skeletal reaction-mechanism diagram for THP flame.

For the three resulting THP-yl radicals, decomposition steps to smaller species were assumed to be more important than O atom addition kinetics, as had been seen in cyclohexane modeling [7]. THP-yls can undergo β-scissions, breaking the ring to form linear, unsaturated radicals, or they can β-scission a C-H bond, forming unsaturated cyclic molecules (analogous to cyclohexene). The linear radicals preferentially β-scission to a two-heavy-atom molecule (C_2H_x or CH_xO species) plus a four-heavy-atom unsaturated radical that may also undergo further β-scission. Alternatively, the six- or four-heavy-atom radicals may yield unsaturated molecules by β-scission of an H-atom. If an unsaturated cyclic molecule is formed, its allylic H is easily abstracted; β-scission then breaks the ring or creates a doubly unsaturated cyclic molecule (analogous to cyclohexadiene).

A reaction set was constructed for THP combustion using this skeletal mechanism. Reaction rate coefficients and fall-off were derived based on analogous reactions from the cyclohexane model [7] but with Arrhenius pre-exponential factors modified for the proper reaction path degeneracy (RPD). The exception was the three hydrogen abstraction routes from THP to distinguish pathways to the three different THP-yl isomers. For THP+H and THP+CH_3, transition states were calculated using CBS-QB3 with Gaussian09 software [36]; rate coefficients were calculated using canonical transition-state theory and fit to an Arrhenius expression; and rate coefficients for THP+C_2H_3, THP+HCO, and THP+CH_3CO abstractions were then estimated by analogy. Abstraction rate coefficients for THP+O_2, THP+O, THP+OH, and THP+HO_2 were estimated by analogy with cyclohexane reactions. Fall-off for THP-yl decompositions was calculated using unimolecular quantum-RRK theory [37]. The acetylene reaction set from [38] was adapted for the hydrocarbon reactions. Direct ring decomposition rate constants were added from Dagaut et al. [5].

Thermochemistry was calculated theoretically for 22 species in the proposed skeletal mechanism using the complete-basis-set method CBS-QB3. Geometry and frequency calculations were completed using tight convergence criteria. If necessary, transport data were estimated by analogy to molecules of similar structure, size, and molecular weight. The resulting reaction set contains 125 species and 1046 reactions (see Appendix E).

Flame simulations were performed using a modified version of the CHEMKIN-II PREMIX flame code [39-42] including thermal and multi-component diffusion. Experimental temperatures were represented by a smoothed curve (see Fig. 7.2). Reaction

pathways and net reaction rates were analyzed using XSenkPlot [43], adapted from the original code to obtain absolute reaction rates (rather than rates divided by density) and integrated reaction fluxes with respect to distance (rather than time).

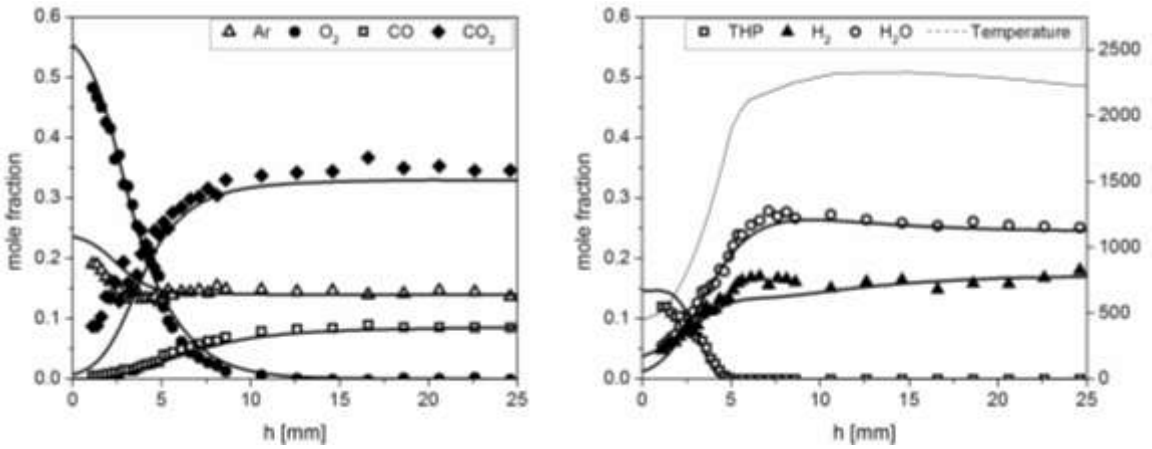

Figure 7.2: Major-species mole-fraction profiles: (left) Ar, O_2, CO, CO_2; (right) THP, H_2, H_2O, temperature. Symbols indicate experimental data (data for the first 1.0 mm have been omitted due to perturbation); lines are from flame model.

7.4 Results and Discussion

Upon detailed analysis, many predicted features of the flame were in quite good agreement with the data set. Simulations of major-species mole fractions (Fig. 7.2) show agreement in peak magnitude, shape, and position, useful indicators of model validity. Post-flame mole fractions (beyond about 6 mm) also agree well with the data. No rate coefficients were adjusted to force such a fit; indeed, the model and predictions were developed independently of the experimental mole-fraction analysis. Agreement is presumably the combined result of a generally valid model, accurate measurements, and accuracy of post-flame temperatures.

Precision is generally estimated as <15% for major-species mole-fraction profiles, 30% for species with reliable photoionization cross sections, and approximately a factor

of two for intermediates with estimated cross sections. Very close to the burner, the flame is significantly perturbed by the probe, so experimental species mole fractions are only reported at h>1 mm, and quantitative comparisons are not encouraged at less than 2 mm.

The following discussion examines how the THP-flame species are formed and destroyed, revealing sensitivity of minor-species predictions to kinetics of the larger intermediates. Aspects of overall THP flame chemistry are addressed first, followed by discussion of intermediate species and the implications of the kinetics of their formation and destruction.

7.4.1 THP destruction pathways

Analysis of the simulation is summarized in Fig. 7.1, showing reaction-arrow line widths scaled proportionally to the integrated reaction fluxes. The thickest lines thus show the major routes of fuel combustion. THP itself is consumed by H-abstraction from the three distinct positions in the proportions THP-2-yl:THP-3-yl:THP-4-yl::10:9:5. The pathway differences can partially be attributed to the differences in C-H bond energies between the three different C-H bonds found in THP. The presence of the oxygen in the ring makes the C-H bonds ortho to the oxygen the weakest C-H bonds at 96.6 kcal, followed by the C-H bonds para to the oxygen at 99.5 kcal. The meta C-H bonds were the most strongly held at 100.9 kcal, making those bonds the hardest to break. These THP-yls are mainly consumed by β-scission of C-C or C-O bonds, opening the ring to form additional mass-85 isomers that β-scission to C_2H_4 or CH_2O plus a four-heavy-atom radical. From the latter radicals, β-scission of C-C or C-O bonds forms C_2H_3, C_2H_4, HCO, and CH_2O, while β-scission of C-H bonds forms 1,3-butadiene or acrolein.

By comparison, β-scission of C-H bonds causes relatively minor THP-yl

destruction channels, forming 3,4-dihydro-2H-pyran and 3,6-dihydro-2H-pyran, the two possible cyclohexene-like C_5H_8O isomers (mass 84). In addition, several open-chain isomers may also contribute to mass 84. The dihydropyran species can undergo H-abstraction to form cyclic mass-83 species, which may β-scission to ring mass-83 species or to form the pyran-diene at mass 82.

The number of isomers expected to contribute at mass 85, 84, 83, and 82 makes experimental identification and quantification difficult, yet the limited comparisons for these species and the good comparisons for smaller species lend support to the model's validity. Eleven mass-85 species and five mass-84 species may contribute, and they could not be resolved experimentally. Model results for THP-diene (mass 82) were only about a factor of two lower than the experimental data, which is acceptably within the range of uncertainty.

7.4.2 Kinetics of THP-yl decomposition intermediates

7.4.2.1 Four-heavy-atom intermediates.

It was possible to identify and provide estimates for the mole fractions of some species featuring four heavy atoms that result from the further fuel breakdown. From the skeletal mechanism in Fig. 7.1, key species in this mass range include $\bullet CH_2CH_2CH{=}O$ and $\bullet CH_2OCH{=}CH_2$ (mass 57), acrolein ($CH_2{=}CH\text{-}CH{=}O$, mass 56), $\bullet CH_2CH_2CH{=}CH_2$ (C_4H_7, mass 55), and 1,3-butadiene ($CH_2{=}CHCH{=}CH_2$, mass 54). All these four-heavy-atom segments of the original ring structure preserve the sequence of heavy atoms, coming from decomposition rather than molecular-weight-growth processes.

The mass-57 radicals could not be resolved, but mass 56 was identified as acrolein and is predicted reasonably well by the model (Fig. 7.3h). The peak magnitude is

predicted well, although the predicted peak is shifted from the experimental profile by approximately 1 mm away from the burner.

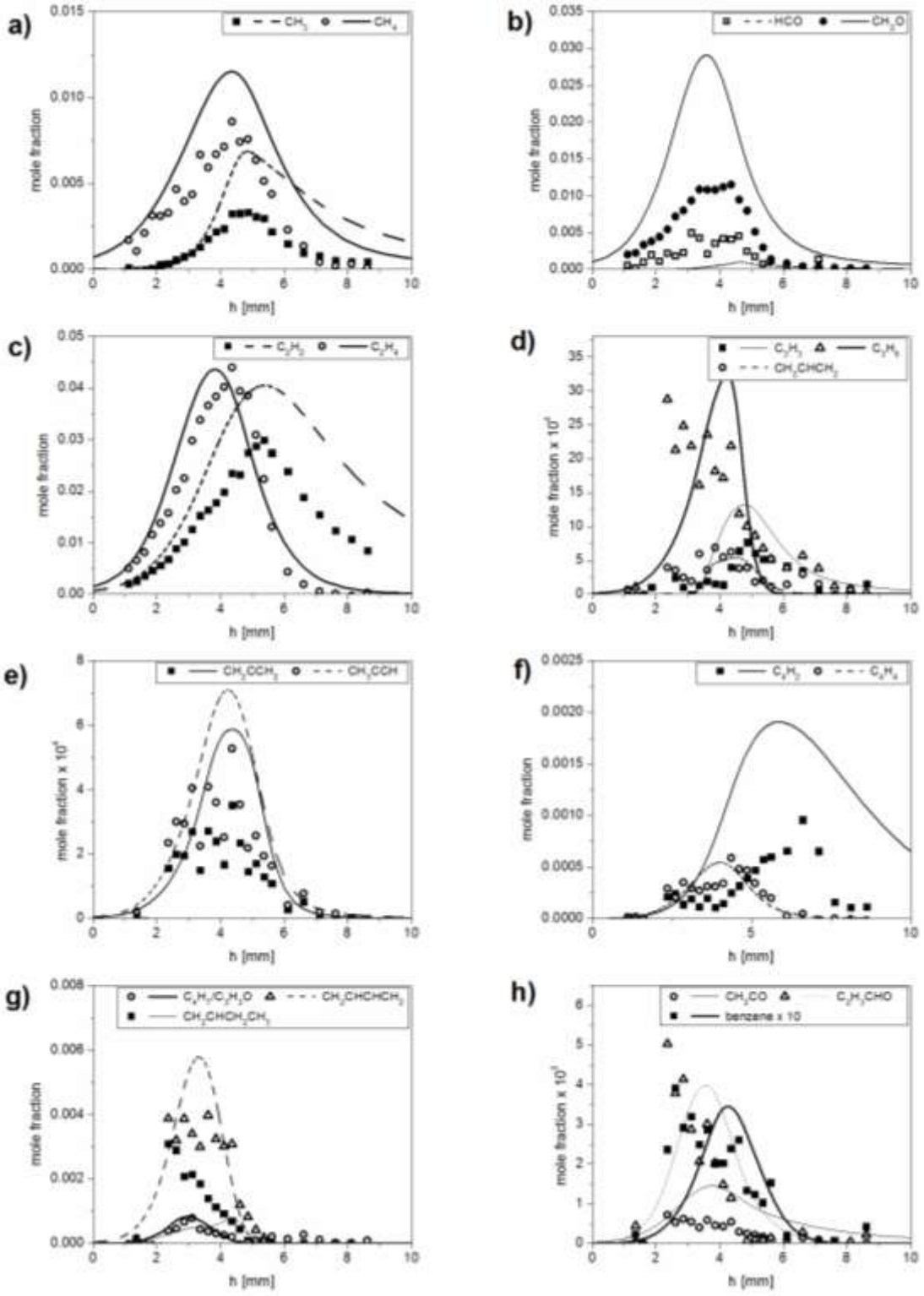

Figure 7.3: Mole-fraction profiles of intermediate species including a) CH_3 and CH_4, b) HCO and CH_2O, c) C_2H_2 and C_2H_4, d) $C_3H_{5\text{-}7}$ e) C_3H_4's, f) C_4H_2 and C_4H_4, g) $C_4H_{6\text{-}8}$, and C_3H_3O, and h) CH_2CO, C_2H_3CHO, and benzene. Symbols indicate experimental data (data for the first 1.0 mm have been omitted due to perturbation); lines are from flame model.

A signal at mass 55 was also observed, but species of molecular formulas C_4H_7 and C_3H_3O could not be distinguished. To propose what mass 55 could be, the model predictions for mass-55 species were compared. The only C_4 species in the decomposition routes, C_4H_7, was predicted to be dominant over all other mass-55 species. The model prediction of mass 55 was quite good, supporting its origin as being THP-yl decomposition. Additional indirect support comes from the good prediction of 1,3-butadiene, which is formed primarily from C_4H_7 by decomposition or H-abstraction. Butadiene is predicted to be about 50% higher than that which was observed experimentally (Fig. 7.3g).

7.4.2.2 Two-heavy-atom intermediates.

The skeletal fuel-decomposition mechanism leads to a number of stable and radical species with two heavy atoms (bottom of Fig. 7.1), including C_2H_2, C_2H_3, C_2H_4, HCO, and CH_2O. They result from more than one pathway, though.

Experimental and predicted mole-fraction profiles for C_2H_4 and C_2H_2 are presented in Fig. 7.3c. The simulation shows good agreement for C_2H_4, matching profile magnitude, and shape well though the model is shifted slightly towards the burner. Analysis of the reaction rates (Fig. 7.4) show that C_2H_4 is produced almost entirely from the THP-yl decomposition routes. The same is true for C_2H_4 production in cyclohexane flames (from cyclohexyl). Of the multiple routes for C_2H_4 formation, the principal formation paths are:

$$THP \rightarrow C_2H_4 + C_3H_6O$$

$$\bullet OCHCH_2CH_2 \rightarrow C_2H_4 + HCO$$

$$\bullet CH_2CH_2CH_2CH_2CHO \rightarrow C_2H_4 + \bullet CH_2CH_2CHO$$

•$CH_2CH_2OCH_2CHCH_2 \rightarrow C_2H_4 + \bullet OCH_2CHCH_2$

•$CH_2CH_2CH_2OCHCH_2 \rightarrow C_2H_4 + \bullet CH_2OCHCH_2$.

The prediction for the C_2H_2 mole-fraction profile captures its peak position and profile shape quite accurately, and its peak magnitude agrees within expected uncertainty. It is produced by decomposition of C_2H_3, which is formed through the THP-yl decomposition paths.

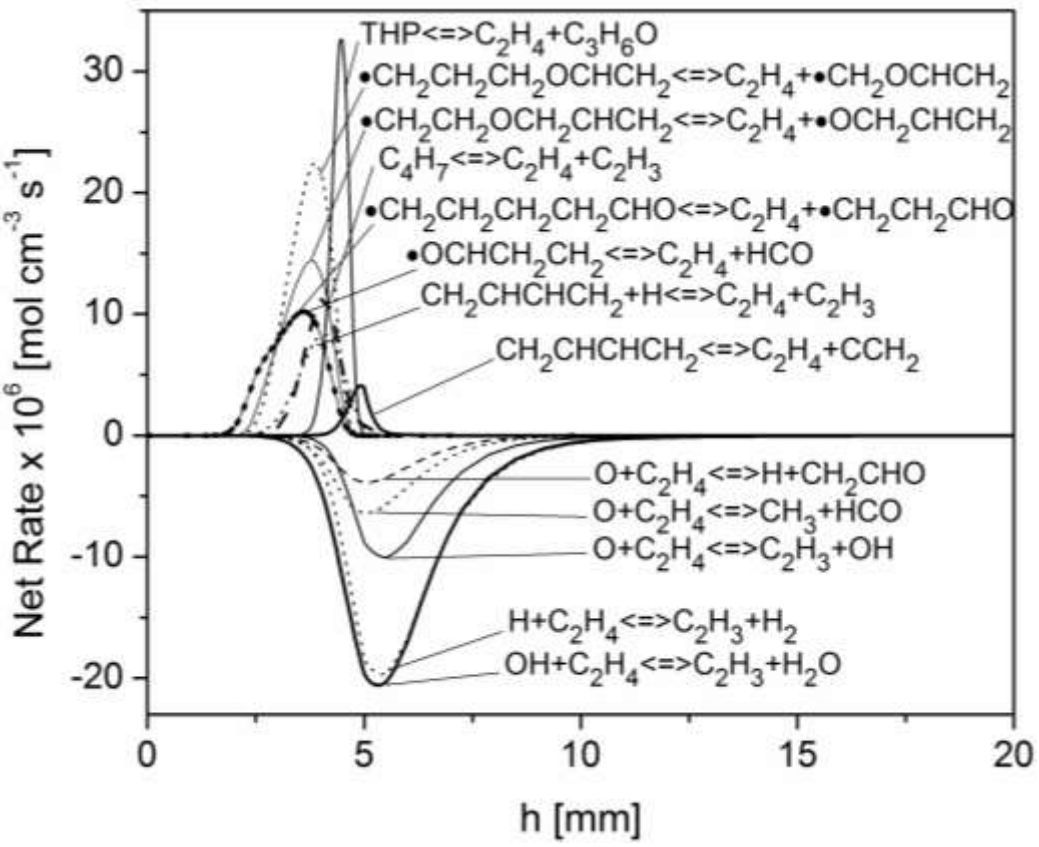

Figure 7.4: Reaction-rate diagram for C_2H_4.

By comparison, CH_2O appears over-predicted by a factor of 2.5, and HCO is under-predicted by a factor of four, although the peak positions and shapes are in good agreement (Fig. 7.3b). The inconsistencies are most likely due to greater HCO calibration uncertainty or its being converted too fast in the model, as many radicals abstract its H.

In the THP flame, CH_2O is predominantly formed directly from the THP-yl decomposition reaction steps, based on the model analysis presented in Fig. 7.5, where net rates of CH_2O formation and destruction are graphed for the main contributors in the THP flame. CH_2O is predominantly formed from decomposition of six-heavy-atom radicals $\bullet CH_2OCH_2CH_2CH=CH_2$ and $\bullet OCH_2CH_2CH_2CH=CH_2$ and a four-heavy-atom radical $\bullet CH_2OCH=CH_2$ that are from the THP-yl decomposition sequence. It can also be formed by direct ring decomposition via $THP \rightarrow CH_2O+C_4H_8$. The reactions $C_2H_3+O_2 \rightleftarrows HCO+CH_2O$ and $\rightleftarrows H+CO+CH_2O$ contribute as well, where C_2H_3 and its precursor C_2H_4 (via $C_2H_4+R \rightleftarrows C_2H_3+RH$, where R is a radical) come mainly from THP-yl decomposition. CH_2O is destroyed by H-abstraction, mainly by H and OH, so accuracy of those radicals' predictions will affect the relative CH_2O and HCO.

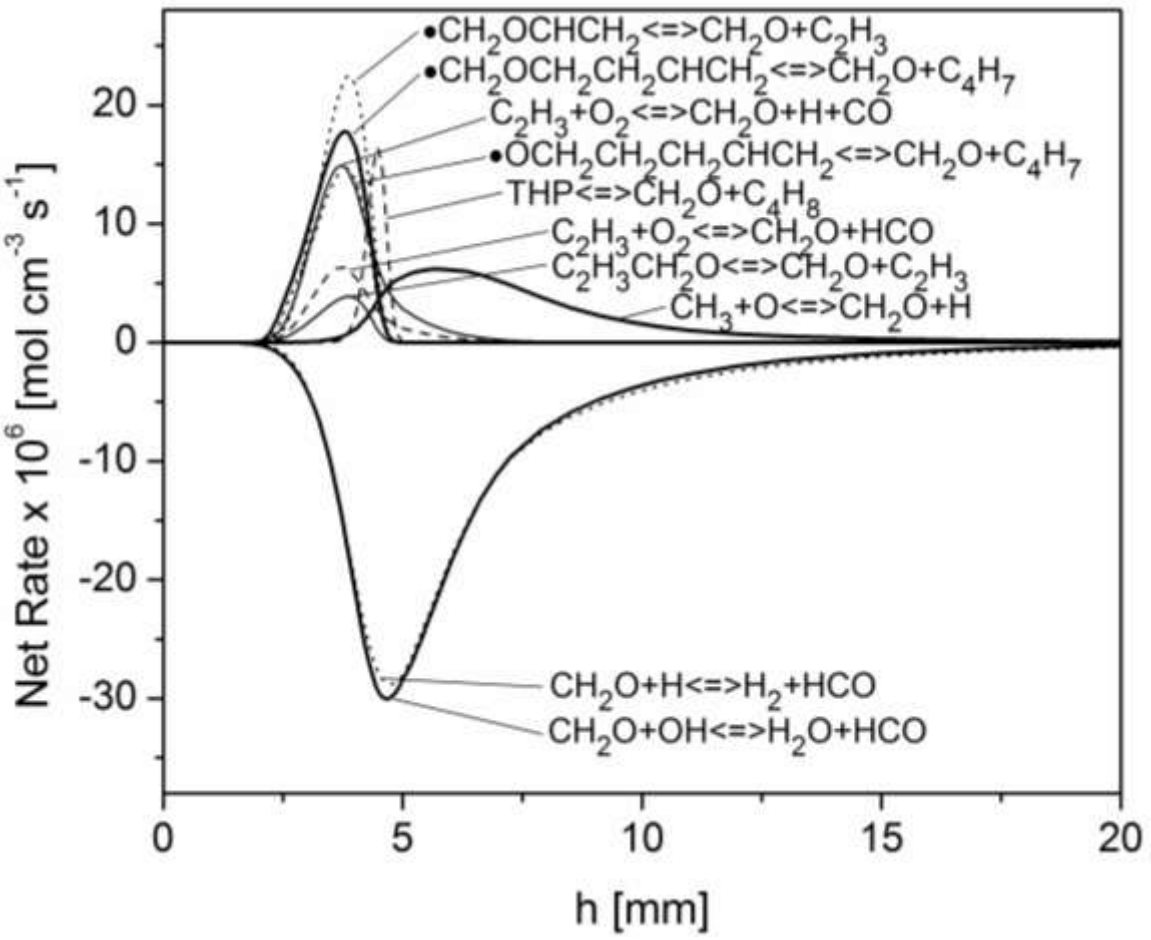

Figure 7. 5: Reaction-rate diagram for CH_2O.

A key insight is that the prediction of CH_2O formation in the THP flame is not strongly related to predictive capability for C_1 and C_2 oxidation reactions. Methyl is not the main source of CH_2O here, unlike CH_4 flames where $CH_3+O \rightleftarrows H+CH_2O$ predominates. The THP situation is more like that of cyclohexane flames [7], where C_2H_3 and C_2H_4 are produced as cyclohexyl ring-decomposition products, but for THP, CH_2O and HCO are also produced. Thus, uncertainty in the predicted CH_2O and HCO profiles may be attributed to the more complex decomposition chemistry of the heterocyclic THP fuel.

7.4.3 Other intermediates and pathways

As discussed above, species with an even number of heavy atoms can form from THP through abstractions and β-scissions. By contrast, species with an odd number of heavy atoms can form from a mix of decomposition and chemically activated oxidation and radical-addition and combination reactions.

7.4.3.1 CH3 and CH4.

The good predictions of CH_3 and CH_4 (Fig. 7.3a) strongly support the model because of the complex routes by which CH_3 is formed. The positions of the maxima are reproduced well by the model (within a factor of two); also, the general shapes of the profiles are in reasonable agreement with the experiment. Prediction of the CH_4 mole-fraction profile is within 30%, the onset of CH_3 is well-described in shape and magnitude, and the CH_3 peak and high-temperature behavior are acceptable.

CH_3 chemistry is the key to both profiles, as the CH_4 is mainly from reversible $CH_3+RH \rightleftarrows CH_4+R$ abstractions. At $h<4.5$ mm where CH_3 formation chemistry dominates its profile, the three main formation reactions are $CH_2CHO(+M) \rightarrow CH_3+CO(+M)$ from Senosiain *et al.* [44], $i\text{-}C_4H_5+H \rightarrow CH_3+C_3H_3$, and $CH_2CHO+H \rightarrow CH_3+HCO$. The C/H/O reactants result from channels in the THP-yl decomposition sequences (Fig. 7.1). CH_2CHO (“vinoxy”) is predicted to be from decomposition of 4-pentenal and vinylallyl ether, the two mono-oxygen analogs of 1,5-hexadiene. In turn, these two oxygenates are formed by secondary decomposition channels of the linear radicals formed from ring-opening of THP-2-yl and THP-3-yl. The $i\text{-}C_4H_5$ is formed by H-abstraction from 1,3-butadiene, a direct product of the THP-4-yl decomposition sequence. Some CH_3 destruction occurs in this region, mainly H-abstraction from the decomposition-generated

HCO.

The CH_3 profile at h>4.5 mm is dominated by the higher-temperature formation reactions of $C_2H_4+O \rightleftarrows CH_3+HCO$ and production from CH_4 and by destruction through CH_3+O and OH. Note that because CH_4 is formed from and destroyed to CH_3, the accurately predicted CH_4 profile depends on correct rate coefficients, temperature, and concentrations of CH_3, RH, and R.

7.4.3.2 C_3H_x compounds.

Profiles of propargyl (C_3H_3), propyne and allene (C_3H_4 isomers), allyl (C_3H_5), and propene (C_3H_6) are presented in Fig. 7.3d-e. These species are significant in part because C_3H_3 is a precursor to phenyl and benzene, which are thought to be precursors of polycyclic aromatic hydrocarbons and soot.

C_3H_3 has a peak mole fraction of $8 \bullet 10^{-4}$ in the ϕ=1.75 THP flame, approximately half of the peak observed in a ϕ=2.0 cyclohexane flame [7]. The presence of the oxygen atom in THP reduces the possibilities of forming a three-carbon chain in the fuel breakdown and reduces the yield of C_3H_3. The predicted propargyl mole fraction is somewhat higher than the experimental profile (within a 70%) and it is accurate with regard to profile peak position and shape, as shown in Fig. 7.3d. Its formation is dominated by i-$C_4H_5+H \rightleftarrows CH_3+C_3H_3$, which is also important for CH_3 formation.

Mole-fraction profiles of allene and propyne are both predicted well by the model (Fig. 7.3e). Reaction analysis shows that propyne formation is dominated by H-catalyzed interconversion from allene, the abstraction C_3H_3+HCO, and $C_2H_2+CH_3$. Allene formation, on the other hand, has significant contributions from abstraction and

decomposition reactions of allyl, the only C_3H_x isomer formed directly from THP decomposition. The model is well within a factor of two (higher) than the experimental data.

Propene has a peak mole fraction of 0.003. The prediction is slightly lower than the experimental data (about 20%). In the model, C_3H_6 is almost entirely formed by H-atom combination with allyl.

7.4.3.3 C_4H_x compounds.

In addition to 1,3-butadiene, discussed earlier, C_4H_2, C_4H_4, and C_4H_8 were measured, and their mole-fraction profiles are presented in Fig. 7.3f-g. Like 1,3-butadiene, these species are generally derived from C_4H_7. C_4H_8 is formed dominantly from C_4H_7+H and C_4H_7+HCO, although the model under-predicts C_4H_8 by a factor of four. H-abstraction from 1,3-butadiene yields the C_4H_5 isomers and vinylacetylene. C_4H_4 is formed primarily from hydrogen abstraction from C_4H_5. Its mole-fraction profile is predicted quite well, including peak magnitude and position. The contribution of C_4H_2 is over-predicted by a factor of two. C_4H_2 is predicted to be formed via hydrogen abstraction from C_4H_3 species.

7.4.3.4 Ketene and benzene.

Ketene CH_2CO is formed predominantly from CH_2CHO and from C_2H_2+OH. Prediction of its mole-fraction profile is within a factor of 2.5 (Fig. 7.3h) of the experimental data. Benzene is detected in the flame, formed by molecular-weight growth because unlike cyclohexane, THP cannot dehydrogenate to a phenyl ring. The predicted maximum of the benzene mole fraction, $6.9 \cdot 10^{-5}$, is close to the experimental data peak of $7.8 \cdot 10^{-5}$ (Fig. 7.3h). Upon analysis, *i*-C_4H_5+C_2H_2→fulvene(+H→benzene+H),

$C_3H_3+C_3H_3 \rightarrow$benzene, and *n*-$C_4H_5+C_2H_2 \rightarrow$benzene+H appear to be the dominant formation routes.

7.5 Conclusions

THP combustion has been analyzed in a low-pressure premixed flat flame at ϕ=1.75. From VUV-PI-MBMS measurements, 31 species with up to six heavy atoms are quantified. A newly developed kinetic mechanism for THP starts from recent modeling of cyclohexane combustion and adds rate coefficients and thermochemistry from quantum chemistry. This model predicts the general flame structure well. Analyzing the predictions shows that THP consumption in the flame is by abstractions of the three different H atoms in THP, followed by logical sequences of decomposition steps from the THP-yl radicals. These radicals then β-scission to six-, four-, and two-heavy-atom species by a logical sequence. Other species are formed by decomposition and oxidation of these intermediates. Although little molecular-weight growth was observed, benzene is produced, and routes are identified to produce it.

THP is studied here as a small C/H/O-containing model biofuel with the aim of contributing to the understanding of the mechanistic pathways for THP combustion and the formation of potential pollutants. The reaction set and kinetic pathways identified in this study will aid design of efficient, low-polluting combustors. THP is an ether variant of cyclohexane and the non-nitrogen equivalent of morpholine, and the present flame data and predictions provide insights into mechanistic similarities and differences from these other fuels.

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CHAPTER 8

HETEROATOMIC FUELS: MORPHOLINE MBMS FLAME STUDY AND MODEL DEVELOPMENT[1]

Use of oxygen-containing fuels is increasing as more biofuels are introduced. Accordingly, the effects of oxygen-containing functional groups on emissions from the combustion of transportation biofuels has been increasingly studied, both in terms of reduced pollutants such as carbon dioxide, aromatic hydrocarbons and soot and in terms of increased formation of other pollutants such as carbonyl and formaldehyde compounds [1-16]. However, combustion of biomass-derived fuels also involves additional heteroatoms, notably nitrogen [17]. NO_x is formed in modern power generation fired with coal and/or biomass by the high-temperature Z'eldovich path of $O+N_2 \rightarrow N+NO$ or via fuel-bound nitrogen [18-20], and NH_3 and HCN accepted to be the major volatile fuel-nitrogen intermediates that are NO_x precursors [18,21-25]. It is thought that heterocyclic compounds in coal lead preferentially to HCN, while amines and proteins in biomass predominantly yield NH_3 [26-27], depending on the stoichiometry of combustion.

The combustion of morpholine (1-oxa-4-aza-cyclohexane) provides a cyclic model compound that contains both nitrogen and oxygen [28-30]. Our collaborative work has identified numerous intermediates and products by photoionization (PI) and electron ionization (EI) molecular-beam mass spectrometry (MBMS), combined with cavity ringdown spectroscopy (CRDS). Morpholine is used as a a fuel additive and a versatile industrial chemical used as an intermediate in syntheses, solvent, corrosion inhibitor, crop

[1] Based in part on A. Lucassen, N.J. Labbe, P.R. Westmoreland, K. Kohse-Höinghaus, *Combust. Flame* **158** (2011) 1647-1666 (cited here as Ref. 30, where Lucassen and Labbe were identified as receiving equal credit as first authors). Model-data comparisons are all new.

protection agent, fungicide, and defoaming agent for paper and pulp [28,31]. For this polyfunctional compound, the ether linkage may increase the reactivity in comparison with corresponding hydrocarbons, while the additional nitrogen function may have an effect on the reactivity of cyclic ethers [31]. Detailed combustion experiments and flame modeling have also become available for cyclohexane, the corresponding hydrocarbon [32-36].

On this basis, quantitative mole fraction profiles were sampled using a powerful combination of EI-MBMS and PI-MBMS. Even with this combination of high mass resolution in the EI-MBMS experiment and excellent energy resolution permitting isomer identification in the PI-MBMS experiment, the quantification proved quite challenging, considering a multitude of stable and radical species with different heavy atoms, their isotopomers, and fragments. The resulting species mole-fraction profiles are discussed with respect to key fuel-decomposition pathways and to intermediates leading to potentially harmful emissions. The analysis is complemented with simulations from a dedicated combustion model being developed for this purpose. Regarding the limited literature knowledge of the thermochemistry, transport data and kinetics for this cyclic N- and O-containing compound, this model is thought to be a nucleus for the further development of reliable mechanisms representing fuel-nitrogen conversion and pollutant formation pertinent to combustion of H/C/N/O-containing fuels.

8.1 Experiments and Procedures

8.1.1 Mass spectrometry

The experiments were carried out with two similar MBMS instruments employing different ionization methods. The PI-MBMS set-up is located at the Advanced Light

Source (ALS) at Lawrence Berkeley (California) National Laboratory and uses tunable VUV radiation to ensure high energy resolution. The EI-MBMS instrument in Bielefeld is equipped with an electron ionization (EI) source and a reflectron time-of-flight (TOF) mass analyzer for high mass resolution. Both experimental arrangements have been described previously [9,37-39], and relevant details regarding the morpholine flame investigations have been given before [28-30]. For the present study, further PI-MBMS and extensive EI-MBMS measurements were made in addition to those reported in [28], supporting the earlier analysis but permitting quantitative mole-fraction evaluation.

A laminar, premixed flat morpholine-oxygen flame diluted with 25% argon was investigated at 40 mbar with $\Phi = 1.3$ (C/O = 0.41) and 0.32 m/s cold gas velocity at 293 K. The flame was stabilized on movable, water-cooled McKenna-type burners. Gas flows were controlled with calibrated mass flow controllers, and liquid morpholine was metered by a syringe pump, evaporated quantitatively, and added to the gas stream. The flame conditions for both experiments are given in Table 8.1; total flow rates were increased in the EI-MBMS experiment to match the slightly larger burner surface.

Table 8.1: Flame conditions; flow rates were adapted to the slightly different burner diameters (63.4 mm in EI-MBMS vs. 60 mm in the PI-MBMS experiment).

Experiment	ϕ	C/O	flow O_2 [slm]	flow Ar [slm]	flow fuel (l) [ml/min]	flow fuel (g) [slm]	total flow [slm]
EI-MBMS	1.3	0.41	1.37	0.56	1.206	0.31	2.23
PI-MBMS	1.3	0.41	1.22	0.5	1.08	0.28	2.0

Samples were withdrawn in the EI-MBMS experiment with a quartz cone with a 0.50-mm-diameter (PI-MBMS: 0.40 mm) orifice at the tip and an angle of 25° (PI-MBMS: 40°). The wall thickness of the probes is near 50 µm (PI-MBMS: 100 µm) at the

tip. The gas sample was expanded to ~10^{-4} mbar in the first pumping stage. The center of the gas cloud was extracted by a skimmer, and the molecular beam then entered the ionization region of the mass spectrometer, kept at a pressure of ~10^{-6} mbar.

In the EI-MBMS experiment, the sample was ionized with a pulsed electron beam (~10^{9} electrons/pulse) using four different energies (10.5 eV, 12.0 eV, 15 eV, and 17.5 eV) to analyze the flame and minimize fragmentation; the energy distribution of the electrons was 1 eV (FWHM). Mass spectra were obtained with a mass resolution of $m/\Delta m$ = 4000. The PI-MBMS instrument has been described in [38,40-41]. Photoionization was performed with a continuous photon beam of ~10^{13} photons/s at energies between 8.00 and 17.00 eV; the energy resolution was about 0.05 eV. Analysis relied on a linear TOF mass spectrometer with a mass resolution of $m/\Delta m$ = 400.

In both experiments, ions were detected by a multichannel plate and integrated with a multichannel scaler with a sensitivity of ~10^{-5}. Mass spectra were collected for at least 10^{5} ionization pulses, either as function of the distance *h* to the burner (burner scan) or as a function of the ionization energy at a fixed distance (energy scan). Spectra were corrected for fragmentation and isotopic contributions of ^{13}C and ^{18}O. The identification of the species took previous assignments in [28] into account. Mole fractions were derived from the independent measurements with both instruments using procedures described below.

8.1.2 Determination of mole fractions

8.1.2.1 Major species

Major species mole fractions were determined based on the elemental balances of carbon, hydrogen, oxygen, and nitrogen. A previously reported approach [39] was thus

adopted and extended regarding the nitrogen balance. For the morpholine flame here, the gas composition at the burner surface is assumed to have the same ratios of fuel, oxygen, and argon as in the feed gas.[2] At the highest distance from the burner, the products are considered to be CO, CO_2, H_2, H_2O, N_2, and NO; contributions of NO_2 and O_2 at this position are negligible. Based on these approximations, the mole fractions of these major species can be calculated in the exhaust gas from the measured ratios of CO/CO_2 and NO/N_2 using the respective element balances. The remaining oxygen is then bound in H_2O, and with the H_2O mole fraction given, the remaining hydrogen is bound in H_2. H, O, and OH mole fractions were neglected in the analysis. It is estimated that this procedure results in an uncertainty of less than 30%.

8.1.2.2 Minor species

The signal $S_i(E)$ of a species i at the energy E is associated with its partial pressure or its respective mole fraction at the corresponding flame position through the following equation:

$$S_i = p_i \cdot c \cdot SW \cdot D_i \cdot \varphi \cdot FKT(h) \cdot \int \sigma_i(E) \cdot f(E) dE \qquad (1),$$

where p_i is the partial pressure of species i (note that p_i is proportional to the mole fraction x_i), c is an instrument factor, SW the number of sweeps, D_i the mass discrimination factor of species i, φ is the number of ionizing particles (photons or electrons), $FKT(h)$ a temperature- and thus position-dependent sampling function, $\sigma_i(E)$ is the ionization cross section of species i at energy E, and $f(E)$ is the energy distribution of the ionizing particles.

[2] Note that in Ref. 30, the composition at the burner had instead been treated as equal to the feed-gas composition.

For the PI-MBMS experiment, the energy distribution is negligibly small. Therefore, convolution of ionization cross section and energy distribution is not necessary, and tabulated photoionization cross sections can be used directly:

$$S_i = p_i \cdot c \cdot SW \cdot D_i \cdot \varphi \cdot FKT(h) \cdot \sigma_i(E) \qquad (2).$$

For a given measurement, *SW* is known and φ is measured; D_i is determined from calibration measurements. *FKT(h)* and *c* can be derived from the argon signal and mole fraction, which are accessible from the major species calculation. With all parameters known, Eq. 2 is then used to calculate species mole fractions based on literature photoionization cross sections for a given photon energy. Note that the instrument factor *c* may differ for measurements made at different times, necessitating further correction in some cases. Details can be found in [39,42].

In the EI-MBMS experiment with its broader energy distribution, all signals can be normalized by the argon signal at all energies. Equation 1 then simplifies to:

$$\frac{S_i}{S_{Ar}} = \frac{x_i}{x_{Ar}} \cdot \frac{D_i}{D_{Ar}} \cdot \frac{\int \sigma_i(E) \cdot f(E) dE}{\int \sigma_{Ar}(E) \cdot f(E) dE} = \frac{x_i}{x_{Ar}} \cdot k_i(E) \qquad (3).$$

With this normalization, all parameters can be condensed into a calibration factor $k_i(E)$. Once this factor $k_i(E)$ is known for a given energy *E*, the mole fraction x_i of an intermediate species can be calculated based on the argon mole-fraction profile from the major species calculation. Derivation of the calibration factor can be achieved by different methods. Here, the method from [43], extended in [44], was adopted. It relies on the simulation of the signal for the different ionization energies, taking literature electron-ionization cross sections and the convolution of cross section and electron energy distribution into account.

8.1.3 Temperature

The temperature profile was measured following the procedures in [45]. The undisturbed temperature was obtained from planar laser-induced fluorescence (PLIF) of NO in the A-X (0-0) band. To account for the distortion caused by the sampling cone [45-46], the temperature profile used for the model calculations was determined from the temperature dependence of the sampling rate through the probe orifice. Assuming a constant pumping speed, the sampling rate can be expressed by the pressure of the first-stage chamber (p_{1st}). This dependence is described by

$$p_{1st} = C\sqrt{\frac{\gamma}{\overline{M}\cdot T}}\left(\frac{2}{\gamma+1}\right)^{Z} \qquad (4),$$

with $Z = \frac{\gamma+1}{2(\gamma-1)}$; $\overline{M}$ is the mean molar mass, γ is the adiabaticity coefficient (C_p/C_V), and C is a device-specific constant which is determined by solving Eq. 4 with the exhaust gas temperature taken from the NO-PLIF measurement. Using this temperature profile, which is measured under conditions that may reflect the actual probe distortion more closely, could plausibly eliminate the need to shift experimental versus modeled species profiles, even though this is a local perturbation applied throughout the whole flame. Shifts as used in [46] and earlier literature were thus not applied, the experimental uncertainty in absolute position being of the order of 0.5 mm. The temperature is seen to decrease slightly in the exhaust gas region due to heat loss, with the experiment not reflecting ideal adiabatic conditions. Temperature sensitivity was examined by performing model calculations with a profile exhibiting a 150 K lower temperature

maximum, and changes of the order of 20% or below occurred in the reported mole-fraction profiles, which is within experimental error.

8.2. Model Development and Simulations

8.2.1 Flame model

A reaction set for morpholine combustion was developed here by analogy to cyclohexane combustion. Dominant fuel decomposition pathways in the morpholine flame, had been proposed before and found in general agreement with the species identified in [28]. In a more systematic approach, investigations of cyclohexane combustion in laminar flat flames [32,34-35, 47] are now used as a starting point for the present morpholine model.

There are six saturated heavy atoms (C, N, O) in the morpholine ring, so it is proposed that, by analogy with cyclohexane, morpholine destruction is through hydrogen abstraction. The key difference is that while each position on a cyclohexane ring is equivalent, morpholine has three different sites from which an H-atom may be abstracted: the carbon *ortho* ("*o*") to the ether oxygen, the *meta* ("*m*") carbon, and the *para* ("*p*") amine nitrogen. Three distinct hydrogen-abstraction routes thus exist, with different rate constants due to different local N-H and C-H bond energies and to the number of H-atoms per site.

Decomposition steps to smaller species were assumed to be more important than direct oxidation by oxygen atoms for the large morphyl radicals, as had been shown in cyclohexane modeling. The resulting *o*-, *m*- and *p*-morphyl radicals can then undergo β-scission by ring-breaking, forming linear, unsaturated radicals, or they can β-scission to

H and unsaturated cyclic molecules. The linear radicals β-scission preferentially to two-heavy-atom molecules (C_2H_4, CH_2NH, or CH_2O) plus a four-heavy-atom unsaturated radical that then again may undergo further β-scission. Alternatively, the six- or four-heavy-atom radicals may yield unsaturated molecules by β-scission of an H-atom. If an unsaturated cyclic molecule is formed, the π bond creates an allylic H that may easily be abstracted. β-Scission then breaks the ring or creates a doubly unsaturated cyclic molecule.

A reaction set was constructed for morpholine combustion using this skeletal mechanism. Key steps for breaking down to two-heavy-atom species are shown in Fig. 8.1. Reaction rate coefficients and fall-off in the reactions of [28] were derived based on analogous reactions from the cyclohexane model but with Arrhenius pre-exponential factors modified for the proper reaction path degeneracy (RPD). This procedure was used for all reactions with the exception of those involving initial hydrogen abstractions from morpholine itself, which were calculated with *ab initio* quantum-chemistry methods. Small-species nitrogen chemistry and the hydrocarbon chemistry were added using the H/C/N/O set presented in Chapter 6. The full morpholine reaction set may be found in Appendix F.

Thermochemistry was calculated theoretically using the complete-basis-set method CBS-QB3 [48] for 29 species in the proposed skeletal mechanism [28], as were new reaction rate constants for the initial hydrogen abstractions from morpholine. Geometry and frequency calculations were completed with Gaussian09 software [49] using the CBS-QB3 method and tight convergence criteria. Transition-state theory was used to calculate rate constants for the abstraction reactions (Table 8.2).

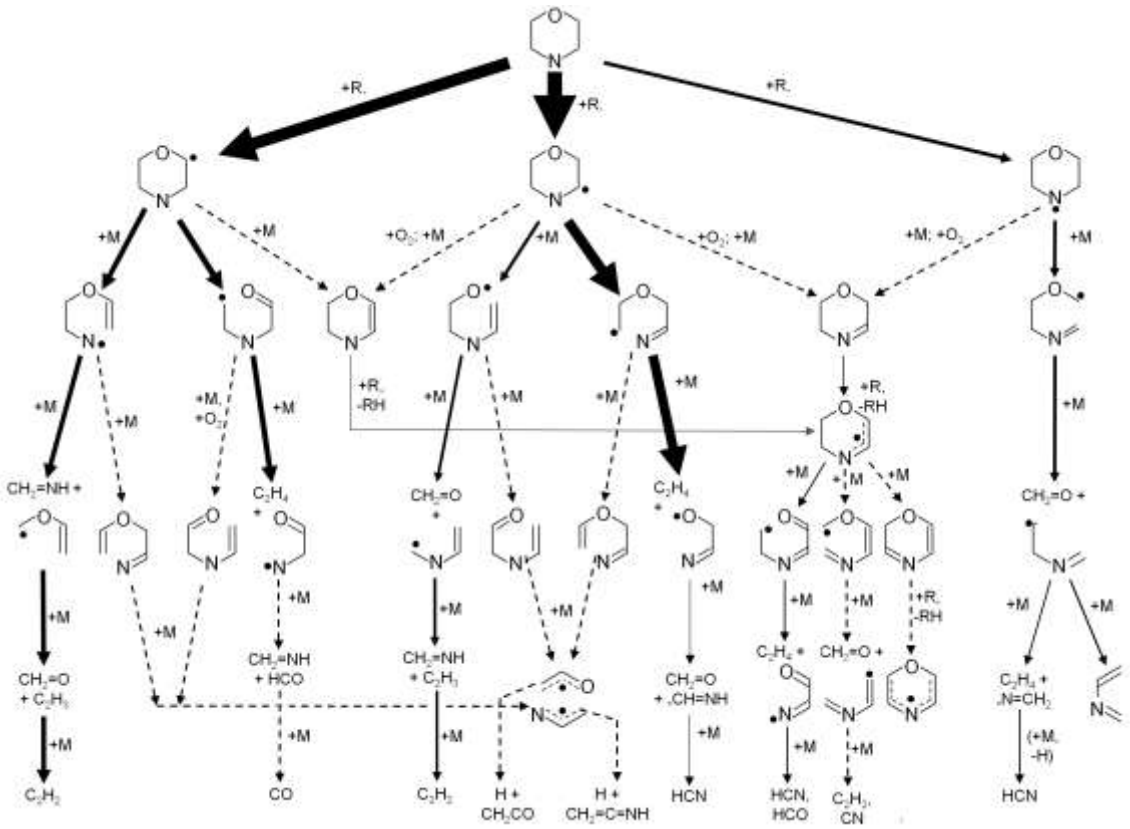

Figure 8.1: Proposed morpholine reaction pathways for model development.

Table 8.2: Rate constants used for hydrogen abstraction from morpholine in the format *A*×exp (-*E*/*RT*) (1 atm, 500-2000 K) from explicit CBS-QB3 computation and extensions to additional reactions by analogies.

Radical, products	*A* [mol s^{-1} cm^{-3}]	*E* [cal mol^{-1}]	Source
H to *o*-morphyl + H_2	2.09E15	15000	Computed
to *m*-morphyl + H_2	1.74E15	13800	Computed
to *p*-morphyl + H_2	2.04E14	11500	Computed
O to *o*-morphyl + OH	7.70E15	10800	Estimated
to *m*-morphyl + OH	6.42E15	9880	Estimated
to *p*-morphyl + OH	7.52E14	8240	Estimated
OH to *o*-morphyl + H_2O	6.18E14	8410	Computed
to *m*-morphyl + H_2O	4.83E14	5970	Estimated
to *p*-morphyl + H_2O	5.63E14	7220	Computed
HO_2 to *o*-morphyl + H_2O_2	4.19E13	8350	Estimated
to *m*-morphyl + H_2O_2	3.49E13	7810	Estimated
to *p*-morphyl + H_2O_2	4.09E12	6520	Estimated

Flame simulations were performed using the CHEMKIN-Pro PREMIX flame code [50-52], including both thermal and multi-component diffusion. The temperature profile used in the model is included in Fig. 8.2 as a dashed line; it was based on the data analyzed with Eq. 4, matched with the NO PLIF measurements at high temperature. The implied burner-surface temperature of 360 K was considered reasonable. Reaction pathways and net reaction rates were analyzed.

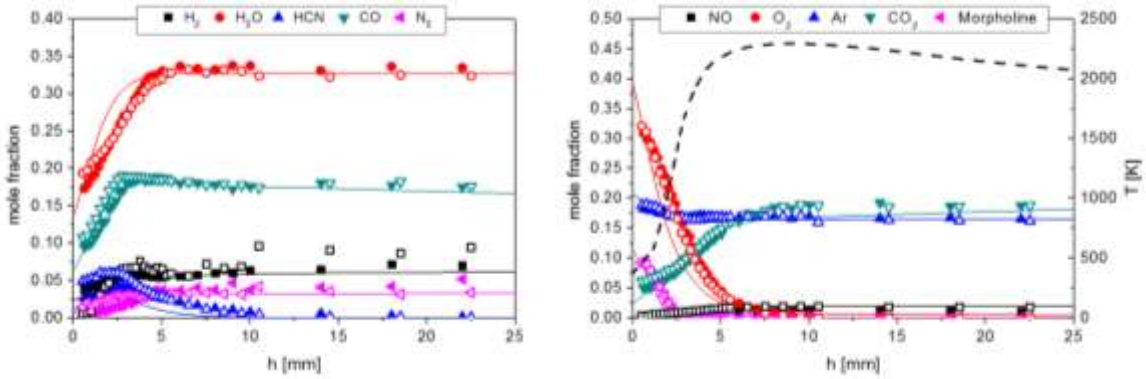

Figure 8.2: Major species mole-fraction profiles. Solid symbols are from EI-MBMS, open symbols from PI-MBMS experiments; solid lines are from flame model, the broken line is the temperature profile used in the simulation.

8.2.2 Tests against non-morpholine flames

It was thought useful to complement the simulations with model calculations for some related flames, including the stoichiometric and fuel-rich ($\Phi = 2.0$) cyclohexane flames with an Ar mole fraction x_{Ar} of 0.325 in [32,34-35,47] and the $\Phi = 1.16$ dimethyl ether (DME) flame with $x_{Ar} = 0.254$ from [14]. For all these cases, the performance of the model used here was compared to those from the respective original papers. This approach was adopted to test whether the morpholine model was capable of adequately capturing the small-hydrocarbon-intermediate chemistry as well as the reaction pathways leading to small oxygenated and nitrogenated compounds.

For the cyclohexane flames, the model from [32,34-35,47] was used with and without the morpholine additions in the present work. As a test, the simulation for the stoichiometric cyclohexane flame from [32] was performed with the full morpholine model, and no differences were seen to the simulation with the cyclohexane subset. This analysis versus the cyclohexane chemistry was thought especially relevant regarding the comparison of fuel decomposition and formation of hydrocarbon intermediates.

In the simulation of the DME flame, the reaction set for DME decomposition was added to the morpholine model from [14]. This well-studied DME flame was chosen to analyze whether the morpholine model could adequately represent the fuel breakdown and especially the formation of small oxygenated intermediates for this simple ether fuel. Again, model calculations were compared with those in the original paper and found in good agreement.

8.3 Results and Discussion

8.3.1 Combination of results from both experiments

An overview is presented in Table 8.3 of species mole fractions from both EI-MBMS and PI-MBMS experiments; peak mole fractions and their respective positions are reported as well as estimated experimental error levels. Major species mole fractions from both experiments, including argon, fuel, O_2, CO, H_2, CO_2, and H_2O are given in Fig. 8.2, which also includes N_2, NO, and HCN mole fractions.

Table 8.3: Intermediate species identification from PI-MBMS and EI-MBMS experiment; peak values of mole-fractions (*x* at h_{max}) and the location of the maximum (h_{max}) are indicated for both experiments as well as for the simulations. Literature references for the ionization cross sections (*xs*) are given, and in the EI-MBMS experiments, the method of calibration is reported.

					PI-MBMS experiment			EI-MBMS experiment				Simulation	
m/z [Th]	formula	species	IE [eV]	mass [amu]	source of *xs*	*x* at h_{max}	h_{max} [mm]	*m*	source of *xs*	*x* at h_{max}	h_{max} [mm]	*x* at h_{max}	h_{max} [mm]
15	CH_3	methyl	9.83	15.023	[53]	1.90E-03[a]	2.3	0.101	[54]	2,95E-03[a]	2.4	1.02E-03	2.7
16	CH_4	methane	12.61	16.031	[55]	2.79E-03[a]	1.5	0.120	meas.	2.73E-03[a]	2.2	2.57E-03	1.6
17	NH_3	ammonia	10.07	17.027	[56]	2.05E-03[b]	2.5	0.080	meas.	2.18E-03[a]	2.6	4.91E-03	1.4
26	C_2H_2	acetylene	11.4	26.016	[57]	6.62E-03[a]	2.5	0.183	meas.	1.36E-02[a]	3.0	6.89E-03	2.4
27	HCN	hydrogen cyanide	13.6	27.011	est.	6.06E-02[b]	1.5	0.111	[58]	4.15E-02[b]	2.4	3.49E-02	2.2
	C_2H_3	ethenyl		27.024	[59]	1.13E-05[a]	2.5	0.157	[60]	1.21E-04[b]	2.2	2.41E-04	2.5
28	CH_2N	methylene amidogen	9.40/9.70 [83]	28.019	est.	7.74E-04[c]	1.8	0.134	[58]	2.44E-03[c]	1.8	5.27E-05	2.3
	C_2H_4	ethene	10.51	28.031	[57]	1.82E-02[a]	1.8	0.116	meas.	2.09E-02[a]	2.2	1.32E-02	1.7
29	HCO	formyl	8.12	29.003	n.a.	n.a.	n.a.	0.066	[60]	5.05E-04[b]	2.4	3.25E-04	2.3
	CH_2NH	methanimine	9.88	29.027	est.	6.57E-03[c]	1.8	0.144	[60]	7.89E-03[b]	2.0	3.18E-04	1.8
	C_2H_5	ethyl	8.12	29.039	n.a.	n.a.	n.a.	0.137	[58]	6.84E-04[b]	1.8	4.24E-05	1.6
30	CH_2O	formaldehyde	10.88	30.011	[61]	1.45E-02[a]	1.8	0.106	[60]	1.38E-02[a]	1.8	4.62E-03	2.1
	CH_4N	n.i.	n.a.	30.034	n.a.	n.a.	n.a.	0.164	[58]	2.57E-04[c]	0.8	1.16E-05	2.2
	C_2H_6	ethane	11.52	30.047	n.a.	n.a.	n.a.	0.271	[60]	4.32E-04[a]	2.2	1.35E-04	1.5
31	HNO	nitrosyl hydride	10.1	31.006	n.a.	n.a.	n.a.	0.062	[58]	2.62E-04[c]	3.8	1.08E-04	1.7
	CH_3NH_2	methylamine	8.9	31.042	est.	2.25E-04[c]	1.3	0.186	[58]	3.08E-04[b]	1.4	6.34E-05	1.6
	CH_3O	methoxy	10.72	31.019	n.a.	n.a.	n.a.	0.140	[58]	2.78E-04[c]	1.2	6.82E-05	1.5

32	CH_3OH	methanol	10.84	32.026	n.a.	n.a.	n.a.	0.130	[62]	6.30E-04[b]	0.8	4.01E-04	1.3
34	H_2O_2	hydrogen peroxide	10.7	34.005	n.a.	n.a.	n.a.	0.063	[60]	5.14E-04[b]	1.8	6.69E-04	1.3
39	C_3H_3	propargyl	8.67	39.023	[59]	3.96E-05[b]	2.0	0.251	[63]	3.94E-05[b]	2.8	1.19E-05	2.2
40	C_2H_2N	n.i.	n.a.	40.0188	n.a.	n.a.	n.a.	0.036	[58]	6.33E-05[c]	2.4	3.87E-04	1.5
	C_3H_4	propyne	10.36	40.031	[57]	9.43E-05[a]	2.8	0.276	[63]	9.89E-05[a]	2.2	9.58E-06	2.1
41	C_2H_3N	2*H*-azirine	10.58	41.027	est.	9.57E-04[c]	0.5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
	CH_3CN	acetonitrile	12.2	41.027	est.	4.82E-03[c]	1.5	0.041	[58]	1.27E-03[c]	1.4	3.87E-04	1.5
	C_3H_5	allyl	8.1	41.0391	n.a.	n.a.	n.a.	0.238	[58]	5.18E-05[c]	2.2	6.17E-06	1.4
42	CH_2CO	ketene	9.61	42.011	meas.	1.63E-04[b]	2.5	0.218	[58]	2.83E-04[b]	2.4	2.52E-04	2.4
	C_2H_4N	n.i.	n.i.	42.034	est.	3.26E-04[c]	2.5	0.084	[58]	1.22E-03[c]	1.4	3.57E-05	2.3
	C_3H_6	propene	9.73	42.047	[41]	5.17E-04[a]	2.5	0.350	[63]	2.35E-04[a]	1.6	8.01E-05	1.5
43	HNCO	isocyanic acid	11.6	43.006	est.	4.29E-03[c]	0.5	n.a.	n.a.	n.a.	n.a.	3.16E-03	3.3
	CH_2CHO	vinyloxy	10.85	43.018	n.a.	n.a.	n.a.	0.197	[60]	2.20E-04[c]	3.0	2.06E-04	2.3
	$C_2H_3NH_2$	ethenamine	8.2	43.042	est.	2.70E-04[c]	0.5	n.a.	n.a.	n.a.	n.a.	2.70E-04	2.1
	CH_3CHNH	acetaldimine	9.7	43.042	est.	3.26E-03[c]	0.8	0.051	[58]	4.25E-03[c]	1.2	1.73E-04	2.3
44	C_2H_3OH	ethenol	9.33	44.026	[57]	3.51E-04[b]	1.5	n.a.	n.a.	n.a.	n.a.	5.21E-06	2.4
	CH_3CHO	acetaldehyde	10.23	44.026	[57]	1.63E-03[a]	0.5	0.138	[58]	8.06E-04[b]	1.6	7.99E-04	1.4
45	CH_3NO	nitrosomethane	9.3	45.021	est.	1.43E-04[c]	1.8	0.237	[58]	1.46E-04[c]	1.6	3.41E-05	1.1
	$C_2H_5NH_2$	ethylamine	9.1	45.058	est.	1.43E-04[c]	1.8	0.060	meas.	3.04E-04[a]	1.0	6.45E-06	1.6
46	NO_2	nitrogen dioxide	9.58	45.993	est.	1.45E-04[b]	1.0	0.101	[60]	1.32E-04[a]	0.6	8.80E-04	0.7
	H_2CO_2	formic acid	11.33	46.005	[41]	3.97E-04[a]	0.5	0.150	[60]	1.90E-04[b]	1.2	n.a.	n.a.
	C_2H_5OH	ethanol	10.48	46.042	n.a.	n.a.	n.a.	0.289	[62]	4.78E-05[a]	1.0	4.55E-07	1.5
47	HNO_2	nitrous acid	11	47.001	n.a.	n.a.	n.a.	0.122	[58]	3.38E-05[b]	0.8	9.79E-07	0.3
51	C_2HCN	2-propynenitrile	11.62	51.011	est.	4.04E-04[c]	0.5	0.184	[58]	4.45E-04[c]	3.2	n.a.	n.a.

52	C_4H_4	vinylacetylene	9.58	52.031	[57]	6.59E-05[a]	3.0	0.345	[58]	4.60E-05[b]	2.6	3.62E-06	2.3
53	C_2H_3CN	2-propenenitrile	10.91	53.027	est.	9.88E-04[b]	2.6	0.226	[58]	1.25E-03[b]	2.4	n.a.	n.a.
54	C_4H_6	butadiene	9.03	54.047	[57]	8.88E-05[a]	2.3	0.337	[58]	1.28E-04[b]	2.2	2.32E-06	2.3
56	C_4H_8	butene	n.i.	56.063	est.	2.20E-04[b]	1.5	0.297	[58]	1.40E-04[b]	1.8	2.72E-06	1.3
71	$C_2H_3CONH_2$	acrylamide	9.6	71.037	n.a.	n.a.	n.a.	0.278	[58]	2.32E-04[c]	1.2	n.a.	n.a.
85	C_4H_7NO		n.a.	85.052	n.a	n.a.	n.a.	0.299	[58]	4.96E-04[c]	0.6	3.54E-03	1.4
86	C_4H_8NO	morphyl	n.a.	86.061	n.a..	n.a.	n.a.	0.315	[58]	1.42E-03[c]	0.6	1.16E-03	1.4

n.i.: not identified, n.a.: not applicable, est.: estimated, meas.: measured in this work, *m* is the slope of the EI cross section. a) uncertainty of 20-40% ; b) uncertainty of factor 2-3; c) uncertainty possibly larger than factor 2-3.

Most importantly, for species where cross sections are available from both photoionization and electron ionization, such as methyl, methane, acetylene, ethene, and propargyl, agreement within a factor of two is found. This agreement is in line with earlier comparisons of species measurements from these independent instruments [9,39].

Species identification [28] and quantification are much more involved than for typical hydrocarbon flames due to the presence of C, N, and O in the fuel and, consequently, to the occurrence of multiple combinations of heavy atoms in the intermediate species. It has been noted before [28] that the H-abstraction / β-scission decomposition pattern leads to groups of species with a mass-to-charge ratio *m/z* of 26-30 (two heavy atoms) and of 40-43 (three heavy atoms); also, some species with 4 heavy atoms with *m/z* of 56-58 had been rationalized from this decomposition scheme (compare Fig. 2 in [28]). The quantitative analysis thus required elaborate calibration procedures, and it would not have been possible without the superior mass resolution of the EI-MBMS instrument in combination with the excellent energy resolution of the PI-MBMS machine. For example, *m/z* 30 represents possible contributions from CH_2O, CH_4N, C_2H_6, and NO. They could be separated by mass in the EI-MBMS experiment and identified, with the exception of CH_4N, by ionization energy in the PI-MBMS experiment. For CH_2O, where a cross section is known for both experiments, the results are in good agreement. Ethane was taken from the EI-MBMS experiment where it could be easily separated.

As evident from Table 8.3, some species were only accessible by the EI-MBMS experiment, particularly when nearly isobaric species with similar ionization thresholds and/or highly different intensities could not be separated reliably in the PI-MBMS

experiment. It is also seen from Fig. 8.2 that the element balance is somewhat more complex here than for hydrocarbon or oxygenate flames. Major N-containing products persisting towards the exhaust are N_2 and NO, with mole fractions of 0.037 and 0.023, respectively, confirming that the calibration approach using the NO/N_2 ratio in the burnt gases is reasonable. HCN also attains a high peak mole fraction of about 0.06 but is ultimately consumed in the flame.

In view of the larger errors associated with the greater chemical complexity of the morpholine flame versus hydrocarbon or oxygenate counterparts, the good agreement of both experiments for major components and many intermediate species provides a reliable basis for comparison with the simulations.

8.3.2 General model performance

For a direct comparison with both experiments, results from the simulation are included in the last columns of Table 8.3. In some cases, several isomers were considered in the model, whereas an unambiguous assignment was not possible in the experiments; such details will be given in the discussion of individual species further below. Upon detailed analysis, many features of the flame were represented by the simulation in quite good agreement with the two data sets, including the quantitative prediction of NO_x.

Simulations of major-species mole fractions in Fig. 8.2, including N_2, show very good agreement in peak magnitude and shape, both key indicators of model validity. Post-flame mole fractions (beyond about 6 mm) also agree well. No parameters were adjusted to force such a fit; indeed, the initial model used purely cyclohexane-based rate constants and predicted the profiles well before the experimental profiles were evaluated. Such agreement is the result both of accuracy in post-flame temperatures and of

quantitatively accurate conversion of intermediates to H_2 and CO.

Some computed profiles appear to be slightly shifted toward the burner. This shift could be partially due to uncertainty in the temperature rather than to chemistry. Probe effects can be natural sources of such uncertainty, which are particularly relevant at small distances from the burner [45-46]. However, another reason here may be the uncertainty associated with the background correction for the water signal. This appears reasonable because predominantly these two profiles are affected. More significant correction of the H_2O background signal would lead to a steeper rise of the H_2O profile, while exhaust-gas values would remain the same. With the oxygen profile coupled to water via the element balance, the O_2 profile would then exhibit lower values. Depending on the magnitude of this correction, both profiles may appear shifted downstream compared to the modelling results. That this influence may be dominant here is also confirmed by the good agreement of peak positions of a large number of minor species, evident from Table 8.3 and from the graphical comparisons between experiment and simulation given further below. However, probe sampling effects may still alter the temperature very close to the burner, affecting thermal diffusion of H and H_2. Therefore, we report experimental species mole fractions only for $h > 0.6$ mm, and quantitative comparisons are not encouraged at less than 1 mm.

The following discussion examines how the morpholine-flame species are formed and destroyed, revealing the sensitivity of minor-species predictions to kinetics of the larger intermediates. Aspects of the morpholine flame chemistry involving the overall system are addressed first, followed by a discussion of C_1-C_4 and selected oxygenated species, and finally, a number of nitrogen-containing species are discussed with

implications for nitrogen conversion for this model biofuel.

In this subsequent discussion, it will be shown that many minor species are well predicted in shape and peak location but not in magnitude; some are not predicted well at all. This finding is in striking contrast to the strong agreement of predictions for major species, HCN, NO, and N_2. The discrepancy will be explained by consideration of experimental uncertainties, particularly photoionization cross-sections, and by careful analysis of the reaction paths in this morpholine flame and in literature flames of cyclohexane (for the hydrocarbon chemistry), dimethyl ether (for oxygenate chemistry), and CH_4/NH_3 (for small-molecular nitrogen chemistry). The modeling discussion will show that many of the deviations are in side products from the fuel-destruction pathways, differing substantially from the sources of these species in the comparison flames. As a consequence, the good prediction of HCN forms a sound basis for interpretation of NO vs. N_2 formation from morpholine.

8.3.3 Morpholine combustion pathways

As given as a result already in Fig. 8.1, analysis of the simulation shows that morpholine itself is consumed by H-abstraction from the three distinct positions. From the integrated reaction flux, contribution of the three morphyl-forming pathways is *m*-morphyl : *o*-morphyl : *p*-morphyl :: 10:8.5:2.6. The simulated mole-fraction profiles of the three morphyl radicals are provided in Fig. 8.3, with relative maxima of *m*-, *o*- and *p*-morphyl as 10:1.3:3.3. Ring opening provides a number of further isomers of *m*/*z* 86, the very minor contributions ($<10^{-5}$) of which are also included in the sum from the simulation. The sum of the mass 86 mole fractions is in very good agreement with the mole-fraction profile determined at *m*/*z* 86 from the EI-MBMS signal. However, this

agreement should not be overstated in view of the fragmentation correction that was necessary for contributions from the fuel at *m*/*z* 87. The PI-MBMS experiment is less prone to fragmentation interferences; nevertheless, a quantitative calibration was not possible here because of unknown ionization cross sections. The different abstraction channels can lead to two stable ring isomers of constitution C_4H_7NO at *m*/*z* 85 (compare Fig. 8.1), one from *m*- and *o*-morphyl featuring a C=C bond, and one from *m*- and *p*-morphyl featuring a C=N bond. In addition, several open-chain isomers contribute to *m*/*z* 85. The sum for all C_4H_7NO species from the simulations, also given in Fig. 8.3, is about an order of magnitude higher than in the experiment, compared to an estimated error of about a factor of 3. A reason for this could be incomplete or too slow consumption kinetics.

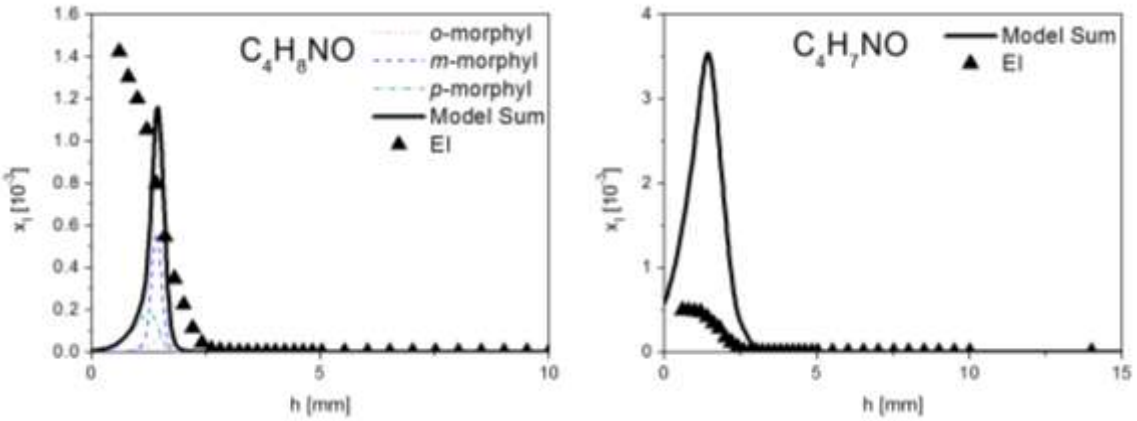

Figure 8.3: Mole-fraction profiles for morphyl and C_4H_7NO species featuring six heavy atoms. Model sum for C_4H_8NO includes *o*-, *m*-, and *p*-morphyl.

With the combined mass and energy resolution, it was possible to identify and provide estimates for the mole fractions of some species featuring four heavy atoms that result from the further fuel breakdown. From the skeletal mechanism in Fig. 8.1, key species that should be present in this mass range include (from left to right)

•$CH_2OCH=CH_2$ at *m*/*z* 57 and •$NHCH_2CH=O$ at *m*/*z* 58 from *o*-morphyl, •$CH_2NHCH=CH_2$ at *m*/*z* 56 and •$OCH_2CH=NH$ at *m*/*z* 58 from *m*-morphyl, and from *p*-morphyl, •$CH_2CH_2N=CH_2$ at *m*/*z* 56, which then yields the doubly unsaturated $CH_2=CHN=CH_2$ at *m*/*z* 55 from further H-abstraction. Also, from *m*- and *p*-morphyl, •$N=CHCH=O$ at *m*/*z* 56 and •$CH=CHN=CH_2$ at *m*/*z* 54 can be formed. All these four-heavy-atom segments of the original ring structure preserve the sequence of heavy atoms and are thus illustrative of the decomposition rather than of build-up processes. While it would be interesting to test the skeletal mechanism experimentally by direct evidence for all decomposition products, even the combination of EI-MBMS and PI-MBMS measurements does not provide a complete experimental inventory of all possible structures featuring four heavy atoms. For example, from known ionization thresholds, assignment to individual species of elemental composition C_2H_3NO, separated by mass in the EI-MBMS experiment at *m*/*z* 57, suggests presence of previously identified species [28], including nitrosoethene (8.55 eV) and isocyanatomethane (10.67 eV); also at *m*/*z* 57, $C_3H_4N_2$ may include 2,2-diazabutadiene (8.9 eV), C_3H_5O may include propionyl radical (<8.2 eV), and 1-methylethenylamine (9.43 eV) may contribute to C_3H_7N. Also present at *m*/*z* 57 is butene, C_4H_8, which can be unambiguously identified by mass. Quantitative analysis is further complicated not only by lack of information on ionization cross sections, but also by the fact that fuel decomposition products and species formed through build-up reactions from smaller intermediates may contribute to a given mass.

A limited comparison of experiment and simulation for some of the four-heavy-atom intermediates, provided in Fig. 8.4, is thus of quite preliminary character, given the combined challenges of providing mole-fraction estimates as well as suitable kinetics for

the fuel decomposition; it is thought to illustrate the main pathways of forming smaller, stable molecules that are more easily detected. Upper and lower mole-fraction limits from the EI-MBMS experiment are indicated in Fig. 8.4, taking the uncertainties from fragmentation corrections for these species into account. Lower limits are provided by assuming that the fragmentation correction must result in a mole fraction near zero at the burner surface, while upper limits use the fuel fragmentation pattern observed for cold-gas samples. Consecutive fragmentation from intermediates (as e.g. from morphyl radical) may occur but could not be quantitatively assessed. Simulated mole-fraction profiles are scaled so that profile shapes and peak positions may be compared; these positions are found in reasonable agreement with the experiment, although peak values are clearly different.

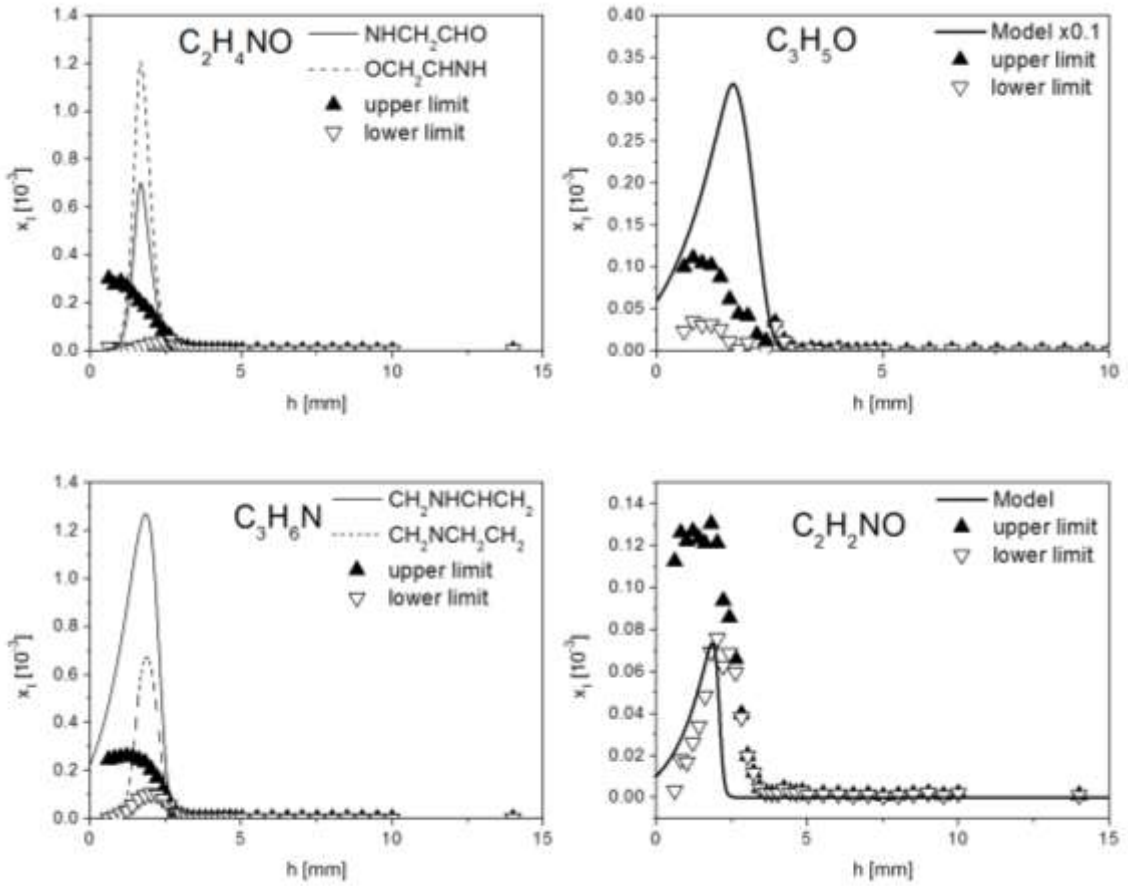

Figure 8.4: Mole-fraction profiles for selected species featuring four heavy atoms. Simulated values were multiplied with factors indicated in the individual panel.

The top left panel in Fig. 8.4 shows the result for C_2H_4NO at *m*/z 58, compared with the sum of the simulated mole fractions from •$NH{=}CH_2CH{=}O$ and •$OCH_2CH{=}NH$. While the shape is in good agreement, the model significantly over-predicts the experimental values. Because these species are direct products from morphyl, where experiment and simulation are in good agreement, the discrepancy is probably caused by incomplete destruction kinetics. The upper right panel compares the experiment for C_3H_5O at *m*/*z* 57 with the simulation for •$CH_2OCH{=}CH_2$, which is again over-predicted.

Also shown in Fig. 8.4 is C_3H_6N at *m*/*z* 56 (bottom left panel), which is compared with the sum of the simulated mole fractions for •$CH_2CH_2N{=}CH_2$ and •$CH_2NHCH{=}CH_2$,

the former from *p*-morphyl and the latter from *m*-morphyl. Again, the over-prediction may hint at too slow consumption reactions. The bottom right panel shows C_2H_2NO at *m*/*z* 56. It is compared with •N=CHCH=O, a product of *m*/*z* 85 which originates from all three morphyl radicals by H-abstraction (see Fig. 8.1, second-right column, precursor to HCN, HCO). In contrast to all other species in Fig. 8.4, this intermediate is very well predicted by the model.

Consequent further analysis of the skeletal fuel decomposition mechanism leads to a number of stable and radical species with two heavy atoms evident at the bottom of Fig. 8.1, including CH_2O, C_2H_3, C_2H_2, C_2H_4, HCO, CO, HCN, CN, CH_2N, and CH_2NH. They may be the result of more than one pathway and will be included in further discussion below.

8.3.4 Details of morpholine flame chemistry involving hydrocarbon and oxygenated species

8.3.4.1 Selected C_1 compounds

Mole-fraction profiles for selected C_1 species are given in Fig. 8.5, including CH_3, CH_4, HCO, and CH_2O. These intermediates are ubiquitous in hydrocarbon and oxygenate combustion. Very good agreement of EI-MBMS and PI-MBMS results is seen. HCO was not separable from ethyl and methanimine (CH_2=NH) in the PI-MBMS experiment and is thus only reported from EI-MBMS. The flame front is close to the burner near 2 mm, and the initial rise of the profile is only observed for methyl. The position of the maxima is well reproduced by the model; also, the general shapes of the profiles are in reasonable agreement with the experiment. While the absolute mole fractions for HCO and CH_4 are reasonably well predicted, methyl and formaldehyde mole fractions are under-predicted

by the model. Regarding the significant over-prediction of parent four-heavy-atom species, this may be a consequence of slow consumption reactions of these precursors. However, it is at first glance intriguing that small-molecule chemistry should not be in better agreement. To investigate this effect further, the respective trends for the cyclohexane [32,34-35,47], DME [14] and CH_4/NH_3 [64] flames were inspected, as explained before in 8.2.2.

Methyl mole fractions from the experiment are of similar magnitude in the cyclohexane and morpholine flames and only slightly higher in the DME flame, while methane mole fractions exhibit differences, especially for the CH_4/NH_3 flame where it is a fuel. The less-than-satisfactory prediction quality of the methyl and methane profiles for the morpholine flame is thus a consequence of the very different formation pathways, as evident from a reaction rate analysis. For the morpholine flame, CH_3 formation is mostly via $C_2H_4 + O \leftrightharpoons CH_3 + HCO$ and $C_2H_5 + H \leftrightharpoons CH_3 + CH_3$, with some smaller contributions also from $CH2CHO \leftrightharpoons CH_3 + CO$ and $H + CH_2CO \leftrightharpoons CH_3 + CO$, and CH_4 is formed from CH_3. Methyl and methane levels thus are both partially determined by C_2 species formation from fuel-decomposition pathways. For the DME flame, CH_3 is an immediate product, jointly with CH_2O, from the fuel consumption. Its singularly most important formation reaction is $CH_3OCH_2 \leftrightharpoons CH_2O + CH_3$, and CH_4 is formed from CH_3 reactions with CH_2O, HCO, and the fuel itself. Interconversion of CH_3 and CH_4 by the reaction of H-atoms with CH_4 and contributions of the methyl recombination reaction to C_2H_5 are important in the cyclohexane flames, along with reactions involving higher hydrocarbons, particularly in the rich flame. CH_3 is a direct product from the fuel via H-abstraction by H and OH in the CH_4/NH_3 flame.

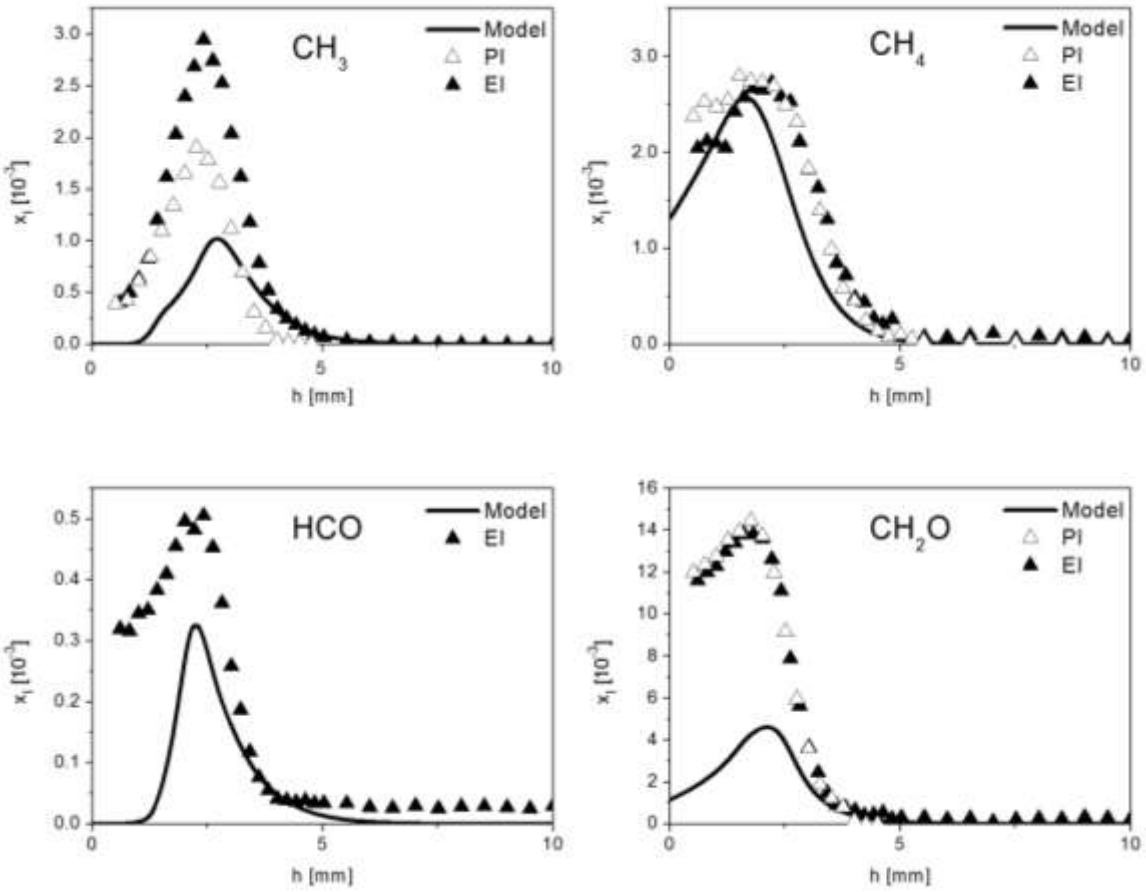

Figure 8.5: Mole-fraction profiles of selected C_1 species.

The formaldehyde and formyl reaction patterns are also quite different for these flames of different fuels. Here again, though, the morpholine predictions depend on fuel decomposition steps. The peak mole fraction of formaldehyde for the morpholine flame is of the order of 2×10^{-2}, similar to that in the DME and the rich cyclohexane flame and about an order of magnitude higher than in the stoichiometric cyclohexane flame. In the DME flame, CH_2O is linked to the formation of CH_3 from the fuel after H-abstraction, and it is also produced from $O + CH_3 \rightleftharpoons H + CH_2O$, while HCO is formed via H-abstraction from formaldehyde by OH, H-, and O-atoms. This pattern is also evident from Fig. 8.3 in [14]. Reactions to formaldehyde in the cyclohexane flames involve mostly

$C_2H_3 + O_2 \leftrightharpoons HCO + CH_2O$, especially under fuel-rich conditions where higher C_2 species concentrations are available. For morpholine as an ether resembling cyclohexane, a plausible assumption would be that the additional amine function should not play a major role in the formation of these C_1 intermediates. However, as shown in the reaction rate diagram in Fig. 8.6, direct relations to N-containing ring fragments are seen with the largest contribution towards formaldehyde formation from $\bullet CH_2CHO{=}CH_2 \leftrightharpoons CH_2O + C_2H_3$ and formaldehyde consumption by reactions with OH and H to form HCO. Also, as evident from Fig. 8.1, formaldehyde is a product of several other morpholine decomposition reactions. The underprediction of CH_3, CH_4 and CH_2O in the morpholine flame is thus not primarily a function of insufficient predictive capability for C_1 species reactions, but it is owed to the more complex decomposition chemistry of this heterocyclic, polyfunctional fuel where a number of steps are involved to provide these small intermediates. This sequence is quite different from the DME or CH_4/NH_3 flames, where CH_3 and/or CH_2O are formed directly from the fuel. More thoroughly examined reaction pathways, rate expressions, and thermochemical and transport parameters are thus needed for these heterocyclic fuels, as was recently also observed in a study of pyrrolidine combustion [65].

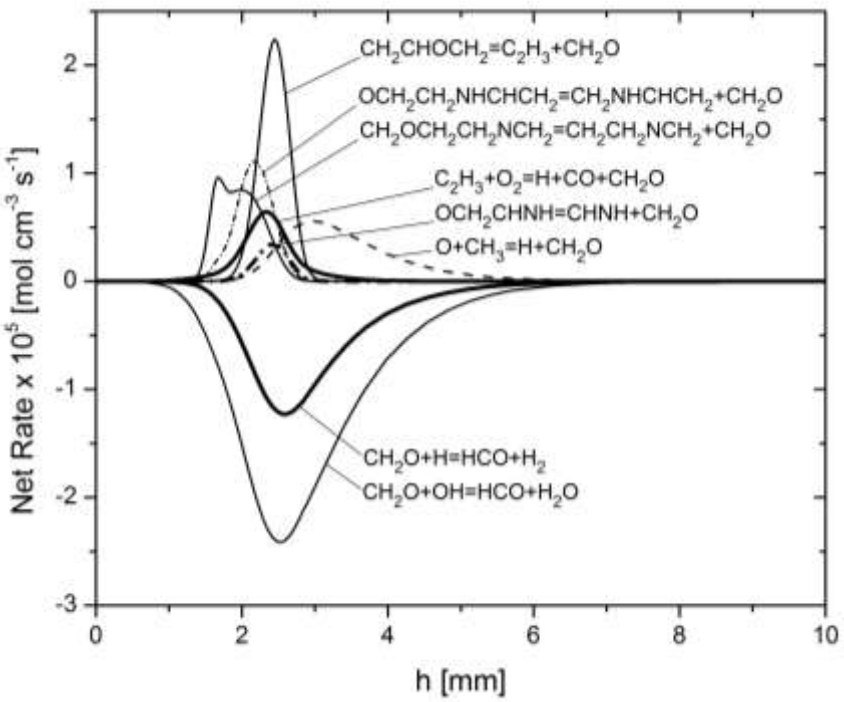

Figure 8.6: **Reaction rate diagram for CH_2O.**

8.3.4.2 Selected C_2 compounds

The mole-fraction profiles for C_2H_2, C_2H_4, C_2H_5, and C_2H_6 are shown in Fig. 8.7. For ethylene, EI-MBMS and PI-MBMS measurements are in good agreement only slightly underpredicted, and for acetylene, peak mole fractions are in line with the PI data. In the PI-MBMS experiment, ethyl and formyl could not be separated quantitatively because of similar ionization thresholds and unknown cross sections; similarly, ethane could not be determined unambiguously because of several contributions to *m*/*z* 30 and high formaldehyde mole fractions. Both profiles are thus only reported from the EI-MBMS measurements. The simulation matches peak position and profile shape for C_2H_5 and C_2H_6 species, although under-predicting their mole fractions by a factor of 10 and 3 respectively.

As a direct product from several pathways in the skeletal mechanism in Fig. 8.1,

C_2H_4 is represented quite well by the simulation. Accordingly, the reaction rate diagram in Fig. 8.8 reflects several fuel decomposition reactions as principal formation paths for

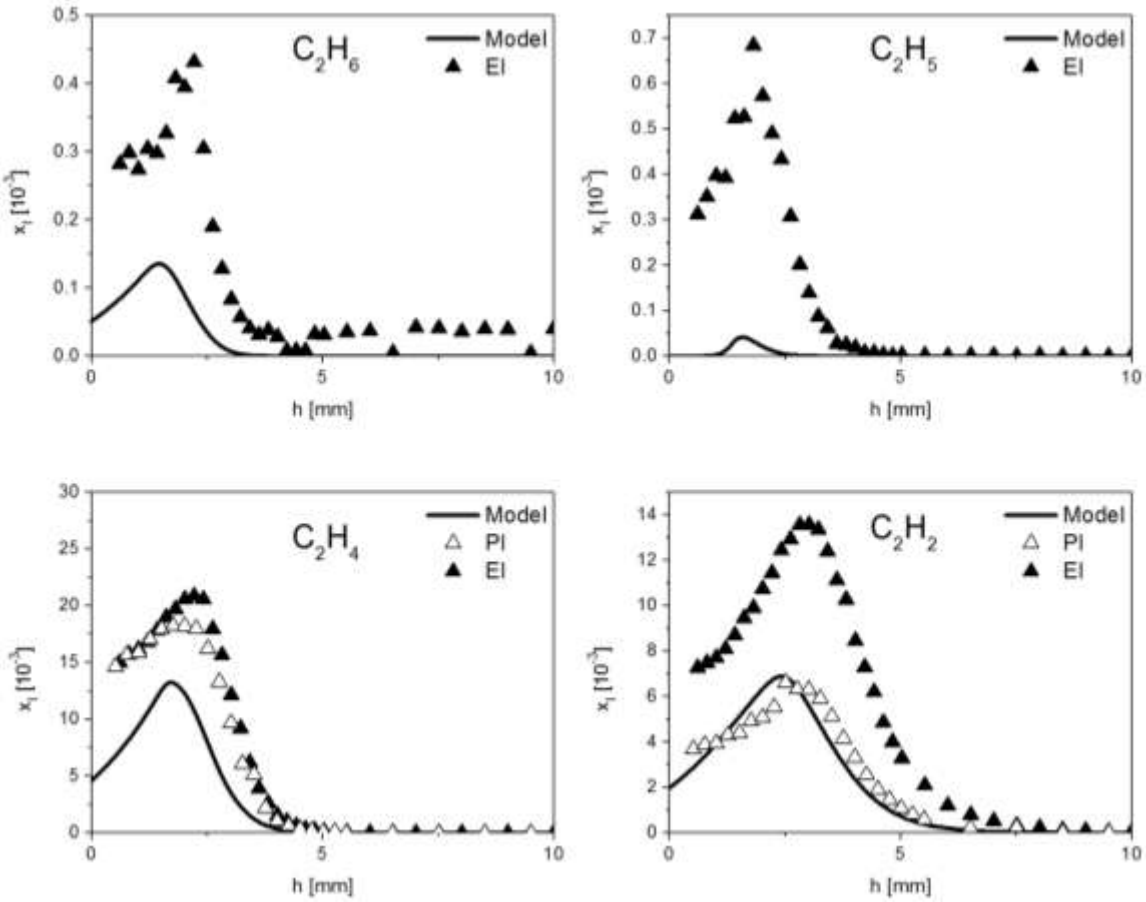

Figure 8.7: Mole-fraction profiles of selected C_2 species.

C_2H_4, with dominant contributions from $\bullet CH_2CH_2OCH_2CH{=}NH \leftrightharpoons C_2H_4 + \bullet OCH_2CH{=}NH$ (from *m*-morphyl), followed by $\bullet CH_2CH_2NCH_2CH{=}O \leftrightharpoons C_2H_4 + \bullet NCH_2CH{=}O$ (originating from *o*-morphyl), $\bullet CH_2CH_2NCH_2 \leftrightharpoons C_2H_4 + \bullet NCH_2$ (originating from *p*-morphyl), and $\bullet CH_2CH_2N{=}CHCH{=}O \leftrightharpoons C_2H_4 + \bullet N{=}CHCH{=}O$ (from the cyclic morphyl-ene species). In contrast, pathways forming the other C_2 species in Fig. 8.7 involve build-up reactions including $CH_3 + CH_3$ (+M) as the main formation reaction for C_2H_6, sequential H-abstraction reactions including $C_2H_4 + OH \leftrightharpoons C_2H_3 +$

H_2O, and $C_2H_3 + H \leftrightharpoons C_2H_2 + H_2$, and further reactions within this small-intermediates pool.

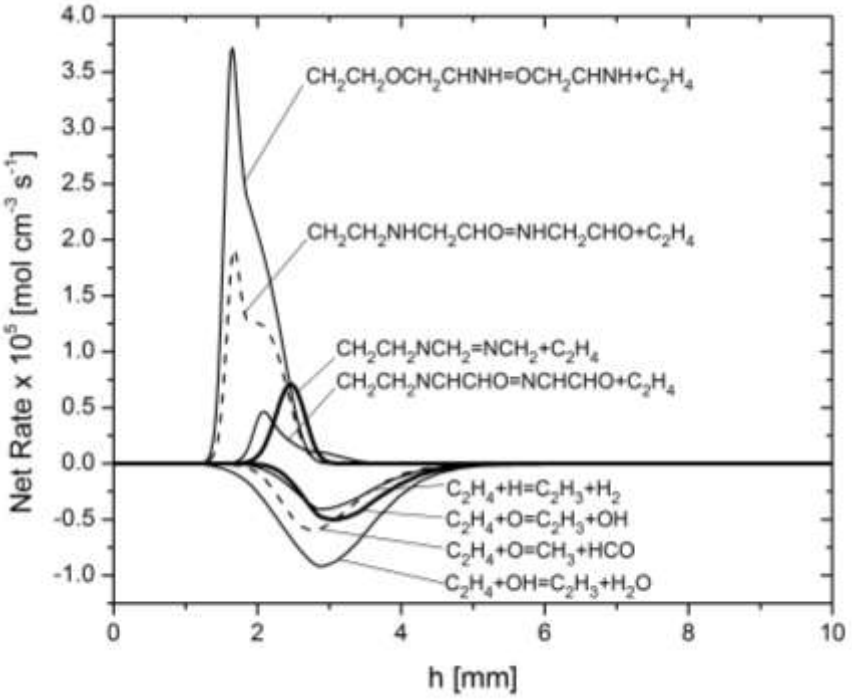

Figure 8.8: Reaction rate diagram for C_2H_4.

Again, it is instructive to compare the main reaction paths in the cyclohexane [32,34-35,47], DME [14], and CH_4/NH_3 [64] flames to those for morpholine. For cyclohexane, C_2H_4 is also formed in the early decomposition steps, with predicted peak mole fractions in the 0.01 (Φ = 1.0) to 0.04 (Φ = 2.0) range, quite comparable to 0.025 found in the morpholine flame. The most important C_2H_4 formation reactions in both cyclohexane flames are $C_6H_{11} \leftrightharpoons C_4H_7 + C_2H_4$ and $C_4H_6 + H \leftrightharpoons C_2H_4 + C_2H_3$, with some further reactions contributing in the fuel-rich flame. In contrast, important reactions determining C_2H_4 formation in the DME flame are C_2H_5 (+M) $\leftrightharpoons$ H + C_2H_4 (+M) and $CH_2 + CH_3 \leftrightharpoons C_2H_4 + H$; the latter is also the most important pathway to C_2H_4 in the

CH_4/NH_3 flame. A decisive difference for the two six-membered-ring fuels versus DME and CH_4/NH_3 combustion is thus the formation of C_2H_4 as a direct product from β-scission reactions in the fuel decomposition. For all flames, build-up reactions like $CH_3 + CH_3 (+M) \leftrightharpoons C_2H_6 (+M)$ are mainly responsible for ethane formation, and interconversion reactions of C_2 species like $C_2H_3 (+M) \leftrightharpoons C_2H_2 + H (+M)$ dominate C_2H_2 formation.

8.3.4.3 Selected C_3 and C_4 compounds

Morpholine's structure presents only two-carbon sequences, and all C_3 and C_4 species are thus the result of build-up reactions. Some of these species are known as precursors to benzene, which in turn is commonly accepted to be an important intermediate in the formation of polycyclic aromatic hydrocarbons and soot. Selected C_3 and C_4 species including C_3H_3, C_3H_4, C_3H_6, and C_4H_4 are presented in Fig. 8.9. Results from EI-MBMS and PI-MBMS are seen in quite good agreement, especially for propargyl and for C_3H_4, which is only propyne as determined by PI-MBMS.

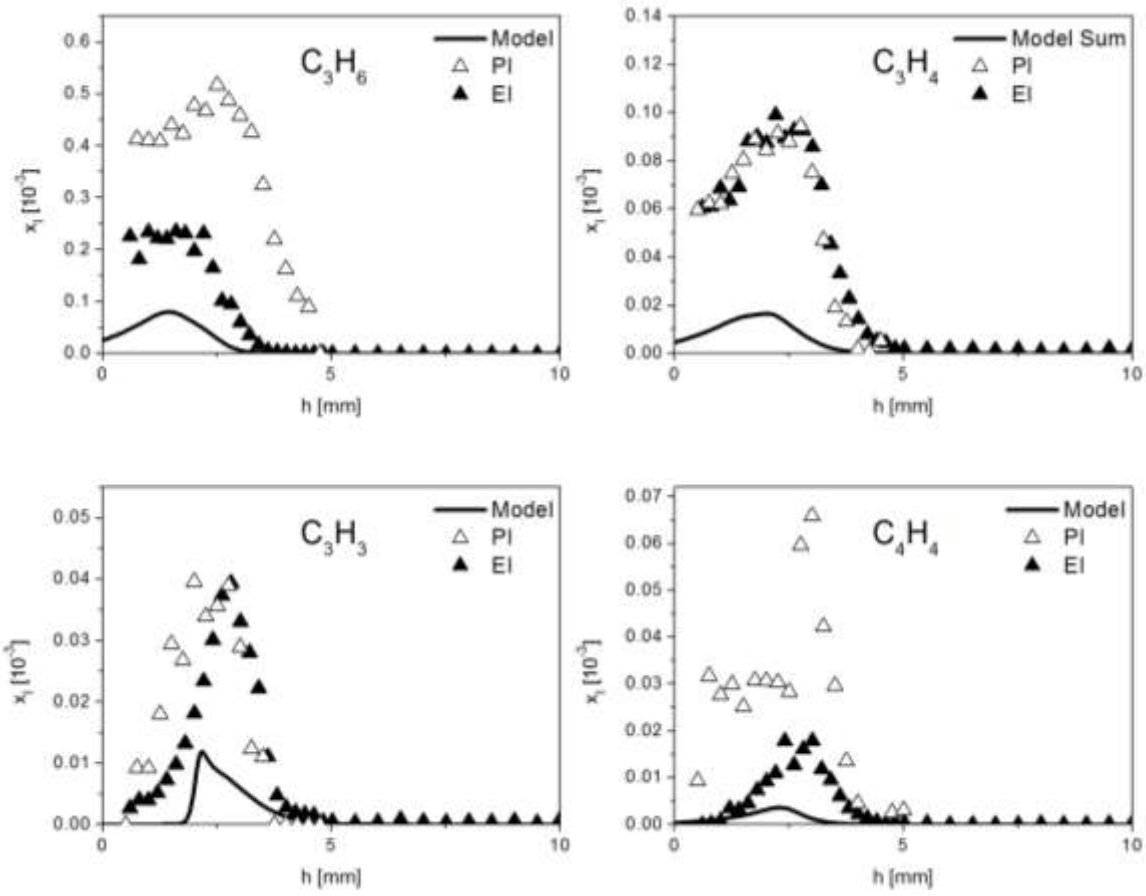

Figure 8.9: Mole-fraction profiles of selected C_3 and C_4 species.

In comparison with rich flames of some hydrocarbon and oxygenate fuels, the peak mole fractions given in Fig. 8.9 are quite low. The mole fraction of C_3H_6 ($\sim 6\times10^{-4}$) is significantly lower than the observed peak mole fractions in fuel-rich flames of cyclohexane ($\sim 4\times10^{-3}$) and 1-hexene ($\sim 10^{-2}$) under comparable combustion conditions [36]. Also, oxygenate fuels may present high C_3H_6 mole fractions, as e.g. of $2\times10^{-3} - 10^{-2}$ for different butanol isomers [9], where the carbon backbone provides easier access to these compounds than morpholine. Propargyl as an important benzene precursor presents with 5×10^{-5}, a much lower peak mole fraction in the morpholine flame than that of $\sim 10^{-3}$ in a fuel-rich propene flame [66] with easy pathways to C_3 intermediates; oxygenate

(DME or ethanol) replacement of propene decreases C_3H_3 by a factor of 2-3 [66], which is still considerably higher than in the morpholine flame. Similarly, C_3H_3 mole fractions are of order 6×10^{-4} and 7×10^{-4} in fuel-rich butanol [9] and ethanol [67] flames, respectively. The propyne mole fraction in the morpholine flame is 1.2×10^{-4}, comparable to peak values of ~7×10^{-5} – 10^{-4} in fuel-rich flames of small esters [68] and somewhat lower than in butanol flames with peak mole fractions of ~2 – 8×10^{-3}. The vinylacetylene mole fraction is also quite low with <5×10^{-5}, while it is up to 4×10^{-4} in the fuel-rich ester flames [68], and 4×10^{-4} – 1.5×10^{-3} in the fuel-rich butanol flames [9]. In view of the generally low concentrations of benzene precursor species, soot formation is expected to be less important for morpholine as a substituted cyclohexane fuel than for cyclohexane itself or for other C_6-hydrocarbon fuels [36].

The model agrees in terms of maximum positions and profile shapes but under-predicts all four species presented in Fig. 8.9 significantly, similarly to some of their important C_1 and C_2 precursors that were discussed above and apparently for similar reasons. For example, propargyl is predominantly formed from $C_2H_2 + {}^1CH_2 \leftrightharpoons C_3H_3 + H$, propene by $CH_2{=}C{=}CH_2 + H \leftrightharpoons C_2H_6$ and $C_2H_3 + CH_3 \leftrightharpoons C_3H_6$, propyne is formed in interconversion reactions involving C_3H_5 and allene as well as from $C_3H_3 + H \leftrightharpoons HCCCH_3$, and vinylacetylene by $C_2H_2 + C_2H_3 \leftrightharpoons C_4H_4 + H$.

8.3.4.4 Oxygenated species

Because of the ether function in the morpholine molecule, it is informative to analyze the small oxygenated intermediate species, also in comparison with their respective amounts in fuel-rich flames of other oxygenated fuels. Figure 8.10 presents results for ketene, methanol, methoxy radical and ethenol/acetaldehyde. Methoxy and

methanol were only quantified from EI-MBMS because a photoionization cross section for the former was not available and the latter was obscured by O_2 signal. For C_2H_4O, the sum of the mole fractions of the isomers acetaldehyde and ethenol, determined individually by PI-MBMS, is in reasonable agreement with the sum from EI-MBMS.

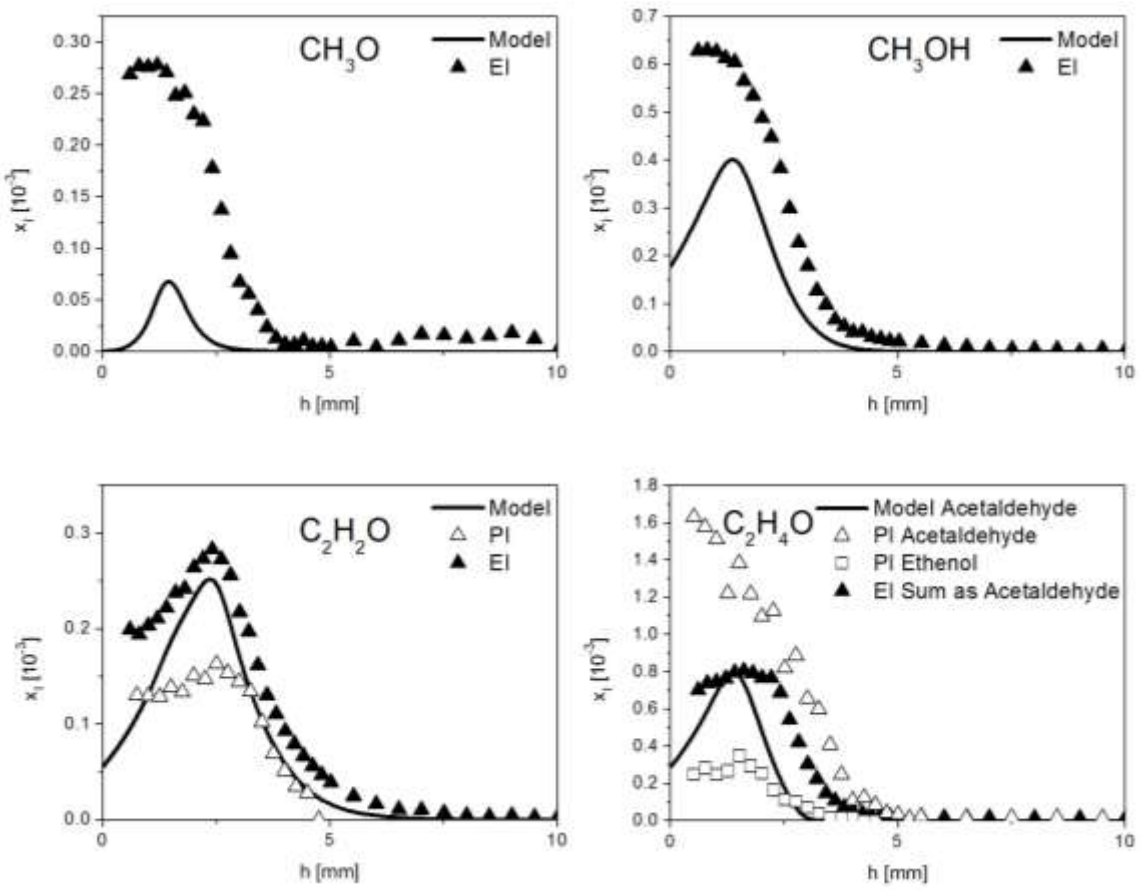

Figure 8.10: Mole-fraction profiles of selected oxygenated species.

In the premixed fuel-rich low-pressure DME flames of [14], ketene, methanol, and acetaldehyde (as the dominant C_2H_4O isomer) mole fractions were reported to be about 10^{-4}, 10^{-3}, and 6×10^{-4}, respectively, compared with 3×10^{-4}, 7×10^{-4}, and $\sim10^{-3}$ in the morpholine flame. These are quite similar trends, also with respect to much higher formaldehyde than acetaldehyde concentrations of the order of 2×10^{-2} in both flames. In

premixed fuel-rich low-pressure ethanol combustion [67], peak CH_3O mole fractions were determined to be ~4×10^{-4}, compared to 3×10^{-4} for the morpholine flame, and C_2H_2O was ~1×10^{-3}, again similar to both DME and morpholine flames.

C_2H_4O (mostly acetaldehyde) was distinctly higher in the ethanol flame with ~9×10^{-3}, compared to the isomeric DME flames, a trend explained with the different fuel structure and breakdown patterns [66]. In fuel-rich flames of the propanol isomers [39], peak acetaldehyde mole fractions were 2 – 6×10^{-3}, and in fuel-rich butanol flames, mole fractions of ketene of 1 – 3×10^{-3} and of acetaldehyde up to 1.7×10^{-2} were noted, depending on butanol isomer [9], whereas peak formaldehyde mole fractions were again lower with 3 – 7×10^{-3}. From these trends, it seems that the ether function in morpholine gives rise to the formation of some small oxygenates in a fashion quite similar to DME. Both ether and alcohol fuels exhibit higher mole fractions of aldehydes than related hydrocarbons, and morpholine is not an exception in that general sense.

Predictions of the oxygenate mole fractions in Fig. 8.10 are in good agreement to the experimental data; they are within experimental error for all but methoxy which is slightly under-predicted. A rate analysis shows that methoxy is predicted to be formed from $HO_2 + CH_3 \leftrightharpoons OH + CH_3O$ with some contributions from nitrogenated intermediates through $NO_2 + CH_3 \leftrightharpoons NO + CH_3O$ and $CH_3NH + O_2 \leftrightharpoons CH_3O + HNO$. Methanol is formed via $CH_3 + OH\ (+M) \leftrightharpoons CH_3OH\ (+M)$, $^1CH_2 + H_2O\ (+M) \leftrightharpoons CH_3OH\ (+M)$ and by the reaction of CH_3O with HCO, yielding methanol and CO as the products. C_2H_4O results mainly form $CH_3 + HCO$, while ketene is formed via $O + C_2H_3$ and $OH + C_2H_2$. Under-prediction of methoxy and slight under-prediction of methanol may thus be connected to the under-estimation of CH_3 discussed before.

The influence of CH_2CHO motivated its evaluation from the *m*/*z* 43 signal, and its mole fraction is presented together with the simulation in Fig. 8.11. Again, an upper and

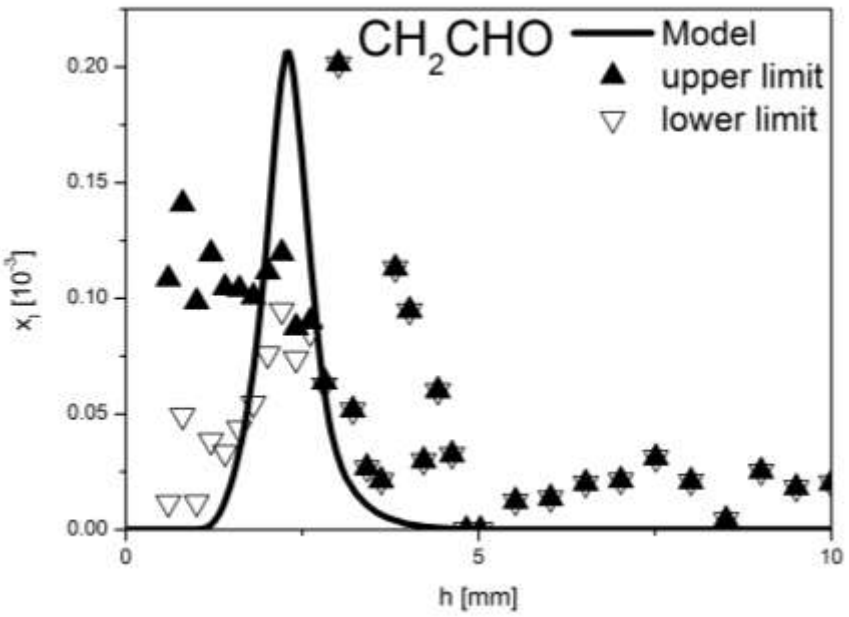

Figure 8.11: Mole-fraction profile of *m*/*z* 43 C_2H_3O, evaluated as CH_2CHO.

lower limit was derived from the EI-MBMS experiment where it could be separated by mass from isocyanic acid, ethenimine and acetaldimine at *m*/*z* 43; fragmentation was corrected from acetaldehyde. The estimated peak mole fraction of 1×10^{-4} is somewhat lower than that of $4\times10^{-4} – 4\times10^{-3}$ found for C_2H_3O in rich butanol [9] and of ~5×10^{-3} in ethanol [67] flames, where the acetaldehyde concentrations are also higher. The prediction is quite good, given the uncertainties in experiment. Further oxygenated intermediates identified in morpholine combustion include formic acid and ethanol, whose role was not analyzed specifically. Traces of further carbonyl compounds as typically seen in oxygenate-fuel combustion cannot be excluded but will have mole fractions below ~10 ppm.

8.3.5 Fuel-nitrogen conversion chemistry in morpholine flames

The previous analysis has focused on morpholine fuel decomposition and on the formation of hydrocarbon and oxygenated intermediates. Although the fuel breakdown sequences were conceived in analogy to cyclohexane, the resulting balance of hydrocarbon intermediates for the heterocyclic morpholine is quite different due to the short carbon sequences in the fuel structure. Measured concentrations for benzene precursors are generally less significant in the morpholine flame than for combustion of hydrocarbons and large alcohols under similar conditions. The ether function in morpholine gives rise to aldehyde formation, with concentrations of the same order of magnitude as those from fuel-rich DME or other oxygenate flames. With respect to the formation of NO from this model biofuel, the identity and amount of small nitrogen-containing species remains to be discussed, expecting the formation of NH_3 and HCN as potential precursors to NO.

8.3.5.1 Small nitrogenated compounds

From recent work combining CRDS and EI-MBMS in the investigation of the morpholine flame [29], NH_2 (from CRDS) has been noted to appear at low heights, followed by NH_3 and HCN, whose peak mole fractions are reached in the flame front, represented by the CH_3 profile. These maxima precede those of CN (from CRDS) and HNCO which both appear further from the burner surface and persist well into the exhaust, where NO reaches its maximum concentration. This sequence, which was also noted in flames of dimethylamine and ethylamine under similar conditions [29], seems to suggest that NH_2, which is closely linked to NH_3, may be formed as precursor to CN/HCN and NO early in the fuel decomposition, in line with perceptions on the

importance of NH_3 for fuel-NO formation from biofuels discussed in the introduction. To analyze the small nitrogen-containing species pool in more detail, Fig. 8.12 presents mole-fraction profiles of NH_3, HCN, NO, NO_2, and HNCO. All species were measured

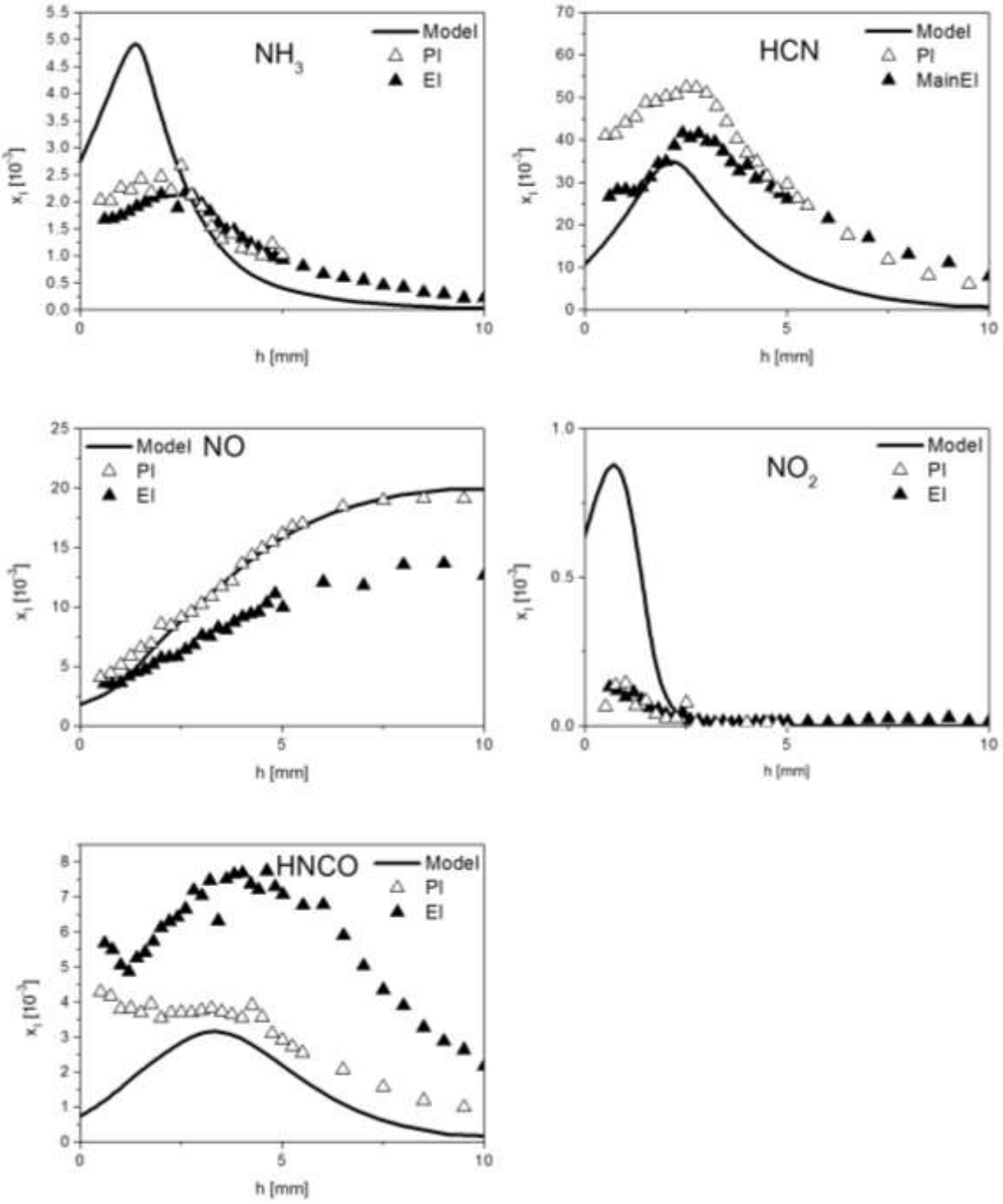

Figure 8.12: Mole-fraction profiles of small nitrogen-containing compounds.

with both PI-MBMS and EI-MBMS, the results of which are found in very good to excellent agreement. NO_2 was separated at *m*/*z* 46 from H_2CO_2 and C_2H_6O in the EI-MBMS experiment; these were identified by PI-MBMS as formic acid (at 11.33 eV) and ethanol (at 10.48 eV) while NO_2 was detected at 9.58 eV. N_2O could not be quantified in the EI-MBMS experiment because of interference with the strong CO_2 signal, which differs only by two thousands of an atomic mass unit. In the PI-MBMS experiment, a strong overlap with acetaldehyde with a large cross section at the ionization threshold of N_2O prevented its quantitative detection. N_2O mole fractions are estimated to be lower than 1×10^{-4}.

Mole fractions of the detected small nitrogen compounds are quite large with 2.5×10^{-2} for NH_3, $\sim6\times10^{-2}$ for HCN, $\sim8\times10^{-3}$ for HNCO, and 2.5×10^{-2} for NO; the NO_2 peak is very close to the burner surface with $\sim2\times10^{-4}$. It is difficult, however, to compare the present results quantitatively to the limited number of earlier studies in premixed flames of nitrogenated fuels, as some previous work reported only a few species accessible by laser methods [69-70]. Furthermore, addition of NH_3 or other nitrogen-containing fuels to hydrocarbon (often methane) base flames was used [64,71], enhancing different aspects of the combustion chemistry. Some recent studies of nitrogenated fuel combustion under premixed low-pressure conditions reported species identification [65,72] but did not derive quantitative concentrations of intermediates. A detailed recent study providing quantitative mole fractions of a large number of species has been devoted to flames of pyrrole [73], a heterocyclic compound usually seen as more representative of coal than of biofuel combustion. In the rich pyrrole flame of [73], the NH_3 profile appears as that of a product rather than intermediate, attaining a plateau similar to NO. The HCN

mole fraction was found to be of similar magnitude as in the morpholine flame with ~10^{-2}, and HNCO was almost an order of magnitude lower with ~4×10^{-3}. Numerous nitrogen-containing intermediates including higher-mass species with 5 to 8 carbon atoms were detected (e.g. pyridine and tolunitrile), mostly in mole fractions of the order of 10^{-4} or below. Furthermore, benzene precursors and benzene were detected in higher amounts than in the morpholine flame where benzene was below the detection limit. Fuel decomposition steps in [73] that rationalize the detected species are quite different from those of morpholine, which makes a more detailed quantitative comparison not useful. A recent experimental and modeling study of nitromethane combustion [74-75] as that of a simple C/H/N/O fuel shows that the CH_3NO_2 molecule easily forms CH_3 and NO_2, enhancing different intermediates and reactions channels from those seen here for morpholine. For the rich nitromethane flame [74-75], the mole fraction of HCN as an intermediate was observed to be ~10^{-2} [74], while NH_3 was not detected [75].

The small-nitrogen-compound chemistry in the morpholine flame can be analyzed further in light of simulations with the flame model. The model predictions for the species in Fig. 8.12 agree well regarding shapes and peak positions; absolute values are in excellent agreement for NO and HCN and are in reasonable agreement for NO_2, NH_3 and HNCO. From the skeletal mechanism in Fig. 8.1, it is evident that species with two heavy atoms are formed as a result of several preceding steps. The formation sequences for the small nitrogenated compounds can thus be analyzed in more detail from a reaction rate analysis, part of which is given for NH_3 and HCN in Fig. 8.13.

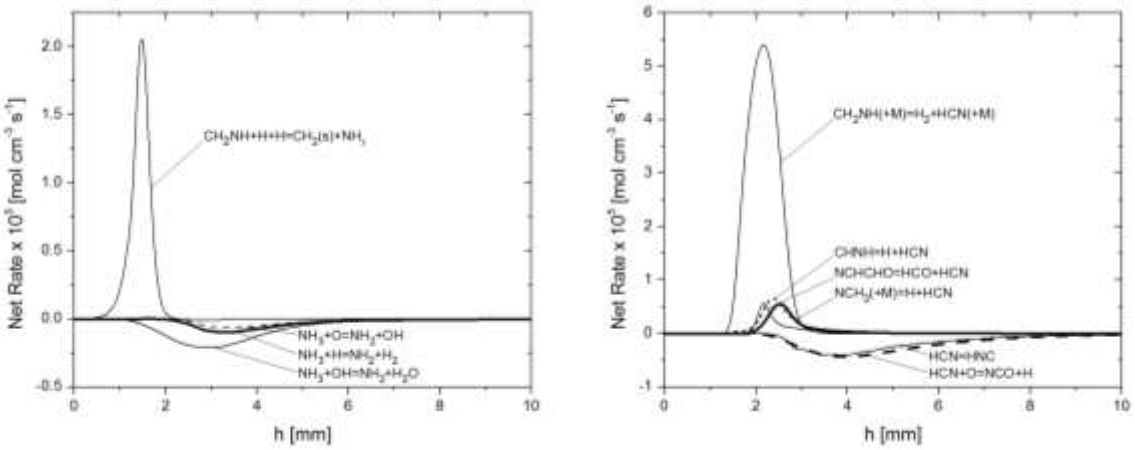

Figure 8.13: Reaction rate diagram for NH_3 and HCN.

According to this analysis, NH_3 is mainly produced from NH_2 through the morpholine decomposition intermediate CH_2NH. NH_2 in turn is produced predominantly from HNCO + H ⇋ NH_2 + CO, with some contributions from H abstraction reactions from NH_3. HNCO is produced via HNC + OH ⇋ HNCO + H, and HNC and HCN are easily interconverted. Unlike the structure in HNCO, N and O are separated by two carbons in the fuel and its breakdown products. NO_2 is produced early in the flame through HO_2 + NO ⇋ NO_2 + OH, where HO_2 is available and can react as soon as NO is formed.

The reaction rate plot for HCN in Fig. 8.13 shows pathways from CH_2=NH (+M) ⇋ HCN + H_2 (+M) as well as contributions from •CH=NH and •N=CH_2 decomposition. Further, a pathway to HCN is seen from •N=CHCH=O ⇋ HCN + HCO, with •N=CHCH=O as a direct morphyl decomposition product.

The main routes from morpholine to N_2 and NO are summarized in Fig. 8.14. The fuel decomposition to species with two heavy atoms provides mostly methanimine, CH_2=NH, from *o*- and *m*-morphyl (compare Fig. 8.1), as well as the related radicals

CH_2=N• and •CH=NH from *p*-morphyl and *m*-morphyl, respectively. According to the model, 1/4 of the NO is formed from HNO by abstraction, where HNO formation reactions $NH_2 + O \rightarrow HNO$ and $NH + OH \rightarrow HNO + H$ are analogous to $CH_3 + O$ and $CH_2 + OH$ chemistry. Important direct pathways lead via $HCN \rightarrow NCO \rightarrow NH$ or $HCN \rightarrow HNC \rightarrow HNCO \rightarrow NH_2$ to NO or N_2.

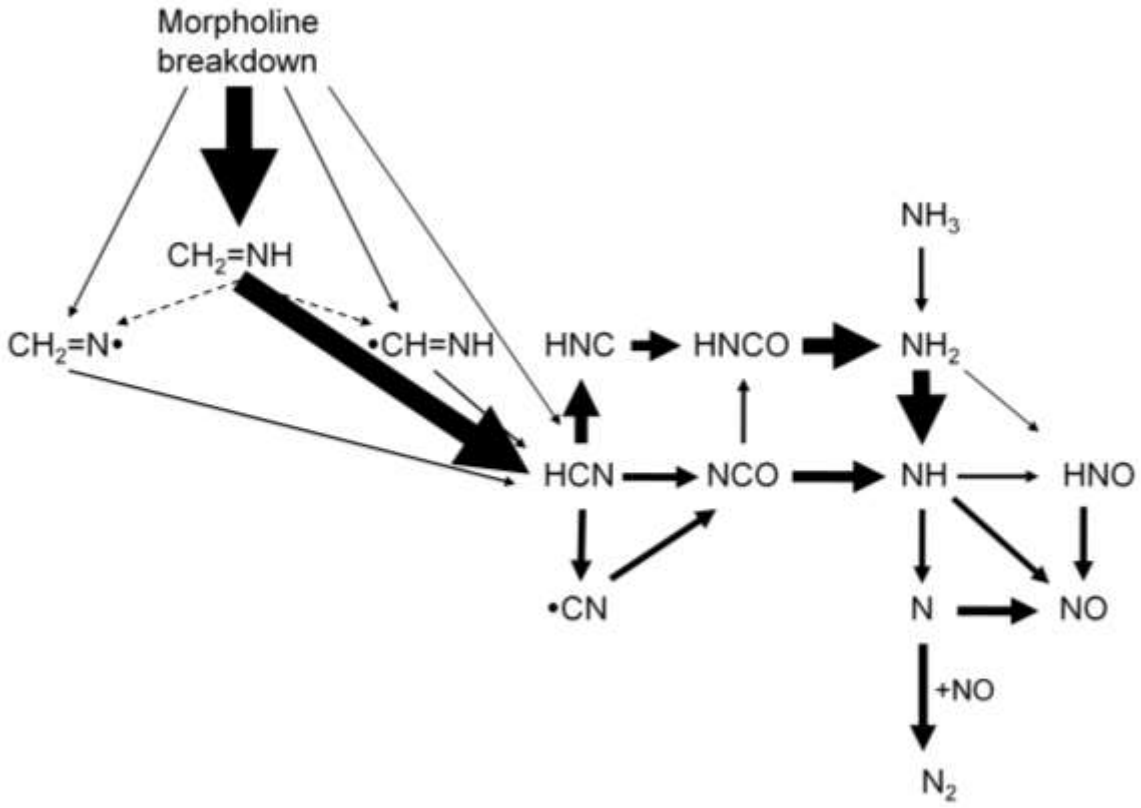

Figure 8.14: Reaction mechanism diagram for NO and N_2 formation.

From both experiment and model, it may be concluded that HCN is a pivotal intermediate in fuel-nitrogen conversion for morpholine with contributions also from NH_2 chemistry, the relative importance of which is linked to the fuel structure and early decomposition steps. Modeling of the present flame and through the literature back to Miller and Bowman [76] also shows that N_2 and NO formation is substantially through

N-atom, and the present flame modeling shows NO is also formed via a non-Miller-Bowman route through HNO. The agreement of the model predictions of N_2 and NO with experimental data implies both an adequately valid rate of HCN formation from fuel breakdown and a valid major-radical-pool concentration.

8.3.5.2 Selected further nitrogenated species

As seen from Table 8.3, a number of further nitrogen-containing species were identified, and Fig. 8.15 presents some nitrogenated C_1 intermediates including CH_2N,

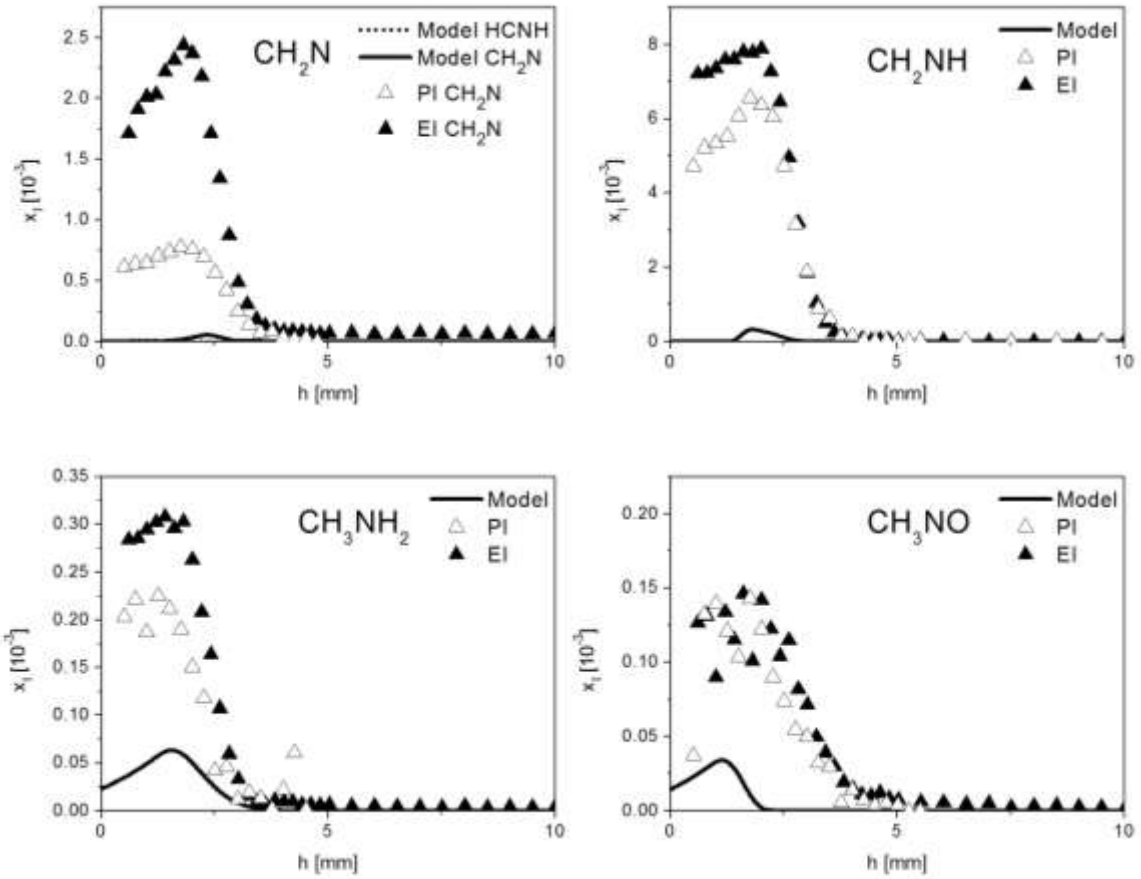

Figure 8. 15: Mole-fraction profiles of nitrogenated C_1 intermediates.

CH_2NH, CH_3NH_2, and CH_3NO. The radicals with formula CH_2N may be CH_2=N• and •CH=NH and were discussed above as precursors to HCN. In the experiment, EI-MBMS

did not discriminate between the two structures, and from PI-MBMS it was determined dominantly to be methylene amidogen, CH_2=N•; peak mole fractions are near 2×10^{-3}. The sum of the model predictions, which favor •CH=NH over CH_2=N•, is in reasonable agreement with the experiment. The stable precursor to both radicals, methaninime, CH_2NH, reaches a peak mole fraction of ~6×10^{-3} and is predicted well in shape and peak location but is under-predicted by an order of magnitude by the model as one of the links between morpholine decomposition and HCN formation. Main formation reactions for CH_2NH are NHCHCHO + H ⇋ CH_2NH + HCO and, to lesser extent, •$NHCH_2CH_2OCHCH_2$ ⇋ CH_2NH + •CH_2OCHCH_2 as well as •$CH_2NHCHCH_2$ ⇋ CH_2NH + C_2H_3.

Also given in Fig. 8.15 is methylamine, where EI-MBMS and PI-MBMS measurements are in excellent agreement but which the model underpredicts. It is not a direct decomposition product from the fuel breakdown but is mainly produced from NH_2 + CH_3 (+M) ⇋ CH_3NH_2 (+M); methyl (compare Fig. 8.5) was also somewhat under-predicted.

Furthermore, the mole fraction of the mass-45 C/H/N/O species is presented in the bottom right panel of Fig. 8.15 as a nitrogenated C_1 species, again with very good agreement between both experiments. In this work, it was inferred from its ionization threshold of 9.3 eV to be nitrosomethane, which is formed in the present mechanism by CH_3NO_2 + H ⇋ CH_3NO + OH and consumed by CH_3NO + H ⇋ CH_2NO + OH; the model predicts within a factor of 3, which is reasonable considering the experimental error. Formamide (NH_2CH=O, 11.16 eV) and the corresponding oxime (CH_2NOH, 11.1 eV) were not identified. In [75], a species of overall formula CH_3NO and a proposed

structure CH_2=NH=O (9.44 eV) was suggested as a potential result of O attack to H_2C=NH. A previous summary on the combustion chemistry of nitrogen [77] has discussed the potential energy diagram for the reaction of CH_3 + NO with CH_3NO, CH_2NHO, and CH_2NOH as (transient) products towards H_2CN + OH and HCN + H_2O, though their inclusion did not affect the prediction.

The mole-fraction profile for CH_4N at *m*/*z* 30 is given in Fig. 8.16. It could be separated from CH_2O, HNO, and C_2H_6 by mass in the EI-MBMS experiment and presents a peak with ~3×10^{-5} in the flame front. The model predictions for CH_3NH and CH_2NH_2 are of the same order of magnitude. Potentially, both may contribute to the measured profile. CH_2NH_2 is formed via H-abstraction from methylamine (compare Fig. 8.15) by CH_3NH_2 + (H, O, OH) ⇋ CH_2NH_2 + (H_2, OH, H_2O), while CH_3NH is from CH_3 + NH ⇋ CH_3NH. Both are thus build-up products from small radicals.

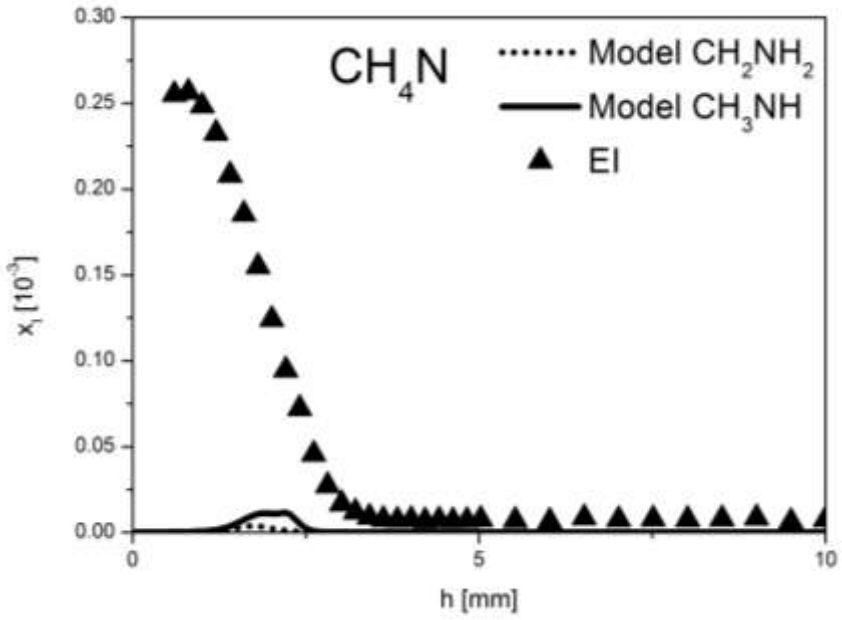

Figure 8.16: Mole-fraction profile of CH_4N.

From the wealth of further nitrogenated intermediates, Fig. 8.17 shows the tautomer pair C_2H_5N, ethenamine and acetaldimine, at *m*/*z* 43, which had already been identified in [28] in analogy to the tautomeric set of formula C_2H_4O, ethenol and acetaldehyde, at *m*/*z* 44. The PI-MBMS experiment permitted separate detection with dominant contribution from ethenamine, and the EI-MBMS experiment which detects the sum of both is seen as being in excellent agreement. Isocyanic acid (compare Fig. 8.12), also at *m*/*z* 43, was clearly identified and quantified both by mass and ionization threshold.

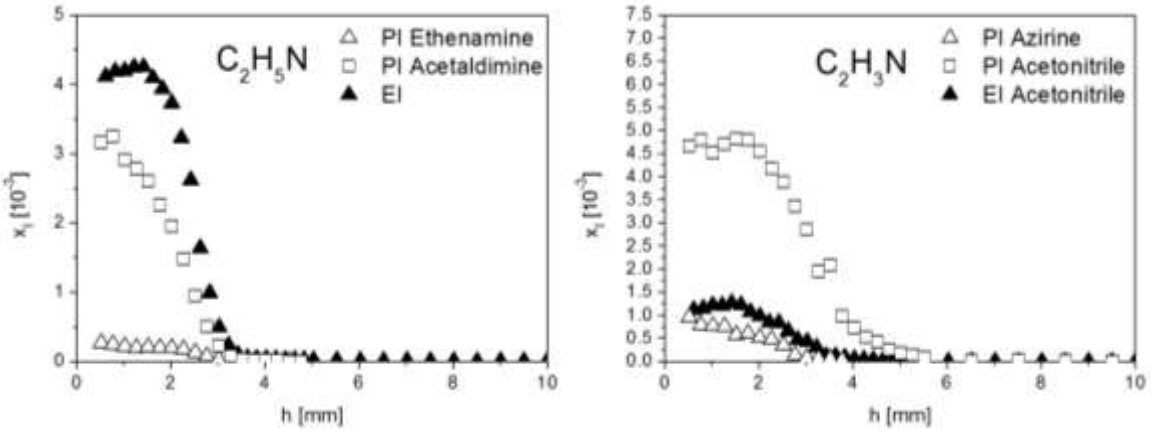

Figure 8. 17: Mole-fraction profiles of some nitrogenated C_2 species.

Also given in Fig. 8.17 is the mole-fraction profile for C_2H_3N at *m*/*z* 41, which was discussed in [28] as 2*H*-azirine and detected near 10.5 eV. The peak mole fraction of this species is 9×10^{-4}. Ketenimine (CH_2=C=NH, 9.28 eV) was not observed. The dominant C_2H_3N species, however, is acetonitrile (CH_3CN, 12.2 eV) with a peak mole fraction of 7×10^{-3}. From the experiment it is evident that toxic acetonitrile is formed as an intermediate in quite substantial concentrations.

Further highly toxic nitrogen-containing species have also been observed, including acrylamide (prop-2-enamide, CH_2=CHC=ONH_2) at *m*/*z* 71 and 2-propenenitrile

(acrylonitrile, CH_2=CHCN) at *m*/*z* 53. Their mole-fraction profiles are presented in Fig. 8.18. Both show typical intermediate-species behavior with maxima of 2.5×10^{-4} from EI-MBMS for acrylamide and 1.3×10^{-3} for propenenitrile, where both PI-MBMS and EI-MBMS are in excellent agreement. The model has not yet included reactions of these larger nitrogen-containing species, which are most probably produced from smaller precursors.

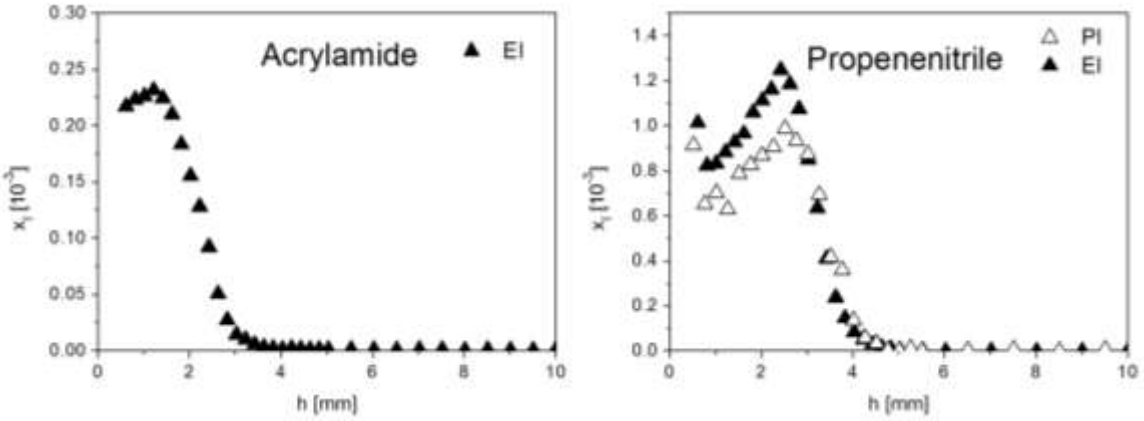

Figure 8. 18: Mole-fraction profiles of selected larger N-containing species.

8.4 Summary and Perspectives

Morpholine combustion has been analyzed in detail under fuel-rich premixed low-pressure flame conditions and a detailed reaction set has been created for modeling morpholine flames. From a combination of PI-MBMS and EI-MBMS, a large number of species with up to six heteroatoms was quantified, relying in part on previous identification [28] and using systematic additional measurements with both systems for a reliable separation and calibration. The two sets of experiments are in good general agreement. A modeling attempt used a newly conceived reaction scheme, starting from recent modeling of cyclohexane combustion, and a dedicated scheme for morpholine decomposition; it was seen to predict the general flame structure and reaction pathways

reasonably well, especially including NO_x formation. The polyfunctional cyclic fuel molecule gives rise to a wealth of combustion intermediates. From the fuel breakdown, especially species with four and two heavy atoms were postulated, many of which were observed; in most cases, mole fractions could be derived or estimated. Also, intermediate build-up and oxidation products were detected quantitatively. This accomplishment would not have been possible without the combined energy and mass resolution of this study.

Morpholine was chosen as a small C/H/N/O-containing model biofuel with the aim of contributing to the understanding of fuel-nitrogen conversion and of the formation of potential hazardous emissions from such compounds. The small-hydrocarbon chemistry was seen to exhibit distinct differences from that seen in flames of the related cyclic hydrocarbon fuel cyclohexane, as well as from that of oxygenated fuels such as DME and of ammonia/methane combustion under low-pressure premixed conditions. These differences are in part owed to the morpholine structure and early fuel breakdown sequences. Build-up of C_3 and C_4 hydrocarbons including typical benzene precursors is less probable than for combustion of hydrocarbons and larger oxygenates, and lower concentrations of polycyclic aromatic compounds and soot can thus be expected.

Aldehydes are formed as intermediates, and especially formaldehyde was observed to reach mole fractions quite similar to that for DME combustion under similar conditions, while acetaldehyde mole fractions were less important. Carbonyl compounds featuring more than two carbon atoms have not been detected, again a probable consequence of the early morpholine breakdown reactions.

The fuel nitrogen is finally converted to N_2 and NO, which present mole fractions

of about 4% and 2%. Major small nitrogen-containing intermediates include HCN, NH_3, HNCO, and NO_2, of which HNCO and NH_3 may persist into the burnt-gas region. The HCN mole fraction was surprisingly high with a peak of about 6%, and NH_3, expected to be a major volatile product, was seen with more than an order of magnitude lower peak mole fraction. The model suggests that HCN is formed from breakdown products of the morpholine ring, with NH_x compounds as further products once HCN is formed and converted rapidly in the small-nitrogen-species pool. However, a direct pathway to NH_x species also seems possible, in agreement with the observation of an early NH_2 maximum [29]. Toxic nitrogen-containing intermediates include also acetonitrile, acrylamide, and 2-propenenitrile.

As a perspective, consequences of these results for C/H/N/O-containing fuels from biogenic sources should be analyzed with care. The complicated breakdown sequence of morpholine resulting from the polyfunctional fuel structure suggests that an easy correlation cannot be given regarding the potential importance of HCN and NH_3. Combustion of nitromethane, an even simpler C/H/N/O fuel [74-75], was observed to produce percent levels of HCN but no NH_3, a consequence of its molecular structure which permits easy C-N bond rupture. Other recent studies of cyclic C/H/N fuels including pyridine [72], pyrrolidine [65], and pyrrole [73], seen as potentially more representative of coal than of biomass combustion, have reported different, but large respective numbers of N-containing intermediates, some of them toxic. Because the simultaneous presence of several structures with different hetero-elements at a given nominal mass presents already a challenge to qualitative analysis, not all of these studies reported a complete species spectrum and quantitative mole fractions. In most cases, a

fuel breakdown scheme was provided, derived from species identification, which would need corroboration by combustion modeling.

Since most studies of fuel-nitrogen conversion have concentrated on the reactions within the small-nitrogen-species pool and on HCN and NH_3 oxidation, a systematic approach that encompasses the combustion chemistry of functionally different fuel-nitrogen is needed, in analogy to the recent efforts that address the combustion chemistry of oxygenated compounds including the alcohol, ether, and ester families and their hydrocarbon relatives. From such a more general, systematic model, prediction of fuel-NO_x and other undesired products and intermediates should be expected for different C/H/N/O fuel structures. As an alert for increased attention when discussing non-hydrocarbon fuels for their perceived potential in reducing CO_2, combustion even of small fuel molecules containing N and O as hetero-elements may give rise to a number of undesirable combustion intermediates and products, including carbonyl compounds and, for example, toxic nitrogen-containing species (NO_x, HCN, NH_3, and others). Assessment of the potential suitability of a chemical as a fuel should thus include not only considerations of its availability, physico-chemical properties, and socio-economic consequences of its use, but analysis also should consider its combustion chemistry.

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CHAPTER 9

HETEROATOMIC FUELS: MODELING LASER DIAGNOSTICS EXPERIMENTS FOR MORPHOLINE FLAME AND SHOCK-TUBE APPLICATIONS[4]

Modeling results are presented in this chapter for a laser-diagnostic experimental study [4] on the same morpholine flat-flame experiment as in [1-2] to determine the mole fraction profiles for CH, CN, and NH_2, as well as HCO for a consistency check between the two studies. As seen in Chapter 8, morpholine is a species well suited for studying the combustion chemistry of biomass-derived fuels, where molecularly bound nitrogen and oxygen play a larger role. Through the experimental work of a morpholine/O_2/Ar flame with $\Phi = 1.3$ using MBMS [1-2], several key combustion pathways were determined and a reaction set for morpholine was developed and validated [2]. However, still several aspects of morpholine combustion have not been tested, including determining the mole fraction profiles of additional key intermediate species, ignition properties, and pyrolysis chemistry.

For example, as illustrated by Miller and Bowman [3] and corroborated in the morpholine modeling study [2], NO_x and N_2 key formation pathways have a direct link with HCN through radical species CN and NH_2. Unfortunately, these radical species were not detected in the MBMS experimental study, and thus no additional information could be gleaned about the kinetic pathways besides what was suggested through the model.

[4] Based in part on S. Li, D. F. Davidson, R. K. Hanson, N. J. Labbe, P. R. Westmoreland, Patrick Oßwald, K. Kohse-Höinghaus. "Shock Tube Measurements and Model Development for Morpholine Pyrolysis and Oxidation at High Pressures," prepared for submission to *Combustion and Flame*, December 2012.

Additionally, the probe cone in the MBMS experiments introduces flame perturbations, which affect flame structure. Laser diagnostics avoid this physical perturbation.

Additionally, the morpholine combustion experimental database still needs to be augmented, as no data have been published for morpholine pyrolysis and oxidation at high pressures. In this chapter, shock-tube measurements are reported and analyzed for morpholine-pyrolysis time histories and for ignition delay times. The morpholine combustion reaction set developed in Chapter 8 was updated and used to simulate the pyrolysis and ignition conditions for comparison to these experimental data.

9.1 Experimental and Modeling methods

9.1.1 Laser diagnostics for morpholine flames

Mimicking the conditions of the morpholine experiment in [1], the laser diagnostics experimental study for morpholine combustion, conducted by colleagues at Bielefeld University, was on a laminar, premixed flat morpholine-oxygen flame diluted with 25% argon was investigated at 40 mbar with $\Phi = 1.3$ (C/O = 0.41) and 0.32 m/s cold gas velocity at 293 K. The flame was stabilized on movable, water-cooled McKenna-type burners. Gas flows were controlled with calibrated mass-flow controllers, and liquid morpholine was metered by a syringe pump, evaporated quantitatively, and added to the gas stream [4].

Mole fraction profiles were measured via chemiluminescence using laser diagnostics using a pulsed dye laser, pumped with a Nd:YAG laser with a spectral bandwidth in the UV of 0.15 cm^{-1}. CH was detected in the $B^2\Sigma$-–$X^2\Pi$ 0-0 band and CN in the $B^2\Sigma^+ – X^2\Sigma^+$ 0-0 band using a Quinolon 390 dye in methanol near 388 nm. NH_2 was detected in the $A^2A_1–X^2B_1$ (090-000) $^PQ_{1,N}(7)$ transition using Rhodamine B dye in

methanol at 597 nm and the laser was run in a double-grating configuration with a bandwidth of 0.1 cm^{-1}. The temperature profile was also sampled using chemiluminescence and was the unshifted profile of Chapter 8, given the lack of probe perturbations by the laser. Further details on the prior experimental work and the apparatus may be found in [4].

9.1.2 Shock-tube experiments

In a second experimental study conducted at Stanford University, morpholine decomposition time histories were measured in morpholine/argon mixtures, and ignition delay times in morpholine/air or morpholine/oxygen/argon mixtures behind reflected shock waves using the Stanford University high-pressure shock tube (HPST). This shock tube has a stainless-steel driven section of 5 m length with a 5-cm inner diameter and a driver section that is 3 m long with an inner diameter of 7.5 cm. Shock-tube driver inserts were used to achieve uniform test conditions at lower temperatures where facility effects at long test times (dP/dt and dT/dt) are most significant [5]. The incident shock speed were determined using five piezoelectric pressure. Temperatures and pressures in the post-shock region were determined from the incident shock speed at the end wall using standard normal shock relations. Ignition delay times were determined by extrapolating, back to the baseline pressure, the steep increase in pressure concurrent with ignition. Other details concerning this shock tube can be found in [6].

Prior to each experiment, morpholine mixtures were manometrically prepared in a 12.8 L, magnetically stirred stainless steel mixing tank. The test mixtures were stirred using a magnetically driven vane assembly for at least 1 hour before actual shock tube experiments. Based on the vapor pressure data [7], morpholine will remain in the vapor

phase inside the tank, mixing assembly and the shock-tube driven section. Initial fuel concentrations were monitored using the 3.39 μm emission of a Spectral Physics model 124B He-Ne laser during both oxidation and pyrolysis experiments. Common mode rejection was used to reduce laser intensity noise. The absorption cross section of morpholine at 3.39 μm and 86 °C was also measured using an FTIR instrument. Details on the FTIR measurement technique can be found in [8]. Fuel-decomposition time histories during the morpholine pyrolysis process were also measured using the same setup.

9.1.3 Model development and simulations: morpholine reaction set and modeling

A new reaction set is proposed for morpholine oxidation based on cyclohexane oxidation [9] (Table 9.1) and for morpholine pyrolysis based on cyclohexane [10] and 1,4-dioxane pyrolysis [11] (see Table 9.2). A reaction set for morpholine flame chemistry has been previously presented in earlier work, constructed using certain analogies with cyclohexane combustion [2]; however, this set did not consider shock tube oxidation and pyrolysis chemistry. In addition to the changes above, the H/C/O chemistry was updated to reflect recent work on acetylene [12] and THP [13].

Table 9. 1: Morpholine oxidation set

Oxidation Reaction Set	* indicated OOH group attached to the preceding group					
Reaction	**A (mol-cm-s-K)**	**n**	**Ea (cal/mol)**	**Ref.**	**Estimation method**	**Parent Molecule**
OrthoMorphyl+O2=cyclic-OrthoOOMorphyl	3.000E+12	0.00	0.0	[9]	RPD	cyclohexane
MetaMorphyl+O2=cyclic-MetaOOMorphyl	3.000E+12	0.00	0.0	[9]	RPD	cyclohexane
ParaMorphyl+O2=cyclic-ParaOOMorphyl	3.000E+12	0.00	0.0	[9]	RPD	cyclohexane
cyclic-OrthoOOMorphyl=cyclic-OCHCHNHCH2CH2+HO2	1.925E+12	0.00	29000.0	[9]	RPD	cyclohexane
cyclic-MetaOOMorphyl=cyclic-OCHCHNHCH2CH2+HO2	1.925E+12	0.00	29000.0	[9]	RPD	cyclohexane
cyclic-MetaOOMorphyl=cyclic-OCH2CHNCH2CH2+HO2	9.625E+11	0.00	29000.0	[9]	RPD	cyclohexane
cyclic-ParaOOMorphyl=cyclic-OCH2CHNCH2CH2+HO2	3.850E+12	0.00	29000.0	[9]	RPD	cyclohexane
cyclic-OrthoOOMorphyl=cyclic-Ortho*Morph3yl	2.470E+11	0.00	31000.0	[9]	RPD	cyclohexane
cyclic-MetaOOMorphyl=cyclic-Meta*Morph2yl	2.470E+11	0.00	31000.0	[9]	RPD	cyclohexane
cyclic-MetaOOMorphyl=cyclic-Meta*Morph4yl	1.235E+11	0.00	31000.0	[9]	RPD	cyclohexane
cyclic-ParaOOMorphyl=cyclic-Para*Morph3yl	4.940E+11	0.00	31000.0	[9]	RPD	cyclohexane
cyclic-OrthoOOMorphyl=cyclic-Ortho*Morph6yl	9.300E+10	0.00	24077.0	[9]	RPD	cyclohexane
cyclic-OrthoOOMorphyl=cyclic-Ortho*Morph4yl	4.650E+10	0.00	24077.0	[9]	RPD	cyclohexane
cyclic-MetaOOMorphyl=cyclic-Meta*Morph5yl	9.300E+10	0.00	24077.0	[9]	RPD	cyclohexane
cyclic-ParaOOMorphyl=cyclic-Para*Morph2yl	1.860E+11	0.00	24077.0	[9]	RPD	cyclohexane
cyclic-OrthoOOMorphyl=cyclic-Ortho*Morph5yl	1.080E+10	0.00	24356.0	[9]	RPD	cyclohexane
cyclic-MetaOOMorphyl=cyclic-Meta*Morph6yl	1.080E+10	0.00	24356.0	[9]	RPD	cyclohexane
CH2CH2OCH*CHNH=cyclic-Ortho*Morph3yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
CH2CH2NHCH*CHO=cyclic-Meta*Morph2yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane

CH2OCH2CH*NCH2=cyclic-Meta*Morph4yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
OCH2CH2N*CHCH2=cyclic-Para*Morph3yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
OCH2CH2NHCHCH*=cyclic-Ortho*Morph3yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
NHCH2CH2OCHCH*=cyclic-Meta*Morph2yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
CH2OCH2CH2NCH*=cyclic-Meta*Morph4yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
CH2CH2OCH2CHN*=cyclic-Para*Morph3yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
cyclic-OCHCHNHCH2CH2+HO2=cyclic-Ortho*Morph3yl	8.000E+10	0.00	6000.0	[9]	RPD	cyclohexane
cyclic-OCHCHNHCH2CH2+HO2=cyclic-Meta*Morph2yl	8.000E+10	0.00	6000.0	[9]	RPD	cyclohexane
cyclic-OCH2CHNCH2CH2+HO2=cyclic-Meta*Morph4yl	8.000E+10	0.00	6000.0	[9]	RPD	cyclohexane
cyclic-OCH2CHNCH2CH2+HO2=cyclic-Para*Morph3yl	8.000E+10	0.00	6000.0	[9]	RPD	cyclohexane
CH2OCH*CH2NCH2=cyclic-Ortho*Morph4yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
NHCH2CH*OCHCH2=cyclic-Ortho*Morph6yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
OCH2CH*NHCHCH2=cyclic-Meta*Morph5yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
CH2CH2N*CH2CHO=cyclic-Para*Morph2yl	2.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
CH*OCH2CH2NCH2=cyclic-Ortho*Morph4yl	5.000E+07	0.86	5900.0	[9]	RPD	cyclohexane
CH*CH2NHCH2CHO=cyclic-Ortho*Morph6yl	5.000E+07	0.86	5900.0	[9]	RPD	cyclohexane
CH*CH2OCH2CHNH=cyclic-Meta*Morph5yl	5.000E+07	0.86	5900.0	[9]	RPD	cyclohexane
N*CH2CH2OCHCH2=cyclic-Para*Morph2yl	5.000E+07	0.86	5900.0	[9]	RPD	cyclohexane
CH2CH*OCH2CHNH=cyclic-Ortho*Morph5yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
OCH*CH2NHCHCH2=cyclic-Ortho*Morph5yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
CH2CH*NHCH2CHO=cyclic-Meta*Morph6yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
NHCH*CH2OCHCH2=cyclic-Meta*Morph6yl	1.000E+08	0.86	5900.0	[9]	RPD	cyclohexane
OCH*CHNH+C2H4=CH2CH2OCH*CHNH	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
NHCH*CHO+C2H4=CH2CH2NHCH*CHO	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2CH*NCH2+CH2O=CH2OCH2CH*NCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2NHCHCH*+CH2O=OCH2CH2NHCHCH*	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane

CH2OCHCH*+CH2NH=NHCH2CH2OCHCH*	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2CH2NCH*+CH2O=CH2OCH2CH2NCH*	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
OCH2CHN*+C2H4=CH2CH2OCH2CHN*	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH*CH2NCH2+CH2O=CH2OCH*CH2NCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH*OCHCH2+CH2NH= NHCH2CH*OCHCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH*NHCHCH2+CH2O= OCH2CH*NHCHCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
N*CH2CHO+C2H4= CH2CH2N*CH2CHO	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
OCHOOH+CH2CH2NCH2= CH*OCH2CH2NCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2CHOOH+NHCH2CHO= CH*CH2NHCH2CHO	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2CHOOH+OCH2CHNH= CH*CH2OCH2CHNH	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2NOOH+CH2CHOCH2= N*CH2CH2OCHCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2CHOOH+OCH2CHNH= CH2CH*OCH2CHNH	1.890E+03	2.67	6850.0	[9]	RPD	cyclohexane
OCHOOH+CH2NHCHCH2= OCH*CH2NHCHCH2	1.890E+03	2.67	6850.0	[9]	RPD	cyclohexane
CH2CHOOH+NHCH2CHO= CH2CH*NHCH2CHO	1.890E+03	2.67	6850.0	[9]	RPD	cyclohexane
NHCHOOH+CH2CHOCH2= NHCH*CH2OCHCH2	1.890E+03	2.67	6850.0	[9]	RPD	cyclohexane
CH2CHOCH2CHNH+HO2= CH2CH*OCH2CHNH	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane
CH2CHOCH2CHNH+HO2= NHCH*CH2OCHCH2	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane
OCHCH2NHCHCH2+HO2= OCH*CH2NHCHCH2	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane
OCHCH2NHCHCH2+HO2=	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane

CH2CH*NHCH2CHO						
NHCHCHO+HO2=OCH*CHNH	2.000E+11	0.00	7600.0	[9]	RPD	cyclohexane
NHCHCHO+HO2=NHCH*CHO	2.000E+11	0.00	7600.0	[9]	RPD	cyclohexane
CH2CHNCH2+HO2=CH2CH*NCH2	2.000E+11	0.00	7600.0	[9]	RPD	cyclohexane
CH2CHNCH2+HO2+CH2O= OCH2CH2N*CHCH2	2.000E+11	0.00	7600.0	[9]	RPD	cyclohexane
CHCHOOH+CH2NH=CH2NHCHCH*	2.000E+11	0.00	2010.0	[9]	RPD	cyclohexane
CHCHOOH+CH2O=CH2OCHCH*	2.000E+11	0.00	2010.0	[9]	RPD	cyclohexane
NCHOOH+C2H4=CH2CH2NCH*	2.000E+11	0.00	2010.0	[9]	RPD	cyclohexane
CHNOOH+CH2O=OCH2CHN*	2.000E+11	0.00	2010.0	[9]	RPD	cyclohexane
NCH2+CH2CHOOH=CH*CH2NCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
C2H3+OCHOOH=CH*OCHCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
C2H3+NHCHOOH=CH*NHCHCH2	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
HCO+CH2NOOH=N*CH2CHO	1.320E+04	2.48	6130.0	[9]	RPD	cyclohexane
CH2NOOH+OH=CHNOOH+H2O	1.800E+06	2.00	-1133.0	[9]	RPD	cyclohexane
NHCHOOH+OH=NCHOOH+H2O	9.000E+05	2.00	-1133.0	[9]	RPD	cyclohexane
CH2NOOH+H=CHNOOH+H2	1.150E+06	2.49	4124.0	[9]	RPD	cyclohexane
NHCHOOH+H=NCHOOH+H2	5.750E+05	2.49	4124.0	[9]	RPD	cyclohexane
CH2NOOH+CH3=CHNOOH+CH4	5.420E+04	2.26	7287.0	[9]	RPD	cyclohexane
NHCHOOH+CH3=NCHOOH+CH4	2.710E+04	2.26	7287.0	[9]	RPD	cyclohexane
CH2NOOH+HO2=CHNOOH+H2O2	1.120E+13	0.00	17686.0	[9]	RPD	cyclohexane
NHCHOOH+HO2=NCHOOH+H2O2	5.600E+12	0.00	17686.0	[9]	RPD	cyclohexane
HCN+HO2=CHNOOH	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane
HCN+HO2=NCHOOH	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane
HCO+HO2=OCHOOH	2.000E+11	0.00	12500.0	[9]	RPD	cyclohexane
CH2CHOOH+OH=CHCHOOH+H2O	1.800E+06	2.00	-1133.0	[9]	direct	cyclohexane
CH2CHOOH+H=CHCHOOH+H2	1.150E+06	2.49	4124.0	[9]	direct	cyclohexane
CH2CHOOH+CH3=CHCHOOH+CH4	5.420E+04	2.26	7287.0	[9]	direct	cyclohexane
CH2CHOOH+HO2=CHCHOOH+H2O2	1.120E+13	0.00	17686.0	[9]	direct	cyclohexane
C2H2+HO2=CHCHOOH	2.000E+11	0.00	12500.0	[9]	direct	cyclohexane

CHNH+HCO=NHCHCHO	7.000E+57	-13.82	17629.0	[12]	RPD	1,3-butadiene
NCHCHO+HCO=NHCHCHO+CO	5.000E+12	0.00	0.0	[12]	RPD	1,3-butadiene
NCHCHO+H2O2=NHCHCHO+HO2	1.210E+10	0.00	-596.0	[12]	RPD	1,3-butadiene
NCHCHO+HO2=NHCHCHO+O2	6.000E+11	0.00	0.0	[12]	RPD	1,3-butadiene
NHCHCHO=NCHCHO+H	3.500E+61	-13.87	129677.0	[12]	RPD	1,3-butadiene
NHCHCHO+H=NCHCHO+H2	3.000E+07	2.00	13000.0	[12]	RPD	1,3-butadiene
CH2NH+HCO=NHCHCHO+H	7.400E+14	-0.66	8420.0	[12]	RPD	1,3-butadiene
CH2O+CHNH=NHCHCHO+H	7.400E+14	-0.66	8420.0	[12]	RPD	1,3-butadiene
NHCHCHO+O=NCHCHO+OH	7.500E+06	1.90	3740.0	[12]	RPD	1,3-butadiene
NHCHCHO+OH=NCHCHO+H2O	2.000E+07	2.00	5000.0	[12]	RPD	1,3-butadiene
NHCHCHO+CH3=NCHCHO+CH4	2.000E+14	0.00	22800.0	[12]	RPD	1,3-butadiene
NHCHCHO+C2H3=NCHCHO+C2H4	5.000E+13	0.00	22800.0	[12]	RPD	1,3-butadiene
NHCHCHO+C3H3=NCHCHO+AC3H4	1.000E+13	0.00	22500.0	[12]	RPD	1,3-butadiene
NHCHCHO+AC3H5=NCHCHO+C3H6	1.000E+13	0.00	22500.0	[12]	RPD	1,3-butadiene
NHCH2CHO=NHCHCHO+H	1.270E+24	-4.75	23777.0	[12]	RPD	1,3-butadiene
OCH2CHNH=NHCHCHO+H	1.270E+24	-4.75	23777.0	[12]	RPD	1,3-butadiene
NHCH2CHO+H=NHCHCHO+H2	1.800E+12	0.00	0.0	[12]	RPD	1,3-butadiene
OCH2CHNH+H=NHCHCHO+H2	1.800E+12	0.00	0.0	[12]	RPD	1,3-butadiene
NHCH2CHO+O2=NHCHCHO+HO2	1.000E+11	0.00	0.0	[12]	RPD	1,3-butadiene
OCH2CHNH+O2=NHCHCHO+HO2	1.000E+11	0.00	0.0	[12]	RPD	1,3-butadiene
NHCH2CHO+CH3=NHCHCHO+CH4	1.100E+13	0.00	0.0	[12]	RPD	1,3-butadiene
OCH2CHNH+CH3=NHCHCHO+CH4	1.100E+13	0.00	0.0	[12]	RPD	1,3-butadiene

Table 9. 2: Morpholine pyrolyis set.

Pyrolysis Reaction Set							
	Reaction	**A (mol-cm-s-K)**	**n**	**Ea (cal/mol)**	**Ref.**	**Estimation method**	**Parent Molecule**
P1	morpholine=C2H4OH+CH2CHNH	1.774E+55	-12.72	78800	[11]	RPD	1,4-dioxane
P2	morpholine=CH2CH2NH2+CH2CHO	1.774E+55	-12.72	78800	[11]	RPD	1,4-dioxane
P3	morpholine=CH3CH2NH+CH2CHO	2.233E+55	-12.72	78400	[11]	RPD	1,4-dioxane
P4	morpholine=CH2CHNH+C2H5O	2.233E+55	-12.72	78400	[11]	RPD	1,4-dioxane
P5	OrthoMorphyl=HCO+C2H4+CH2NH	3.155E+15	-2.00	23000	[11]	RPD	1,4-dioxane
P6	MetaMorphyl=CH2O+C2H4+CHNH	3.155E+15	-2.00	23000	[11]	RPD	1,4-dioxane
P7	ParaMorphyl=NCH2+C2H4+CH2O	1.052E+15	-2.00	23000	[11]	RPD	1,4-dioxane
P8	OrthoMorphyl=CH3CH2NH+CH2CO	7.843E+08	0.00	23000	[11]	RPD	1,4-dioxane
P9	MetaMorphyl=CH2CNH+C2H5O	7.843E+08	0.00	23000	[11]	RPD	1,4-dioxane
P10	morpholine=CH3CH2NHCH2CHO	6.404E+65	-15.32	88293	[11]	RPD & Ea -8 kcal	1,4-dioxane
P11	morpholine=NH2CH2CH2OCHCH2	6.231E+63	-14.83	85767	[11]	RPD & Ea -8 kcal	1,4-dioxane
P12	morpholine=CH3CH2OCH2CHNH	6.404E+65	-15.32	88293	[11]	RPD & Ea -8 kcal	1,4-dioxane
P13	morpholine=OHCH2CH2NHCHCH2	6.231E+63	-14.83	85767	[11]	RPD & Ea -8 kcal	1,4-dioxane
P14	morpholine=CH3OCH2CH2NCH2	3.358E+15	0.37	82760	[10]	RPD & Ea -8 kcal	cyclohexane
P15	CH3CH2NHCH2CHO= CH3CH2NH+CH2CHO	1.464E+27	-3.03	78550	[10]	RPD	cyclohexane
P16	NH2CH2CH2OCHCH2= CH2CH2NH2+CH2CHO	1.464E+27	-3.03	78550	[10]	RPD	cyclohexane
P17	CH3CH2OCH2CHNH= C2H5O+CH2CHNH	1.464E+27	-3.03	78550	[10]	RPD	cyclohexane
P18	OHCH2CH2NHCHCH2= C2H4OH+CH2CHNH	1.464E+27	-3.03	78550	[10]	RPD	cyclohexane

P19	CH3OCH2CH2NCH2= CH3OCH2+CH2NCH2	1.464E+27	-3.03	78550	[10]	RPD	cyclohexane
P20	CH3CH2NHCH2CHO= CH3CHNH+CH2CHOH	3.981E+12	0.00	57392	[22]	RPD	1-hexene
P21	NH2CH2CH2OCHCH2= CH2CHNH+CH3CHOH	3.981E+12	0.00	57392	[22]	RPD	1-hexene
P22	CH3CH2OCH2CHNH= CH3CHO+CH2CHNH2	3.981E+12	0.00	57392	[22]	RPD	1-hexene
P23	OHCH2CH2NHCHCH2= CH2CHOH+CH3CHNH	3.981E+12	0.00	57392	[22]	RPD	1-hexene

Rate coefficients for morpholine will be different from those for cyclohexane or other 6-membered ring species, but the transition-state structures have useful similarities. There are six saturated heavy atoms (C, N, O) in the morpholine ring, so it is proposed that, by analogy with cyclohexane, morpholine oxidation in the shock tube occurs by O_2 addition to a radical site. The key difference is that while each hydrogen on a cyclohexane ring is symmetrically equivalent, morpholine has three different sites from which an H-atom may be abstracted: the carbon ortho to the ether oxygen, the meta carbon, and the para amine nitrogen. Thus, three distinct hydrogen-abstraction routes exist. Once an RO_2 morpholine species is formed, like in cyclohexane, the O_2 group can internally abstract a hydrogen atom from the ring and either form HO_2 + an unsaturated morpholine-ene cyclic species or one of several morpholine QOOH species. The resulting QOOH radicals can then undergo β-scission by ring-breaking, forming linear and branched, unsaturated radicals. The linear and branched radicals can undergo further β-scission reactions until small products with 2 to 3-heavy-atoms are formed. Reaction rate coefficients for the oxidation reactions for morpholine were derived based on analogous reactions from the cyclohexane model for oxidation [10].

Accounting for thermal decomposition of the ring requires assumptions about product channels and a rate constant based on the present data. There are no previous data in the literature, and the products and rate constants are not settled in the literature for similar ring species that might provide analogies. However, for cyclohexane, Tsang [22] detected only 1-hexene as an experimental product.

Initially, in this work the initial ring decomposition was assumed analogous to the mechanism proposed for 1,4-dioxane [11] and cyclohexane [10], modifying Arrhenius

pre-exponential factors for the proper reaction-path degeneracy (RPD). In the set of Ref [16], three decomposition routes were proposed from theoretical studies: 1) homolytic cleavage of the ring into three 2-heavy-atom species, 2) opening of the ring into a diradical species which can then internally abstract a hydrogen in a 6-centered transition state, then decomposing into two 3-heavy-atom radicals, and 3) 1,3-hydrogen shift reaction, breaking the ring into a 6-heavy-atom linear species with a single π bond at the end, such as the 1-hexene from cyclohexane observed by Tsang [22]. As proposed in a recent cyclohexane pyrolysis mechanism [10], the 6-heavy-atom linear species can also thermally dissociate into two 3-heavy-atom radicals.

Reaction rate coefficients for the oxidation and pyrolysis reactions for morpholine were generally derived based on analogous reactions from the cyclohexane [9] model for oxidation and cyclohexane [10] and 1,4-dioxane [11] models for pyrolysis, but with pre-exponential factors modified for the proper reaction path degeneracy (RPD). For the pyrolysis data, adopting these analogies resulted in much too slow morpholine consumption. Instead, the molecular product channels (to 1-hexene-like compounds, reactions P10-P14 in Table 9.2 were assumed to constitute the principal decomposition route, and the activation energies were empirically lowered by Δ=8 kcal/mol (from 90-96 kcal) to fit the experimental data.

Thermochemistry was calculated theoretically using the complete-basis-set method CBS-QB3 [23] for the 28 species introduced in [2], as well as five further species from the new pyrolysis reaction set and 41 additional species from the oxidation reaction set. Geometry and frequency calculations were completed with Gaussian 09 software [24] using the tight convergence criteria and rigid-rotor approximations. Thermochemistry

was estimated for an additional nine radical species for the oxidation set based on their non-radical analogues. The resulting reaction set is 290 species and 2130 reactions (see Appendix F). Shock tube simulations were performed using the Senkin code in ChemkinPro [25-26] assuming constant pressure and adiabatic conditions.

9.2 Results and discussion

9.2.1 Morpholine intermediates detected via laser diagnostics

In the chemiluminescence experiments, compared to the MBMS flame experiment, the flame is much closer to the burner, starting to plateau at around 3 mm away from the burner in the optical experiment as opposed to 6 mm in the MBMS flame. As a result, profiles are much closer to the burner surface than observed in the MBMS flame experiment at the same conditions. The experimental temperature profile and profiles for CH and CN radicals are shown in Fig. 9.1. CH, an important hydrocarbon

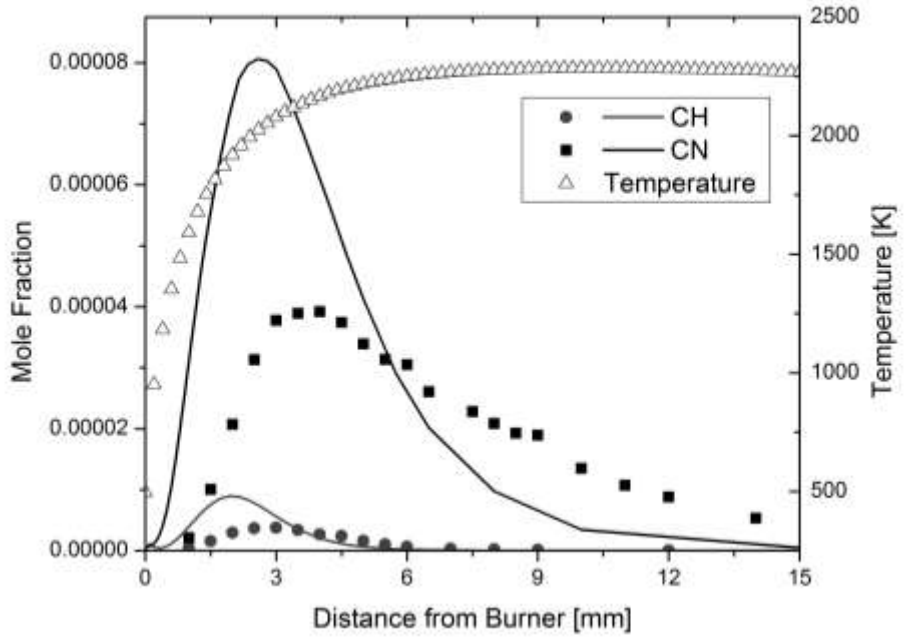

Figure 9.1: Experimental mole fraction profiles for CH and CN with modeling results. The experimental temperature profile is also given.

radical, has a peak mole fraction of approximately 4×10^{-6}. CN is also an important radical in the context of NO_x production and has an order of magnitude higher peak experimental mole fraction of 4×10^{-5}. For the model predictions (see Fig. 9.1), the profiles for CH and CN are both overpredicted only by about a factor of two.

The experimental profiles for HCO and NH_2 are presented in Fig. 9.2. HCO is an important precursor in CO production and peaks quite close to the burner (~1.5 mm) at about 2.5×10^{-4}. The model profile is also quite close to the burner but overpredicts the data to peak at 4×10^{-4}. The experimental profile for NH_2, another important NO_x precursor, is a much broader profile, peaking also at 2.5×10^{-4}. The model overpredicts this profile as well to peak at 4×10^{-4}, well within a factor of two.

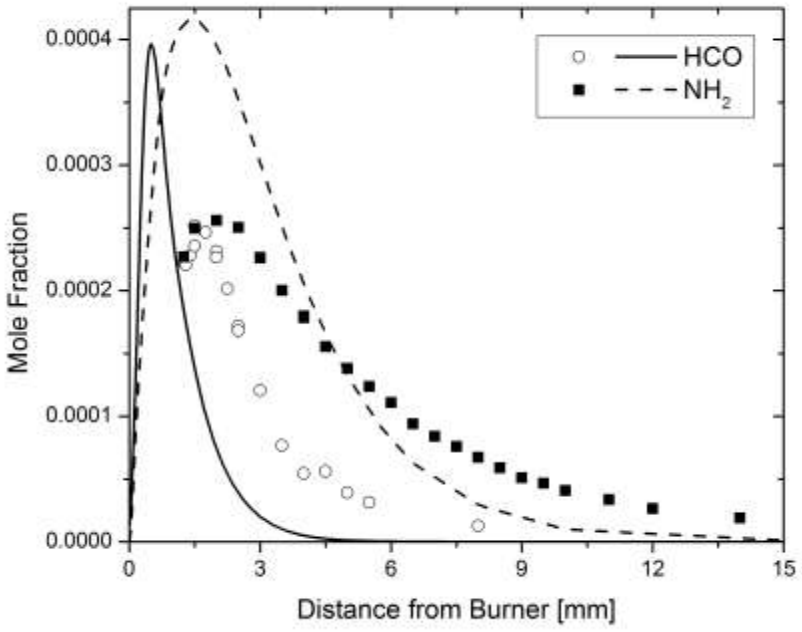

Figure 9.2: Experimental mole fraction profiles for HCO and NH_2 with model results.

A suggested error bound for this experiment is approximately 25%; however, the true experimental error may be larger. The EI-MBMS experiment was performed on the same apparatus as the optical experiment, differing only in the use of a probe. Relative peaks of the same species should be comparable, though shifts between the two sets of data would be expected. In contrast to the peak mole fraction observed in the optical experiment (2.5×10^{-4}), the EI-MBMS peak mole fraction was found to be 5.0×10^{-4}, a factor of two higher, suggesting the errors may be in reality at least a factor of two or higher. This difference suggests that the model results, though appearing to be overpredicted, are in reality quite reasonable.

9.2.2 Morpholine pyrolysis

Morpholine pyrolysis experiments were carried out in 5000 ppm morpholine/argon mixtures. A 3.39 μm He-Ne laser was used to monitor the initial fuel concentration and fuel-decomposition time histories. Because the pyrolysis products can also absorb at 3.39 μm, the same assumption as in [27] that the interfering products form at the same rate as the fuel decays was made to correct the time histories. In other words, the pyrolysis process was modeled using the following overall reaction

$$\text{Morpholine} \rightarrow \text{products} \tag{9.1}$$

With this assumption and the ideal gas law, the fuel mole fraction can be determined from Eq. 9.2

$$X_{fuel}(t) = \frac{\alpha_{meas}(t)-\alpha_{meas}(\infty)}{\alpha_{meas}(0)-\alpha_{meas}(\infty)} X_{fuel}(0) \tag{9.2}$$

where α(t) is the absorbance. The morpholine mole fraction time histories determined using Eq. 9.2 are shown in Fig. 9.3. The temperature range of the pyrolysis study is 1086-1404 K with a pressure range 20-23.6 atm.

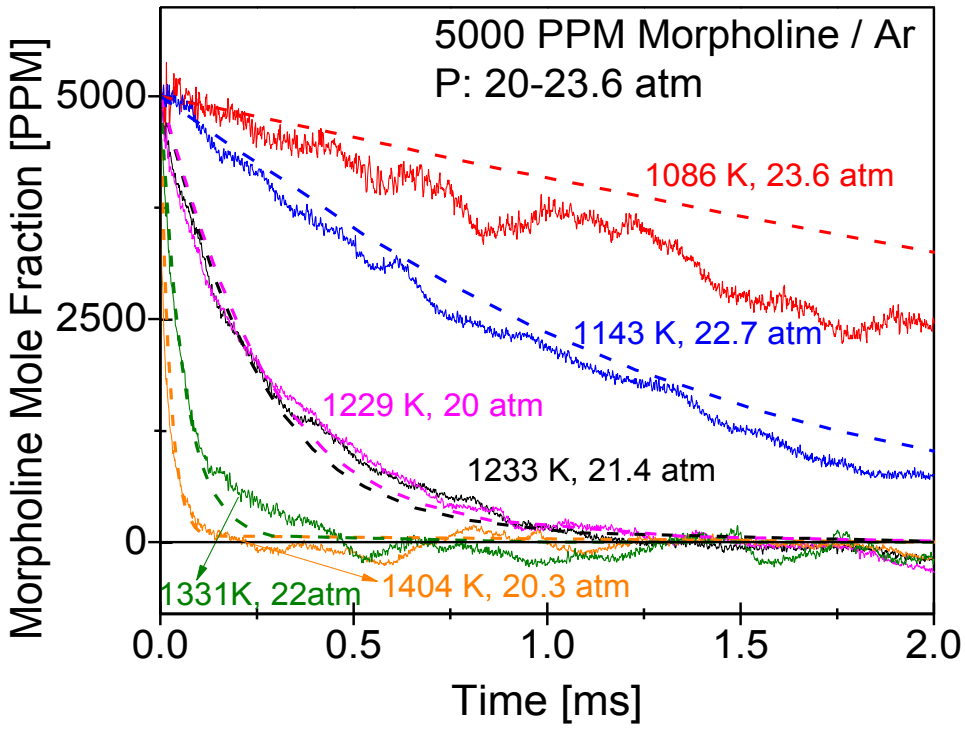

Figure 9.3: Morpholine decay time histories in 5000 ppm morpholine/argon mixtures in the temperature range of 1086-1404 K and pressure range 20-23.6 atm compared to model predictions. Dashed lines: simulation results using current reaction set.

The fuel decay curves were fitted using an exponential decay equation: $y = A \cdot exp(-kt) + C$ to get the overall removal rate for morpholine at different temperatures. The Arrhenius plot for the overall morpholine removal rate is shown in Fig. 9.4, with a best linear fit to the experimental data (R^2=0.97). The following rate constant (20-23.6 atm, 1086-1404 K) was determined for the overall morpholine removal rate:

$$k = 1.42 \times 10^{12} \exp\left(-\frac{49.5 \pm 8\%(1\sigma)\left[\frac{kcal}{mol}\right]}{RT}\right) s^{-1} \quad (9.3)$$

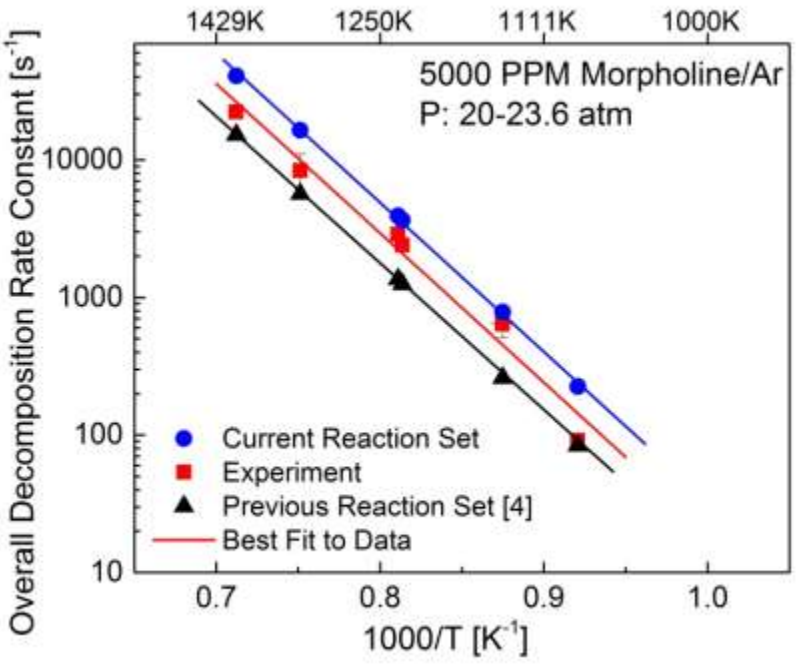

Figure 9.4: Arrhenius plot for the overall morpholine removal rate (20-23.6 atm, 1086-1404 K).

In Fig. 9.3, the model predictions are shown as dashed lines for morpholine-pyrolysis time histories in 5000-ppm morpholine/argon mixtures, together with the shock tube experimental data. The adjustable parameter Δ was varied from 0 to 11 kcal/mol, giving an optimum prediction among the different data sets at 8 kcal/mol. The simulation results using the current reaction set and thermochemistry data then match with experiments very well at all temperatures. Likewise, the sum of rate-constant values for P10-P14 in Table 9.2 gives points that agree well with the direct Arrhenius fit in Eq. 9.3. Because only morpholine consumption was measured, verification that the model predicts accurate product channels will have to come from future work by product speciation and/or theory.

9.2.3 Morpholine oxidation

Ignition delay times were measured during morpholine oxidation experiments under different conditions behind the reflected shock waves and are shown in Figs. 9.5-7 and listed in Table 9.3.

Table 9.3: Shock tube ignition delay times. Test gas mixture: morpholine/O_2/argon.

T_5 [K]	$1000/T_5$ [1/K]	P_5 [atm]	Φ	X_{O2}	IDT [μs]
1097	0.912	13.02	1	0.21	115
1062	0.942	13.77	1	0.21	197
1009	0.991	14.04	1	0.21	374
938	1.066	14.66	1	0.21	1000
910	1.099	14.71	1	0.21	1350
966	1.035	14.79	1	0.21	636
925	1.081	15.83	1	0.21	1070
915	1.093	15.76	1	0.21	1130
1168	0.856	12.53	0.5	0.21	97
1110	0.901	13.19	0.5	0.21	192
1023	0.978	13.37	0.5	0.21	547
983	1.017	13.94	0.5	0.21	1030
921	1.086	13.79	0.5	0.21	1970
875	1.143	16.45	2	0.21	969
901	1.110	16.60	2	0.21	775
935	1.070	16.29	2	0.21	562
965	1.036	15.25	2	0.21	402
994	1.006	16.13	2	0.21	223
1041	0.961	15.08	2	0.21	136
1197	0.835	15.56	1	0.04	145
1139	0.878	15.94	1	0.04	244
1091	0.917	16.30	1	0.04	430
1042	0.960	16.64	1	0.04	845
1027	0.974	16.50	1	0.04	1150
1074	0.931	26.36	1	0.21	82
1046	0.956	27.05	1	0.21	117

994	1.006	27.02	1	0.21	241
986	1.014	26.70	1	0.21	279
955	1.047	29.18	1	0.21	389
932	1.073	25.21	1	0.21	625
917	1.091	13.42	0.5	0.21	2130
910	1.099	14.10	0.5	0.21	2210
899	1.112	14.70	0.5	0.21	2310
882	1.134	14.97	0.5	0.21	3260
878	1.139	14.66	0.5	0.21	4270
869	1.151	13.76	0.5	0.21	4600
870	1.149	15.42	0.5	0.21	5480
866	1.155	14.64	0.5	0.21	5680

In Fig. 9.5, ignition delay times in morpholine/air mixtures at pressure near 15 atm are shown for different equivalence ratios. The stoichiometric case was defined with the following reaction:

$$C_4H_9NO + 5.75(O_2 + 3.76N_2) \rightarrow 4CO_2 + 4.5H_2O + 22.62N_2 \qquad (9.4)$$

As can be seen from Fig. 9.5, in morpholine/air mixtures, when other conditions are held the same, auto-ignition occurs faster with increasing equivalence ratio. The model predictions for the morpholine oxidation system are shown using dashed lines in Figs. 9.5-8, to be compared with the shock tube experiment data. As can be seen in Fig. 9.5, for the equivalence ratio dependence of the ignition delay time, the current reaction model captures the same trend as the experiment. Also shown in the figure are the simulation results using the reaction set of [2], represented by solid lines. It is evident that the current model matches much better with the experimental data than the model in [2] because of the addition of the O_2 addition chemistry. The current reaction set is quite good at equivalence ratio 0.5 but overpredicts the ignition delay times as richness increases.

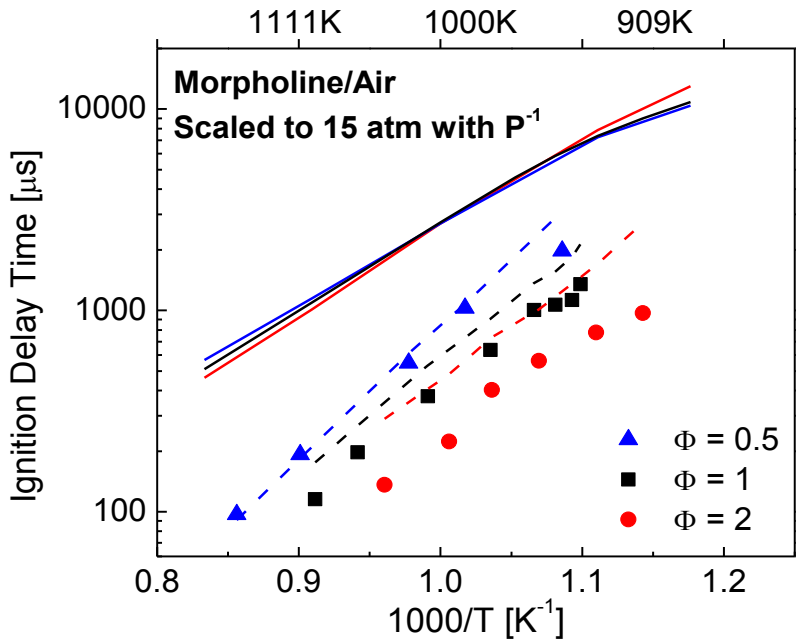

Figure 9.5: Comparison of model predictions to morpholine/air ignition delay time measurements around 15 atm and with equivalence ratios of 0.5, 1 and 2. Solid lines: simulation results using the previous reaction set [2]. Dashed lines: simulation results using current reaction set.

The ignition delay times in morpholine/air mixtures are shown in Fig. 9.6 for an equivalence ratio of 1 and pressures around 15 and 25 atm. The ignition delay time near 25 atm is shorter than that near 15 atm, as expected. Also shown in Fig. 9.6 are the simulated ignition delay times at 15 and 25 atm, using both the current reaction set (dashed lines) and reaction set published in [2] (solid lines). Significant improvement is evident in the modeling results using the current reaction set.

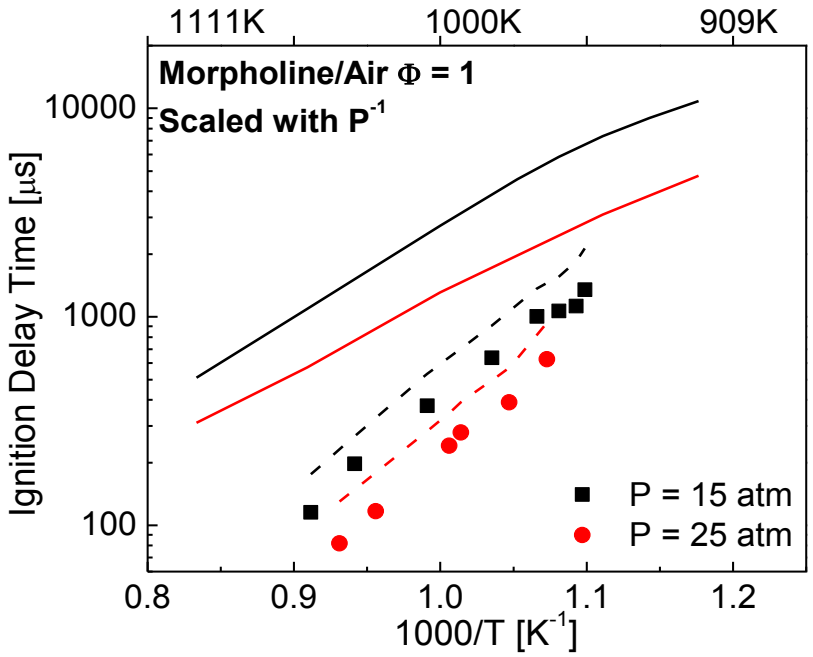

Figure 9.6: Comparison of model predictions to morpholine/air ignition delay time measurements for stoichiometric mixtures around 15 and 25 atm respectively. Solid lines: simulation results using the previous reaction set [2]. Dashed lines: simulation results using current reaction set.

To study the effects of oxidizer concentration, ignition delay times were measured in morpholine/4% O_2/argon mixtures as well, and compared with morpholine/air mixtures in Fig. 9.7. The ignition delay time decreases with increasing oxygen concentration. The model predicted influence of oxidizer concentration on ignition delay time can be also seen in Fig. 9.7. The current model is quite good but still overpredicts the ignition delay times by about 50% in stoichiometric morpholine mixtures with 4% O_2 or 21% O_2, while the reaction set used in [2] overpredicts by a factor of 5. Future experimental and modeling work will need to be be carried out to improve the reaction set further.

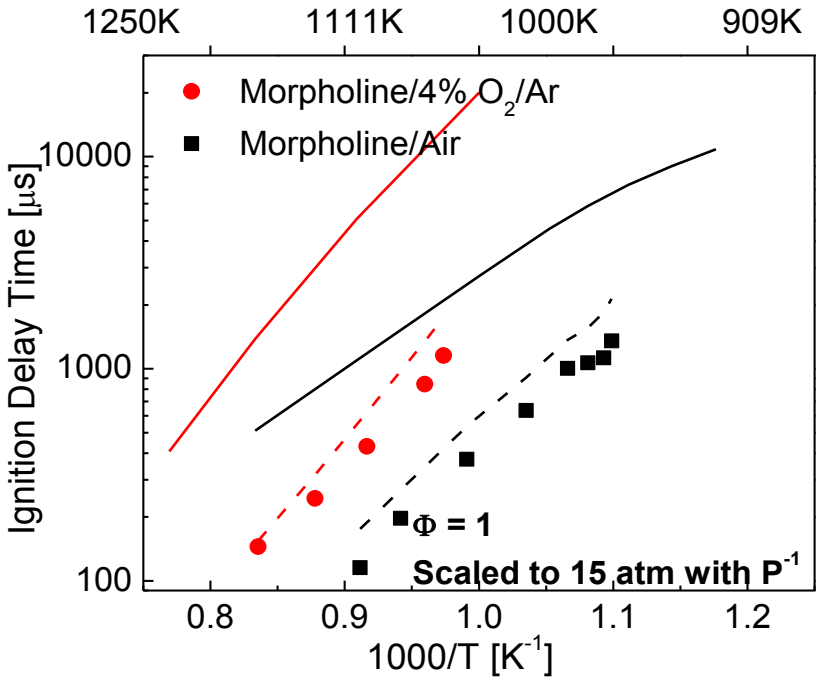

Figure 9.7: Comparison of model predictions to morpholine ignition delay time measurements around 15 atm for morpholine/4% O_2/argon and morpholine/air mixtures. Solid lines: simulation results using the previous reaction set [2]. Dashed lines: simulation results using current reaction set.

A regression analysis was carried out based on all the experimental data reported in this section, and the following scaling relation was found for morpholine ignition delay time

$$\tau \sim \phi^{-0.8} P^{-0.9} {x_{O2}}^{-0.84} \tag{9.5}$$

over a range of temperatures of 866-1197 K, of pressures 15-25 atm, and of equivalence ratios 0.5-2.

9.3 Summary and Conclusions

Several different experiments were conducted using laser diagnostic techniques for morpholine combustion. In one experiment, chemiluminescence was employed to capture the mole fraction profiles for important intermediate reactants CH, CN, HCO,

and NH_2 on a flame identical to the EI-MBMS flame experiments discussed in Chapter 8. Experimental profiles were much closer to the burner in the unperturbed optical flame than in the MBMS flame experiment. The difference between peak mole fractions for HCO in both experiments was a factor of two, suggesting at least a factor of two experimental error. The modeling results using the model from Chapter 8 is well within the factor of two bounds, though it over predicts all four radical species.

Morpholine pyrolysis was studied in 5000 ppm morpholine/argon mixtures behind reflected shock waves at temperatures from 1086 to 1404 K and pressures 20-23.6 atm. An IR He-Ne laser at 3.39 μm was used to measure morpholine concentration time-histories assuming that interfering products form at the same rate as morpholine decays. Ignition delay times were measured under a wide range of conditions in the same shock tube, covering temperatures form 866 to 1197 K, equivalence ratios of 0.5, 1 and 2, two pressure groups (around 15 and 25 atm) and two oxygen concentration values (4% O_2 and 21% O_2). The current shock tube work extended the morpholine combustion experimental database.

The morpholine reaction set originally developed for low-pressure flames in [2] significantly overpredicts the fuel decay and ignition delay times under all conditions. With the current updated set, though, the model predictions match with the measured fuel-decomposition time histories quite well for the pyrolysis experiments. In terms of ignition delay time results, current model predictions match much better with the experimental data than when using the previous mechanism developed in [2] and can successfully capture the equivalence ratio dependence near 15 atm. Future shock-tube

measurements of different species time histories will help to further improve the current reaction set for even better agreement with experimental data.

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CHAPTER 10

HYPERGOLIC ROCKET FUELS: MODELING THE CHEMISTRY OF MONOMETHYLHYDRAZINE + RED FUMING NITRIC ACID

In continuing the trend of exploring nitrogen-containing fuels, several hypergolic rocket propellants have been developed for use in rocket thrusters [1-3]. Hypergolicity implies that ignition occurs upon contact of the fuel and oxidizer, requiring no ignitor. Many of these fuels have high amounts of fuel nitrogen and are often amine-based compounds, furfurylidine ketones, tetraformaltrisazines, and phenyl- and dimethyl-hydrazones [4]. The drawback of using hypergolic propellants is that they are hazardous materials. Hydrazine is known to be a toxic substance and has been identified as an environmental contaminant and pollutant [5]. Monomethyl hydrazine (CH_3NHNH_2) is a popular hypergolic fuel choice, but it is lethal at high exposure and is thought to be carcinogenic when exposed long-term [6].

Despite the environmental and health concerns, hypergolic fuels are particularly attractive for use in rockets. Hypergolicity is also useful in space applications, where engines are used primarily for directional steering and are needed in short small bursts. A potential approach is that the fuel be gelled, the splash hazard to workers and averting vaporization of the fuel in the case of a leak, which would greatly reduce the dangers of accidental rocket ignition.

Previous work on hypergolic rocket-fuel combustion has been limited. Much of the work has been in the context of hydrazine as another hypergolic propellant [7-9], with some additional work on unsymmetrical dimethyl hydrazine (UDMH) [10]. Catoire et al. produced a reaction set for monomethyl hydrazine (MMH) combustion and characterized

the fuel experimentally, though much of the work was for combustion with oxygen [11-14]. The work of Catoire et al. was expanded by the theoretical kinetics work of Sun et al. for better kinetic rate constant calculation for several MMH combustion reactions [3, 15-17]. A second reaction set for MMH combustion has been proposed as well via Army Research Laboratories [1]. Lastly, a study for MMH pyrolysis in a shock tube was reported in [18].

In this chapter, combustion of monomethyl hydrazine (MMH) with red fuming nitric acid is examined to determine the chemistry of combustion. The intent is to shed light on why MMH is hypergolic and to introduce alternative hypergols that are potentially less toxic and non-carcinogenic. Additionally, the reaction set is refined to reduced sets for use in computational fluid dynamics (CFD) codes.

10.1 Justification for focus on gas-phase chemistry

In hypergolic rocket engines, ignition and reaction is assumed to occur spontaneously when a droplet of fuel makes contact with an oxidizer droplet. In the context of this study, the fuel is a gelled monomethyl hydrazine (MMH; mixture contains ~94-97% MMH, 3-6% gelling agent) and the oxidizer is red fuming nitric acid (RFNA; ~84% HNO_3, ~13% N_2O_4, ~3% H_2O). The chemistry in these hypergolic rockets may be described in three categories, the first of which is liquid-liquid chemistry. The liquid-liquid chemistry occurs as a droplet of oxidizer mixes with a droplet of fuel. It is proposed that reaction in mixed liquid phase is nearly instantaneous. The second category is liquid-gas chemistry. Once enough heat is generated to vaporize some of the oxidizer or fuel, the vapor phase can react with the surfaces of droplets. This reaction is

thought to be mass-transfer-limited chemistry. The last category of chemistry is the gas-phase chemistry, which is thought to dominate reaction.

To test the theory that gas-phase chemistry dominates in hypergolic rocket engines due to the fast, highly exothermic liquid-liquid chemistry, the following estimation for heat release is proposed.

10.1.1 Ideal reaction of MMH with RFNA

RFNA is a composite of HNO_3, N_2O_4, and water. Ideal stoichiometric reaction of MMH with RFNA follows:

$$CH_3NHNH_2 + 2\ HNO_3 \Leftrightarrow CO_2 + 4\ H_2O + 2\ N_2 \qquad (10.1)$$

$$4\ CH_3NHNH_2 + 5\ N_2O_4 \Leftrightarrow 4\ CO_2 + 12\ H_2O + 9\ N_2 \qquad (10.2)$$

With a proposed RFNA composition of 84% HNO_3, 13% N_2O_4, and 3% H_2O, the overall reaction becomes

$$CH_3NHNH_2 + 1.9084\ RFNA \Leftrightarrow CO_2 + 3.859\ H_2O + 2.050\ N_2 \qquad (10.3)$$

From this an estimated heat of reaction for a stoichiometric mixture of MMH and RFNA can be calculated. Table 10.1 contains a list of necessary physical parameters for these calculations for all reactants and products.

Table10. 1: Physical parameters for reactants and products

Species	Molecular Weight	Density	T_b	Heat of Formation	Heat of Vaporization	Thermal Conductivity
	g/mol	kg/m^3	C	kJ/mol	kJ/kg	W/m-K
MMH	46.072	874[19]	87.5[19]	54.1[19]	709 ± 5[19]	0.246[19]
HNO_3	63.013	1480[20]	100[20]	-207.36[21]	620.51[22]	
N_2O_4	92.011	1477[19]	21.15[19]	-19.564[19]	413[19]	0.131[19]
H_2O	18.015	997[21]	100[21]	-285.83[21] (l) -241.82[21] (g)	2259.2[21]	0.5606[23]
CO_2	44.010			-393.51[21]	573.28[21]	
N_2	28.013	1.25[22]	-195.79[22]	-	-	0.02583[22]

From these values, the heat of reaction per mole of MMH for a stoichiometric mixture of MMH and RFNA can be estimated as follows.

$$\Delta H_{rxn} = \sum_n^{prod} x_n H_{f,n}^{\circ} - \sum_m^{rxt} H_{f,m}^{\circ} \tag{10.4}$$

$$\sum_n^{prod} x_n H_{f,n}^{\circ} =$$

$$\left(-393.51\,\frac{kJ}{mol}\right) + 3.859 * \left(-241.82\,\frac{kJ}{mol}\right) + 2.050 * 0\,\frac{kJ}{mol}$$

$$\sum_n^{prod} x_n H_{f,n}^{\circ} = -1327\,\frac{kJ}{mol} \tag{10.5}$$

$$\sum_n^{rxt} x_n H_{f,n}^{\circ} = 54.1\,\frac{kJ}{mol} + 1.603 * \left(-207.36\,\frac{kJ}{mol}\right)$$

$$+0.248 * \left(-19.564\,\frac{kJ}{mol}\right) + 0.057 * \left(-241.82\,\frac{kJ}{mol}\right)$$

$$\sum_n^{rxt} x_n H_{f,n}^{\circ} = -297\,\frac{kJ}{mol} \tag{10.6}$$

$$\Delta H_{rxn} = -1030\,\frac{kJ}{mol} \tag{10.7}$$

Likewise, the heat of vaporization of MMH and RFNA can be calculated.

$$\Delta H_{vap,MMH} = 709\,\frac{kJ}{kg} * 0.001\,\frac{kg}{g} * 46.072\,\frac{g}{mol} = 32.67\,\frac{kJ}{mol} \tag{10.8}$$

$$\Delta H_{vap,HNO3} = 620.51\,\frac{kJ}{kg} * 0.001\,\frac{kg}{g} * 63.013\,\frac{g}{mol} = 39.10\,\frac{kJ}{mol} \tag{10.9}$$

$$\Delta H_{vap,N2O4} = 413\,\frac{kJ}{kg} * 0.001\,\frac{kg}{g} * 92.011\,\frac{g}{mol} = 38.00\,\frac{kJ}{mol} \tag{10.10}$$

$$\Delta H_{vap,H2O} = 2259.2\,\frac{kJ}{kg} * 0.001\,\frac{kg}{g} * 18.015\,\frac{g}{mol} = 40.70\,\frac{kJ}{mol} \tag{10.11}$$

$$\Delta H_{vap,RFNA} = 0.84 * \Delta H_{vap,HNO3} + 0.13 * \Delta H_{vap,N2O4}$$

$$+0.03 * \Delta H_{vap,H2O}$$

$$\Delta H_{vap,RFNA} = 39.01\,\frac{kJ}{mol} \tag{10.12}$$

10.1.2 Comparison of estimated MMH properties to CFD model.

An adaptive gridding code has been developed in the Schmidt group at UMass to model the mixing of 2 droplets. In this code, the average cell size is on the order of 10^{-15} m^3. Looking at an individual cell basis, heat release for a cell with a stoichiometric mixture of fuel and oxidizer can be estimated.

$$\rho_{MMH\ drop} = 10^{-15} m^3 * 874 \frac{kg}{m^3} * 1000 \frac{g}{kg} * \frac{1}{46.072} \frac{mol}{g}$$

$$= 1.897 * 10^{-11} \frac{mol}{m^3} \quad (10.13)$$

$$\rho_{HNO3\ drop} = 10^{-15} m^3 * 1480 \frac{kg}{m^3} * 1000 \frac{g}{kg} * \frac{1}{63.013} \frac{mol}{g}$$

$$= 2.349 * 10^{-11} \frac{mol}{m^3} \quad (10.14)$$

$$\rho_{N2O4\ drop} = 10^{-15} m^3 * 1477 \frac{kg}{m^3} * 1000 \frac{g}{kg} * \frac{1}{92.011} \frac{mol}{g}$$

$$= 1.605 * 10^{-11} \frac{mol}{m^3} \quad (10.15)$$

$$\rho_{H2O\ drop} = 10^{-15} m^3 * 997 \frac{kg}{m^3} * 1000 \frac{g}{kg} * \frac{1}{18.015} \frac{mol}{g}$$

$$= 5.534 * 10^{-11} \frac{mol}{m^3} \quad (10.16)$$

$$\rho_{RFNAdrop} = 0.84 * \rho_{HNO3} + 0.13 * \rho_{N2O4} + 0.03 * \rho_{H2O}$$

$$= 2.348 * 10^{-11} \frac{mol}{m^3} \quad (10.17)$$

$$\rho_{stoich\ drop} = \frac{1}{2.9084} \rho_{MMH} + \frac{1.9084}{2.9084} \rho_{RFNA}$$

$$= 2.193 * 10^{-11} \frac{mol}{m^3} \quad (10.18)$$

$$\Delta H_{rxn\ per\ cell} = -1030 \frac{kJ}{mol\ MMH} * \frac{1}{2.9084} \frac{mol\ MMH}{mol\ stoich} * 2.193 * 10^{-11} \frac{mol}{m^3}$$

$$\Delta H_{rxn\ per\ cell} = -7.766 * 10^{-9} \frac{kJ}{m^3} \quad (10.19)$$

$$H_{vap\ MMH\ cell} = 32.67\frac{kJ}{mol} * 1.897 * 10^{-11}\frac{mol}{m^3}$$

$$= 6.198 * 10^{-10}\frac{kJ}{m^3} \quad (10.20)$$

$$H_{vap\ RFNA\ cell} = 39.01\frac{kJ}{mol} * 2.348 * 10^{-11}\frac{mol}{m^3}$$

$$= 9.160 * 10^{-10}\frac{kJ}{m^3} \quad (10.21)$$

$$H_{vap\ stoich\ cell} = \frac{\left(32.67\frac{kJ}{mol} + 1.9084 * 39.01\frac{kJ}{mol}\right)}{2.9084} * 2.193 * 10^{-11}\frac{mol}{m^3}$$

$$H_{vap\ stoich\ cell} = 8.077 * 10^{-10}\frac{kJ}{m^3} \quad (10.22)$$

The heat release can then be compared to the heat necessary to vaporize droplets of the same size, indicating how much mixing would would need to occur before enough heat is generated to vaporize droplets.

For MMH: $\frac{H_{vap\ MMH\ cell}}{H_{rxn\ per\ cell}} = \frac{6.198 * 10^{-10}\frac{kJ}{m^3}}{7.366 * 10^{-9}\frac{kJ}{m^3}} = 0.080$ (10.23)

For RFNA: $\frac{H_{vap\ RFNA\ cell}}{H_{rxn\ per\ cell}} = \frac{9.160 * 10^{-10}\frac{kJ}{m^3}}{7.366 * 10^{-9}\frac{kJ}{m^3}} = 0.118$ (10.24)

For stoichiometric cell: $\frac{H_{vap\ stoich\ cell}}{H_{rxn\ per\ cell}} = \frac{8.077 * 10^{-10}\frac{kJ}{m^3}}{7.366 * 10^{-9}\frac{kJ}{m^3}} = 0.104$ (10.25)

Because MMH degrades over time, heat of vaporization can be recalculated using the same numbers if 65% of the MMH is degraded. Density and heat of vaporization for the degraded MMH solution are assumed the same as MMH itself. The results are:

$$\rho_{stoich\ drop\ 65\%} = \frac{1}{1 + 0.35 * 1.9084}\rho_{MMH} + \frac{0.35 * 1.9084}{1 + 0.35 * 1.9084}\rho_{RFNA}$$

$$\rho_{stoich\ drop\ 65\%} = 2.077 * 10^{-11}\frac{mol}{m^3} \quad (10.26)$$

$$\Delta H_{rxn\ per\ cell\ 65\%} =$$

$$-1030\,\frac{kJ}{mol\ MMH} * \frac{0.35}{1+0.35*1.9084}\,\frac{mol\ MMH}{mol\ stoich} * 2.077 * 10^{-11}\,\frac{mol}{m^3}$$

$$\Delta H_{rxn\ per\ cell\ 65\%} = -4.489 * 10^{-9}\,\frac{kJ}{m^3} \tag{10.27}$$

$$H_{vap\ stoich\ cell\ 65\%} = \frac{\left(32.67\frac{kJ}{mol}+0.35*1.9084*39.01\frac{kJ}{mol}\right)}{1+0.35*1.9084} * 2.077 * 10^{-11}\,\frac{mol}{m^3}$$

$$H_{vap\ stoich\ cell\ 65\%} = 7.313 * 10^{-10}\,\frac{kJ}{m^3} \tag{10.28}$$

For MMH 65%: $\frac{H_{vap\ MMH\ cell}}{H_{rxn\ per\ cell\ 65\%}} = \frac{6.198*10^{-10}\frac{kJ}{m^3}}{4.489*10^{-9}\frac{kJ}{m^3}} = 0.138$ (10.29)

For RFNA 65%: $\frac{H_{vap\ RFNA\ cell}}{H_{rxn\ per\ cell\ 65\%}} = \frac{9.160*10^{-10}\frac{kJ}{m^3}}{4.489*10^{-9}\frac{kJ}{m^3}} = 0.204$ (10.30)

For stoichiometric cell 65%: $\frac{H_{vap\ stoich\ cell\ 65\%}}{H_{rxn\ per\ cell\ 65\%}} = \frac{7.313*10^{-10}\frac{kJ}{m^3}}{4.489*10^{-9}\frac{kJ}{m^3}} = 0.163$ (10.31)

From these calculations it is estimated that 12-21% mixing would have to occur before enough heat would be generated to vaporize the fuel and oxidizer. As a visual, percent of mixing can be related to a scalar mixing coefficient, α, used in the droplet collision code developed by the Schmidt group at the University of Massachusetts Amherst. In their code, α = 1 represents a completely unmixed system and α =0 represents a completely mixed system. In Fig. 10.1 are snapshots for both head-on and oblique collisions of two drops at 10% mixing (α = 0.9). This extent of mixing is at the lower threshold for total vaporization.

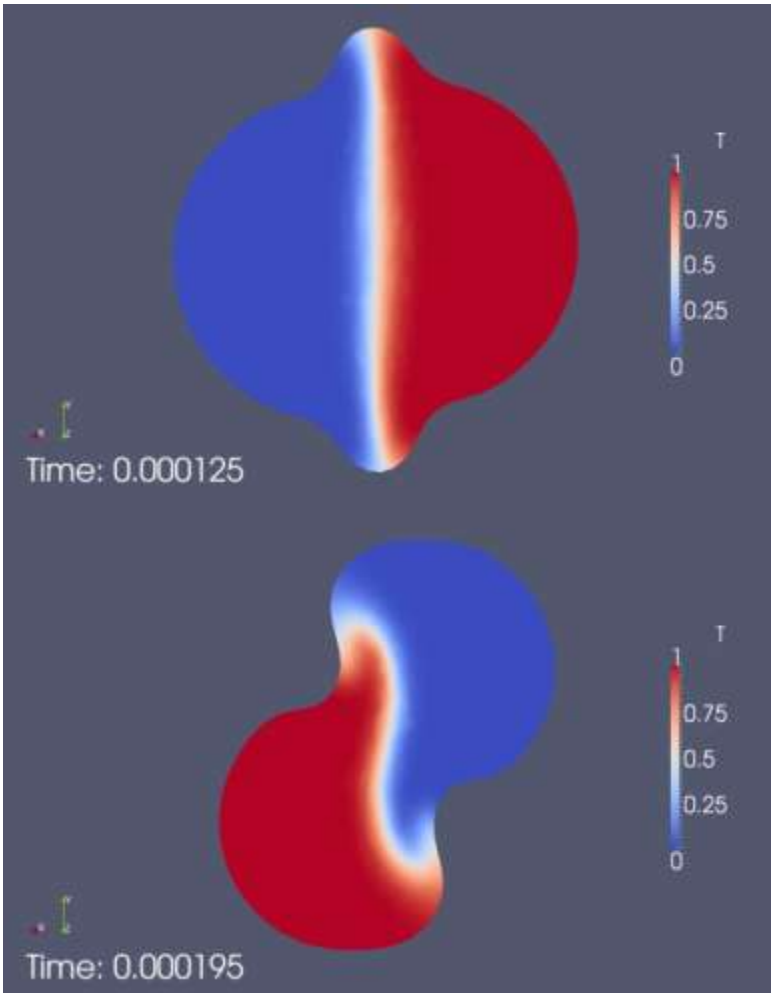

Figure 10.1: Snapshots of the Schmidt droplet mixing code for head-on and oblique droplet collisions at α = 0.9 (10% overall mixing). [Kyle Mooney Personal Communication 2011]

10.2 Development of an MMH/RFNA reaction set

In this study, a MMH/RFNA reaction set was developed, building from the base H/C/N/O mechanism of Chapter 6. Additional reactions for MMH combustion were added from the reaction set proposed by researchers at the Army Research Laboratories [1] as well as the kinetics calculated for MMH pyrolysis from Sun et al. [3]. The decomposition of MMH via hydrogen abstraction can follow three routes, as seen in Fig. 10.2: Abstraction from the methyl group, abstraction from the central nitrogen atom, and

abstraction from the terminal nitrogen atom. In the ARL reaction set, the only abstraction route considered was the abstraction of the hydrogen atom from the central nitrogen atom. Direct hydrogen abstractions from the methyl group or the terminal nitrogen were neglected. In the Sun reaction set, these routes were included, but given the nature of the study being for pyrolysis, several key abstraction partners were neglected. To account for the missing abstraction routes using the rates from Sun et al. [3], linear free energy relationships were used here to estimate the kinetics for the missing abstraction reactions. The resulting new reaction set is comprised of 177 species and 1619 reactions (see Appendix G).

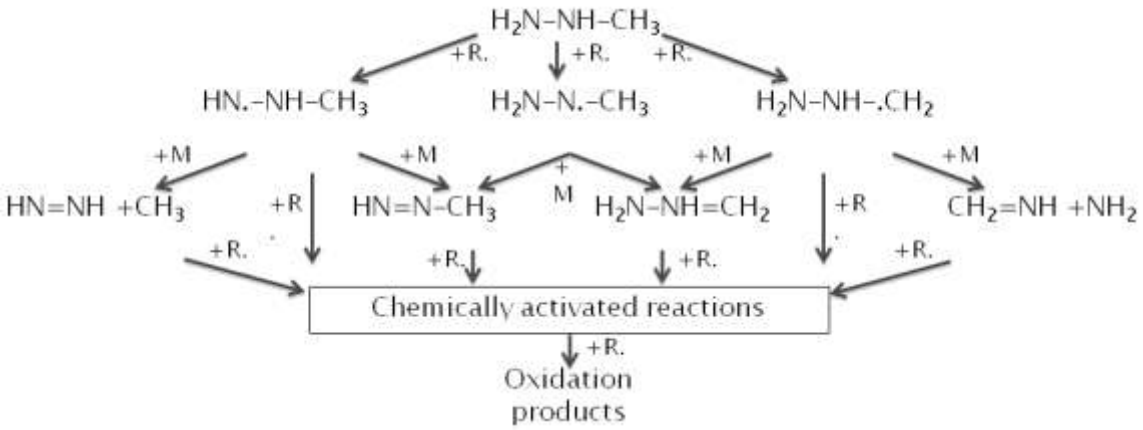

Figure 10.2: Reaction mechanism showing possible hydrogen abstraction routes for MMH combustion and their subsequent products.

10.3 Testing of the MMH/RFNA model

To test the new reaction set, combustion of MMH with RFNA was modeled using an adiabatic, constant-pressure, perfectly stirred reactor using the Chemkin PRO code [24]. Starting temperatures were slightly elevated to 600 K to aid ignition. The following is a discussion of the modeling results and their implications for model reductions for use in CFD codes.

10.3.1 Base case test: 1 atm stoichiometric MMH/RFNA ignition

As a base case, a stoichiometric ($\Phi = 1$) MMH/RFNA mixture was modeled in a zero-D reactor. Figure 10.3 shows the resulting mole fractions of the major species in the stoichiometric flame versus time. Reactants HNO_3 and MMH are consumed within the first 100 μs of reaction, and products NO, N_2, H_2O, and CO are being formed. NO_2 was found to be a significant intermediate species, resulting from immediate fissure of N_2O_4 to 2 NO_2, growing through secondary reactions, and eventually being consumed as an abstraction partner and conversion to NO and N_2.

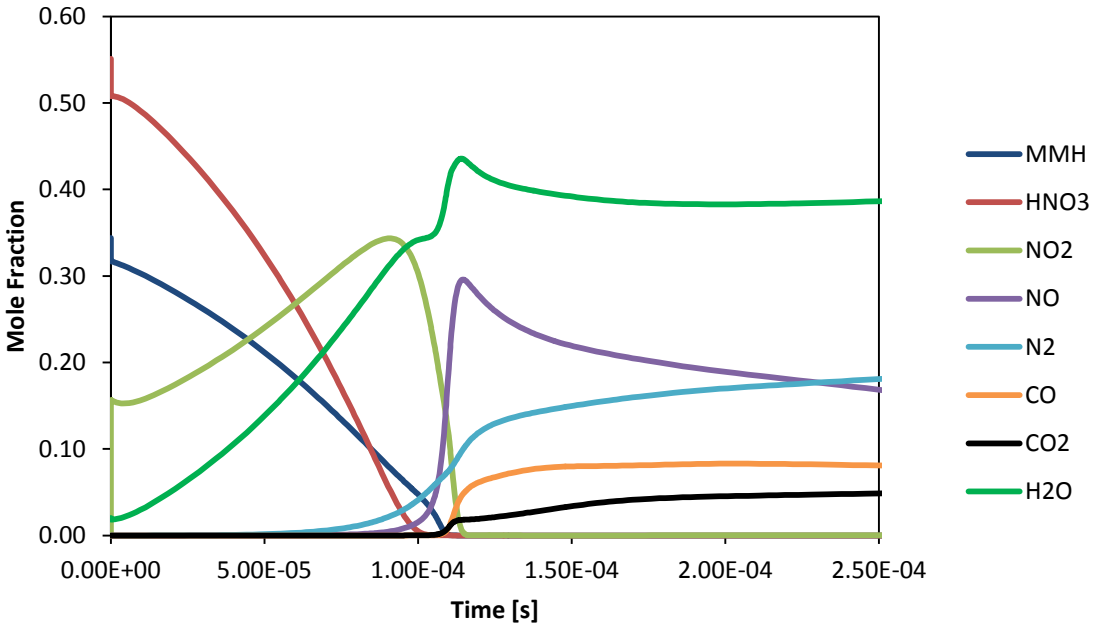

Figure 10.3: Time history profiles for major reactants and products in stoichiometric, P = 1 atm MMH/RFNA igniton.

Study of the reaction flux diagram (Fig. 10.4) shows the dominant reaction pathway for MMH/RFNA. NO_2, as stated before, is initially formed by the rapid decomposition of N_2O_4 at low temperatures. As the system heats up, HNO_3 predominantly decomposes into OH and additional NO_2. MMH is first attacked by a

radical, R, to form CH_3-$N^{\cdot}$-NH_2, which is further attacked by another radical to form CH_3NNH. Often the abstraction partner is NO_2, forming HONO. Once formed, HONO then decomposes to form NO and regenerate OH radicals. The CH_3NNH is attacked once again by a radical abstraction partner to form CH_3NN. CH_3NN decomposes into CH_3 and N_2. The methyl radical then undergoes subsequent reactions to form CO.

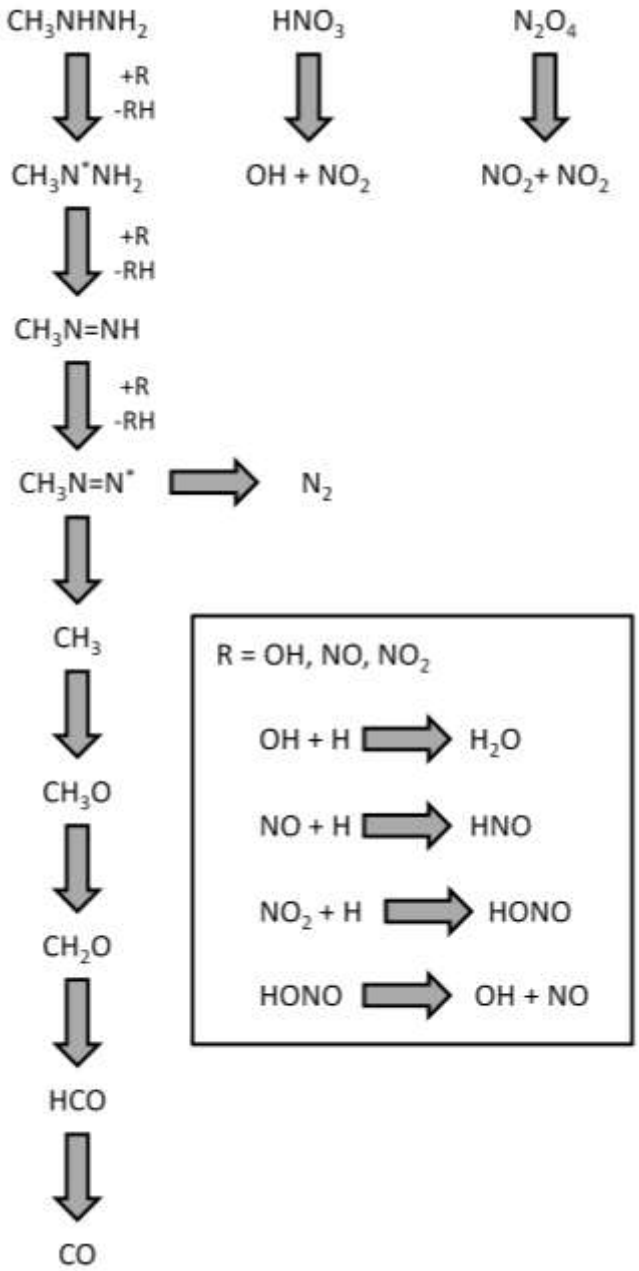

Figure 10.4: Dominant reaction pathways for MMH/RFNA stoichiometric combustion.

10.3.2 Trends with change in stoichiometry

In combustion in real engines, the fuel and oxidizer are not always perfectly mixed. Instead there are regions where the gas mixture is fuel-lean and others where the mixture is fuel-rich. It is thus necessary to examine the mechanism at varying conditions then to observe its performance. Modeling tests were run at conditions identical to the base-case stoichiometric reactor at P = 1 atm, this time varying the compositions from fuel-lean to fuel-rich (Φ = 0.8 to 1.3). Mixture compositions may be found in Table 10.2.

Table 10.2: Fuel/oxidizer compositions for different fuel equivalence ratios.

Φ	x_{MMH}	x_{HNO3}	x_{N2O4}	x_{H2O}
0.8	0.2863	0.5995	0.0928	0.0214
0.9	0.3163	0.5743	0.0889	0.0205
1.0	0.3438	0.5512	0.0853	0.0197
1.15	0.3812	0.5198	0.0804	0.0186
1.3	0.4146	0.4917	0.0761	0.0176

Model results as a function of fuel equivalence ratio are presented in Figs. 10.5-10. For the base case test, the ignition delay time was about 1.1×10^{-4} seconds. As seen in Fig. 10.5, for the fuel equivalence ratios studied, ignition delay times are longer at fuel-lean conditions and shorter for fuel-rich conditions.

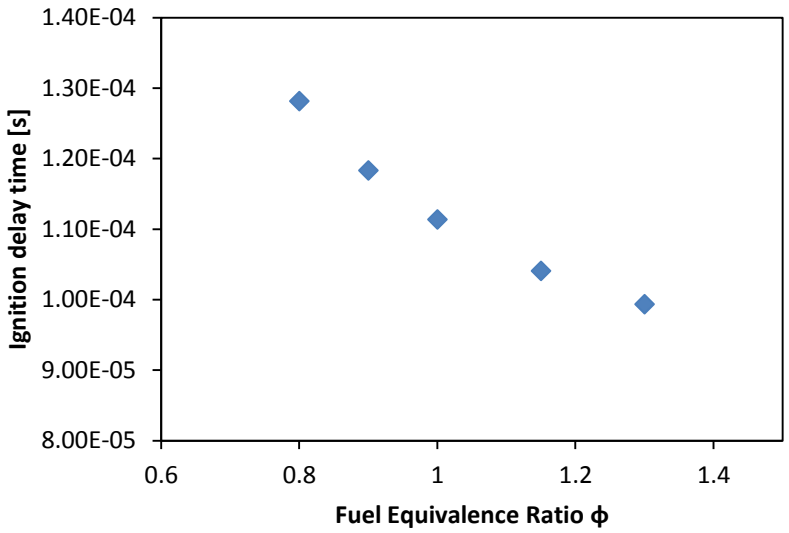

Figure 10.5: Ignition delay times dependence on fuel equivalence ratio.

This shift in ignition delay times with fuel equivalence ratios can also be observed in the temperature profiles (see Fig. 10.6). The initial spike in temperature occurs earliest at the richest of the test cases. Likewise, the initial spike in temperature occurs at the latest times for the leanest of the test cases.

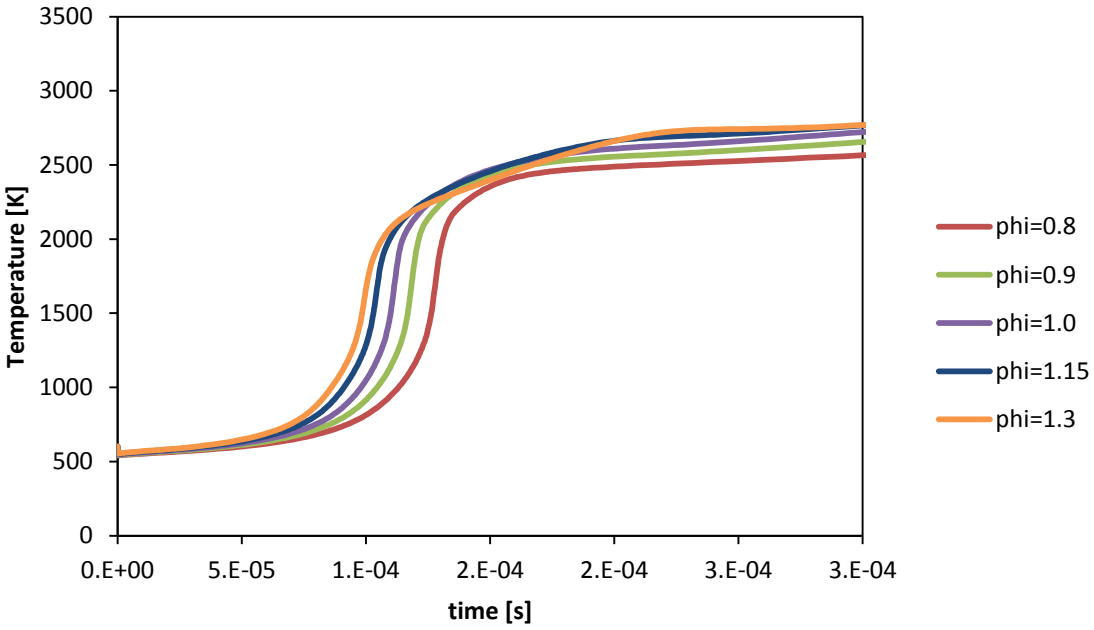

Figure 10.6: The variance of temperature profiles as functions of time with the change in fuel equivalence ratio.

Figures 10.7 to 10.10 show mole fraction profiles for MMH, NO_2, CO and OH for each of the different fuel equivalence ratios. Although the profiles rise to different maximum concentrations, behavior is similar for all five cases. The MMH profile (Fig. 10.7) is seen to decay over the first 100 μs with the profile slope changing largely as a factor of different inlet concentrations of MMH due to the different feed mixtures. Similarly, NO_2 profiles are seen to vary in peak and slope as a function of amount of inlet N_2O_4 in Fig. 10.8. Also observed is a shift in consumption, happening at shorter times for the fuel-rich cases that have the least amount of NO_2 and the shortest ignition time delays, and happening at longer times for the fuel-lean cases that have the most NO_2 and the longest ignition time delays.

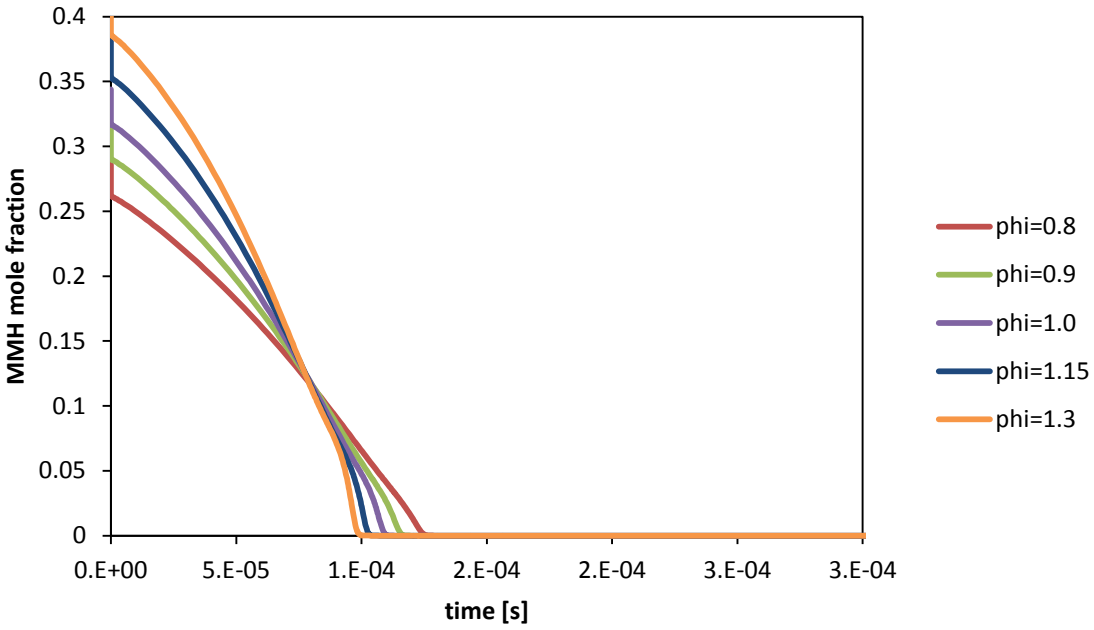

Figure 10.7: The variance of MMH mole fraction profiles as functions of time with the change in fuel equivalence ratio.

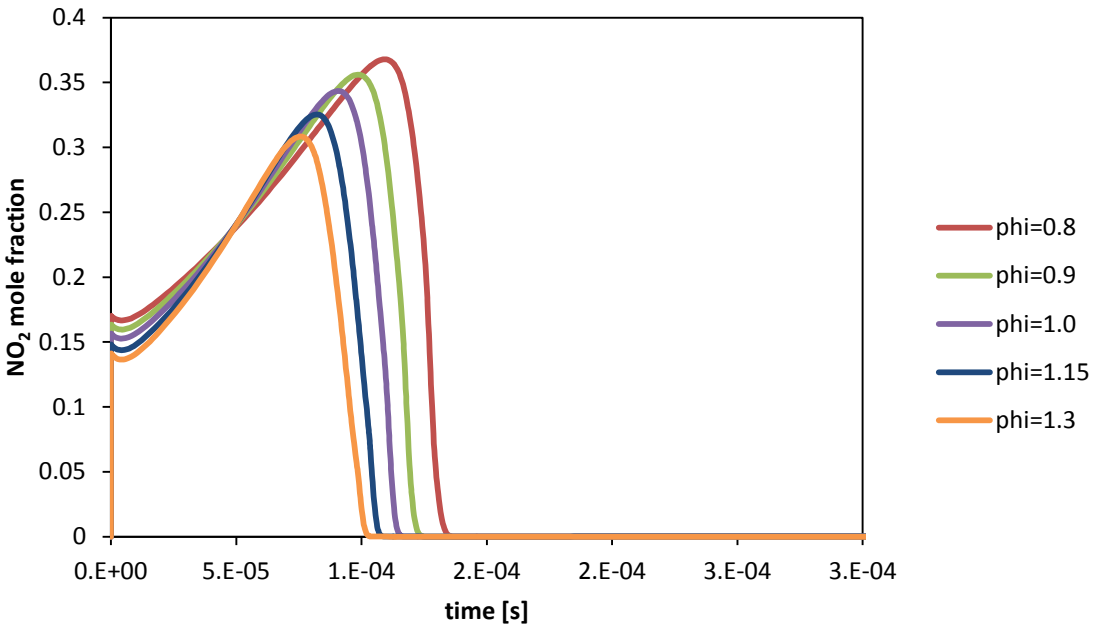

Figure 10.8: The variance of NO_2 mole fraction profiles as functions of time with the change in fuel equivalence ratio.

With the mole fraction profiles for CO and OH, there is a larger variance between the profiles for different fuel equivalence ratios, but still they are similar. Figure 10.9 shows the profiles for CO. In general, the profiles are the same in shape and behavior. Again a shift is observed between the fuel equivalence ratios corresponding to the shift in ignition delay times, and ultimate concentrations vary with the amount of fuel in the feed mixtures. There is a slight shape discrepancy at the highest fuel equivalence ratio as oxygen atoms in the system become most scarce. Fig. 10.10 shows the change in OH profile with fuel equivalence ratio. All five profiles begin to peak at the same time, and as expected, the smallest concentrations correspond with the richest of flames. A turnover seems to occur at a fuel equivalence ratio of 0.9. Below that, OH production changes slightly as the amount of oxidizer increases likely due to lower temperatures.

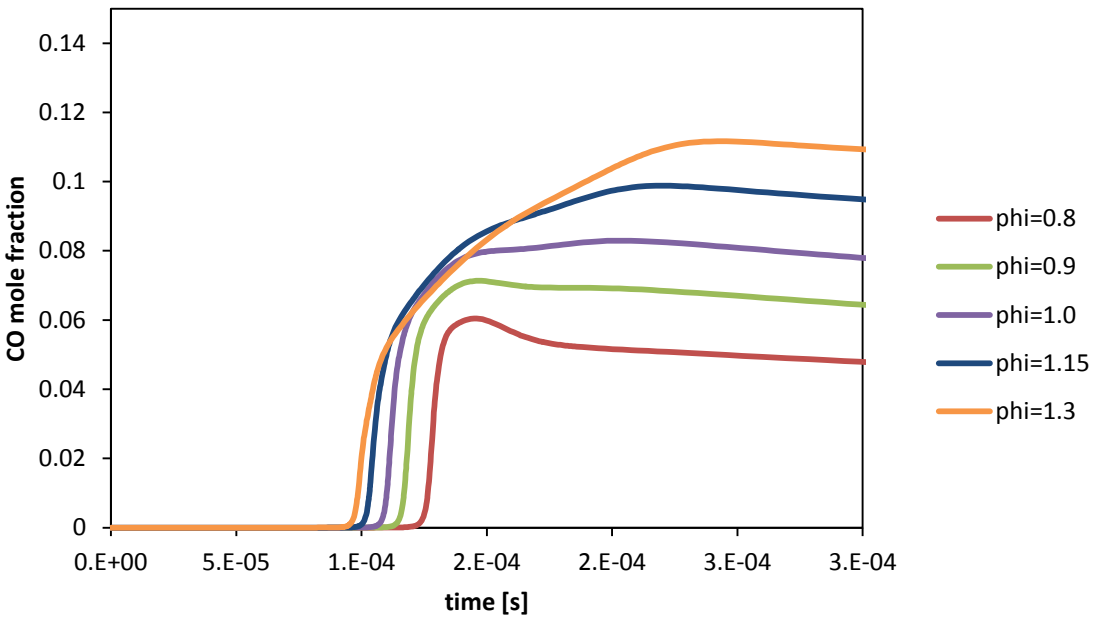

Figure 10.9: The variance of CO mole fraction profiles as functions of time with the change in fuel equivalence ratio.

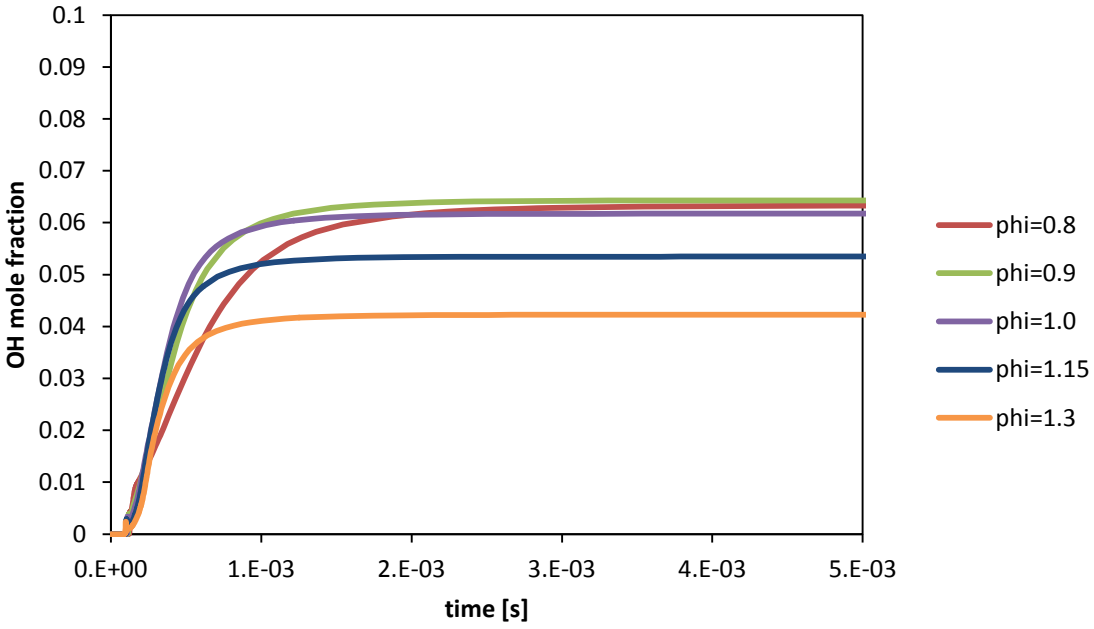

Figure 10.10: The variance of OH mole fraction profiles as functions of time with the change in fuel equivalence ratio.

One important feature of this mechanism is that the NO_2 hydrogen-abstraction reaction forming HONO regenerates OH through HONO decomposition. Because of the abundance of OH and NO_2 from the reactants and the OH regeneration via HONO, there are only minor differences in the dominant reactions when comparing flames with fuel equivalence ratios (Φ) ranging from 0.8 to 1.3, even though the resulting profiles are altered by the fuel mixture. For this reason, it is hypothesized that separate mechanisms for fuel-rich and fuel-lean conditions are unnecessary.

10.3.3 Trends with change in pressure

In practical applications for MMH combustion (i.e., combustion in an engine), operating pressures are much higher than atmospheric pressure. Experimental studies tend to be at lower pressures for simplicity and safety. To model both experimental studies as well as predict behavior in real engines, the model should be able to perform at a range of different pressures. Figures 10.11 to 10.16 show the behavior of the model as pressure is increased from 1 atm to 100 atm while keeping fuel equivalence ratio at stoichiometric and inlet temperature at 600 K.

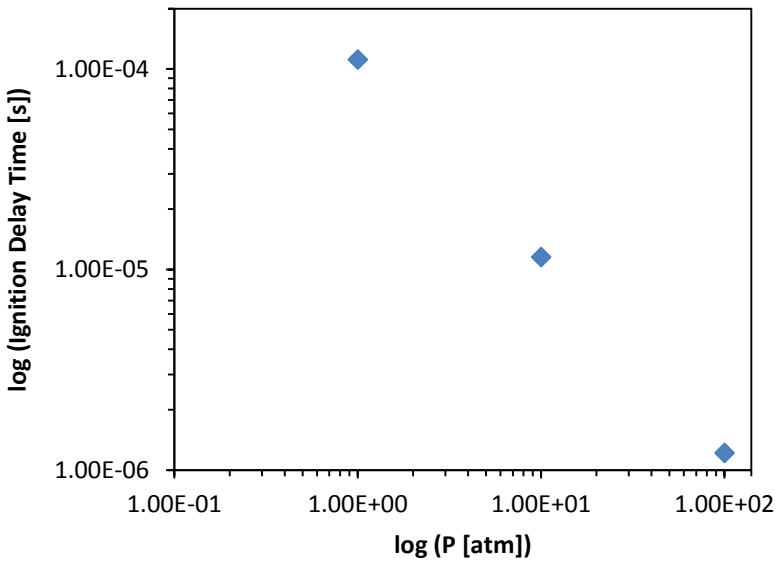

Figure 10.11: Ignition delay times as a function of pressure.

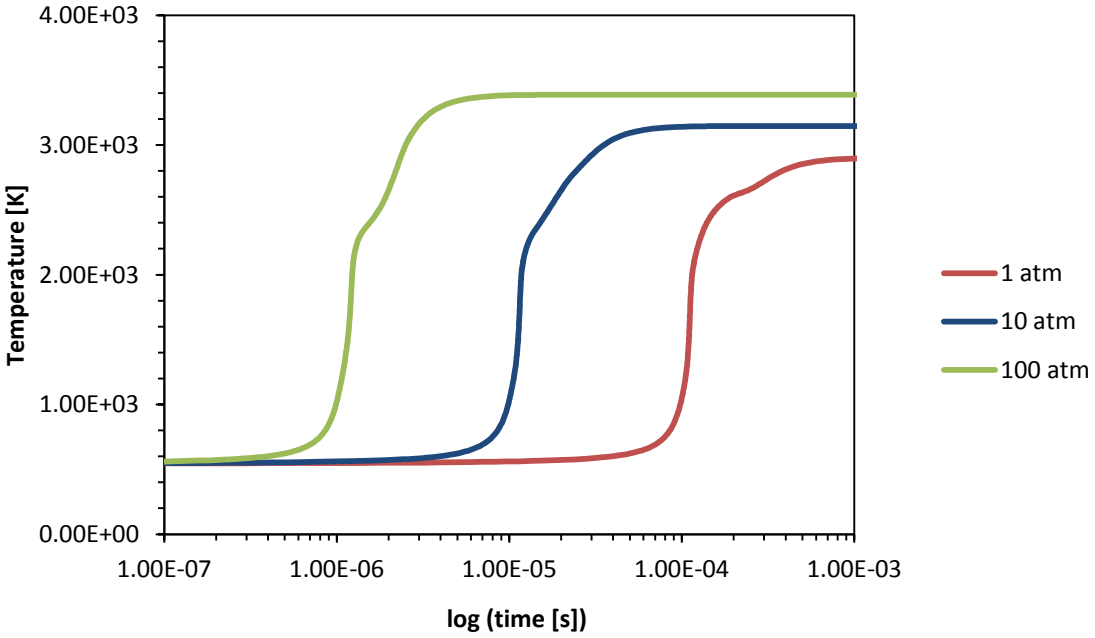

Figure 10.12: The variance of temperature profiles as functions of time with the change in pressure.

The largest difference in the three different studies is the change in ignition delay time. Figure 10.11 shows the ignition delay times as a function of pressure. As the

pressure increases by an order of magnitude, the ignition delay time decreases by an order of magnitude. This trend is observed in the temperature profiles in Fig. 10.12. Shifts are observed for the three temperature profiles corresponding to the ignition time delays. The higher pressures also produce higher temperatures, as expected from the ideal gas law.

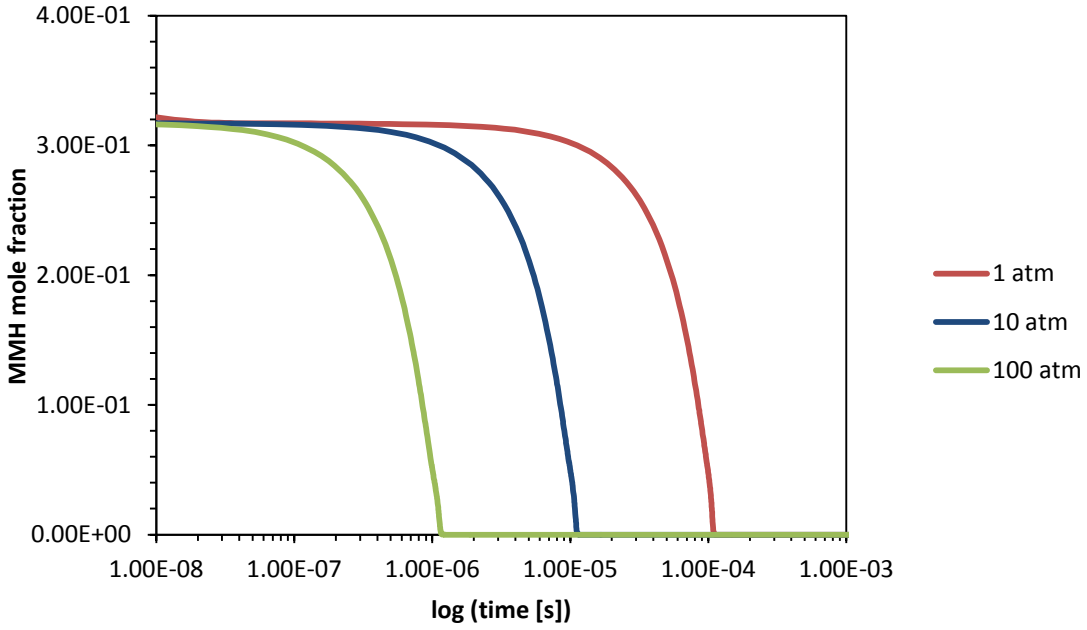

Figure 10.13: The variance of MMH mole fraction profiles as functions of time with the change in pressure.

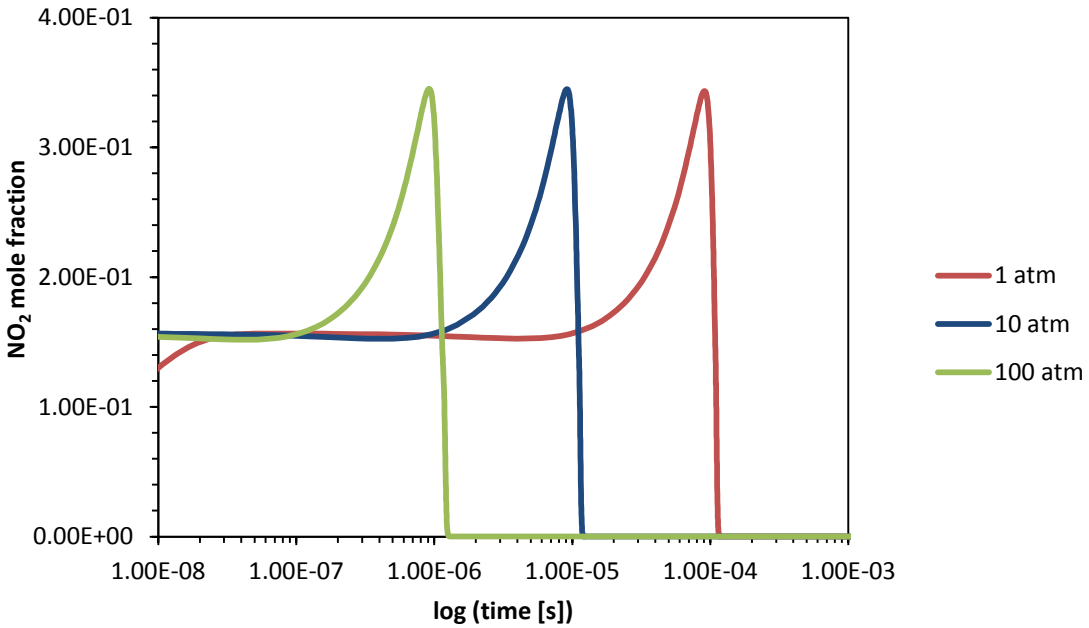

Figure 10.14: The variance of NO_2 mole fraction profiles as functions of time with the change in pressure.

Behavior for the different pressure cases is remarkably similar for species profiles. Figure 10.13 shows the mole fraction profiles for MMH which only differ in shift corresponding to the change in ignition delay times. The same can be said about NO_2 (Fig. 10.14). Larger differences are observed with CO and OH. Final concentrations for the CO profiles (Fig. 10.15) decrease as pressure is increased, and the same behavior is observed for OH (Fig. 10.16). Again, with the same trends observed over the range of pressures sampled in this parameter study, it is reasonable to suggest that a single reduced mechanism should be able to capture the chemistry of MMH with RFNA at different pressure conditions as well as different fuel equivalence ratios.

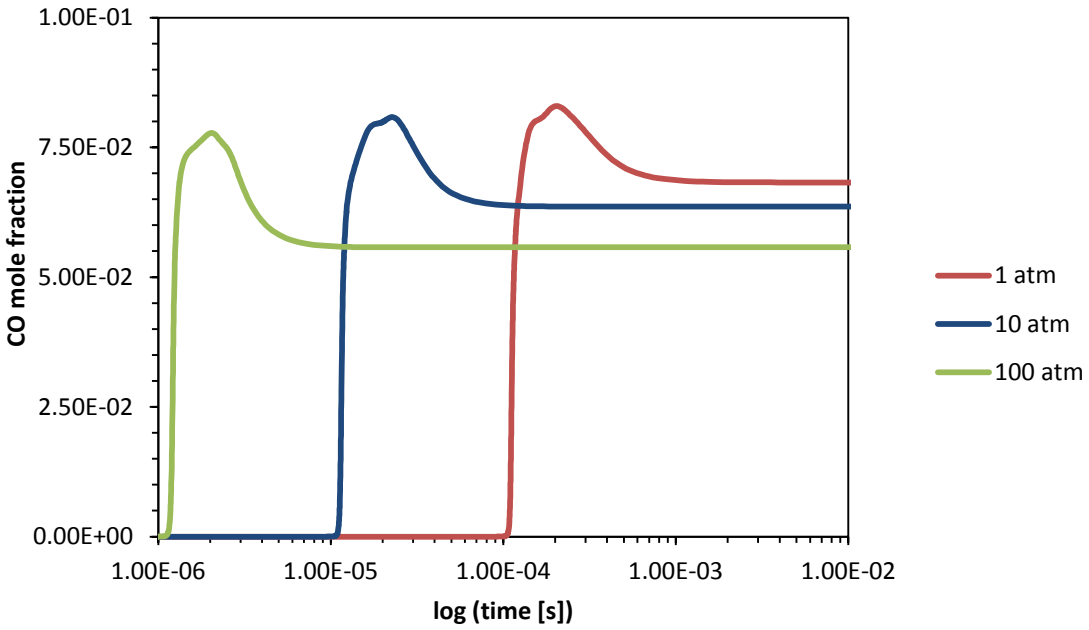

Figure 10.15: The variance of CO mole fraction profiles as functions of time with the change in pressure.

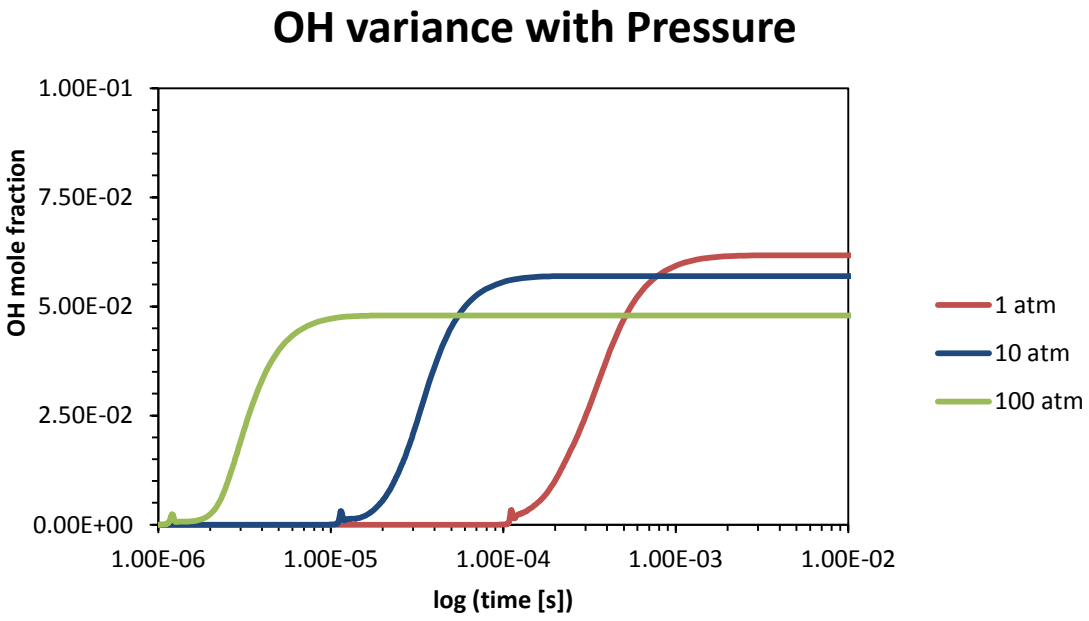

Figure 10. 16: The variance of OH mole fraction profiles as a function of time with the change in pressure.

10.4 Reducing the MMH/RFNA model

CFD models are often employed to model real combustion systems, such as engines. With the increased computational challenges of incorporating advanced fluid dynamics and transport into these models, the size of the reaction set that can be included in these models is highly restricted. Therefore, reduced reaction sets are needed for these types of models.

10.4.1 Procedure for model reduction

The full reaction set included 177 species and 1619 reactions, which is far too large for many CFD models. To reduce the reaction set, a rate of production analysis through time was performed for each species included in the model and each reaction rate included in the model for the base-case system (stoichiometric, P = 1 atm). Peak rates of production were summed for every reaction included in the model to determine relative contributions to the overall model. The reactions with minimal contributions were iteratively eliminated until a first reduced reaction set with 87 species and 482 reactions was developed, which may be found in Appendix H. This reduced reaction set will be referred to as "reduced set 1."

While some CFD models may be able to incorporate such a large model, others need a further reduced model. To eliminate reactions and species further, overall contribution to the model for each species was considered and species were iteratively eliminated to make a further reduced set with 41 species and 200 reactions, which may be found in Appendix I. This reduced reaction set will be referred to as "reduced set 2." This further reduced set had to eliminate some important chemistry, and performance of reduced set 2 is expected to be inferior to that of reduced set 1. However, given

computational constraints of some CFD codes, the second set should give a good estimate. These two sets both contain only elementary-reaction rate constants. Further reduction could be achieved through the introduction of composite rate constants.

10.4.2 Comparison to full model

To highlight the performance of the reduced sets, Figs. 10.17 to 10.21 show the two reduced sets in comparison to the full set. Reduced set 1 predictions are indistinguishable from that of the full set, while reduced set 2 performs similarly, but more slowly than what is observed in the full set. Specifically, the ignition time delay for reduced set 1 is 110 μs (same as for the full set) compared to the ignition time delay for reduced set 2 of 1620 μs. The difference of a factor of about 15 is significant and should be considered when it is necessary to use such a reduced set. The shift is observed in the temperature profiles (Fig. 10.17). While the reduced set 1 temperature profile is indistinguishable from the full set, reduced set 2's profile is shifted by the same shift in ignition time delay.

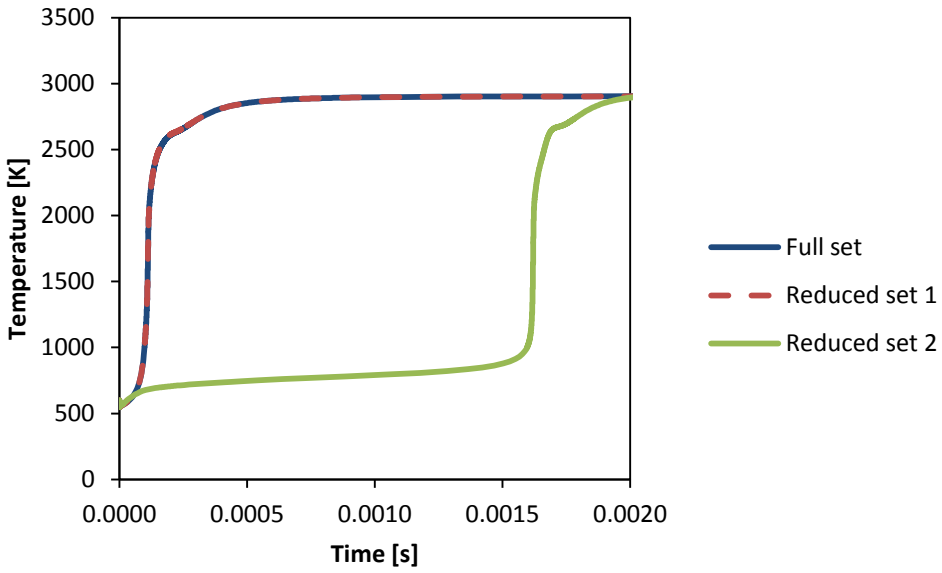

Figure 10.17: Temperature profile predictions for the full reaction set vs. the two reduced sets.

Mole fraction profiles for MMH (Fig. 10.18) and for NO_2 (Fig. 10.19) for the full and reduced set 1 are again identical. In the reduced set 2 profile, there is a two-step decay observed for MMH, largely due to an initial jump in radicals primarily from the immediate N_2O_4 dissociation reducing the overall mole fraction of MMH. The largest phenomenological difference between the reaction set 2 and the full set is observed in the NO_2 profile. In the full set and reduced set 1, NO_2 increases after the initial N_2O_4 decomposition, but that chemistry is eliminated in reduced set 2, so no gradual increase of NO_2 is observed past the initial generation from N_2O_4. Given the importance of NO_2 as a reaction partner in the full set, this explanation could be the key for the large difference between the full set and reduced set 2.

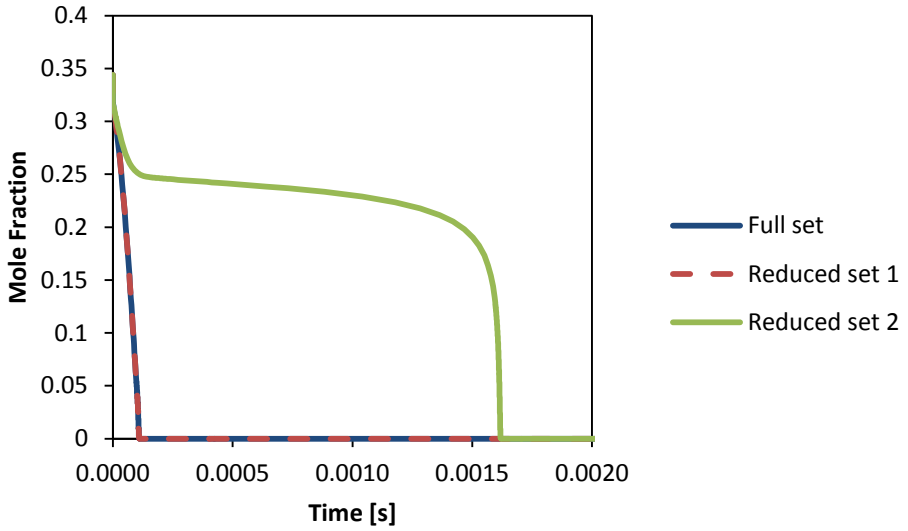

Figure 10.18: MMH mole fraction profile predictions for the full reaction set vs. the two reduced sets.

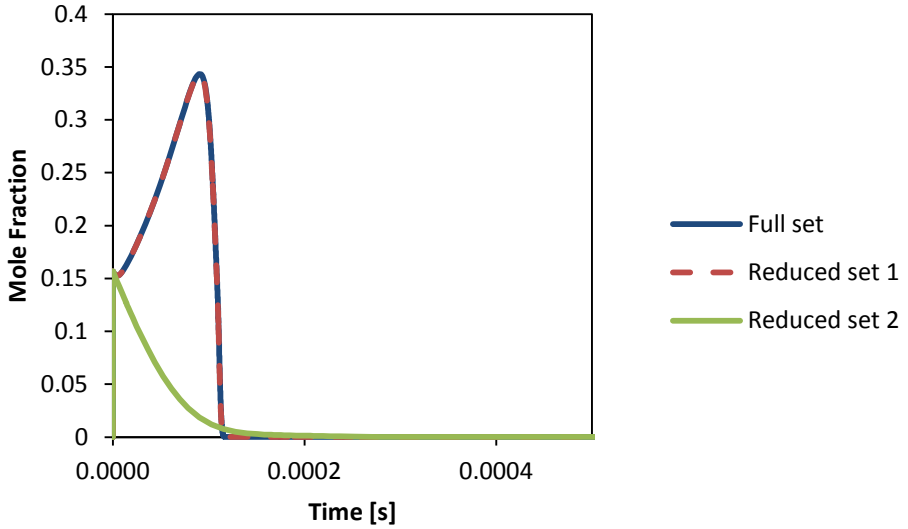

Figure 10.19: NO_2 mole fraction profile predictions for the full reaction set vs. the two reduced sets.

Again, for CO (Fig. 10.20) and OH (Fig. 10.12), the full set and reduced set 1 predictions are identical. For CO and OH, the primary difference between reduced set 2 and the full set is the shift due to difference in ignition time delay. For reduced set 2, CO

is predicted to be lower than from the full set and OH is predicted to be higher than from the full set.

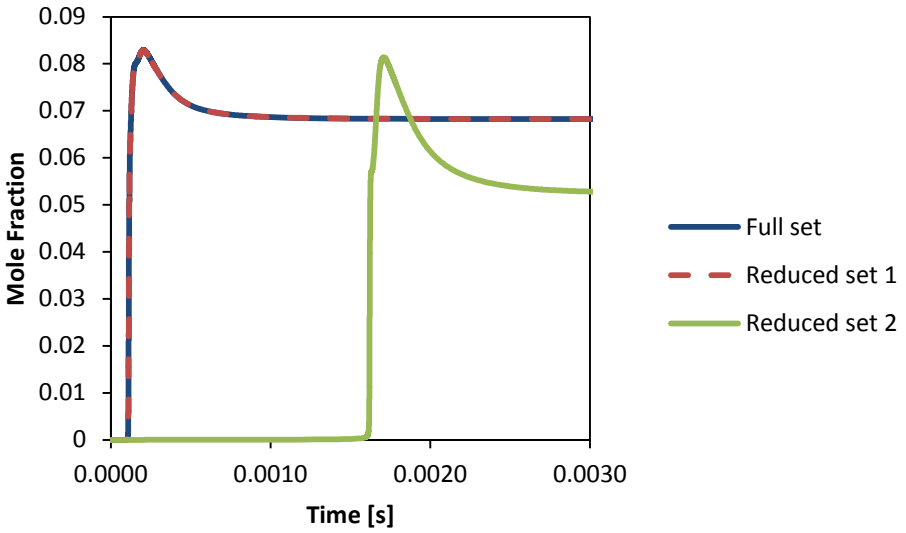

Figure 10.20: CO mole fraction profile predictions for the full reaction set vs. the two reduced sets.

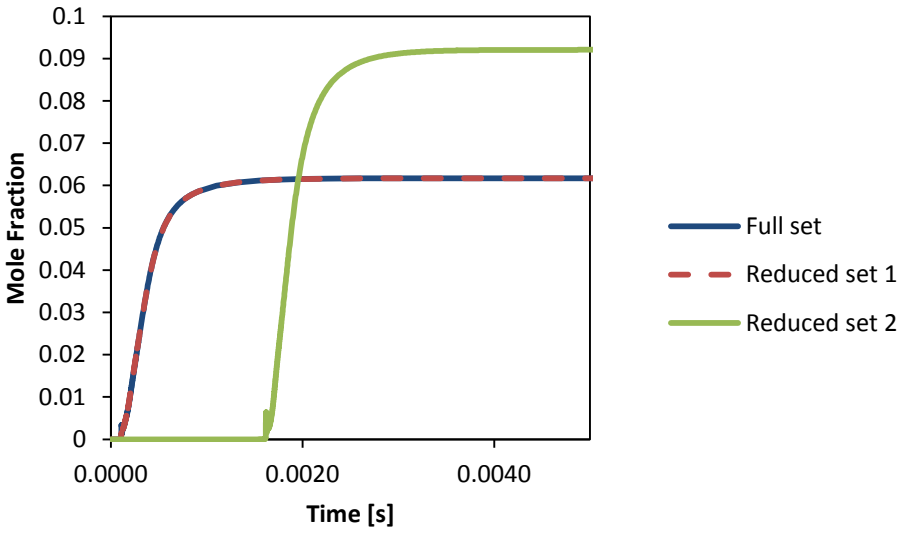

Figure 10. 21: OH mole fraction profile predictions for the full reaction set vs. the two reduced sets.

10.5 Summary and conclusions

MMH combustion with RFNA is a highly reactive system with complicated kinetics. As shown through estimates of heats of vaporization, liquid-liquid chemistry for these systems should be largely unimportant beyond initial heat generation because the droplets generate gas quickly upon contact. Instead, gas-phase chemistry is likely most important to consider for these hypergolic systems. Accordingly, a new reaction set for gas-phase combustion chemistry of MMH/RFNA was developed.

From observation of the modeling results, MMH is destroyed mainly by abstraction of the central hydrogen atom. The resulting intermediates then are destroyed by abstractions, especially abstractions by NO_2 and OH, until CH_3NN is formed, which further reacts to form products N_2, CO, and H_2O. Consequently, NO_2 and OH are the main drivers of reaction. The NO_2 comes from N_2O_4 decomposition and HNO_3 decomposition. OH also comes from the HNO_3 decomposition and is also regenerated through a minor reaction, $NO_2 + H$ ($\rightarrow$ HONO $\rightarrow$ OH + NO). This regeneration allows adiabatic flames with fuel equivalence ratios (Φ) ranging from 0.8 to 1.3 to follow the same combustion reaction pathway, unlike hydrocarbon flames.

Two reduced sets were developed for MMH/RFNA for use in CFD models. The larger set has 87 species and 482 reactions, down from the full set of 177 species and 1619 reactions. It is able to capture the chemistry of the full set perfectly. A second reduced set of 41 species and 200 reactions was developed for more restricted CFD models and was found to capture many of the same trends as the full mechanism, though ignition delay times were a factor of 15 longer than those calculated in the full set. Use of the more heavily reduced set should consider the longer time delays.

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CHAPTER 11

HYPERGOLIC ROCKET FUELS: DEVELOPING A REACTION SET FOR TETRAMETHYLETHYLDIAMINE + RED FUMING NITRIC ACID

As explained with MMH/RFNA in Chapter 10, hypergolic rocket fuels are attractive for use because they require no ignitor. A potential improvement is that they may be gelled and still easily ignited, reducing the potential for accidental ignition by reducing the ability of the fuel to vaporize. The drawback of using hypergolic propellants is that they are hazardous materials, and gelation would improve their handling. Hydrazine is known to be a toxic substance and has been identified as an environmental contaminant and pollutant [1]. Monomethyl hydrazine is a popular hypergolic fuel choice, but it is lethal under high exposure and is thought to be carcinogenic in the long term [2].

Two promising alternative hypergols have been proposed: dimethylamino-2-ethylazide (DMAZ) and tetramethylethanediamine (TMEDA). DMAZ and TMEDA have been found to be less toxic than hydrazine, and they also have been shown to be non-mutagenic in mouse studies, in contrast to hydrazine and monomethyl hydrazine [1]. DMAZ has been shown to have competitive performance to hydrazine but has not met ignition-delay standards in application tests thus far [3]. TMEDA has faster ignition times but lower thrust capabilities compared to DMAZ. Blends of DMAZ and TMEDA may resolve ignition delay concerns while still having comparable performance to monomethyl hydrazine.

11.1 Formulation of the Skeletal Mechanism and Reaction Set

An initial skeletal set has been developed for TMEDA combustion using analogies to the reactions of traditional hydrocarbon fuel combustion. It is proposed that like hydrocarbon fuels, TMEDA first reacts predominantly via hydrogen abstraction. TMEDA has two structurally distinct H-abstraction sites: the methyl groups and the two CH_2 groups. The two resulting TMEDA radicals can undergo β-scissions; the TMEDA radical with a radical site on a methyl group can eliminate either a neighboring methyl group or CH_3NCH_2 while the other TMEDA radical can either eliminate a methyl group, CH_3NCH_3 radical, or a hydrogen atom to form a TMEDA-ene species. The products of these β-scissions can further undergo chemically activated reactions. Figure 11.1 illustrates the possible TMEDA abstraction paths and the possible reactions that follow.

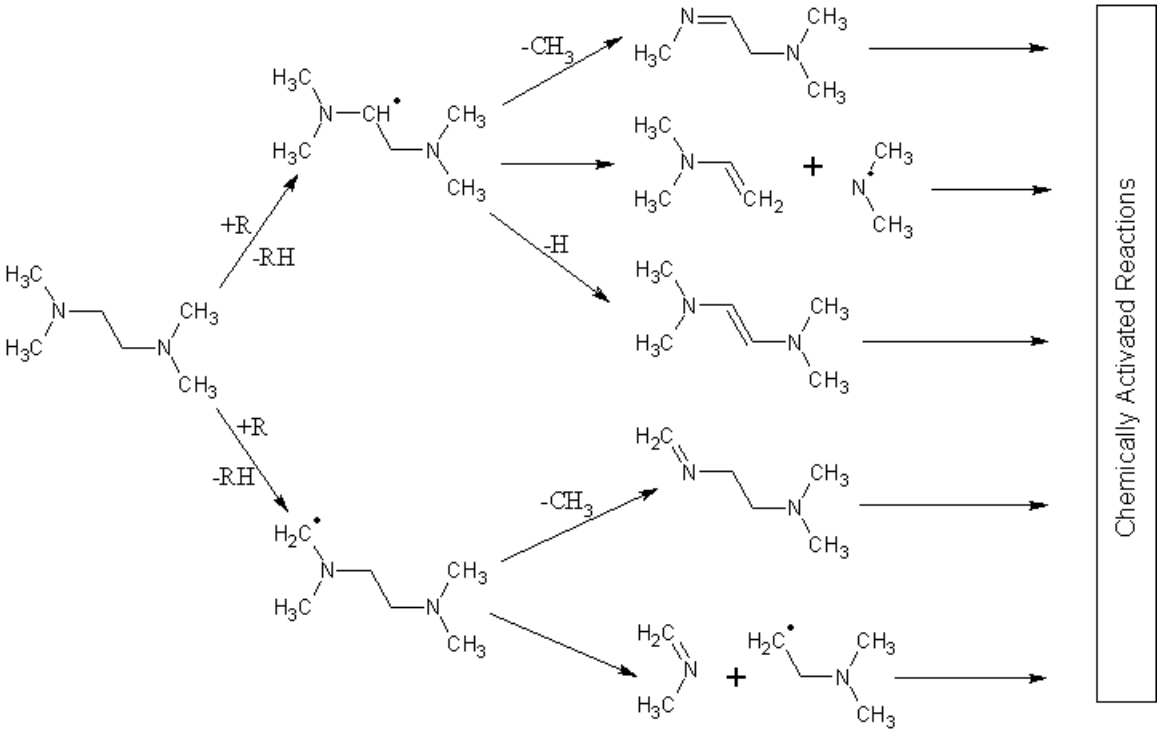


Figure 11.1: Proposed abstraction reactions in TMEDA combustion. First, either a primary or secondary hydrogen can be abstracted from TMEDA. The resultant TMEDA radicals then undergo various β-scission and chemically activated reactions.

While it is expected that abstraction reactions dominate steady-state TMEDA destruction, thermal decomposition may also be important, especially for ignition. Figure 11.2 shows the skeletal mechanism for three possible TMEDA thermal decomposition reactions by fission of either the C-C or one of the two types of C-N bonds, resulting in two radical species. These radicals can all undergo β-scission and chemically activated reactions.

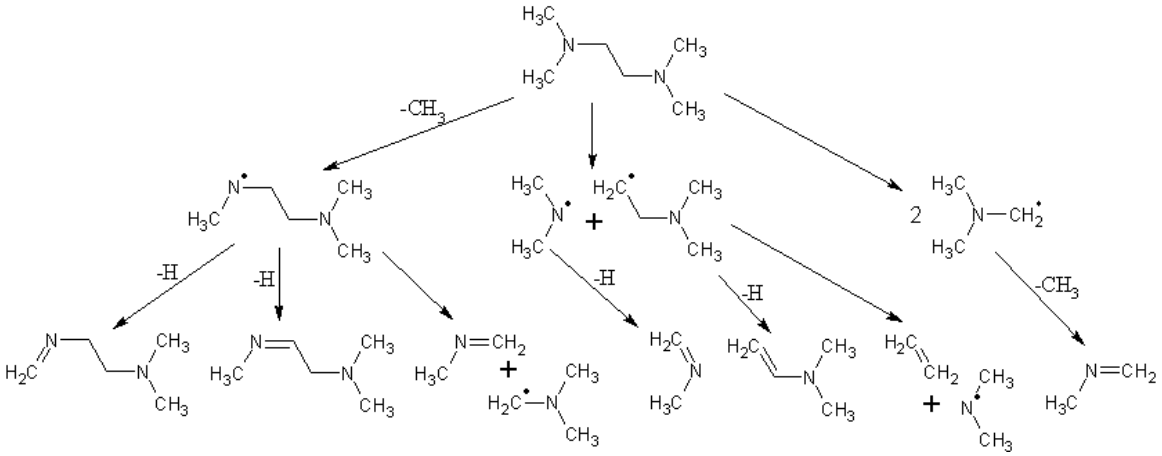
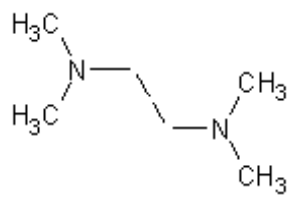
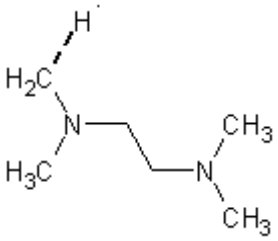
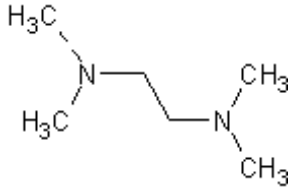
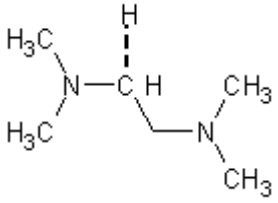
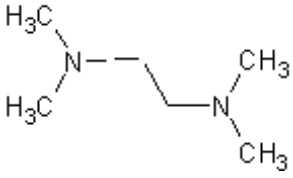


Figure 11.2: Proposed thermal decomposition pathways for TMEDA.

Thermochemistry was calculated for all 21 new TMEDA species in the proposed skeletal mechanism, accounting for hindered rotors. Geometries, frequencies, and transition states were calculated using the Gaussian 09 software [4] and thermodynamic fits were calculated with ChemRate [5]. All simulations used Petersson's complete basis method CBS-QB3 [6] and tight convergence criteria.

Table 11.1: Bond dissociation energies for TMEDA. Analysis shows that the weakest bond is the central C-C bond.

Bond (Indicated by broken line)	Bond Dissociation Energy (kcal/mol)	Bond (Indicated by broken line)	Bond Dissociation Energy (kcal/mol)
	72.01		91.76
	78.50		93.01
	79.08		

From the calculated thermochemistry, bond dissociation energies were calculated for all structurally unique bonds in TMEDA (Table 11.1). From this analysis, the C-H bonds are the most tightly held while the central C-C bond is the weakest, suggesting severance of the C-C bond is the most likely TMEDA thermal dissociation pathway. The two structurally different C-N bonds are similar in bond dissociation energy (differing by half a kcal), are significantly stronger than the central C-C bond with a difference of 6.5-7 kcal/mol.

Reaction rate constants were generally derived by analogy to 2-methylheptane reactions [7-8] for reactions involving 4-7 heavy atom species, correcting Arrhenius pre-exponential factors for reaction path degeneracy. Additional reactions involving 3-4

heavy atom species were estimated using analogous reactions found in the reaction sets of Law [9-10] and Li [11]. The TMEDA reaction rate constants were added to the MMH/RFNA full reaction set developed in Chapter 10. In all, a total of 141 new reaction rates for TMEDA combustion have been included in the mechanism. With the addition of these reactions and species, the TMEDA mechanism is comprised of a total of 198 species and 1760 reactions. The reaction set may be found in Appendix J.

11.2 Modeling TMEDA ignition using a stoichiometric TMEDA/RFNA mixture

To test the new reaction set, combustion of TMEDA with RFNA was modeled using an adiabatic, zero-D, constant-pressure, perfectly stirred reactor using the Chemkin PRO code [12]. Starting temperatures were elevated to 1000 K to aid ignition. As a base case, TMEDA/RFNA mixture at stoichiometric ($\Phi = 1$) conditions. The model predicted an ignition delay time at these conditions of 233 μsec. Figure 11.3 shows a predicted temperature profile for the stoichiometric flame versus time. There is an initial dip in the temperature below the starting temperature of 1000 K. This effect is due to the dissociation of N_2O_4 to 2 NO_2, which acts as a heat sink initially. Post-ignition, the temperature of the adiabatic reactor rises to a peak temperature of 2756 K.

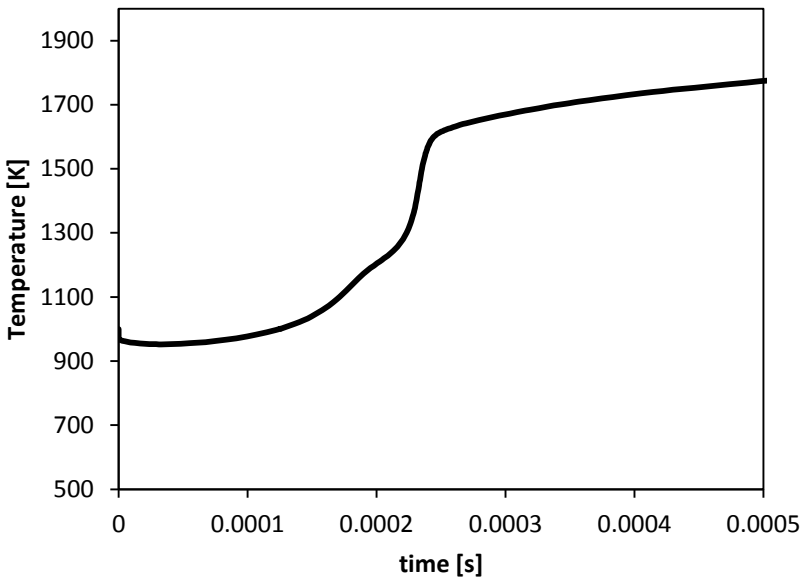


Figure 11.3: Temperature profile from a 0-D constant pressure reactor model using a stoichiometric TMEDA/RFNA mixture at P= 1 atm and initial temperature of 1000 K.

Mole fraction profiles for several major species are presented in Fig. 11.4. Upon first inspection, the mole fraction profiles are not smooth, suggesting some instabilities within the model and perhaps that the analogies to the 2-methylheptane reaction set of [7-8] are not sufficient for TMEDA modeling. Regardless, trends are easily observed. Reactants HNO_3 and TMEDA are consumed steadily over the first 250 μs of reaction. The NO_2 profile rises sharply at the outset corresponding to N_2O_4 decomposition and then steadily declines. Product species H_2O, CO, H_2, and NO all rise steadily. Surprisingly, HCN concentrations rise above 10% total mole fraction and persist for some time. Eventually HCN is consumed, but consumption reactions are delayed for a period of about 100 μs.

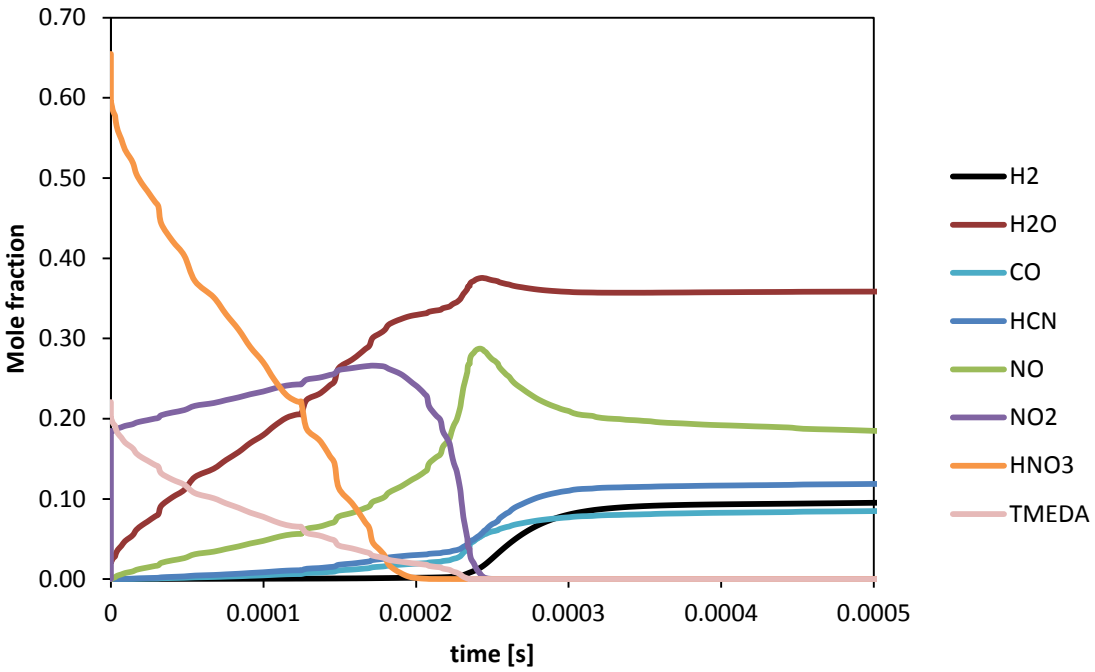


Figure 11.4: Mole fraction profiles for H_2, H_2O, CO, HCN, NO, NO_2, HNO_3 and TMEDA from a 0-D constant pressure reactor model using a stoichiometric TMEDA/RFNA mixture at P = 1 atm and initial temperature of 1000 K.

Additional mole fraction profiles for CH_4, C_2H_2, CO_2, N_2, HONO, and CH_3NCH_2 are provided in Fig. 11.5. In contrast to combustion with MMH, small carbon species play a much larger role than the small nitrogen species due to the fact the carbon to nitrogen ratio in TMEDA is 6:2 compared to the carbon to nitrogen ratio in MMH of 1:2. As such, significant concentrations of methane and acetylene are found as intermediate species. These species persist similarly to HCN, only to be consumed approximately 100 μs later. CO_2 and N_2 are also formed, with N_2 being the main nitrogen-containing product of combustion. HONO is also found in appreciable concentrations as a result of the high concentrations of NO_2 at the onset of combustion. CH_3NCH_2 was also found in high concentrations, suggesting it may play an important role in combustion of TMEDA.

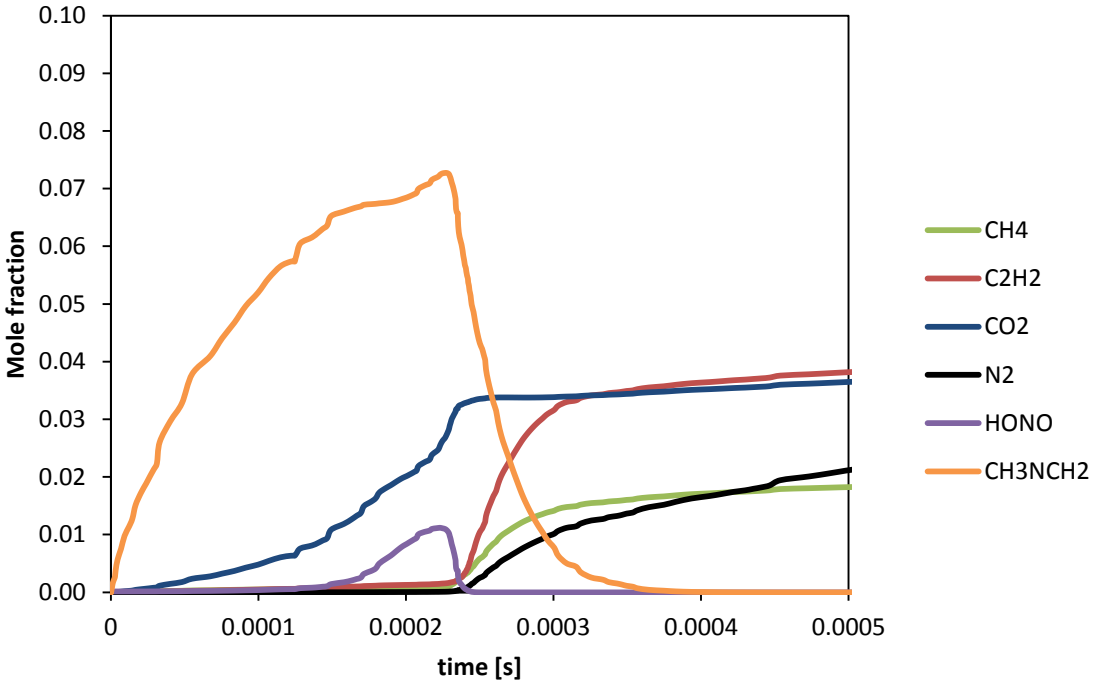


Figure 11.5: Mole fraction profiles for CH_4, C_2H_2, CO_2, N_2, HONO, and CH_3NCH_2 from a 0-D constant pressure reactor model using a stoichiometric TMEDA/RFNA mixture at P = 1 atm and initial temperature of 1000 K.

From the model results, dominant reaction pathways may be determined and are illustrated in Fig. 11.6. Primarily, TMEDA first loses a hydrogen atom via abstraction reaction, resulting in one of two different TMEDA radicals. Once a radical is formed, both different TMEDA radicals then preferentially β-scission the C-N bond adjacent to the ethane bridge, forming a three-heavy-atom species (either radical species CH_3-N-CH_3 or CH_3-N=CH_2) and a five-heavy-atom species. The CH_3-N-CH_3 radical then β-scissions a hydrogen to form CH_3-N=CH_2. The five-heavy-atom species, through subsequent reactions, also each form CH_3-N=CH_2 as an eventual product of reaction. Hence, each TMEDA molecule generally produces two CH_3-N=CH_2 molecules, resulting in the large spike in concentration of CH_3-N=CH_2 during reaction.

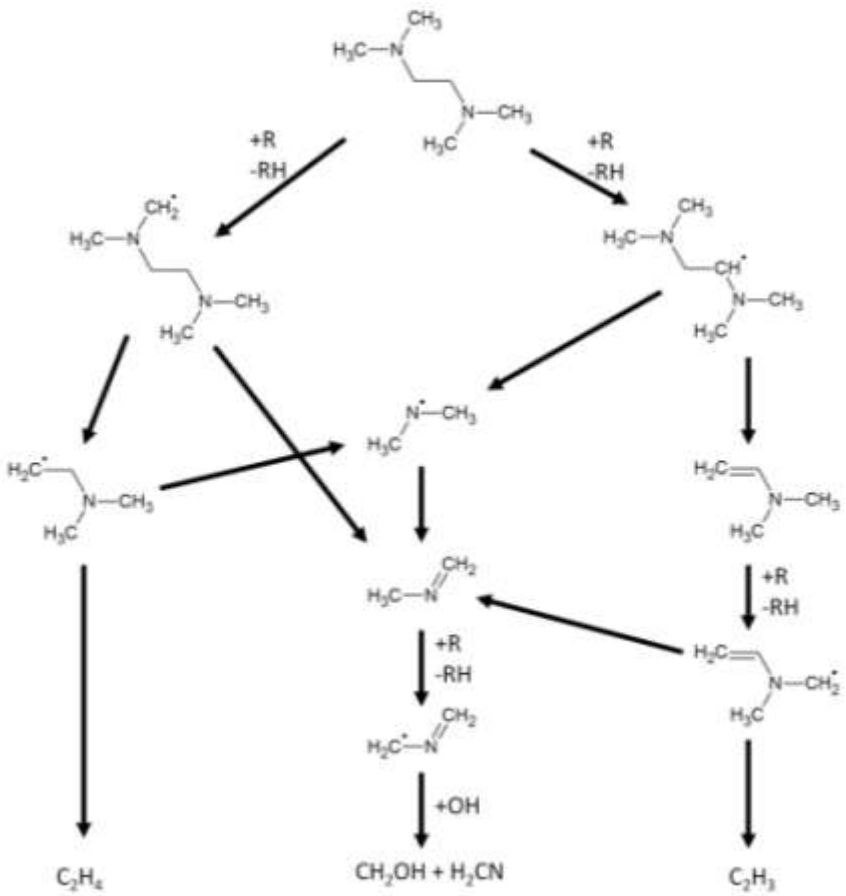


Figure 11.6: Major reaction route for stoichiometric TMEDA/RFNA combustion at P = 1 atm.

11.3 Summary and Conclusions

A new reaction mechanism and corresponding thermochemistry for the combustion of TMEDA with RFNA has been assembled using a combination of careful estimations based on analogous hydrocarbon combustion reactions and quantum chemistry calculations. From a bond dissociation energy analysis, it is expected that the severance of the C-C bond TMEDA is the most likely thermal dissociation pathway. However, abstraction reactions from TMEDA dominated in TMEDA/RFNA combustion. Subsequent β-scission reactions yield two CH_3NCH_2 molecules for every TMEDA

molecule generally, and a corresponding high mole fraction peak of CH_3NCH_2 is observed around time of ignition.

Despite the success of using kinetic analogies for other nitrogen-containing fuels, use of a 2-methylheptane reaction set for analogy appears to have some issues. Mole fraction profiles were not smooth, suggesting instabilities that must stem from the TMEDA reactions since the same characteristics were not observed using the same core set in studies of other fuels. Additionally, intermediate species such as HCN persist for long periods of time (about 100 μs) before being consumed which is unusual behavior. Future work should include additional quantum-chemistry calculations and explore other options for the basis of analogy to TMEDA.

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CHAPTER 12

CONCLUSIONS AND FUTURE WORK

With the introduction of new biofuels for transportation, it is necessary to have a fundamental understanding of the combustion chemistry of heteroatoms such as oxygen and nitrogen beyond our understanding of hydrocarbon combustion chemistry. These heteroatoms could have a profound impact on emissions, both contributing to and hindering the formation of toxic pollutants. In this work, chemical kinetic models were developed and tested against experimental data to predict kinetic pathways for several different nitrogen- and oxygen- containing fuels, providing a better understanding of hetreoatomic fuel combustion in a broader context. These models may be used as a nucleus of kinetics and thermochemistry to model other heteroatomic fuels.

12.1 Conclusions

Key results of the research are new reaction sets that provide a hierarchy of molecular complexities from single-nitrogen fuels to the highly reactive di-nitrogen fuels used as hypergolic rocket propellants:

- A new H/N/O reaction set was developed and tested successfully, becoming the largest and most accurate elementary-reaction set for H/N/O combustion currently available (Chapter 5).
- A new H/C/N/O reaction set was developed using recent literature contributions including improved cyclohexane and acetylene chemistry. This new set was tested against stoichiometric NH_3/CH_4, ethylamine, and dimethylamine flames, matching or bettering most predictions by existing reaction sets (Chapter 6).

- A new reaction set was developed and tested successfully for tetrahydropyran combustion. THP is a mono-oxygen ether analogue to cyclohexane, and its study reveals the extent and limits on useful analogies to cyclohexane kinetics (Chapter 7).
- A new reaction set was developed for morpholine combustion and tested successfully against detailed flame data (Chapter 8) and laser-diagnostics and shock-tube data (Chapter 9). Morpholine extends the analogy approach, as it is like THP but with an amine NH in the ring opposite to the oxygen's position.
- Three new reaction sets were developed for gas-phase combustion chemistry of the hypergolic combination of monomethylhydrazine (MMH) and red fuming nitric acid (RFNA). One set was fully detailed, while two were reduced sets. No composition data are available for testing the models, but prediction of experimental ignition delays provided a basis for examination (Chapter 10).
- Skeletal reaction sets were developed for the alternative hypergolics dimethylamino-2-ethylazide (DMAZ) and tetramethylethanediamine (TMEDA). Thermochemistry and kinetics were developed for the TMEDA set, and ignition times were modeled (Chapter 11)

12.2 Discussion of conclusions

The key component to chemical kinetic models for combustion is the reaction set, a database of reactions and elementary rate constants. These models rely on the reaction sets to describe what reactions are allowed and, thus, cannot allow reactions to occur unless there is a rate constant explicitly provided for that reaction. Experimental studies have provided measurements for many rate constants for reactions occurring in combustion. Difficulties arise when measurements are not available over a wide enough

temperature range sufficient for reaction conditions. Often it is too difficult to measure rate constants for radical species, leaving experimental databases for reaction rate constant incomplete for combustion.

Advances in computational chemistry and computing power have made quantum-chemistry calculations feasible using large enough basis sets that reaction rate constants may be calculated fairly reliably. These methods have been employed to determine rate constants for many instances where experimental data were not available for use. Despite the numerous advances in computational chemistry however, reaction sets often contain thousands of reaction rate constants. Computing that many reaction rates with today's computing power is not feasible, so identification of key steps is important for using computing resources most effectively.

In this work, reaction sets for combustion were developed for several heteroatomic fuels, including novel fuels where reaction sets had not been previously published, introducing the need for rate coefficients for many reactions where data were not previously published. The large number of unknown reaction rate constants made quantum calculations for each of these reaction sets too impractical. Thus, rate-constant estimation techniques were employed in conjunction with quantum chemistry calculations to develop reaction sets for these different heteroatomic fuels. Reaction rate constants were estimated by analogy to reactions of hydrocarbons, adjusting A-factors using reaction path degeneracy. Not only did these techniques provide reasonable estimations to the rate constants, but the resultaing reaction sets performed well against experimental data validation tests. The following is a summary of the development of

several combustion reaction sets and the modeling results obtained with these reaction sets in comparison to experimental data.

12.2.1 Building a small-molecule nitrogen reaction set

In an effort to better model H/N/O combustion globally over several experimental conditions, a new H/N/O reaction set was developed, currently the largest elementary-reaction set available for H/N/O combustion. This model was compiled as an extensive database of available elementary rate constants that was optimized via sensitivity analysis over the currently available H/N/O models. The new reaction set has 43 species and 307 reactions and was tested over twelve experimental MBMS flame data sets and compared against six different models. Additionally, the new reaction set was compared against a pyrolysis shock-tube study. The results showed overall agreement with the experimental data, providing generally model results that were as good as or better than the current models available. Major improvements on N_2 and NO modeling results were achieved, and intermediate radical species were generally predicted within a factor of 2.

The H/N/O reaction set was then expanded to include carbon chemistry. The hydrocarbon chemistry was included largely from published studies on cyclohexane and acetylene and was generally unmodified, as the kinetics had been previously tested. H/C/N/O chemistry was added from several previously published sources and compiled into one master database and reaction set. This new set was tested against three different stoichiometric flames, including an NH_3/CH_4 flame, an ethylamine flame, and a dimethylamine flame.

The overall agreement of the new reaction set versus the experimental data and the model results published in the experimental flame studies was good. The largest

issues arose in the predictions of intermediate species and often were predicted poorly by both models in those cases. While some intermediate species were predicted more poorly than the published models, other predictions were improved.

12.2.2 Combustion of heterocyclic fuels

The combustion of several heterocyclic fuels was studied as model biofuels. Tetrahydropyran (THP) combustion has been analyzed in a low-pressure premixed flat flame at ϕ=1.75. From VUV-PI-MBMS measurements, 31 species with up to six heavy atoms were quantified. A newly developed kinetic mechanism for THP was based on recent modeling of cyclohexane combustion with additional rate coefficients and thermochemistry added from quantum chemistry calculations and analogies. This model predicts the general flame structure well. Analyzing the predictions shows that THP consumption in the flame is by abstractions of the three different H atoms in THP, followed by logical sequences of decomposition steps from the THP-yl radicals. These radicals then β-scission to six-, four-, and two-heavy-atom species by a logical sequence. Other species are formed by decomposition and oxidation of these intermediates. Although little molecular-weight growth was observed, benzene is produced, and routes are identified to produce it.

THP is studied here as a small C/H/O-containing model biofuel with the aim of contributing to the understanding of the mechanistic pathways for THP combustion and the formation of potential pollutants. The reaction set and kinetic pathways identified in this study will aid design of efficient, low-polluting combustors. THP is an ether variant of cyclohexane and the non-nitrogen equivalent of morpholine, and the present flame data and predictions provide insights into mechanistic similarities and differences from

these other fuels.

Morpholine combustion has been analyzed in detail under fuel-rich premixed low-pressure flame conditions and a detailed reaction set has been created for modeling morpholine flames. From a combination of PI-MBMS and EI-MBMS, a large number of species with up to six heteroatoms was quantified, relying in part on previous identification [28] and using systematic additional measurements with both systems for a reliable separation and calibration. The two sets of experiments are in good general agreement. A modeling attempt used a newly conceived reaction scheme, starting from recent modeling of cyclohexane combustion, and a dedicated scheme for morpholine decomposition; it was seen to predict the general flame structure and reaction pathways reasonably well, especially including NO_x formation. The polyfunctional cyclic fuel molecule gives rise to a wealth of combustion intermediates. From the fuel breakdown, four and two heavy atom species were observed. Also, intermediate build-up and oxidation products were detected quantitatively. Aldehydes were formed as intermediates, and especially formaldehyde was observed to reach mole fractions quite similar to that for DME combustion under similar conditions, while acetaldehyde mole fractions were less important. Carbonyl compounds featuring more than two carbon atoms have not been detected, again a probable consequence of the early morpholine breakdown reactions.

The fuel nitrogen is finally converted to N_2 and NO, which present mole fractions of about 4% and 2%. Major small nitrogen-containing intermediates include HCN, NH_3, HNCO, and NO_2, of which HNCO and NH_3 may persist into the burnt-gas region. The HCN mole fraction was surprisingly high with a peak of about 6%, and NH_3, expected to

be a major volatile product, was seen with more than an order of magnitude lower peak mole fraction. The model suggests that HCN is formed from breakdown products of the morpholine ring, with NH_x compounds as further products once HCN is formed and converted rapidly in the small-nitrogen-species pool. Toxic nitrogen-containing intermediates observed include acetonitrile, acrylamide, and 2-propenenitrile.

In addition to the MBMS flat-flame study, several different experiments were conducted using laser diagnostic techniques for morpholine combustion. In one experiment, chemiluminescence was employed to capture the mole fraction profiles for important intermediate reactants CH, CN, HCO, and NH_2 on a flame identical to the EI-MBMS flame experiments. Experimental profiles were much closer to the burner in the unperturbed optical flame than in the MBMS flame experiment. The difference between peak mole fractions for HCO in both experiments was a factor of two, suggesting at least a factor of two experimental error. The modeling is well within the factor of two bounds, though it overpredicts all four radical species.

Morpholine pyrolysis was studied in 5000 ppm morpholine/argon mixtures behind reflected shock waves at temperatures from 1086 to 1404 K and pressures 20-23.6 atm. An IR He-Ne laser at 3.39 μm was used to measure morpholine concentration time-histories assuming that interfering products form at the same rate as morpholine decays. Ignition delay times were measured under a wide range of conditions in the same shock tube, covering temperatures form 866 to 1197 K, equivalence ratios of 0.5, 1 and 2, two pressure groups (around 15 and 25 atm) and two oxygen concentration values (4% O_2 and 21% O_2). The current shock tube work extended the morpholine combustion experimental database.

The morpholine reaction set, the model predictions match with the measured fuel decomposition time-histories quite well for the pyrolysis experiments. In terms of ignition delay time results, the model can successfully capture the equivalence ratio dependence near 15 atm. Future shock tube measurements of different species time-histories will help to further improve the current reaction set for even better agreement with experimental data.

As a perspective, consequences of these results for C/H/N/O-containing fuels from biogenic sources should be analyzed with care. The complicated breakdown sequence of morpholine resulting from the polyfunctional fuel structure suggests that an easy correlation cannot be given regarding the potential importance of HCN and NH_3. Because the simultaneous presence of several structures with different hetero-elements at a given nominal mass presents already a challenge to qualitative analysis, studies often do not report a complete species spectrum and quantitative mole fractions. Because most studies of fuel-nitrogen conversion have concentrated on the reactions within the small-nitrogen-species pool and on HCN and NH_3 oxidation, a systematic approach that encompasses the combustion chemistry of functionally different fuel-nitrogen is needed, by analogy to the recent efforts that address the combustion chemistry of oxygenated compounds including the alcohol, ether, and ester families and their hydrocarbon relatives.

12.2.3 Combustion of hypergolic rocket fuels

MMH combustion with RFNA is a highly reactive system with complicated kinetics. As shown through estimates of heats of vaporization, liquid-liquid chemistry for these systems is largely unimportant beyond initial heat generation as the droplets

generate gas quickly upon contact. Instead, gas phase chemistry is likely most important to consider for these hypergolic systems. As such, a new reaction set was developed for gas-phase combustion chemistry of MMH/RFNA.

From observation of the modeling results, MMH is destroyed mainly by abstraction of the central hydrogen atom. The resulting intermediates then are destroyed by abstractions, especially NO_2 and OH abstractions, until CH_3NN is formed, which further reacts to form products N_2, CO, and H_2O. Consequently, NO_2 and OH are the main drivers of reaction. The NO_2 comes from N_2O_4 decomposition and HNO_3 decomposition. OH also comes from the HNO_3 decomposition and is also regenerated through a minor reaction, $NO_2 + H$ ($\rightarrow$ HONO $\rightarrow$ OH + NO). This regeneration allows adiabatic flames with fuel equivalence ratios (Φ) ranging from 0.8 to 1.3 to follow the same combustion reaction pathway.

Further, two reduced sets for MMH/RFNA were developed for use in CFD models. The larger reaction set has 87 species and 482 reactions (down from the full set of 177 species and 1619 reactions) and is able to capture the chemistry of the full set perfectly. A second reduced set of 41 species and 200 reactions was developed for more restricted CFD models and was found to capture many of the same trends as the full mechanism, though ignition delay times were a factor of 15 longer than those calculated in the full set. Use of the more heavily reduced set is cautioned and should consider the longer time delays.

As a less toxic, non-carcinogenic alternative hypergol to MMH, kinetics for TMEDA were estimated and assembled into a new reaction set, including corresponding thermochemistry based on analogous hydrocarbon combustion reactions and quantum

chemistry calculations. From a bond dissociation energy analysis, it is expected that the severance of the C-C bond TMEDA is the most likely thermal dissociation pathway. However, abstraction reactions from TMEDA dominated in TMEDA/RFNA combustion. Subsequent β-scission reactions yield two CH_3NCH_2 molecules for every TMEDA molecule generally, and a corresponding high mole fraction peak of CH_3NCH_2 is observed around time of ignition.

Despite the success of using kinetic analogies for other nitrogen-containing fuels, use of a 2-methylheptane reaction set for analogy appears to have some issues. Mole fraction profiles were not smooth, suggesting instabilities that must stem from the TMEDA reactions since the same characteristics were not observed using the same core set in studies of other fuels. Additionally, intermediate species such as HCN persist for long periods of time (about 100 μs) before being consumed, which is unusual behavior. Future work should consider performing quantum chemistry calculations or explore other options for the basis of analogy to TMEDA.

12.3 Recommendations for future work

While the reaction sets presented in this dissertation have been tested against numerous experimental data sets and have shown to predict experimental mole fraction profiles and reaction pathways reasonably well, additional work is needed to refine the reaction models to make the models more accurate across wider ranges of conditions. Additionally, further focus on heterocyclic compounds and hypergolic rocket fuels could provide better insight to the chemistry of these fuels. The following is a discussion of possible directions for future work in these areas of study.

12.3.1 Directions for developing a small molecule nitrogen chemistry reaction set

Perhaps one of the largest challenges with refining the H/N/O reaction set was selection of which reaction rates to use. With hundreds of reactions, several with numerous possibilities for reaction rate constants, selection of the best rate constants for a wide range of experimental data is both difficult and introduces issues of human bias. Despite the large number of reactions in the H/N/O model, the reaction set is small enough that development of an automated computer program for selection of a best-fit reaction set is possible. Reaction sets could be iteratively generated for each possible combination of reaction rate constants and tested by modeling the experimental data sets described in Chapter 5. Those with the largest relative errors could be eliminated, narrowing the number of possible mechanisms from thousands to a few.

Additionally, obtaining experimental data over a wider range of experiments for H/N/O reaction set validation would be helpful. Of the 12 flame studies, only two had more than six species identified for comparison to the reaction sets. Closer attention to radical species is critical for H/N/O set validation. Expanding the tests to additional types of experiments such as flow reactors would be beneficial as well.

Future work on the new H/C/N/O model is needed on three fronts. First, more reliable experimental data must be obtained for comparison and model validation, as there are too many questions with the current studies and broad enough range of conditions is not sampled. There is extensive opportunity for flame studies in this area. Secondly, the chemistry in the hydrocarbon part of the set needs further testing and validation. Evidence from the study suggests there are issues in the H/C/O chemistry that could possibly affect the H/C/N/O set. Further testing and refinement of that base set

would improve model predictions significantly. Lastly, with a wider range of data for comparison, the H/C/N/O set should be further refined on the same basis as the H/N/O model was refined. Until a large enough experimental data database is assembled however, growth of this part of the model is limited.

12.3.2 Directions for modeling heterocyclic fuels

Assuming that the base H/C/N/O reaction set is fully developed based on the recommendations of the previous section, the largest improvements to the heterocyclic models for THP and morpholine could best be served through additional quantum-chemistry calculations and inclusion of fall-off to the reaction sets for direct fuel decomposition reactions. While estimation techniques were quite successful in the model development for THP and morpholine, many of the intermediate species with the widest discrepancies between the data and the model link directly to fuel decomposition reactions. This deficiency is especially apparent in the morpholine pyrolysis study where analogies to 1,4-dioxane and cyclohexane do not appear sufficient to capture the experimental data.

Also of note is the limited testing of the THP and morpholine reaction sets versus experimental data. Both flame studies were conducted at a single fuel-rich condition. As demonstrated with hydrocarbon fuels, combustion chemistry changes as flame conditions vary from fuel-lean to fuel-rich. Conducting complementary MBMS-flame experiments would be helpful for model development, varying the stoichiometries for these two fuels. Additionally, experimental studies of THP and morpholine, as well as of cyclohexane and piperidine (the THP analog with a single nitrogen in the ring instead of an oxygen) would provide direct comparison of the four analogous fuels to compare the chemistry of these

four six-member cyclic fuels more directly. Since the flames are not at the same conditions, currently the data can only be compared approximately to describe the effects of the addition of heteroatoms to the ring.

12.2.3 Directions for modeling hypergolic rocket fuels

Unfortunately, due to the reactive nature of hypergolic fuels, kinetic studies of these fuels are both difficult and dangerous. Few quantitative data for speciation in MMH/RFNA or TMEDA/RFNA combustion are available. However, greater reliability for the MMH/RFNA and TMEDA/RFNA reaction sets may be obtained through additional quantum-chemistry work. Previous work on MMH combustion either did not consider all abstraction sites from MMH (focusing specifically on abstraction from the central nitrogen) or did not consider key abstraction partners due to the nature of the exotic oxidizer RFNA such as NO, NO_2, NH_2, or NH. Additionally, evidence from the instabilities in the TMEDA modeling work suggests that analogies to 2-methylheptane are not appropriate for modeling TMEDA combustion. These two reaction sets would benefit greatly from quantum-chemistry calculations to determine more accurate kinetic rate expressions for the decomposition of these fuels.

APPENDIX A

THERMODYNAMIC DATABASE

The following the thermodynamic database that may be used for all reaction sets developed in the work of this dissertation. Details on the format may be found in Chapter 4.

```
THERMO
   300.000  1000.000  5000.000
H                 L 7/88H   1              G   200.000  3500.000  1000.000    1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22    2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15    3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01                   4
H2                TPIS78H   2              G   200.000  3500.000  1000.000    1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14    2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05    3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01                   4
HE REF ELEMENT    g 5/97HE 1.   0.   0.   0.G   200.000  6000.000 1000.       1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01 0.00000000E+00    4
C                 L11/88C   1              G   200.000  3500.000  1000.000    1
 2.49266888E+00 4.79889284E-05-7.24335020E-08 3.74291029E-11-4.87277893E-15    2
 8.54512953E+04 4.80150373E+00 2.55423955E+00-3.21537724E-04 7.33792245E-07    3
-7.32234889E-10 2.66521446E-13 8.54438832E+04 4.53130848E+00                   4
CH                JUN03 C   1H   1          G   200.000  6000.000  1000.000    1
 0.25209369E+01 0.17653639E-02-0.46147660E-06 0.59289675E-10-0.33474501E-14    2
 0.70946769E+05 0.74051829E+01 0.34897583E+01 0.32432160E-03-0.16899751E-05    3
 0.31628420E-08-0.14061803E-11 0.70612646E+05 0.20842841E+01 0.71658188E+05    4
N                 120186N   1              G   300.00   5000.00  1000.00      1
 0.02450268E+02 0.01066146E-02-0.07465337E-06 0.01879652E-09-0.01025984E-13    2
 0.05611604E+06 0.04448758E+02 0.02503071E+02-0.02180018E-03 0.05420529E-06    3
-0.05647560E-09 0.02099904E-12 0.05609890E+06 0.04167566E+02                   4
CH2               JUN03 C   1H   2          G   200.000  6000.000  1000.000    1
 0.31463189E+01 0.30367126E-02-0.99647444E-06 0.15048358E-09-0.85733552E-14    2
```

```
 0.46041260E+05 0.47234171E+01 0.37175785E+01 0.12739126E-02 0.21734725E-05    3
-0.34885850E-08 0.16520887E-11 0.45872387E+05 0.17529794E+01 0.47050492E+05    4
CH2SING           JUN03 C   1H   2          G   200.000  6000.000  1000.000    1
 0.31350169E+01 0.28959393E-02-0.81666809E-06 0.11357270E-09-0.63626284E-14    2
 0.50504050E+05 0.40603062E+01 0.41933133E+01-0.23310518E-02 0.81567645E-05    3
-0.66298598E-08 0.19323320E-11 0.50366225E+05-0.74673431E+00 0.51572728E+05    4
NH                      N   1H   1    0    0G   200.00   6000.00  1000.0      1
 0.27836929E+01 0.13298429E-02-0.42478047E-06 0.78348504E-10-0.55044470E-14    2
 0.42134514E+05 0.57407798E+01 0.34929084E+01 0.31179197E-03-0.14890484E-05    3
 0.24816442E-08-0.10356967E-11 0.41894294E+05 0.18483277E+01 0.42940822E+05    4
CH3               JUN03 C   1H   3          G   200.000  6000.000  1000.000    1
 0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-13    2
 0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-05    3
-0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01 0.17643935E+05    4
O                 L 1/90O   1              G   200.000  3500.000  1000.000    1
 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15    2
 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00                   4
NH2               121686N   1H   2          G   300.00   5000.00  1000.00     1
 0.02961311E+02 0.02932699E-01-0.09063600E-05 0.01617257E-08-0.01204200E-12    2
 0.02191977E+06 0.05777878E+02 0.03432493E+02 0.03299540E-01-0.06613600E-04    3
 0.08590947E-07-0.03572047E-10 0.02177228E+06 0.03090111E+02                   4
CH4               L 8/88C   1H   4          G   200.000  3500.000  1000.000    1
 7.48514950E-02 1.33909467E-02-5.73285809E-06 1.22292535E-09-1.01815230E-13    2
-9.46834459E+03 1.84373180E+01 5.14987613E+00-1.36709788E-02 4.91800599E-05    3
-4.84743026E-08 1.66693956E-11-1.02466476E+04-4.64130376E+00                   4
OH                JUN03 O   1H   1          G   200.000  6000.000  1000.000    1
 0.28385303E+01 0.11074129E-02-0.29400021E-06 0.42069873E-10-0.24228989E-14    2
 0.36978081E+04 0.58449465E+01 0.39919842E+01-0.24010666E-02 0.46166403E-05    3
-0.38791631E-08 0.13631950E-11 0.33688984E+04-0.10399848E+00 0.44861538E+04    4
NH3               121386N   1H   3          G   300.00   5000.00  1000.00     1
 0.02461904E+02 0.06059166E-01-0.02004977E-04 0.03136003E-08-0.01938317E-12    2
-0.06493270E+05 0.07472097E+02 0.02204352E+02 0.01011476E+00-0.01465265E-03    3
 0.01447235E-06-0.05328509E-10-0.06525488E+05 0.08127138E+02                   4
H2O               L 8/89H   2O   1          G   200.000  3500.000  1000.000    1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11 1.68200992E-14    2
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-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03 6.52040211E-06    3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01                   4
C2H               L 1/91C   2H   1          G   200.000  3500.000  1000.000    1
 3.16780652E+00 4.75221902E-03-1.83787077E-06 3.04190252E-10-1.77232770E-14    2
 6.71210650E+04 6.63589475E+00 2.88965733E+00 1.34099611E-02-2.84769501E-05    3
 2.94791045E-08-1.09331511E-11 6.68393932E+04 6.22296438E+00                   4
CN                      C   1N   1    0    0G   200.00   6000.00  1000.0      1
 3.39912871E+00 7.46548271E-04-1.41493637E-07 1.86747261E-11-1.26032174E-15    2
 5.14665281E+04 4.67150296E+00 3.61256066E+00-9.53015376E-04 2.13757148E-06    3
-3.05000108E-10-4.70518899E-13 5.15179601E+04 3.98240466E+00 5.25707468E+04    4
C2H2              L 1/91C   2H   2          G   200.000  3500.000  1000.000    1
 4.14756964E+00 5.96166664E-03-2.37294852E-06 4.67412171E-10-3.61235213E-14    2
 2.59359992E+04-1.23028121E+00 8.08681094E-01 2.33615629E-02-3.55171815E-05    3
 2.80152437E-08-8.50072974E-12 2.64289807E+04 1.39397051E+01                   4
H2CC              L12/89H   2C   2    0    0G   200.000  6000.000  1000.000    1
 0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-13    2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-05    3
-0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01 0.49887266E+05    4
HCN               110193H   1C   1N   1     G  0300.00   4000.00  1000.00     1
 0.03426457E+02 0.03924190E-01-0.01601138E-04 0.03161966E-08-0.02432850E-12    2
 0.01485552E+06 0.03607795E+02 0.02417787E+02 0.09031856E-01-0.01107727E-03    3
 0.07980141E-07-0.02311141E-10 0.01501044E+06 0.08222891E+02                   4
HNC        46.8         H   1C   1N   1     G  0300.00   5000.00  1500.00     1
 0.05283464E+02 0.01092476E-01-0.01170865E-05-0.02308672E-09 0.03950673E-13    2
 2.16142302E+04-0.06388218E+02 0.03592377E+02 0.05561340E-01-0.05936823E-04    3
 0.03782329E-07-0.09365092E-11 2.22826802E+04 0.02732160E+02                   4
C2H3                    0C   2H   3    0    0G   200.000  5000.000 1100.00    0 1
 0.44767928E+01 0.72667722E-02-0.25458602E-05 0.40524242E-09-0.24034979E-13    2
 0.33868175E+05-0.70126031E-01 0.23280072E+01 0.99989781E-02 0.65780491E-06    3
-0.57360094E-08 0.23261669E-11 0.34648342E+05 0.11898753E+02                   4
CO                TPIS79C   1O   1          G   200.000  3500.000  1000.000    1
 2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-2.03647716E-14    2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04 1.01681433E-06    3
 9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00                   4
N2        BUR0302 G 8/02N   2    0    0    0G   200.00   6000.00  1000.       1
 2.95257637E+00 1.39690040E-03-4.92631603E-07 7.86010195E-11-4.60755204E-15    2
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-9.23948688E+02 5.87188762E+00 3.53100528E+00-1.23660988E-04-5.02999433E-07    3
 2.43530612E-09-1.40881235E-12-1.04697628E+03 2.96747038E+00 0.00000000E+00    4
CHNH               41687C   1H   2N   1     G  0300.00   4000.00  1000.00      1
 0.04923293E+02 0.03332897E-01-0.03370897E-05-0.01901619E-08 0.03531825E-12    2
 0.03132669E+06-0.01632509E+02 0.02759456E+02 0.06103387E-01 0.07713149E-05    3
-0.02063094E-07 0.01931920E-11 0.03217247E+06 0.01057489E+03                   4
NCH2               41687H   2C   1N   1     G  0300.00   4000.00  1000.00      1
 0.05209703E+02 0.02969291E-01-0.02855589E-05-0.01635550E-08 0.03043259E-12    2
 0.02767711E+06-0.04444478E+02 0.02851661E+02 0.05695233E-01 0.01071140E-04    3
-0.01622612E-07-0.02351108E-11 0.02863782E+06 0.08992751E+02                   4
C2H4              L 1/91C   2H   4          G   200.000  3500.000  1000.000    1
 2.03611116E+00 1.46454151E-02-6.71077915E-06 1.47222923E-09-1.25706061E-13    2
 4.93988614E+03 1.03053693E+01 3.95920148E+00-7.57052247E-03 5.70990292E-05    3
-6.91588753E-08 2.69884373E-11 5.08977593E+03 4.09733096E+00                   4
HCO               L12/89H   1C   1O   1     G   200.000  3500.000  1000.000    1
 2.77217438E+00 4.95695526E-03-2.48445613E-06 5.89161778E-10-5.33508711E-14    2
 4.01191815E+03 9.79834492E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00                   4
NNH               T 1/06N   2H   1    0    0G   200.000  6000.000 1000.       1 ! burcat
2010
 3.42744423E+00 3.23295234E-03-1.17296299E-06 1.90508356E-10-1.14491506E-14    2
 2.88067740E+04 6.39209233E+00 4.25474632E+00-3.45098298E-03 1.37788699E-05    3
-1.33263744E-08 4.41023397E-12 2.88323793E+04 3.28551762E+00 3.02815661E+04    4
CH2NH       MELIUS 88   H   3C   1N   1    0G   300.000  5000.000 1577.000    01 ! DB00
 4.54737795E+00 7.17720948E-03-2.47935299E-06 3.87692351E-10-2.26113075E-14    2
 8.64056516E+03-1.16687427E+00 2.81849510E+00 5.11983235E-03 6.38887146E-06    3
-6.61374671E-09 1.65531940E-12 9.88442597E+03 1.03390629E+01                   4
C2H5              L12/92C   2H   5          G   200.000  3500.000  1000.000    1
 1.95465642E+00 1.73972722E-02-7.98206668E-06 1.75217689E-09-1.49641576E-13    2
 1.28575200E+04 1.34624343E+01 4.30646568E+00-4.18658892E-03 4.97142807E-05    3
-5.99126606E-08 2.30509004E-11 1.28416265E+04 4.70720924E+00                   4
NO                RUS 89N   1O   1    0    0G   200.00   6000.00  1000.       1 !
 3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15    2
9.89456954E+03 6.36900469E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05    3
-9.34055507E-09 2.80554874E-12 9.81823786E+03 2.28060952E+00                   4 !Cp
[BURCAT]
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CH2O              L 8/88H   2C   1O   1     G   200.000  3500.000  1000.000    1
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14    2
-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05    3
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01                   4
N2H2              121286N   2H   2          G   300.00   5000.00  1000.00      1
 0.03371185E+02 0.06039968E-01-0.02303854E-04 0.04062789E-08-0.02713144E-12    2
 0.02418172E+06 0.04980585E+02 0.01617999E+02 0.01306312E+00-0.01715712E-03    3
 0.01605608E-06-0.06093639E-10 0.02467526E+06 0.01379467E+03                   4
H2NN  DBOZ00M93/JBPM3 96N   2H   2    0    0G   300.000  5000.000 1695.000     1
 3.13531032E+00 5.68632569E-03-1.93983467E-06 3.01290501E-10-1.74978144E-14    2
 3.33678346E+04 7.04815840E+00 2.88544262E+00 4.69495999E-03 7.01983230E-07    3
-1.53359038E-09 3.79345858E-13 3.36030690E+04 8.95096779E+00                   4
CH3NH       THERM92     H   4C   1N   1    0G   300.000  5000.000 1404.000    11 ! DB00
 4.90528413E+00 8.50385569E-03-2.82356461E-06 4.29267836E-10-2.45297886E-14    2
 1.94541503E+04-1.35290137E+00 1.53882571E+00 1.62436539E-02-9.89573425E-06    3
 3.49954504E-09-5.53823621E-13 2.06715086E+04 1.68295527E+01                   4
CH2NH2      THERM92     H   4C   1N   1    0G   300.000  5000.000 1397.000    11 ! DB00
 6.11432288E+00 7.69126269E-03-2.59025729E-06 3.97713575E-10-2.28883272E-14    2
 1.55835138E+04-8.93053780E+00 2.56157769E+00 1.60730713E-02-1.05960335E-05    3
 4.07638829E-09-6.95570548E-13 1.68563722E+04 1.01987687E+01                   4
C2H6              L 8/88C   2H   6          G   200.000  3500.000  1000.000    1
 1.07188150E+00 2.16852677E-02-1.00256067E-05 2.21412001E-09-1.90002890E-13    2
-1.14263932E+04 1.51156107E+01 4.29142492E+00-5.50154270E-03 5.99438288E-05    3
-7.08466285E-08 2.68685771E-11-1.15222055E+04 2.66682316E+00                   4
HNO           ATcT/A     H   1N   1O   1    0G   200.00   6000.00  1000.       1 !BURCAT
 3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07602668E-15    2
 1.17654289E+04 7.64513642E+00 4.53525574E+00-5.68543377E-03 1.85198540E-05    3
-1.71881225E-08 5.55818157E-12 1.16110981E+04 1.74318356E+00                   4 !
HON           HF MELIUS93H   1N   1O   1    0G   300.00   5000.00  1671.000    01
 3.78577430E+00 2.86062728E-03-1.02423922E-06 1.64463139E-10-9.77943616E-15    2
 2.93319701E+04 3.12193293E+00 3.33656431E+00 2.67682939E-03 5.61801303E-07    3
-1.11362279E-09 2.84076438E-13 2.95979751E+04 5.96343188E+00                   4
CH2OH             JUN03 C   1H   3O   1     G   200.000  6000.000  1000.000    1
 0.50931437E+01 0.59476126E-02-0.20649746E-05 0.32300817E-09-0.18812590E-13    2
-0.40340964E+04-0.18469149E+01 0.44783436E+01-0.13507031E-02 0.27848498E-04    3
-0.36486906E-07 0.14790745E-10-0.35007289E+04 0.33091350E+01-0.20446277E+04    4
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CH3O              JUN03 C   1H   3O   1     G   200.000  6000.000  1000.000    1
 0.47577924E+01 0.74414247E-02-0.26970518E-05 0.43809050E-09-0.26353710E-13    2
 0.37811194E+03-0.19668003E+01 0.37118050E+01-0.28046331E-02 0.37655097E-04    3
-0.47307209E-07 0.18658842E-10 0.12956976E+04 0.65724086E+01 0.25257166E+04    4
N2H3              120186N   2H   3          G   300.00   5000.00  1000.00      1
 0.04441846E+02 0.07214271E-01-0.02495684E-04 0.03920565E-08-0.02298950E-12    2
 0.01664221E+06-0.04275205E+01 0.03174204E+02 0.04715907E-01 0.01334867E-03    3
-0.01919685E-06 0.07487564E-10 0.01727270E+06 0.07557224E+02                   4
CH3NH2      SWS         H   5C   1N   1    0G   300.000  5000.000 1387.000    11 ! DB00
 5.23365618E+00 1.08525479E-02-3.65205276E-06 5.60552543E-10-3.22553444E-14    2
-5.52829576E+03-5.21507359E+00 1.69170293E+00 1.60389160E-02-4.99028441E-06    3
-3.83481304E-10 3.57345746E-13-3.94057426E+03 1.49835076E+01                   4
O2                TPIS89O   2              G   200.000  3500.000  1000.000    1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14    2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06    3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00                   4
NH2O              102290H   2N   1O   1     G   300.00   4000.00  1500.00      1
 0.05673346E+02 0.02298837E-01-0.01774446E-05-0.01103482E-08 0.01859762E-12    2
 0.05569325E+05-0.06153540E+02 0.02530590E+02 0.08596035E-01-0.05471030E-04    3
 0.02276249E-07-0.04648073E-11 0.06868030E+05 0.01126651E+03                   4
HNOH trans & Equ  T11/11H   2N   1O   1    0G   200.000  6000.000 1000.       1
 3.98321933E+00 4.88846374E-03-1.65086637E-06 2.55371446E-10-1.48308561E-14    2
 1.05780106E+04 3.62582838E+00 3.95608248E+00-3.02611020E-03 2.56874396E-05    3
-3.15645120E-08 1.24084574E-11 1.09199790E+04 5.55950983E+00 1.21354115E+04    4
CH3OH             L 8/88C   1H   4O   1     G   200.000  3500.000  1000.000    1
 1.78970791E+00 1.40938292E-02-6.36500835E-06 1.38171085E-09-1.17060220E-13    2
-2.53748747E+04 1.45023623E+01 5.71539582E+00-1.52309129E-02 6.52441155E-05    3
-7.10806889E-08 2.61352698E-11-2.56427656E+04-1.50409823E+00                   4
N2H4              121286N   2H   4          G   300.00   5000.00  1000.00      1
 0.04977317E+02 0.09595519E-01-0.03547639E-04 0.06124299E-08-0.04029795E-12    2
 0.09341219E+05-0.02962990E+02 0.06442606E+00 0.02749730E+00-0.02899451E-03    3
 0.01745240E-06-0.04422282E-10 0.01045192E+06 0.02127789E+03                   4
NH2OH        JWB/SAND88 N   1H   3O   1    0G   300.000  5000.000 1412.000    1
 5.12276969E+00 5.73428233E-03-1.86277359E-06 2.78938290E-10-1.57685159E-14    2
-7.42648110E+03-3.34064363E+00 1.59842441E+00 1.54722273E-02-1.24132635E-05    3
 5.50996715E-09-1.00114333E-12-6.34935610E+03 1.50585859E+01                   4
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HO2               L 5/89H   1O   2          G   200.000  3500.000  1000.000    1
 4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-1.07908535E-14    2
 1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05    3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00                   4
H2O2              L 7/88H   2O   2          G   200.000  3500.000  1000.000    1
 4.16500285E+00 4.90831694E-03-1.90139225E-06 3.71185986E-10-2.87908305E-14    2
-1.78617877E+04 2.91615662E+00 4.27611269E+00-5.42822417E-04 1.67335701E-05    3
-2.15770813E-08 8.62454363E-12-1.77025821E+04 3.43505074E+00                   4
C3H2              121686C   3H   2          G  0300.00   5000.00  1000.00     1
 0.06530853E+02 0.05870316E-01-0.01720777E-04 0.02127498E-08-0.08291910E-13    2
 0.05115214E+06-0.01122728E+03 0.02691077E+02 0.01480366E+00-0.03250551E-04    3
-0.08644363E-07 0.05284878E-10 0.05219072E+06 0.08757391E+02                   4
C3H3              T 5/99C   3H   3    0    0G   200.000  6000.000              1
 7.14221880E+00 7.61902005E-03-2.67459950E-06 4.24914801E-10-2.51475415E-14    2
 3.89087427E+04-1.25848436E+01 1.35110927E+00 3.27411223E-02-4.73827135E-05    3
 3.76309808E-08-1.18540923E-11 4.01057783E+04 1.52058924E+01 4.16139977E+04    4
AR                120186AR  1               G   300.000  5000.000  1000.000    1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02                   4
NCN               103190C   1N   2          G  0300.00   4000.00  1500.00     1
 0.06652121E+02 0.06108034E-02-0.01389727E-05 0.02695549E-10 0.01669944E-13    2
 0.05172403E+06-0.01138517E+03 0.03101270E+02 0.09981674E-01-0.09920701E-04    3
 0.04758919E-07-0.08968626E-11 0.05285757E+06 0.07317579E+02                   4
AC3H4             L 8/89C   3H   4    0    0G   200.000  6000.000              1
 0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-13    2
 0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-04    3
-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02 0.22962267E+05    4
PC3H4             T 2/90H   4C   3    0    0G   200.000  6000.000              1
 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-13    2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-05    3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01 0.22302059E+05    4
HCCO              SRIC91H   1C   2O   1     G   300.00   4000.00   1000.000    1
 0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-0.19407832E-13    2
 0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-0.23729101E-04    3
 0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02                   4
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HCNN              SRI/94C   1N   2H   1     G   300.000  5000.000  1000.000    1
 0.58946362E+01 0.39895959E-02-0.15982380E-05 0.29249395E-09-0.20094686E-13    2
 0.53452941E+05-0.51030502E+01 0.25243194E+01 0.15960619E-01-0.18816354E-04    3
 0.12125540E-07-0.32357378E-11 0.54261984E+05 0.11675870E+02                   4
CH2CNH            NL0512H   3C   2N   1    0g    200.00  5000.00  1000.00      1
 5.66216832E+00 9.26107024E-03-3.48651570E-06 6.07628542E-10-4.01043359E-14    2
 1.97095267E+04-5.55742628E+00 1.86949849E+00 1.78925908E-02-5.52740583E-06    3
-7.02394385E-09 4.78548967E-12 2.08046216E+04 1.43621039E+01                   4
AC3H5             PD5/98C   3H   5    0    0G   300.000  3000.000             1
 0.65007877E+01 0.14324731E-01-0.56781632E-05 0.11080801E-08-0.90363887E-13    2
 0.17482449E+05-0.11243050E+02 0.13631835E+01 0.19813821E-01 0.12497060E-04    3
-0.33355555E-07 0.15846571E-10 0.19245629E+05 0.17173214E+02                   4
TC3H5             PD5/98C   3H   5    0    0G   300.000  3000.000             1
 0.54255528E+01 0.15511072E-01-0.56678350E-05 0.79224388E-09-0.16878034E-13    2
 0.27843027E+05-0.33527184E+01 0.17329209E+01 0.22394620E-01-0.51490611E-05    3
-0.67596466E-08 0.38253211E-11 0.29040498E+05 0.16568878E+02                   4
SC3H5             PD5/98C   3H   5    0    0G   300.000  3000.000             1
 0.53725281E+01 0.15780509E-01-0.59922850E-05 0.93089664E-09-0.36550966E-13    2
 0.29614760E+05-0.34186478E+01 0.91372931E+00 0.26432343E-01-0.11758950E-04    3
-0.23035678E-08 0.27715488E-11 0.30916867E+05 0.19989269E+02                   4
NCO                     C   1H   0N   1O   1G   300.00   5000.00  1000.00     1
 0.51511740E+01 0.25379660E-02-0.10948080E-05 0.21129870E-09-0.15056170E-13    2
 0.13463290E+05-0.33718940E+01 0.45124190E+01-0.32980770E-02 0.21963190E-04    3
-0.26656140E-07 0.10269190E-10 0.13994080E+05 0.17322690E+01                   4
CH2CO             L 5/90C   2H   2O   1     G   200.000  3500.000  1000.000    1
 4.51129732E+00 9.00359745E-03-4.16939635E-06 9.23345882E-10-7.94838201E-14    2
-7.55105311E+03 6.32247205E-01 2.13583630E+00 1.81188721E-02-1.73947474E-05    3
 9.34397568E-09-2.01457615E-12-7.04291804E+03 1.22156480E+01                   4
CH2CHNH           NL0512H   4C   2N   1    0g    200.00  5000.00  1000.00      1
 5.50102729E+00 1.17702172E-02-4.46657421E-06 7.83031653E-10-5.19089322E-14    2
 2.19556791E+04-3.60212879E+00 3.10187116E+00 6.36614579E-03 3.03829741E-05    3
-4.49078917E-08 1.85867428E-11 2.31285075E+04 1.15129893E+01                   4
C3H6              120186C   3H   6          G  0300.00   5000.00  1000.00      1
 0.06732257E+02 0.01490834E+00-0.04949899E-04 0.07212022E-08-0.03766204E-12    2
-0.09235703E+04-0.01331335E+03 0.01493307E+02 0.02092518E+00 0.04486794E-04    3
-0.01668912E-06 0.07158146E-10 0.01074826E+05 0.01614534E+03                   4
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HCNO                    C   1H   1N   1O   1G   300.00   5000.00  1000.00      1
 0.60356200E+01 0.40593330E-02-0.15887770E-05 0.29204810E-09-0.20230570E-13    2
 0.18339880E+05-0.91024050E+01 0.24825640E+01 0.14813560E-01-0.13687980E-04    3
 0.60469050E-08-0.87705910E-12 0.19281540E+05 0.90325330E+01                   4
HNCO                    C   1H   1N   1O   1G   300.00   5000.00  1000.00      1
 0.53288440E+01 0.42143370E-02-0.16473930E-05 0.30184220E-09-0.20844800E-13    2
-0.15892150E+05-0.34500500E+01 0.34991880E+01 0.62636580E-02 0.31257680E-05    3
-0.86252000E-08 0.39133720E-11-0.15233280E+05 0.67449930E+01                   4
HOCN                    C   1H   1N   1O   1G   300.00   5000.00  1000.00      1
 0.48074750E+01 0.41918370E-02-0.16199240E-05 0.29436220E-09-0.20214190E-13    2
-0.33443110E+04 0.84660710E+00 0.47161980E+01-0.12249760E-02 0.15769070E-04    3
-0.18447440E-07 0.68406900E-11-0.30276870E+04 0.27314860E+01                   4
CH3CO             JUN03 C   2H   3O   1    0G   200.000  6000.000  1000.0      1
 0.53137165E+01 0.91737793E-02-0.33220386E-05 0.53947456E-09-0.32452368E-13    2
-0.36450414E+04-0.16757558E+01 0.40358705E+01 0.87729487E-03 0.30710010E-04    3
-0.39247565E-07 0.15296869E-10-0.26820738E+04 0.78617682E+01-0.12388039E+04    4
CH2CHO            SAND86O   1H   3C   2     G   300.000  5000.000  1000.000    1
 0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12    2
 0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04    3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02                   4
CH3NN    CH3-N=N  T01/07C  1.H  3.N  2.   0.G   200.000  6000.000 1000.       1
 5.03058624E+00 1.01655807E-02-3.80821408E-06 6.28676801E-10-3.81266093E-14    2
 2.60782020E+04-1.37768696E+00 3.03556733E+00 7.89116568E-03 1.45352429E-05    3
-2.24777249E-08 8.99425199E-12 2.70660675E+04 1.09501412E+01 2.84101033E+04    4
nC3H7             P11/94C   3H   7    0    0G   300.000  3000.000             1
 0.77097479E+01 0.16031485E-01-0.52720238E-05 0.75888352E-09-0.38862719E-13    2
 0.79762236E+04-0.15515297E+02 0.10491173E+01 0.26008973E-01 0.23542516E-05    3
-0.19595132E-07 0.93720207E-11 0.10312346E+05 0.21136034E+02                   4
iC3H7             P11/94C   3H   7    0    0G   300.000  3000.000             1
 0.65192741E+01 0.17220104E-01-0.57364217E-05 0.84130732E-09-0.44565913E-13    2
 0.73227193E+04-0.90830215E+01 0.14449199E+01 0.20999112E-01 0.77036222E-05    3
-0.18476253E-07 0.71282962E-11 0.94223724E+04 0.20116317E+02                   4
CO2               L 7/88C   1O   2          G   200.000  3500.000  1000.000    1
 3.85746029E+00 4.41437026E-03-2.21481404E-06 5.23490188E-10-4.72084164E-14    2
-4.87591660E+04 2.27163806E+00 2.35677352E+00 8.98459677E-03-7.12356269E-06    3
 2.45919022E-09-1.43699548E-13-4.83719697E+04 9.90105222E+00                   4
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N2O               121286N   2O   1          G   300.00   5000.00  1000.00      1
 0.04718977E+02 0.02873714E-01-0.01197496E-04 0.02250552E-08-0.01575337E-12    2
 0.08165811E+05-0.01657250E+02 0.02543058E+02 0.09492193E-01-0.09792775E-04    3
 0.06263845E-07-0.01901826E-10 0.08765100E+05 0.09511222E+02                   4
C2H4O             J 9/65C   2H   4O   1    0G   300.000  5000.000             1
 0.59249249E 01 0.11120714E-01-0.37434083E-05 0.55413918E-09-0.29549886E-13    2
-0.93028008E 04-0.93792849E 01-0.24173594E 00 0.20761095E-01 0.21481201E-05    3
-0.16948157E-07 0.81075771E-11-0.71720117E 04 0.24432190E 02                   4
CH3CHO            L 8/88C   2H   4O   1     G   200.000  6000.000  1000.000    1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01                   4
CH3NNH                 0C   1H   4N   2O   0G   200.000  6000.000 1000.00      1
 5.48334026D+00 1.17117818D-02-4.12106147D-06 6.54262200D-10-3.86199590D-14    2
 1.86890527D+04-4.73384237D+00 3.51484036D+00 5.56200324D-03 2.14472257D-05    3
-2.41589770D-08 7.32461054D-12 1.99403457D+04 8.65997982D+00                   4
C3H8              P11/94C   3H   8    0    0G   300.000  3000.000             1
 0.75244152E+01 0.18898282E-01-0.62921041E-05 0.92161457E-09-0.48684478E-13    2
-0.16564394E+05-0.17838375E+02 0.92851093E+00 0.26460566E-01 0.60332446E-05    3
-0.21914953E-07 0.94961544E-11-0.14057907E+05 0.19225538E+02                   4
HOCO              103190C   1H   1O   2     G  0300.00   4000.00  1500.00      1
 0.07517634E+02 0.01259029E-01-0.01910901E-05-0.03136391E-09 0.07547673E-13    2
-0.02634121E+06-0.01448392E+03 0.02285122E+02 0.01351435E+00-0.01160407E-03    3
 0.05047011E-07-0.09032231E-11-0.02448416E+06 0.01367874E+03                   4
HNNO          MELIUS    N   2H   1O   1    0G   300.000  5000.000 1389.000     1
 6.24922910E+00 3.26983002E-03-1.14794284E-06 1.81383141E-10-1.06538637E-14    2
 2.53822106E+04-7.09495778E+00 2.40143922E+00 1.26718648E-02-1.00828306E-05    3
 4.10522736E-09-6.79228705E-13 2.66782646E+04 1.34257436E+01                   4
CH3NO             103190C   1H   3N   1O   1G  0300.00   4000.00  1500.00      1
 0.08820547E+02 0.03706233E-01-0.02894741E-05-0.01897910E-08 0.03237544E-12    2
 0.05362862E+05-0.02213220E+03 0.02109955E+02 0.01517822E+00-0.07071789E-04    3
 0.01510611E-07-0.01604204E-11 0.08293612E+05 0.01569702E+03                   4
C2H5O            JUN03  C   2O   1H   5     G   200.000  6000.000 1000.00      1
 0.66889982E+01 0.13125676E-01-0.47038840E-05 0.75858552E-09-0.45413306E-13    2
-0.47457832E+04-0.96983755E+01 0.43074268E+01 0.64147205E-02 0.31139714E-04    3
-0.43314083E-07 0.17276184E-10-0.34027524E+04 0.59025837E+01-0.16357022E+04    4
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CH3NNH2                0C   1H   5N   2O   0G   200.000  6000.000 1000.00      1
 6.48248625D+00 1.31416200D-02-4.55408099D-06 7.15495219D-10-4.19235501D-14    2
 2.18344199D+04-9.10020638D+00 2.89725447D+00 1.52571928D-02 5.46573210D-06    3
-1.13299263D-08 3.45334525D-12 2.33342324D+04 1.16815443D+01                   4
HNNNH2      MOPAC/JWB   N   3H   3    0    0G   300.000  5000.000 1387.000     1
 6.69002957E+00 7.47314756E-03-2.57645360E-06 4.02077699E-10-2.34100069E-14    2
 2.41665871E+04-1.12237235E+01 1.77934210E+00 1.84512489E-02-1.22068382E-05    3
 4.40169354E-09-6.88479465E-13 2.59657722E+04 1.53992810E+01                   4
NO2               L 7/88N   1O   2    0    0G   200.00   6000.00  1000.        1 !
 4.88475400E+00 2.17239550E-03-8.28069090E-07 1.57475100E-10-1.05108950E-14    2
 2.29397777E+03-1.17416951E-01 3.94403120E+00-1.58542900E-03 1.66578120E-05    3
-2.04754260E-08 7.83505640E-12 2.87409757E+03 6.31199190E+00                   4 !Cp
[BURCAT]
NH2NO  H2NN=O     T 1/12H   2N   2O   1    0G   200.000  6000.000 1000.        1
 5.78592771E+00 6.03964151E-03-2.08624357E-06 3.28153040E-10-1.92960549E-14    2
 7.61382696E+03-5.32127808E+00 3.68835855E+00 5.97978170E-03 1.22601857E-05    3
-2.07157226E-08 8.83557926E-12 8.44917678E+03 6.85576793E+00 9.88619462E+03    4
NHNHO           M/B686  N   2H   2O   1    0G   300.000  5000.000 1382.000     1
 6.87844514E+00 5.97768876E-03-2.32835297E-06 3.91753162E-10-2.40352995E-14    2
 9.95321692E+03-1.33617968E+01 5.11596626E-01 1.95396787E-02-1.31481264E-05    3
 4.26547517E-09-5.54657119E-13 1.23230195E+04 2.13441672E+01                   4
CH3NHNH2               0C   1H   6N   2    0G   298.150  6000.000 1000.00      1
 6.46195602D+00 1.54661452D-02-5.29188310D-06 8.22877488D-10-4.78182997D-14    2
 8.08517920D+03-1.06506405D+01-1.55617356D-01 3.41164172D-02-3.21289044D-05    3
 2.50164209D-08-9.43703969D-12 1.01527490D+04 2.41129608D+01                   4
HONO          RUS 89     H   1N   1O   2    0G   200.00   6000.00  1000.        1 !BURCAT
 0.57919018E+01 0.36515212E-02-0.12928936E-05 0.20688716E-09-0.12315254E-13    2
-0.11565589E+05-0.40558233E+01 0.32141709E+01 0.81276869E-02 0.16602559E-05    3
-0.95285182E-08 0.48715058E-11-0.10753237E+05 0.98219504E+01-0.94355439E+04    4 !
HNO2          103190     H   1N   1O   2     G   300.00   4000.00  1500.00      1
!RAS/GLA08a
 6.47963000E+00 1.99527400E-03-1.74038700E-07-9.69587200E-11 1.70148000E-14    2 !
-7.80950291E+03-1.06771518E+01 1.93483800E+00 1.01003600E-02-4.96461600E-06    3
 8.70112000E-10-2.32413500E-15-5.91571591E+03 1.47282082E+01                   4 !
HNOO        MELIUS88     N   1H   1O   2    0G   300.000  5000.000 1685.000     1
 6.22843297E+00 3.99232107E-03-1.71329587E-06 3.09055124E-10-1.99408751E-14    2
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 2.57303316E+04-7.82004870E+00 2.82368890E+00 9.26020228E-03-3.10307876E-06    3
-6.57987763E-10 3.64688961E-13 2.71092460E+04 1.13391387E+01                    4
NH2NHO     m93/jwb96pm3 N   2H   3O   1    0G   300.000  5000.000 1405.000     1
 6.76839963E+00 6.93278545E-03-2.28605862E-06 3.45978133E-10-1.97094457E-14    2
 1.42869505E+04-9.16405703E+00 2.56091917E+00 1.79916569E-02-1.37740397E-05    3
 5.87277161E-09-1.04140760E-12 1.56384602E+04 1.30177571E+01                    4
HONHO       M/JB86      N   1H   2O   2    0G   300.000  5000.000 1416.000     1
 9.01087354E+00 3.23941301E-03-1.18327845E-06 1.91943898E-10-1.14815574E-14    2
-1.48028338E+03-2.30114112E+01 1.05169569E-02 2.58437554E-02-2.25307323E-05    3
 9.16861679E-09-1.42700071E-12 1.39517739E+03 2.46124525E+01                    4
C4H               P 1/93C   4H   1    0    0G   300.000  3000.000              1
 0.77697593E+01 0.49829976E-02-0.17628546E-05 0.28144284E-09-0.16689869E-13    2
 0.94345900E+05-0.14165274E+02 0.13186295E+01 0.38582956E-01-0.71385623E-04    3
 0.65356359E-07-0.22617666E-10 0.95456106E+05 0.15567583E+02                    4
C4H2              P 1/93C   4H   2    0    0G   300.000  3000.000              1
 0.86637708E+01 0.67247189E-02-0.23593397E-05 0.37506380E-09-0.22230940E-13    2
 0.53252275E+05-0.21093503E+02-0.39201030E+00 0.51937565E-01-0.91737340E-04    3
 0.80471986E-07-0.26898218E-10 0.54845266E+05 0.20957794E+02                    4
iC4H3                  0C   4H   3    0    0G   200.000  5000.000 1200.00    0 1
 0.87092233E+01 0.88631021E-02-0.31303011E-05 0.50137975E-09-0.29878650E-13    2
 0.57500575E+05-0.18391950E+02 0.37694948E+01 0.23256639E-01-0.18531943E-04    3
 0.76188028E-08-0.12128742E-11 0.58835310E+05 0.69616708E+01                    4
nC4H3              82489C   4H   3          G  0300.00   4000.00  1000.00      1
 0.10752738E+02 0.05381153E-01-0.05549637E-05-0.03052266E-08 0.05761740E-12    2
 0.61979123E+05-0.02973025E+03 0.04153881E+02 0.01726287E+00-0.02389374E-05    3
-0.10187000E-07 0.04340504E-10 0.64145633E+05 0.06036506E+02                    4
C4H4              H6W/94C   4H   4    0    0G   300.000  3000.000              1
 0.66507092E+01 0.16129434E-01-0.71938875E-05 0.14981787E-08-0.11864110E-12    2
 0.31195992E+05-0.97952118E+01-0.19152479E+01 0.52750878E-01-0.71655944E-04    3
 0.55072423E-07-0.17286228E-10 0.32978504E+05 0.31419983E+02                    4
C2N2 Dicyanogen   ATcT/AC  2.N  2.   0.   0.G   200.000  6000.000 1000.         1
 6.70549520E+00 3.64271185E-03-1.30939702E-06 2.16421413E-10-1.31193815E-14    2
 3.48824335E+04-1.04803146E+01 2.32928126E+00 2.61540993E-02-4.90009889E-05    3
 4.61923035E-08-1.64325831E-11 3.56900732E+04 9.86348075E+00 3.71976220E+04    4
n-C4H5             82489C   4H   5          G  0300.00   4000.00  1000.00      1
 0.12865971E+02 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12    2
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 0.38695564E+05-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04    3
-0.11482454E-07 0.03197823E-10 0.42282224E+05 0.12894539E+02                    4
i-C4H5             82489C   4H   5          G  0300.00   4000.00  1000.00      1
 0.11997762E+02 0.07990580E-01-0.08098172E-05-0.04568733E-08 0.08636911E-12    2
 0.33423896E+05-0.03528494E+03 0.03879443E+02 0.01997663E+00 0.01872777E-04    3
-0.09306953E-07 0.02386116E-10 0.36407556E+05 0.09842152E+02                    4
CHCHNCH2           NL0512H   4C   3N   1    0g    200.00  5000.00 1000.00      1
 7.02829199E+00 1.35098428E-02-5.23747631E-06 9.32145327E-10-6.24710034E-14    2
 4.76681967E+04-9.71920936E+00 2.28897829E+00 1.73684484E-02 1.33889942E-05    3
-3.07663318E-08 1.38741396E-11 4.93973364E+04 1.69179788E+01                    4
iiC4H6             A 8/83C   4H   6    0    0G   300.     3000.     1000.0     1
  0.1781557E 02 -0.4257502E-02  0.1051185E-04 -0.4473844E-08  0.5848138E-12    2
  0.1267342E 05 -0.6982662E 02  0.1023467E 01  0.3495919E-01 -0.2200905E-04    3
  0.6942272E-08 -0.7879187E-12  0.1811799E 05  0.1975066E 02  0.1950807E+05    4
iiiC4H6            H6W/94C   4H   6    0    0G   300.000  3000.000             1
 0.88673134E+01 0.14918670E-01-0.31548716E-05-0.41841330E-09 0.15761258E-12    2
 0.91338516E+04-0.23328171E+02 0.11284465E+00 0.34369022E-01-0.11107392E-04    3
-0.92106660E-08 0.62065179E-11 0.11802270E+05 0.23089996E+02                    4
C2H3CO C3H3O       T05/99C   3H   3O   1    0G   200.000  6000.000             1
 6.95842227E+00 1.07193211E-02-3.85218494E-06 6.22009064E-10-3.72401640E-14    2
 5.64826498E+03-1.14745786E+01 3.21169467E+00 1.18422105E-02 1.67462582E-05    3
-3.06947176E-08 1.33048816E-11 7.12815750E+03 1.00881663E+01 8.70564832E+03    4
CH2CHNCH2          NL0512H   5C   3N   1    0g    200.00  5000.00  1000.00     1
 6.46267020E+00 1.67980010E-02-6.50097404E-06 1.15557676E-09-7.73743161E-14    2
 1.64952732E+04-7.60355530E+00 2.70686712E+00 1.09849355E-02 3.70034076E-05    3
-5.58051692E-08 2.29301182E-11 1.82832281E+04 1.56229034E+01                    4
C4H7               AM1/94C   4H   7    0    0G   300.000  3000.000  1000.000    1
 0.11963392E+02 0.11425305E-01 0.78948909E-06-0.19858872E-08 0.36873645E-12    2
 0.16962977E+05-0.37542908E+02 0.28698254E+00 0.36964495E-01-0.86277441E-05    3
-0.15051821E-07 0.89891263E-11 0.20551301E+05 0.24484467E+02                    4
NCNO                92789C   1N   2O   1    0G   300.000  4000.000 1000.00      1
 0.73266358E+01 0.17882655E-02-0.20288753E-06-0.94724527E-10 0.18667134E-13    2
 0.36704793E+05-0.10886014E+02 0.49251637E+01 0.53706546E-02 0.27844874E-06    3
-0.21986761E-08 0.46036536E-12 0.37592273E+05 0.24706030E+01                    4
NCHCHO             NL0512H   2C   2N   1O   1g    200.00  5000.00  1000.00     1
 6.44159689E+00 8.76156545E-03-3.47897897E-06 6.29479906E-10-4.26839588E-14    2
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 1.29189347E+04-5.19292137E+00 3.28273760E+00 1.07949442E-02 9.12178960E-06    3
-1.91878297E-08 8.28309072E-12 1.41429825E+04 1.28099292E+01                    4
C2H3CHO           T 6/92C   3H   4O   1    0G   298.150  3000.0    1000.0      1
 0.48353180E+01 0.19772601E-01-0.10426628E-04 0.26525803E-08-0.26278207E-12    2
-0.11557837E+05 0.18853144E+01 0.11529584E+01 0.28040214E-01-0.15072153E-04    3
 0.15905842E-08 0.84930371E-12-0.10417694E+05 0.21453279E+02-0.89572567E+04    4
CH2NHCHCH2        NL0512H   6C   3N   1    0g    200.00  5000.00  1000.00      1
 7.50196587E+00 1.74773808E-02-6.58383837E-06 1.14807651E-09-7.58107388E-14    2
 2.33814706E+04-1.07082718E+01 2.57728607E+00 2.24497938E-02 1.01983386E-05    3
-2.94479134E-08 1.36722613E-11 2.51162220E+04 1.66980623E+01                    4
CH2CH2NCH2        NL0512H   6C   3N   1    0g    200.00  5000.00  1000.00      1
 6.83108119E+00 1.87496609E-02-7.24470207E-06 1.28609137E-09-8.60231248E-14    2
 2.76999696E+04-7.71271290E+00 3.26656995E+00 1.24529614E-02 3.59690850E-05    3
-5.44100284E-08 2.22352278E-11 2.94559526E+04 1.45710410E+01                    4
IC4H8             T 6/83C   4H   8    0    0G   300.000  5000.000              1
 0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12    2
-0.21397231E+04 0.15543201E+02 0.11811380E+01 0.30853380E-01 0.50865247E-05    3
-0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21062469E+02                    4
nC4H9      BURCAT T 6/93C   4H   9    0     G   200.000  6000.000 1000.        1
 8.97401527E+00 2.39704154E-02-8.48703645E-06 1.35644127E-09-8.06234913E-14    2
 5.19161526E+03-2.31075609E+01 4.73737837E+00 9.69051565E-03 6.63846383E-05    3
-9.24799302E-08 3.74006099E-11 7.57382332E+03 4.91063455E+00 9.83838903E+03    4
C2H3CH2O          96PRW1C   3H   5O   1    0G   300.00   3000.00  1000.00      1
+2.75835879D+00+2.71781452D-02-1.44239030D-05+3.66635155D-09-3.64832209D-13    2
+1.09685129D+04+1.15870981D+01+4.48935705D-01+3.24335892D-02-1.58843257D-05    3
+4.03948822D-10+1.43106465D-12+1.15934429D+04+2.36532883D+01                    4
CH2CHOCH2         T 9/92C   3H   5O   1    0G   298.150  3000.000              1
 0.91206991E+01 0.12196117E-01-0.42929777E-05 0.12616892E-08-0.15705367E-12    2
 0.91765012E+04-0.22071447E+02 0.70599393E+00 0.25629797E-01 0.71080411E-05    3
-0.29693495E-07 0.14360721E-10 0.11909268E+05 0.23610039E+02 0.13269823E+05    4
NHCH2CHO          NL0512H   4C   2N   1O   1g    200.00  5000.00  1000.00      1
 6.65451690E+00 1.34611580E-02-5.23712324E-06 9.34385840E-10-6.27315718E-14    2
 5.41174749E+03-5.10878592E+00 3.92385121E+00 7.15579388E-03 3.25906178E-05    3
-4.68246266E-08 1.88885802E-11 6.82584683E+03 1.23163070E+01                    4
OCH2CHNH          NL0512H   4C   2N   1O   1g    200.00  5000.00  1000.00      1
 6.88692946E+00 1.37500525E-02-5.36155188E-06 9.58262578E-10-6.44217673E-14    2
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 1.09153616E+04-8.85641597E+00 3.10309188E+00 9.14738168E-03 3.45167980E-05    3
-5.20699744E-08 2.14575673E-11 1.26500440E+04 1.42283131E+01                   4
CH3NNCH3        C&S-02  C   2N   2H   6    0G   300.000  4000.000  1000.00     1
 0.49863152E+01 0.24070809E-01-0.10732555E-04 0.22441162E-08-0.17961655E-12    2
 0.15409582E+05-0.15606158E+01 0.19013815E+01 0.27280859E-01-0.53752194E-05    3
-0.57609693E-08 0.23430172E-11 0.16600457E+05 0.15898338E+02 1.83222625E+04    4
C2H3OO            PRW84 C   2O   2H   3     G  0300.00   5000.00  1000.00      1
+1.07095497D+00+2.93293018D-02-2.26481331D-05+8.68753392D-09-1.30462650D-12    2
+1.27909845D+04+2.07891307D+01+3.93381061D+00+1.98311250D-02-1.14186387D-05    3
+3.09270357D-09-3.22330856D-13+1.21364287D+04+6.51468027D+00                   4
H2CNO2            103190C   1H   2N   1O   2G  0300.00   4000.00  1500.00      1
 0.01127481E+03 0.02584711E-01-0.03934331E-05-0.05614969E-09 0.01392400E-12    2
 0.01360470E+06-0.03461951E+03 0.01165696E+02 0.02890490E+00-0.02817663E-03    3
 0.01387569E-06-0.02727595E-10 0.01694546E+06 0.01888293E+03                   4
CH3NO2            103190C   1H   3N   1O   2G  0300.00   4000.00  1500.00      1
 0.01090158E+03 0.04326381E-01-0.04203548E-05-0.01893071E-08 0.03417444E-12    2
-0.01370862E+06-0.03073183E+03 0.03224717E+01 0.02665147E+00-0.01930574E-03    3
 0.07762620E-07-0.01398746E-10-0.09597527E+05 0.02726156E+03                   4
CH3ONO            103190C   1H   3N   1O   2G  0300.00   4000.00  1500.00      1
 0.01136129E+03 0.04159349E-01-0.04145670E-05-0.01695140E-08 0.03028732E-12    2
-0.01281482E+06-0.03545435E+03 0.01490345E+02 0.02645433E+00-0.02112332E-03    3
 0.09414399E-07-0.01811205E-10-0.09125782E+05 0.01813766E+03                   4
C2H5OO            PW3/94C   2O   2H   5     G  0300.00   5000.00  1000.00      1
+2.10630563D+00+2.77943799D-02-1.44630852D-05+3.25545688D-09-2.46592854D-13    2
-2.64777663D+03+1.80691037D+01+2.10630563D+00+2.77943799D-02-1.44630852D-05    3
+3.25545688D-09-2.46592854D-13-2.64767408D+03+1.80671959D+01                   4
C5H2                  0C   5H   2    0    0G   200.000  5000.000  900.00    0 1
 0.10912226E+02 0.77090390E-02-0.28335089E-05 0.46991021E-09-0.28842258E-13    2
 0.85484262E+05-0.29829361E+02 0.25183751E+01 0.44292500E-01-0.62601709E-04    3
 0.43850625E-07-0.11831256E-10 0.87024418E+05 0.99443064E+01                   4
NO3               ATcT/AN   1O   3    0    0G   200.00   6000.00  1000.       1 !BURCAT
 7.48347702E+00 2.57772064E-03-1.00945831E-06 1.72314063E-10-1.07154008E-14    2
 6.12990474E+03-1.41618136E+01 2.17359330E+00 1.04902685E-02 1.10472669E-05    3
-2.81561867E-08 1.36583960E-11 7.81290905E+03 1.46022090E+01 8.97563416E+03    4 !
NH2NO2 NITRAMIDE  tpis89N   2H   2O   2     G   200.000  6000.000 1000.00      1
 7.38890844E+00 7.65188287E-03-2.75087184E-06 4.44623197E-10-2.66488354E-14    2
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-6.21766970E+03-1.32736914E+01 2.17310160E+00 1.43162238E-02 1.09031816E-05    3
-2.76714916E-08 1.29868784E-11-4.45906123E+03 1.53831146E+01-3.12706341E+03    4
H2CCCCCH               0C   5H   3    0    0G   200.000  5000.000 1000.00    0 1
 0.10024302E+02 0.10655411E-01-0.38709251E-05 0.63462431E-09-0.38550202E-13    2
 0.65691196E+05-0.25065161E+02 0.23963519E+01 0.36748178E-01-0.36381526E-04    3
 0.17889326E-07-0.32474675E-11 0.67437737E+05 0.12840045E+02                   4
HCCCHCCH               0C   5H   3    0    0G   200.000  5000.000 1000.00    0 1
 0.10313636E+02 0.10278554E-01-0.37086568E-05 0.60568664E-09-0.36721455E-13    2
 0.65859508E+05-0.26380088E+02 0.10442368E+01 0.44574721E-01-0.50980758E-04    3
 0.29338989E-07-0.65246891E-11 0.67852460E+05 0.19034765E+02                   4
HNO3         T 8/03     H   1N   1O   3    0G   200.00   6000.00  1000.        1 !BURCAT
 8.03098942E+00 4.46958589E-03-1.72459491E-06 2.91556153E-10-1.80102702E-14    2
-1.92821685E+04-1.62616720E+01 1.69329154E+00 1.90167702E-02-8.25176697E-06    3
6.06113827E-09 4.65236978E-12-1.73882411E+04 1.71839655E+01                   4 !
C5H5       HR 6/01BLYP00C   5H   5    0     G   300.000  5000.000 1403.000     1
 1.26805871E+01 1.27575785E-02-4.34788920E-06 6.73442111E-10-3.90092992E-14    2
 2.55507801E+04-4.67103980E+01-3.35979212E+00 5.80041481E-02-5.41839461E-05    3
 2.56964859E-08-4.80036435E-12 3.03384665E+04 3.66689604E+01                   4
l-C5H5            BurcatC   5H   5    0    0G   300.000  5000.000 1402.000    01
 1.38816308E+01 1.14454546E-02-3.83729159E-06 5.88208430E-10-3.38379570E-14    2
 4.27127349E+04-4.87035050E+01-8.60045246E-01 5.18320271E-02-4.67951024E-05    3
 2.14122502E-08-3.87182913E-12 4.71932361E+04 2.82849534E+01                   4
H2C4O             120189H   2C   4O   1     G   300.000  4000.000 1000.00      1
 1.02688800e+01 4.89616400e-03-4.88508100e-07-2.70856600e-10 5.10701300e-14    2
 2.34690300e+04-2.81598500e+01 4.81097100e+00 1.31399900e-02 9.86507300e-07    3
-6.12072000e-09 1.64000300e-12 2.54580300e+04 2.11342400e+00                   4
C5H6       HR11/99BLYP00C   5H   6    0     G   300.000  5000.000 1402.000     1
 1.26575005E+01 1.53301203E-02-5.23821364E-06 8.12867095E-10-4.71504821E-14    2
 1.03083446E+04-4.75386061E+01-4.78259036E+00 6.09873033E-02-5.17363931E-05    3
 2.25173536E-08-3.92621113E-12 1.58382836E+04 4.43226201E+01                   4
CH2CHCH2CCH             C   5H   6          G   300.000  5000.000  1000.000    1
 2.27091750E+01-3.00201330E-03 3.55710540E-06-9.23306040E-10 7.65447070E-14    2
 2.29371430E+04-9.59871140E+01 3.25148510E+00 3.10524290E-02-1.09708150E-05    3
-1.24545210E-09 4.37795310E-13 3.02185390E+04 1.16484310E+01                   4
CH2CHCHCCH2             C   5H   6          G   300.000  5000.000  1000.000    1
 1.16185120E+01 1.61550680E-02-5.49912650E-06 8.78380530E-10-5.41899260E-14    2
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 2.53440310E+04-3.52899400E+01 1.21979650E-01 4.73406170E-02-3.22280940E-05    3
 7.08673830E-09 7.66264600E-13 2.84412680E+04 2.40296630E+01                   4
C6H2              P 1/93C   6H   2    0    0G   300.000  3000.000              1
 0.13226281E+02 0.73904302E-02-0.22715381E-05 0.25875217E-09-0.55356741E-14    2
 0.80565258E+05-0.41201176E+02-0.15932624E+01 0.80530145E-01-0.14800649E-03    3
 0.13300031E-06-0.45332313E-10 0.83273227E+05 0.27980873E+02                   4
C6H3              H6W/94C   6H   3    0    0G   300.000  3000.000              1
 0.58188343E+01 0.27933408E-01-0.17825427E-04 0.53702536E-08-0.61707627E-12    2
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-04    3
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02                   4
l-C6H4            H6W/94C   6H   4    0    0G   300.000  3000.000              1
 0.12715182E+02 0.13839662E-01-0.43765440E-05 0.31541636E-09 0.46619026E-13    2
 0.57031148E+05-0.39464600E+02 0.29590225E+00 0.58053318E-01-0.67766756E-04    3
 0.43376762E-07-0.11418864E-10 0.60001371E+05 0.22318970E+02                   4
c-C6H4            H6W/94C   6H   4    0    0G   300.000  3000.000              1
 0.13849209E+02 0.78807920E-02 0.18243836E-05-0.21169166E-08 0.37459977E-12    2
 0.47446340E+05-0.50404953E+02-0.30991268E+01 0.54030564E-01-0.40839004E-04    3
 0.10738837E-07 0.98078490E-12 0.52205711E+05 0.37415207E+02                   4
n-C6H5            H6W/94C   6H   5    0    0G   300.000  3000.000              1
 0.16070068E+02 0.81899539E-02 0.17325165E-05-0.20624185E-08 0.36292345E-12    2
 0.64616867E+05-0.56163742E+02-0.61135769E+00 0.65082610E-01-0.78262397E-04    3
 0.53030828E-07-0.14946683E-10 0.68805375E+05 0.27635468E+02                   4
i-C6H5            H6W/94C   6H   5    0    0G   300.000  3000.000              1
 0.22501663E+02-0.81009977E-02 0.15955695E-04-0.72310371E-08 0.10310424E-11    2
 0.58473410E+05-0.91224777E+02-0.78585434E+00 0.60221825E-01-0.62890264E-04    3
 0.36310730E-07-0.87000259E-11 0.64942270E+05 0.28658905E+02                   4
CH3ONO2           103190C   1H   3N   1O   3G  0300.00   4000.00  1500.00     1
 0.01436189E+03 0.04112243E-01-0.05113052E-05-0.01496436E-08 0.03012156E-12    2
-0.01972440E+06-0.05131842E+03 0.07803354E+01 0.03454204E+00-0.02822328E-03    3
 0.01232324E-06-0.02302164E-10-0.01465346E+06 0.02245752E+03                   4
A1                H6W/94C   6H   5    0    0G   300.000  3000.000              1
 0.14493439E+02 0.75712688E-02 0.37894542E-05-0.30769500E-08 0.51347820E-12    2
 0.33189977E+05-0.54288940E+02-0.49076147E+01 0.59790771E-01-0.45639827E-04    3
 0.14964993E-07-0.91767826E-12 0.38733410E+05 0.46567780E+02                   4
l-C6H6            H6W/94C   6H   6    0    0G   300.000  3000.000              1
 0.17584442E+02 0.64486600E-02 0.48933980E-05-0.34696221E-08 0.56150749E-12    2
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 0.34111988E+05-0.66017838E+02-0.10170622E+01 0.61794821E-01-0.59461061E-04    3
 0.31873491E-07-0.71717693E-11 0.39202707E+05 0.29460373E+02                    4
C4H5C2H                0C   6H   6    0    0G   200.000  5000.000 1100.00    0 1
 0.13903605E+02 0.17453182E-01-0.63026581E-05 0.10316520E-08-0.63440931E-13    2
 0.35975470E+05-0.47671401E+02-0.23220260E+00 0.54092928E-01-0.36134322E-04    3
 0.69104632E-08 0.13734168E-11 0.39978520E+05 0.25932864E+02                    4
A                 H6W/94C   6H   6    0    0G   300.000  3000.000              1
 0.17246994E+02 0.38420164E-02 0.82776232E-05-0.48961120E-08 0.76064545E-12    2
 0.26646055E+04-0.71945175E+02-0.48998680E+01 0.59806932E-01-0.36710087E-04    3
 0.32740399E-08 0.37600886E-11 0.91824570E+04 0.44095642E+02                    4
FC6H6             T03/97C   6H   6    0     G   200.000  6000.000  1000.0      1
 1.19233607E+01 1.98993861E-02-7.21223888E-06 1.17141499E-09-7.04278845E-14    2
 2.27199368E+04-4.13488172E+01 1.25853571E-01 3.04056534E-02 4.01806332E-05    3
-8.27651456E-08 3.77645005E-11 2.68838408E+04 2.44628931E+01 2.84820633E+04    4
CYC6H7     BURCAT T 6/93C   6H   7    0     G   200.000  6000.000 1000.        1
 0.12801758E+02 0.21924749E-01-0.79713001E-05 0.12972935E-08-0.78100416E-13    2
 0.17889539E+05-0.45804341E+02-0.10303140E+00 0.34393354E-01 0.39788466E-04    3
-0.85116612E-07 0.39012224E-10 0.22425515E+05 0.26022350E+02 0.24125213E+05    4
n-C6H7            H6W/94C   6H   7    0    0G   300.000  3000.000              1
 0.22577469E+02-0.30737517E-02 0.14225234E-04-0.69880848E-08 0.10232874E-11    2
 0.41228980E+05-0.91568619E+02 0.13248032E+00 0.57103366E-01-0.43712644E-04    3
 0.15538603E-07-0.12976356E-11 0.47730512E+05 0.25339081E+02                    4
i-C6H7            H6W/94C   6H   7    0    0G   300.000  3000.000              1
 0.20481506E+02 0.79439697E-03 0.11450761E-04-0.60991177E-08 0.91756724E-12    2
 0.37728426E+05-0.81812073E+02-0.17099094E+01 0.62486034E-01-0.54290707E-04    3
 0.26959682E-07-0.58999090E-11 0.44086621E+05 0.33344772E+02                    4
C6H8              H6W/94C   6H   8    0    0G   300.000  3000.000              1
 0.28481979E+02-0.15702948E-01 0.26771697E-04-0.11780109E-07 0.16573427E-11    2
 0.93346445E+04-0.12500226E+03 0.15850439E+01 0.40215142E-01 0.78439543E-05    3
-0.38761325E-07 0.18545207E-10 0.17949613E+05 0.19112625E+02                    4
CY13C6H8   BURCAT T 2/90C   6H   8    0     G   200.000  6000.000 1000.        1
 0.11779870E+02 0.25519980E-01-0.92666947E-05 0.15068122E-08-0.90658701E-13    2
 0.65486686E+04-0.41618805E+02 0.17265319E+01 0.14887612E-01 0.94809230E-04    3
-0.14083394E-06 0.58859873E-10 0.11021297E+05 0.19130886E+02 0.12784878E+05    4
C5H4O     10/00BURCBLYP C   5H   4O   1     G   300.000  5000.000 1402.000     1
 1.37907739E+01 1.19738147E-02-4.11436106E-06 6.40954643E-10-3.72821366E-14    2
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 2.74553951E+02-5.06296371E+01-3.01174376E+00 5.82012965E-02-5.36527132E-05    3
 2.48757306E-08-4.54630764E-12 5.38127213E+03 3.70844611E+01                    4
C5H5O     ZHONG/BOZ1998 C   5H   5O   1     G   300.000  5000.000 1395.000     1
 1.49072105E+01 1.36369619E-02-4.70762207E-06 7.36028654E-10-4.29314124E-14    2
 1.43724130E+04-5.69296345E+01-4.14628450E+00 6.23584874E-02-5.28374678E-05    3
 2.24628793E-08-3.80136191E-12 2.04992627E+04 4.37921058E+01                    4
C5H4OH    ALZUETA 2000  C   5H   5O   1     G   300.000  5000.000 1417.000     1
 1.54616992E+01 1.21543874E-02-3.97713729E-06 5.99530783E-10-3.40841280E-14    2
 1.18008962E+03-5.80092304E+01-3.36507049E+00 6.65211552E-02-6.40907012E-05    3
 3.04663074E-08-5.61147666E-12 6.55733089E+03 3.92124189E+01                    4
C6H9       BURCAT T 2/92C   6H   9    0     G   298.150  3000.000 1000.        1
 0.21786938E+02 0.11894129E-01-0.21209124E-05 0.00000000E+00 0.00000000E+00    2
 0.20013752E+05-0.89218982E+02 0.20594889E+01 0.46753513E-01-0.18644505E-04    3
 0.00000000E+00 0.00000000E+00 0.27665639E+05 0.20293525E+02 0.30193000E+05    4
CYC6H9     BURCAT T 2/92C   6H   9    0     G   298.150  3000.000 1000.        1
 0.26295828E+02 0.86828857E-02-0.15770376E-05 0.00000000E+00 0.00000000E+00    2
 0.20863563E+04-0.12573825E+03-0.35714300E+01 0.61696043E-01-0.26928803E-04    3
 0.00000000E+00 0.00000000E+00 0.13657039E+05 0.39986250E+02 0.15096500E+05    4
CYC6H10    BURCAT T 2/90C   6H  10    0     G   200.000  6000.000 1000.        1
 0.11773904E+02 0.30947360E-01-0.11234330E-04 0.18262494E-08-0.10985119E-12    2
-0.72028376E+04-0.42658688E+02 0.23662378E+01 0.10681712E-01 0.11822112E-03    3
-0.16567854E-06 0.67612802E-10-0.24824973E+04 0.16769357E+02-0.55324968E+03    4
C6H10      BURCAT T 2/92C   6H  10    0     G   298.150  3000.000 1000.        1
 0.23903966E+02 0.12046216E-01-0.19588306E-05 0.00000000E+00 0.00000000E+00    2
-0.43733937E+04-0.10376594E+03-0.96299362E+00 0.60880377E-01-0.28062414E-04    3
 0.00000000E+00 0.00000000E+00 0.45722054E+04 0.32010145E+02 0.67431033E+04    4
CYC6H11    BURCAT 12/98 C   6H  11    0     G   298.150  5000.000 1000.        1
 1.28647309E+01 3.52600147E-02-1.39450525E-05 2.51808759E-09-1.70899213E-13    2
 6.15531214E+02-4.88786148E+01-3.76580647E+00 5.88838077E-02 1.22955158E-07    3
-3.30729397E-08 1.42142299E-11 6.76556720E+03 4.36106643E+01 8.20243165E+03    4
C6H11-12                C   6H  110   00   0G   300.00   5000.00  1000.00      1
 0.15903220E+02 0.23659610E-01-0.67095560E-05 0.94231160E-09-0.53289920E-13    2
 0.15837710E+05-0.54096690E+02 0.14245270E+00 0.61529150E-01-0.39403020E-04    3
 0.13625820E-07-0.21393720E-11 0.20807860E+05 0.29545670E+02                    4
C6H11-15                C   6H  110   00   0G   300.00   5000.00  1000.00      1
 0.16511810E+02 0.23103710E-01-0.65196350E-05 0.91279680E-09-0.51533620E-13    2
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 0.11020680E+05-0.57226020E+02-0.65185990E+00 0.69069390E-01-0.55091450E-04    3
 0.26728390E-07-0.60813550E-11 0.16144180E+05 0.32558910E+02                    4
C6H11-13                C   6H  110   00   0G   300.00   5000.00  1000.00      1
 0.15939530E+02 0.24454600E-01-0.71328250E-05 0.10237720E-08-0.58843450E-13    2
 0.27317560E+04-0.56236800E+02-0.18343630E+00 0.62924820E-01-0.39494870E-04    3
 0.12901540E-07-0.19206490E-11 0.78098810E+04 0.29353710E+02                    4
C6H11-14                C   6H  11O   00   0G   300.00   5000.00  1000.00      1
 1.32786E+01    2.79515E-02   -8.47472E-06    1.23752E-09   -7.12640E-14       2
 1.22232E+04   -3.88114E+01   -1.06617E+00    7.16134E-02   -5.85771E-05       3
 2.71262E-08   -5.15786E-12    1.59829E+04    3.43102E+01                      4
C6H11      BURCAT  2/92 C   6H  11    0     G   298.150  3000.000 1000.       1
 0.24938654E+02 0.13258801E-01-0.23302223E-05 0.00000000E+00 0.00000000E+00    2
 0.51145941E+04-0.10690338E+03 0.63802451E+00 0.56209452E-01-0.23047424E-04    3
 0.00000000E+00 0.00000000E+00 0.14624427E+05 0.28133981E+02 0.17109367E+05    4
CYC6H12    BURCAT 2/90  C   6H  12    0     G   200.000  5000.000 1000.       1
 0.10209166E+02 0.41894173E-01-0.17234045E-04 0.32239024E-08-0.22540929E-12    2
-0.21742125E+05-0.38990666E+02 0.40402264E+01-0.61827997E-02 0.17662080E-03    3
-0.22300383E-06 0.86393385E-10-0.16919808E+05 0.85269500E+01-0.14829497E+05    4
hexene1    BURCAT T 6/93C   6H  12    0     G   200.000  6000.000 1000.       1
 1.60616093E+01 2.75650562E-02-9.32973368E-06 1.49349013E-09-8.98810268E-14    2
-1.28042951E+04-5.69925586E+01 7.31509054E+00 3.71150329E-03 1.27250318E-04    3
-1.71556964E-07 6.89805935E-11-8.20916507E+03-5.94354365E-01-5.04539654E+03    4
hex1yl     BURCAT T 6/93C   6H  13    0     G   200.000  6000.000 1000.       1
 1.39163141E+01 3.48510892E-02-1.26898935E-05 2.07144196E-09-1.24756674E-13    2
-4.01785625E+03-4.33071846E+01 8.76348959E+00 2.16244832E-03 1.31674686E-04    3
-1.73828247E-07 6.92518175E-11-5.42630596E+02-5.91729689E+00 3.01881891E+03    4
hex2yl     BURCAT T 6/93C   6H  13    0     G   200.000  6000.000 1000.       1
 1.41986473E+01 3.46787125E-02-1.25515738E-05 2.02767674E-09-1.21224274E-13    2
-3.68102477E+03-4.23012097E+01 7.58145549E+00 1.89615514E-02 8.16571755E-05    3
-1.18091545E-07 4.81236008E-11-2.27328454E+02 5.28216352E-05 3.38664816E+03    4
hex3yl                  C   6H  130   00   0G   300.00   5000.00  1000.00      1
 0.18621920E+02 0.24911520E-01-0.68681720E-05 0.94495470E-09-0.52683770E-13    2
-0.51170230E+04-0.69174640E+02-0.17466440E+01 0.81867340E-01-0.74301960E-04    3
 0.43594630E-07-0.11843740E-10 0.94735310E+03 0.37018690E+02                    4
cyCHOCHCHNCH      NL0512H   4C   4N   1O   1g    200.00  5000.00  1000.00      1
 1.03705295E+01 1.68075131E-02-6.61865393E-06 1.19161020E-09-8.05474290E-14    2
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9.67068671E+03-3.13371480E+01 3.67481839E-01 2.72420856E-02 2.73087786E-05 3
-6.12972824E-08 2.80352020E-11 1.31318307E+04 2.41467476E+01 4
cyOCHCHNCHCH2 NL0512H 5C 4N 1O 1g 200.00 5000.00 1000.00 1
9.76552055E+00 2.02657471E-02-7.98168483E-06 1.43674533E-09-9.70897569E-14 2
2.84807107E+02-2.85557941E+01 1.16612804E+00 2.16650486E-02 4.45062449E-05 3
-7.69829934E-08 3.30130453E-11 3.65457986E+03 2.10458988E+01 4
cyNCH2CH2OCHCH NL0512H 6C 4N 1O 1g 200.00 5000.00 1000.00 1
9.97152024E+00 2.28761402E-02-8.99290464E-06 1.61649943E-09-1.09121631E-13 2
1.60990018E+03-3.00221894E+01 1.66539922E+00 1.95697562E-02 5.65836534E-05 3
-9.03888845E-08 3.79072249E-11 5.08978152E+03 1.90149637E+01 4
cyCHCH2OCH2CHN NL0512H 6C 4N 1O 1g 200.00 5000.00 1000.00 1
1.04023579E+01 2.25422296E-02-8.88080545E-06 1.59862300E-09-1.08020089E-13 2
5.31436341E+03-3.05589738E+01 1.98370077E+00 2.06090929E-02 5.29123058E-05 3
-8.64542761E-08 3.64783370E-11 8.77929416E+03 1.88141517E+01 4
CH2CH2NCHCHO NL0512H 6C 4N 1O 1g 200.00 5000.00 1000.00 1
1.00065027E+01 2.12590310E-02-8.31100940E-06 1.48775653E-09-1.00118748E-13 2
1.21780377E+04-1.93320698E+01 4.33376118E+00 1.86085860E-02 3.55081766E-05 3
-5.83047758E-08 2.41648557E-11 1.46495593E+04 1.44416372E+01 4
CH2OCHCHNCH2 NL0512H 6C 4N 1O 1g 200.00 5000.00 1000.00 1
1.03605553E+01 2.06456475E-02-7.99918574E-06 1.42319844E-09-9.53626274E-14 2
1.96067184E+04-2.13482013E+01 3.72756375E+00 2.38804018E-02 2.39881369E-05 3
-4.83222462E-08 2.10324917E-11 2.21567964E+04 1.65262174E+01 4
CH2CHOCH2CHNH NL0512H 7C 4N 1O 1g 200.00 5000.00 1000.00 1
9.43983097E+00 2.43022381E-02-9.41764568E-06 1.67592431E-09-1.12319107E-13 2
-4.75041182E+03-1.64775948E+01 3.72389545E+00 1.38728098E-02 6.19611809E-05 3
-9.06265414E-08 3.69314827E-11-1.96325859E+03 1.92328019E+01 4
OCHCH2NHCHCH2 NL0512H 7C 4N 1O 1g 200.00 5000.00 1000.00 1
9.51050292E+00 2.42544440E-02-9.40389507E-06 1.67405636E-09-1.12220969E-13 2
-1.05680496E+04-1.66197033E+01 3.42017416E+00 1.87512420E-02 4.73591100E-05 3
-7.43155583E-08 3.06779216E-11-7.82478385E+03 2.01847716E+01 4
cyOCHCHNHCH2CH2 NL0512H 7C 4N 1O 1g 200.00 5000.00 1000.00 1
9.96793833E+00 2.53402066E-02-9.85898966E-06 1.75969237E-09-1.18197555E-13 2
-1.16516760E+04-3.03807434E+01 1.21602259E+00 2.35404585E-02 5.39979642E-05 3
-8.96195781E-08 3.79292297E-11-8.06933954E+03 2.08719874E+01 4
cyOCH2CHNCH2CH2 NL0512H 7C 4N 1O 1g 200.00 5000.00 1000.00 1
9.33224514E+00 2.64207014E-02-1.04038145E-05 1.87193808E-09-1.26439658E-13 2

-1.23029574E+04-2.70916446E+01 2.49837851E+00 1.28784770E-02 7.73276547E-05 3
-1.10046453E-07 4.44047025E-11-8.88976270E+03 1.59397184E+01 4
NHCH2CH2OCHCH2 NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
9.68514907E+00 2.63704105E-02-1.02072196E-05 1.81470963E-09-1.21528697E-13 2
7.77400194E+03-1.57389988E+01 4.66014797E+00 9.74899317E-03 7.73358783E-05 3
-1.07446350E-07 4.32187645E-11 1.05573351E+04 1.73860355E+01 4
CH2CH2NHCH2CHO NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
9.63125770E+00 2.65728138E-02-1.03260369E-05 1.84083887E-09-1.23517420E-13 2
1.11522710E+03-1.56168502E+01 4.58706944E+00 1.29143845E-02 6.58248031E-05 3
-9.30880660E-08 3.73253324E-11 3.82891071E+03 1.70693852E+01 4
OCH2CH2NHCHCH2 NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
1.02790961E+01 2.62562858E-02-1.01579159E-05 1.80548429E-09-1.20895234E-13 2
7.62616153E+03-2.11386698E+01 3.01769742E+00 2.23810637E-02 5.00400721E-05 3
-8.16538191E-08 3.42477167E-11 1.07319447E+04 2.20035773E+01 4
CH2CH2OCH2CHNH NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
9.69346283E+00 2.64566136E-02-1.02654930E-05 1.82814406E-09-1.22574898E-13 2
5.79069027E+03-1.59166130E+01 5.00481411E+00 1.02546298E-02 7.21573999E-05 3
-9.95032423E-08 3.96464100E-11 8.46664878E+03 1.52754770E+01 4
CH2OCH2CH2NCH2 NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
9.19762303E+00 2.70086271E-02-1.05012971E-05 1.87264019E-09-1.25671746E-13 2
7.15236012E+03-1.35395043E+01 4.90847630E+00 9.21835654E-03 7.37451907E-05 3
-9.99089152E-08 3.94556163E-11 9.76473253E+03 1.57658288E+01 4
cyOrthoMorphyl NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
1.00887739E+01 2.82096961E-02-1.10180966E-05 1.97161497E-09-1.32664086E-13 2
-1.23231840E+03-3.15337889E+01 2.05875485E+00 1.90415609E-02 7.10034306E-05 3
-1.06937795E-07 4.39210066E-11 2.43624755E+03 1.73572200E+01 4
cyMetaMorphyl NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
1.01394481E+01 2.81012751E-02-1.09599640E-05 1.95928556E-09-1.31743233E-13 2
-3.46128688E+03-3.17383673E+01 1.86240736E+00 2.14671652E-02 6.42559456E-05 3
-9.97807063E-08 4.12699685E-11 1.94265168E+02 1.80014282E+01 4
cyParaMorphyl NL0512H 8C 4N 1O 1g 200.00 5000.00 1000.00 1
9.81857071E+00 2.87092590E-02-1.12748460E-05 2.02488549E-09-1.36588144E-13 2
-2.55902949E+03-3.03711366E+01 2.49291590E+00 1.36616039E-02 8.52467307E-05 3
-1.21418965E-07 4.91270481E-11 1.10200123E+03 1.58247257E+01 4
cyMorph NL0512H 9C 4N 1O 1g 200.00 5000.00 1000.00 1
9.31663792E+00 3.18026464E-02-1.24290335E-05 2.22486836E-09-1.49735740E-13 2

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-2.42647198E+04-2.86792745E+01 2.42819448E+00 1.18580482E-02 9.64514708E-05    3
-1.33245554E-07 5.32368692E-11-2.05315873E+04 1.61901809E+01                    4
N2O4              ATcT AN   2O   4    0    0G   200.00   6000.00  1000.        1 !BURCAT
 1.15752932E+01 4.01615532E-03-1.57178022E-06 2.68273657E-10-1.66921538E-14    2
-2.96184070E+03-3.19488531E+01 3.02002271E+00 2.95904359E-02-3.01342572E-05    3
 1.42360526E-08-2.44100411E-12-6.79967151E+02 1.18059714E+01                    4 !
C2H4OH            T 4/83H   5C   2O   1    0G   300.000  5000.    1000.        1
 0.75944014E+01 0.93229339E-02-0.30303854E-05 0.43216319E-09-0.21970039E-13    2
-0.57727852E+04-0.13955572E+02 0.14019508E+01 0.21543175E-01-0.22326512E-05    3
-0.14464092E-07 0.80488420E-11-0.38464519E+04 0.19148981E+02-0.25154820E+04    4
CH3CHOH           T 4/83C   2O   1H   5    0G   300.000  5000.    1000.        1
 0.67665424E+01 0.11634436E-01-0.37790651E-05 0.53828875E-09-0.27315345E-13    2
-0.56092969E+04-0.93980442E+01 0.24813328E+01 0.16790036E-01 0.37755499E-05    3
-0.13923497E-07 0.60095193E-11-0.40120054E+04 0.14581622E+02-0.25172860E+04    4
C2H5OH            L 8/88C   2H   6O   1    0G   200.000  6000.000 1000.        1
 0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13    2
-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04    3
-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05    4
CH3OCH3           AK0904C   2H   6O   1    0G   270.000  3000.000  710.00      1
 8.30815546E-01 2.69173263E-02-1.38874777E-05 3.47515079E-09-3.41706784E-13    2
-2.34120975E+04 2.02174360E+01 5.68097447E+00-5.39434751E-03 6.49472750E-05    3
-8.05065318E-08 3.27474018E-11-2.39755455E+04-6.36955496E-01                    4
CH3OCH2    7/20/98 THERMC   2H   5O   1    0G   300.000  5000.000 1376.000    21
 8.17137842E+00 1.10086181E-02-3.82352277E-06 5.99637202E-10-3.50317513E-14    2
-3.41941605E+03-1.78650856E+01 2.91327415E+00 2.03364659E-02-9.59712342E-06    3
 2.07478525E-09-1.71343362E-13-1.18844240E+03 1.16066817E+01                    4
CH3OCH2O   2/ 9/96 THERMC   2H   5O   2    0G   300.000  5000.000 2012.000    21
 8.60261845E+00 1.35772195E-02-4.84661602E-06 7.77766193E-10-4.62633624E-14    2
-2.13762444E+04-1.75775023E+01 3.25889339E+00 2.22146359E-02-7.78556340E-06    3
-2.41484158E-10 4.51914496E-13-1.92377212E+04 1.23680069E+01                    4
CH3OCHO    4/20/99 THERMC   2H   4O   2    0G   300.000  5000.000 1686.000    21
 8.69123518E+00 1.15503122E-02-4.27782486E-06 7.02533059E-10-4.24333552E-14    2
-4.64364769E+04-1.89301478E+01 3.08839783E+00 2.03760048E-02-6.84777040E-06    3
-7.28186203E-10 5.62130216E-13-4.41855167E+04 1.25364719E+01                    4
CH3OCO     4/20/99 THERMC   2H   3O   2    0G   300.000  5000.000 1362.000    21
 1.30877600E+01 4.53544950E-03-1.65096364E-06 2.67197277E-10-1.59576863E-14    2
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-2.46616400E+04-3.27914051E+01 3.94199159E+00 2.43434884E-02-1.65595560E-05   3
 4.58537411E-09-3.31795708E-13-2.14404829E+04 1.66954362E+01   4
OCHO   2/14/95 THERMC   1H   1O   2   0G   300.000 5000.000 1690.000   01
 6.12628782E+00 3.75602932E-03-1.42010352E-06 2.36429200E-10-1.44167651E-14   2
-2.17698466E+04-8.01574694E+00 1.35213452E+00 1.50082004E-02-1.09896141E-05   3
 3.73679840E-09-4.81014498E-13-2.02253647E+04 1.74373147E+01   4
CH2NCH2   1104 C   2H   4N   1O   0G   298.150 3000.000 1000.00   1
 3.32004739E+00 1.85256567E-02-9.56913297E-06 2.33791748E-09-2.22816553E-13   2
 2.51357839E+04 6.51880960E+00 8.69061323E-01 2.52857715E-02-1.51435611E-05   3
 3.01037347E-09 3.70026806E-13 2.57781726E+04 1.91043579E+01   4
CH3CH2OCH2CHNH   NL0512H   9C   4N   1O   1g   200.00 5000.00 1000.00   1
 8.36000200E+00 3.06389215E-02-1.19217691E-05 2.12710396E-09-1.42805755E-13   2
-1.92820605E+04-9.98252697E+00 6.10346035E+00-3.66483343E-03 1.12168585E-04   3
-1.38733317E-07 5.31527398E-11-1.67028344E+04 1.14681226E+01   4
CH3OCH2CH2NCH2   NL0512H   9C   4N   1O   1g   200.00 5000.00 1000.00   1
 8.05415179E+00 3.11255928E-02-1.21622491E-05 2.17616891E-09-1.46388264E-13   2
-1.55439366E+04-8.60414956E+00 6.20974625E+00-5.18178680E-03 1.14720181E-04   3
-1.39910256E-07 5.31704738E-11-1.30042686E+04 1.10095350E+01   4
OHCH2CH2NHCHCH2   NL0512H   9C   4N   1O   1g   200.00 5000.00 1000.00   1
 9.59411279E+00 2.87385506E-02-1.09953106E-05 1.93953570E-09-1.29179308E-13   2
-1.92057654E+04-1.58976491E+01 4.33461015E+00 1.22408435E-02 7.74855054E-05   3
-1.08614992E-07 4.36754430E-11-1.63320526E+04 1.85695490E+01   4
CH3CH2NHCH2CHO   NL0512H   9C   4N   1O   1g   200.00 5000.00 1000.00   1
 8.37917027E+00 3.06041482E-02-1.19039388E-05 2.12339984E-09-1.42532279E-13   2
-2.35334995E+04-1.01585630E+01 5.60458654E+00 5.92374408E-04 1.01275767E-04   3
-1.27517982E-07 4.90685747E-11-2.09329223E+04 1.33156783E+01   4
NH2CH2CH2OCHCH2   NL0512H   9C   4N   1O   1g   200.00 5000.00 1000.00   1
 9.24017968E+00 2.92252711E-02-1.12209141E-05 1.98384906E-09-1.32333667E-13   2
-1.72651475E+04-1.35100265E+01 4.73403778E+00 8.03702900E-03 8.77461142E-05   3
-1.18729852E-07 4.72834190E-11-1.44781450E+04 1.76832014E+01   4
CH2CHOH   NL0512H   4C   2O   1   0g   200.00 5000.00 1000.00   1
 5.42272094E+00 1.15933167E-02-4.33696384E-06 7.52881119E-10-4.95662269E-14   2
-1.69295063E+04-2.60547080E+00 3.06992485E+00 6.70489764E-03 2.86649911E-05   3
-4.28687590E-08 1.78068027E-11-1.58054191E+04 1.21037066E+01   4
C2   ATCT/AC 2.   0.   0.   0.G   200.000 6000.000 1000.   1
 4.12492246E+00 1.08348338E-04 1.57252585E-07-4.24046828E-11 3.25059373E-15   2

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 9.81882961E+04 7.97432262E-01-1.96261001E+00 5.76822247E-02-1.58039636E-04    3
 1.72462711E-07-6.57913199E-11 9.82538219E+04 2.33201223E+01 9.91459509E+04    4
C2O               110203C   2O   1    0    0G   300.000  4000.000 1000.00    0 1 ! Melius
2003; see WIL/FLE07
 0.50266479E+01 0.28918227E-02-0.13913841E-05 0.30703546E-09-0.25567905E-13    2 !
 0.44888900E+05-0.17853398E+01 0.29665556E+01 0.10513229E-01-0.13516489E-04    3
 0.99333965E-08-0.30881376E-11 0.45385915E+05 0.84432753E+01                   4
OCHCHO    SAND    120596H   2C   2O   2    0G   300.00   3000.00  1000.00      1
 0.49087462E+01 0.13182673E-01-0.71416730E-05 0.18461316E-08-0.18525858E-12    2
-0.27116386E+05 0.59148768E+00 0.25068862E+01 0.18899139E-01-0.10302623E-04    3
 0.62607508E-09 0.88114253E-12-0.26427374E+05 0.13187043E+02                   4
CHCNH             1107  C   2H   2N   1O   0G   298.150  3000.000 1000.00      1
 5.54662620E+00 7.65157744E-03-3.57997666E-06 8.31108900E-10-7.71666875E-14    2
 4.53945633E+04-3.17646312E+00 2.87300918E+00 1.98561384E-02-2.41519574E-05    3
 1.60558556E-08-4.26087659E-12 4.58537821E+04 9.34467032E+00                   4
CH2CN   BUR0302   T01/03C  2.H  2.N  1.   0.G   200.000  6000.000 1000.        1
 6.14873620E+00 6.06600240E-03-2.17174620E-06 3.49750387E-10-2.09004207E-14    2
 2.86491222E+04-6.59235995E+00 2.63064017E+00 1.73644377E-02-1.70284117E-05    3
 9.86551140E-09-2.46033517E-12 2.95791691E+04 1.12776223E+01 3.10031788E+04    4
CH2CHN            1110  C   2H   3N   1O   0G   298.150  3000.000 1000.00      1
 4.14453572E+00 1.31731672E-02-6.28186453E-06 1.43989655E-09-1.30842159E-13    2
 4.10389141E+04 3.75755189E+00 3.85114887E-01 2.63155652E-02-2.31525336E-05    3
 1.07917240E-08-1.99497769E-12 4.18855625E+04 2.23684056E+01                   4
CH2CHN(S)         1110  C   2H   3N   1O   0G   298.150  3000.000 1000.00      1
 4.14453572E+00 1.31731672E-02-6.28186453E-06 1.43989655E-09-1.30842159E-13    2
 4.85873563E+04 3.75755189E+00 3.85114887E-01 2.63155652E-02-2.31525336E-05    3
 1.07917240E-08-1.99497769E-12 4.94340048E+04 2.23684056E+01                   4
CHCNH2            1107  C   2H   3N   1O   0G   298.150  3000.000 1000.00      1
 4.67245309E+00 1.04989910E-02-4.62630454E-06 1.01345924E-09-8.92616681E-14    2
 2.60712723E+04-5.77430843E-01 1.34809615E+00 2.60893264E-02-3.14511691E-05    3
 2.11896099E-08-5.70652625E-12 2.66214983E+04 1.48874428E+01                   4
CH3CN  BUR0302    T01/03C  2.H  3.N  1.   0.G   200.000  6000.000 1000.        1
 5.09921882E+00 9.69585649E-03-3.48051966E-06 5.61420173E-10-3.35835856E-14    2
 6.60967324E+03-3.36087178E+00 3.82392803E+00 4.08201943E-03 2.16209537E-05    3
-2.89807789E-08 1.12962700E-11 7.44430382E+03 5.52656156E+00 8.90492212E+03    4
c-C2H3N           1110  C   2H   3N   1O   0G   298.150  3000.000 1000.00      1
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 2.80979324E+00 1.50201816E-02-7.58141908E-06 1.85246807E-09-1.77642437E-13    2
 3.06581771E+04 8.95343001E+00 8.28524446E-02 2.20080656E-02-1.21834261E-05    3
 1.00059353E-09 1.01529601E-12 3.13995593E+04 2.30893128E+01                   4
CH3NCH            1106  C   2H   4N   1O   0G   298.150  3000.000 1000.00      1
 3.29670257E+00 1.69750507E-02-8.65108533E-06 2.12635860E-09-2.04492818E-13    2
 2.51028107E+04 8.60277030E+00 2.23655533E+00 1.58044545E-02 1.22158661E-06    3
-9.86660781E-09 4.14654507E-12 2.55853994E+04 1.50701642E+01                   4
CH3CNH            1106  C   2H   4N   1O   0G   298.150  3000.000 1000.00      1
 3.29670257E+00 1.69750507E-02-8.65108533E-06 2.12635860E-09-2.04492818E-13    2
 2.51028107E+04 8.60277030E+00 2.23655533E+00 1.58044545E-02 1.22158661E-06    3
-9.86660781E-09 4.14654507E-12 2.55853994E+04 1.50701642E+01                   4
CH3CHN            1106  C   2H   4N   1O   0G   298.150  3000.000 1000.00      1
 2.67758316E+00 1.76421637E-02-8.68916543E-06 2.06973359E-09-1.93574323E-13    2
 2.23928599E+04 1.20240438E+01 2.81409484E+00 1.32950847E-02 3.53300166E-06    3
-9.87941013E-09 3.74396969E-12 2.25556092E+04 1.23157119E+01                   4
CH2CNH2           1107  C   2H   4N   1O   0G   298.150  3000.000 1000.00      1
 4.21874005E+00 1.56980617E-02-7.75730038E-06 1.84326074E-09-1.71837565E-13    2
 3.03905504E+04 4.69611801E+00 2.01233456E+00 2.56068048E-02-2.42450966E-05    3
 1.39182460E-08-3.46136416E-12 3.07776754E+04 1.50699688E+01                   4
CHCHNH2           1104  C   2H   4N   1O   0G   298.150  3000.000 1000.00      1
 4.77534564E+00 1.46041683E-02-6.78153232E-06 1.55237043E-09-1.41604244E-13    2
 3.54379126E+04 3.02319529E-01 5.83297823E-01 3.10085354E-02-3.08423467E-05    3
 1.72290892E-08-3.96982789E-12 3.62945134E+04 2.06174831E+01                   4
CH3CHNH           1104  C   2H   5N   1O   0G   298.150  3000.000 1000.00      1
 1.99419246E+00 2.12775413E-02-1.02686597E-05 2.40039260E-09-2.20647891E-13    2
 4.56273305E+03 1.43228859E+01 2.24230513E+00 1.46071399E-02 8.25386853E-06    3
-1.56259103E-08 5.70541553E-12 4.79700805E+03 1.45453734E+01                   4
CH3NCH2           1104  C   2H   5N   1O   0G   298.150  3000.000 1000.00      1
 1.74096270E+00 2.20935014E-02-1.09102093E-05 2.60523608E-09-2.44224882E-13    2
 7.19229187E+03 1.52596427E+01 2.12431227E+00 1.61641640E-02 4.57770566E-06    3
-1.21159798E-08 4.53506389E-12 7.33541892E+03 1.45091874E+01                   4
CH2CHNH2          1104  C   2H   5N   1O   0G   298.150  3000.000 1000.00      1
 4.59217082E+00 1.72595719E-02-7.93920737E-06 1.79644782E-09-1.61748720E-13    2
 2.46743039E+03-8.63800108E-02-7.10306111E-01 3.74245041E-02-3.66191425E-05    3
 1.98714291E-08-4.41925018E-12 3.58017455E+03 2.57562499E+01                   4
CH3CH2NH          1104  C   2H   6N   1O   0G   298.150  3000.000 1000.00      1
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 3.09795233E+00 2.24757903E-02-1.07197166E-05 2.48313682E-09-2.26728211E-13    2
 1.65130465E+04 1.02924690E+01 1.92365746E+00 2.38729244E-02-7.86534966E-06    3
-2.71981984E-09 1.89902230E-12 1.69129077E+04 1.67827743E+01                   4
CH3CHNH2          1104  C   2H   6N   1O   0G   298.150  3000.000 1000.00      1
 4.08789216E+00 2.05227724E-02-9.45003681E-06 2.12694610E-09-1.89705755E-13    2
 1.19396821E+04 5.24987703E+00 1.64074549E+00 2.85826810E-02-1.89468825E-05    3
 6.72949839E-09-9.08174290E-13 1.25155453E+04 1.74881147E+01                   4
CH2CH2NH2         1104  C   2H   6N   1O   0G   298.150  3000.000 1000.00      1
 4.10302792E+00 2.03084588E-02-9.25456057E-06 2.06112265E-09-1.81949714E-13    2
 1.70234069E+04 5.55411391E+00 1.25928611E+00 3.01867188E-02-2.18268895E-05    3
 8.94596797E-09-1.52898422E-12 1.76669906E+04 1.96477011E+01                   4
CH3CH2NH2         1104  C   2H   7N   1O   0G   298.150  3000.000 1000.00      1
 2.82804839E+00 2.53750154E-02-1.18740298E-05 2.70990740E-09-2.44590811E-13    2
-8.03920733E+03 1.01771802E+01 6.44080211E-01 3.14866800E-02-1.71052145E-05    3
 3.57315578E-09 1.95649123E-13-7.47120329E+03 2.13696162E+01                   4
H2NCO             T09/96H   2N   1C   1O   1G   200.000  6000.000 1000.00      1 ! Burcat
 0.57886741D+01 0.60938325D-02-0.21165797D-05 0.33404486D-09-0.19684582D-13    2
-0.50210948D+04-0.44063740D+01 0.35677914D+01 0.10193381D-01-0.15289951D-05    3
-0.47571551D-08 0.26052647D-11-0.42980380D+04 0.75824281D+01-0.28029168D+04    4
H2NCHO            T12/92N   1C   1H   3O   1G   200.000  6000.000 1000.00      1 ! Burcat
 0.50996641E+01 0.96197778E-02-0.33675100E-05 0.52625772E-09-0.30639100E-13    2
-0.25835964E+05-0.22514334E+01 0.31136723E+01 0.29491209E-02 0.32396676E-04    3
-0.44756760E-07 0.18144841E-10-0.24750380E+05 0.10806345E+02-0.23484619E+05    4
CH3NHCH2          1104  C   2H   6N   1O   0G   298.150  3000.000 1000.00      1
 3.95751097E+00 2.09452232E-02-9.75570653E-06 2.21626118E-09-1.99156129E-13    2
 1.60587518E+04 4.96297406E+00 1.71401860E+00 2.75573004E-02-1.61309839E-05    3
 4.10455384E-09-8.07562261E-14 1.66255449E+04 1.63770009E+01                   4
CH3NCH3           1104  C   2H   6N   1O   0G   298.150  3000.000 1000.00      1
 1.54968373E+00 2.47836253E-02-1.20302906E-05 2.81641066E-09-2.58540173E-13    2
 1.73453147E+04 1.93447983E+01 3.61164557E+00 9.06653308E-03 2.27492150E-05    3
-2.78391712E-08 9.27266651E-12 1.73063845E+04 1.12643356E+01                   4
CH3NHCH3          1104  C   2H   7N   1O   0G   298.150  3000.000 1000.00      1
 2.13913083E+00 2.68643078E-02-1.28763453E-05 2.99663495E-09-2.74772023E-13    2
-4.17331872E+03 1.29759199E+01 1.22882380E+00 2.60430675E-02-4.95078244E-06    3
-6.74954202E-09 3.27738931E-12-3.76813390E+03 1.84832422E+01                   4
NCCN                    C   2N   2O   0O   0G   300.00   5000.00  1000.00      1
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 0.65480000E+01 0.39847100E-02-0.16342200E-05 0.30386000E-09-0.21110000E-13    2
 0.34907200E+05-0.97360000E+01 0.42654600E+01 0.11922570E-01-0.13420140E-04    3
 0.91923000E-08-0.27789400E-11 0.35478900E+05 0.17130000E+01                   4
CH2NN H2C=N=N     T09/09C  1.H  2.N  2.   0.G   200.000  6000.000 1000.       1
 5.48509574E+00 6.47548090E-03-2.27700420E-06 3.62251938E-10-2.14627058E-14    2
 3.01582071E+04-4.44806421E+00 2.70017481E+00 1.53945741E-02-1.42688481E-05    3
 8.44885976E-09-2.25039897E-12 3.09049980E+04 9.72801485E+00 3.22838652E+04    4
CH2NO  H2C=N-O*   T06/08C  1.H  2.N  1.O  1.G   200.000  6000.000 1000.       1
 5.41478025E+00 6.68230119E-03-2.38625695E-06 3.83764001E-10-2.29149657E-14    2
 1.63459530E+04-3.03719498E+00 3.00389272E+00 6.88209471E-03 1.26563213E-05    3
-2.17579528E-08 9.28731765E-12 1.73161337E+04 1.09485576E+01 1.85908365E+04    4
CH3N              NL0512H   3C   1N   1    0g    200.00  5000.00  1000.00      1
 3.47435316E+00 8.90511141E-03-3.45265524E-06 6.14249201E-10-4.11440888E-14    2
 3.58953250E+04 4.68744026E+00 4.05938864E+00-6.37703777E-03 4.24396060E-05    3
-4.91579210E-08 1.85297277E-11 3.63766007E+04 4.92297238E+00                   4
CH2NHNH2          NL0512H   5C   1N   2    0g    200.00  5000.00  1000.00      1
 5.38918485E+00 1.36677756E-02-5.06038159E-06 8.71303083E-10-5.69969006E-14    2
 2.88735149E+04 3.79464404E-01 3.56810411E+00 7.39883066E-03 2.89039288E-05    3
-4.26008614E-08 1.75343624E-11 2.98509598E+04 1.23314054E+01                   4
CH2NNH2           NL0512H   4C   1N   2    0g    200.00  5000.00  1000.00      1
 5.03931713E+00 1.20256813E-02-4.52114259E-06 7.87423335E-10-5.19552431E-14    2
 1.65652364E+04-2.48661011E-01 3.07990856E+00 7.44662359E-03 2.37048127E-05    3
-3.55412708E-08 1.45796497E-11 1.75548321E+04 1.21966403E+01                   4
CH3NHNH           NL0512H   5C   1N   2    0g    200.00  5000.00  1000.00      1
 4.63174083E+00 1.47871383E-02-5.60045843E-06 9.80256309E-10-6.49014119E-14    2
 2.23321958E+04 3.18439809E+00 5.04587002E+00-3.20775711E-03 4.93020757E-05    3
-5.82273135E-08 2.18060409E-11 2.30346875E+04 5.12706947E+00                   4
CH2CHOOH   4/25/ 6 thermC   2H   4O   2    0g   300.000  5000.000 1397.000    21
 1.15749951e+01 8.09909174e-03-2.81808668e-06 4.42697954e-10-2.58998042e-14    2
-8.85355935e+03-3.43859117e+01 1.35644398e+00 3.37002447e-02-2.75988500e-05    3
 1.14222854e-08-1.89488886e-12-5.50499964e+03 1.98354466e+01                   4
CHCHOOH    4/25/ 6 thermC   2H   3O   2    0g   300.000  5000.000 1398.000    21
 1.14545496e+01 5.70488492e-03-2.00315570e-06 3.16596832e-10-1.86008264e-14    2
 2.12557351e+04-3.18525958e+01 2.29523631e+00 3.00886042e-02-2.72416044e-05    3
 1.22702909e-08-2.18203315e-12 2.41142608e+04 1.62401413e+01                   4
CH*CH2NHCH2CHO NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
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 1.30164816E+01 2.80109857E-02-1.08741014E-05 1.93802554E-09-1.30043635E-13    2
-1.16546837E+04-2.48070328E+01 5.42040565E+00 1.88068691E-02 6.82656239E-05    3
-1.02615169E-07 4.20518143E-11-8.15501883E+03 2.15806945E+01                   4
CH2CH*NCH2     NL0512   H   6C   3N   1O   2g    200.00   5000.00 1000.00      1
 1.10263776E+01 1.92266713E-02-7.36564355E-06 1.30050347E-09-8.66782140E-14    2
 1.48722617E+04-2.21910608E+01 3.35068539E+00 2.94352732E-02 1.01622407E-05    3
-3.60568146E-08 1.71869326E-11 1.74736591E+04 1.99785496E+01                   4
CH2CH*NHCH2CHO NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.40465661E+01 2.66858117E-02-1.02641634E-05 1.81759017E-09-1.21404761E-13    2
-1.27783905E+04-3.12450536E+01 4.01476630E+00 3.63117104E-02 2.38107787E-05    3
-5.84599747E-08 2.64529437E-11-9.18082726E+03 2.48175037E+01                   4
CH2CH*OCH2CHNH NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.40062755E+01 2.67439268E-02-1.02921034E-05 1.82323617E-09-1.21815680E-13    2
-1.00990260E+04-3.11807636E+01 4.33637567E+00 3.12375346E-02 3.92601547E-05    3
-7.58887531E-08 3.31854325E-11-6.44480528E+03 2.39032338E+01                   4
CH2CH2N*CH2CHO NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.43298921E+01 2.66279222E-02-1.02932659E-05 1.82885000E-09-1.22439348E-13    2
-7.56828280E+02-3.22917241E+01 4.34641135E+00 3.58416230E-02 2.48370467E-05    3
-5.96169809E-08 2.69284262E-11 2.84302255E+03 2.35913156E+01                   4
CH2CH2NCH*     NL0512   H   6C   3N   1O   2g    200.00   5000.00 1000.00      1
 1.07415634E+01 1.96049391E-02-7.54215785E-06 1.33561647E-09-8.92082500E-14    2
 1.17770921E+04-2.02938447E+01 4.55218264E+00 2.10948298E-02 2.80592757E-05    3
-5.21784900E-08 2.24998609E-11 1.42023644E+04 1.53464850E+01                   4
CH2CH2NHCH*CHO NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.39177909E+01 2.69352936E-02-1.03947453E-05 1.84498100E-09-1.23437476E-13    2
-1.21139348E+04-3.08542226E+01 4.31928289E+00 3.27643759E-02 3.32594468E-05    3
-6.81791196E-08 2.99826668E-11-8.51476305E+03 2.35875495E+01                   4
CH2CH2OCH*CHNH NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.39841286E+01 2.68473912E-02-1.03540469E-05 1.83694761E-09-1.22862498E-13    2
-7.49192309E+03-3.12875790E+01 4.93155036E+00 2.80235738E-02 4.55169594E-05    3
-8.10850759E-08 3.47748839E-11-3.91850160E+03 2.10288051E+01                   4
CH2CH2OCH2CHN* NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.38305676E+01 2.72323278E-02-1.05645345E-05 1.88172948E-09-1.26204325E-13    2
 4.68495732E+03-2.99185206E+01 5.33303875E+00 2.57673014E-02 4.93770536E-05    3
-8.35210041E-08 3.52644673E-11 8.18787198E+03 1.98723445E+01                   4
CH2CHCHhO      NL0512   H   5C   3O   3    0g    200.00   5000.00 1000.00      1
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 1.13317066E+01 1.67319420E-02-6.43469628E-06 1.13960394E-09-7.61353298E-14    2
-6.25190487E+03-2.51050816E+01 3.08845462E+00 2.74265239E-02 1.45812538E-05    3
-4.25715682E-08 2.01523137E-11-3.49086614E+03 2.01343963E+01                   4
N*CH2CH2OCHCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.31127368E+01 2.78836158E-02-1.08125627E-05 1.92537665E-09-1.29108102E-13    2
 2.83867075E+01-2.47108351E+01 5.65560427E+00 1.63244277E-02 7.64947642E-05    3
-1.12744930E-07 4.62242315E-11 3.53914880E+03 2.13180178E+01                   4
CH2NOOH        NL0512   H   3C   1N   1O   2g    200.00   5000.00 1000.00      1
 7.17582349E+00 9.79263705E-03-3.71946961E-06 6.52992770E-10-4.33523400E-14    2
 6.82963103E+03-7.13181609E+00 3.15036645E+00 1.35715816E-02 1.15310867E-05    3
-2.65245945E-08 1.21229787E-11 8.23708842E+03 1.52814276E+01                   4
CH2OCH*CH2NCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.35820823E+01 2.73236615E-02-1.05637153E-05 1.87720255E-09-1.25695193E-13    2
-8.81756260E+03-2.94341643E+01 4.47710974E+00 2.88018273E-02 4.41123322E-05    3
-7.93251300E-08 3.39947812E-11-5.21935493E+03 2.31601299E+01                   4
CH2OCH2CH*NCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.34620945E+01 2.74988677E-02-1.06479392E-05 1.89416533E-09-1.26924720E-13    2
-6.99738127E+03-2.87092643E+01 4.97554314E+00 2.60642602E-02 4.88869557E-05    3
-8.27593539E-08 3.48786455E-11-3.49531052E+03 2.10252758E+01                   4
CH2OCH2CH2NCH* NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.30784904E+01 2.78970237E-02-1.08131229E-05 1.92491950E-09-1.29051131E-13    2
-9.00870949E+03-2.61182406E+01 6.02328824E+00 1.85725386E-02 6.44918395E-05    3
-9.64751511E-08 3.93113397E-11-5.70056608E+03 1.72066346E+01                   4
CH2OCHCH*      NL0512   H   5C   3O   3    0g    200.00   5000.00 1000.00      1
 1.12483668E+01 1.61273413E-02-6.14165814E-06 1.08005797E-09-7.17860356E-14    2
-2.66635615E+03-2.21385221E+01 3.92166702E+00 2.81579238E-02 3.49502879E-06    3
-2.69389309E-08 1.35880864E-11-3.04097256E+02 1.75373003E+01                   4
CHNOOH         NL0512   H   2C   1N   1O   2g    200.00   5000.00 1000.00      1
 7.80042897E+00 6.40552192E-03-2.40515771E-06 4.18901008E-10-2.76544439E-14    2
 3.39008772E+04-9.43082516E+00 2.60123962E+00 2.34626502E-02-2.31820252E-05    3
 1.10678507E-08-1.76655034E-12 3.51793443E+04 1.66965104E+01                   4
cyMeta*Morph2yl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.44936260E+01 2.84174553E-02-1.10130662E-05 1.96075052E-09-1.31481905E-13    2
-1.75139579E+04-4.61749827E+01 2.85460413E+00 3.47108929E-02 4.58139450E-05    3
-8.84256420E-08 3.87426690E-11-1.31631576E+04 1.99033209E+01                   4
cyMeta*Morph4yl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
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 1.40033433E+01 2.92910380E-02-1.14606805E-05 2.05376880E-09-1.38349845E-13    2
-1.79211949E+04-4.49087515E+01 3.48965388E+00 2.51688611E-02 7.13937282E-05    3
-1.14226316E-07 4.78915530E-11-1.35236855E+04 1.71376235E+01                   4
cyMeta*Morph5yl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.44092626E+01 2.85603054E-02-1.10876144E-05 1.97658231E-09-1.32672377E-13    2
-1.80920027E+04-4.64954956E+01 3.05337416E+00 3.22718540E-02 5.17972652E-05    3
-9.39861692E-08 4.05573759E-11-1.37222731E+04 1.85841574E+01                   4
cyMeta*Morph6yl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.42811521E+01 2.87517833E-02-1.11807730E-05 1.99549274E-09-1.34050797E-13    2
-1.55544397E+04-4.59761819E+01 3.31230094E+00 2.89368322E-02 6.08024541E-05    3
-1.03344033E-07 4.39751277E-11-1.11814296E+04 1.76774595E+01                   4
cyMetaOOMorphyl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.34256646E+01 3.05058652E-02-1.19859435E-05 2.15387694E-09-1.45372407E-13    2
-2.02548603E+04-4.43498328E+01 3.19764079E+00 2.28944790E-02 7.92420820E-05    3
-1.21708190E-07 5.02915820E-11-1.57771252E+04 1.69491455E+01                   4
cyOrtho*Morph3yl NL0512 H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.43813934E+01 2.85914794E-02-1.11005523E-05 1.97894351E-09-1.32831719E-13    2
-1.95955185E+04-4.60547527E+01 2.77886114E+00 3.42731564E-02 4.67991048E-05    3
-8.88417849E-08 3.86756711E-11-1.52115669E+04 2.00076157E+01                   4
cyOrtho*Morph4yl NL0512 H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.40670573E+01 2.92187586E-02-1.14295978E-05 2.04788683E-09-1.37939904E-13    2
-1.85486652E+04-4.48488250E+01 3.70708125E+00 2.43215815E-02 7.30279111E-05    3
-1.15752226E-07 4.84308955E-11-1.41794651E+04 1.64811958E+01                   4
cyOrtho*Morph5yl NL0512 H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.43585773E+01 2.86262145E-02-1.11175743E-05 1.98241316E-09-1.33085330E-13    2
-1.97719027E+04-4.64166304E+01 2.87434461E+00 3.32590726E-02 4.94614281E-05    3
-9.15756165E-08 3.96642141E-11-1.53885119E+04 1.92027980E+01                   4
cyOrtho*Morph6yl NL0512 H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.43413148E+01 2.87036271E-02-1.11638036E-05 1.99264499E-09-1.33866837E-13    2
-1.73152303E+04-4.62804717E+01 2.87622151E+00 3.20463318E-02 5.36776820E-05    3
-9.64406960E-08 4.15481657E-11-1.28852074E+04 1.95191682E+01                   4
cyOrthoOOMorphyl NL0512 H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.34466865E+01 3.04892931E-02-1.19806733E-05 2.15311303E-09-1.45330662E-13    2
-2.11677212E+04-4.48218647E+01 2.95386103E+00 2.44607933E-02 7.56095403E-05    3
-1.18042498E-07 4.89435730E-11-1.66509885E+04 1.76572080E+01                   4
cyPara*Morph2yl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
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 1.47102177E+01 2.83961643E-02-1.10519010E-05 1.97340093E-09-1.32600818E-13    2
-3.64746991E+03-4.78982998E+01 2.55437348E+00 3.78704072E-02 3.80416173E-05    3
-8.02865143E-08 3.56803063E-11 7.87841849E+02 2.04920295E+01                   4
cyParaOOMorphyl NL0512  H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.36300476E+01 3.04519141E-02-1.19984403E-05 2.15997110E-09-1.45956292E-13    2
-8.87940963E+03-4.56742592E+01 2.79542102E+00 2.73891189E-02 6.79938461E-05    3
-1.10279161E-07 4.61586986E-11-4.35342225E+03 1.81096207E+01                   4
NCHOOH        NL0512    H   2C   1N   1O   2g    200.00   5000.00 1000.00      1
 7.10570171E+00 7.19161595E-03-2.74797378E-06 4.84767950E-10-3.23061095E-14    2
 1.51061797E+04-6.07644452E+00 3.74118310E+00 1.03240545E-02 9.72734050E-06    3
-2.15309443E-08 9.73393078E-12 1.62918435E+04 1.26861875E+01                   4
NHCH*CH2OCHCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.40550909E+01 2.66804501E-02-1.02631256E-05 1.81757914E-09-1.21414362E-13    2
-6.55580797E+03-3.17317087E+01 3.32439456E+00 3.39748652E-02 3.85084033E-05    3
-7.87538466E-08 3.50903365E-11-2.64736165E+03 2.87460439E+01                   4
NHCH*CHO       NL0512   H   4C   2N   1O   3g    200.00   5000.00 1000.00      1
 1.08834987E+01 1.39364479E-02-5.36548409E-06 9.51136725E-10-6.35927285E-14    2
-7.61189374E+03-1.96122436E+01 4.44731671E+00 2.09870104E-02 1.46881216E-05    3
-3.66476905E-08 1.68526989E-11-5.37874098E+03 1.60627465E+01                   4
NHCH2CH*OCHCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.41215687E+01 2.66566036E-02-1.02636180E-05 1.81883384E-09-1.21552853E-13    2
-9.73098248E+03-3.18788658E+01 4.28533096E+00 2.91580811E-02 4.81909202E-05    3
-8.74330598E-08 3.79872753E-11-5.95766516E+03 2.45406587E+01                   4
NHCH2CH2OCHCH* NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.37181650E+01 2.71811666E-02-1.05059024E-05 1.86673563E-09-1.24990383E-13    2
-3.96420344E+03-2.97215086E+01 4.69972662E+00 2.61459466E-02 5.25333871E-05    3
-8.91156072E-08 3.78427651E-11-3.08411468E+02 2.29044430E+01                   4
NHCHCHO       NL0512    H   3C   2N   1O   1g    200.00   5000.00 1000.00      1
 6.06110214E+00 1.17315660E-02-4.58245457E-06 8.20065433E-10-5.51835208E-14    2
-6.71499719E+03-3.93068633E+00 3.66909704E+00 5.30244554E-03 3.07387433E-05    3
-4.26415871E-08 1.68900909E-11-5.41456528E+03 1.16018000E+01                   4
NHCHOOH       NL0512    H   3C   1N   1O   2g    200.00   5000.00 1000.00      1
 6.97204150E+00 9.85204326E-03-3.71095118E-06 6.47859126E-10-4.28456257E-14    2
-8.50754478E+03-6.04757205E+00 3.58188558E+00 9.23867044E-03 2.18529170E-05    3
-3.66413746E-08 1.56809911E-11-7.16056328E+03 1.36940577E+01                   4
OCH*CH2NHCHCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
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1.44473084E+01 2.66987605E-02-1.02498668E-05 1.81283474E-09-1.20987251E-13 2
-9.81285088E+03-3.58238308E+01 2.28019125E+00 4.30569383E-02 1.78101658E-05 3
-5.83943085E-08 2.78060133E-11-5.72981492E+03 3.09016390E+01 4
OCH*CHNH NL0512 H 4C 2N 1O 3g 200.00 5000.00 1000.00 1
1.11063015E+01 1.42173081E-02-5.48184513E-06 9.72926411E-10-6.51105684E-14 2
-4.83909000E+03-2.36269923E+01 2.97333270E+00 2.66600442E-02 8.98499815E-06 3
-3.50419505E-08 1.71598540E-11-2.20140198E+03 2.05640924E+01 4
OCH2CH*NHCHCH2 NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.45742148E+01 2.66561292E-02-1.02535445E-05 1.81599074E-09-1.21318258E-13 2
-8.57671485E+03-3.64424404E+01 3.02570077E+00 4.00653041E-02 2.30154756E-05 3
-6.24782673E-08 2.90138138E-11-4.59418218E+03 2.74144568E+01 4
OCH2CH2N*CHCH2 NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.48058721E+01 2.66024711E-02-1.02732732E-05 1.82428256E-09-1.22094157E-13 2
6.45678993E+03-3.74286417E+01 3.00050291E+00 4.05458330E-02 2.31961795E-05 3
-6.35628437E-08 2.96284231E-11 1.05119923E+04 2.77780948E+01 4
OCH2CH2NHCHCH* NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.43367527E+01 2.70324643E-02-1.04397282E-05 1.85404209E-09-1.24100858E-13 2
-3.52196182E+03-3.44009184E+01 4.05664603E+00 3.38473722E-02 3.48119332E-05 3
-7.17391346E-08 3.16499012E-11 2.91335126E+02 2.37361430E+01 4
OCH2CHN* NL0512 H 4C 2N 1O 3g 200.00 5000.00 1000.00 1
1.10300682E+01 1.45184852E-02-5.65716043E-06 1.01114507E-09-6.79990668E-14 2
1.01731294E+04-2.27953442E+01 3.54243352E+00 2.46766429E-02 1.07538024E-05 3
-3.45468820E-08 1.63904561E-11 1.26981966E+04 1.82890149E+01 4
N*CH2CHO NL0512 H 4C 2N 1O 3g 200.00 5000.00 1000.00 1
1.00051943E+01 1.50715838E-02-5.88652810E-06 1.05364933E-09-7.09219581E-14 2
-9.84274147E+02-1.43535163E+01 4.86607433E+00 1.37414053E-02 3.16707895E-05 3
-5.18684616E-08 2.17445312E-11 1.15680407E+03 1.58712857E+01 4
OCHOOH NL0512 H 2C 1O 3 0g 200.00 5000.00 1000.00 1
6.59570455E+00 7.71138318E-03-2.96087667E-06 5.24049901E-10-3.50043803E-14 2
-3.67925907E+04-3.36287842E+00 4.12675703E+00 6.35427459E-03 1.75788334E-05 3
-2.77785835E-08 1.15459444E-11-3.57375164E+04 1.13121420E+01 4
cyPara*Morph3yl NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.54166324E+01 2.81691005E-02-1.10840504E-05 1.99450306E-09-1.34769408E-13 2
2.26750237E+04-5.28862611E+01 2.84806241E+00 3.18532543E-02 5.91337653E-05 3
-1.04088922E-07 4.45800368E-11 2.75500178E+04 1.92961907E+01 4
CH*CH2OCH2CHNH NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1

```
 1.43927498E+01 2.74549524E-02-1.08625213E-05 1.96219978E-09-1.32955189E-13    2
 6.87350101E+03-3.27794818E+01 7.29744474E+00 1.12182087E-03 1.19723674E-04    3
-1.57232030E-07 6.18725468E-11 1.09797900E+04 1.48081111E+01                   4
CH2NHCHCH*   NL0512     H   6C   3N   1O   2g    200.00   5000.00 1000.00      1
 1.13162338E+01 1.85103901E-02-6.97320497E-06 1.21677780E-09-8.04147624E-14    2
 1.37277095E+04-2.32257879E+01 3.59085639E+00 3.15936836E-02 2.11982510E-06    3
-2.73622171E-08 1.40277919E-11 1.61934065E+04 1.84972072E+01                   4
CH*CH2NCH2   NL0512     H   6C   3N   1O   2g    200.00   5000.00 1000.00      1
 1.16785871E+01 1.96070016E-02-7.78699082E-06 1.41045208E-09-9.57580059E-14    2
 2.48851949E+04-2.65236022E+01 4.63740383E+00 8.84713781E-03 7.22066789E-05    3
-1.01983568E-07 4.10812971E-11 2.82370817E+04 1.70278372E+01                   4
CH*OCH2CH2NCH2 NL0512   H   8C   4N   1O   3g    200.00   5000.00 1000.00      1
 1.35296823E+01 2.80081240E-02-1.10036466E-05 1.97765559E-09-1.33507372E-13    2
 1.18128499E+04-2.88704692E+01 5.85599616E+00 1.07507540E-02 9.43258839E-05    3
-1.31148909E-07 5.25622949E-11 1.57249325E+04 1.99048334E+01                   4
CH*OCHCH2      NL0512   H   5C   3O   3    0g    200.00   5000.00 1000.00      1
 1.14821134E+01 1.64350154E-02-6.40711507E-06 1.14601429E-09-7.71243035E-14    2
 1.08000752E+04-2.46800638E+01 3.19973238E+00 2.05901841E-02 3.59399245E-05    3
-6.59932095E-08 2.88282279E-11 1.38796089E+04 2.23418535E+01                   4
CH*NHCHCH2     NL0512   H   6C   3N   1O   2g    200.00   5000.00 1000.00      1
 1.16713205E+01 1.87336990E-02-7.21354447E-06 1.27919413E-09-8.55599211E-14    2
 2.44423797E+04-2.59814895E+01 2.88962207E+00 2.47255506E-02 3.25458850E-05    3
-6.42362362E-08 2.84441742E-11 2.76341655E+04 2.34988397E+01                   4
CH2CHCH2CH2CH2O         H   9C   5O   1    0g    200.00   5000.00 1000.00      1
 9.95800640E+00 2.96191538E-02-1.15270602E-05 2.05686802E-09-1.38097093E-13    2
 1.28158232E+03-1.97769057E+01 4.15233137E+00 1.34930482E-02 7.83259946E-05    3
-1.10480936E-07 4.44454497E-11 4.39561293E+03 1.78683941E+01                   4
CH2CHCH2CH2OCH2         H   9C   5O   1    0g    200.00   5000.00 1000.00      1
 9.59464358E+00 2.92067681E-02-1.12914003E-05 2.00552911E-09-1.34206342E-13    2
 1.38106589E+03-1.54328835E+01 4.49117160E+00 1.23575797E-02 7.66057421E-05    3
-1.07020765E-07 4.29168170E-11 4.23646406E+03 1.82772149E+01                   4
CH2CHCH2OCH2CH2         H   9C   5O   1    0g    200.00   5000.00 1000.00      1
 9.91865355E+00 2.90098252E-02-1.12429688E-05 2.00035454E-09-1.34023886E-13    2
 3.41257205E+03-1.70551963E+01 4.52063420E+00 1.36812732E-02 7.34923404E-05    3
-1.04079051E-07 4.19050308E-11 6.32162807E+03 1.80203080E+01                   4
CH2CHCHCHCH2O           H   7C   5O   1    0g    200.00   5000.00 1000.00      1
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1.02584659E+01 2.41294259E-02-9.38244543E-06 1.67348043E-09-1.12334013E-13 2

1.50832103E+04-2.32092537E+01 3.86727394E+00 1.59690636E-02 5.94865728E-05 3

-8.98247756E-08 3.70439943E-11 1.80237928E+04 1.58548804E+01 4

CH2CHCHCHOCH2 H 7C 5O 1 0g 200.00 5000.00 1000.00 1

1.06036390E+01 2.30054370E-02-8.85678777E-06 1.56870409E-09-1.04771830E-13 2

1.34916570E+04-2.24512000E+01 3.41804992E+00 2.57010665E-02 2.96902101E-05 3

-5.78750926E-08 2.52554463E-11 1.62541579E+04 1.86727180E+01 4

CH2CHOCH2CH2CH2 H 9C 5O 1 0g 200.00 5000.00 1000.00 1

1.00354122E+01 2.87433752E-02-1.10978334E-05 1.96934349E-09-1.31697779E-13 2

1.50688024E+03-1.76344562E+01 4.01296525E+00 1.73380308E-02 6.57406937E-05 3

-9.75049224E-08 3.99025757E-11 4.46142840E+03 2.00799967E+01 4

CH2CHOCH2CHCH2 H 8C 5O 1 0g 200.00 5000.00 1000.00 1

9.65992226E+00 2.68535369E-02-1.03925401E-05 1.84744221E-09-1.23710295E-13 2

-7.28616842E+03-1.82865813E+01 3.23394758E+00 1.73203369E-02 6.32569095E-05 3

-9.51854564E-08 3.91923828E-11-4.26726587E+03 2.13040991E+01 4

OCHCH2CH2CH2CH2 H 9C 5O 1 0g 200.00 5000.00 1000.00 1

9.44843525E+00 2.95457440E-02-1.14753216E-05 2.04464316E-09-1.37128420E-13 2

-6.92759623E+03-1.44821661E+01 4.63848079E+00 1.19429683E-02 7.58808469E-05 3

-1.04765349E-07 4.16944283E-11-4.11942170E+03 1.77897611E+01 4

OCHCH2CH2CHCH2 H 8C 5O 1 0g 200.00 5000.00 1000.00 1

9.07249258E+00 2.76874063E-02-1.07904362E-05 1.92738301E-09-1.29500029E-13 2

-1.64906010E+04-1.50894328E+01 3.90667924E+00 1.16718795E-02 7.38510193E-05 3

-1.02729757E-07 4.10347428E-11-1.36195683E+04 1.88604741E+01 4

OCHCHCHCH2CH2 H 7C 5O 1 0g 200.00 5000.00 1000.00 1

1.00865859E+01 2.38245801E-02-9.26260561E-06 1.65175179E-09-1.10851331E-13 2

5.92357395E+03-1.97520739E+01 4.15133580E+00 1.86634038E-02 4.53038024E-05 3

-7.15061140E-08 2.95464328E-11 8.59181286E+03 1.60770532E+01 4

OCHCHCHCHCH2 H 6C 5O 1 0g 200.00 5000.00 1000.00 1

9.63030095E+00 2.20112320E-02-8.58742285E-06 1.53528188E-09-1.03231886E-13 2

-5.65130686E+03-1.97633991E+01 3.86403335E+00 1.56174506E-02 4.89640964E-05 3

-7.45525296E-08 3.05653860E-11-3.00008301E+03 1.53628061E+01 4

THP H 10C 5O 1 0g 200.00 5000.00 1000.00 1

9.20537986E+00 3.48397906E-02-1.36377768E-05 2.44351206E-09-1.64544021E-13 2

-3.27017440E+04-2.87282160E+01 2.62932191E+00 9.94376161E-03 1.09026105E-04 3

-1.47458768E-07 5.85060003E-11-2.88508553E+04 1.55300438E+01 4

THP-2-4-ene H 6C 5O 1 0g 200.00 5000.00 1000.00 1

```
 9.97327764E+00 2.27305813E-02-8.89843829E-06 1.59499332E-09-1.07456349E-13    2
-4.91256156E+03-3.00504300E+01 9.91851546E-01 2.36136943E-02 4.83306448E-05    3
-8.35452380E-08 3.58797368E-11-1.37950235E+03 2.18554220E+01                   4
THP-2-ene               H   8C   5O   1    0g    200.00   5000.00 1000.00      1
 9.57224784E+00 2.87670745E-02-1.12519276E-05 2.01522876E-09-1.35675392E-13    2
-1.94661550E+04-2.91620431E+01 1.87623925E+00 1.63758484E-02 7.96228631E-05    3
-1.16562910E-07 4.76248051E-11-1.57959623E+04 1.85136525E+01                   4
THP-2-yl                H   9C   5O   1    0g    200.00   5000.00 1000.00      1
 9.94579606E+00 3.12545526E-02-1.22238987E-05 2.18899067E-09-1.47351411E-13    2
-1.02479271E+04-3.14581743E+01 2.16371809E+00 1.75248957E-02 8.28254607E-05    3
-1.20543344E-07 4.90116083E-11-6.45669208E+03 1.70964482E+01                   4
THP-3-ene               H   8C   5O   1    0g    200.00   5000.00 1000.00      1
 9.54821274E+00 2.88864513E-02-1.13235369E-05 2.03107019E-09-1.36883728E-13    2
-1.73887515E+04-2.90051113E+01 2.09475742E+00 1.53414112E-02 8.11913852E-05    3
-1.17327791E-07 4.76735269E-11-1.37460528E+04 1.75761827E+01                   4
THP-3-yl                H   9C   5O   1    0g    200.00   5000.00 1000.00      1
 1.01937872E+01 3.10858714E-02-1.21748661E-05 2.18225847E-09-1.46994451E-13    2
-8.16191263E+03-3.21975676E+01 2.80208383E+00 1.56296472E-02 8.57391013E-05    3
-1.22674405E-07 4.96077471E-11-4.44079616E+03 1.45137704E+01                   4
THP-4-yl                H   9C   5O   1    0g    200.00   5000.00 1000.00      1
 1.02134277E+01 3.10339312E-02-1.21457377E-05 2.17595532E-09-1.46518301E-13    2
-8.86016357E+03-3.23181344E+01 2.77920888E+00 1.59416832E-02 8.49794853E-05    3
-1.22004001E-07 4.93991538E-11-5.14281917E+03 1.45441639E+01                   4
THP-5yl                 H   5C   5O   1    0g    200.00   5000.00 1000.00      1
 1.08320763E+01 1.89690619E-02-7.39998208E-06 1.32352482E-09-8.90416868E-14    2
 4.43652751E+03-3.42148749E+01-6.04097939E-01 3.62685089E-02 1.40482665E-05    3
-5.10821873E-08 2.49885563E-11 8.14443813E+03 2.79413240E+01                   4
THP-234-enyl            H   7C   5O   1    0g    200.00   5000.00 1000.00      1
 1.04118853E+01 2.50912489E-02-9.80403193E-06 1.75484245E-09-1.18100764E-13    2
-3.74058647E+03-3.28701654E+01 8.79576349E-01 2.68617993E-02 4.77980714E-05    3
-8.47322915E-08 3.65017751E-11-1.58207013E+01 2.20563432E+01                   4
THP-345-enyl            H   7C   5O   1    0g    200.00   5000.00 1000.00      1
 1.04498256E+01 2.51728058E-02-9.86646722E-06 1.76974619E-09-1.19280089E-13    2
-5.48370180E+02-3.27209406E+01 1.45017712E+00 2.33592113E-02 5.57236398E-05    3
-9.22197653E-08 3.90665496E-11 3.13502546E+03 1.99749234E+01                   4
C3H6O Propionald  T05/10C  3.H  6.O  1.   0.G   200.000  6000.000 1000.       1
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 7.44085690E+00 1.77301764E-02-6.34081568E-06 1.02040803E-09-6.09461714E-14    2
-2.60055814E+04-1.44195446E+01 4.24529681E+00 6.68296706E-03 4.93337933E-05    3
-6.71986124E-08 2.67262347E-11-2.41473007E+04 6.90738560E+00-2.22688471E+04    4
C3H5O  *CH2C2H3O  A11/04C  3.H  5.O  1.   0.G   200.000  6000.000 1000.        1
 8.15052559E+00 1.42542561E-02-5.05387276E-06 8.08732845E-10-4.81184188E-14    2
 8.72987262E+03-1.69520239E+01 3.53458477E+00 8.02398508E-03 4.85256807E-05    3
-7.23549959E-08 3.03822687E-11 1.08059525E+04 1.11545728E+01 1.25165081E+04    4
HOC2H4O2               C   2H   5O   3    0G   300.000  5000.000 1391.000    01
 1.00941573E+01 1.23879015E-02-3.73811683E-06 5.46874551E-10-3.09943951E-14    2
-2.37710522E+04-2.00956526E+01 4.44209543E+00 2.52880383E-02-1.51605275E-05    3
 5.24921198E-09-7.91470852E-13-2.17507126E+04 1.04122371E+01                   4
TMEDA                  H  16C   6N   2    0g    200.00   5000.00 1000.00      1
 1.02798013E+01 5.28689120E-02-2.05899972E-05 3.67534121E-09-2.46803201E-13    2
-1.00055382E+04-1.32913333E+01 8.67828380E+00-8.72815512E-03 1.83300281E-04    3
-2.20049981E-07 8.27156042E-11-6.26727165E+03 1.12142773E+01                   4
TMEDA-1                H  15C   6N   2    0g    200.00   5000.00 1000.00      1
 1.13176118E+01 4.88094297E-02-1.89402722E-05 3.37242970E-09-2.26061521E-13    2
 1.05891995E+04-1.78763459E+01 7.42551904E+00 5.56995146E-03 1.41668817E-04    3
-1.78829647E-07 6.84324886E-11 1.43502267E+04 1.54745619E+01                   4
TMEDA-3                H  15C   6N   2    0g    200.00   5000.00 1000.00      1
 1.09230369E+01 4.93888440E-02-1.92206699E-05 3.42921085E-09-2.30194825E-13    2
 1.00205044E+04-1.55544713E+01 8.32472997E+00-2.04123609E-03 1.58714028E-04    3
-1.94278577E-07 7.35035699E-11 1.36680145E+04 1.22853821E+01                   4
TMEDA-2                H  13C   5N   2    0g    200.00   5000.00 1000.00      1
 9.62401232E+00 4.27381686E-02-1.66625532E-05 2.97654180E-09-1.99986947E-13    2
 1.25631028E+04-1.16241739E+01 7.57628074E+00-6.20767915E-03 1.51547146E-04    3
-1.84533138E-07 7.00401380E-11 1.58126459E+04 1.22693378E+01                   4
N(CH3)2CH2CH2          H  10C   4N   1    0g    200.00   5000.00 1000.00      1
 7.64141738E+00 3.10900513E-02-1.20324193E-05 2.13829129E-09-1.43128244E-13    2
 1.37089754E+04-7.23921114E+00 5.37293090E+00 4.47726761E-03 8.64620779E-05    3
-1.09869932E-07 4.22118942E-11 1.59628604E+04 1.25197388E+01                   4
N(CH3)2CH2             H   8C   3N   1    0g    200.00   5000.00 1000.00      1
 5.93336346E+00 2.45652452E-02-9.45434371E-06 1.67348187E-09-1.11693004E-13    2
 1.31661964E+04-5.62644077E-01 5.29553381E+00 5.44001000E-04 7.03031732E-05    3
-8.61269607E-08 3.25589719E-11 1.46294564E+04 9.06705239E+00                   4
TMEDA-0-5              H  12C   5N   2    0g    200.00   5000.00 1000.00      1
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9.44594673E+00 4.05666131E-02-1.58213980E-05 2.82708838E-09-1.89988929E-13 2

3.39218373E+03-1.32802879E+01 6.33741102E+00 1.61654311E-04 1.31295350E-04 3

-1.63379100E-07 6.23589255E-11 6.67697264E+03 1.47699396E+01 4

N(CH3)2CHCH2 H 9C 4N 1 0g 200.00 5000.00 1000.00 1

7.26011505E+00 2.90352218E-02-1.12177343E-05 1.99128095E-09-1.33187615E-13 2

1.79860036E+03-7.48853562E+00 4.69708429E+00 5.22168404E-03 8.06828839E-05 3

-1.03856653E-07 4.01549226E-11 4.02002577E+03 1.32675789E+01 4

TMEDA-0-4 H 12C 5N 2 0g 200.00 5000.00 1000.00 1

9.52309107E+00 4.04929877E-02-1.57915302E-05 2.82152336E-09-1.89600843E-13 2

1.17242173E+03-1.36356738E+01 7.43199730E+00-3.17214569E-03 1.34505249E-04 3

-1.63880975E-07 6.19164337E-11 4.22277893E+03 9.33297678E+00 4

TMEDA-0-3 H 14C 6N 2 0g 200.00 5000.00 1000.00 1

1.12265286E+01 4.67075940E-02-1.81654021E-05 3.23955645E-09-2.17400624E-13 2

2.19898143E+03-1.97171957E+01 8.03645283E+00 1.64827174E-03 1.43408594E-04 3

-1.78077140E-07 6.77103577E-11 5.77189584E+03 1.00102178E+01 4

TMEDA-1-3 H 13C 6N 2 0g 200.00 5000.00 1000.00 1

1.23916314E+01 4.25215080E-02-1.64649610E-05 2.92745596E-09-1.96036777E-13 2

2.16700103E+04-2.55885134E+01 6.15065645E+00 2.01894442E-02 9.24477715E-05 3

-1.28026290E-07 5.03572206E-11 2.53722538E+04 1.63779832E+01 4

TMEDA-1-4 H 11C 5N 2 0g 200.00 5000.00 1000.00 1

1.05254751E+01 3.64843594E-02-1.41664762E-05 2.52363825E-09-1.69227244E-13 2

2.20192210E+04-1.87405022E+01 5.56661494E+00 1.40335431E-02 8.72407466E-05 3

-1.17643421E-07 4.59483213E-11 2.51944429E+04 1.57583389E+01 4

TMEDA-1-5 H 11C 5N 2 0g 200.00 5000.00 1000.00 1

1.04821143E+01 3.65121855E-02-1.41746635E-05 2.52484584E-09-1.69298961E-13 2

2.40441688E+04-1.82158036E+01 4.71725536E+00 1.64608967E-02 8.54839701E-05 3

-1.18271980E-07 4.67353406E-11 2.74083144E+04 2.03383510E+01 4

TMEDA-3-5 H 11C 5N 2 0g 200.00 5000.00 1000.00 1

1.01544558E+01 3.70098612E-02-1.44181374E-05 2.57439560E-09-1.72915616E-13 2

2.41393577E+04-1.58886090E+01 5.97803117E+00 7.80642918E-03 1.03677163E-04 3

-1.34211458E-07 5.18461841E-11 2.73188846E+04 1.56766155E+01 4

N(CH3)2CHCH H 8C 4N 1 0g 200.00 5000.00 1000.00 1

7.90263916E+00 2.57651649E-02-9.98514539E-06 1.77631089E-09-1.18993097E-13 2

3.54370242E+04-9.96100430E+00 4.51154310E+00 9.26561988E-03 6.39469337E-05 3

-8.63765778E-08 3.39596758E-11 3.76389328E+04 1.38415423E+01 4

N(CH3CH2)CHCH2 H 8C 4N 1 0g 200.00 5000.00 1000.00 1

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 8.49665814E+00 2.47640779E-02-9.47945531E-06 1.67184504E-09-1.11303420E-13    2
 2.15609720E+04-1.32438129E+01 3.10397455E+00 2.26737572E-02 3.16763327E-05    3
-5.55367393E-08 2.33930841E-11 2.38665320E+04 1.86958578E+01                   4
N(CH3)2CCH2             H   8C   4N   1    0g    200.00   5000.00 1000.00      1
 7.67414873E+00 2.59149436E-02-1.00258559E-05 1.78136164E-09-1.19224875E-13    2
 2.95450342E+04-8.63609219E+00 4.88735505E+00 7.92702159E-03 6.42406219E-05    3
-8.48424804E-08 3.29784303E-11 3.15896038E+04 1.20491773E+01                   4
N(CH3)2CCH              H   7C   4N   1    0g    200.00   5000.00 1000.00      1
 7.69321417E+00 2.28757286E-02-8.78762352E-06 1.55348815E-09-1.03588271E-13    2
 2.60117169E+04-1.12125623E+01 4.64474768E+00 1.31622473E-02 4.03139122E-05    3
-5.78682682E-08 2.29497269E-11 2.78047728E+04 9.08474434E+00                   4
N(CH3CH2)CH2CH3         H  10C   4N   1    0g    200.00   5000.00 1000.00      1
 7.36554415E+00 3.11755856E-02-1.20200788E-05 2.13047885E-09-1.42336654E-13    2
 9.41138600E+03-5.70104775E+00 5.22624406E+00 4.79252842E-03 8.51012400E-05    3
-1.08247222E-07 4.15973720E-11 1.15949277E+04 1.32333507E+01                   4
CH3CH2NCH2              H   7C   3N   1    0g    200.00   5000.00 1000.00      1
 5.54210513E+00 2.28743500E-02-8.87491249E-06 1.57999891E-09-1.05897409E-13    2
 2.39148781E+03-1.01474749E+00 4.23314943E+00-6.66626151E-04 7.44510203E-05    3
-9.23887517E-08 3.53600096E-11 4.07890744E+03 1.23432131E+01                   4
CH3CHNCH2               H   6C   3N   1    0g    200.00   5000.00 1000.00      1
 6.73741195E+00 1.88536562E-02-7.28958182E-06 1.29466092E-09-8.66260046E-14    2
 1.87970065E+04-7.25431622E+00 3.55962901E+00 9.53243058E-03 4.32647258E-05    3
-6.16706324E-08 2.48017462E-11 2.05350945E+04 1.34928457E+01                   4
CH2CHNCH3               H   6C   3N   1    0g    200.00   5000.00 1000.00      1
 6.53085284E+00 1.90486934E-02-7.36667404E-06 1.30864800E-09-8.75792161E-14    2
 1.96461864E+04-6.37902880E+00 3.74426499E+00 5.92591408E-03 5.33134119E-05    3
-7.22911818E-08 2.87219539E-11 2.13926074E+04 1.29686415E+01                   4
END
```

APPENDIX B

TRANSPORT DATABASE

The following the thermodynamic database that may be used for all reaction sets developed in the work of this dissertation. Details on the format may be found in Chapter 4.

```
HE                0    10.200     2.576     0.000     0.000     0.000 !(*)
AR                0   136.500     3.330     0.000     0.000     0.000 !
H                 0   145.000     2.050     0.000     0.000     0.000 !
H2                1    38.000     2.920     0.000     0.790   280.000 !
C                 0    71.400     3.298     0.000     0.000     0.000 !(*)
CH                1    80.000     2.750     0.000     0.000     0.000 !
CH2               1   144.000     3.800     0.000     0.000     0.000 !
CH2SING           1   144.000     3.800     0.000     0.000     0.000 !
CH3               1   144.000     3.800     0.000     0.000     0.000 !
CH4               2   141.400     3.746     0.000     2.600    13.000 !
O                 0    80.000     2.750     0.000     0.000     0.000 !
OH                1    80.000     2.750     0.000     0.000     0.000 !
H2O               2   572.400     2.605     1.844     0.000     4.000 !
C2H               1   209.000     4.100     0.000     0.000     2.500 !
C2H2              1   209.000     4.100     0.000     0.000     2.500 !
C2H3              2   209.000     4.100     0.000     0.000     1.000 !(*)
C2H4              2   280.800     3.971     0.000     0.000     1.500 !
C2H5              2   252.300     4.302     0.000     0.000     1.500 !
C2H6              2   252.300     4.302     0.000     0.000     1.500 !
CO                1    98.100     3.650     0.000     1.950     1.800 !
HCO               2   498.000     3.590     0.000     0.000     0.000 !
CH2O              2   498.000     3.590     0.000     0.000     2.000 !
CH3O              2   417.000     3.690     1.700     0.000     2.000 !
CH2OH             2   417.000     3.690     1.700     0.000     2.000 !
CH3OH             2   481.800     3.626     0.000     0.000     1.000 !(SVE)
O2                1   107.400     3.458     0.000     1.600     3.800 !
HO2               2   107.400     3.458     0.000     0.000     1.000 !(*)
H2O2              2   107.400     3.458     0.000     0.000     3.800 !
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C3H2            2   209.000     4.100     0.000     0.000     1.000 !(*)
C3H3            2   252.000     4.760     0.000     0.000     1.000 !(JAM)
AC3H4           2   252.000     4.760     0.000     0.000     1.000
PC3H4           2   252.000     4.760     0.000     0.000     1.000
SC3H5           2   260.000     4.850     0.000     0.000     1.000 !(JAM)
TC3H5           2   260.000     4.850     0.000     0.000     1.000 !(JAM)
AC3H5           2   260.000     4.850     0.000     0.000     1.000 !(JAM)
C3H6            2   266.800     4.982     0.000     0.000     1.000 !
nC3H7           2   266.800     4.982     0.000     0.000     1.000
iC3H7           2   266.800     4.982     0.000     0.000     1.000
C3H8            2   266.800     4.982     0.000     0.000     1.000 !
HCCO            2   150.000     2.500     0.000     0.000     1.000 !(*)
CH2CO           2   436.000     3.970     0.000     0.000     2.000 !
CH2CHO          2   436.000     3.970     0.000     0.000     2.000 !est.
CH3CO           2   436.000     3.970     0.000     0.000     2.000 !
CH3CHO          2   436.000     3.970     0.000     0.000     2.000 !
CO2             1   244.000     3.763     0.000     2.650     2.100 !
C2H4O           2   436.000     3.970     0.000     0.000     2.000 !guess
C2H5O           2   436.000     3.970     0.000     0.000     2.000 !est
C4H2            1   357.000     5.180     0.000     0.000     1.000 !
nC4H3           2   357.000     5.180     0.000     0.000    1.000 !guess
iC4H3           2   357.000     5.180     0.000     0.000    1.000 !TC from Wang
C4H4            2   357.000     5.180     0.000     0.000     1.000 !(JAM)
n-C4H5          2   357.000     5.180     0.000     0.000     1.000 !AB/97
i-C4H5          2   357.000     5.180     0.000     0.000     1.000 !AB/97
iiC4H6          2   357.000     5.176     0.000     0.000     1.000
iiiC4H6         2   357.000     5.176     0.000     0.000     1.000
C4H7            2   357.000     5.176     0.000     0.000     1.000
IC4H8           2   357.000     5.176     0.000     0.000     1.000
nC4H9           2   357.000     5.176     0.000     0.000     1.000 !
CH3CHOH         2   470.600     4.410     0.000     0.000     1.500 !From LLNL Marinov
CH2CHOCH2       2   357.000     5.176     0.000     0.000     1.000 !est
C2H4OH          2   470.600     4.410     0.000     0.000     1.500 !From LLNL Marinov
C3H6O           2   357.000     5.176     0.000     0.000     1.000
H2C4O           2   357.521     4.459     0.000     0.000     1.000 ! LJcjp
CH3CH2O         2   470.600     4.410     0.000     0.000     1.500 ! From LLNL
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C2H5OH          2   470.600     4.410     0.000     0.000     1.500 ! From LLNL
C2H3CO          2   429.000     4.999     2.9       0.        1.    !est
C2H3CHO         2   429.000     4.999     2.9       0.        1.    !PRW2/93
C2H3CH2O        2   429.000     4.999     2.9       0.        1.    !PRW5/93
C5H2            1   386.805     4.852     0.000     0.000     1.000 ! LJcjp
C5H5            1   357.000     5.180     0.000     0.000     1.000 ! same as C5H3
l-C5H5          1   357.000     5.180     0.000     0.000     1.000    !
H2CCCCCH        2   389.341     5.055     0.000     0.000     1.000 ! LJcjp
HCCCHCCH        2   378.067     5.021     0.000     0.000     1.000 ! LJcjp
C5H6            2   354.700     5.13      0.000     0.000     1.000 !ab
CH2CHCH2CCH     2   357.000     5.176     0.000     0.000     1.000
CH2CHCHCCH2     2   357.000     5.176     0.000     0.000     1.000
C6H3            2   412.300     5.349     0.000     0.000     1.000 !ab/97
n-C6H5          2   412.300     5.349     0.000     0.000     1.000 !ab/97
i-C6H5          2   412.300     5.349     0.000     0.000     1.000 !ab/97
n-C6H7          2   412.300     5.349     0.000     0.000     1.000 !ab/97
i-C6H7          2   412.300     5.349     0.000     0.000     1.000 !ab/97
A1              2   412.300     5.349     0.000     0.000     1.000 !ab/97
A               2   412.300     5.349     0.000     0.000     1.000 !ab/97
l-C6H4          2   367.700     5.36      0.000     0.000     1.000 !ab/97
c-C6H4          2   367.700     5.36      0.000     0.000     1.000 !ab/97
C6H8            2   412.300     5.349     0.000     0.000     1.000 !ab/97
FC6H6           2   412.300     5.349     0.000     0.000     1.000 !ab/97
C6H9            2   324.        6.093     0.000     0.000     1.000 !ab/97
C6H2            1   357.000     5.180     0.000     0.000     1.000 !
l-C6H6          2   412.300     5.349     0.000     0.000     1.000 !ab/97
C4H5C2H         2   412.3       5.349     0.00      0.00      1.00  ! JAM(12/02)
CYC6H7          2   412.300     5.349     0.000     0.000     1.000 ! same as benzene
C6H11-13        2   412.300     5.349     0.000     0.000     1.00  ! same as benzene
C6H11-12        2   399.3       5.949     0.000     0.000     1.000 !est from C6H10
C6H11-14        2   399.3       5.949     0.000     0.000     1.000 !est from C6H10
C6H11-15        2   399.3       5.949     0.000     0.000     1.000 !est from C6H10
CYC6H9          2   324.        6.093     0.000     0.000     1.000 ! BSL60
CYC6H10         2   324.        6.093     0.000     0.000     1.000 ! BSL60
C6H10           2   399.3       5.949     0.000     0.000     1.000 !est
CYC6H11         2   324.        6.093     0.000     0.000     1.000 ! BSL60
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C6H11            2   412.300     5.349     0.000     0.000     1.000 ! same as benzene
CYC6H12          2   324.        6.093     0.000     0.000     1.000 ! BSL60
CY13C6H8         2   412.300     5.349     0.000     0.000     1.000 ! same benzene
C5H4O            2   450.000     5.500     0.000     0.000     1.000 !    !
C5H4OH           2   450.000     5.500     0.000     0.000     1.000 !    !
C5H5O            2   450.000     5.500     0.000     0.000     1.000 !    !
hexene1          2   413.        5.909     0.000     0.000     1.000 ! BSL60 for nC6H14
hex1yl           2   413.        5.909     0.000     0.000     1.000 ! BSL60 for nC6H14
hex2yl           2   413.        5.909     0.000     0.000     1.000 ! BSL60 for nC6H14
hex3yl           2   413.        5.909     0.000     0.000     1.000 ! BSL60 for nC6H14
N                0    71.400     3.298     0.000     0.000     0.000 !(*)
N2               1    97.530     3.621     0.000     1.760     4.000 !
N2H2             2    71.400     3.798     0.000     0.000     1.000 !(*)
N2H3             2   200.000     3.900     0.000     0.000     1.000 !(*)
N2H4             2   205.000     4.230     0.000     4.260     1.500 !
N2O              1   232.400     3.828     0.000     0.000     1.000 !(*)
NCN              1   232.400     3.828     0.000     0.000     1.000 !(OIS)
NCO              1   232.400     3.828     0.000     0.000     1.000 !(OIS)
NH               1    80.000     2.650     0.000     0.000     4.000 !
NH2              2    80.000     2.650     0.000     2.260     4.000 !
NH3              2   481.000     2.920     1.470     0.000    10.000 !
NNH              2    71.400     3.798     0.000     0.000     1.000 !(*)
NO               1    97.530     3.621     0.000     1.760     4.000 !
NCNO             2   232.400     3.828     0.000     0.000     1.000 !(OIS)
NO2              2   200.000     3.500     0.000     0.000     1.000 !(*)
NO3              2   200.000     3.500     0.000     0.000     1.000 !
HCN              1   569.000     3.630     0.000     0.000     1.000 !(OIS)
CN               1    75.000     3.856     0.000     0.000     1.000 !(OIS)
H2CN             1   569.000     3.630     0.000     0.000     1.000 !(os/jm)
HCNO             2   232.400     3.828     0.000     0.000     1.000 !(JAM)
HOCN             2   232.400     3.828     0.000     0.000     1.000 !(JAM)
HNCO             2   232.400     3.828     0.000     0.000     1.000 !(OIS)
HOCO             2   232.400     3.828     0.000     0.000     1.000 !
HONO             2   232.400     3.828     0.000     0.000     1.000 !
HNO3             2   232.400     3.828     0.000     0.000     1.000 !
HNO              2   116.700     3.492     0.000     0.000     1.000 !(*)
```

HNNO	2	232.400	3.828	0.000	0.000	1.000	!(*)
cyMorph	2	412.300	5.349	0.000	0.000	1.000	!same as benzene
cyOrthoMorphyl	2	412.300	5.349	0.000	0.000	1.000	!same as Benzenyl
cyMetaMorphyl	2	412.300	5.349	0.000	0.000	1.000	!same as Benzenyl
cyParaMorphyl	2	412.300	5.349	0.000	0.000	1.000	!same as Benzenyl
NHCH2CH2OCHCH2	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
CH2CH2NHCH2CHO	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
OCH2CH2NHCHCH2	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
CH2CH2OCH2CHNH	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
CH2OCH2CH2NCH2	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
CH2OCHCH2	2	357.000	5.176	0.000	0.000	1.000	!same CH2COCH3
NHCH2CHO	2	429.000	4.999	2.9	0.	1.	!same as CH3CHCHO
CH2NHCHCH2	2	357.000	5.180	0.000	0.000	1.000	!CH2CHCHCH
OCH2CHNH	2	429.000	4.999	2.9	0.	1.	!same as C2H3CH2O
CH2CH2NCH2	2	357.000	5.176	0.000	0.000	1.000	!same as C4H7
CHNH	2	569.000	3.630	0.000	0.000	1.000	!same as HCN
CH2NH	2	569.000	3.630	0.000	0.000	1.000	!same as CH2N
CH2CHOCH2CHNH	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
CH2CHNH	2	436.000	3.970	0.000	0.000	2.000	!same as CH2CHO
CH2CNH	2	436.000	3.970	0.000	0.000	2.000	!same as CH2CO
OCHCH2NHCHCH2	2	399.3	5.949	0.000	0.000	1.000	!same as C6H10
cyOCHCHNHCH2CH2	2	324.	6.093	0.000	0.000	1.000	!same CYC6H10
cyNCH2CH2OCHCH	2	324.	6.093	0.000	0.000	1.000	!same as CYC6H9
CH2CH2NCHCHO	2	324.	6.093	0.000	0.000	1.000	!same as C6H9
CH2OCHCHNCH2	2	324.	6.093	0.000	0.000	1.000	!same as C6H9
cyOCHCHNCHCH2	2	412.300	5.349	0.000	0.000	1.000	!sameCY13C6H8
cyCHOCHCHNCH	2	412.300	5.349	0.000	0.000	1.000	!same as CYC6H7
cyOCH2CHNCH2CH2	2	324.	6.093	0.000	0.000	1.000	!same CYC6H10
CH2CHNCH2	2	357.000	5.176	0.000	0.000	1.000	!same as iiiC4H6
NCHCHO	2	429.000	4.999	2.9	0.	1.	!same as CH3CHCHO
CHCHNCH2	2	357.000	5.176	0.000	0.000	1.000	!same as iiiC4H6
HNC	1	569.000	3.630	0.000	0.000	1.000	! same as HCN
HNO2	2	232.400	3.828	0.000	0.000	1.000	! same as HONO
NH2O	2	116.700	3.492	0.000	0.000	1.000	! same as HNO (*)
HNOH	2	116.700	3.492	0.000	0.000	1.000	! JAM
CH3ONO2	2	232.400	3.828	0.000	0.000	1.000	! same as HOONO

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CH3ONO              2   232.400     3.828     0.000     0.000     1.000 ! same as HOONO
CH3NO               2   436.000     3.970     0.000     0.000     2.000 ! same as CH3OO
H2CNO2              2   576.7       4.549     0.000     0.000     1.000 ! Same as CH3CO2
CH3NO2              2   576.7       4.549     0.000     0.000     1.000 ! Same as CH3CO2
N2O4                2   232.400     3.828     0.000     0.000     1.000 ! same as HNO3
CH3NHNH2            2   266.800     4.982     0.000     0.000     1.000 ! same as C3H6
CH3NNH2             2   260.000     4.850     0.000     0.000     1.000 ! same as C3H5
CH3NH               2   569.000     3.630     0.000     0.000     1.000 ! same as H2CN
CH3NNH              2   232.400     3.828     0.000     0.000     1.000 ! same as CNN
CH3NN               2   232.400     3.828     0.000     0.000     1.000 ! same as CNN
CH3NNCH3            2   357.000     5.180     0.000     0.000     1.000 ! same as CH3CCCH2
HCNN                2   232.400     3.828     0.000     0.000     1.000 ! Same as HCNO
CH2CN               2   436.000     3.970     0.000     0.000     2.000 !same as CH2CO
CH3CN               2   436.000     3.970     0.000     0.000     2.000 !same as CH3CO
CH3NH2              1   569.000     3.630     0.000     0.000     1.000 ! same as H2CN
CH2NH2              1   569.000     3.630     0.000     0.000     1.000 ! same as H2CN
TMEDA             2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-1           2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-3           2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-2           2     546.85      5.99      0      0          1 !same as c7h16-2
CH3NCH3           2     266.800     4.982     0.000  0.000      1 !same as iC3H7
N(CH3)2CH2CH2     2     523.2       5.664     1.7    0.0        1 !same as dc5h11
N(CH3)2CH2        2     295.8       5.392     0.1    0.0        1 !same as ic4h10
CH3NCH2           2     260.000     4.850     0.000  0.000      1 !same as AC3H5
TMEDA-0-5         2     546.85      5.99      0      0          1 !same as c7h16-2
N(CH3)2CHCH2      2     523.2       5.664     1.7    0.0        1 !same as dc5h11
TMEDA-0-4         2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-0-3         2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-1-3         2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-1-4         2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-1-5         2     546.85      5.99      0      0          1 !same as c7h16-2
TMEDA-3-5         2     546.85      5.99      0      0          1 !same as c7h16-2
N(CH3)2CHCH       2     523.2       5.664     1.7    0.0        1 !same as dc5h11
CH2CHNCH3         2     357.000     5.176     0.000  0.000      1 !same as C4H7
CH2NCH2           2     260.000     4.850     0.000  0.000      1 !same as AC3H5
N(CH3CH2)CHCH2    2     523.2       5.664     1.7    0.0        1 !same as dc5h11
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N(CH3)2CCH2       2     523.2      5.664    1.7   0.0       1 !same as dc5h11
N(CH3)2CCH        2     523.2      5.664    1.7   0.0       1 !same as dc5h11
CH2CHNCH          2     357.000    5.180    0.000 0.000     1 !same as CH2CHCHCH
CH3NCH            2     260.000    4.850    0.000 0.000     1 !same as AC3H5
N(CH3CH2)CH2CH3   2     523.2      5.664    1.7   0.0       1 !same as dc5h11
CH3CH2NCH2        2     357.000    5.176    0.000 0.000     1 !same as nC4H8-1
CH3CHNCH2         2     357.000    5.176    0.000 0.000     1 !same as C4H7
CH2NCH            2     252.000    4.760    0.000 0.000     1 !same as PC3H4
CH3N(NH2)NO2      2     523.2      5.664    1.7   0.0       1 !same as dc5h11
CH3N(NH2)ONO      2     523.2      5.664    1.7   0.0       1 !same as dc5h11
H2NN               2    71.400     3.798     0.000     0.000     1.000 ! same as N2H2
HON                2   116.700     3.492     0.000     0.000     1.000 ! same as HNO
HNNNH2             2   252.000     4.760     0.000     0.000     1.000 ! same as H2CCCH
HNOO               2   232.400     3.828     0.000     0.000     1.000 ! same as HONO
HONHO              2   232.400     3.828     0.000     0.000     1.000 ! same as HONO
NH2NO2             2   232.400     3.828     0.000     0.000     1.000 ! same as HNO3
NCH2               1   569.000     3.630     0.000     0.000     1.000 !(os/jm)
NH2NO              2   232.400     3.828     0.000     0.000     1.000 ! same as HNNO (*)
NHNHO              2   232.400     3.828     0.000     0.000     1.000 ! same as HNNO (*)
NH2NHO             2   232.400     3.828     0.000     0.000     1.000 ! same as HNNO (*)
NH2OH              2   116.700     3.492     0.000     0.000     1.000 ! same as HNO (*)
CH3OCH3            2   329.400     4.624     0.000     0.000     1.000 !loc_est
CH3OCH2            2   329.400     4.624     0.000     0.000     1.000 !=CH3OCH3
CH3OCH2O           2   470.900     4.862     0.000     0.000     1.000 !loc_est
CH3OCHO            2   406.500     4.709     0.000     0.000     1.000 !loc_est
CH3OCO             2   406.500     4.709     0.000     0.000     1.000 !=CH3OCH
OCHO               2   485.400     4.410     0.000     0.000     1.000 !loc_est
C2                 1    97.530     3.621     0.000     1.760     4.000
CHCNH              1   252.000     4.760     0.000     0.000     1.000 ! = c3h4
CH3CH2NH2          2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
CH3NHCH3           2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
CH2CH2NH2          2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
CH3NHCH2           2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
CH3CHNH2           2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
CH3CH2NH           2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
CH2CHNH2           2   303.400     4.810     0.000     0.000     1.000 ! = c3h7
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CH3CHNH            2   303.400     4.810     0.000     0.000     1.000 ! = c3h7
CHCHNH2            2   307.800     4.140     0.000     0.000     1.000 ! = c3h6
CH3CHN             2   307.800     4.140     0.000     0.000     1.000 ! = c3h6
CH3CNH             2   307.800     4.140     0.000     0.000     1.000 ! = c3h6
CH2CNH2            2   307.800     4.140     0.000     0.000     1.000 ! = c3h6
CH2CHN             2   260.000     4.850     0.000     0.000     1.000 ! = c3h5
CH2CHN(S)          2   260.000     4.850     0.000     0.000     1.000 ! = c3h5
c-C2H3N            2   260.000     4.850     0.000     0.000     1.000 ! = c3h5
CHCNH2             2   260.000     4.850     0.000     0.000     1.000 ! = c3h5
H2NCHO             2   307.800     4.140     0.000     0.000     1.000 ! = c3h6
H2NCO              2   307.800     4.140     0.000     0.000     1.000 ! = c3h6
NCCN               1   349.000     4.361     0.000     0.000     1.000  !(OIS)
CH2CHOH            2   436.000     3.970     0.000     0.000     2.000 ! = CH3CHO
OCHCHO             2   406.937     4.823     0.000     0.000     2.000 ! LJcjp
CH3N               2   569.000     3.630     0.000     0.000     1.000 ! same as
CH2NN              2   232.400     3.828     0.000     0.000     1.000 ! same as CNN
CH2NNH2            2   260.000     4.850     0.000     0.000     1.000 ! same as C3H5
CH2NO              2   232.400     3.828     0.000     0.000     1.000 ! same as HCNO
CH2NHNH2           2   260.000     4.850     0.000     0.000     1.000 ! same as C3H5
CH3NHNH            2   260.000     4.850     0.000     0.000     1.000 ! same as C3H5
CH3CH2NHCH2CHO     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
NH2CH2CH2OCHCH2    2   413.        5.909     0.000     0.000     1.000 ! same 1hexene
CH3CH2OCH2CHNH     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
OHCH2CH2NHCHCH2    2   413.        5.909     0.000     0.000     1.000 ! same 1hexene
CH3OCH2CH2NCH2     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
cyOrthoOOMorphyl   2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyMetaOOMorphyl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyParaOOMorphyl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyOrtho*Morph3yl   2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyOrtho*Morph4yl   2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyOrtho*Morph5yl   2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyOrtho*Morph6yl   2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyMeta*Morph2yl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyMeta*Morph4yl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyMeta*Morph5yl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyMeta*Morph6yl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
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cyPara*Morph2yl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
cyPara*Morph3yl    2   475.7       5.916     0.0       0.0       1.0   !methylcyclohexane
CH2CH2OCH*CHNH     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH2CH2NHCH*CHO     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH2OCH2CH*NCH2     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
OCH2CH2N*CHCH2     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
OCH2CH2NHCHCH*     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
NHCH2CH2OCHCH*     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH2OCH2CH2NCH*     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH2CH2OCH2CHN*     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH2OCH*CH2NCH2     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
NHCH2CH*OCHCH2     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
OCH2CH*NHCHCH2     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH2CH2N*CH2CHO     2   413.        5.909     0.000     0.000     1.000 ! 1hexene
CH*OCH2CH2NCH2     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH*CH2NHCH2CHO     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH*CH2OCH2CHNH     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
N*CH2CH2OCHCH2     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2CH*OCH2CHNH     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
OCH*CH2NHCHCH2     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2CH*NHCH2CHO     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
NHCH*CH2OCHCH2     2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
OCH*CHNH           2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
NHCH*CHO           2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2CH*NCH2         2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2N*CHCH2         2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2NHCHCH*         2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2OCHCH*          2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH2CH2NCH*         2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
OCH2CHN*           2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH*CH2NCH2         2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH*OCHCH2          2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
CH*NHCHCH2         2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
N*CH2CHO           2   413.        5.909     0.000     0.000     1.000 ! same as 1hexene
OCHOOH             2   428.8       4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
CH2CHOOH           2   428.8       4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
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CH2NOOH          2   428.8      4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
NHCHOOH          2   428.8      4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
CHCHOOH          2   428.8      4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
NCHOOH           2   428.8      4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
CHNOOH           2   428.8      4.958     2.9       0.0       1.0   !   WJP: C2H3CHO
NHCHCHO          2   429.000    4.999     2.9       0.        1.    !same as CH3CHCHO
H2CC             2   238.       4.07      0.0       0.0       2.5   ! JAM(1/02)
C2O              2   232.400    3.828     0.000     0.000     1.000 !(TC,no data)
HOC2H4O2         2   470.600    4.410     0.000     0.000     1.500 !same as c2h5oh
C4H              1   357.000    5.180     0.000     0.000     1.000 !
C2H5OO           2   576.7      4.549     0.000     0.000     1.000 !est.
C2H3OO           2   556.000    4.610     0.000     0.000     0.000 !(Hennessy?)
CH2CHCH2CH2CH2O  2   399.3      5.949     0.000     0.000     1.000 ! C6H10
CH2CHCH2CH2OCH2  2   399.3      5.949     0.000     0.000     1.000 ! C6H10
CH2CHCH2OCH2CH2  2   399.3      5.949     0.000     0.000     1.000 ! C6H10
CH2CHOCH2CH2CH2  2   399.3      5.949     0.000     0.000     1.000 ! C6H10
CH2CHOCH2CHCH2   2   399.3      5.949     0.000     0.000     1.000 ! C6H10
OCHCH2CH2CH2CH2  2   399.3      5.949     0.000     0.000     1.000 ! C6H10
OCHCH2CH2CHCH2   2   399.3      5.949     0.000     0.000     1.000 ! C6H10
OCHCHCHCH2CH2    2   399.3      5.949     0.000     0.000     1.000 ! C6H10
OCHCHCHCHCH2     2   399.3      5.949     0.000     0.000     1.000 ! C6H10
THP              2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-2-4-ene      2   412.300    5.349     0.000     0.000     1.000 ! same as benzene
THP-2-ene        2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-2-yl         2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-3-ene        2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-3-yl         2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-4-yl         2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-5yl          2   412.300    5.349     0.000     0.000     1.000 ! same as benzene
THP-234-enyl     2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
THP-345-enyl     2   324.       6.093     0.000     0.000     1.000 ! same as CYC6H12
CH2CHCHCHOCH2    2   399.3      5.949     0.000     0.000     1.000 ! same as C6H10
C3H5O            2   429.000    4.999     2.9       0.        1.    ! same as C2H3CHO
CH2CHCHCHCH2O    2   399.3      5.949     0.000     0.000     1.000 ! same as C6H10
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APPENDIX C

H/N/O REACTION SET

The following is the reaction set for H/N/O combustion described in Chapter 5, and used in Chapters 6, 8, 9, 10, and 11. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	HE	C	O	N	AR
1	H	G	0	1.01E+00	300	5000	1	0	0	0	0	0
2	H2	G	0	2.02E+00	300	5000	2	0	0	0	0	0
3	N	G	0	1.40E+01	200	6000	0	0	0	1	0	0
4	NH	G	0	1.50E+01	200	6000	1	0	0	1	0	0
5	NH2	G	0	1.60E+01	200	3000	2	0	0	1	0	0
6	NH3	G	0	1.70E+01	200	6000	3	0	0	1	0	0
7	N2	G	0	2.80E+01	300	5000	0	0	0	2	0	0
8	NNH	G	0	2.90E+01	200	6000	1	0	0	2	0	0
9	N2H2	G	0	3.00E+01	200	6000	2	0	0	2	0	0
10	H2NN	G	0	3.00E+01	200	6000	2	0	0	2	0	0
11	N2H3	G	0	3.10E+01	200	6000	3	0	0	2	0	0
12	N2H4	G	0	3.20E+01	200	6000	4	0	0	2	0	0
13	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0
14	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
15	HON	G	0	3.10E+01	200	6000	1	0	0	1	1	0
16	HNOH	G	0	3.20E+01	200	6000	2	0	0	1	1	0
17	NH2O	G	0	3.20E+01	200	6000	2	0	0	1	1	0
18	NH2OH	G	0	3.30E+01	200	6000	3	0	0	1	1	0
19	HNNNH2	G	0	4.50E+01	300	5000	3	0	0	3	0	0
20	N2O	G	0	4.40E+01	200	6000	0	0	0	2	1	0
21	HNNO	G	0	4.50E+01	300	5000	1	0	0	2	1	0
22	NH2NO	G	0	4.60E+01	200	6000	2	0	0	2	1	0
23	NHNHO	G	0	4.60E+01	300	5000	2	0	0	2	1	0

24	NH2NHO	G	0	4.70E+01	300	5000	3	0	0	2	1	0
25	NO2	G	0	4.60E+01	200	6000	0	0	0	1	2	0
26	HONO	G	0	4.70E+01	200	6000	1	0	0	1	2	0
27	HNO2	G	0	4.70E+01	200	6000	1	0	0	1	2	0
28	HNOO	G	0	4.70E+01	300	5000	1	0	0	1	2	0
29	HONHO	G	0	4.80E+01	300	5000	2	0	0	1	2	0
30	NH2NO2	G	0	6.20E+01	200	6000	2	0	0	2	2	0
31	NO3	G	0	6.20E+01	200	6000	0	0	0	1	3	0
32	HNO3	G	0	6.30E+01	200	6000	1	0	0	1	3	0
33	N2O4	G	0	9.20E+01	200	6000	0	0	0	2	4	0
34	O	G	0	1.60E+01	300	5000	0	0	0	0	1	0
35	OH	G	0	1.70E+01	200	6000	1	0	0	0	1	0
36	H2O	G	0	1.80E+01	300	5000	2	0	0	0	1	0
37	O2	G	0	3.20E+01	300	5000	0	0	0	0	2	0
38	HO2	G	0	3.30E+01	200	3500	1	0	0	0	2	0
39	H2O2	G	0	3.40E+01	300	5000	2	0	0	0	2	0
40	HE	G	0	4.00E+00	300	5000	0	1	0	0	0	0
41	AR	G	0	3.99E+01	300	5000	0	0	0	0	0	1
42	CO	G	0	2.80E+01	300	5000	0	0	1	0	1	0
43	CO2	G	0	4.40E+01	300	5000	0	0	1	0	2	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. 2O+M=O2+M			6.16E+15	-0.5	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
2. 2O+AR=O2+AR			1.89E+13	0.0	-1790.0
3. O+H+M=OH+M			4.71E+18	-1.0	0.0
H2O	Enhanced by	1.200E+01			

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    H2              Enhanced by    2.500E+00
    AR              Enhanced by    7.500E-01
 4. H2+M=2H+M                                      4.58E+19   -1.4   104380.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    0.000E+00
 5. H2+AR=2H+AR                                    5.84E+18   -1.1   104380.0
 6. H+OH+M=H2O+M                                   2.21E+22   -2.0        0.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    0.000E+00
 7. H+OH+AR=H2O+AR                                 8.41E+21   -2.0        0.0
 8. H2O2(+M)=2OH(+M)                               2.95E+14    0.0    48400.0
    Low pressure limit:  0.12000E+18  0.00000E+00  0.45500E+05
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    1.600E-01
 9. H2O+O=OH+OH                                    2.97E+06    2.0    13400.0
10. O+H2=H+OH                                      5.08E+04    2.7     6290.0
11. OH+H2=H+H2O                                    2.16E+08    1.5     3430.0
12. H+O2(+M)=HO2(+M)                               1.48E+12    0.6        0.0
    Low pressure limit:  0.35000E+17 -0.41000E+00 -0.11200E+04
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    5.000E-02
13. H+O2=O+OH                                      4.49E+08    1.3    16191.0
    Declared duplicate reaction...
14. H+O2=O+OH                                      2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
15. O+HO2=OH+O2                                    3.25E+13    0.0        0.0
16. H+HO2=O2+H2                                    1.66E+13    0.0      820.0
17. H+HO2=2OH                                      7.08E+13    0.0      300.0
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18.	OH+HO2=O2+H2O	4.64E+13	0.0	-500.0
19.	2HO2=O2+H2O2	1.30E+11	0.0	-1630.0
	Declared duplicate reaction...			
20.	2HO2=O2+H2O2	4.20E+14	0.0	11980.0
	Declared duplicate reaction...			
21.	O+H2O2=OH+HO2	9.55E+06	2.0	3970.0
22.	H+H2O2=HO2+H2	4.82E+13	0.0	7950.0
23.	H+H2O2=OH+H2O	2.41E+13	0.0	3970.0
24.	OH+H2O2=HO2+H2O	1.00E+12	0.0	0.0
	Declared duplicate reaction...			
25.	OH+H2O2=HO2+H2O	5.80E+14	0.0	9560.0
	Declared duplicate reaction...			
26.	NH+M=N+H+M	2.65E+14	0.0	75500.0
27.	NH+H=N+H2	3.20E+13	0.0	325.0
28.	NH+O=N+OH	1.70E+08	1.5	3368.0
29.	NH+OH=N+H2O	1.60E+07	1.7	-576.0
30.	NH2+M=NH+H+M	3.16E+23	-2.0	91400.0
31.	NH2+H=NH+H2	4.00E+13	0.0	3650.0
32.	NH2+O=NH+OH	7.00E+12	0.0	0.0
	Declared duplicate reaction...			
33.	NH2+O=NH+OH	8.60E-01	4.0	1673.0
	Declared duplicate reaction...			
34.	NH2+OH=NH+H2O	3.30E+06	1.9	-217.0
35.	NH2+O2=NH+HO2	1.00E+14	0.0	49997.0
36.	NH+NH=NH2+N	5.70E-01	3.9	342.0
37.	NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
38.	NH3+M=NH+H2+M	6.30E+14	0.0	93390.0
39.	NH3+H=NH2+H2	6.36E+05	2.4	10171.0
40.	NH3+O=NH2+OH	2.80E+02	3.3	4471.0
41.	NH3+OH=NH2+H2O	2.00E+06	2.0	566.0
42.	NH2+HO2=NH3+O2	9.20E+05	1.9	-1152.0
43.	NH3+HO2=NH2+H2O2	3.00E+11	0.0	22000.0

44.	NH2+NH=NH3+N			9.60E+03	2.5	107.0
45.	NH2+NH2=NH3+NH			5.60E+00	3.5	552.0
46.	N2+M=N+N+M			1.00E+28	-3.3	225000.0
47.	NH+N=N2+H			3.00E+13	0.0	0.0
48.	NH+NH=N2+H+H			2.50E+13	0.0	0.0
49.	NH2+N=N2+H+H			7.10E+13	0.0	0.0
50.	NH+NH=N2+H2			1.00E+08	1.0	0.0
51.	NNH=N2+H			1.00E+09	0.0	0.0
52.	NNH+H=N2+H2			1.00E+14	0.0	0.0
53.	NH+NH=NNH+H			5.10E+13	0.0	0.0
54.	NNH+O=N2+OH			1.20E+13	0.1	-217.0
55.	NNH+OH=N2+H2O			5.00E+13	0.0	0.0
56.	NNH+O2=N2+HO2			5.60E+14	-0.4	-13.0
57.	NNH+O2=N2+H+O2			5.00E+13	0.0	0.0
58.	NNH+HO2=N2+H2O2			1.40E+04	2.7	-1599.0
59.	NNH+N=NH+N2			3.00E+13	0.0	2000.0
60.	NNH+NH=N2+NH2			5.00E+13	0.0	0.0
61.	NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
62.	N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
	H2O	Enhanced by	1.500E+01			
	O2	Enhanced by	2.000E+00			
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
63.	N2H2+M=NH+NH+M			3.16E+16	0.0	99400.0
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
64.	NH2+NH=N2H2+H			4.30E+14	-0.3	-77.0
65.	N2H2+H=NNH+H2			8.50E+04	2.6	230.0
66.	NH2+NH2=N2H2+H2			1.70E+08	1.6	11783.0
67.	N2H2+O=NNH+OH			3.30E+08	1.5	496.0
68.	N2H2+OH=NNH+H2O			5.90E+01	3.4	1360.0
69.	N2H2+N=NNH+NH			1.00E+06	2.0	0.0

70. N2H2+NH=NNH+NH2	1.00E+13	0.0	6000.0
71. N2H2+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
72. NNH+NNH=N2H2+N2	1.00E+13	0.0	4000.0
73. H2NN=NNH+H	3.40E+26	-4.8	46228.0
74. N2H2=H2NN	2.00E+41	-9.4	68413.0
75. H2NN+H=N2H2+H	7.00E+13	0.0	0.0
76. H2NN+H=NNH+H2	4.80E+08	1.5	-894.0
77. NH2+NH2=H2NN+H2	7.20E+04	1.9	8802.0
78. H2NN+O=OH+NNH	3.30E+08	1.5	-894.0
79. H2NN+OH=NNH+H2O	2.40E+06	2.0	-1192.0
80. H2NN+HO2=NNH+H2O2	2.90E+04	2.7	-1599.0
81. H2NN+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
82. N2H3=N2H2+H	3.60E+47	-10.4	68970.0
83. N2H3+M=NH2+NH+M	5.00E+16	0.0	60000.0
84. NH2+NH2=N2H3+H	1.20E+12	0.0	10078.0
85. N2H3+H=N2H2+H2	2.40E+08	1.5	0.0
86. N2H3+H=NH+NH3	1.00E+11	0.0	0.0
87. NH3+NH2=N2H3+H2	1.00E+11	0.5	21600.0
88. N2H3+O=N2H2+OH	1.70E+08	1.5	-645.0
89. N2H3+OH=N2H2+H2O	1.20E+06	2.0	-1192.0
90. N2H3+OH=H2NN+H2O	3.00E+13	0.0	0.0
91. N2H3+HO2=N2H2+H2O2	1.40E+04	2.7	-1600.0
92. N2H3+N=N2H2+NH	1.00E+06	2.0	0.0
93. N2H3+NH=N2H2+NH2	2.00E+13	0.0	0.0
94. N2H3+NH2=N2H2+NH3	9.20E+05	1.9	-1152.0
95. N2H3+NH2=H2NN+NH3	3.00E+13	0.0	0.0
96. N2H3+NNH=N2H2+N2H2	1.00E+13	0.0	4000.0
97. N2H3+N2H3=NH3+NH3+N2	3.00E+12	0.0	0.0
98. NH2+NH2(+M)=N2H4(+M)	5.60E+14	-0.4	66.0
Low pressure limit: 0.16000E+35 -0.54900E+01 0.19870E+04			
TROE centering: 0.31000E+00 0.10000E-29 0.10000E+31 0.10000E+31			
99. N2H4+M=N2H3+H+M	1.00E+15	0.0	63600.0

	N2	Enhanced by	2.400E+00			
	NH3	Enhanced by	3.000E+00			
	N2H4	Enhanced by	4.000E+00			
100.	N2H4=H2NN+H2			5.30E+39	-8.3	69267.0
101.	N2H4+H=N2H3+H2			7.00E+12	0.0	2500.0
102.	N2H4+H=NH2+NH3			2.40E+09	0.0	3100.0
103.	N2H4+O=N2H3+OH			6.70E+08	1.5	2850.0
104.	N2H4+O=N2H2+H2O			4.40E+11	0.0	-1270.0
105.	N2H4+OH=N2H3+H2O			4.00E+13	0.0	0.0
106.	N2H3+HO2=N2H4+O2			9.20E+05	1.9	2125.0
107.	N2H4+N=N2H3+NH			1.00E+10	1.0	2000.0
108.	N2H4+NH=NH2+N2H3			1.00E+09	1.5	2000.0
109.	N2H4+NH2=N2H3+NH3			3.90E+12	0.0	1500.0
110.	N2H3+N2H2=N2H4+NNH			1.00E+13	0.0	6000.0
111.	N2H3+N2H3=N2H4+N2H2			1.20E+13	0.0	0.0
112.	NO+M=N+O+M			1.40E+15	0.0	148430.0
	N2	Enhanced by	1.000E+00			
	H2	Enhanced by	2.200E+00			
	H2O	Enhanced by	6.700E+00			
	CO2	Enhanced by	3.000E+00			
	N2O	Enhanced by	2.200E+00			
113.	N+OH=NO+H			3.80E+13	0.0	0.0
114.	NH+O=NO+H			9.20E+13	0.0	0.0
115.	NH2+O=NO+H2			5.00E+12	0.0	0.0
116.	NH+OH=NO+H2			2.00E+13	0.0	0.0
117.	NO+O=O2+N			1.81E+09	1.0	38725.0
118.	NH+O2=NO+OH			1.30E+06	1.5	100.0
119.	N+NO=N2+O			3.30E+12	0.3	0.0
120.	NH+NO=N2+OH			2.20E+13	-0.2	0.0
121.	NNH+O=NH+NO			5.20E+11	0.4	-409.0
122.	NH2+NO=N2+H2O			2.80E+20	-2.7	1258.0
123.	NH2+NO=NNH+OH			2.29E+10	0.4	-814.0

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124. N2H2+O=NH2+NO                                    1.00E+13    0.0        0.0
125. H2NN+O=NH2+NO                                    7.00E+13    0.0        0.0
126. H2NN+OH=>NH2+NO+H                                2.00E+12    0.0        0.0
127. N2H3+O=>NH2+NO+H                                 3.00E+13    0.0        0.0
128. H2NN+HO2=>NH2+NO+OH                              9.00E+12    0.0        0.0
129. NO+H(+M)=HNO(+M)                                 1.50E+15   -0.4        0.0
     Low pressure limit:  0.24000E+15  0.20600E+00 -0.15500E+04
     TROE centering:      0.82000E+00  0.10000E-29  0.10000E+31  0.10000E+31
     N2              Enhanced by    1.600E+00
130. HNO+H=H2+NO                                      4.50E+11    0.7      655.0
131. NH+OH=HNO+H                                      3.20E+14   -0.4      -46.0
132. NH2+O=HNO+H                                      6.63E+14   -0.5        0.0
133. NH+H2O=HNO+H2                                    2.00E+13    0.0    13850.0
134. HNO+O=OH+NO                                      1.81E+13    0.0        0.0
135. NH+O2=HNO+O                                      4.60E+05    2.0     6494.0
136. HNO+OH=NO+H2O                                    3.60E+13    0.0        0.0
137. NH2+O2=HNO+OH                                    2.90E-02    3.8    18185.0
138. NH2+HO2=HNO+H2O                                  5.68E+15   -1.1      707.0
139. HNO+O2=NO+HO2                                    2.00E+13    0.0    15887.0
140. NH2+HNO=NH3+NO                                   3.60E+06    1.6    -1250.0
141. N2H3+O=NH2+HNO                                   3.00E+13    0.0        0.0
142. N2H3+OH=NH3+HNO                                  1.00E+12    0.0    15000.0
143. NNH+NO=N2+HNO                                    5.00E+13    0.0        0.0
144. H+NO+N2=HNO+N2                                   4.00E+20   -1.8        0.0
145. HON+M=NO+H+M                                     5.10E+19   -1.7    16045.0
     AR              Enhanced by    7.000E-01
     H2O             Enhanced by    7.000E+00
     CO2             Enhanced by    2.000E+00
146. HON+H=HNO+H                                      2.00E+13    0.0        0.0
147. HON+H=OH+NH                                      2.00E+13    0.0        0.0
148. HON+O=OH+NO                                      7.00E+13    0.0        0.0
149. HNOH+M=H+HNO+M                                   2.00E+24   -2.8    58901.0
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150. HNOH+H=NH2+OH                                    4.00E+13    0.0        0.0
151. HNOH+H=HNO+H2                                    4.80E+08    1.5      377.0
152. HNOH+O=HNO+OH                                    7.00E+13    0.0        0.0
     Declared duplicate reaction...
153. HNOH+O=HNO+OH                                    3.30E+08    1.5     -357.0
     Declared duplicate reaction...
154. HNOH+OH=HNO+H2O                                  2.40E+06    2.0    -1192.0
155. HNOH+O2=HNO+HO2                                  3.00E+12    0.0    25000.0
156. HNOH+HO2=HNO+H2O2                                2.90E+04    2.7    -1599.0
157. HNOH+NH2=N2H3+OH                                 1.00E+01    3.5     -467.0
158. HNOH+NH2=H2NN+H2O                                8.80E+16   -1.1     1113.0
159. HNOH+NH2=HNO+NH3                                 1.80E+06    1.9    -1152.0
160. NH2O+M=HNO+H+M                                   2.80E+24   -2.8    64915.0
     H2O             Enhanced by    1.000E+01
161. NH2O+M=HNOH+M                                    1.10E+29   -4.0    44000.0
     H2O             Enhanced by    1.000E+01
162. NH2O+H=NH2+OH                                    5.00E+13    0.0        0.0
163. NH2O+H=HNO+H2                                    3.00E+07    2.0     2000.0
164. NH2O+O=HNO+OH                                    3.00E+07    2.0     2000.0
165. NH2+O2=NH2O+O                                    2.50E+11    0.5    29570.0
166. NH2O+OH=HNO+H2O                                  2.00E+07    2.0     1000.0
167. NH2+HO2=NH2O+OH                                  5.00E+13    0.0        0.0
168. NH2O+O2=HNO+HO2                                  3.00E+12    0.0    25000.0
169. NH2O+HO2=HNO+H2O2                                2.90E+04    2.7    -1599.0
170. NH2O+NH2=HNO+NH3                                 3.00E+12    0.0     1000.0
171. NH2O+NO=HNO+HNO                                  2.00E+04    2.0    13000.0
172. NH2OH(+M)=NH2+OH(+M)                             1.40E+20   -1.3    64080.0
     Low pressure limit:  0.54000E+38 -0.59600E+01  0.66783E+05
     TROE centering:      0.31000E+00  0.10000E-29  0.10000E+31  0.10000E+31
173. NH2OH+H=HNOH+H2                                  4.80E+08    1.5     6246.0
174. NH2OH+H=NH2O+H2                                  2.40E+08    1.5     5064.0
175. NH2OH+O=HNOH+OH                                  3.30E+08    1.5     3863.0
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176. NH2OH+O=NH2O+OH                                  1.70E+08    1.5     3009.0
177. NH2OH+OH=HNOH+H2O                                1.50E+04    2.6    -3537.0
178. NH2OH+OH=NH2O+H2O                                1.50E+05    2.3    -1296.0
179. NH2O+HO2=O2+NH2OH                                2.90E+04    2.7    -1599.0
180. HNOH+HO2=NH2OH+O2                                2.90E+04    2.7    -1599.0
181. NH2OH+HO2=HNOH+H2O2                              2.90E+04    2.7     9552.0
182. NH2OH+HO2=NH2O+H2O2                              1.40E+04    2.7     6414.0
183. N2H4+O=NH2OH+NH                                  2.90E+11    0.0    -1270.0
184. NH2OH+NH=HNOH+NH2                                2.90E-03    4.4     1564.0
185. NH2OH+NH=NH2O+NH2                                1.50E-03    4.6     2424.0
186. NH2OH+NH2=HNOH+NH3                               1.10E-01    4.0      -97.0
187. NH2OH+NH2=NH2O+NH3                               9.50E+00    3.4    -1013.0
188. H2NN+NH2=HNNNH2+H                                7.90E+06    1.9    -1331.0
189. N2O(+M)=N2+O(+M)                                 1.30E+12    0.0    62570.0
     Low pressure limit:  0.40000E+15  0.00000E+00  0.56600E+05
     N2              Enhanced by    1.700E+00
     O2              Enhanced by    1.400E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    1.200E+01
190. N2O+H=N2+OH                                      3.30E+10    0.0     4729.0
     Declared duplicate reaction...
191. N2O+H=N2+OH                                      4.40E+14    0.0    19254.0
     Declared duplicate reaction...
192. NH+NO=N2O+H                                      2.90E+14   -0.4        0.0
     Declared duplicate reaction...
193. NH+NO=N2O+H                                     -2.20E+13   -0.2        0.0
     Declared duplicate reaction...
194. NNH+O=N2O+H                                      1.00E+14    0.0        0.0
195. NH2+NO=H2+N2O                                    1.00E+13    0.0    33700.0
196. NO+NO=N2O+O                                      3.61E+12    0.0    65335.0
     Declared duplicate reaction...
197. N2O+O=NO+NO                                      6.62E+13    0.0    26611.0
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Declared duplicate reaction...

198.	N2O+O=O2+N2	1.02E+14	0.0	28001.0
199.	N2O+OH=HNO+NO	1.20E-04	4.3	25080.0
200.	N2O+OH=N2+HO2	1.00E+14	0.0	30000.0
201.	NNH+O2=N2O+OH	2.90E+11	-0.3	149.0
202.	HNO+HNO=N2O+H2O	9.00E+08	0.0	3100.0
203.	NH+N2O=N2+HNO	2.00E+12	0.0	6000.0
204.	N2H2+NO=N2O+NH2	3.00E+10	0.0	0.0
205.	HNNO+M=H+N2O+M	2.20E+15	0.0	21600.0
206.	HNNO+M=N2+OH+M	1.00E+15	0.0	25600.0
207.	HNNO+H=H2+N2O	2.00E+13	0.0	0.0
208.	NH2+NO=HNNO+H	8.00E+13	0.0	28000.0
209.	NNH+HO2=HNNO+OH	2.40E+13	0.0	1698.0
210.	HNNO+NO=N2O+HNO	1.00E+12	0.0	0.0
211.	NH2+NO=NH2NO	3.50E+31	-6.8	3724.0
212.	NH2NO=N2+H2O	3.10E+34	-7.1	36262.0
213.	NH2NO+H=HNNO+H2	4.80E+08	1.5	7407.0
214.	N2H3+O=NH2NO+H	3.00E+13	0.0	0.0
215.	H2NN+OH=NH2NO+H	2.00E+12	0.0	0.0
216.	NH2NO+O=HNNO+OH	3.30E+08	1.5	4697.0
217.	NH2NO+OH=HNNO+H2O	2.40E+06	2.0	-70.0
218.	H2NN+HO2=NH2NO+OH	6.60E+05	1.9	7050.0
219.	NH2NO+HO2=HNNO+H2O2	2.90E+04	2.7	12620.0
220.	NH2NO+NH2=HNNO+NH3	1.80E+06	1.9	4538.0
221.	NH2NHO=NH2+HNO	2.40E+40	-8.7	41584.0
222.	NH2NHO+H=NHNHO+H2	4.80E+08	1.5	-894.0
223.	NH2NHO+O=NHNHO+OH	3.30E+08	1.5	-894.0
224.	NH2NHO+OH=NHNHO+H2O	2.40E+06	2.0	-1192.0
225.	N2H3+HO2=NH2NHO+OH	3.00E+13	0.0	0.0
226.	NH2NHO+HO2=NHNHO+H2O2	2.90E+04	2.7	-1599.0
227.	NH2NHO+NH2=NHNHO+NH3	1.80E+06	1.9	-1152.0
228.	NO2(+M)=NO+O(+M)	7.60E+18	-1.3	73245.0

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     Low pressure limit:  0.24700E+29 -0.33700E+01  0.74756E+05
     TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.49816E+04
     N2O             Enhanced by    1.500E+00
     H2O             Enhanced by    4.400E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    2.300E+00
     Declared duplicate reaction...
229. NO+O(+M)=NO2(+M)                                1.30E+15   -0.8        0.0
     Low pressure limit:  0.47100E+25 -0.28700E+01  0.15510E+04
     TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.46816E+04
     Declared duplicate reaction...
230. NO2+H=NO+OH                                     1.30E+14    0.0      357.0
231. NH+O2=H+NO2                                     2.30E+10    0.0     2482.0
232. NO2+O=O2+NO                                     3.91E+12    0.0     -238.0
233. NO2+OH=HO2+NO                                   1.81E+13    0.0     6673.0
234. HON+O2=NO2+OH                                   1.00E+12    0.0     4968.0
235. NO2+N=N2O+O                                     3.49E+12    0.0     -437.0
236. NH+NO2=N2O+OH                                   4.10E+12    0.0        0.0
237. NH+NO2=HNO+NO                                   5.90E+12    0.0        0.0
238. NH2+NO2=N2O+H2O                                 3.00E+14   -0.8      242.0
239. NH2+NO2=NH2O+NO                                 1.30E+15   -0.8      242.0
240. H2NN+O2=NH2+NO2                                 1.50E+12    0.0     5958.0
241. HNNO+NO=NNH+NO2                                 3.20E+12    0.0      270.0
242. N2O+NO=NO2+N2                                   5.30E+05    2.2    46280.0
243. NO+NO+NO=N2O+NO2                                1.07E+10    0.0    26800.0
244. HNO+NO+NO=HNNO+NO2                              1.70E+11    0.0     2100.0
245. NO2+NO2=NO+NO+O2                                1.63E+12    0.0    26108.0
246. HONO(+M)=OH+NO(+M)                              1.20E+19   -1.2    49667.0
     Low pressure limit:  0.30100E+31 -0.38000E+01  0.50322E+05
     TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
     Declared duplicate reaction...
247. NO+OH(+M)=HONO(+M)                              1.99E+12   -0.1     -721.0
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     Low pressure limit:  0.50800E+24 -0.25100E+01 -0.68000E+02
     TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
     Declared duplicate reaction...
248. NO2+H2=HONO+H                                  1.30E+04    2.8    29770.0
249. HONO+H=H2O+NO                                  8.10E+06    1.9     3843.0
250. HONO+H=OH+HNO                                  5.60E+10    0.9     4965.0
251. HON+OH=HONO+H                                  4.00E+13    0.0        0.0
252. HONO+O=OH+NO2                                  1.20E+13    0.0     5958.0
253. HON+O2=HONO+O                                  1.00E+12    0.0     4965.0
254. HONO+OH=H2O+NO2                                1.26E+10    1.0      135.0
255. NO2+HO2=HONO+O2                                6.30E+08    1.2     5000.0
256. NH+HONO=NH2+NO2                                1.00E+13    0.0        0.0
257. NH2+HONO=NH3+NO2                               7.10E+01    3.0    -4940.0
258. HNNO+NO=N2+HONO                                2.60E+11    0.0      810.0
259. HNO+NO2=HONO+NO                                4.40E+04    2.6     4040.0
260. NH2O+NO2=HONO+HNO                              6.00E+11    0.0     2000.0
261. HNOH+NO2=HONO+HNO                              6.00E+11    0.0     2000.0
262. HNNO+NO2=N2O+HONO                              1.00E+12    0.0        0.0
263. HONO+HONO=NO+NO2+H2O                           3.50E-01    3.6    12140.0
264. HNO2(+M)=HONO(+M)                              2.50E+14    0.0    32300.0
     Low pressure limit:  0.31000E+19  0.00000E+00  0.31500E+05
     TROE centering:      0.11490E+01  0.10000E-29  0.31250E+04  0.10000E+31
265. NO2+H2=HNO2+H                                  2.40E+00    3.7    32400.0
266. HNO2+O=OH+NO2                                  1.70E+08    1.5     2363.0
267. HNO2+OH=H2O+NO2                                1.20E+06    2.0     -794.0
268. NO2+HO2=HNO2+O2                                1.90E+01    3.3     4983.0
269. HNO2+NH2=NO2+NH3                               9.20E+05    1.9      874.0
270. HNO+NO2=HNO2+NO                                6.02E+11    0.0     1986.0
271. NH+O2=HNOO                                     3.70E+24   -5.0     2294.0
272. NH+O2+M=HNOO+M                                 3.00E+26   -4.0     2274.0
273. HNOO+M=OH+NO+M                                 1.50E+36   -6.2    31119.0
274. HNOH+HO2=HONHO+OH                              4.00E+13    0.0        0.0
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275. NH2+NO2=NH2NO2 3.50E+31 -6.8 3726.0

276. NO2+O(+M)=NO3(+M) 1.32E+13 0.0 0.0

Low pressure limit: 0.14900E+29 -0.40800E+01 0.24660E+04

TROE centering: 0.32600E+00 0.50000E+03 0.62049E+04 0.26060E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

N2 Enhanced by 1.000E+00

HNO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

277. NO3+H=NO2+OH 6.00E+13 0.0 0.0

278. NO3+O=NO2+O2 1.00E+13 0.0 0.0

279. NO3+OH=NO2+HO2 1.40E+13 0.0 0.0

280. NO3+HO2=NO2+O2+OH 1.50E+12 0.0 0.0

281. NO3+NH=HNO+NO2 1.50E+13 0.0 0.0

282. NO3+NH2=NH2O+NO2 9.00E+05 0.0 100.0

283. HNNO+NO2=NNH+NO3 1.00E+13 0.0 0.0

284. NO2+NO2=NO3+NO 9.60E+09 0.7 20900.0

285. NO3+NO2=NO+NO2+O2 5.00E+10 0.0 2940.0

286. NO3+NO3=NO2+NO2+O2 5.12E+11 0.0 4870.0

287. NO2+OH(+M)=HNO3(+M) 2.41E+13 0.0 0.0

Low pressure limit: 0.64200E+33 -0.54900E+01 0.23490E+04

TROE centering: 0.40000E+00 0.45070E+03 0.15840E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

N2 Enhanced by 1.000E+00

HNO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

288. HNO3+H=NO3+H2 5.60E+08 1.5 16400.0

289. HNO3+H=H2O+NO2 6.10E+01 3.3 6285.0

290. HNO3+H=OH+HONO 3.80E+05 2.3 6976.0

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291. HNO3+H=HNO2+OH                                   6.00E+13    0.0     7000.0
292. HNO3+O=OH+NO3                                    1.80E+07    0.0        0.0
293. HNO3+OH=H2O+NO3                                  9.00E+10    0.0        0.0
294. HNO3+OH(+M)=H2O+NO3(+M)                          2.47E+08    0.0    -2860.0
     Low pressure limit:  0.68900E+15  0.00000E+00 -0.14400E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     HNO3            Enhanced by    5.000E+00
     NO3             Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
295. NO3+H2O2=HNO3+HO2                                1.00E+12    0.0     8500.0
296. NO3+NH=HNO3+N                                    1.00E+12    0.0     5000.0
297. NO3+NH2=HNO3+NH                                  1.00E+12    0.0    10000.0
298. HNO3+NH=HNOH+NO2                                 1.50E+13    0.0     6000.0
299. HNO3+NH2=NO3+NH3                                 9.00E+05    2.0     7300.0
300. HNO3+NH2=NH2O+HNO2                               3.00E+12    0.0     9000.0
301. HNO3+NH3=NH2O+H2O+NO                             2.32E+01    3.5    44930.0
302. NH3+HNO3=H2O+NH2NO2                              8.00E-01    3.5    43100.0
303. HONO+NO2=HNO3+NO                                 2.00E+11    0.0    32700.0
304. HONO+NO3=HNO3+NO2                                1.00E+12    0.0     6000.0
305. HNO2+NO3=HNO3+NO2                                1.00E+12    0.0     5000.0
306. N2O4(+M)=NO2+NO2(+M)                             4.05E+18   -1.1    12840.0
     Low pressure limit:  0.19600E+29 -0.38000E+01  0.12840E+05
307. N2O4+H2O=HONO+HNO3                               2.52E+14    0.0    11586.0
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UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX D

H/C/N/O REACTION SET

The following is the reaction set for H/C/N/O combustion described in Chapter 6, and used in Chapters 8, 9, 10, and 11. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	HE	C	O	N	AR
1	H	G	0	1.01E+00	200	3500	1	0	0	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0	0	0
3	C	G	0	1.20E+01	200	3500	0	0	1	0	0	0
4	O	G	0	1.60E+01	200	3500	0	0	0	1	0	0
5	O2	G	0	3.20E+01	200	3500	0	0	0	2	0	0
6	OH	G	0	1.70E+01	200	6000	1	0	0	1	0	0
7	H2O	G	0	1.80E+01	200	3500	2	0	0	1	0	0
8	HO2	G	0	3.30E+01	200	3500	1	0	0	2	0	0
9	H2O2	G	0	3.40E+01	200	3500	2	0	0	2	0	0
10	CH	G	0	1.30E+01	200	6000	1	0	1	0	0	0
11	CH2	G	0	1.40E+01	200	6000	2	0	1	0	0	0
12	CH2SING	G	0	1.40E+01	200	6000	2	0	1	0	0	0
13	CH3	G	0	1.50E+01	200	6000	3	0	1	0	0	0
14	CH4	G	0	1.60E+01	200	3500	4	0	1	0	0	0
15	C2	G	0	2.40E+01	200	6000	0	0	2	0	0	0
16	CO	G	0	2.80E+01	200	3500	0	0	1	1	0	0
17	HCO	G	0	2.90E+01	200	3500	1	0	1	1	0	0
18	CH2O	G	0	3.00E+01	200	3500	2	0	1	1	0	0
19	CH2OH	G	0	3.10E+01	200	6000	3	0	1	1	0	0
20	CH3O	G	0	3.10E+01	200	6000	3	0	1	1	0	0
21	CH3OH	G	0	3.20E+01	200	3500	4	0	1	1	0	0
22	C2H	G	0	2.50E+01	200	3500	1	0	2	0	0	0
23	C2H2	G	0	2.60E+01	200	3500	2	0	2	0	0	0

24	H2CC	G	0	2.60E+01	200	6000	2	0	2	0	0	0
25	C2H3	G	0	2.70E+01	200	5000	3	0	2	0	0	0
26	C2H4	G	0	2.81E+01	200	3500	4	0	2	0	0	0
27	C2H5	G	0	2.91E+01	200	3500	5	0	2	0	0	0
28	C2H6	G	0	3.01E+01	200	3500	6	0	2	0	0	0
29	C3H2	G	0	3.80E+01	300	5000	2	0	3	0	0	0
30	C3H3	G	0	3.91E+01	200	6000	3	0	3	0	0	0
31	AR	G	0	3.99E+01	300	5000	0	0	0	0	0	1
32	AC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
33	PC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
34	C2O	G	0	4.00E+01	300	4000	0	0	2	1	0	0
35	HCCO	G	0	4.10E+01	300	4000	1	0	2	1	0	0
36	AC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
37	TC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
38	SC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
39	CH2CO	G	0	4.20E+01	200	3500	2	0	2	1	0	0
40	C3H6	G	0	4.21E+01	300	5000	6	0	3	0	0	0
41	CH3CO	G	0	4.30E+01	200	6000	3	0	2	1	0	0
42	CH2CHO	G	0	4.30E+01	300	5000	3	0	2	1	0	0
43	nC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
44	iC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
45	C2H4O	G	0	4.41E+01	300	5000	4	0	2	1	0	0
46	CH3CHO	G	0	4.41E+01	200	6000	4	0	2	1	0	0
47	C3H8	G	0	4.41E+01	300	3000	8	0	3	0	0	0
48	CO2	G	0	4.40E+01	200	3500	0	0	1	2	0	0
49	OCHO	G	0	4.50E+01	300	5000	1	0	1	2	0	0
50	C2H5O	G	0	4.51E+01	200	6000	5	0	2	1	0	0
51	CH3CHOH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
52	C2H4OH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
53	CH3OCH2	G	0	4.51E+01	300	5000	5	0	2	1	0	0
54	CH3OCH3	G	0	4.61E+01	270	3000	6	0	2	1	0	0

55	C2H5OH	G	0	4.61E+01	200	6000	6	0	2	1	0	0
56	CH3OCO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
57	CH3OCHO	G	0	6.01E+01	300	5000	4	0	2	2	0	0
58	CH3OCH2O	G	0	6.11E+01	300	5000	5	0	2	2	0	0
59	HOC2H4O2	G	0	7.71E+01	300	5000	5	0	2	3	0	0
60	C4H	G	0	4.91E+01	300	3000	1	0	4	0	0	0
61	C2H5OO	G	0	6.11E+01	300	5000	5	0	2	2	0	0
62	C2H3CO	G	0	5.51E+01	200	6000	3	0	3	1	0	0
63	C2H3CHO	G	0	5.61E+01	298	3000	4	0	3	1	0	0
64	C2H3CH2O	G	0	5.71E+01	300	3000	5	0	3	1	0	0
65	C4H2	G	0	5.01E+01	300	3000	2	0	4	0	0	0
66	iC4H3	G	0	5.11E+01	200	5000	3	0	4	0	0	0
67	nC4H3	G	0	5.11E+01	300	4000	3	0	4	0	0	0
68	C4H4	G	0	5.21E+01	300	3000	4	0	4	0	0	0
69	n-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
70	i-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
71	iiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
72	iiiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
73	C4H7	G	0	5.51E+01	300	3000	7	0	4	0	0	0
74	IC4H8	G	0	5.61E+01	300	5000	8	0	4	0	0	0
75	nC4H9	G	0	5.71E+01	200	6000	9	0	4	0	0	0
76	OCHCHO	G	0	5.80E+01	300	3000	2	0	2	2	0	0
77	C2H3OO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
78	C5H2	G	0	6.21E+01	200	5000	2	0	5	0	0	0
79	H2CCCCCH	G	0	6.31E+01	200	5000	3	0	5	0	0	0
80	HCCCHCCH	G	0	6.31E+01	200	5000	3	0	5	0	0	0
81	C5H5	G	0	6.51E+01	300	5000	5	0	5	0	0	0
82	l-C5H5	G	0	6.51E+01	300	5000	5	0	5	0	0	0
83	H2C4O	G	0	6.61E+01	300	4000	2	0	4	1	0	0
84	C5H6	G	0	6.61E+01	300	5000	6	0	5	0	0	0
85	CH2CHCH2CCH	G	0	6.61E+01	300	5000	6	0	5	0	0	0

86	CH2CHCHCCH2	G	0	6.61E+01	300	5000	6	0	5	0	0	0
87	C6H2	G	0	7.41E+01	300	3000	2	0	6	0	0	0
88	C6H3	G	0	7.51E+01	300	3000	3	0	6	0	0	0
89	l-C6H4	G	0	7.61E+01	300	3000	4	0	6	0	0	0
90	c-C6H4	G	0	7.61E+01	300	3000	4	0	6	0	0	0
91	n-C6H5	G	0	7.71E+01	300	3000	5	0	6	0	0	0
92	i-C6H5	G	0	7.71E+01	300	3000	5	0	6	0	0	0
93	A1	G	0	7.71E+01	300	3000	5	0	6	0	0	0
94	A	G	0	7.81E+01	300	3000	6	0	6	0	0	0
95	FC6H6	G	0	7.81E+01	200	6000	6	0	6	0	0	0
96	l-C6H6	G	0	7.81E+01	300	3000	6	0	6	0	0	0
97	C4H5C2H	G	0	7.81E+01	200	5000	6	0	6	0	0	0
98	CYC6H7	G	0	7.91E+01	200	6000	7	0	6	0	0	0
99	n-C6H7	G	0	7.91E+01	300	3000	7	0	6	0	0	0
100	i-C6H7	G	0	7.91E+01	300	3000	7	0	6	0	0	0
101	C5H4O	G	0	8.01E+01	300	5000	4	0	5	1	0	0
102	C6H8	G	0	8.01E+01	300	3000	8	0	6	0	0	0
103	CY13C6H8	G	0	8.01E+01	200	6000	8	0	6	0	0	0
104	C5H5O	G	0	8.11E+01	300	5000	5	0	5	1	0	0
105	C5H4OH	G	0	8.11E+01	300	5000	5	0	5	1	0	0
106	C6H9	G	0	8.11E+01	298	3000	9	0	6	0	0	0
107	CYC6H9	G	0	8.11E+01	298	3000	9	0	6	0	0	0
108	CYC6H10	G	0	8.21E+01	200	6000	10	0	6	0	0	0
109	C6H10	G	0	8.21E+01	298	3000	10	0	6	0	0	0
110	CYC6H11	G	0	8.32E+01	298	5000	11	0	6	0	0	0
111	C6H11-12	G	0	8.32E+01	300	5000	11	0	6	0	0	0
112	C6H11-13	G	0	8.32E+01	300	5000	11	0	6	0	0	0
113	C6H11-14	G	0	8.32E+01	300	5000	11	0	6	0	0	0
114	C6H11-15	G	0	8.32E+01	300	5000	11	0	6	0	0	0
115	C6H11	G	0	8.32E+01	298	3000	11	0	6	0	0	0
116	CYC6H12	G	0	8.42E+01	200	5000	12	0	6	0	0	0

117	hexene1	G	0	8.42E+01	200	6000	12	0	6	0	0	0
118	hex1yl	G	0	8.52E+01	200	6000	13	0	6	0	0	0
119	hex2yl	G	0	8.52E+01	200	6000	13	0	6	0	0	0
120	hex3yl	G	0	8.52E+01	300	5000	13	0	6	0	0	0
121	N	G	0	1.40E+01	300	5000	0	0	0	0	1	0
122	NH	G	0	1.50E+01	200	6000	1	0	0	0	1	0
123	NH2	G	0	1.60E+01	300	5000	2	0	0	0	1	0
124	NH3	G	0	1.70E+01	300	5000	3	0	0	0	1	0
125	N2	G	0	2.80E+01	200	6000	0	0	0	0	2	0
126	NNH	G	0	2.90E+01	200	6000	1	0	0	0	2	0
127	N2H2	G	0	3.00E+01	300	5000	2	0	0	0	2	0
128	H2NN	G	0	3.00E+01	300	5000	2	0	0	0	2	0
129	N2H3	G	0	3.10E+01	300	5000	3	0	0	0	2	0
130	N2H4	G	0	3.20E+01	300	5000	4	0	0	0	2	0
131	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0
132	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
133	HON	G	0	3.10E+01	300	5000	1	0	0	1	1	0
134	HNOH	G	0	3.20E+01	200	6000	2	0	0	1	1	0
135	NH2O	G	0	3.20E+01	300	4000	2	0	0	1	1	0
136	NH2OH	G	0	3.30E+01	300	5000	3	0	0	1	1	0
137	HNNNH2	G	0	4.50E+01	300	5000	3	0	0	0	3	0
138	N2O	G	0	4.40E+01	300	5000	0	0	0	1	2	0
139	HNNO	G	0	4.50E+01	300	5000	1	0	0	1	2	0
140	NH2NO	G	0	4.60E+01	200	6000	2	0	0	1	2	0
141	NHNHO	G	0	4.60E+01	300	5000	2	0	0	1	2	0
142	NH2NHO	G	0	4.70E+01	300	5000	3	0	0	1	2	0
143	NO2	G	0	4.60E+01	200	6000	0	0	0	2	1	0
144	HONO	G	0	4.70E+01	200	6000	1	0	0	2	1	0
145	HNO2	G	0	4.70E+01	300	4000	1	0	0	2	1	0
146	HNOO	G	0	4.70E+01	300	5000	1	0	0	2	1	0
147	HONHO	G	0	4.80E+01	300	5000	2	0	0	2	1	0

148	NH2NO2	G	0	6.20E+01	200	6000	2	0	0	2	2	0
149	NO3	G	0	6.20E+01	200	6000	0	0	0	3	1	0
150	HNO3	G	0	6.30E+01	200	6000	1	0	0	3	1	0
151	N2O4	G	0	9.20E+01	200	6000	0	0	0	4	2	0
152	HE	G	0	4.00E+00	200	6000	0	1	0	0	0	0
153	CN	G	0	2.60E+01	200	6000	0	0	1	0	1	0
154	HCN	G	0	2.70E+01	300	4000	1	0	1	0	1	0
155	HNC	G	0	2.70E+01	300	5000	1	0	1	0	1	0
156	CHNH	G	0	2.80E+01	300	4000	2	0	1	0	1	0
157	NCH2	G	0	2.80E+01	300	4000	2	0	1	0	1	0
158	CH2NH	G	0	2.90E+01	300	5000	3	0	1	0	1	0
159	CH3N	G	0	2.90E+01	200	5000	3	0	1	0	1	0
160	CH3NH	G	0	3.01E+01	300	5000	4	0	1	0	1	0
161	CH2NH2	G	0	3.01E+01	300	5000	4	0	1	0	1	0
162	CH3NH2	G	0	3.11E+01	300	5000	5	0	1	0	1	0
163	NCN	G	0	4.00E+01	300	4000	0	0	1	0	2	0
164	CHCNH	G	0	4.00E+01	298	3000	2	0	2	0	1	0
165	CH2CN	G	0	4.00E+01	200	6000	2	0	2	0	1	0
166	HCNN	G	0	4.10E+01	300	5000	1	0	1	0	2	0
167	CH2CNH	G	0	4.11E+01	200	5000	3	0	2	0	1	0
168	CH2CHN	G	0	4.11E+01	298	3000	3	0	2	0	1	0
169	CH2CHN(S)	G	0	4.11E+01	298	3000	3	0	2	0	1	0
170	CHCNH2	G	0	4.11E+01	298	3000	3	0	2	0	1	0
171	CH3CN	G	0	4.11E+01	200	6000	3	0	2	0	1	0
172	c-C2H3N	G	0	4.11E+01	298	3000	3	0	2	0	1	0
173	CH2NN	G	0	4.20E+01	200	6000	2	0	1	0	2	0
174	NCO	G	0	4.20E+01	300	5000	0	0	1	1	1	0
175	CH3NCH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
176	CH3CHN	G	0	4.21E+01	298	3000	4	0	2	0	1	0
177	CH3CNH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
178	CH2CNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0

179	CHCHNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
180	CH2NCH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
181	CH2CHNH	G	0	4.21E+01	200	5000	4	0	2	0	1	0
182	CH3CHNH	G	0	4.31E+01	298	3000	5	0	2	0	1	0
183	CH3NCH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
184	CH2CHNH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
185	CH3CH2NH	G	0	4.41E+01	298	3000	6	0	2	0	1	0
186	CH3CHNH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
187	CH2CH2NH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
188	CH3CH2NH2	G	0	4.51E+01	298	3000	7	0	2	0	1	0
189	HCNO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
190	HNCO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
191	HOCN	G	0	4.30E+01	300	5000	1	0	1	1	1	0
192	CH3NN	G	0	4.30E+01	200	6000	3	0	1	0	2	0
193	H2NCO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
194	CH3NNH	G	0	4.41E+01	200	6000	4	0	1	0	2	0
195	H2NCHO	G	0	4.50E+01	200	6000	3	0	1	1	1	0
196	CH2NNH2	G	0	4.41E+01	200	5000	4	0	1	0	2	0
197	CH3NCH3	G	0	4.41E+01	298	3000	6	0	2	0	1	0
198	CH3NHCH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
199	CH2NO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
200	HOCO	G	0	4.50E+01	300	4000	1	0	1	2	0	0
201	CH3NO	G	0	4.50E+01	300	4000	3	0	1	1	1	0
202	CH3NHCH3	G	0	4.51E+01	298	3000	7	0	2	0	1	0
203	NCCN	G	0	5.20E+01	300	5000	0	0	2	0	2	0
204	CHCHNCH2	G	0	5.41E+01	200	5000	4	0	3	0	1	0
205	CH2CHNCH2	G	0	5.51E+01	200	5000	5	0	3	0	1	0
206	NCNO	G	0	5.60E+01	300	4000	0	0	1	1	2	0
207	NCHCHO	G	0	5.60E+01	200	5000	2	0	2	1	1	0
208	CH2NHCHCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
209	CH2CH2NCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0

210	NHCH2CHO	G	0	5.81E+01	200	5000	4	0	2	1	1	0
211	OCH2CHNH	G	0	5.81E+01	200	5000	4	0	2	1	1	0
212	CH3NNCH3	G	0	5.81E+01	300	4000	6	0	2	0	2	0
213	H2CNO2	G	0	6.00E+01	300	4000	2	0	1	2	1	0
214	CH3NO2	G	0	6.10E+01	300	4000	3	0	1	2	1	0
215	CH3ONO	G	0	6.10E+01	300	4000	3	0	1	2	1	0
216	CH3ONO2	G	0	7.70E+01	300	4000	3	0	1	3	1	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. 2O+M=O2+M			6.16E+15	-0.5	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
2. 2O+AR=O2+AR			1.89E+13	0.0	-1790.0
3. O+H+M=OH+M			4.71E+18	-1.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	7.500E-01			
4. H2+M=2H+M			4.58E+19	-1.4	104380.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
5. H2+AR=2H+AR			5.84E+18	-1.1	104380.0
6. H+OH+M=H2O+M			2.21E+22	-2.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
7. H+OH+AR=H2O+AR			8.41E+21	-2.0	0.0
8. H2O2(+M)=2OH(+M)			2.95E+14	0.0	48400.0

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    Low pressure limit:  0.12000E+18  0.00000E+00  0.45500E+05
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    1.600E-01
 9. H2O+O=OH+OH                                    2.97E+06    2.0    13400.0
10. O+H2=H+OH                                      5.08E+04    2.7     6290.0
11. OH+H2=H+H2O                                    2.16E+08    1.5     3430.0
12. H+O2(+M)=HO2(+M)                               1.48E+12    0.6        0.0
    Low pressure limit:  0.35000E+17 -0.41000E+00 -0.11200E+04
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    5.000E-02
13. H+O2=O+OH                                      4.49E+08    1.3    16191.0
    Declared duplicate reaction...
14. H+O2=O+OH                                      2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
15. O+HO2=OH+O2                                    3.25E+13    0.0        0.0
16. H+HO2=O2+H2                                    1.66E+13    0.0      820.0
17. H+HO2=2OH                                      7.08E+13    0.0      300.0
18. OH+HO2=O2+H2O                                  4.64E+13    0.0     -500.0
19. 2HO2=O2+H2O2                                   1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
20. 2HO2=O2+H2O2                                   4.20E+14    0.0    11980.0
    Declared duplicate reaction...
21. O+H2O2=OH+HO2                                  9.55E+06    2.0     3970.0
22. H+H2O2=HO2+H2                                  4.82E+13    0.0     7950.0
23. H+H2O2=OH+H2O                                  2.41E+13    0.0     3970.0
24. OH+H2O2=HO2+H2O                                1.00E+12    0.0        0.0
    Declared duplicate reaction...
25. OH+H2O2=HO2+H2O                                5.80E+14    0.0     9560.0
    Declared duplicate reaction...
26. O+CO(+M)=CO2(+M)                               1.80E+10    0.0     2385.0
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    Low pressure limit:  0.60200E+15  0.00000E+00  0.30000E+04
    H2              Enhanced by    2.000E+00
    O2              Enhanced by    6.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    3.500E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    5.000E-01
27. O2+CO=O+CO2                                    2.50E+12    0.0    47800.0
28. H2+CO(+M)=CH2O(+M)                             4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
29. OH+CO=H+CO2                                    4.10E+04    2.1    -1578.0
30. HO2+CO=OH+CO2                                  1.50E+14    0.0    23600.0
31. O+HCO=OH+CO                                    3.00E+13    0.0        0.0
32. O+HCO=H+CO2                                    3.00E+13    0.0        0.0
33. H+HCO(+M)=CH2O(+M)                             1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
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    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
34. H+HCO=H2+CO                                  7.30E+13    0.0        0.0
35. OH+HCO=H2O+CO                                3.00E+13    0.0        0.0
36. HCO+M=H+CO+M                                 1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
37. HCO+O2=HO2+CO                                4.22E+12    0.0        0.0
38. HCO+HO2=CO2+OH+H                             3.00E+13    0.0        0.0
39. O+CH2O=OH+HCO                                1.81E+13    0.0     3078.0
40. O2+CH2O=HO2+HCO                              2.05E+13    0.0    38920.0
41. H+CH2O=HCO+H2                                5.18E+07    1.7     1834.0
42. H+CH2O(+M)=CH2OH(+M)                         5.40E+11    0.5     3600.0
    Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
    TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
43. H+CH2O(+M)=CH3O(+M)                          5.40E+11    0.5     2600.0
    Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
    TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
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CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

44.	OH+CH2O=HCO+H2O	3.43E+09	1.2	-447.0
45.	HO2+CH2O=HCO+H2O2	1.47E+13	0.0	15200.0
46.	O+CH2OH=OH+CH2O	4.20E+13	0.0	0.0
47.	H+CH2OH=H2+CH2O	6.00E+12	0.0	0.0
48.	H+CH2OH=OH+CH3	9.63E+13	0.0	0.0
49.	OH+CH2OH=H2O+CH2O	2.40E+13	0.0	0.0
50.	CH2OH+O2=HO2+CH2O	2.41E+14	0.0	5017.0
	Declared duplicate reaction...			
51.	CH2OH+O2=HO2+CH2O	1.51E+15	-1.0	0.0
	Declared duplicate reaction...			
52.	CH2OH+HO2=CH2O+H2O2	1.20E+13	0.0	0.0
53.	CH2OH+HCO=CH3OH+CO	1.20E+14	0.0	0.0
54.	CH2OH+HCO=CH2O+CH2O	1.80E+14	0.0	0.0
55.	2CH2OH=CH3OH+CH2O	3.00E+12	0.0	0.0
56.	CH2OH+CH3O=CH3OH+CH2O	2.40E+13	0.0	0.0
57.	O+CH3O=OH+CH2O	6.00E+12	0.0	0.0
58.	H+CH3O=H2+CH2O	2.00E+13	0.0	0.0
59.	H+CH3O=OH+CH3	3.20E+13	0.0	0.0
60.	OH+CH3O=H2O+CH2O	1.80E+13	0.0	0.0
61.	CH3O+O2=HO2+CH2O	9.03E+13	0.0	11980.0
	Declared duplicate reaction...			
62.	CH3O+O2=HO2+CH2O	2.20E+10	0.0	1748.0
	Declared duplicate reaction...			
63.	CH3O+HO2=CH2O+H2O2	3.00E+11	0.0	0.0
64.	CH3O+CO=CH3+CO2	1.57E+13	0.0	11800.0
65.	CH3O+HCO=CH3OH+CO	9.00E+13	0.0	0.0
66.	2CH3O=CH3OH+CH2O	6.00E+13	0.0	0.0
67.	O+CH3OH=OH+CH2OH	3.88E+05	2.5	3080.0
68.	H+CH3OH=CH2OH+H2	1.44E+13	0.0	6095.0

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69. H+CH3OH=CH3O+H2                                   3.60E+12    0.0     6095.0
70. OH+CH3OH=CH2OH+H2O                                7.10E+06    1.8     -596.0
71. OH+CH3OH=CH3O+H2O                                 1.00E+06    2.1      496.5
72. CH3+CH3OH=CH2OH+CH4                               3.19E+01    3.2     7172.0
73. O2+CH3OH=CH2OH+HO2                                2.05E+13    0.0    44900.0
74. HCO+CH3OH=CH2OH+CH2O                              9.63E+03    2.9    13110.0
75. HO2+CH3OH=CH2OH+H2O2                              3.98E+13    0.0    19400.0
76. CH3O+CH3OH=CH2OH+CH3OH                            3.00E+11    0.0     4060.0
77. CH3OH(+M)=CH3+OH(+M)                              1.90E+16    0.0    91730.0
    Low pressure limit:  0.29500E+45 -0.73500E+01  0.95460E+05
    TROE centering:      0.41400E+00  0.27900E+03  0.54590E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
78. CH3OH(+M)=CH2OH+H(+M)                             2.69E+16   -0.1    98940.0
    Low pressure limit:  0.23400E+41 -0.63300E+01  0.10310E+06
    TROE centering:      0.77300E+00  0.69300E+03  0.53330E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
79. O+CH4=OH+CH3                                      1.02E+09    1.5     8600.0
80. H+CH4=CH3+H2                                      6.60E+08    1.6    10840.0
81. OH+CH4=CH3+H2O                                    1.00E+08    1.6     3120.0
82. CH+CH4=H+C2H4                                     6.00E+13    0.0        0.0
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83. CH2SING+CH4=2CH3                                  1.60E+13    0.0     -570.0
84. CH2+CH4=2CH3                                      2.46E+06    2.0     8270.0
85. O+CH3=H+CH2O                                      5.06E+13    0.0        0.0
86. O+CH3=H+H2+CO                                     3.37E+13    0.0        0.0
87. H+CH3(+M)=CH4(+M)                                 1.39E+16   -0.5      536.0
    Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
    TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
88. OH+CH3=CH2+H2O                                    5.60E+07    1.6     5420.0
89. OH+CH3=CH2SING+H2O                                6.44E+17   -1.3     1417.0
90. HO2+CH3=O2+CH4                                    1.00E+12    0.0        0.0
91. HO2+CH3=OH+CH3O                                   2.00E+13    0.0        0.0
92. CH+CH3=H+C2H3                                     3.00E+13    0.0        0.0
93. CH2SING+CH3=H+C2H4                                1.20E+13    0.0     -570.0
94. CH3+O2=O+CH3O                                     3.56E+13    0.0    30480.0
95. CH3+O2=OH+CH2O                                    2.31E+12    0.0    20315.0
96. CH3+H2O2=HO2+CH4                                  2.45E+04    2.5     5180.0
97. 2CH3(+M)=C2H6(+M)                                 6.77E+16   -1.2      654.0
    Low pressure limit:  0.34000E+42 -0.70300E+01  0.27630E+04
    TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
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     AR              Enhanced by    7.000E-01
 98. 2CH3=H+C2H5                                  6.84E+12    0.1    10600.0
 99. CH3+HCO=CH4+CO                               1.21E+14    0.0        0.0
100. CH3+CH2O=HCO+CH4                             3.32E+03    2.8     5860.0
101. CH2+CH3=H+C2H4                               4.00E+13    0.0        0.0
102. O+CH2=H+HCO                                  8.00E+13    0.0        0.0
103. O+CH2SING=H2+CO                              1.50E+13    0.0        0.0
104. O+CH2SING=H+HCO                              1.50E+13    0.0        0.0
105. H+CH2(+M)=CH3(+M)                            6.00E+14    0.0        0.0
     Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
     TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
106. H+CH2SING=CH+H2                              3.00E+13    0.0        0.0
107. OH+CH2=H+CH2O                                2.00E+13    0.0        0.0
108. OH+CH2=CH+H2O                                1.13E+07    2.0     3000.0
109. OH+CH2SING=H+CH2O                            3.00E+13    0.0        0.0
110. HO2+CH2=OH+CH2O                              2.00E+13    0.0        0.0
111. CH+CH2=H+C2H2                                4.00E+13    0.0        0.0
112. CH2+O2=OH+H+CO                               5.00E+12    0.0     1500.0
113. CH2+O2=CO2+2H                                5.80E+12    0.0     1500.0
114. CH2+O2=O+CH2O                                2.40E+12    0.0     1500.0
115. CH2+H2=H+CH3                                 5.00E+05    2.0     7230.0
116. 2CH2=H2+C2H2                                 1.60E+15    0.0    11944.0
117. 2CH2=H+H+C2H2                                2.00E+14    0.0    10989.0
118. CH2SING+CO=CH2+CO                            9.00E+12    0.0        0.0
119. CH2SING+AR=CH2+AR                            9.00E+12    0.0      600.0
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120. CH2SING+CO2=CH2+CO2                              7.00E+12    0.0        0.0
121. CH2SING+CO2=CO+CH2O                              1.40E+13    0.0        0.0
122. CH2+CO(+M)=CH2CO(+M)                             8.10E+11    0.5     4510.0
     Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
123. CH2SING+O2=H+OH+CO                               2.80E+13    0.0        0.0
124. CH2SING+O2=CO+H2O                                1.20E+13    0.0        0.0
125. CH2SING+H2=CH3+H                                 7.00E+13    0.0        0.0
126. CH2SING+H2O(+M)=CH3OH(+M)                        4.82E+17   -1.2     1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
127. CH2SING+H2O=CH2+H2O                              3.00E+13    0.0        0.0
128. CH2SING+H2O=H2+CH2O                              6.82E+10    0.2     -935.0
129. O+CH=H+CO                                        5.70E+13    0.0        0.0
130. OH+CH=H+HCO                                      3.00E+13    0.0        0.0
131. CH+O2=O+HCO                                      6.71E+13    0.0        0.0
132. CH+H2=H+CH2                                      1.08E+14    0.0     3110.0
133. CH+H2O=H+CH2O                                    5.71E+12    0.0     -755.0
134. CH+CO(+M)=HCCO(+M)                               5.00E+13    0.0        0.0
     Low pressure limit:  0.26900E+29 -0.37400E+01  0.19360E+04
```

TROE centering: 0.57570E+00 0.23700E+03 0.16520E+04 0.50690E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

135. CH+CO2=HCO+CO 1.90E+14 0.0 15792.0

136. CH+CH2O=H+CH2CO 9.46E+13 0.0 -515.0

137. CH+HCCO=CO+C2H2 5.00E+13 0.0 0.0

138. O+C2H6=OH+C2H5 3.00E+07 2.0 5115.0

139. H+C2H6=C2H5+H2 5.40E+02 3.5 5210.0

140. OH+C2H6=C2H5+H2O 7.26E+06 2.0 864.0

141. CH3+C2H6=C2H5+CH4 5.50E-01 4.0 8300.0

142. CH2SING+C2H6=CH3+C2H5 4.00E+13 0.0 -550.0

143. C2H6+O2=C2H5+HO2 4.04E+13 0.0 50872.0

144. C2H6+CH2OH=CH3OH+C2H5 1.99E+02 3.0 13976.0

145. C2H6+CH3O=CH3OH+C2H5 2.41E+11 0.0 7094.0

146. C2H6+C2H=C2H2+C2H5 3.61E+12 0.0 0.0

147. C2H6+C2H3=C2H4+C2H5 6.01E+02 3.3 10502.0

148. C2H6+CH3CO=CH3CHO+C2H5 1.81E+04 2.8 17527.0

149. C2H6+HCO=CH2O+C2H5 4.70E+04 2.7 18235.0

150. O+C2H5=CH3+CH2O 2.24E+13 0.0 0.0

151. O+C2H5=H+CH3CHO 1.10E+14 0.0 0.0

152. H+C2H5=H2+C2H4 2.00E+12 0.0 0.0

153. H+C2H5(+M)=C2H6(+M) 5.21E+17 -1.0 1580.0

Low pressure limit: 0.19900E+42 -0.70800E+01 0.66850E+04

TROE centering: 0.84220E+00 0.12500E+03 0.22190E+04 0.68820E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

```
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
154. C2H5+O2=HO2+C2H4                                1.92E+07    1.0    -2035.0
155. C2H5+HO2=C2H5O+OH                               3.00E+13    0.0        0.0
156. C2H5+HO2=C2H4+H2O2                              3.01E+11    0.0        0.0
157. C2H5+OH=C2H4+H2O                                2.41E+13    0.0        0.0
158. C2H5+CH3=CH4+C2H4                               1.13E+12   -0.5        0.0
159. CH3+C2H5(+M)=C3H8(+M)                           9.60E+14   -0.5        0.0
     Low pressure limit:  0.68000E+62 -0.13420E+02  0.60000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.14339E+04  0.53288E+04
160. C2H5+CH2OH=C2H4+CH3OH                           2.41E+12    0.0        0.0
161. C2H5+CH2OH=C2H6+CH2O                            2.41E+12    0.0        0.0
162. C2H5+CH3O=C2H6+CH2O                             2.41E+13    0.0        0.0
163. C2H5+C2H=C2H2+C2H4                              1.81E+12    0.0        0.0
164. CH2+C2H5=C2H4+CH3                               1.81E+13    0.0        0.0
165. CH2SING+C2H5=C2H4+CH3                           9.00E+12    0.0        0.0
166. C2H5+CH2SING=C3H6+H                             9.00E+12    0.0        0.0
167. C2H5+H2O2=C2H6+HO2                              8.73E+09    0.0      974.0
168. H+C2H4(+M)=C2H5(+M)                             1.37E+09    1.5     1355.0
     Low pressure limit:  0.20260E+40 -0.66420E+01  0.57690E+04
     TROE centering:     -0.56900E+00  0.29900E+03 -0.91470E+04  0.15240E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
169. H+C2H4=C2H3+H2                                  1.12E+07    2.1    13366.0
170. OH+C2H4=C2H3+H2O                                1.31E-01    4.2     -860.0
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171. OH+C2H4=CH3+CH2O 3.19E+01 2.7 -1172.0

172. OH+C2H4=CH3CHO+H 8.73E-05 4.6 -618.0

173. CH3+C2H4=C2H3+CH4 2.27E+05 2.0 9200.0

174. CH3+C2H4(+M)<=>nC3H7(+M) 2.55E+06 1.6 5700.0

Low pressure limit: 0.30000E+64 -0.14600E+02 0.18170E+05

TROE centering: 0.18940E+00 0.27700E+03 0.87480E+04 0.78910E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

175. C2H4(+M)=H2+C2H2(+M) 8.00E+12 0.4 88770.0

Low pressure limit: 0.15800E+52 -0.93000E+01 0.97800E+05

TROE centering: 0.73450E+00 0.18000E+03 0.10350E+04 0.54170E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

176. C2H4+CH2SING=AC3H5+H 4.53E+13 0.0 -556.0

177. C2H4+HO2=C2H4O+OH 6.03E+09 0.0 7949.0

178. C2H4+O=H+CH2CHO 7.33E+07 1.6 1260.0

179. C2H4+O=CH3+HCO 1.13E+08 1.6 1020.0

180. C2H4+O=C2H3+OH 2.15E+06 2.5 11900.0

181. C2H4+O2=C2H3+HO2 4.22E+13 0.0 60800.0

182. C2H4+CO=C2H3+HCO 1.51E+14 0.0 90616.0

183. C2H4+C2H=C4H4+H 1.21E+13 0.0 0.0

184. C2H4+C2H2=C2H3+C2H3 2.41E+13 0.0 68360.0

185. C2H4+C2H4=C2H5+C2H3 4.82E+14 0.0 71539.0

186. H+C2H3(+M)=C2H4(+M) 6.08E+12 0.3 280.0

Low pressure limit: 0.14000E+31 -0.38600E+01 0.33200E+04

TROE centering: 0.78200E+00 0.20750E+03 0.26630E+04 0.60950E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

187. H+C2H2(+M)=C2H3(+M) 1.71E+10 1.3 2709.0

Low pressure limit: 0.63480E+32 -0.46639E+01 0.37800E+04

TROE centering: 0.00000E+00 0.78784E+05 -0.10210E+05 0.10000E-29

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

188. H+C2H3=H2+C2H2 9.64E+13 0.0 0.0

189. OH+C2H3=H2O+C2H2 5.00E+12 0.0 0.0

190. C2H3+O2=C2H2+HO2 1.34E+06 1.6 -383.0

Declared duplicate reaction...

191. C2H3+O2=C2H2+HO2 1.37E+02 3.4 3663.0

Declared duplicate reaction...

192. C2H3+O2=HCO+CH2O 9.33E+13 -0.7 268.7

193. C2H3+O2=H+CO+CH2O 2.19E+14 -0.7 268.7

194. C2H3+O2=CH2CHO+O 7.52E+08 1.0 -137.4

195. C2H3+HO2=OH+CH2CO+H 3.01E+13 0.0 0.0

196. C2H3+CH3=C2H2+CH4 3.92E+11 0.0 0.0

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197. C2H3+O=CH2CO+H                                   1.00E+14    0.0        0.0
198. C2H3OO+H=CH2CHO+OH                               1.00E+14    0.0        0.0
199. C2H3OO+CH2=CH2CHO+CH2O                           2.00E+13    0.0        0.0
200. C2H3OO+OH=CH2CHO+HO2                             2.00E+13    0.0        0.0
201. C2H3OO+O=CH2CHO+O2                               2.00E+13    0.0        0.0
202. C2H3+CH2OH=C2H4+CH2O                             3.01E+13    0.0        0.0
203. C2H3+CH3O=C2H4+CH2O                              2.41E+13    0.0        0.0
204. C2H3+CH3OH=C2H4+CH3O                             1.44E+01    3.1     6935.0
205. C2H3+CH3OH=C2H4+CH2OH                            3.19E+01    3.2     7172.0
206. C2H3+CO=C2H3CO                                   1.51E+11    0.0     4809.0
207. C2H3+C2H=C4H4                                    1.00E+14    0.0        0.0
208. C2H3+C2H=C2H2+C2H2                               9.64E+11    0.0        0.0
209. C2H3+CH3CO=C2H3CO+CH3                            1.81E+13    0.0        0.0
210. C2H5+C2H3=AC3H5+CH3                              8.00E+25   -3.5    11775.0
211. C2H3+C2H5(+M)=IC4H8(+M)                          1.50E+13    0.0        0.0
     Low pressure limit:  0.15500E+57 -0.11790E+02  0.89845E+04
     TROE centering:      0.19800E+00  0.22779E+04  0.60000E+05  0.57232E+04
212. C2H3+C2H5=C2H2+C2H6                              4.82E+11    0.0        0.0
213. C2H3+CH2SING=C2H2+CH3                            1.81E+13    0.0        0.0
214. C2H3+CH2=C2H2+CH3                                1.81E+13    0.0        0.0
215. C2H3+H2O2=C2H4+HO2                               1.21E+10    0.0     -596.0
216. C2H3+CH2O=C2H4+HCO                               5.43E+03    2.8     5862.0
217. C2H3+CH2=AC3H4+H                                 3.00E+13    0.0        0.0
218. C2H3+C2H3=i-C4H5+H                               1.50E+30   -5.0    13000.0
219. C2H3+C2H3=n-C4H5+H                               1.10E+24   -3.3    12400.0
220. H2CC+C2H2(+M)=C4H4(+M)                           3.50E+05    2.1    -2400.0
     Low pressure limit:  0.14000E+61 -0.12599E+02  0.74170E+04
     TROE centering:      0.98000E+00  0.56000E+02  0.58000E+03  0.41640E+04
     H2              Enhanced by    2.000E+00
     CH4             Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     C2H2            Enhanced by    3.000E+00
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     CO              Enhanced by    1.500E+00
     C2H4            Enhanced by    3.000E+00
     C2H6            Enhanced by    3.000E+00
     CO2             Enhanced by    2.000E+00
221. C2H2(+M)=H2CC(+M)                              8.00E+14   -0.5    50750.0
     Low pressure limit:  0.24500E+16 -0.64000E+00  0.49700E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H4            Enhanced by    2.500E+00
222. H2CC+C2H4=iiiC4H6                              1.00E+12    0.0        0.0
223. H2CC+O2=CH2+CO2                                1.00E+13    0.0        0.0
224. H2CC+H=C2H2+H                                  1.00E+14    0.0        0.0
225. H2CC+OH=CH2CO+H                                2.00E+13    0.0        0.0
226. C2H2+O=C2H+OH                                  4.60E+19   -1.4    28950.0
227. C2H2+O=CH2+CO                                  2.35E+08    1.4     2204.5
228. C2H2+O=HCCO+H                                  9.40E+08    1.4     2204.5
229. OH+C2H2=C2H+H2O                                2.63E+06    2.1    17060.0
230. OH+C2H2=H+CH2CO                                1.52E+04    2.3     -292.0
231. OH+C2H2=CH3+CO                                 4.37E+06    1.4      227.0
232. C2H2+CH=C3H2+H                                 1.10E+13    0.0        0.0
233. C2H2+CH2=C3H3+H                                1.20E+13    0.0     6620.0
234. C2H2+CH3=C2H+CH4                               1.81E+11    0.0    17289.0
235. C2H2+O2=2HCO                                   1.00E+12    0.0    28000.0
236. C2H2+CH2OH=C2H3+CH2O                           7.23E+11    0.0     9004.0
237. C2H2+CO=C2H+HCO                                4.82E+14    0.0   106713.0
238. C2H2+C2H=C4H2+H                                3.00E+13    0.0        0.0
239. C2H2+C2H(+M)=nC4H3(+M)                         8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
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     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
240. C2H2+C2H(+M)=iC4H3(+M)                          8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
241. C2H2+CH2SING=C3H3+H                             3.42E+15   -0.6     -230.7
242. C2H2+CH2SING=CH2+C2H2                           8.55E+14   -0.6     -230.7
243. HCCO+C2H2=C3H3+CO                               1.00E+11    0.0     3000.0
244. C2H2+C2H3=n-C4H5                                1.10E+32   -7.3     6200.0
245. C2H2+C2H3=i-C4H5                                2.10E+36   -8.8     9100.0
246. C2H3+C2H2=C4H4+H                                5.00E+14   -0.7     6700.0
247. O+C2H=CH+CO                                     1.00E+13    0.0        0.0
248. H+C2H(+M)=C2H2(+M)                              1.00E+17   -1.0        0.0
     Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
     TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
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	CH4	Enhanced by	2.000E+00		
	CO	Enhanced by	1.500E+00		
	CO2	Enhanced by	2.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	7.000E-01		
249.	OH+C2H=H+HCCO		2.00E+13	0.0	0.0
250.	C2H+O2=HCO+CO		1.00E+13	0.0	-775.0
251.	C2H+H2=H+C2H2		5.68E+10	0.9	1993.0
252.	C2H+HO2=HCCO+OH		1.81E+13	0.0	0.0
253.	C2H+CH3=C3H3+H		2.41E+13	0.0	0.0
254.	C2H+O2=HCCO+O		6.03E+11	0.0	0.0
255.	C2H+CH2OH=C2H2+CH2O		3.61E+13	0.0	0.0
256.	C2H+CH2OH=C3H3+OH		1.21E+13	0.0	0.0
257.	C2H+CH3OH=C2H2+CH2OH		6.03E+12	0.0	0.0
258.	C2H+CH3O=CH2O+C2H2		2.41E+13	0.0	0.0
259.	C2H+CH3OH=C2H2+CH3O		1.21E+12	0.0	0.0
260.	C2H+CH2=CH+C2H2		1.81E+13	0.0	0.0
261.	C2H+CH2SING=C2H2+CH		1.81E+13	0.0	0.0
262.	O+HCCO=H+2CO		1.00E+14	0.0	0.0
263.	H+HCCO=CH2SING+CO		5.00E+13	0.0	0.0
264.	CH2+HCCO=C2H3+CO		3.00E+13	0.0	0.0
265.	HCCO+O2=CO2+CO+H		4.78E+12	-0.1	1150.0
266.	HCCO+O2=CO+CO+OH		1.91E+11	0.0	1023.0
267.	HCCO+O2=O+CO+HCO		2.18E+02	2.7	3541.0
268.	2HCCO=2CO+C2H2		1.00E+13	0.0	0.0
269.	HCCO+CH3=C2H4+CO		5.00E+13	0.0	0.0
270.	O+CH2CO=OH+HCCO		1.00E+13	0.0	8000.0
271.	O+CH2CO=CH2+CO2		1.75E+12	0.0	1350.0
272.	H+CH2CO=HCCO+H2		5.00E+13	0.0	8000.0
273.	CH2CO+H=CH3+CO		7.77E+08	1.4	2780.0
274.	CH2CHO=H+CH2CO		2.48E+27	-5.2	44304.0
275.	CH2CHO=CH3+CO		1.54E+31	-6.3	42478.0

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276. OH+CH2CO=HCCO+H2O                                7.50E+12    0.0     2000.0
277. CH2CO+OH=CH2OH+CO                                1.00E+13    0.0        0.0
278. CH3CO=CH3+CO                                     2.40E+15   -2.0    14805.0
279. CH2CHO+H=CH3CHO                                  6.40E+35   -7.6     5215.0
280. CH2CHO+H=CH3+HCO                                 4.99E+14   -0.3      912.0
281. CH2CHO+O=CH2O+HCO                                5.00E+13    0.0        0.0
282. CH2CHO+OH=H2O+CH2CO                              1.20E+13    0.0        0.0
283. CH2CHO+OH=HCO+CH2OH                              3.01E+13    0.0        0.0
284. CH2CHO+O2=CH2CO+HO2                              1.57E+11    0.0        0.0
285. CH3CHO=CH3+HCO                                   9.59E+14    0.0    74180.0
286. CH3CHO+O2=CH3CO+HO2                              2.00E+13    0.5    42200.0
287. CH3CHO+H=CH2CHO+H2                               4.10E+09    1.2     2405.0
288. CH3CHO+OH=CH3CO+H2O                              2.35E+10    0.7    -1113.0
289. CH3CHO+O=CH2CHO+OH                               5.85E+12    0.0     1808.0
290. CH3CHO+HO2=CH3CO+H2O2                            1.70E+12    0.0    10700.0
291. CH3CHO+CH3=CH3CO+CH4                             1.70E+12    0.0     8440.0
292. CH3CHO+HCO=CH3CO+CH2O                            7.80E+13    0.0     8440.0
293. C2H5+O2(+M)=C2H5OO(+M)                           2.02E+10    1.0      -63.6
     Low pressure limit:  0.84900E+30 -0.42900E+01  0.22000E+03
     TROE centering:      0.10300E+00  0.60100E+03  0.10000E-09
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
294. C2H5OO(+M)=C2H4+HO2(+M)                          7.14E+04    2.3    27955.0
     Low pressure limit:  0.83100E+22 -0.65100E+00  0.22890E+05
     TROE centering:      0.00000E+00  0.10600E+03  0.10600E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
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CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

295.	C2H5OO+HO2=C2H5O+OH+O2	1.75E+10	0.0	-3275.0
296.	C2H5O=CH3+CH2O	1.00E+15	0.0	21523.0
297.	C2H5O=CH3CHO+H	2.00E+14	0.0	23215.0
298.	C2H5O+O2=CH3CHO+HO2	6.03E+10	0.0	1643.0
299.	C2H4O+O2=CH2CHO+HO2	4.00E+13	0.0	61500.0
300.	C2H4O+H=CH2CHO+H2	2.00E+13	0.0	8300.0
301.	C2H4O+H=C2H3+H2O	5.00E+09	0.0	5000.0
302.	C2H4O+H=C2H4+OH	9.51E+10	0.0	5000.0
303.	C2H4O+OH=CH2CHO+H2O	4.79E+13	0.0	5955.0
304.	C2H4O+O=CH2CHO+OH	1.91E+12	0.0	5250.0
305.	C2H4O+HO2=CH2CHO+H2O2	4.00E+12	0.0	17000.0
306.	C2H4O=CH3CHO	6.00E+13	0.0	57167.0
307.	C2H4O=CH3+HCO	4.90E+13	0.0	57167.0
308.	C2H4O=CH4+CO	1.21E+13	0.0	57167.0
309.	C3H8+H=nC3H7+H2	1.30E+06	2.5	6756.0
310.	C3H8+H=iC3H7+H2	1.30E+06	2.4	4471.0
311.	C3H8+O=nC3H7+OH	1.90E+05	2.7	3716.0
312.	C3H8+O=iC3H7+OH	4.76E+04	2.7	2106.0
313.	C3H8+OH=iC3H7+H2O	1.40E+03	2.8	-310.0
314.	C3H8+OH=nC3H7+H2O	1.37E+03	2.7	580.0
315.	C3H8+O2=nC3H7+HO2	3.97E+13	0.0	50872.0
316.	C3H8+O2=iC3H7+HO2	3.97E+13	0.0	47693.0
317.	C3H8+HO2=nC3H7+H2O2	4.76E+04	2.5	16494.0
318.	C3H8+HO2=iC3H7+H2O2	9.64E+03	2.6	13910.0
319.	C3H8+CH3=nC3H7+CH4	9.04E-01	3.6	7154.0
320.	C3H8+CH3=iC3H7+CH4	1.51E+00	3.5	5481.0
321.	C3H8+CH2OH=nC3H7+CH3OH	1.99E+02	3.0	3976.0

322. C3H8+CH3O=nC3H7+CH3OH 4.34E+11 0.0 6458.0

323. C3H8+CH2SING=nC3H7+CH3 9.04E-01 3.6 7154.0

324. C3H8+C2H3=nC3H7+C2H4 6.03E+02 3.3 10502.0

325. C3H8+C2H=nC3H7+C2H2 3.61E+12 0.0 0.0

326. C3H8+C2H5=nC3H7+C2H6 9.04E-02 3.6 9141.0

327. C3H8+HCO=nC3H7+CH2O 2.05E+05 2.5 18431.0

328. C3H8+iC3H7=nC3H7+C3H8 8.40E-03 4.2 8716.0

329. C3H8+CH3CO=nC3H7+CH3CHO 4.22E+04 2.6 17658.0

330. C3H8+CH2=nC3H7+CH3 9.03E-01 3.6 7154.0

331. C3H8+CH2OH=iC3H7+CH3OH 6.03E+01 3.0 11989.0

332. C3H8+CH3O=iC3H7+CH3OH 1.45E+11 0.0 4571.0

333. C3H8+CH2SING=iC3H7+CH3 1.51E+00 3.5 7472.0

334. C3H8+C2H3=iC3H7+C2H4 1.02E+03 3.1 8829.0

335. C3H8+C2H=iC3H7+C2H2 1.21E+12 0.0 0.0

336. C3H8+C2H5=iC3H7+C2H6 1.21E+00 3.5 7468.0

337. C3H8+HCO=iC3H7+CH2O 1.08E+07 1.9 17006.0

338. C3H8+CH3CO=iC3H7+CH3CHO 5.30E+06 2.0 16241.0

339. C3H8+CH2=iC3H7+CH3 1.51E+00 3.5 7472.0

340. nC3H7+H=C3H6+H2 1.81E+12 0.0 0.0

341. nC3H7+H(+M)=C3H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+59 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

342. nC3H7+H=C2H5+CH3 3.40E+18 -1.3 5386.0

343. nC3H7+O=C2H5+CH2O 9.60E+13 0.0 0.0

344. nC3H7+O2=C3H6+HO2 9.04E+10 0.0 0.0

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345. nC3H7+HO2=C2H5+OH+CH2O                          2.41E+13    0.0        0.0
346. nC3H7+OH=C3H6+H2O                               2.41E+13    0.0        0.0
347. nC3H7+CH3=CH4+C3H6                              1.14E+13   -0.3        0.0
348. nC3H7+C2H5=C3H6+C2H6                            1.45E+12    0.0        0.0
349. nC3H7+C2H5=C3H8+C2H4                            1.15E+12    0.0        0.0
350. nC3H7+C2H3=C3H8+C2H2                            1.21E+12    0.0        0.0
351. nC3H7+C2H2=AC3H5+C2H4                           7.23E+11    0.0     9004.0
352. nC3H7+C2H=C3H3+C2H5                             1.21E+13    0.0        0.0
353. nC3H7+C2H=C3H6+C2H2                             6.03E+12    0.0        0.0
354. nC3H7+iC3H7=C3H8+C3H6                           5.13E+13   -0.3        0.0
355. nC3H7+HCO=CO+C3H8                               6.03E+13    0.0        0.0
356. nC3H7+CH3O=C3H8+CH2O                            2.41E+13    0.0        0.0
357. nC3H7+CH2SING=C2H5+C2H4                         2.58E+13    0.0        0.0
358. nC3H7+CH2SING=C3H6+CH3                          1.03E+13    0.0        0.0
359. nC3H7+CH2=C2H4+C2H5                             1.81E+13    0.0        0.0
360. nC3H7+CH2=C3H6+CH3                              1.81E+12    0.0        0.0
361. nC3H7+CH2OH=C3H6+CH3OH                          4.82E+11    0.0        0.0
362. iC3H7=CH3+C2H4                                  1.00E+14    0.0    45000.0
363. iC3H7+H=C3H6+H2                                 3.61E+12    0.0        0.0
364. iC3H7+H(+M)=C3H8(+M)                            2.40E+13    0.0        0.0
     Low pressure limit:  0.17000E+59 -0.12080E+02  0.11264E+05
     TROE centering:      0.64900E+00  0.12131E+04  0.12131E+04  0.13370E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
365. iC3H7+H=CH3+C2H5                                5.90E+23   -2.8    10009.0
366. iC3H7+O=CH3CHO+CH3                              9.60E+13    0.0        0.0
367. iC3H7+O2=C3H6+HO2                               1.26E+11    0.0        0.0
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368. iC3H7+HO2=CH3CHO+OH+CH3                          2.41E+13    0.0        0.0
369. iC3H7+OH=C3H6+H2O                                2.41E+13    0.0        0.0
370. iC3H7+CH3=CH4+C3H6                               2.19E+14   -0.7        0.0
371. iC3H7+C2H5=C3H6+C2H6                             2.30E+13   -0.3        0.0
372. iC3H7+C2H5=C3H8+C2H4                             1.84E+13   -0.3        0.0
373. iC3H7+C2H3=C2H4+C3H6                             1.52E+14   -0.7        0.0
374. iC3H7+C2H3=C3H8+C2H2                             1.52E+14   -0.7        0.0
375. iC3H7+C2H2=CH3+iiiC4H6                           2.77E+10    0.0     6504.0
376. iC3H7+C2H=C3H6+C2H2                              3.60E+12    0.0        0.0
377. iC3H7+iC3H7=C3H8+C3H6                            2.11E+14   -0.7        0.0
378. iC3H7+HCO=CO+C3H8                                1.20E+14    0.0        0.0
379. iC3H7+CH3O=C3H8+CH2O                             1.21E+13    0.0        0.0
380. iC3H7+CH2SING=C3H6+CH3                           1.04E+13    0.0        0.0
381. iC3H7+CH2=C3H6+CH3                               3.01E+13    0.0        0.0
382. iC3H7+CH2OH=C3H6+CH3OH                           2.89E+12    0.0        0.0
383. iC3H7+CH2OH=C3H8+CH2O                            2.35E+12    0.0        0.0
384. CH3+C2H3(+M)=C3H6(+M)                            2.50E+13    0.0        0.0
     Low pressure limit:  0.42700E+59 -0.11940E+02  0.97700E+04
     TROE centering:      0.17500E+00  0.13410E+04  0.60000E+05  0.10140E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H2            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
385. C3H6+H=H2+AC3H5                                  1.70E+05    2.5     2492.0
386. C3H6+H=C2H4+CH3                                  8.80E+16   -1.1     6461.0
387. C3H6+H=SC3H5+H2                                  7.81E+05    2.5    12285.0
388. C3H6+H(+M)=nC3H7(+M)                             1.33E+13    0.0     3260.7
     Low pressure limit:  0.62600E+39 -0.66600E+01  0.70000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.13100E+04  0.48097E+05
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     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
389. C3H6+H(+M)=iC3H7(+M)                          1.33E+13    0.0     1559.8
     Low pressure limit:  0.87000E+43 -0.75000E+01  0.47218E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.64540E+03  0.68443E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
390. C3H6+H=TC3H5+H2                               3.90E+05    2.5     5821.0
391. C3H6=H2+AC3H4                                 4.00E+13    0.0    80000.0
392. C3H6=CH4+C2H2                                 3.50E+12    0.0    70000.0
393. C3H6+O=C2H5+HCO                               3.50E+07    1.6     -972.0
394. C3H6+O=AC3H5+OH                               1.75E+11    0.7     5884.0
395. C3H6+O=SC3H5+OH                               1.21E+11    0.7     8960.0
396. C3H6+O=TC3H5+OH                               6.03E+10    0.7     7633.0
397. C3H6+O=CH3+H+CH2CO                            1.20E+08    1.6      327.0
398. C3H6+OH=AC3H5+H2O                             3.12E+06    2.0     -298.0
399. C3H6+OH=SC3H5+H2O                             2.14E+06    2.0     2778.0
400. C3H6+OH=TC3H5+H2O                             1.11E+06    2.0     1451.0
401. C3H6+HO2=AC3H5+H2O2                           9.63E+03    2.6    13910.0
402. C3H6+O2=AC3H5+HO2                             6.03E+13    0.0    47590.0
403. C3H6+CH3=AC3H5+CH4                            2.20E+00    3.5     5675.0
404. C3H6+CH3=TC3H5+CH4                            8.40E-01    3.5    11660.0
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405. C3H6+C2H5=AC3H5+C2H6 2.23E+00 3.5 6637.0

406. C3H6+C2H2=AC3H5+C2H3 4.04E+13 0.0 46818.0

407. C3H6+C2H3=AC3H5+C2H4 2.21E+00 3.5 4682.0

408. C3H6+C2H3=SC3H5+C2H4 1.35E+00 3.5 10842.0

409. C3H6+C2H3=TC3H5+C2H4 8.40E-01 3.5 9670.0

410. C3H6+C2H3=iiiC4H6+CH3 7.23E+11 0.0 5008.0

411. C3H6+C2H4=AC3H5+C2H5 5.78E+13 0.0 51584.0

412. C3H6+C2H4=nC3H7+C2H3 6.03E+13 0.0 75446.0

413. C3H6+CH2OH=AC3H5+CH3OH 6.03E+01 3.0 12000.0

414. C3H6+nC3H7=AC3H5+C3H8 2.23E+00 3.5 6637.0

415. C3H6+nC3H7=IC4H8+C2H5 2.23E+00 3.5 -2000.0

416. C3H6+iC3H7=C3H8+AC3H5 6.62E-02 4.0 8066.0

417. C3H6+C3H6=AC3H5+nC3H7 2.53E+14 0.0 55179.0

418. C3H6+C3H6=AC3H5+iC3H7 4.88E+13 0.0 52309.0

419. CH3+C2H3=AC3H5+H 1.50E+24 -2.8 18618.0

420. CH3+C2H3=SC3H5+H 3.20E+35 -7.8 13300.0

421. CH3+C2H3=TC3H5+H 4.99E+22 -4.4 18850.0

422. AC3H5+H(+M)=C3H6(+M) 2.00E+14 0.0 0.0

Low pressure limit: 0.13300E+61 -0.12000E+02 0.59678E+04

TROE centering: 0.20000E-01 0.10970E+04 0.10967E+05 0.68600E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

423. AC3H5+H=AC3H4+H2 1.80E+13 0.0 0.0

424. TC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

425. SC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

426. AC3H5+O=C2H3CHO+H 6.00E+13 0.0 0.0

427. AC3H5+O=C2H3+CH2O 1.80E+14 0.0 0.0

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428. SC3H5+O=CH2CO+CH3                                1.81E+14    0.0        0.0
429. TC3H5+O=H+HCCO+CH3                               1.81E+14    0.0        0.0
430. AC3H5+OH=C2H3CHO+H+H                             5.30E+37   -6.7    29306.0
431. AC3H5+OH=AC3H4+H2O                               6.00E+12    0.0        0.0
432. AC3H5+O2=AC3H4+HO2                               4.99E+15   -1.4    22428.0
433. AC3H5+O2=CH2O+CH3CO                              1.19E+15   -1.0    20128.0
434. AC3H5+O2=OH+C2H3CHO                              1.82E+13   -0.4    22859.0
435. SC3H5+O2=CH3CHO+HCO                              4.34E+12    0.0        0.0
436. TC3H5+O2=CH3CHO+HCO                              4.34E+12    0.0        0.0
437. AC3H5+HO2=C2H3+CH2O+OH                           6.60E+12    0.0        0.0
438. AC3H5+CH3=AC3H4+CH4                              3.00E+12   -0.3     -131.0
439. AC3H5+CH3(+M)=IC4H8(+M)                          1.00E+14   -0.3     -262.0
     Low pressure limit:  0.35100E+61 -0.12970E+02  0.60000E+04
     TROE centering:      0.89600E+00  0.60000E+05  0.16060E+04  0.61180E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
440. SC3H5+CH3=AC3H4+CH4                              1.00E+11    0.0        0.0
441. TC3H5+CH3=AC3H4+CH4                              1.00E+11    0.0        0.0
442. AC3H5+C2H3=AC3H4+C2H4                            1.00E+12    0.0        0.0
443. SC3H5+C2H3=AC3H4+C2H4                            1.00E+11    0.0        0.0
444. TC3H5+C2H3=AC3H4+C2H4                            1.00E+11    0.0        0.0
445. AC3H5+CH2O=C3H6+HCO                              1.26E+08    1.9    18191.0
446. AC3H5+HCO=C3H6+CO                                6.00E+13    0.0        0.0
447. AC3H5+AC3H5=AC3H4+C3H6                           8.43E+10    0.0     -262.0
448. AC3H5+CH2=iiiC4H6+H                              3.00E+13    0.0        0.0
449. AC3H5+nC3H7=AC3H4+C3H8                           7.23E+11    0.0     -131.0
450. AC3H5+iC3H7=AC3H4+C3H8                           4.58E+12   -0.3     -131.0
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451.	AC3H5=TC3H5	3.90E+59	-15.4	75400.0
452.	AC3H5=SC3H5	1.30E+55	-14.5	73800.0
453.	TC3H5=SC3H5	1.60E+44	-12.2	52200.0
454.	AC3H4=PC3H4	6.03E+53	-12.2	84276.0
455.	AC3H4+H=AC3H5	1.24E+52	-12.0	17839.0
	Declared duplicate reaction...			
456.	AC3H4+H=AC3H5	6.92E+36	-8.2	7462.0
	Declared duplicate reaction...			
457.	AC3H4+H=TC3H5	1.55E+53	-13.1	14472.0
	Declared duplicate reaction...			
458.	AC3H4+H=TC3H5	9.88E+44	-11.2	8212.0
	Declared duplicate reaction...			
459.	PC3H4+H=TC3H5	3.17E+52	-12.7	14226.0
	Declared duplicate reaction...			
460.	PC3H4+H=TC3H5	2.59E+45	-11.2	8046.0
	Declared duplicate reaction...			
461.	PC3H4+H=SC3H5	3.38E+49	-12.8	14072.0
	Declared duplicate reaction...			
462.	PC3H4+H=SC3H5	2.98E+43	-11.4	8736.0
	Declared duplicate reaction...			
463.	AC3H4+H=PC3H4+H	1.48E+13	0.3	4103.0
464.	AC3H4+H=CH3+C2H2	2.72E+09	1.2	6834.0
465.	PC3H4+H=CH3+C2H2	3.89E+10	1.0	4114.0
466.	C2H2+CH3=SC3H5	-6.81E+48	-12.3	16642.0
	Declared duplicate reaction...			
467.	C2H2+CH3=SC3H5	1.52E+44	-10.7	15256.0
	Declared duplicate reaction...			
468.	C2H2+CH3=TC3H5	6.80E+20	-4.2	18000.0
469.	C2H2+CH3=AC3H5	8.20E+53	-13.3	33200.0
470.	AC3H4+H=C3H3+H2	6.60E+03	3.1	5522.0
471.	AC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
472.	PC3H4+H=C3H3+H2	3.57E+04	2.8	4821.0

473.	AC3H4+O=C2H4+CO	2.00E+07	1.8	1000.0
474.	AC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
475.	AC3H4+CH3=C3H3+CH4	1.30E+12	0.0	7700.0
476.	PC3H4+O=HCCO+CH3	7.30E+12	0.0	2250.0
477.	PC3H4+O=C2H4+CO	1.00E+13	0.0	2250.0
478.	PC3H4+O=C3H3+OH	3.44E+04	2.2	4830.0
479.	PC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
480.	PC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
481.	PC3H4+CH3=C3H3+CH4	1.80E+12	0.0	7700.0
482.	C3H3+H=PC3H4	3.63E+36	-7.4	6039.0
483.	C3H3+H=AC3H4	3.39E+36	-7.4	6337.0
484.	C3H3+CH3=iiC4H6	3.61E+13	0.0	0.0
485.	C2H3+C2H3=iiiC4H6	7.00E+57	-13.8	17629.0
486.	C3H3+H=C3H2+H2	2.14E+05	2.5	7453.0
487.	C3H3+O=>C2H2+HCO	1.38E+14	0.0	0.0
488.	C3H3+O=C2H3+CO	4.62E+13	0.0	0.0
489.	C3H3+O=C2H+CH2O	4.62E+13	0.0	0.0
490.	C3H3+O=>C2H2+CO+H	4.62E+13	0.0	0.0
491.	C3H3+OH=C3H2+H2O	2.00E+13	0.0	8000.0
492.	C3H3+HCO=AC3H4+CO	2.50E+13	0.0	0.0
493.	C3H3+HCO=PC3H4+CO	2.50E+13	0.0	0.0
494.	C3H3+CH=iC4H3+H	5.00E+13	0.0	0.0
495.	C3H3+CH2=C4H4+H	5.00E+13	0.0	0.0
496.	C3H3+O2=CH2CO+HCO	1.70E+05	1.7	1500.0
497.	C3H3+HCCO=C4H4+CO	2.50E+13	0.0	0.0
498.	C3H3+HO2=OH+CO+C2H3	8.00E+11	0.0	0.0
499.	C3H3+HO2=AC3H4+O2	3.00E+11	0.0	0.0
500.	C3H3+HO2=PC3H4+O2	2.50E+12	0.0	0.0
501.	C3H2+O2=H+CO+HCCO	2.00E+12	0.0	1000.0
502.	C3H2+O=C2H2+CO	6.80E+13	0.0	0.0
503.	C3H2+OH=C2H2+HCO	6.80E+13	0.0	0.0
504.	C3H2+H=C3H3	1.10E+40	-8.0	84700.0

505. C3H2+CH=C4H2+H	5.00E+13	0.0	0.0
506. C3H2+CH2=nC4H3+H	5.00E+13	0.0	0.0
507. C3H2+CH3=C4H4+H	5.00E+12	0.0	0.0
508. C3H2+HCCO=nC4H3+CO	1.00E+13	0.0	0.0
509. C2H3CO+M=>C2H3+CO+M	8.51E+15	0.0	23000.0
510. C2H3+CO+M=>C2H3CO+M	1.58E+11	0.0	6000.0
511. C2H3CHO+HO2=>C2H3CH2O+O2	1.29E+11	0.0	32000.0
512. C2H3CH2O=>C2H3CHO+H	1.00E+14	0.0	19000.0
513. C2H3CHO+H=>C2H3CH2O	1.00E+08	0.0	10000.0
514. C2H3CHO+OH=>C2H3CO+H2O	1.00E+13	0.0	0.0
515. C2H3CO+H2O=>C2H3CHO+OH	1.91E+13	0.0	36620.0
516. C2H3CHO+H=>C2H3CO+H2	3.98E+13	0.0	4200.0
517. C2H3CO+H2=>C2H3CHO+H	1.78E+13	0.0	23670.0
518. C2H3CHO+O=>C2H3CO+OH	5.01E+12	0.0	1790.0
519. C2H3CO+OH=>C2H3CHO+O	1.00E+12	0.0	19160.0
520. C2H3CHO+HO2=>C2H3CO+H2O2	1.70E+12	0.0	10700.0
521. C2H3CO+H2O2=>C2H3CHO+HO2	1.00E+12	0.0	14100.0
522. C2H3CHO+CH3=>C2H3CO+CH4	1.74E+12	0.0	8440.0
523. C2H3CO+CH4=>C2H3CHO+CH3	1.51E+13	0.0	28000.0
524. C2H3CH2O+O2=>C2H3CHO+HO2	1.74E+11	0.0	1750.0
525. C2H3CH2O=>CH2O+C2H3	1.00E+14	0.0	21600.0
526. CH2O+C2H3=>C2H3CH2O	1.00E+11	0.0	0.0
527. C4H+H2=C4H2+H	2.00E+13	0.0	5000.0
528. C4H+O2=CO+CO+C2H	1.20E+12	0.0	0.0
529. C4H2+OH=H2O+C4H	9.15E+09	1.0	21746.0
530. H2C4O+OH=C2H2+CO+HCO	1.00E+13	0.0	0.0
531. iC4H3+O=H2C4O+H	2.00E+13	0.0	0.0
532. C4H2+OH=H+H2C4O	1.63E+15	-1.1	2549.0
533. C4H2+OH=CO+C3H3	1.69E+28	-4.6	20140.0
534. C4H2+H=nC4H3	1.44E+63	-15.7	24018.0
Declared duplicate reaction...			
535. C4H2+H=nC4H3	4.16E+32	-6.5	9726.1

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     Declared duplicate reaction...
536. C4H2+H(+M)=iC4H3(+M)                              4.31E+10    1.2     1752.9
     Low pressure limit:  0.23000E+46 -0.80950E+01  0.25066E+04
     TROE centering:      0.74800E-01  0.10000E-49 -0.42159E+04  0.10000E+51
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
537. C4H2+O=C3H2+CO                                    2.70E+13    0.0     1720.0
538. C4H2+C2H=C6H2+H                                   9.60E+13    0.0        0.0
539. C4H2+C2H=C6H3                                     1.10E+30   -6.3     2790.0
540. nC4H3=iC4H3                                       3.70E+61  -15.8    54890.0
541. nC4H3+H=iC4H3+H                                   2.40E+11    0.8     2410.0
542. nC4H3+H=C2H2+H2CC                                 1.60E+19   -1.6     2220.0
543. nC4H3+H=C4H4                                      1.10E+42   -9.7     7000.0
544. nC4H3+H=C4H2+H2                                   3.00E+13    0.0        0.0
545. nC4H3+OH=C4H2+H2O                                 2.00E+12    0.0        0.0
546. nC4H3+C2H2=l-C6H4+H                               3.70E+16   -1.2    11100.0
547. nC4H3+C2H2=A1                                     2.30E+68  -17.6    24400.0
548. nC4H3+C2H2=c-C6H4+H                               1.90E+36   -7.2    17900.0
549. iC4H3+H=C2H2+H2CC                                 2.40E+19   -1.6     2800.0
550. iC4H3+H=C4H4                                      4.20E+44  -10.3     7890.0
551. iC4H3+H=C4H2+H2                                   5.00E+13    0.0        0.0
552. iC4H3+OH=C4H2+H2O                                 4.00E+12    0.0        0.0
553. iC4H3+O2=HCCO+CH2CO                               7.86E+16   -1.8        0.0
554. C4H4+H=n-C4H5                                     4.20E+50  -12.3    12500.0
555. C4H4+H=i-C4H5                                     9.60E+52  -12.8    14300.0
556. C4H4+H=nC4H3+H2                                   6.65E+05    2.5    12240.0
557. C4H4+H=iC4H3+H2                                   3.33E+05    2.5     9240.0
558. C4H4+OH=nC4H3+H2O                                 3.10E+07    2.0     3430.0
559. C4H4+OH=iC4H3+H2O                                 1.55E+07    2.0      430.0
560. C4H4+O=C3H3+HCO                                   6.00E+08    1.4     -860.0
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561. C4H4+C2H=l-C6H4+H	1.20E+13	0.0	0.0
562. n-C4H5=i-C4H5	1.30E+62	-16.4	49600.0
563. n-C4H5+H=i-C4H5+H	1.00E+36	-6.3	17486.0
564. n-C4H5+H=C4H4+H2	1.50E+13	0.0	0.0
565. n-C4H5+OH=C4H4+H2O	2.00E+12	0.0	0.0
566. n-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
567. n-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
568. n-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
569. n-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
570. n-C4H5+O2=HCO+C2H3CHO	9.20E+16	-1.4	1010.0
571. i-C4H5+H=C4H4+H2	3.00E+13	0.0	0.0
572. i-C4H5+H=C3H3+CH3	1.00E+14	0.0	0.0
573. i-C4H5+OH=C4H4+H2O	4.00E+12	0.0	0.0
574. i-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
575. i-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
576. i-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
577. i-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
578. i-C4H5+O2=CH2CO+CH2CHO	2.16E+10	0.0	2500.0
579. n-C4H5+C5H6=iiiC4H6+C5H5	6.00E+12	0.0	0.0
580. i-C4H5+C5H6=iiiC4H6+C5H5	6.00E+12	0.0	0.0
581. iiiC4H6=i-C4H5+H	8.20E+51	-10.9	118409.0
582. iiiC4H6=n-C4H5+H	3.50E+61	-13.9	129677.0
583. iiiC4H6=C4H4+H2	2.50E+15	0.0	94700.0
584. iiiC4H6+H=n-C4H5+H2	3.00E+07	2.0	13000.0
585. iiiC4H6+H=i-C4H5+H2	3.00E+07	2.0	6000.0
586. C2H4+C2H3=iiiC4H6+H	7.40E+14	-0.7	8420.0
587. iiiC4H6+H=PC3H4+CH3	2.00E+12	0.0	7000.0
588. iiiC4H6+H=AC3H4+CH3	2.00E+12	0.0	7000.0
589. iiiC4H6+O=n-C4H5+OH	7.50E+06	1.9	3740.0
590. iiiC4H6+O=i-C4H5+OH	7.50E+06	1.9	3740.0
591. iiiC4H6+O=HCO+AC3H5	6.02E+08	1.4	-858.0
592. iiiC4H6+OH=CH3CHO+C2H3	6.30E+12	0.0	-874.0

593.	iiiC4H6+OH=AC3H5+CH2O	6.30E+12	0.0	-874.0
594.	iiiC4H6+OH=n-C4H5+H2O	2.00E+07	2.0	5000.0
595.	iiiC4H6+OH=i-C4H5+H2O	2.00E+07	2.0	2000.0
596.	iiiC4H6+CH3=n-C4H5+CH4	2.00E+14	0.0	22800.0
597.	iiiC4H6+CH3=i-C4H5+CH4	1.00E+14	0.0	19800.0
598.	iiiC4H6+C2H3=n-C4H5+C2H4	5.00E+13	0.0	22800.0
599.	iiiC4H6+C2H3=i-C4H5+C2H4	2.50E+13	0.0	19800.0
600.	iiiC4H6+C3H3=n-C4H5+AC3H4	1.00E+13	0.0	22500.0
601.	iiiC4H6+C3H3=i-C4H5+AC3H4	5.00E+12	0.0	19500.0
602.	iiiC4H6+AC3H5=n-C4H5+C3H6	1.00E+13	0.0	22500.0
603.	iiiC4H6+AC3H5=i-C4H5+C3H6	5.00E+12	0.0	19500.0
604.	iiiC4H6+C2H3=A+H2+H	5.62E+11	0.0	3240.0
605.	iiC4H6=i-C4H5+H	4.20E+15	0.0	92600.0
606.	iiC4H6+H=iiiC4H6+H	2.00E+13	0.0	4000.0
607.	iiC4H6+H=i-C4H5+H2	1.70E+05	2.5	2490.0
608.	iiC4H6+H=AC3H4+CH3	2.00E+13	0.0	2000.0
609.	iiC4H6+H=PC3H4+CH3	2.00E+13	0.0	2000.0
610.	iiC4H6+CH3=i-C4H5+CH4	7.00E+13	0.0	18500.0
611.	iiC4H6+O=CH2CO+C2H4	1.20E+08	1.6	327.0
612.	iiC4H6+O=i-C4H5+OH	1.80E+11	0.7	5880.0
613.	iiC4H6+OH=i-C4H5+H2O	3.10E+06	2.0	-298.0
614.	iiC4H6=iiiC4H6	3.00E+13	0.0	65000.0
615.	IC4H8+H=C2H4+C2H5	1.60E+22	-2.4	11180.0
616.	IC4H8+H=C3H6+CH3	3.20E+22	-2.4	11180.0
617.	IC4H8+H=C4H7+H2	6.50E+05	2.5	6756.0
618.	IC4H8+O=nC3H7+HCO	3.30E+08	1.4	-402.0
619.	IC4H8+O=C4H7+OH	1.50E+13	0.0	5760.0
	Declared duplicate reaction...			
620.	IC4H8+O=C4H7+OH	2.60E+13	0.0	4470.0
	Declared duplicate reaction...			
621.	IC4H8+OH=C4H7+H2O	7.00E+02	2.7	527.0
622.	IC4H8+O2=C4H7+HO2	2.00E+13	0.0	50930.0

623. IC4H8+HO2=C4H7+H2O2 1.00E+12 0.0 14340.0

624. IC4H8+CH3=C4H7+CH4 4.50E-01 3.6 7153.0

625. C4H7=iiiC4H6+H 1.27E+24 -4.8 23777.0

626. C4H7+H(+M)=IC4H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+49 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

627. C4H7+H=CH3+AC3H5 2.00E+21 -2.0 11000.0

628. C4H7+H=iiiC4H6+H2 1.80E+12 0.0 0.0

629. C4H7+O2=iiiC4H6+HO2 1.00E+11 0.0 0.0

630. C4H7+HCO=IC4H8+CO 6.00E+13 0.0 0.0

631. C4H7+CH3=iiiC4H6+CH4 1.10E+13 0.0 0.0

632. C2H4+C2H3=C4H7 1.23E+35 -7.8 9930.0

633. IC4H8+H(+M)=nC4H9(+M) 1.33E+13 0.0 3260.7

Low pressure limit: 0.62600E+39 -0.66600E+01 0.70000E+04

TROE centering: 0.10000E+01 0.10000E+04 0.13100E+04 0.48097E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

634. C2H4+C2H5=nC4H9 1.50E+11 0.0 7300.0

635. nC4H9+H=IC4H8+H2 1.80E+12 0.0 0.0

636. nC4H9+O=nC3H7+CH2O 9.60E+13 0.0 0.0

637.	nC4H9+OH=IC4H8+H2O	2.40E+13	0.0	0.0
638.	nC4H9+O2=IC4H8+HO2	2.70E+11	0.0	0.0
639.	nC4H9+HO2=nC3H7+OH+CH2O	2.40E+13	0.0	0.0
640.	nC4H9+CH3=IC4H8+CH4	1.10E+13	0.0	0.0
641.	CH+C4H2=C5H2+H	1.00E+14	0.0	0.0
642.	H2CCCCCH+H=C5H2+H2	1.00E+13	0.0	0.0
643.	HCCCHCCH+H=C5H2+H2	1.00E+13	0.0	0.0
644.	H2CCCCCH+CH3=C5H2+CH4	3.00E+12	0.0	5000.0
645.	HCCCHCCH+CH3=C5H2+CH4	3.00E+12	0.0	5000.0
646.	C3H3+C2H=H2CCCCCH+H	1.00E+13	0.0	0.0
647.	CH2+C4H2=H2CCCCCH+H	1.30E+13	0.0	4326.0
648.	CH2SING+C4H2=H2CCCCCH+H	2.54E+16	-0.9	0.0
649.	HCCCHCCH+H=H2CCCCCH+H	1.00E+13	0.0	0.0
650.	H2CCCCCH+CH3=FC6H6	1.00E+11	0.0	0.0
651.	H2CCCCCH+CH3=A1+H	1.00E+11	0.0	0.0
652.	H2CCCCCH+CH3=A	5.00E+10	0.0	0.0
653.	C3H2+C2H2=HCCCHCCH+H	5.00E+12	0.0	5000.0
654.	C3H3+C2H=HCCCHCCH+H	3.00E+13	0.0	0.0
655.	CH2SING+C4H2=HCCCHCCH+H	2.54E+16	-0.9	0.0
656.	C3H3+C3H3=HCCCHCCH+CH3	5.00E+11	0.0	0.0
657.	HCCCHCCH+CH3=FC6H6	1.00E+11	0.0	0.0
658.	HCCCHCCH+CH3=A1+H	1.00E+11	0.0	0.0
659.	iC4H3+CH3=l-C5H5+H	3.00E+13	0.0	0.0
660.	C5H5=l-C5H5	4.09E+47	-10.4	54874.0
661.	C3H3+C2H2=l-C5H5	5.62E+32	-7.3	6758.0
662.	C5H5+H=C5H6	2.71E+63	-14.8	21050.0
663.	C5H5=C3H3+C2H2	2.79E+79	-18.3	130834.0
664.	C5H5+O=n-C4H5+CO	7.27E+13	-0.3	470.0
665.	C5H5+O=C5H5O	1.84E+03	1.0	-6960.0
666.	C5H5+O=C5H4O+H	6.71E+13	0.0	40.0
667.	C5H5+HO2=C5H5O+OH	3.00E+13	0.0	0.0
668.	C5H5O=n-C4H5+CO	2.51E+11	0.0	43900.0

669.	C5H5O=C5H4O+H	2.90E+32	-6.5	21220.0
670.	C5H5O=i-C4H5+CO	1.10E+79	-19.6	66250.0
671.	C5H5+OH=iiiC4H6+CO	1.20E+14	0.0	4500.0
672.	C5H5+OH=C5H4OH+H	2.15E+30	-4.6	25050.0
673.	C5H4O+H=C5H4OH	1.10E+69	-16.0	37130.0
674.	C5H4OH+O2=C5H4O+HO2	3.00E+13	0.0	5000.0
675.	C5H4O+H=n-C4H5+CO	2.10E+61	-13.3	40810.0
676.	C5H4O+O=C4H4+CO2	1.00E+13	0.0	2000.0
677.	C5H4O=2C2H2+CO	1.10E+47	-9.6	99500.0
678.	C5H6+H=C5H5+H2	2.80E+13	0.0	2259.0
679.	C5H6+H=AC3H5+C2H2	6.60E+14	0.0	12345.0
680.	C5H6+OH=C5H5+H2O	3.08E+06	2.0	0.0
681.	C5H6+O=C5H5+OH	4.77E+04	2.7	1106.0
682.	C5H6+O2=C5H5+HO2	4.00E+13	0.0	37150.0
683.	C5H6+HO2=C5H5+H2O2	1.10E+04	2.6	12900.0
684.	C5H6+CH3=C5H5+CH4	1.80E-01	4.0	0.0
685.	C5H6+C2H3=C5H5+C2H4	1.20E-01	4.0	0.0
686.	C5H6+A1=C5H5+A	1.00E-01	4.0	0.0
687.	C5H6=CH2CHCHCCH2	1.35E+15	0.0	80450.0
688.	CH2CHCHCCH2=PC3H4+C2H2	2.88E+13	0.0	66550.0
689.	C5H6=C2H2+AC3H4	3.80E+17	0.0	104000.0
690.	C5H6=CH2CHCH2CCH	8.50E+14	0.0	90540.0
691.	CH2CHCH2CCH=C2H2+AC3H4	3.55E+13	0.0	63360.0
692.	C6H2+H=C6H3	4.30E+45	-10.2	13250.0
693.	C6H3+H=C4H2+C2H2	2.40E+19	-1.6	2800.0
694.	C6H3+H=l-C6H4	4.20E+44	-10.3	7890.0
695.	C6H3+H=C6H2+H2	3.00E+13	0.0	0.0
696.	C6H3+OH=C6H2+H2O	5.00E+12	0.0	0.0
697.	C6H3+O2=>CO+C3H2+HCCO	5.00E+11	0.0	0.0
698.	l-C6H4+H=n-C6H5	3.30E+44	-10.0	18800.0
699.	l-C6H4+H=A1	3.60E+77	-20.1	28100.0
700.	A1(+M)=c-C6H4+H(+M)	4.30E+12	0.6	77313.0

Low pressure limit: 0.10000E+85 -0.18866E+02 0.90064E+05

TROE centering: 0.90200E+00 0.69600E+03 0.35800E+03 0.38560E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

701. A1+H=c-C6H4+H2 2.00E+11 1.1 24500.0

702. l-C6H4+H=C6H3+H2 6.65E+06 2.5 9240.0

703. l-C6H4+OH=C6H3+H2O 3.10E+06 2.0 430.0

704. n-C6H5=A1 1.30E+62 -15.9 35800.0

705. n-C6H5=c-C6H4+H 2.70E+65 -15.9 59700.0

706. n-C6H5+H=i-C6H5+H 2.40E+11 0.8 2410.0

707. n-C6H5+H=l-C6H6 1.10E+42 -9.7 7000.0

708. i-C6H5+H=l-C6H6 4.20E+44 -10.3 7890.0

709. n-C6H5+H=l-C6H4+H2 1.50E+13 0.0 0.0

710. i-C6H5+H=l-C6H4+H2 3.00E+13 0.0 0.0

711. n-C6H5+OH=l-C6H4+H2O 2.50E+12 0.0 0.0

712. i-C6H5+OH=l-C6H4+H2O 5.00E+12 0.0 0.0

713. n-C6H5+O2=>C4H4+HCO+CO 4.16E+10 0.0 2500.0

714. i-C6H5+O2=>CH2CO+CH2CO+C2H 7.86E+16 -1.8 0.0

715. nC4H3+C2H2=n-C6H5 6.00E+33 -7.4 13700.0

716. l-C6H6+H+M=n-C6H7+M 2.90E+17 -0.5 1000.0

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

CH4 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

717. l-C6H6+H+M=CYC6H7+M 1.70E+28 -4.7 2800.0

H2 Enhanced by 2.000E+00

	H2O	Enhanced by	6.000E+00		
	CO	Enhanced by	1.500E+00		
	CO2	Enhanced by	2.000E+00		
	CH4	Enhanced by	2.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	7.000E-01		
718.	l-C6H6+H=n-C6H5+H2		6.65E+05	2.5	12240.0
719.	l-C6H6+H=i-C6H5+H2		3.33E+05	2.5	9240.0
720.	l-C6H6+OH=n-C6H5+H2O		6.20E+06	2.0	3430.0
721.	l-C6H6+OH=i-C6H5+H2O		3.10E+06	2.0	430.0
722.	n-C6H7=CYC6H7		4.10E+24	-7.1	3900.0
723.	n-C6H7=A+H		8.40E+21	-4.2	11300.0
724.	n-C6H7+H=i-C6H7+H		4.00E+41	-8.1	19200.0
725.	i-C6H7+H=C6H8		1.20E+60	-13.9	21000.0
726.	n-C6H7+H=C6H8		8.70E+69	-17.0	24000.0
727.	n-C6H7+H=l-C6H6+H2		1.50E+13	0.0	0.0
728.	i-C6H7+H=l-C6H6+H2		3.00E+13	0.0	0.0
729.	n-C6H7+OH=l-C6H6+H2O		2.50E+12	0.0	0.0
730.	i-C6H7+OH=l-C6H6+H2O		5.00E+12	0.0	0.0
731.	n-C6H7+O2=>iiiC4H6+CO+HCO		4.16E+10	0.0	2500.0
732.	i-C6H7+O2=>CH2CO+CH2CO+C2H3		7.86E+16	-1.8	0.0
733.	C6H8+H=n-C6H7+H2		1.33E+06	2.5	12240.0
734.	C6H8+H=i-C6H7+H2		6.65E+05	2.5	9240.0
735.	C6H8+OH=n-C6H7+H2O		6.20E+06	2.0	3430.0
736.	C6H8+OH=i-C6H7+H2O		3.10E+06	2.0	430.0
737.	A1+O=C5H5+CO		9.00E+13	0.0	0.0
738.	CH2SING+A=A1+CH3		1.70E+14	0.0	0.0
739.	C3H3+C3H3=C4H5C2H		6.48E+68	-16.7	2872.0
	Declared duplicate reaction...				
740.	C3H3+C3H3=C4H5C2H		1.54E+36	-7.8	5580.0
	Declared duplicate reaction...				
741.	C3H3+C3H3=FC6H6		7.25E+65	-16.0	25035.0

	Declared duplicate reaction...			
742.	C3H3+C3H3=FC6H6	4.19E+39	-9.0	6098.0
	Declared duplicate reaction...			
743.	C3H3+C3H3=A	1.64E+66	-15.9	27529.0
	Declared duplicate reaction...			
744.	C3H3+C3H3=A	1.20E+35	-7.4	5058.0
	Declared duplicate reaction...			
745.	C3H3+C3H3=A1+H	2.02E+33	-6.0	15940.0
746.	C3H3+AC3H5=FC6H6+H+H	3.26E+29	-5.4	3390.0
747.	nC4H3+C2H3=A	2.87E+14	0.0	817.0
748.	n-C4H5+C2H3=A+H2	2.80E-07	5.6	-1890.0
749.	n-C4H5+C2H3=CY13C6H8	5.50E+15	-1.7	1470.0
750.	iiiC4H6+C2H3=CY13C6H8+H	2.28E+12	-0.2	9920.0
751.	n-C4H5+C2H2=A+H	2.94E+16	-1.1	9257.0
752.	n-C4H5+C2H2=l-C6H6+H	1.14E+09	1.4	17338.0
753.	n-C4H5+C2H2=FC6H6+H	1.52E+15	-0.8	8762.0
754.	C2H2+n-C4H5=CYC6H7	2.85E+48	-12.3	15693.4
	Declared duplicate reaction...			
755.	C2H2+n-C4H5=CYC6H7	3.49E-06	4.0	-5112.0
	Declared duplicate reaction...			
756.	i-C4H5+C2H2=A+H	1.47E+23	-3.3	24907.0
757.	i-C4H5+C2H2=FC6H6+H	1.01E+34	-5.9	28786.0
758.	i-C4H5+C2H2=C4H5C2H+H	5.70E+18	-1.4	30351.0
759.	C2H2+i-C4H5=CYC6H7	1.14E+31	-9.2	19403.0
	Declared duplicate reaction...			
760.	C2H2+i-C4H5=CYC6H7	4.34E+39	-9.1	19210.0
	Declared duplicate reaction...			
761.	C5H5+CH3=FC6H6+H2	9.26E+01	2.2	8811.4
762.	FC6H6=A	5.62E+81	-19.4	121500.0
763.	FC6H6=A1+H	2.57E+97	-23.2	153470.0
764.	FC6H6+H=A+H	3.00E+12	0.5	2000.0
765.	CY13C6H8=A+H2	4.39E+37	-7.3	71949.0

766.	CY13C6H8=CYC6H7+H	2.42E+59	-13.3	96147.0
767.	CYC6H7=A+H	2.64E+59	-14.3	44929.0
768.	A=A1+H	1.35+108	-25.8	181750.0
769.	A+H=A1+H2	2.50E+14	0.0	16000.0
770.	A+OH=A1+H2O	1.63E+08	1.4	1450.0
771.	A+O2=A1+HO2	6.30E+13	0.0	60000.0
772.	A+O=A1+OH	2.00E+13	0.0	14704.0
773.	hexene1+H=hex1yl	2.92E+41	-9.3	9784.0
	Declared duplicate reaction...			
774.	hexene1+H=hex1yl	1.24E+62	-15.6	22448.0
	Declared duplicate reaction...			
775.	hexene1+H=hex2yl	1.68E+63	-15.8	21543.0
	Declared duplicate reaction...			
776.	hexene1+H=hex2yl	3.53E+47	-11.0	11174.0
	Declared duplicate reaction...			
777.	hex1yl=hex2yl	2.00E+11	0.0	11100.0
778.	hex1yl=hex3yl	2.00E+11	0.0	18100.0
779.	hex2yl+O2=>CH3CHO+IC4H8+OH	2.10E+11	0.0	6858.0
780.	hex2yl+HO2=>CH3CHO+nC4H9+OH	1.00E+13	0.0	0.0
781.	hex2yl+OH=hexene1+H2O	3.64E+13	0.0	0.0
782.	hex2yl+O=CH3CHO+nC4H9	1.61E+13	0.0	0.0
783.	hex3yl=IC4H8+C2H5	6.00E+13	0.0	29700.0
784.	hex2yl=C3H6+nC3H7	5.00E+13	0.0	28700.0
785.	hex1yl=C2H4+nC4H9	1.00E+13	0.0	28700.0
786.	hex1yl+H=hexene1+H2	1.81E+12	0.0	0.0
787.	hex2yl+O2=hexene1+HO2	3.00E+12	0.0	4500.0
788.	hex1yl+O2=hexene1+HO2	2.00E+12	0.0	2000.0
789.	hex1yl+OH=hexene1+H2O	2.43E+13	0.0	0.0
790.	hex1yl+CH3=hexene1+CH4	1.00E+12	0.0	0.0
791.	hex1yl+C2H5=hexene1+C2H6	1.00E+12	0.0	0.0
792.	hex1yl+C2H3=hexene1+C2H4	1.00E+12	0.0	0.0
793.	hex1yl+AC3H5=hexene1+C3H6	1.00E+12	0.0	0.0

794.	hex2yl+CH3=hexene1+CH4	1.00E+12	0.0	0.0
795.	hex2yl+C2H5=hexene1+C2H6	1.00E+12	0.0	0.0
796.	hex2yl+C2H3=hexene1+C2H4	1.00E+12	0.0	0.0
797.	hex2yl+AC3H5=hexene1+C3H6	1.00E+12	0.0	0.0
798.	hexene1=AC3H5+nC3H7	1.08E+80	-19.3	95177.0
799.	hexene1=C4H7+C2H5	2.71E+80	-19.3	107015.0
800.	C2H3+nC4H9=hexene1	1.00E+13	0.0	0.0
801.	hexene1+O2=C6H11-13+HO2	4.00E+12	0.0	40000.0
802.	hexene1+O2=C6H11-15+HO2	2.80E+13	0.0	48300.0
803.	hexene1+O2=C6H11-14+HO2	2.80E+13	0.0	48300.0
804.	hexene1+O2=C6H11+HO2	2.10E+13	0.0	51300.0
805.	hexene1+HO2=C6H11-14+H2O2	6.80E+12	0.0	17000.0
806.	hexene1+HO2=C6H11-15+H2O2	6.80E+12	0.0	17000.0
807.	hexene1+HO2=C6H11+H2O2	5.60E+12	0.0	19400.0
808.	hexene1+HO2=C6H11-13+H2O2	1.00E+11	0.0	17060.0
809.	hexene1+O=C6H11+OH	4.20E+02	3.5	3092.0
810.	hexene1+O=C6H11-15+OH	2.25E+03	3.3	1653.0
811.	hexene1+O=C6H11-14+OH	2.25E+03	3.3	1653.0
812.	hexene1+O=C6H11-13+OH	4.00E+13	0.0	4000.0
813.	hexene1+H=C6H11+H2	2.80E+07	2.0	7700.0
814.	hexene1+H=C6H11-15+H2	9.10E+06	0.0	5000.0
815.	hexene1+H=C6H11-14+H2	9.10E+06	0.0	5000.0
816.	hexene1+H=C6H11-13+H2	6.55E+12	0.0	4445.0
817.	hexene1+OH=C6H11+H2O	2.85E+05	2.3	236.0
818.	hexene1+OH=C6H11-15+H2O	6.35E+06	2.0	-500.0
819.	hexene1+OH=C6H11-14+H2O	6.35E+06	2.0	-500.0
820.	hexene1+OH=C6H11-13+H2O	6.00E+13	0.0	1230.0
821.	hexene1+CH3=C6H11+CH4	1.47E+12	0.0	11722.0
822.	hexene1+CH3=C6H11-15+CH4	6.60E+11	0.0	10120.0
823.	hexene1+CH3=C6H11-14+CH4	6.60E+11	0.0	10120.0
824.	hexene1+CH3=C6H11-13+CH4	2.00E+11	0.0	6800.0
825.	hexene1+C2H3=C6H11-13+C2H4	2.00E+11	0.0	6800.0

826.	hexene1+C2H3=C6H11-14+C2H4	6.60E+12	0.0	10120.0
827.	hexene1+C2H3=C6H11-15+C2H4	6.60E+12	0.0	10120.0
828.	hexene1+C2H3=C6H11+C2H4	2.94E+12	0.0	11722.0
829.	C6H11-13+H=hexene1	1.00E+13	0.0	0.0
830.	hexene1+nC3H7=C6H11-13+C3H8	1.00E+11	0.0	8300.0
831.	C6H11-13+HO2=>nC3H7+C2H3CHO+OH	1.00E+12	0.0	8000.0
832.	C6H11=C6H11-12	1.00E+11	0.0	20320.0
833.	C6H11-12=C6H11-15	2.00E+11	0.0	18100.0
834.	C6H11-12=nC3H7+AC3H4	1.00E+12	0.0	33000.0
835.	C6H11-14=C2H3+IC4H8	4.00E+13	0.0	35500.0
836.	C6H11-15=AC3H5+C3H6	4.00E+13	0.0	35500.0
837.	CYC6H12=hexene1	5.88+157	-40.2	180653.2
838.	CYC6H12+M=CYC6H11+H+M	3.00E+16	0.0	95000.0
839.	CYC6H12+O2=CYC6H11+HO2	7.50E+13	0.0	49000.0
840.	CYC6H12+HO2=CYC6H11+H2O2	1.20E+13	0.0	17057.0
841.	CYC6H12+O=CYC6H11+OH	2.60E+06	2.6	2563.0
842.	CYC6H12+H=CYC6H11+H2	6.00E+14	0.0	8373.0
843.	CYC6H12+CH3=CYC6H11+CH4	1.35E+12	0.0	9540.0
844.	CYC6H12+C2H3=CYC6H11+C2H4	1.35E+12	0.0	9540.0
845.	CYC6H12+C2H5=CYC6H11+C2H6	1.35E+12	0.0	9540.0
846.	CYC6H12+AC3H5=CYC6H11+C3H6	1.35E+12	0.0	9540.0
847.	CYC6H12+SC3H5=CYC6H11+C3H6	1.35E+12	0.0	9540.0
848.	CYC6H12+TC3H5=CYC6H11+C3H6	1.35E+12	0.0	9540.0
849.	CYC6H12+CH3O=CYC6H11+CH3OH	4.32E+11	0.0	4473.0
850.	CYC6H12+HCO=CYC6H11+CH2O	1.35E+12	0.0	9540.0
851.	CYC6H11=C6H11	1.26E+92	-24.4	54251.0
852.	CYC6H11=C6H11-13	3.40E+97	-25.6	64287.0
853.	CYC6H11=CYC6H10+H	3.93E+56	-13.8	48532.0
854.	CYC6H11=C4H7+C2H4	4.11E+70	-17.1	63299.0
855.	CYC6H11=iiiC4H6+C2H5	1.95E+89	-22.5	77468.0
856.	C6H11=C4H7+C2H4	8.13E+51	-12.2	41926.0
857.	C6H11=CYC6H10+H	1.39E+59	-15.1	40495.0

858. C6H11=C6H11-13	1.42E+80	-21.3	41217.0
859. C6H11=C2H5+iiiC4H6	5.41E+78	-19.9	59833.0
860. C6H11-13=C4H7+C2H4	8.18E+84	-21.4	72373.0
861. C6H11-13=CYC6H10+H	7.01E+83	-21.8	67519.0
862. C6H11-13=C2H5+iiiC4H6	8.36E+68	-16.6	62898.0
863. CYC6H11+O2=CYC6H10+HO2	2.40E+11	0.0	0.0
864. CYC6H11+HO2=CYC6H10+H2O2	2.00E+12	0.0	2000.0
865. CYC6H11+OH=CYC6H10+H2O	4.80E+13	0.0	0.0
866. CYC6H11+O=CYC6H10+OH	9.64E+13	0.0	0.0
867. CYC6H11+H=CYC6H10+H2	2.00E+11	0.0	0.0
868. CYC6H11+CH3=CYC6H10+CH4	4.00E+12	0.0	0.0
869. CYC6H11+HCO=CYC6H10+CH2O	4.00E+12	0.0	0.0
870. CYC6H10=iiiC4H6+C2H4	1.01E+44	-8.7	78963.0
871. CYC6H10=CY13C6H8+H2	2.26E+38	-7.4	70907.0
872. CYC6H10=CYC6H9+H	5.98E+53	-11.5	95520.0
873. CYC6H10+O2=CYC6H9+HO2	7.20E+13	0.0	34800.0
874. CYC6H10+HO2=CYC6H9+H2O2	2.00E+11	0.0	17060.0
875. CYC6H10+OH=CYC6H9+H2O	6.00E+13	0.0	300.0
876. CYC6H10+O=CYC6H9+OH	6.20E+12	0.0	4445.0
877. CYC6H10+H=CYC6H9+H2	6.20E+12	0.0	4445.0
878. CYC6H10+CH3=CYC6H9+CH4	1.65E+11	0.0	4118.0
879. CYC6H10+HCO=CYC6H9+CH2O	1.65E+11	0.0	4118.0
880. CYC6H9=CY13C6H8+H	1.62E+57	-13.0	66036.0
881. CYC6H9=C6H9	5.36E+50	-11.9	48276.0
882. CYC6H9=n-C4H5+C2H4	2.77E+73	-17.3	89006.0
883. CYC6H9=C6H8+H	4.44E+73	-17.3	89006.0
884. C6H9=CY13C6H8+H	3.21E+52	-12.5	41221.0
885. C6H9=n-C4H5+C2H4	2.45E+52	-12.1	51404.0
886. C6H9=C6H8+H	3.92E+52	-12.1	51404.0
887. CYC6H9+O2=CY13C6H8+HO2	1.60E+12	0.0	15160.0
888. CYC6H9+HO2=CY13C6H8+H2O2	1.00E+12	0.0	0.0
889. CYC6H9+OH=CY13C6H8+H2O	6.02E+12	0.0	0.0

890.	CYC6H9+O=CY13C6H8+OH	1.80E+13	0.0	0.0
891.	CYC6H9+H=CY13C6H8+H2	3.16E+13	0.0	0.0
892.	CYC6H9+CH3=CY13C6H8+CH4	8.00E+12	0.0	0.0
893.	CYC6H9+HCO=CY13C6H8+CH2O	4.00E+12	0.0	0.0
894.	CY13C6H8+O2=CYC6H7+HO2	8.31E+11	0.0	24858.0
895.	CY13C6H8+HO2=CYC6H7+H2O2	4.00E+12	0.0	17057.0
896.	CY13C6H8+OH=CYC6H7+H2O	6.00E+06	2.0	-1520.0
897.	CY13C6H8+O=CYC6H7+OH	1.40E+13	0.0	-795.0
898.	CY13C6H8+H=CYC6H7+H2	1.10E+05	2.5	-1900.0
899.	CY13C6H8+CH3=CYC6H7+CH4	1.23E+11	0.0	5201.0
900.	CY13C6H8+C2H3=CYC6H7+C2H4	1.23E+11	0.0	5201.0
901.	CY13C6H8+HCO=CYC6H7+CH2O	1.23E+11	0.0	5201.0
902.	CY13C6H8+C2H2=A+C2H4	3.10E+10	0.0	27200.0
903.	CYC6H7+O2=A+HO2	1.00E+12	0.0	0.0
904.	CYC6H7+HO2=A+H2O2	1.00E+12	0.0	0.0
905.	CYC6H7+HO2=C5H6+HCO+OH	4.50E+12	0.0	0.0
906.	CYC6H7+OH=A+H2O	6.02E+12	0.0	0.0
907.	CYC6H7+O=A+OH	1.80E+13	0.0	0.0
908.	CYC6H7+O=C5H6+HCO	8.26E+13	0.0	0.0
909.	CYC6H7+H=A+H2	3.16E+13	0.0	0.0
910.	CYC6H7+CH3=A+CH4	8.00E+12	0.0	0.0
911.	CYC6H7+HCO=A+CH2O	4.00E+12	0.0	0.0
912.	C6H11+H=C6H10+H2	1.80E+12	0.0	0.0
913.	C6H11+O2=C6H10+HO2	1.00E+11	0.0	0.0
914.	C6H11+CH3=C6H10+CH4	1.10E+13	0.0	0.0
915.	C6H11+O=C6H10+OH	4.82E+13	0.0	0.0
916.	C6H11+OH=C6H10+H2O	2.41E+13	0.0	0.0
917.	C6H10+H=C4H7+C2H4	1.46E+30	-4.3	21647.0
918.	C6H10+O=CH2CO+C4H7+H	1.20E+08	1.6	327.0
919.	C6H9+O2=C6H8+HO2	1.60E+12	0.0	5000.0
920.	C6H9+H=C6H8+H2	1.80E+12	0.0	0.0
921.	C6H9+CH3=C6H8+CH4	1.10E+13	0.0	0.0

922. C6H9+O=C6H8+OH	4.82E+13	0.0	0.0
923. C6H9+OH=C6H8+H2O	2.41E+13	0.0	0.0
924. C6H8+O=CH2CO+n-C4H5+H	1.20E+08	1.6	327.0
925. C2H5OH=CH3+CH2OH	1.26E+51	-10.6	100869.0
926. C2H5OH=C2H4+H2O	8.80E+25	-3.7	70799.0
927. C2H5OH+OH=C2H4OH+H2O	1.81E+11	0.4	716.5
928. C2H5OH+OH=CH3CHOH+H2O	3.09E+10	0.5	-379.8
929. C2H5OH+OH=C2H5O+H2O	1.05E+10	0.8	716.9
930. C2H5OH+H=C2H4OH+H2	1.90E+07	1.8	5098.0
931. C2H5OH+H=CH3CHOH+H2	2.58E+07	1.6	2827.0
932. C2H5OH+H=C2H5O+H2	1.50E+07	1.6	3038.0
933. C2H5OH+O=C2H4OH+OH	9.41E+07	1.7	5459.0
934. C2H5OH+O=CH3CHOH+OH	1.88E+07	1.9	1824.0
935. C2H5OH+O=C2H5O+OH	1.58E+07	2.0	4448.0
936. C2H5OH+CH3=C2H4OH+CH4	2.19E+02	3.2	9622.0
937. C2H5OH+CH3=CH3CHOH+CH4	7.28E+02	3.0	7948.0
938. C2H5OH+CH3=C2H5O+CH4	1.45E+02	3.0	7649.0
939. C2H5OH+HO2=CH3CHOH+H2O2	8.20E+03	2.5	10750.0
940. C2H5OH+HO2=C2H4OH+H2O2	2.43E+04	2.5	15750.0
941. C2H5OH+HO2=C2H5O+H2O2	3.80E+12	0.0	24000.0
942. C2H5O+M=CH3CHO+H+M	5.60E+34	-5.9	25274.0
943. C2H5O+M=CH3+CH2O+M	5.35E+37	-7.0	23800.0
944. C2H5O+CO=C2H5+CO2	4.68E+02	3.2	5380.0
945. C2H5O+H=CH3+CH2OH	3.00E+13	0.0	0.0
946. C2H5O+H=C2H4+H2O	3.00E+13	0.0	0.0
947. C2H5O+OH=CH3CHO+H2O	1.00E+13	0.0	0.0
948. CH3CHOH+O2=CH3CHO+HO2	4.82E+13	0.0	5017.0
Declared duplicate reaction...			
949. CH3CHOH+O2=CH3CHO+HO2	8.43E+14	-1.2	0.0
Declared duplicate reaction...			
950. CH3CHOH+O=CH3CHO+OH	1.00E+14	0.0	0.0
951. CH3CHOH+H=C2H4+H2O	3.00E+13	0.0	0.0

952.	CH3CHOH+H=CH3+CH2OH	3.00E+13	0.0	0.0
953.	CH3CHOH+HO2=CH3CHO+OH+OH	4.00E+13	0.0	0.0
954.	CH3CHOH+OH=CH3CHO+H2O	5.00E+12	0.0	0.0
955.	CH3CHOH+M=CH3CHO+H+M	1.00E+14	0.0	25000.0
956.	C2H4+OH=C2H4OH	2.41E+11	0.0	-2385.0
957.	C2H4OH+O2=HOC2H4O2	1.00E+12	0.0	-1100.0
958.	HOC2H4O2=CH2O+CH2O+OH	1.80E+11	0.0	24500.0
959.	CH3OCH3=CH3+CH3O	1.88E+49	-10.4	93453.5
960.	CH3OCH3+OH=CH3OCH2+H2O	6.71E+06	2.0	-629.9
961.	CH3OCH3+H=CH3OCH2+H2	2.97E+07	2.0	4033.6
962.	CH3OCH3+O=CH3OCH2+OH	1.86E-03	5.3	-109.0
963.	CH3OCH3+HO2=CH3OCH2+H2O2	1.68E+13	0.0	17690.0
964.	CH3OCH3+CH3=CH3OCH2+CH4	3.86E-08	6.2	2513.9
965.	CH3OCH3+O2=CH3OCH2+HO2	4.10E+13	0.0	44910.0
966.	CH3OCH3+CH3O=CH3OCH2+CH3OH	6.02E+11	0.0	4074.0
967.	CH3OCH2=CH2O+CH3	1.60E+13	0.0	25500.0
968.	CH3OCH2+CH3O=CH3OCH3+CH2O	2.41E+13	0.0	0.0
969.	CH3OCH2+CH2O=CH3OCH3+HCO	5.49E+03	2.8	5862.0
970.	CH3OCH2+O2=>CH2O+CH2O+OH	5.02E+23	-3.8	3100.0
971.	CH3OCH2+HO2=CH3OCH2O+OH	9.00E+12	0.0	0.0
972.	CH3OCH2O=CH3OCHO+H	1.74E+16	-0.7	11720.0
973.	CH3OCHO=CH3+OCHO	1.39E+18	-1.0	79140.0
974.	CH3OCHO+O2=CH3OCO+HO2	1.00E+13	0.0	49700.0
975.	CH3OCHO+OH=CH3OCO+H2O	2.34E+07	1.6	-35.0
976.	CH3OCHO+HO2=CH3OCO+H2O2	1.22E+12	0.0	17000.0
977.	CH3OCHO+O=CH3OCO+OH	2.35E+05	2.5	2230.0
978.	CH3OCHO+H=CH3OCO+H2	4.55E+06	2.0	5000.0
979.	CH3OCHO+CH3=CH3OCO+CH4	7.55E-01	3.5	5481.0
980.	CH3OCHO+CH3O=CH3OCO+CH3OH	5.48E+11	0.0	5000.0
981.	CH3OCO=CH3O+CO	7.45E+12	-1.8	17150.0
982.	CH3OCO=CH3+CO2	1.51E+12	-1.8	13820.0
983.	OCHO+M=H+CO2+M	2.44E+15	-0.5	26500.0

984.	NH+M=N+H+M	2.65E+14	0.0	75500.0
985.	NH+H=N+H2	3.20E+13	0.0	325.0
986.	NH+O=N+OH	1.70E+08	1.5	3368.0
987.	NH+OH=N+H2O	1.60E+07	1.7	-576.0
988.	NH2+M=NH+H+M	3.16E+23	-2.0	91400.0
989.	NH2+H=NH+H2	4.00E+13	0.0	3650.0
990.	NH2+O=NH+OH	7.00E+12	0.0	0.0
	Declared duplicate reaction...			
991.	NH2+O=NH+OH	8.60E-01	4.0	1673.0
	Declared duplicate reaction...			
992.	NH2+OH=NH+H2O	3.30E+06	1.9	-217.0
993.	NH2+O2=NH+HO2	1.00E+14	0.0	49997.0
994.	NH+NH=NH2+N	5.70E-01	3.9	342.0
995.	NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
996.	NH3+M=NH+H2+M	6.30E+14	0.0	93390.0
997.	NH3+H=NH2+H2	6.36E+05	2.4	10171.0
998.	NH3+O=NH2+OH	2.80E+02	3.3	4471.0
999.	NH3+OH=NH2+H2O	2.00E+06	2.0	566.0
1000.	NH2+HO2=NH3+O2	9.20E+05	1.9	-1152.0
1001.	NH3+HO2=NH2+H2O2	3.00E+11	0.0	22000.0
1002.	NH2+NH=NH3+N	9.60E+03	2.5	107.0
1003.	NH2+NH2=NH3+NH	5.60E+00	3.5	552.0
1004.	N2+M=N+N+M	1.00E+28	-3.3	225000.0
1005.	NH+N=N2+H	3.00E+13	0.0	0.0
1006.	NH+NH=N2+H+H	2.50E+13	0.0	0.0
1007.	NH2+N=N2+H+H	7.10E+13	0.0	0.0
1008.	NH+NH=N2+H2	1.00E+08	1.0	0.0
1009.	NNH=N2+H	1.00E+09	0.0	0.0
1010.	NNH+H=N2+H2	1.00E+14	0.0	0.0
1011.	NH+NH=NNH+H	5.10E+13	0.0	0.0
1012.	NNH+O=N2+OH	1.20E+13	0.1	-217.0
1013.	NNH+OH=N2+H2O	5.00E+13	0.0	0.0

1014.	NNH+O2=N2+HO2			5.60E+14	-0.4	-13.0
1015.	NNH+O2=N2+H+O2			5.00E+13	0.0	0.0
1016.	NNH+HO2=N2+H2O2			1.40E+04	2.7	-1599.0
1017.	NNH+N=NH+N2			3.00E+13	0.0	2000.0
1018.	NNH+NH=N2+NH2			5.00E+13	0.0	0.0
1019.	NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
1020.	N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
	H2O	Enhanced by	1.500E+01			
	O2	Enhanced by	2.000E+00			
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
1021.	N2H2+M=NH+NH+M			3.16E+16	0.0	99400.0
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
1022.	NH2+NH=N2H2+H			4.30E+14	-0.3	-77.0
1023.	N2H2+H=NNH+H2			8.50E+04	2.6	230.0
1024.	NH2+NH2=N2H2+H2			1.70E+08	1.6	11783.0
1025.	N2H2+O=NNH+OH			3.30E+08	1.5	496.0
1026.	N2H2+OH=NNH+H2O			5.90E+01	3.4	1360.0
1027.	N2H2+N=NNH+NH			1.00E+06	2.0	0.0
1028.	N2H2+NH=NNH+NH2			1.00E+13	0.0	6000.0
1029.	N2H2+NH2=NH3+NNH			1.80E+06	1.9	-1152.0
1030.	NNH+NNH=N2H2+N2			1.00E+13	0.0	4000.0
1031.	H2NN=NNH+H			3.40E+26	-4.8	46228.0
1032.	N2H2=H2NN			2.00E+41	-9.4	68413.0
1033.	H2NN+H=N2H2+H			7.00E+13	0.0	0.0
1034.	H2NN+H=NNH+H2			4.80E+08	1.5	-894.0
1035.	NH2+NH2=H2NN+H2			7.20E+04	1.9	8802.0
1036.	H2NN+O=OH+NNH			3.30E+08	1.5	-894.0
1037.	H2NN+OH=NNH+H2O			2.40E+06	2.0	-1192.0
1038.	H2NN+HO2=NNH+H2O2			2.90E+04	2.7	-1599.0
1039.	H2NN+NH2=NH3+NNH			1.80E+06	1.9	-1152.0

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1040. N2H3=N2H2+H                                     3.60E+47  -10.4    68970.0
1041. N2H3+M=NH2+NH+M                                 5.00E+16    0.0    60000.0
1042. NH2+NH2=N2H3+H                                  1.20E+12    0.0    10078.0
1043. N2H3+H=N2H2+H2                                  2.40E+08    1.5        0.0
1044. N2H3+H=NH+NH3                                   1.00E+11    0.0        0.0
1045. NH3+NH2=N2H3+H2                                 1.00E+11    0.5    21600.0
1046. N2H3+O=N2H2+OH                                  1.70E+08    1.5     -645.0
1047. N2H3+OH=N2H2+H2O                                1.20E+06    2.0    -1192.0
1048. N2H3+OH=H2NN+H2O                                3.00E+13    0.0        0.0
1049. N2H3+HO2=N2H2+H2O2                              1.40E+04    2.7    -1600.0
1050. N2H3+N=N2H2+NH                                  1.00E+06    2.0        0.0
1051. N2H3+NH=N2H2+NH2                                2.00E+13    0.0        0.0
1052. N2H3+NH2=N2H2+NH3                               9.20E+05    1.9    -1152.0
1053. N2H3+NH2=H2NN+NH3                               3.00E+13    0.0        0.0
1054. N2H3+NNH=N2H2+N2H2                              1.00E+13    0.0     4000.0
1055. N2H3+N2H3=NH3+NH3+N2                            3.00E+12    0.0        0.0
1056. NH2+NH2(+M)=N2H4(+M)                            5.60E+14   -0.4       66.0
      Low pressure limit:  0.16000E+35 -0.54900E+01  0.19870E+04
      TROE centering:      0.31000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1057. N2H4+M=N2H3+H+M                                 1.00E+15    0.0    63600.0
      N2              Enhanced by    2.400E+00
      NH3             Enhanced by    3.000E+00
      N2H4            Enhanced by    4.000E+00
1058. N2H4=H2NN+H2                                    5.30E+39   -8.3    69267.0
1059. N2H4+H=N2H3+H2                                  7.00E+12    0.0     2500.0
1060. N2H4+H=NH2+NH3                                  2.40E+09    0.0     3100.0
1061. N2H4+O=N2H3+OH                                  6.70E+08    1.5     2850.0
1062. N2H4+O=N2H2+H2O                                 4.40E+11    0.0    -1270.0
1063. N2H4+OH=N2H3+H2O                                4.00E+13    0.0        0.0
1064. N2H3+HO2=N2H4+O2                                9.20E+05    1.9     2125.0
1065. N2H4+N=N2H3+NH                                  1.00E+10    1.0     2000.0
1066. N2H4+NH=NH2+N2H3                                1.00E+09    1.5     2000.0
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1067.	N2H4+NH2=N2H3+NH3		3.90E+12	0.0	1500.0
1068.	N2H3+N2H2=N2H4+NNH		1.00E+13	0.0	6000.0
1069.	N2H3+N2H3=N2H4+N2H2		1.20E+13	0.0	0.0
1070.	NO+M=N+O+M		1.40E+15	0.0	148430.0
	N2	Enhanced by 1.000E+00			
	H2	Enhanced by 2.200E+00			
	H2O	Enhanced by 6.700E+00			
	CO2	Enhanced by 3.000E+00			
	N2O	Enhanced by 2.200E+00			
1071.	N+OH=NO+H		3.80E+13	0.0	0.0
1072.	NH+O=NO+H		9.20E+13	0.0	0.0
1073.	NH2+O=NO+H2		5.00E+12	0.0	0.0
1074.	NH+OH=NO+H2		2.00E+13	0.0	0.0
1075.	NO+O=O2+N		1.81E+09	1.0	38725.0
1076.	NH+O2=NO+OH		1.30E+06	1.5	100.0
1077.	N+NO=N2+O		3.30E+12	0.3	0.0
1078.	NH+NO=N2+OH		2.20E+13	-0.2	0.0
1079.	NNH+O=NH+NO		5.20E+11	0.4	-409.0
1080.	NH2+NO=N2+H2O		2.80E+20	-2.7	1258.0
1081.	NH2+NO=NNH+OH		2.29E+10	0.4	-814.0
1082.	N2H2+O=NH2+NO		1.00E+13	0.0	0.0
1083.	H2NN+O=NH2+NO		7.00E+13	0.0	0.0
1084.	H2NN+OH=>NH2+NO+H		2.00E+12	0.0	0.0
1085.	N2H3+O=>NH2+NO+H		3.00E+13	0.0	0.0
1086.	H2NN+HO2=>NH2+NO+OH		9.00E+12	0.0	0.0
1087.	NO+H(+M)=HNO(+M)		1.50E+15	-0.4	0.0
	Low pressure limit: 0.24000E+15 0.20600E+00 -0.15500E+04				
	TROE centering: 0.82000E+00 0.10000E-29 0.10000E+31 0.10000E+31				
	N2	Enhanced by 1.600E+00			
1088.	HNO+H=H2+NO		4.50E+11	0.7	655.0
1089.	NH+OH=HNO+H		3.20E+14	-0.4	-46.0
1090.	NH2+O=HNO+H		6.63E+14	-0.5	0.0

1091.	NH+H2O=HNO+H2			2.00E+13	0.0	13850.0
1092.	HNO+O=OH+NO			1.81E+13	0.0	0.0
1093.	NH+O2=HNO+O			4.60E+05	2.0	6494.0
1094.	HNO+OH=NO+H2O			3.60E+13	0.0	0.0
1095.	NH2+O2=HNO+OH			2.90E-02	3.8	18185.0
1096.	NH2+HO2=HNO+H2O			5.68E+15	-1.1	707.0
1097.	HNO+O2=NO+HO2			2.00E+13	0.0	15887.0
1098.	NH2+HNO=NH3+NO			3.60E+06	1.6	-1250.0
1099.	N2H3+O=NH2+HNO			3.00E+13	0.0	0.0
1100.	N2H3+OH=NH3+HNO			1.00E+12	0.0	15000.0
1101.	NNH+NO=N2+HNO			5.00E+13	0.0	0.0
1102.	H+NO+N2=HNO+N2			4.00E+20	-1.8	0.0
1103.	HON+M=NO+H+M			5.10E+19	-1.7	16045.0
	AR	Enhanced by	7.000E-01			
	H2O	Enhanced by	7.000E+00			
	CO2	Enhanced by	2.000E+00			
1104.	HON+H=HNO+H			2.00E+13	0.0	0.0
1105.	HON+H=OH+NH			2.00E+13	0.0	0.0
1106.	HON+O=OH+NO			7.00E+13	0.0	0.0
1107.	HNOH+M=H+HNO+M			2.00E+24	-2.8	58901.0
1108.	HNOH+H=NH2+OH			4.00E+13	0.0	0.0
1109.	HNOH+H=HNO+H2			4.80E+08	1.5	377.0
1110.	HNOH+O=HNO+OH			7.00E+13	0.0	0.0
	Declared duplicate reaction...					
1111.	HNOH+O=HNO+OH			3.30E+08	1.5	-357.0
	Declared duplicate reaction...					
1112.	HNOH+OH=HNO+H2O			2.40E+06	2.0	-1192.0
1113.	HNOH+O2=HNO+HO2			3.00E+12	0.0	25000.0
1114.	HNOH+HO2=HNO+H2O2			2.90E+04	2.7	-1599.0
1115.	HNOH+NH2=N2H3+OH			1.00E+01	3.5	-467.0
1116.	HNOH+NH2=H2NN+H2O			8.80E+16	-1.1	1113.0
1117.	HNOH+NH2=HNO+NH3			1.80E+06	1.9	-1152.0

1118.	NH2O+M=HNO+H+M		2.80E+24	-2.8	64915.0
	H2O	Enhanced by 1.000E+01			
1119.	NH2O+M=HNOH+M		1.10E+29	-4.0	44000.0
	H2O	Enhanced by 1.000E+01			
1120.	NH2O+H=NH2+OH		5.00E+13	0.0	0.0
1121.	NH2O+H=HNO+H2		3.00E+07	2.0	2000.0
1122.	NH2O+O=HNO+OH		3.00E+07	2.0	2000.0
1123.	NH2+O2=NH2O+O		2.50E+11	0.5	29570.0
1124.	NH2O+OH=HNO+H2O		2.00E+07	2.0	1000.0
1125.	NH2+HO2=NH2O+OH		5.00E+13	0.0	0.0
1126.	NH2O+O2=HNO+HO2		3.00E+12	0.0	25000.0
1127.	NH2O+HO2=HNO+H2O2		2.90E+04	2.7	-1599.0
1128.	NH2O+NH2=HNO+NH3		3.00E+12	0.0	1000.0
1129.	NH2O+NO=HNO+HNO		2.00E+04	2.0	13000.0
1130.	NH2OH(+M)=NH2+OH(+M)		1.40E+20	-1.3	64080.0
	Low pressure limit:	0.54000E+38 -0.59600E+01 0.66783E+05			
	TROE centering:	0.31000E+00 0.10000E-29 0.10000E+31 0.10000E+31			
1131.	NH2OH+H=HNOH+H2		4.80E+08	1.5	6246.0
1132.	NH2OH+H=NH2O+H2		2.40E+08	1.5	5064.0
1133.	NH2OH+O=HNOH+OH		3.30E+08	1.5	3863.0
1134.	NH2OH+O=NH2O+OH		1.70E+08	1.5	3009.0
1135.	NH2OH+OH=HNOH+H2O		1.50E+04	2.6	-3537.0
1136.	NH2OH+OH=NH2O+H2O		1.50E+05	2.3	-1296.0
1137.	NH2O+HO2=O2+NH2OH		2.90E+04	2.7	-1599.0
1138.	HNOH+HO2=NH2OH+O2		2.90E+04	2.7	-1599.0
1139.	NH2OH+HO2=HNOH+H2O2		2.90E+04	2.7	9552.0
1140.	NH2OH+HO2=NH2O+H2O2		1.40E+04	2.7	6414.0
1141.	N2H4+O=NH2OH+NH		2.90E+11	0.0	-1270.0
1142.	NH2OH+NH=HNOH+NH2		2.90E-03	4.4	1564.0
1143.	NH2OH+NH=NH2O+NH2		1.50E-03	4.6	2424.0
1144.	NH2OH+NH2=HNOH+NH3		1.10E-01	4.0	-97.0
1145.	NH2OH+NH2=NH2O+NH3		9.50E+00	3.4	-1013.0

1146.	H2NN+NH2=HNNNH2+H	7.90E+06	1.9	-1331.0
1147.	N2O(+M)=N2+O(+M)	1.30E+12	0.0	62570.0
	Low pressure limit: 0.40000E+15 0.00000E+00 0.56600E+05			
	N2 Enhanced by 1.700E+00			
	O2 Enhanced by 1.400E+00			
	CO2 Enhanced by 3.000E+00			
	H2O Enhanced by 1.200E+01			
1148.	N2O+H=N2+OH	3.30E+10	0.0	4729.0
	Declared duplicate reaction...			
1149.	N2O+H=N2+OH	4.40E+14	0.0	19254.0
	Declared duplicate reaction...			
1150.	NH+NO=N2O+H	2.90E+14	-0.4	0.0
	Declared duplicate reaction...			
1151.	NH+NO=N2O+H	-2.20E+13	-0.2	0.0
	Declared duplicate reaction...			
1152.	NNH+O=N2O+H	1.00E+14	0.0	0.0
1153.	NH2+NO=H2+N2O	1.00E+13	0.0	33700.0
1154.	NO+NO=N2O+O	3.61E+12	0.0	65335.0
	Declared duplicate reaction...			
1155.	N2O+O=NO+NO	6.62E+13	0.0	26611.0
	Declared duplicate reaction...			
1156.	N2O+O=O2+N2	1.02E+14	0.0	28001.0
1157.	N2O+OH=HNO+NO	1.20E-04	4.3	25080.0
1158.	N2O+OH=N2+HO2	1.00E+14	0.0	30000.0
1159.	NNH+O2=N2O+OH	2.90E+11	-0.3	149.0
1160.	HNO+HNO=N2O+H2O	9.00E+08	0.0	3100.0
1161.	NH+N2O=N2+HNO	2.00E+12	0.0	6000.0
1162.	N2H2+NO=N2O+NH2	3.00E+10	0.0	0.0
1163.	HNNO+M=H+N2O+M	2.20E+15	0.0	21600.0
1164.	HNNO+M=N2+OH+M	1.00E+15	0.0	25600.0
1165.	HNNO+H=H2+N2O	2.00E+13	0.0	0.0
1166.	NH2+NO=HNNO+H	8.00E+13	0.0	28000.0

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1167. NNH+HO2=HNNO+OH                                 2.40E+13    0.0     1698.0
1168. HNNO+NO=N2O+HNO                                 1.00E+12    0.0        0.0
1169. NH2+NO=NH2NO                                    3.50E+31   -6.8     3724.0
1170. NH2NO=N2+H2O                                    3.10E+34   -7.1    36262.0
1171. NH2NO+H=HNNO+H2                                 4.80E+08    1.5     7407.0
1172. N2H3+O=NH2NO+H                                  3.00E+13    0.0        0.0
1173. H2NN+OH=NH2NO+H                                 2.00E+12    0.0        0.0
1174. NH2NO+O=HNNO+OH                                 3.30E+08    1.5     4697.0
1175. NH2NO+OH=HNNO+H2O                               2.40E+06    2.0      -70.0
1176. H2NN+HO2=NH2NO+OH                               6.60E+05    1.9     7050.0
1177. NH2NO+HO2=HNNO+H2O2                             2.90E+04    2.7    12620.0
1178. NH2NO+NH2=HNNO+NH3                              1.80E+06    1.9     4538.0
1179. NH2NHO=NH2+HNO                                  2.40E+40   -8.7    41584.0
1180. NH2NHO+H=NHNHO+H2                               4.80E+08    1.5     -894.0
1181. NH2NHO+O=NHNHO+OH                               3.30E+08    1.5     -894.0
1182. NH2NHO+OH=NHNHO+H2O                             2.40E+06    2.0    -1192.0
1183. N2H3+HO2=NH2NHO+OH                              3.00E+13    0.0        0.0
1184. NH2NHO+HO2=NHNHO+H2O2                           2.90E+04    2.7    -1599.0
1185. NH2NHO+NH2=NHNHO+NH3                            1.80E+06    1.9    -1152.0
1186. NO2(+M)=NO+O(+M)                                7.60E+18   -1.3    73245.0
      Low pressure limit:  0.24700E+29 -0.33700E+01  0.74756E+05
      TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.49816E+04
      N2O             Enhanced by    1.500E+00
      H2O             Enhanced by    4.400E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    2.300E+00
      Declared duplicate reaction...
1187. NO+O(+M)=NO2(+M)                                1.30E+15   -0.8        0.0
      Low pressure limit:  0.47100E+25 -0.28700E+01  0.15510E+04
      TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.46816E+04
      Declared duplicate reaction...
1188. NO2+H=NO+OH                                     1.30E+14    0.0      357.0
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1189. NH+O2=H+NO2                                   2.30E+10    0.0     2482.0
1190. NO2+O=O2+NO                                   3.91E+12    0.0     -238.0
1191. NO2+OH=HO2+NO                                 1.81E+13    0.0     6673.0
1192. HON+O2=NO2+OH                                 1.00E+12    0.0     4968.0
1193. NO2+N=N2O+O                                   3.49E+12    0.0     -437.0
1194. NH+NO2=N2O+OH                                 4.10E+12    0.0        0.0
1195. NH+NO2=HNO+NO                                 5.90E+12    0.0        0.0
1196. NH2+NO2=N2O+H2O                               3.00E+14   -0.8      242.0
1197. NH2+NO2=NH2O+NO                               1.30E+15   -0.8      242.0
1198. H2NN+O2=NH2+NO2                               1.50E+12    0.0     5958.0
1199. HNNO+NO=NNH+NO2                               3.20E+12    0.0      270.0
1200. N2O+NO=NO2+N2                                 5.30E+05    2.2    46280.0
1201. NO+NO+NO=N2O+NO2                              1.07E+10    0.0    26800.0
1202. HNO+NO+NO=HNNO+NO2                            1.70E+11    0.0     2100.0
1203. NO2+NO2=NO+NO+O2                              1.63E+12    0.0    26108.0
1204. HONO(+M)=OH+NO(+M)                            1.20E+19   -1.2    49667.0
      Low pressure limit:  0.30100E+31 -0.38000E+01  0.50322E+05
      TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
      Declared duplicate reaction...
1205. NO+OH(+M)=HONO(+M)                            1.99E+12   -0.1     -721.0
      Low pressure limit:  0.50800E+24 -0.25100E+01 -0.68000E+02
      TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
      Declared duplicate reaction...
1206. NO2+H2=HONO+H                                 1.30E+04    2.8    29770.0
1207. HONO+H=H2O+NO                                 8.10E+06    1.9     3843.0
1208. HONO+H=OH+HNO                                 5.60E+10    0.9     4965.0
1209. HON+OH=HONO+H                                 4.00E+13    0.0        0.0
1210. HONO+O=OH+NO2                                 1.20E+13    0.0     5958.0
1211. HON+O2=HONO+O                                 1.00E+12    0.0     4965.0
1212. HONO+OH=H2O+NO2                               1.26E+10    1.0      135.0
1213. NO2+HO2=HONO+O2                               6.30E+08    1.2     5000.0
1214. NH+HONO=NH2+NO2                               1.00E+13    0.0        0.0
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1215. NH2+HONO=NH3+NO2                                7.10E+01    3.0    -4940.0
1216. HNNO+NO=N2+HONO                                 2.60E+11    0.0      810.0
1217. HNO+NO2=HONO+NO                                 4.40E+04    2.6     4040.0
1218. NH2O+NO2=HONO+HNO                               6.00E+11    0.0     2000.0
1219. HNOH+NO2=HONO+HNO                               6.00E+11    0.0     2000.0
1220. HNNO+NO2=N2O+HONO                               1.00E+12    0.0        0.0
1221. HONO+HONO=NO+NO2+H2O                            3.50E-01    3.6    12140.0
1222. HNO2(+M)=HONO(+M)                               2.50E+14    0.0    32300.0
      Low pressure limit:  0.31000E+19  0.00000E+00  0.31500E+05
      TROE centering:      0.11490E+01  0.10000E-29  0.31250E+04  0.10000E+31
1223. NO2+H2=HNO2+H                                   2.40E+00    3.7    32400.0
1224. HNO2+O=OH+NO2                                   1.70E+08    1.5     2363.0
1225. HNO2+OH=H2O+NO2                                 1.20E+06    2.0     -794.0
1226. NO2+HO2=HNO2+O2                                 1.90E+01    3.3     4983.0
1227. HNO2+NH2=NO2+NH3                                9.20E+05    1.9      874.0
1228. HNO+NO2=HNO2+NO                                 6.02E+11    0.0     1986.0
1229. NH+O2=HNOO                                      3.70E+24   -5.0     2294.0
1230. NH+O2+M=HNOO+M                                  3.00E+26   -4.0     2274.0
1231. HNOO+M=OH+NO+M                                  1.50E+36   -6.2    31119.0
1232. HNOH+HO2=HONHO+OH                               4.00E+13    0.0        0.0
1233. NH2+NO2=NH2NO2                                  3.50E+31   -6.8     3726.0
1234. NO2+O(+M)=NO3(+M)                               1.32E+13    0.0        0.0
      Low pressure limit:  0.14900E+29 -0.40800E+01  0.24660E+04
      TROE centering:      0.32600E+00  0.50000E+03  0.62049E+04  0.26060E+04
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      N2              Enhanced by    1.000E+00
      HNO3            Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
      NO3             Enhanced by    5.000E+00
1235. NO3+H=NO2+OH                                    6.00E+13    0.0        0.0
1236. NO3+O=NO2+O2                                    1.00E+13    0.0        0.0
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1237. NO3+OH=NO2+HO2 1.40E+13 0.0 0.0

1238. NO3+HO2=NO2+O2+OH 1.50E+12 0.0 0.0

1239. NO3+NH=HNO+NO2 1.50E+13 0.0 0.0

1240. NO3+NH2=NH2O+NO2 9.00E+05 0.0 100.0

1241. HNNO+NO2=NNH+NO3 1.00E+13 0.0 0.0

1242. NO2+NO2=NO3+NO 9.60E+09 0.7 20900.0

1243. NO3+NO2=NO+NO2+O2 5.00E+10 0.0 2940.0

1244. NO3+NO3=NO2+NO2+O2 5.12E+11 0.0 4870.0

1245. NO2+OH(+M)=HNO3(+M) 2.41E+13 0.0 0.0

Low pressure limit: 0.64200E+33 -0.54900E+01 0.23490E+04

TROE centering: 0.40000E+00 0.45070E+03 0.15840E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

N2 Enhanced by 1.000E+00

HNO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

1246. HNO3+H=NO3+H2 5.60E+08 1.5 16400.0

1247. HNO3+H=H2O+NO2 6.10E+01 3.3 6285.0

1248. HNO3+H=OH+HONO 3.80E+05 2.3 6976.0

1249. HNO3+H=HNO2+OH 6.00E+13 0.0 7000.0

1250. HNO3+O=OH+NO3 1.80E+07 0.0 0.0

1251. HNO3+OH=H2O+NO3 9.00E+10 0.0 0.0

1252. HNO3+OH(+M)=H2O+NO3(+M) 2.47E+08 0.0 -2860.0

Low pressure limit: 0.68900E+15 0.00000E+00 -0.14400E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

HNO3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

1253. NO3+H2O2=HNO3+HO2 1.00E+12 0.0 8500.0

1254. NO3+NH=HNO3+N 1.00E+12 0.0 5000.0

1255.	NO3+NH2=HNO3+NH	1.00E+12	0.0	10000.0
1256.	HNO3+NH=HNOH+NO2	1.50E+13	0.0	6000.0
1257.	HNO3+NH2=NO3+NH3	9.00E+05	2.0	7300.0
1258.	HNO3+NH2=NH2O+HNO2	3.00E+12	0.0	9000.0
1259.	HNO3+NH3=NH2O+H2O+NO	2.32E+01	3.5	44930.0
1260.	NH3+HNO3=H2O+NH2NO2	8.00E-01	3.5	43100.0
1261.	HONO+NO2=HNO3+NO	2.00E+11	0.0	32700.0
1262.	HONO+NO3=HNO3+NO2	1.00E+12	0.0	6000.0
1263.	HNO2+NO3=HNO3+NO2	1.00E+12	0.0	5000.0
1264.	N2O4(+M)=NO2+NO2(+M)	4.05E+18	-1.1	12840.0
	Low pressure limit: 0.19600E+29 -0.38000E+01	0.12840E+05		
1265.	N2O4+H2O=HONO+HNO3	2.52E+14	0.0	11586.0
1266.	NH+CH3=CH4+N	8.20E+05	1.9	5848.0
1267.	C2H5+N=C2H4+NH	4.30E+13	0.0	0.0
1268.	CH3+NH2=CH4+NH	2.80E+06	1.9	9205.0
1269.	CH3+NH2=CH2+NH3	1.60E+06	1.9	7566.0
1270.	CH2SING+NH3=CH3+NH2	1.00E+14	0.0	0.0
1271.	CH4+NH2=CH3+NH3	1.50E+03	3.0	9940.0
1272.	C2H+NH3=C2H2+NH2	7.20E+12	0.0	-735.0
1273.	C2H4+NH2=C2H3+NH3	5.30E+12	0.0	10274.0
1274.	C2H6+NH2=C2H5+NH3	4.50E+01	3.5	5600.0
1275.	NNH+CH3<=>CH4+N2	2.50E+13	0.0	0.0
1276.	N2H2+CH3=NNH+CH4	1.60E+06	1.9	2969.0
1277.	H2NN+CH3=CH4+NNH	1.60E+06	1.9	129.0
1278.	N2H3+CH3=N2H2+CH4	8.20E+05	1.9	1817.0
1279.	N2H3+CH3=H2NN+CH4	3.00E+13	0.0	0.0
1280.	N2H4+CH3=N2H3+CH4	3.30E+06	1.9	5322.0
1281.	CH2SING+NO=CH2+NO	1.00E+14	0.0	0.0
1282.	C+NO<=>CO+N	2.90E+13	0.0	0.0
1283.	CH+NO=HCO+N	6.80E+12	0.0	0.0
1284.	CH+NO=CO+NH	9.10E+12	0.0	0.0
1285.	CH2+NO=NH2+CO	2.30E+16	-1.4	1331.0

1286.	C2+NO=C2O+N	2.30E+13	0.0	8640.0
1287.	N+CO2<=>NO+CO	3.00E+12	0.0	11300.0
1288.	NH+CO2<=>HNO+CO	1.00E+13	0.0	14350.0
1289.	HNO+CH3=NO+CH4	8.20E+05	1.9	480.0
1290.	C2H3+NO=C2H2+HNO	1.00E+12	0.0	1000.0
1291.	HCO+NO=HNO+CO	7.23E+12	0.0	0.0
1292.	HCO+HNO=CH2O+NO	6.00E+11	0.0	2000.0
1293.	CH3O+NO=HNO+CH2O	7.50E+12	0.0	2017.0
	Declared duplicate reaction...			
1294.	CH3O+NO=HNO+CH2O	2.50E+18	-2.6	0.0
	Declared duplicate reaction...			
1295.	CH2OH+NO=CH2O+HNO	1.30E+12	0.0	0.0
1296.	CH3O+HNO=NO+CH3OH	3.20E+13	0.0	0.0
1297.	CH2OH+HNO=NO+CH3OH	3.00E+13	0.0	0.0
1298.	CH2CHO+NO=HNO+CH2CO	1.00E+12	0.0	8600.0
1299.	NH2O+CH3=CH3O+NH2	2.00E+13	0.0	0.0
1300.	NH2O+CH3=CH4+HNO	1.60E+06	1.9	2959.0
1301.	HNOH+CH3=CH4+HNO	1.60E+06	1.9	2095.0
1302.	NH2OH+CH3=HNOH+CH4	1.60E+06	1.9	6345.0
1303.	NH2OH+CH3=NH2O+CH4	8.20E+05	1.9	5491.0
1304.	CH+NO2=HCO+NO	1.01E+14	0.0	0.0
1305.	CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
1306.	NO2+CH3=NO+CH3O	1.40E+13	0.0	0.0
1307.	C2H3+NO2=NO+CH2CHO	7.70E+14	-0.6	0.0
1308.	C2H5+NO2=NO+C2H5O	4.00E+13	-0.2	0.0
1309.	CO+NO2=NO+CO2	9.04E+13	0.0	33780.0
1310.	HCO+NO2=CO+NO+OH	1.20E+23	-3.3	2355.0
1311.	HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
1312.	CH3CO+NO2=>CH3+CO2+NO	1.50E+13	0.0	0.0
1313.	CH4+NO2=HONO+CH3	6.50E+14	0.0	45800.0
1314.	C2H4+NO2=HONO+C2H3	6.50E+14	0.0	41400.0
1315.	C2H6+NO2=HONO+C2H5	6.50E+14	0.0	41400.0

1316.	HOCO+NO=CO+HONO		1.50E+12	0.0	0.0
1317.	HCO+NO2=CO+HONO		1.24E+23	-3.3	2355.0
1318.	CH2O+NO2=HCO+HONO		8.02E+02	2.8	13730.0
1319.	CH3O+NO2=CH2O+HONO		6.00E+12	0.0	2285.0
1320.	CH2OH+NO2=HONO+CH2O		5.00E+12	0.0	0.0
1321.	CH3OH+NO2=HONO+CH2OH		1.50E+02	3.3	20035.0
1322.	CH2CHO+NO2=CH2CO+HONO		8.90E+12	0.0	-159.0
1323.	CH3CHO+NO2=HONO+CH2CHO		1.30E+12	0.0	3700.0
1324.	CH4+NO2=HNO2+CH3		6.00E+14	0.0	37600.0
1325.	C2H4+NO2=HNO2+C2H3		6.00E+14	0.0	33200.0
1326.	C2H6+NO2=HNO2+C2H5		6.00E+14	0.0	33200.0
1327.	CH2O+NO2=HNO2+HCO		1.10E-01	4.2	19850.0
1328.	CH3OH+NO2=HNO2+CH2OH		2.40E+03	2.9	27470.0
1329.	CH2SING+N2O=CH2O+N2		3.80E+13	0.0	0.0
1330.	CO+N2O=N2+CO2		2.70E+11	0.0	20237.0
1331.	NH2NO+CH3=HNNO+CH4		1.60E+06	1.9	7179.0
1332.	NH2NHO+CH3=NHNHO+CH4		1.60E+06	1.9	377.0
1333.	CN+M=C+N+M		2.50E+14	0.0	141100.0
	N2	Enhanced by 1.500E+00			
	CO2	Enhanced by 2.400E+00			
1334.	CH+N=CN+H		1.70E+14	-0.1	0.0
1335.	CN+O=CO+N		1.90E+12	0.5	723.0
1336.	NO+C=CN+O		1.10E+13	0.0	0.0
1337.	CH+NO=OH+CN		3.30E+12	0.0	0.0
1338.	CN+O2=NO+CO		2.80E+17	-2.0	0.0
1339.	CN+N=C+N2		1.80E+14	0.0	0.0
1340.	CN+NO=N2+CO		3.90E+11	0.0	27820.0
1341.	C+N2O=CN+NO		4.80E+12	0.0	0.0
1342.	CN+NO2=CO+N2O		4.90E+14	-0.8	344.0
1343.	CN+NO2=N2+CO2		3.70E+14	-0.8	344.0
1344.	C2+N2=CN+CN		1.50E+13	0.0	41730.0
1345.	HCN(+M)=H+CN(+M)		8.30E+17	-0.9	123800.0

Low pressure limit: 0.35700E+27 -0.26000E+01 0.12490E+06

TROE centering: 0.73420E+00 0.11201E+04 0.10000E+06

N2O Enhanced by 5.000E+00

H2O Enhanced by 5.000E+00

N2 Enhanced by 1.000E+00

CO2 Enhanced by 1.600E+00

H2 Enhanced by 2.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

1346.	CH2+N=HCN+H	5.00E+13	0.0	0.0
1347.	CN+H2=HCN+H	3.60E+08	1.6	2999.0
1348.	CH+NH=HCN+H	3.00E+13	0.0	0.0
1349.	CH3+N=HCN+H2	3.70E+12	0.1	-89.0
1350.	C2H3+N=HCN+CH2	2.00E+13	0.0	0.0
1351.	CH4+CN=CH3+HCN	8.60E+05	2.3	-32.0
1352.	C3H3+N=HCN+C2H2	1.00E+13	0.0	0.0
1353.	C2H6+CN=C2H5+HCN	1.20E+08	1.8	-994.0
1354.	CH+N2=HCN+N	4.40E+12	0.0	21964.0
1355.	CH2+N2=HCN+NH	1.00E+13	0.0	73954.0
1356.	CH2SING+N2<=>NH+HCN	1.00E+11	0.0	65000.0
1357.	CN+NH3=HCN+NH2	9.20E+12	0.0	-357.0
1358.	HCN+N2=H+CN+N2	3.60E+26	-2.6	124890.0
1359.	HCN+O=NH+CO	3.50E+03	2.6	4980.0
1360.	HCN+O=CN+OH	4.20E+10	0.4	20663.0
1361.	HCN+OH=CN+H2O	3.90E+06	1.8	10287.0
1362.	OH+HCN=NH2+CO	7.83E-04	4.0	4000.0
1363.	HCN+O2=CN+HO2	3.00E+13	0.0	75100.0
1364.	HCCO+N=HCN+CO	5.00E+13	0.0	0.0
1365.	CH2O+CN=HCO+HCN	1.70E+03	2.7	-1427.0
1366.	CH+NO=HCN+O	5.30E+13	0.0	0.0

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1367. CH2+NO=HCN+OH                                   2.90E+14   -0.7      755.0
1368. CH2SING+NO<=>OH+HCN                             2.90E+14   -0.7      760.0
1369. CH3+NO=HCN+H2O                                  4.90E+08    0.5    12392.0
1370. C2H+NO=HCN+CO                                   6.00E+13    0.0      570.0
1371. C2H3+NO=HCN+CH2O                                7.00E+21   -3.4     1025.0
1372. HCCO+NO=HCN+CO2                                 3.70E+14   -0.8      -90.0
1373. CN+HNO=HCN+NO                                   1.80E+13    0.0        0.0
1374. CN+HONO=HCN+NO2                                 1.20E+13    0.0        0.0
1375. CH+N2O=HCN+NO                                   1.90E+13    0.0     -511.0
1376. HCN=HNC                                         1.50E+23   -4.2    49428.0
1377. HCN+M=HNC+M                                     1.60E+26   -3.2    54600.0
      AR              Enhanced by    7.000E-01
      H2O             Enhanced by    7.000E+00
      CO2             Enhanced by    2.000E+00
      Warning...superceding enhancement factor for AR
      AR              Enhanced by    7.000E-01
      Warning...superceding enhancement factor for H2O
      H2O             Enhanced by    7.000E+00
      Warning...superceding enhancement factor for CO2
      CO2             Enhanced by    2.000E+00
      Warning...superceding enhancement factor for AR
      AR              Enhanced by    7.000E-01
      Warning...superceding enhancement factor for H2O
      H2O             Enhanced by    7.000E+00
      Warning...superceding enhancement factor for CO2
      CO2             Enhanced by    2.000E+00
1378. HNC+H=HCN+H                                     7.80E+13    0.0     3600.0
1379. O+HNC=NH+CO                                     4.60E+12    0.0     2184.0
1380. HNC+OH=CN+H2O                                   1.50E+12    0.0     7680.0
1381. HNC+O2=NH+CO2                                   1.60E+19   -2.2     1777.0
1382. H+HCN(+M)<=>NCH2(+M)                            3.30E+13    0.0        0.0
      Low pressure limit:  0.14000E+27 -0.34000E+01  0.19000E+04
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H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

N2O Enhanced by 5.000E+00

N2 Enhanced by 1.000E+00

1383.	CH+NH3=NCH2+H+H	4.40E+13	0.0	-630.0
1384.	NCH2+H=HCN+H2	2.40E+08	1.5	-894.0
1385.	CH3+N=NCH2+H	6.10E+14	-0.3	288.0
1386.	CH+NH2=NCH2+H	3.00E+13	0.0	0.0
1387.	CH3+NH=NCH2+H2	3.50E+13	0.0	290.0
1388.	NCH2+CH3=HCN+CH4	8.10E+05	1.9	-1112.0
1389.	C2H5+N=CH3+NCH2	2.30E+13	0.0	0.0
1390.	NCH2+N=HCN+NH	7.20E+13	0.0	400.0
1391.	NCH2+N=N2+CH2	6.00E+13	0.0	397.0
1392.	NCH2+NH=HCN+NH2	1.70E+08	1.5	-894.0
1393.	NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0
1394.	CH2+NO=NCH2+O	8.10E+07	1.4	4111.0
1395.	NCH2+O=HCN+OH	1.70E+08	1.5	-894.0
1396.	CH3+NO=NCH2+OH	1.50E-01	3.5	3950.0
1397.	NCH2+OH=HCN+H2O	1.50E+19	-2.2	2166.0
	Declared duplicate reaction...			
1398.	NCH2+OH=HCN+H2O	1.20E+06	2.0	-1192.0
	Declared duplicate reaction...			
1399.	NCH2+O2=CH2O+NO	3.00E+12	0.0	5958.0
1400.	NCH2+O2=HCN+HO2	2.70E+04	2.0	17300.0
1401.	NCH2+HO2=HCN+H2O2	1.40E+04	2.7	-1609.0
1402.	NCH2+NO=HCN+HNO	1.00E+07	2.0	4400.0
1403.	CHNH=HCN+H	6.10E+28	-5.7	24257.0

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1404. CH3+N=CHNH+H                                    1.20E+11    0.5     -367.0
1405. CHNH+H=NCH2+H                                   2.00E+13    0.0        0.0
1406. CHNH+H=HCN+H2                                   2.40E+08    1.5     -894.0
1407. CHNH+O=HCN+OH                                   1.70E+08    1.5     -894.0
1408. CHNH+OH=HCN+H2O                                 1.20E+06    2.0    -1192.0
1409. CHNH+CH3=HCN+CH4                                8.20E+05    1.9    -1112.0
1410. CH2NH+M=HCN+H2+M                                1.00E+14    0.0    10000.0
1411. NH+CH3=CH2NH+H                                  4.00E+13    0.0        0.0
1412. CH2NH+H=NCH2+H2                                 2.40E+08    1.5     7318.0
1413. CH2NH+H=CHNH+H2                                 3.00E+08    1.5     6126.0
1414. CH+NH3=CH2NH+H                                  4.40E+13    0.0     -630.0
1415. CH2SING+NH2=CH2NH+H                             3.00E+13    0.0        0.0
1416. CH2SING+NH3=CH2NH+H+H                           1.00E+14    0.0        0.0
1417. CH3+NH2<=>CH2NH+H2                              2.40E+06    1.2    17369.0
1418. CH2NH+O=NCH2+OH                                 1.70E+08    1.5     4627.0
1419. CH2NH+O=CHNH+OH                                 2.20E+08    1.5     5402.0
1420. CH2NH+O=CH2O+NH                                 1.70E+06    2.1        0.0
1421. CH2NH+OH=NCH2+H2O                               1.20E+06    2.0      -89.0
1422. CH2NH+OH=CHNH+H2O                               2.40E+06    2.0      457.0
1423. CH2NH+OH=CH2O+NH2                               1.80E+05    2.0    14800.0
1424. NCH2+HO2=CH2NH+O2                               1.40E+04    2.7    -1609.0
1425. CH2NH+CH3=NCH2+CH4                              8.20E+05    1.9     7119.0
1426. CH2NH+CH3=CHNH+CH4                              5.30E+05    1.9     9681.0
1427. CH2NH+NH2=NCH2+NH3                              9.20E+05    1.9     4438.0
1428. CH2NH+NH2=CHNH+NH3                              1.80E+06    1.9     6087.0
1429. CH3N(+AR)<=>CH2NH(+AR)                          1.83E+13    0.2    43980.0
      Low pressure limit:  0.22300E+29 -0.44500E+01  0.46000E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
1430. CH3N(+AR)<=>NCH2+H(+AR)                         7.40E+11    0.9    35470.0
      Low pressure limit:  0.18700E+31 -0.45200E+01  0.37950E+05
      TROE centering:      0.74900E+00  0.21800E+03  0.10000E+02  0.26000E+09
1431. CH3NH=CH2NH+H                                   1.30E+42   -9.2    41316.0
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      Declared duplicate reaction...
1432. CH3NH(+AR)<=>CH2NH+H(+AR)                       7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      Declared duplicate reaction...
1433. CH3NH+M=CH3+NH+M                                1.00E+14    0.0    18000.0
1434. CH3+NH2<=>CH3NH+H                               9.08E+13   -0.4    15714.0
1435. CH3NH+H=CH2NH+H2                                7.20E+08    1.5     -894.0
1436. CH3NH+O=CH2NH+OH                                5.00E+08    1.5     -894.0
1437. CH3NH+O=CH3O+NH                                 6.00E+13    0.0        0.0
1438. CH3NH+OH=CH2NH+H2O                              3.60E+06    2.0    -1192.0
1439. CH3NH+OH=CH4+HNO                                6.00E+12    0.0        0.0
1440. HNOH+CH3=CH3NH+OH                               2.00E+13    0.0        0.0
1441. CH3NH+O2=CH2NH+HO2                              1.00E+07    2.0     6300.0
1442. CH3NH+O2=CH3O+HNO                               6.00E+12    0.0     4000.0
1443. CH3NH+CH3=CH2NH+CH4                             2.40E+06    1.9    -1112.0
1444. CH2NH2=CH2NH+H                                  2.40E+48  -10.8    52010.0
      Declared duplicate reaction...
1445. CH2NH2(+AR)<=>CH2NH+H(+AR)                      7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
      Declared duplicate reaction...
1446. CH3+NH2<=>CH2NH2+H                              5.15E+14   -0.6    10155.0
1447. CH2NH2+H=CH2NH+H2                               4.80E+08    1.5     -894.0
1448. CH2NH2+O=CH2O+NH2                               7.00E+13    0.0        0.0
1449. CH2NH2+O=CH2NH+OH                               3.30E+08    1.5     -894.0
1450. CH2NH2+OH=CH2OH+NH2                             4.00E+13    0.0        0.0
1451. CH2NH2+OH=CH2NH+H2O                             2.40E+06    2.0    -1192.0
1452. CH2NH2+O2=CH2NH+HO2                             1.00E+22   -3.1     6752.0
1453. CH2NH2+O2=NH2+CH2O+O                            6.00E+18   -1.6    30175.0
1454. CH2NH2+CH3=C2H5+NH2                             2.00E+13    0.0     2701.0
1455. CH2NH2+CH3=CH2NH+CH4                            1.60E+06    1.9     -626.0
1456. CH3+NH2<=>CH3NH2                                1.03E+33   -6.3     5750.0
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1457. CH3+NH2(+M)=CH3NH2(+M) 7.20E+12 0.4 0.0

Low pressure limit: 0.22000E+31 -0.38500E+01 0.00000E+00

1458. CH3NH2(+AR)<=>CH2NH+H2(+AR) 9.99E+08 1.2 102880.0

Low pressure limit: 0.24600E+31 -0.47500E+01 0.10700E+06

TROE centering: 0.82000E+00 0.15459E+03 0.10000E+01 0.40100E+06

1459. CH3NH2+M=CH2NH+H2+M 2.40E+13 0.0 107260.0

1460. CH3NH2(+AR)<=>CH2NH2+H(+AR) 3.93E+15 -0.1 93820.0

Low pressure limit: 0.68200E+41 -0.70100E+01 0.98400E+05

TROE centering: 0.00000E+00 0.23101E+03 0.10000E+01 0.40100E+06

1461. CH3NH2(+AR)<=>CH3NH+H(+AR) 1.44E+16 -0.3 100940.0

Low pressure limit: 0.11400E+39 -0.63500E+01 0.10500E+06

TROE centering: 0.67000E+00 0.16967E+03 0.10000E+01 0.40100E+06

1462. CH3NH2+H=CH2NH2+H2 5.60E+08 1.5 5461.0

1463. CH3NH2+H=CH3NH+H2 4.80E+08 1.5 9701.0

1464. CH3NH2+O=CH2NH2+OH 4.00E+08 1.5 5193.0

1465. CH3NH2+O=CH3NH+OH 3.30E+08 1.5 6345.0

1466. CH3NH2+OH=CH2NH2+H2O 3.60E+06 2.0 238.0

1467. CH3NH2+OH=CH3NH+H2O 2.40E+06 2.0 447.0

1468. CH3NH2+CH3=CH2NH2+CH4 1.50E+06 1.9 9163.0

1469. CH3NH2+CH3=CH3NH+CH4 1.60E+06 1.9 8837.0

1470. CH3NH2+NH2=CH2NH2+NH3 2.80E+06 1.9 5491.0

1471. CH3NH2+NH2=CH3NH+NH3 1.80E+06 1.9 7139.0

1472. CH3NCH=CH3+HCN 8.10E+15 -2.4 14942.0

1473. CH3NCH+H=CH2NCH2+H 2.00E+13 0.0 0.0

1474. CH2NCH2=CH3NCH 1.30E+45 -10.1 66111.0

1475. CH2NCH2+H=CH3+NCH2 3.00E+13 0.0 0.0

1476. CH2NCH2+O=CH2O+NCH2 3.00E+13 0.0 0.0

1477. CH2NCH2+OH=CH2OH+NCH2 2.00E+13 0.0 0.0

1478. CH2NCH2+H=CH3NCH2 5.80E+13 0.2 -125.0

1479. CH3NCH2+H=CH2NCH2+H2 5.60E+08 1.5 5464.0

1480. CH3NCH2+H=CH3NCH+H2 3.00E+08 1.5 6130.0

1481. CH3NCH2+O=CH2NCH2+OH 4.00E+08 1.5 5196.0

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1482. CH3NCH2+O=CH3NCH+OH                              2.20E+08    1.5     5404.0
1483. CH3NCH2+OH=CH2NCH2+H2O                           8.00E+12    0.0        0.0
1484. CH3NCH2+OH=CH3NCH+H2O                            2.40E+06    2.0      457.0
1485. CH3NCH2+CH3=CH2NCH2+CH4                          1.50E+06    1.9     9170.0
1486. CH3NCH2+CH3=CH3NCH+CH4                           5.30E+05    1.9     9687.0
1487. CH3NCH2+NH2=CH2NCH2+NH3                          2.80E+06    1.9     5494.0
1488. CH3NCH2+NH2=CH3NCH+NH3                           1.80E+06    1.9     6090.0
1489. CH3NCH3=CH3NCH2+H                                1.60E+15   -7.5    38425.0
1490. CH3NCH3+H=CH3NCH2+H2                             3.20E+12    0.0        0.0
1491. CH3NCH3+OH=CH3NCH2+H2O                           2.40E+13    0.0        0.0
1492. CH3NCH3+CH3=CH3NCH2+CH4                          6.00E+12    0.0        0.0
1493. CH3NHCH2=CH3+CH2NH                               9.80E+43  -10.3    37459.0
1494. CH3NHCH2=CH3NCH2+H                               5.90E+44  -10.3    46803.0
1495. CH3NHCH2+H=CH3NCH2+H2                            4.80E+08    1.5     -894.0
1496. CH3NHCH2+O=CH2O+CH3NH                            7.00E+13    0.0        0.0
1497. CH3NHCH2+O=CH3NCH2+OH                            3.30E+08    1.5     -894.0
1498. CH3NHCH2+OH=CH2OH+CH3NH                          4.00E+13    0.0        0.0
1499. CH3NHCH2+OH=CH3NCH2+H2O                          2.40E+06    2.0    -1192.0
1500. CH3NHCH2+CH3=C2H5+CH3NH                          2.00E+13    0.0     2702.0
1501. CH3NHCH2+CH3=CH3NCH2+CH4                         1.60E+06    1.9     -626.0
1502. CH3NHCH2+H(+M)=CH3NHCH3(+M)                      5.20E+17   -1.0     1580.0
      Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
      TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
1503. CH3NCH3+H=CH3NHCH3                               1.00E+12    0.0        0.0
1504. CH3NHCH3+H=CH3NHCH2+H2                           5.60E+08    1.5     5464.0
1505. CH3NHCH3+H=CH3NCH3+H2                            4.80E+08    1.5     9706.0
1506. CH3NHCH3+O=CH3NHCH2+OH                           6.10E+12    0.0      556.0
1507. CH3NHCH3+O=CH3NCH3+OH                            3.00E+12    0.0      556.0
1508. CH3NHCH3+OH=CH3NHCH2+H2O                         2.00E+13    0.0        0.0
1509. CH3NHCH3+OH=CH3NCH3+H2O                          1.90E+13    0.0        0.0
1510. CH3NHCH3+CH3=CH3NHCH2+CH4                        1.50E+06    1.9     9170.0
1511. CH3NHCH3+CH3=CH3NCH3+CH4                         1.60E+06    1.9     8842.0
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1512.	CH3NHCH3+NH2=CH3NHCH2+NH3	2.80E+06	1.9	5494.0
1513.	CH3NHCH3+NH2=CH3NCH3+NH3	1.80E+06	1.9	7143.0
1514.	CHCNH+H=CH2+HNC	1.50E+14	0.0	0.0
1515.	CHCNH+O=H+CO+HNC	1.00E+14	0.0	0.0
1516.	CHCNH+OH=HCO+CHNH	1.00E+13	0.0	0.0
1517.	CHCNH+O2=HNC+CO+OH	1.60E+11	0.0	1020.0
1518.	CHCNH+O2=HNC+HCO+O	2.20E+02	2.7	3540.0
1519.	CH2SING+HCN=CH2CN+H	1.80E+14	0.0	0.0
1520.	CH3+CN=CH2CN+H	1.00E+14	0.0	0.0
1521.	CH2CN+O=CH2O+CN	1.00E+14	0.0	0.0
1522.	CH2OH+CN=CH2CN+OH	5.00E+13	0.0	0.0
1523.	CH3CN=CH2CN+H	7.90E+14	0.0	94940.0
1524.	CH3CN+H=HCN+CH3	4.40E+10	0.8	6800.0
1525.	CH3CN+H=HNC+CH3	2.80E+15	-0.3	20030.0
1526.	CH3CN+H=CH2CN+H2	6.00E+04	3.0	8522.0
1527.	CH3CN+O=CH2CN+OH	4.70E+08	1.2	14360.0
1528.	CH3CN+OH=CH2CN+H2O	2.00E+07	2.0	2000.0
1529.	CH3CN+CH3=CH2CN+CH4	5.00E+12	0.0	7000.0
1530.	CH3CN+CN=CH2CN+HCN	5.00E+13	0.0	2000.0
1531.	c-C2H3N=CH3CN	4.70E+13	0.0	41500.0
1532.	c-C2H3N+H=CH2NCH2	9.80E+09	1.2	1969.0
1533.	c-C2H3N+H=CH2CHNH	1.10E+10	1.2	2422.0
1534.	c-C2H3N+O=>NCH2+HCO	1.00E+13	0.0	0.0
1535.	c-C2H3N+O=>C2H3+NO	1.00E+13	0.0	0.0
1536.	c-C2H3N+OH=>NCH2+CH2O	5.00E+12	0.0	0.0
1537.	CH2CHN(S)+M=CH2CHN+M	1.00E+13	0.0	0.0
	H Enhanced by 0.000E+00			
1538.	CH2CHN(S)+H=CH2CHN+H	1.00E+14	0.0	0.0
1539.	CH2CHN(S)+H=CH3+HCN	3.00E+13	0.0	0.0
1540.	CH2CHN(S)=c-C2H3N	3.00E+13	0.0	4000.0
1541.	CH2CHN(S)=CH3CN	3.00E+13	0.0	8000.0
1542.	CH2CHN(S)+O=>HCO+HCN+H	3.00E+13	0.0	0.0

1543.	CH2CHN(S)+OH=>CH2O+HCN+H	3.00E+13	0.0	0.0
1544.	CH2CNH=CH3CN	2.50E+13	0.0	70300.0
1545.	CH2CNH+H=CH3CN+H	3.00E+13	0.0	0.0
1546.	CH2CNH+H=CH3+HNC	3.30E+10	0.9	2840.0
1547.	CH2CNH+H=CHCNH+H2	3.00E+07	2.0	10000.0
1548.	CH2CNH+H=CH2CN+H2	2.40E+08	1.5	7322.0
1549.	CH2CNH+O=CH2+HNCO	1.80E+12	0.0	1350.0
1550.	CH2CNH+O=CHCNH+OH	2.00E+07	2.0	10000.0
1551.	CH2CNH+O=CH2CN+OH	1.70E+08	1.5	4630.0
1552.	CH2CNH+OH=CH2OH+HNC	1.00E+12	0.0	-1013.0
1553.	CH2CNH+OH=CHCNH+H2O	1.00E+07	2.0	3000.0
1554.	CH2CNH+OH=CH2CN+H2O	1.20E+06	2.0	-89.0
1555.	CH2CNH+CH3=CH2CN+CH4	8.20E+05	1.9	7123.0
1556.	CH2CNH+NH2=CH2CN+NH3	9.20E+05	1.9	4441.0
1557.	CH2CHN+H=CH3+HCN	1.00E+13	0.0	0.0
1558.	CH2CHN+O=CH2O+HCN	5.00E+13	0.0	0.0
1559.	CHCNH2+H=CHCNH+H2	4.80E+08	1.5	9706.0
1560.	CHCNH2+O=CHCNH+OH	3.30E+08	1.5	6348.0
1561.	CHCNH2+O=HCCO+NH2	1.40E+07	2.0	1900.0
1562.	CHCNH2+OH=CHCNH+H2O	2.00E+12	0.0	0.0
1563.	CHCNH2+CH3=CHCNH+CH4	1.60E+06	1.9	8842.0
1564.	CHCNH2+NH2=CHCNH+NH3	1.80E+06	1.9	7143.0
1565.	CH3+HCN=CH3CHN	1.00E+12	0.0	9900.0
1566.	CH3CHN+H=CH3CN+H2	2.40E+08	1.5	-894.0
1567.	CH3CHN+H=CH2CHN+H2	9.00E+13	0.0	15100.0
1568.	CH2CHN(S)+H2=CH3CHN+H	7.20E+13	0.0	0.0
1569.	CH3CHN+O=CH3CN+OH	1.70E+08	1.5	-894.0
1570.	CH3CHN+OH=CH3CN+H2O	1.20E+06	2.0	-1192.0
1571.	CH3CHN+OH=CH2CHN+H2O	1.10E+03	3.0	2780.0
1572.	CH3CHN+OH=CH2CHN(S)+H2O	4.40E+13	-0.3	-727.0
1573.	CH3CHN+NH2=CH3CN+NH3	9.20E+05	1.9	-1152.0
1574.	CH3CNH=CH3+HNC	6.50E+18	-2.5	33000.0

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1575. CH3CNH=CH3CN+H                                  7.70E+25   -5.2    24000.0
1576. CH3CNH+H=CH3+CHNH                               2.10E+13    0.0        0.0
1577. CH3CNH+H=CH2CNH+H2                              1.20E+13    0.0        0.0
1578. CH3CNH+H=CH3CN+H2                               2.40E+08    1.5     -894.0
1579. CH3CNH+O=CH2CNH+OH                              5.30E+13    0.0        0.0
1580. CH3CNH+O=CH3CN+OH                               1.70E+08    1.5     -894.0
1581. CH3CNH+OH=CH2CNH+H2O                            1.20E+13    0.0        0.0
1582. CH3CNH+OH=CH3CN+H2O                             1.20E+06    2.0    -1192.0
1583. CH3CNH+O2=CH2O+CO+NH2                           1.90E+12    0.0        0.0
1584. CH3CNH+CH3=CH2CNH+CH4                           5.30E+13    0.0        0.0
1585. CH3CNH+CH3=CH3CN+CH4                            8.20E+05    1.9    -1113.0
1586. CH2CHNH+H=CH3+CHNH                              1.00E+14    0.0        0.0
1587. CH2CHNH+H=CH3CNH+H                              3.00E+13    0.0        0.0
1588. CH2CHNH+H=CH2CNH+H2                             2.00E+13    0.0        0.0
1589. CH2CHNH+O=CH2CNH+OH                             2.00E+13    0.0        0.0
1590. CH2CHNH+OH=CH2CNH+H2O                           2.00E+13    0.0        0.0
1591. CH2CHNH+OH=CH2OH+CHNH                           1.00E+13    0.0        0.0
1592. CH2CHNH+O2=CH2O+CO+NH2                          5.70E+17   -1.8    11067.0
1593. CHCNH2+H(+M)=CH2CNH2(+M)                        1.70E+10    1.3     2709.0
      Low pressure limit:  0.63000E+32 -0.46640E+01  0.37800E+04
      TROE centering:      0.78780E+00 -0.10212E+05  0.10000E+31
      H2              Enhanced by    2.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
      H2O             Enhanced by    5.000E+00
1594. CH2CNH2+H=CHCNH2+H2                             4.50E+13    0.0        0.0
1595. CH2CNH2+O=CH2CO+NH2                             3.00E+13    0.0        0.0
1596. CH2CNH2+OH=CHCNH2+H2O                           2.00E+13    0.0        0.0
1597. CH2CNH2+O2=OCHCHO+NH2                           4.00E+12    0.0        0.0
1598. CH2CNH2+CH3=CHCNH2+CH4                          2.00E+13    0.0        0.0
1599. NH2+C2H2=CHCHNH2                                7.80E-18    8.3     7430.0
1600. CHCNH2+H(+M)=CHCHNH2(+M)                        1.70E+10    1.3     2709.0
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      Low pressure limit:  0.63000E+32 -0.46640E+01  0.37800E+04
      TROE centering:      0.78780E+00 -0.10212E+05  0.10000E+31
      H2              Enhanced by    2.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
      H2O             Enhanced by    5.000E+00
1601. CHCHNH2+H=CHCNH2+H2                             4.50E+13    0.0        0.0
1602. CHCHNH2+OH=CHCNH2+H2O                           2.00E+13    0.0        0.0
1603. CHCHNH2+O2=OCHCHO+NH2                           4.00E+12    0.0        0.0
1604. CHCHNH2+CH3=CHCNH2+CH4                          2.00E+13    0.0        0.0
1605. CH2CHNH+H=CH3CHNH                               5.80E+13    0.2     -125.0
1606. CH3+CHNH=CH3CHNH                                1.80E+13    0.0        0.0
1607. CH3CHNH+H=CH3CNH+H2                             4.70E+13   -0.3     3000.0
1608. CH3CHNH+H=CH2CHNH+H2                            1.90E+12    0.4     5359.0
1609. CH3CHNH+H=CH3CHN+H2                             2.40E+08    1.5     7322.0
1610. CH3CHNH+O=CH3CNH+OH                             1.80E+18   -1.9     2975.0
1611. CH3CHNH+O=CH2CHNH+OH                            3.70E+13   -0.2     3556.0
1612. CH3CHNH+O=CH3CHN+OH                             1.70E+08    1.5     4630.0
1613. CH3CHNH+OH=CH3CNH+H2O                           2.40E+11    0.3    -1000.0
1614. CH3CHNH+OH=CH2CHNH+H2O                          3.00E+13   -0.6      800.0
1615. CH3CHNH+OH=CH3CHN+H2O                           1.20E+06    2.0      -89.0
1616. CH3CHNH+CH3=CH3CNH+CH4                          3.90E-07    5.8     2200.0
1617. CH3CHNH+CH3=CH2CHNH+CH4                         2.50E+01    3.1     5727.0
1618. CH3CHNH+CH3=CH3CHN+CH4                          8.20E+05    1.9     7123.0
1619. CH3CHNH+NH2=CH3CHN+NH3                          9.20E+05    1.9     4441.0
1620. CHCHNH2+H(+M)=CH2CHNH2(+M)                      3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1621. CH2CNH2+H(+M)=CH2CHNH2(+M)                      3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1622. CH3CHNH=CH2CHNH2                                5.00E+18   -2.5    67995.0
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1623. CH2CHNH2+H=CHCHNH2+H2                          2.40E+02    3.6    11266.0
1624. CH2CHNH2+H=CH2CNH2+H2                          2.40E+02    3.6    11266.0
1625. CH2CHNH2+H=CH2CHNH+H2                          4.80E+08    1.5     9700.0
1626. CH3CHNH+H=CH2CHNH2+H                           3.00E+13    0.0        0.0
1627. CH2CHNH2+O=CH2CHNH+OH                          3.30E+08    1.5     6348.0
1628. CH2CHNH2+OH=CHCHNH2+H2O                        1.30E-01    4.2     -860.0
1629. CH2CHNH2+OH=CH2CNH2+H2O                        1.30E-01    4.2     -860.0
1630. CH2CHNH2+OH=CH2CHNH+H2O                        2.40E+06    2.0      447.0
1631. CH2CHNH2+CH3=CHCHNH2+CH4                       6.00E+07    1.6    16630.0
1632. CH2CHNH2+CH3=CH2CNH2+CH4                       6.00E+07    1.6    16630.0
1633. CH2CHNH2+CH3=CH2CHNH+CH4                       1.60E+06    1.9     8842.0
1634. CH2CHNH2+NH2=CHCHNH2+NH3                       5.30E+12    0.0    10274.0
1635. CH2CHNH2+NH2=CH2CNH2+NH3                       5.30E+12    0.0    10274.0
1636. CH2CHNH2+NH2=CH2CHNH+NH3                       1.80E+06    1.9     7143.0
1637. CH3CH2NH=CH2NH+CH3                             1.90E+10    0.0    23500.0
1638. CH3CH2NH=CH3CHNH+H                             1.60E+36   -7.9    36342.0
1639. CH3CH2NH+H=CH3+CH2NH2                          1.40E+12    0.7      346.0
1640. CH3CH2NH+H=CH3CHNH+H2                          7.20E+08    1.5     -894.0
1641. CH3CH2NH+O=CH3CHNH+OH                          5.00E+08    1.5     -894.0
1642. CH3CH2NH+OH=CH3CHNH+H2O                        3.60E+06    2.0    -1192.0
1643. CH3CH2NH+CH3=CH3CHNH+CH4                       2.40E+06    1.9    -1113.0
1644. CH2CHNH2+H(+M)=CH3CHNH2(+M)                    1.40E+09    1.5     1355.0
      Low pressure limit:  0.20000E+40 -0.66420E+01  0.57690E+04
      TROE centering:     -0.56900E+00  0.29900E+03  0.91470E+04  0.15240E+03
1645. CH3CHNH2=CH3CHNH+H                             1.10E+45  -10.2    47817.0
1646. CH3CHNH2+H=CH2CHNH2+H2                         4.90E+08    1.7      588.0
1647. CH3CHNH2+H=CH3+CH2NH2                          8.40E+16   -0.9     2903.0
1648. CH3CHNH2+H=C2H4+NH3                            4.70E+21   -3.0     2845.0
1649. CH3CHNH2+H=C2H5+NH2                            2.00E+13    0.0        0.0
1650. CH3CHNH2+O=CH2CHNH2+OH                         2.50E+13    0.0        0.0
1651. CH3CHNH2+OH=CH2CHNH2+H2O                       2.40E+13    0.0        0.0
1652. CH3CHNH2+O2=CH2CHNH2+HO2                       6.70E+20   -3.0     2504.0
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1653.	CH3CHNH2+CH3=CH2CHNH2+CH4	1.80E+13	0.0	-769.0
1654.	C2H4+NH2=CH2CH2NH2	1.20E+11	0.0	3955.0
1655.	CH2CH2NH2+H=CH2CHNH2+H2	1.80E+12	0.0	0.0
1656.	CH2CH2NH2+O=CH2O+CH2NH2	9.60E+13	0.0	0.0
1657.	CH2CH2NH2+OH=CH2CHNH2+H2O	2.40E+13	0.0	0.0
1658.	CH2CH2NH2+HO2=>CH2O+OH+CH2NH2	2.40E+13	0.0	0.0
1659.	CH2CH2NH2+O2=CH2CHNH2+HO2	3.70E+16	-1.6	3418.0
1660.	CH2CH2NH2+CH3=CH2CHNH2+CH4	1.20E+13	-0.3	0.0
1661.	CH3CH2NH2=C2H4+NH3	6.20E+67	-15.9	99348.0
1662.	C2H5+NH2(+M)=CH3CH2NH2(+M)	7.20E+12	0.4	0.0
	Low pressure limit: 0.22000E+31 -0.38500E+01	0.00000E+00		
1663.	CH3CHNH2+H=CH3CH2NH2	1.70E+13	0.2	0.0
1664.	CH2CH2NH2+H=CH3CH2NH2	5.40E+13	0.2	0.0
1665.	CH3CH2NH2+H=CH2CH2NH2+H2	1.20E+07	1.8	5100.0
1666.	CH3CH2NH2+H=CH3CHNH2+H2	2.60E+07	1.6	2830.0
1667.	CH3CH2NH2+H=CH3CH2NH+H2	4.80E+08	1.5	9700.0
1668.	CH3CH2NH2+O=CH2CH2NH2+OH	9.40E+07	1.7	5460.0
1669.	CH3CH2NH2+O=CH3CHNH2+OH	6.80E+12	0.0	1275.0
1670.	CH3CH2NH2+O=CH3CH2NH+OH	3.30E+08	1.5	6348.0
1671.	CH3CH2NH2+OH=CH2CH2NH2+H2O	1.60E+12	0.0	1300.0
1672.	CH3CH2NH2+OH=CH3CHNH2+H2O	1.40E+13	0.0	0.0
1673.	CH3CH2NH2+OH=CH3CH2NH+H2O	2.40E+06	2.0	447.0
1674.	CH3CH2NH2+HO2=CH2CH2NH2+H2O2	1.20E+04	2.5	15750.0
1675.	CH3CH2NH2+HO2=CH3CHNH2+H2O2	8.20E+03	2.5	10750.0
1676.	CH3CH2NH2+CH3=CH2CH2NH2+CH4	2.20E+02	3.2	9620.0
1677.	CH3CH2NH2+CH3=CH3CHNH2+CH4	7.30E+02	3.0	7950.0
1678.	CH3CH2NH2+CH3=CH3CH2NH+CH4	1.60E+06	1.9	8842.0
1679.	CH3CH2NH2+NH2=CH2CH2NH2+NH3	2.20E+02	3.2	9620.0
1680.	CH3CH2NH2+NH2=CH3CHNH2+NH3	7.30E+02	3.0	7950.0
1681.	CH3CH2NH2+NH2=CH3CH2NH+NH3	1.80E+06	1.9	7140.0
1682.	CH2CH2NH2+HCO=CH3CH2NH2+CO	6.00E+13	0.0	0.0
1683.	CH3CHNH2+HCO=CH3CH2NH2+CO	1.20E+14	0.0	0.0

1684. CH+N2=NCN+H 3.70E+07 1.4 20723.0

1685. H+NCN=HCN+N 1.89E+14 0.0 8425.0

1686. NCN+O=CN+NO 1.00E+14 0.0 0.0

1687. NCN+OH=HCN+NO 5.00E+13 0.0 0.0

1688. NCN+N=CN+N2 2.00E+13 0.0 0.0

1689. CN+N2O=NCN+NO 3.80E+03 2.6 3700.0

1690. CH+N2=HCNN 3.60E+28 -5.8 2621.0

1691. HCNN+H<=>CH2+N2 1.00E+14 0.0 0.0

1692. HCNN+O<=>CO+H+N2 2.20E+13 0.0 0.0

1693. HCNN+O<=>HCN+NO 2.00E+12 0.0 0.0

1694. HCNN+OH<=>H+HCO+N2 1.20E+13 0.0 0.0

1695. HCNN+O2=H+CO2+N2 4.00E+12 0.0 0.0

1696. HCNN+O2=HCO+N2O 4.00E+12 0.0 0.0

1697. HCNN+O2<=>O+HCO+N2 1.20E+13 0.0 0.0

1698. CH2+N2=CH2NN 1.60E+32 -7.1 19958.0

1699. CH3NN+M=CH3+N2+M 1.00E+11 0.0 5900.0

1700. CH3NNH(+AR)<=>CH3+NNH(+AR) 3.30E+16 -0.1 55000.0

Low pressure limit: 0.18800E+32 -0.45500E+01 0.57500E+05

TROE centering: 0.97000E+00 0.25059E+03 0.10000E+01 0.40100E+06

1701. NCCN+M=CN+CN+M 1.10E+34 -4.3 130079.0

N2 Enhanced by 1.500E+00

O2 Enhanced by 1.500E+00

H2 Enhanced by 1.500E+00

H2O Enhanced by 1.000E+01

CO2 Enhanced by 3.000E+00

1702. CN+HCN=NCCN+H 1.50E+07 1.7 1529.0

1703. HNC+CN=NCCN+H 1.00E+13 0.0 0.0

1704. CH3NNCH3=CH3NN+CH3 6.92E+15 0.0 50875.0

1705. CH3NNCH3=C2H6+N2 2.00E+11 0.0 33000.0

1706. NCO+M=N+CO+M 2.20E+14 0.0 54050.0

N2 Enhanced by 1.500E+00

Warning...superceding enhancement factor for N2

	N2 Enhanced by 1.500E+00			
1707.	CN+OH=NCO+H	4.00E+13	0.0	0.0
1708.	CH+NO=H+NCO	2.00E+13	0.0	0.0
1709.	HCN+O=NCO+H	1.40E+04	2.6	4980.0
1710.	HNC+O=H+NCO	1.60E+01	3.1	-224.0
1711.	NCO+H=NH+CO	5.20E+13	0.0	0.0
1712.	CN+O2=NCO+O	7.20E+12	0.0	-417.0
	Declared duplicate reaction...			
1713.	CN+O2=NCO+O	-2.80E+17	-2.0	0.0
	Declared duplicate reaction...			
1714.	NCO+O=NO+CO	2.00E+15	-0.5	0.0
1715.	NCO+O=N+CO2	8.00E+12	0.0	2502.0
1716.	NCO+OH=HON+CO	5.30E+12	-0.1	5124.0
1717.	NCO+OH=H+CO+NO	8.30E+12	-0.1	18032.0
1718.	NCO+O2=NO+CO2	2.00E+12	0.0	20000.0
1719.	CH3CN+O=CH3+NCO	6.00E+09	1.8	8130.0
1720.	CH3NCH+O=>CH3+NCO+H	7.00E+13	0.0	0.0
1721.	C2H2+NCO=HCCO+HCN	1.40E+12	0.0	1815.0
1722.	CN+CO2=NCO+CO	3.67E+06	2.2	26900.0
1723.	C2O+NO=CO+NCO	1.00E+14	0.0	670.0
1724.	C2O+NO2=CO2+NCO	5.10E+13	0.0	125.0
1725.	NCO+N=N2+CO	2.00E+13	0.0	0.0
1726.	CN+NO=NCO+N	9.60E+13	0.0	42100.0
1727.	CN+NO2=NCO+NO	5.30E+15	-0.8	344.0
1728.	NCO+NO=N2+CO2	1.50E+21	-2.7	1824.0
1729.	NCO+NO=N2O+CO	4.00E+19	-2.2	1743.0
1730.	NCN+O2=NO+NCO	4.40E+09	0.5	24580.0
1731.	N2O+NCO=CO+N2+NO	9.00E+13	0.0	27800.0
1732.	NCO+NO2=CO2+N2O	3.00E+12	0.0	-707.0
1733.	NCO+NO2=CO+NO+NO	2.10E+11	0.0	-874.0
1734.	NCCN+O=NCO+CN	4.60E+12	0.0	8877.0
1735.	CN+NCO=NCN+CO	1.80E+13	0.0	0.0

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1736. NCO+NCO=CO+CO+N2                                1.80E+13    0.0        0.0
1737. HCNO=HCN+O                                      4.20E+31   -6.1    61175.0
1738. CH2+NO=HCNO+H                                   3.80E+13   -0.4      576.0
1739. CH2SING+NO<=>H+HCNO                             3.80E+13   -0.4      580.0
1740. NCH2+O=HCNO+H                                   2.00E+13    0.0        0.0
1741. HCNO+H=HCN+OH                                   7.20E+10    0.8     8612.0
1742. HCNO+H=NH2+CO                                   1.70E+14   -0.8     2889.0
1743. HCNO+O=HCO+NO                                   6.30E+13    0.0        0.0
1744. HCNO+O=NCO+OH                                   7.00E+12    0.0        0.0
1745. HCNO+OH=HCO+HNO                                 4.50E+12    0.0        0.0
1746. HCNO+OH=CH2O+NO                                 1.00E+12    0.0        0.0
1747. HCNO+OH=NO+CO+H2                                6.50E+12    0.0        0.0
1748. HCNO+OH=NCO+H2O                                 3.50E+12    0.0        0.0
1749. HCNO+OH=NCO+H+OH                                4.50E+12    0.0        0.0
1750. NO+HCCO=HCNO+CO                                 4.60E+13    0.0      695.0
1751. HCCO+NO2=HCNO+CO2                               1.60E+13    0.0        0.0
1752. HCNO+CN=HCN+NCO                                 6.00E+13    0.0        0.0
1753. HNCO(+M)=NH+CO(+M)                              6.00E+13    0.0    99800.0
      Low pressure limit:  0.21700E+29 -0.31000E+01  0.10190E+06
      TROE centering:      0.46650E+00  0.10000E+04  0.10000E+07
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    1.600E+00
1754. HNCO+M=H+NCO+M                                  1.00E+17    0.0   112000.0
1755. HCNO+H<=>H+HNCO                                 2.10E+15   -0.7     2850.0
1756. CH2+NO=HNCO+H                                   3.10E+17   -1.4     1271.0
1757. CH2SING+NO<=>H+HNCO                             3.10E+17   -1.4     1270.0
1758. OH+HCN=HNCO+H                                   1.98E-03    4.0     1000.0
1759. OH+HNC=HNCO+H                                   2.80E+13    0.0     3694.0
1760. CHNH+O=HNCO+H                                   7.00E+13    0.0        0.0
1761. HNCO+H=NCO+H2                                   9.00E+07    1.7    13900.0
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1762.	HNCO+H=NH2+CO	3.60E+04	2.5	2343.0
1763.	HNC+O2=HNCO+O	1.50E+12	0.0	4111.0
1764.	HNCO+O=HNO+CO	1.49E+08	1.6	44010.0
1765.	HNCO+O=CO2+NH	9.80E+07	1.4	8524.0
1766.	HNCO+O=NCO+OH	2.20E+06	2.1	11430.0
1767.	HNCO+OH=NH2+CO2	6.30E+10	-0.1	11637.0
1768.	HNCO+OH=NCO+H2O	3.60E+07	1.5	3594.0
1769.	HNCO+O2=HNO+CO2	1.00E+12	0.0	35000.0
1770.	NCO+HO2=HNCO+O2	2.00E+13	0.0	0.0
1771.	HNCO+HO2=NCO+H2O2	3.00E+11	0.0	23700.0
1772.	NCO+CH4=HNCO+CH3	9.80E+12	0.0	8122.0
1773.	CH3CNH+O=CH3+HNCO	1.60E+14	0.0	0.0
1774.	CH2CNH+OH=CH3+HNCO	6.70E+11	0.0	-1013.0
1775.	C2H6+NCO=C2H5+HNCO	1.50E-09	6.9	-2910.0
1776.	NCO+HCO=HNCO+CO	3.60E+13	0.0	0.0
1777.	CH2O+NCO=HNCO+HCO	6.00E+12	0.0	0.0
1778.	CHCNH+O2=HNCO+HCO	4.90E+12	-0.1	1150.0
1779.	CH2CHN+O2=CH2O+HNCO	1.00E+12	0.0	0.0
1780.	HNCO+N=NH+NCO	2.32E+19	0.0	52500.0
1781.	HNCO+NH=NH2+NCO	3.00E+13	0.0	23700.0
1782.	NCO+NH3=HNCO+NH2	2.80E+04	2.5	983.0
1783.	NCO+HNO=HNCO+NO	1.80E+13	0.0	0.0
1784.	HNC+NO2=HNCO+NO	1.00E+12	0.0	32000.0
1785.	NCO+HONO=HNCO+NO2	3.60E+12	0.0	0.0
1786.	HNCO+NO2=HNNO+CO2	2.50E+12	0.0	26000.0
1787.	CN+HNCO=HCN+NCO	1.00E+13	0.0	0.0
1788.	HCN+OH=HOCN+H	5.90E+04	2.4	12500.0
1789.	HCNO+H=HOCN+H	1.40E+11	-0.2	2482.0
1790.	HOCN+H=HNCO+H	3.10E+08	0.8	1916.0
1791.	HOCN+H=NH2+CO	1.20E+08	0.6	2075.0
1792.	HOCN+H=H2+NCO	2.40E+08	1.5	6613.0
1793.	HOCN+O=OH+NCO	1.70E+08	1.5	4131.0

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1794. HOCN+OH=H2O+NCO                                 1.20E+06    2.0     -248.0
1795. HOCN+CH3=CH4+NCO                                8.20E+05    1.9     6613.0
1796. CH3+HOCN=CH3CN+OH                               5.00E+12    0.0     2000.0
1797. HOCN+NH2=NCO+NH3                                9.20E+05    1.9     3644.0
1798. NCCN+OH=HOCN+CN                                 2.00E+12    0.0    18985.0
1799. CH2NO=HNCO+H                                    2.30E+42   -9.1    53807.0
1800. CH2NO+H=CH3+NO                                  4.00E+13    0.0        0.0
1801. CH2NO+H=HCNO+H2                                 4.80E+08    1.5     -894.0
1802. CH2NO+O=CH2O+NO                                 7.00E+13    0.0        0.0
1803. CH2NO+O=HCNO+OH                                 3.30E+08    1.5     -894.0
1804. NCH2+HO2=CH2NO+OH                               3.00E+13    0.0        0.0
1805. CH2NO+OH=CH2OH+NO                               4.00E+13    0.0        0.0
1806. CH2NO+OH=HCNO+H2O                               2.40E+06    2.0    -1192.0
1807. CH2NO+O2=CH2O+NO2                               1.20E+15   -1.0    20117.0
1808. CH2NO+CH3=C2H5+NO                               3.00E+13    0.0        0.0
1809. CH2NO+CH3=HCNO+CH4                              1.60E+06    1.9    -1112.0
1810. CH2NO+NH2=CH2NH2+NO                             3.00E+13    0.0        0.0
1811. CH2NO+NH2=HCNO+NH3                              1.80E+06    1.9    -1152.0
1812. H2NCO(+M)=CO+NH2(+M)                            5.90E+12    0.0    25000.0
      Low pressure limit:  0.10000E+15  0.00000E+00  0.21700E+05
1813. H2NCO+H=HNCO+H2                                 3.00E+13    0.0        0.0
1814. H2NCO+O=HNCO+OH                                 3.00E+13    0.0        0.0
1815. H2NCO+OH=HNCO+H2O                               3.00E+13    0.0        0.0
1816. CH2CHNH2+O=CH3+H2NCO                            3.90E+12    0.0     1494.0
      Declared duplicate reaction...
1817. CH2CHNH2+O=CH3+H2NCO                            6.20E+13    0.0     6855.0
      Declared duplicate reaction...
1818. CH3+NO(+M)=CH3NO(+M)                            9.00E+12    0.0      192.0
      Low pressure limit:  0.25000E+17  0.00000E+00 -0.28410E+04
      TROE centering:      0.50000E+01  0.10000E-29  0.12000E+03  0.10000E+31
1819. CH3+NO=CH3NO                                    1.00E+37   -8.4     5223.0
1820. CH3NO+H=CH2NO+H2                                4.40E+08    1.5      377.0
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1821. CH3NO+H=CH3+HNO                                 1.80E+13    0.0     2780.0
1822. CH3NO+O=CH2NO+OH                                3.30E+08    1.5     3614.0
1823. CH3NO+O=CH3+NO2                                 1.70E+06    2.1        0.0
1824. CH3NO+OH=CH2NO+H2O                              3.60E+06    2.0    -1192.0
1825. CH3NO+OH=CH3+HONO                               2.50E+12    0.0      993.0
1826. CH3NO+CH3=CH2NO+CH4                             7.90E+05    1.9     5412.0
1827. CH3NCH3+O=CH3NO+CH3                             5.00E+13    0.0        0.0
1828. CH3NCH3+O2=CH3NO+CH3O                           1.00E+09    1.0     6000.0
1829. CH3NO+NH2=CH2NO+NH3                             2.80E+06    1.9     1072.0
1830. H2NCHO(+M)=CO+NH3(+M)                           1.00E+14    0.0    75514.0
      Low pressure limit:  0.83000E+15  0.00000E+00  0.49084E+05
1831. H2NCHO+M=HCO+NH2+M                              1.40E+16    0.0    72900.0
1832. H2NCHO+M=H2NCO+H+M                              4.60E+15    0.0    64200.0
1833. H2NCHO+H=H2NCO+H2                               1.30E+13    0.0     6955.0
1834. H2NCHO+H=HCO+NH3                                1.00E+13    0.0    19100.0
1835. H2NCHO+O=H2NCO+OH                               4.00E+08    1.5     5196.0
1836. CH3CHNH2+O=CH3+H2NCHO                           4.00E+13    0.0        0.0
1837. H2NCHO+OH=H2NCO+H2O                             8.00E+12    0.0        0.0
1838. CH3CHNH2+HO2=>CH3+OH+H2NCHO                     2.40E+13    0.0        0.0
1839. H2NCHO+CH3=H2NCO+CH4                            7.00E+05    2.0     9000.0
1840. H2NCHO+NH2=H2NCO+NH3                            2.00E+06    2.0     5000.0
1841. H2CNO2=CH2O+NO                                  1.00E+13    0.0    36000.0
1842. CH3O+NO(+M)=CH3ONO(+M)                          6.60E+14   -0.6        0.0
      Low pressure limit:  0.27000E+28 -0.35000E+01  0.00000E+00
1843. CH3NO2(+M)=CH3+NO2(+M)                          1.80E+16    0.0    58500.0
      Low pressure limit:  0.13000E+18  0.00000E+00  0.42000E+05
      TROE centering:      0.18320E+00  0.10000E+02  0.10000E+07
1844. CH3NO2+H=CH3+HONO                               3.30E+12    0.0     3730.0
1845. CH3NO2+H=CH3NO+OH                               1.40E+12    0.0     3730.0
1846. CH3NO2+H=H2CNO2+H2                              5.40E+02    3.5     5200.0
1847. CH3NO2+O=H2CNO2+OH                              1.50E+13    0.0     5350.0
1848. CH3NO2+OH=H2CNO2+H2O                            5.00E+05    2.0     1000.0
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1849. CH3NO2+OH=CH3OH+NO2                              2.00E+10    0.0    -1000.0
1850. CH3NO2+CH2=H2CNO2+CH3                            6.50E+12    0.0     7900.0
1851. CH3NO2+CH2SING=H2CNO2+CH3                        1.20E+14    0.0        0.0
1852. CH3NO2+CH3=H2CNO2+CH4                            5.50E-01    4.0     8300.0
1853. CN+NO(+M)=NCNO(+M)                               3.98E+13    0.0        0.0
      Low pressure limit:  0.15600E+37 -0.62000E+01  0.48780E+04
      TROE centering:      0.65080E+00  0.10000E+02  0.10000E+07
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    2.000E+00
1854. CH3O+NO2(+M)=CH3ONO2(+M)                         1.20E+13    0.0        0.0
      Low pressure limit:  0.14000E+31 -0.45000E+01  0.00000E+00
```

UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX E

THP REACTION SET

The following is the reaction set for THP combustion described in Chapter 7. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	C	O	AR
1	H	G	0	1.01E+00	200	3500	1	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0
3	O	G	0	1.60E+01	200	3500	0	0	1	0
4	O2	G	0	3.20E+01	200	3500	0	0	2	0
5	OH	G	0	1.70E+01	200	6000	1	0	1	0
6	H2O	G	0	1.80E+01	200	3500	2	0	1	0
7	HO2	G	0	3.30E+01	200	3500	1	0	2	0
8	H2O2	G	0	3.40E+01	200	3500	2	0	2	0
9	CH	G	0	1.30E+01	200	6000	1	1	0	0
10	CH2	G	0	1.40E+01	200	6000	2	1	0	0
11	CH2SING	G	0	1.40E+01	200	6000	2	1	0	0
12	CH3	G	0	1.50E+01	200	6000	3	1	0	0
13	CH4	G	0	1.60E+01	200	3500	4	1	0	0
14	CO	G	0	2.80E+01	200	3500	0	1	1	0
15	HCO	G	0	2.90E+01	200	3500	1	1	1	0
16	CH2O	G	0	3.00E+01	200	3500	2	1	1	0
17	CH2OH	G	0	3.10E+01	200	6000	3	1	1	0
18	CH3O	G	0	3.10E+01	200	6000	3	1	1	0
19	CH3OH	G	0	3.20E+01	200	3500	4	1	1	0
20	C2H	G	0	2.50E+01	200	3500	1	2	0	0
21	C2H2	G	0	2.60E+01	200	3500	2	2	0	0
22	H2CC	G	0	2.60E+01	200	6000	2	2	0	0
23	C2H3	G	0	2.70E+01	200	3500	3	2	0	0

24	C2H4	G	0	2.81E+01	200	3500	4	2	0	0
25	C2H5	G	0	2.91E+01	200	3500	5	2	0	0
26	C2H6	G	0	3.01E+01	200	3500	6	2	0	0
27	C3H2	G	0	3.80E+01	300	5000	2	3	0	0
28	C3H3	G	0	3.91E+01	200	6000	3	3	0	0
29	AR	G	0	3.99E+01	300	5000	0	0	0	1
30	AC3H4	G	0	4.01E+01	200	6000	4	3	0	0
31	PC3H4	G	0	4.01E+01	200	6000	4	3	0	0
32	HCCO	G	0	4.10E+01	300	4000	1	2	1	0
33	AC3H5	G	0	4.11E+01	300	3000	5	3	0	0
34	TC3H5	G	0	4.11E+01	300	3000	5	3	0	0
35	SC3H5	G	0	4.11E+01	300	3000	5	3	0	0
36	CH2CO	G	0	4.20E+01	200	3500	2	2	1	0
37	C3H6	G	0	4.21E+01	300	5000	6	3	0	0
38	CH3CO	G	0	4.30E+01	200	6000	3	2	1	0
39	CH2CHO	G	0	4.30E+01	300	5000	3	2	1	0
40	nC3H7	G	0	4.31E+01	300	3000	7	3	0	0
41	iC3H7	G	0	4.31E+01	300	3000	7	3	0	0
42	C2H4O	G	0	4.41E+01	300	5000	4	2	1	0
43	CH3CHO	G	0	4.41E+01	200	6000	4	2	1	0
44	C3H8	G	0	4.41E+01	300	3000	8	3	0	0
45	CO2	G	0	4.40E+01	200	3500	0	1	2	0
46	C2H5O	G	0	4.51E+01	200	6000	5	2	1	0
47	C4H	G	0	4.91E+01	300	3000	1	4	0	0
48	C2H3CO	G	0	5.51E+01	200	6000	3	3	1	0
49	C2H3CHO	G	0	5.61E+01	298	3000	4	3	1	0
50	C2H3CH2O	G	0	5.71E+01	300	3000	5	3	1	0
51	C3H6O	G	0	5.81E+01	200	6000	6	3	1	0
52	C4H2	G	0	5.01E+01	300	3000	2	4	0	0
53	iC4H3	G	0	5.11E+01	200	5000	3	4	0	0
54	nC4H3	G	0	5.11E+01	300	4000	3	4	0	0

55	C4H4	G	0	5.21E+01	300	3000	4	4	0	0
56	n-C4H5	G	0	5.31E+01	300	4000	5	4	0	0
57	i-C4H5	G	0	5.31E+01	300	4000	5	4	0	0
58	iiC4H6	G	0	5.41E+01	300	3000	6	4	0	0
59	iiiC4H6	G	0	5.41E+01	300	3000	6	4	0	0
60	C4H7	G	0	5.51E+01	300	3000	7	4	0	0
61	IC4H8	G	0	5.61E+01	300	5000	8	4	0	0
62	nC4H9	G	0	5.71E+01	200	6000	9	4	0	0
63	C5H2	G	0	6.21E+01	200	5000	2	5	0	0
64	H2CCCCCH	G	0	6.31E+01	200	5000	3	5	0	0
65	HCCCHCCH	G	0	6.31E+01	200	5000	3	5	0	0
66	C5H5	G	0	6.51E+01	300	5000	5	5	0	0
67	l-C5H5	G	0	6.51E+01	300	5000	5	5	0	0
68	H2C4O	G	0	6.61E+01	300	4000	2	4	1	0
69	C5H6	G	0	6.61E+01	300	5000	6	5	0	0
70	CH2CHCH2CCH	G	0	6.61E+01	300	5000	6	5	0	0
71	CH2CHCHCCH2	G	0	6.61E+01	300	5000	6	5	0	0
72	C6H2	G	0	7.41E+01	300	3000	2	6	0	0
73	C6H3	G	0	7.51E+01	300	3000	3	6	0	0
74	l-C6H4	G	0	7.61E+01	300	3000	4	6	0	0
75	c-C6H4	G	0	7.61E+01	300	3000	4	6	0	0
76	n-C6H5	G	0	7.71E+01	300	3000	5	6	0	0
77	i-C6H5	G	0	7.71E+01	300	3000	5	6	0	0
78	A1	G	0	7.71E+01	300	3000	5	6	0	0
79	A	G	0	7.81E+01	300	3000	6	6	0	0
80	FC6H6	G	0	7.81E+01	200	6000	6	6	0	0
81	l-C6H6	G	0	7.81E+01	300	3000	6	6	0	0
82	C4H5C2H	G	0	7.81E+01	200	5000	6	6	0	0
83	CYC6H7	G	0	7.91E+01	200	6000	7	6	0	0
84	n-C6H7	G	0	7.91E+01	300	3000	7	6	0	0
85	i-C6H7	G	0	7.91E+01	300	3000	7	6	0	0

86	C5H4O	G	0	8.01E+01	300	5000	4	5	1	0
87	C6H8	G	0	8.01E+01	300	3000	8	6	0	0
88	CY13C6H8	G	0	8.01E+01	200	6000	8	6	0	0
89	C5H5O	G	0	8.11E+01	300	5000	5	5	1	0
90	C5H4OH	G	0	8.11E+01	300	5000	5	5	1	0
91	C6H9	G	0	8.11E+01	298	3000	9	6	0	0
92	CYC6H9	G	0	8.11E+01	298	3000	9	6	0	0
93	C6H10	G	0	8.21E+01	298	3000	10	6	0	0
94	C6H11-12	G	0	8.32E+01	300	5000	11	6	0	0
95	C6H11-13	G	0	8.32E+01	300	5000	11	6	0	0
96	C6H11-14	G	0	8.32E+01	300	5000	11	6	0	0
97	C6H11-15	G	0	8.32E+01	300	5000	11	6	0	0
98	C6H11	G	0	8.32E+01	298	3000	11	6	0	0
99	hexene1	G	0	8.42E+01	200	6000	12	6	0	0
100	hex1yl	G	0	8.52E+01	200	6000	13	6	0	0
101	hex2yl	G	0	8.52E+01	200	6000	13	6	0	0
102	hex3yl	G	0	8.52E+01	300	5000	13	6	0	0
103	CH2CHCH2CH2CH2O	G	0	8.51E+01	200	5000	9	5	1	0
104	CH2CHCH2CH2OCH2	G	0	8.51E+01	200	5000	9	5	1	0
105	CH2CHCH2OCH2CH2	G	0	8.51E+01	200	5000	9	5	1	0
106	CH2CHOCH2	G	0	5.71E+01	298	3000	5	3	1	0
107	CH2CHOCH2CH2CH2	G	0	8.51E+01	200	5000	9	5	1	0
108	CH2CHOCH2CHCH2	G	0	8.41E+01	200	5000	8	5	1	0
109	OCHCH2CH2CH2CH2	G	0	8.51E+01	200	5000	9	5	1	0
110	OCHCH2CH2CHCH2	G	0	8.41E+01	200	5000	8	5	1	0
111	THP	G	0	8.61E+01	200	5000	10	5	1	0
112	THP-2-4-ene	G	0	8.21E+01	200	5000	6	5	1	0
113	THP-2-ene	G	0	8.41E+01	200	5000	8	5	1	0
114	THP-2-yl	G	0	8.51E+01	200	5000	9	5	1	0
115	THP-3-ene	G	0	8.41E+01	200	5000	8	5	1	0
116	THP-3-yl	G	0	8.51E+01	200	5000	9	5	1	0

117	THP-4-yl	G	0	8.51E+01	200	5000	9	5	1	0
118	THP-5yl	G	0	8.11E+01	200	5000	5	5	1	0
119	THP-234-enyl	G	0	8.31E+01	200	5000	7	5	1	0
120	THP-345-enyl	G	0	8.31E+01	200	5000	7	5	1	0
121	CH2CHCHCHOCH2	G	0	8.31E+01	200	5000	7	5	1	0
122	C3H5O	G	0	5.71E+01	200	6000	5	3	1	0
123	CH2CHCHCHCH2O	G	0	8.31E+01	200	5000	7	5	1	0
124	OCHCHCHCH2CH2	G	0	8.31E+01	200	5000	7	5	1	0
125	OCHCHCHCHCH2	G	0	8.21E+01	200	5000	6	5	1	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. 2O+M=O2+M			6.16E+15	-0.5	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
2. 2O+AR=O2+AR			1.89E+13	0.0	-1790.0
3. O+H+M=OH+M			4.71E+18	-1.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	7.500E-01			
4. H2+M=2H+M			4.58E+19	-1.4	104380.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
5. H2+AR=2H+AR			5.84E+18	-1.1	104380.0
6. H+OH+M=H2O+M			2.21E+22	-2.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			

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 7. H+OH+AR=H2O+AR                                  8.41E+21   -2.0        0.0
 8. H2O2(+M)=2OH(+M)                                2.95E+14    0.0    48400.0
    Low pressure limit:  0.12000E+18  0.00000E+00  0.45500E+05
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    1.600E-01
 9. H2O+O=OH+OH                                     2.97E+06    2.0    13400.0
10. O+H2=H+OH                                       5.08E+04    2.7     6290.0
11. OH+H2=H+H2O                                     2.16E+08    1.5     3430.0
12. H+O2(+M)=HO2(+M)                                1.48E+12    0.6        0.0
    Low pressure limit:  0.35000E+17 -0.41000E+00 -0.11200E+04
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    5.000E-02
13. H+O2=O+OH                                       4.49E+08    1.3    16191.0
    Declared duplicate reaction...
14. H+O2=O+OH                                       2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
15. O+HO2=OH+O2                                     3.25E+13    0.0        0.0
16. H+HO2=O2+H2                                     1.66E+13    0.0      820.0
17. H+HO2=2OH                                       7.08E+13    0.0      300.0
18. OH+HO2=O2+H2O                                   4.64E+13    0.0     -500.0
19. 2HO2=O2+H2O2                                    1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
20. 2HO2=O2+H2O2                                    4.20E+14    0.0    11980.0
    Declared duplicate reaction...
21. O+H2O2=OH+HO2                                   9.55E+06    2.0     3970.0
22. H+H2O2=HO2+H2                                   4.82E+13    0.0     7950.0
23. H+H2O2=OH+H2O                                   2.41E+13    0.0     3970.0
24. OH+H2O2=HO2+H2O                                 1.00E+12    0.0        0.0
    Declared duplicate reaction...
25. OH+H2O2=HO2+H2O                                 5.80E+14    0.0     9560.0
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    Declared duplicate reaction...
26. O+CO(+M)=CO2(+M)                                1.80E+10    0.0     2385.0
    Low pressure limit:  0.60200E+15  0.00000E+00  0.30000E+04
    H2              Enhanced by    2.000E+00
    O2              Enhanced by    6.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    3.500E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    5.000E-01
27. O2+CO=O+CO2                                     2.50E+12    0.0    47800.0
28. H2+CO(+M)=CH2O(+M)                              4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
29. OH+CO=H+CO2                                     4.10E+04    2.1    -1578.0
30. HO2+CO=OH+CO2                                   1.50E+14    0.0    23600.0
31. O+HCO=OH+CO                                     3.00E+13    0.0        0.0
32. O+HCO=H+CO2                                     3.00E+13    0.0        0.0
33. H+HCO(+M)=CH2O(+M)                              1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
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    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
34. H+HCO=H2+CO                                  7.30E+13    0.0        0.0
35. OH+HCO=H2O+CO                                3.00E+13    0.0        0.0
36. HCO+M=H+CO+M                                 1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
37. HCO+O2=HO2+CO                                4.22E+12    0.0        0.0
38. HCO+HO2=CO2+OH+H                             3.00E+13    0.0        0.0
39. O+CH2O=OH+HCO                                1.81E+13    0.0     3078.0
40. O2+CH2O=HO2+HCO                              2.05E+13    0.0    38920.0
41. H+CH2O=HCO+H2                                5.18E+07    1.7     1834.0
42. H+CH2O(+M)=CH2OH(+M)                         5.40E+11    0.5     3600.0
    Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
    TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
43. H+CH2O(+M)=CH3O(+M)                          5.40E+11    0.5     2600.0
    Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
    TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
    H2              Enhanced by    2.000E+00
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	H2O	Enhanced by	6.000E+00		
	CH4	Enhanced by	2.000E+00		
	CO	Enhanced by	1.500E+00		
	CO2	Enhanced by	2.000E+00		
	C2H6	Enhanced by	3.000E+00		
44.	OH+CH2O=HCO+H2O		3.43E+09	1.2	-447.0
45.	HO2+CH2O=HCO+H2O2		1.47E+13	0.0	15200.0
46.	O+CH2OH=OH+CH2O		4.20E+13	0.0	0.0
47.	H+CH2OH=H2+CH2O		6.00E+12	0.0	0.0
48.	H+CH2OH=OH+CH3		9.63E+13	0.0	0.0
49.	OH+CH2OH=H2O+CH2O		2.40E+13	0.0	0.0
50.	CH2OH+O2=HO2+CH2O		2.41E+14	0.0	5017.0
	Declared duplicate reaction...				
51.	CH2OH+O2=HO2+CH2O		1.51E+15	-1.0	0.0
	Declared duplicate reaction...				
52.	CH2OH+HO2=CH2O+H2O2		1.20E+13	0.0	0.0
53.	CH2OH+HCO=CH3OH+CO		1.20E+14	0.0	0.0
54.	CH2OH+HCO=CH2O+CH2O		1.80E+14	0.0	0.0
55.	2CH2OH=CH3OH+CH2O		3.00E+12	0.0	0.0
56.	CH2OH+CH3O=CH3OH+CH2O		2.40E+13	0.0	0.0
57.	O+CH3O=OH+CH2O		6.00E+12	0.0	0.0
58.	H+CH3O=H2+CH2O		2.00E+13	0.0	0.0
59.	H+CH3O=OH+CH3		3.20E+13	0.0	0.0
60.	OH+CH3O=H2O+CH2O		1.80E+13	0.0	0.0
61.	CH3O+O2=HO2+CH2O		9.03E+13	0.0	11980.0
	Declared duplicate reaction...				
62.	CH3O+O2=HO2+CH2O		2.20E+10	0.0	1748.0
	Declared duplicate reaction...				
63.	CH3O+HO2=CH2O+H2O2		3.00E+11	0.0	0.0
64.	CH3O+CO=CH3+CO2		1.57E+13	0.0	11800.0
65.	CH3O+HCO=CH3OH+CO		9.00E+13	0.0	0.0
66.	2CH3O=CH3OH+CH2O		6.00E+13	0.0	0.0

67. O+CH3OH=OH+CH2OH 3.88E+05 2.5 3080.0

68. H+CH3OH=CH2OH+H2 1.44E+13 0.0 6095.0

69. H+CH3OH=CH3O+H2 3.60E+12 0.0 6095.0

70. OH+CH3OH=CH2OH+H2O 7.10E+06 1.8 -596.0

71. OH+CH3OH=CH3O+H2O 1.00E+06 2.1 496.5

72. CH3+CH3OH=CH2OH+CH4 3.19E+01 3.2 7172.0

73. O2+CH3OH=CH2OH+HO2 2.05E+13 0.0 44900.0

74. HCO+CH3OH=CH2OH+CH2O 9.63E+03 2.9 13110.0

75. HO2+CH3OH=CH2OH+H2O2 3.98E+13 0.0 19400.0

76. CH3O+CH3OH=CH2OH+CH3OH 3.00E+11 0.0 4060.0

77. CH3OH(+M)=CH3+OH(+M) 1.90E+16 0.0 91730.0

Low pressure limit: 0.29500E+45 -0.73500E+01 0.95460E+05

TROE centering: 0.41400E+00 0.27900E+03 0.54590E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

78. CH3OH(+M)=CH2OH+H(+M) 2.69E+16 -0.1 98940.0

Low pressure limit: 0.23400E+41 -0.63300E+01 0.10310E+06

TROE centering: 0.77300E+00 0.69300E+03 0.53330E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

79. O+CH4=OH+CH3 1.02E+09 1.5 8600.0

80. H+CH4=CH3+H2 6.60E+08 1.6 10840.0

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81. OH+CH4=CH3+H2O                                    1.00E+08    1.6     3120.0
82. CH+CH4=H+C2H4                                     6.00E+13    0.0        0.0
83. CH2SING+CH4=2CH3                                  1.60E+13    0.0     -570.0
84. CH2+CH4=2CH3                                      2.46E+06    2.0     8270.0
85. O+CH3=H+CH2O                                      5.06E+13    0.0        0.0
86. O+CH3=H+H2+CO                                     3.37E+13    0.0        0.0
87. H+CH3(+M)=CH4(+M)                                 1.39E+16   -0.5      536.0
    Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
    TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
88. OH+CH3=CH2+H2O                                    5.60E+07    1.6     5420.0
89. OH+CH3=CH2SING+H2O                                6.44E+17   -1.3     1417.0
90. HO2+CH3=O2+CH4                                    1.00E+12    0.0        0.0
91. HO2+CH3=OH+CH3O                                   2.00E+13    0.0        0.0
92. CH+CH3=H+C2H3                                     3.00E+13    0.0        0.0
93. CH2SING+CH3=H+C2H4                                1.20E+13    0.0     -570.0
94. CH3+O2=O+CH3O                                     3.56E+13    0.0    30480.0
95. CH3+O2=OH+CH2O                                    2.31E+12    0.0    20315.0
96. CH3+H2O2=HO2+CH4                                  2.45E+04    2.5     5180.0
97. 2CH3(+M)=C2H6(+M)                                 6.77E+16   -1.2      654.0
    Low pressure limit:  0.34000E+42 -0.70300E+01  0.27630E+04
    TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
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     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
 98. 2CH3=H+C2H5                                  6.84E+12    0.1    10600.0
 99. CH3+HCO=CH4+CO                               1.21E+14    0.0        0.0
100. CH3+CH2O=HCO+CH4                             3.32E+03    2.8     5860.0
101. CH2+CH3=H+C2H4                               4.00E+13    0.0        0.0
102. O+CH2=H+HCO                                  8.00E+13    0.0        0.0
103. O+CH2SING=H2+CO                              1.50E+13    0.0        0.0
104. O+CH2SING=H+HCO                              1.50E+13    0.0        0.0
105. H+CH2(+M)=CH3(+M)                            6.00E+14    0.0        0.0
     Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
     TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
106. H+CH2SING=CH+H2                              3.00E+13    0.0        0.0
107. OH+CH2=H+CH2O                                2.00E+13    0.0        0.0
108. OH+CH2=CH+H2O                                1.13E+07    2.0     3000.0
109. OH+CH2SING=H+CH2O                            3.00E+13    0.0        0.0
110. HO2+CH2=OH+CH2O                              2.00E+13    0.0        0.0
111. CH+CH2=H+C2H2                                4.00E+13    0.0        0.0
112. CH2+O2=OH+H+CO                               5.00E+12    0.0     1500.0
113. CH2+O2=CO2+2H                                5.80E+12    0.0     1500.0
114. CH2+O2=O+CH2O                                2.40E+12    0.0     1500.0
115. CH2+H2=H+CH3                                 5.00E+05    2.0     7230.0
116. 2CH2=H2+C2H2                                 1.60E+15    0.0    11944.0
117. 2CH2=H+H+C2H2                                2.00E+14    0.0    10989.0
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118. CH2SING+CO=CH2+CO                                9.00E+12    0.0        0.0
119. CH2SING+AR=CH2+AR                                9.00E+12    0.0      600.0
120. CH2SING+CO2=CH2+CO2                              7.00E+12    0.0        0.0
121. CH2SING+CO2=CO+CH2O                              1.40E+13    0.0        0.0
122. CH2+CO(+M)=CH2CO(+M)                             8.10E+11    0.5     4510.0
     Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
123. CH2SING+O2=H+OH+CO                               2.80E+13    0.0        0.0
124. CH2SING+O2=CO+H2O                                1.20E+13    0.0        0.0
125. CH2SING+H2=CH3+H                                 7.00E+13    0.0        0.0
126. CH2SING+H2O(+M)=CH3OH(+M)                        4.82E+17   -1.2     1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
127. CH2SING+H2O=CH2+H2O                              3.00E+13    0.0        0.0
128. CH2SING+H2O=H2+CH2O                              6.82E+10    0.2     -935.0
129. O+CH=H+CO                                        5.70E+13    0.0        0.0
130. OH+CH=H+HCO                                      3.00E+13    0.0        0.0
131. CH+O2=O+HCO                                      6.71E+13    0.0        0.0
132. CH+H2=H+CH2                                      1.08E+14    0.0     3110.0
133. CH+H2O=H+CH2O                                    5.71E+12    0.0     -755.0
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134. CH+CO(+M)=HCCO(+M) 5.00E+13 0.0 0.0

Low pressure limit: 0.26900E+29 -0.37400E+01 0.19360E+04

TROE centering: 0.57570E+00 0.23700E+03 0.16520E+04 0.50690E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

135. CH+CO2=HCO+CO 1.90E+14 0.0 15792.0

136. CH+CH2O=H+CH2CO 9.46E+13 0.0 -515.0

137. CH+HCCO=CO+C2H2 5.00E+13 0.0 0.0

138. O+C2H6=OH+C2H5 3.00E+07 2.0 5115.0

139. H+C2H6=C2H5+H2 5.40E+02 3.5 5210.0

140. OH+C2H6=C2H5+H2O 7.26E+06 2.0 864.0

141. CH3+C2H6=C2H5+CH4 5.50E-01 4.0 8300.0

142. CH2SING+C2H6=CH3+C2H5 4.00E+13 0.0 -550.0

143. C2H6+O2=C2H5+HO2 4.04E+13 0.0 50872.0

144. C2H6+CH2OH=CH3OH+C2H5 1.99E+02 3.0 13976.0

145. C2H6+CH3O=CH3OH+C2H5 2.41E+11 0.0 7094.0

146. C2H6+C2H=C2H2+C2H5 3.61E+12 0.0 0.0

147. C2H6+C2H3=C2H4+C2H5 6.01E+02 3.3 10502.0

148. C2H6+CH3CO=CH3CHO+C2H5 1.81E+04 2.8 17527.0

149. C2H6+HCO=CH2O+C2H5 4.70E+04 2.7 18235.0

150. O+C2H5=CH3+CH2O 2.24E+13 0.0 0.0

151. O+C2H5=H+CH3CHO 1.10E+14 0.0 0.0

152. H+C2H5=H2+C2H4 2.00E+12 0.0 0.0

153. H+C2H5(+M)=C2H6(+M) 5.21E+17 -1.0 1580.0

Low pressure limit: 0.19900E+42 -0.70800E+01 0.66850E+04

TROE centering: 0.84220E+00 0.12500E+03 0.22190E+04 0.68820E+04

H2 Enhanced by 2.000E+00

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     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
154. C2H5+O2=HO2+C2H4                                1.92E+07    1.0    -2035.0
155. C2H5+HO2=C2H5O+OH                               3.00E+13    0.0        0.0
156. C2H5+HO2=C2H4+H2O2                              3.01E+11    0.0        0.0
157. C2H5+OH=C2H4+H2O                                2.41E+13    0.0        0.0
158. C2H5+CH3=CH4+C2H4                               1.13E+12   -0.5        0.0
159. CH3+C2H5(+M)=C3H8(+M)                           9.60E+14   -0.5        0.0
     Low pressure limit:  0.68000E+62 -0.13420E+02  0.60000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.14339E+04  0.53288E+04
160. C2H5+CH2OH=C2H4+CH3OH                           2.41E+12    0.0        0.0
161. C2H5+CH2OH=C2H6+CH2O                            2.41E+12    0.0        0.0
162. C2H5+CH3O=C2H6+CH2O                             2.41E+13    0.0        0.0
163. C2H5+C2H=C2H2+C2H4                              1.81E+12    0.0        0.0
164. CH2+C2H5=C2H4+CH3                               1.81E+13    0.0        0.0
165. CH2SING+C2H5=C2H4+CH3                           9.00E+12    0.0        0.0
166. C2H5+CH2SING=C3H6+H                             9.00E+12    0.0        0.0
167. C2H5+H2O2=C2H6+HO2                              8.73E+09    0.0      974.0
168. H+C2H4(+M)=C2H5(+M)                             1.37E+09    1.5     1355.0
     Low pressure limit:  0.20260E+40 -0.66420E+01  0.57690E+04
     TROE centering:     -0.56900E+00  0.29900E+03 -0.91470E+04  0.15240E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
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169. H+C2H4=C2H3+H2 1.12E+07 2.1 13366.0

170. OH+C2H4=C2H3+H2O 1.31E-01 4.2 -860.0

171. OH+C2H4=CH3+CH2O 3.19E+01 2.7 -1172.0

172. OH+C2H4=CH3CHO+H 8.73E-05 4.6 -618.0

173. CH3+C2H4=C2H3+CH4 2.27E+05 2.0 9200.0

174. CH3+C2H4(+M)<=>nC3H7(+M) 2.55E+06 1.6 5700.0

Low pressure limit: 0.30000E+64 -0.14600E+02 0.18170E+05

TROE centering: 0.18940E+00 0.27700E+03 0.87480E+04 0.78910E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

175. C2H4(+M)=H2+C2H2(+M) 8.00E+12 0.4 88770.0

Low pressure limit: 0.15800E+52 -0.93000E+01 0.97800E+05

TROE centering: 0.73450E+00 0.18000E+03 0.10350E+04 0.54170E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

176. C2H4+CH2SING=AC3H5+H 4.53E+13 0.0 -556.0

177. C2H4+HO2=C2H4O+OH 6.03E+09 0.0 7949.0

178. C2H4+O=H+CH2CHO 7.33E+07 1.6 1260.0

179. C2H4+O=CH3+HCO 1.13E+08 1.6 1020.0

180. C2H4+O=C2H3+OH 2.15E+06 2.5 11900.0

181. C2H4+O2=C2H3+HO2 4.22E+13 0.0 60800.0

182. C2H4+CO=C2H3+HCO 1.51E+14 0.0 90616.0

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183. C2H4+C2H=C4H4+H                                  1.21E+13    0.0        0.0
184. C2H4+C2H2=C2H3+C2H3                              2.41E+13    0.0    68360.0
185. C2H4+C2H4=C2H5+C2H3                              4.82E+14    0.0    71539.0
186. H+C2H3(+M)=C2H4(+M)                              6.08E+12    0.3      280.0
     Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
187. H+C2H2(+M)=C2H3(+M)                              1.71E+10    1.3     2709.0
     Low pressure limit:  0.63480E+32 -0.46639E+01  0.37800E+04
     TROE centering:      0.00000E+00  0.78784E+05 -0.10210E+05  0.10000E-29
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
188. H+C2H3=H2+C2H2                                   9.64E+13    0.0        0.0
189. OH+C2H3=H2O+C2H2                                 5.00E+12    0.0        0.0
190. C2H3+O2=C2H2+HO2                                 1.34E+06    1.6     -383.0
     Declared duplicate reaction...
191. C2H3+O2=C2H2+HO2                                 1.37E+02    3.4     3663.0
     Declared duplicate reaction...
192. C2H3+O2=HCO+CH2O                                 9.33E+13   -0.7      268.7
193. C2H3+O2=H+CO+CH2O                                2.19E+14   -0.7      268.7
194. C2H3+O2=CH2CHO+O                                 7.52E+08    1.0     -137.4
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195. C2H3+HO2=OH+CH2CO+H                              3.01E+13    0.0        0.0
196. C2H3+CH3=C2H2+CH4                               3.92E+11    0.0        0.0
197. C2H3+O=CH2CO+H                                  1.00E+14    0.0        0.0
198. C2H3+CH2OH=C2H4+CH2O                            3.01E+13    0.0        0.0
199. C2H3+CH3O=C2H4+CH2O                             2.41E+13    0.0        0.0
200. C2H3+CH3OH=C2H4+CH3O                            1.44E+01    3.1     6935.0
201. C2H3+CH3OH=C2H4+CH2OH                           3.19E+01    3.2     7172.0
202. C2H3+CO=C2H3CO                                  1.51E+11    0.0     4809.0
203. C2H3+C2H=C4H4                                   1.00E+14    0.0        0.0
204. C2H3+C2H=C2H2+C2H2                              9.64E+11    0.0        0.0
205. C2H3+CH3CO=C2H3CO+CH3                           1.81E+13    0.0        0.0
206. C2H5+C2H3=AC3H5+CH3                             8.00E+25   -3.5    11775.0
207. C2H3+C2H5(+M)=IC4H8(+M)                         1.50E+13    0.0        0.0
     Low pressure limit:  0.15500E+57 -0.11790E+02  0.89845E+04
     TROE centering:      0.19800E+00  0.22779E+04  0.60000E+05  0.57232E+04
208. C2H3+C2H5=C2H2+C2H6                             4.82E+11    0.0        0.0
209. C2H3+CH2SING=C2H2+CH3                           1.81E+13    0.0        0.0
210. C2H3+CH2=C2H2+CH3                               1.81E+13    0.0        0.0
211. C2H3+H2O2=C2H4+HO2                              1.21E+10    0.0     -596.0
212. C2H3+CH2O=C2H4+HCO                              5.43E+03    2.8     5862.0
213. C2H3+CH2=AC3H4+H                                3.00E+13    0.0        0.0
214. C2H3+C2H3=i-C4H5+H                              1.50E+30   -5.0    13000.0
215. C2H3+C2H3=n-C4H5+H                              1.10E+24   -3.3    12400.0
216. H2CC+C2H2(+M)=C4H4(+M)                          3.50E+05    2.1    -2400.0
     Low pressure limit:  0.14000E+61 -0.12599E+02  0.74170E+04
     TROE centering:      0.98000E+00  0.56000E+02  0.58000E+03  0.41640E+04
     H2              Enhanced by    2.000E+00
     CH4             Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     C2H2            Enhanced by    3.000E+00
     CO              Enhanced by    1.500E+00
     C2H4            Enhanced by    3.000E+00
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     C2H6            Enhanced by    3.000E+00
     CO2             Enhanced by    2.000E+00
217. C2H2(+M)=H2CC(+M)                              8.00E+14   -0.5    50750.0
     Low pressure limit:  0.24500E+16 -0.64000E+00  0.49700E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H4            Enhanced by    2.500E+00
218. H2CC+C2H4=iiiC4H6                              1.00E+12    0.0        0.0
219. H2CC+O2=CH2+CO2                                1.00E+13    0.0        0.0
220. H2CC+H=C2H2+H                                  1.00E+14    0.0        0.0
221. H2CC+OH=CH2CO+H                                2.00E+13    0.0        0.0
222. C2H2+O=C2H+OH                                  4.60E+19   -1.4    28950.0
223. C2H2+O=CH2+CO                                  2.35E+08    1.4     2204.5
224. C2H2+O=HCCO+H                                  9.40E+08    1.4     2204.5
225. OH+C2H2=C2H+H2O                                2.63E+06    2.1    17060.0
226. OH+C2H2=H+CH2CO                                1.52E+04    2.3     -292.0
227. OH+C2H2=CH3+CO                                 4.37E+06    1.4      227.0
228. C2H2+CH=C3H2+H                                 1.10E+13    0.0        0.0
229. C2H2+CH2=C3H3+H                                1.20E+13    0.0     6620.0
230. C2H2+CH3=C2H+CH4                               1.81E+11    0.0    17289.0
231. C2H2+O2=2HCO                                   1.00E+12    0.0    28000.0
232. C2H2+CH2OH=C2H3+CH2O                           7.23E+11    0.0     9004.0
233. C2H2+CO=C2H+HCO                                4.82E+14    0.0   106713.0
234. C2H2+C2H=C4H2+H                                3.00E+13    0.0        0.0
235. C2H2+C2H(+M)=nC4H3(+M)                         8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
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     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
236. C2H2+C2H(+M)=iC4H3(+M)                          8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
237. C2H2+CH2SING=C3H3+H                             3.42E+15   -0.6     -230.7
238. C2H2+CH2SING=CH2+C2H2                           8.55E+14   -0.6     -230.7
239. HCCO+C2H2=C3H3+CO                               1.00E+11    0.0     3000.0
240. C2H2+C2H3=n-C4H5                                1.10E+32   -7.3     6200.0
241. C2H2+C2H3=i-C4H5                                2.10E+36   -8.8     9100.0
242. C2H3+C2H2=C4H4+H                                5.00E+14   -0.7     6700.0
243. O+C2H=CH+CO                                     1.00E+13    0.0        0.0
244. H+C2H(+M)=C2H2(+M)                              1.00E+17   -1.0        0.0
     Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
     TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
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	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	7.000E-01			
245.	OH+C2H=H+HCCO			2.00E+13	0.0	0.0
246.	C2H+O2=HCO+CO			1.00E+13	0.0	-775.0
247.	C2H+H2=H+C2H2			5.68E+10	0.9	1993.0
248.	C2H+HO2=HCCO+OH			1.81E+13	0.0	0.0
249.	C2H+CH3=C3H3+H			2.41E+13	0.0	0.0
250.	C2H+O2=HCCO+O			6.03E+11	0.0	0.0
251.	C2H+CH2OH=C2H2+CH2O			3.61E+13	0.0	0.0
252.	C2H+CH2OH=C3H3+OH			1.21E+13	0.0	0.0
253.	C2H+CH3OH=C2H2+CH2OH			6.03E+12	0.0	0.0
254.	C2H+CH3O=CH2O+C2H2			2.41E+13	0.0	0.0
255.	C2H+CH3OH=C2H2+CH3O			1.21E+12	0.0	0.0
256.	C2H+CH2=CH+C2H2			1.81E+13	0.0	0.0
257.	C2H+CH2SING=C2H2+CH			1.81E+13	0.0	0.0
258.	O+HCCO=H+2CO			1.00E+14	0.0	0.0
259.	H+HCCO=CH2SING+CO			5.00E+13	0.0	0.0
260.	CH2+HCCO=C2H3+CO			3.00E+13	0.0	0.0
261.	HCCO+O2=CO2+CO+H			4.78E+12	-0.1	1150.0
262.	HCCO+O2=CO+CO+OH			1.91E+11	0.0	1023.0
263.	HCCO+O2=O+CO+HCO			2.18E+02	2.7	3541.0
264.	2HCCO=2CO+C2H2			1.00E+13	0.0	0.0
265.	HCCO+CH3=C2H4+CO			5.00E+13	0.0	0.0
266.	O+CH2CO=OH+HCCO			1.00E+13	0.0	8000.0
267.	O+CH2CO=CH2+CO2			1.75E+12	0.0	1350.0
268.	H+CH2CO=HCCO+H2			5.00E+13	0.0	8000.0
269.	CH2CO+H=CH3+CO			7.77E+08	1.4	2780.0
270.	CH2CHO=H+CH2CO			2.48E+27	-5.2	44304.0
271.	CH2CHO=CH3+CO			1.54E+31	-6.3	42478.0
272.	OH+CH2CO=HCCO+H2O			7.50E+12	0.0	2000.0
273.	CH2CO+OH=CH2OH+CO			1.00E+13	0.0	0.0

274.	CH3CO=CH3+CO	2.40E+15	-2.0	14805.0
275.	CH2CHO+H=CH3CHO	6.40E+35	-7.6	5215.0
276.	CH2CHO+H=CH3+HCO	4.99E+14	-0.3	912.0
277.	CH2CHO+O=CH2O+HCO	5.00E+13	0.0	0.0
278.	CH2CHO+OH=H2O+CH2CO	1.20E+13	0.0	0.0
279.	CH2CHO+OH=HCO+CH2OH	3.01E+13	0.0	0.0
280.	CH2CHO+O2=CH2CO+HO2	1.57E+11	0.0	0.0
281.	CH3CHO=CH3+HCO	9.59E+14	0.0	74180.0
282.	CH3CHO+O2=CH3CO+HO2	2.00E+13	0.5	42200.0
283.	CH3CHO+H=CH2CHO+H2	4.10E+09	1.2	2405.0
284.	CH3CHO+OH=CH3CO+H2O	2.35E+10	0.7	-1113.0
285.	CH3CHO+O=CH2CHO+OH	5.85E+12	0.0	1808.0
286.	CH3CHO+HO2=CH3CO+H2O2	1.70E+12	0.0	10700.0
287.	CH3CHO+CH3=CH3CO+CH4	1.70E+12	0.0	8440.0
288.	CH3CHO+HCO=CH3CO+CH2O	7.80E+13	0.0	8440.0
289.	C2H5O=CH3+CH2O	1.00E+15	0.0	21523.0
290.	C2H5O=CH3CHO+H	2.00E+14	0.0	23215.0
291.	C2H5O+O2=CH3CHO+HO2	6.03E+10	0.0	1643.0
292.	C2H4O+O2=CH2CHO+HO2	4.00E+13	0.0	61500.0
293.	C2H4O+H=CH2CHO+H2	2.00E+13	0.0	8300.0
294.	C2H4O+H=C2H3+H2O	5.00E+09	0.0	5000.0
295.	C2H4O+H=C2H4+OH	9.51E+10	0.0	5000.0
296.	C2H4O+OH=CH2CHO+H2O	4.79E+13	0.0	5955.0
297.	C2H4O+O=CH2CHO+OH	1.91E+12	0.0	5250.0
298.	C2H4O+HO2=CH2CHO+H2O2	4.00E+12	0.0	17000.0
299.	C2H4O=CH3CHO	6.00E+13	0.0	57167.0
300.	C2H4O=CH3+HCO	4.90E+13	0.0	57167.0
301.	C2H4O=CH4+CO	1.21E+13	0.0	57167.0
302.	C3H8+H=nC3H7+H2	1.30E+06	2.5	6756.0
303.	C3H8+H=iC3H7+H2	1.30E+06	2.4	4471.0
304.	C3H8+O=nC3H7+OH	1.90E+05	2.7	3716.0
305.	C3H8+O=iC3H7+OH	4.76E+04	2.7	2106.0

306. C3H8+OH=iC3H7+H2O 1.40E+03 2.8 -310.0

307. C3H8+OH=nC3H7+H2O 1.37E+03 2.7 580.0

308. C3H8+O2=nC3H7+HO2 3.97E+13 0.0 50872.0

309. C3H8+O2=iC3H7+HO2 3.97E+13 0.0 47693.0

310. C3H8+HO2=nC3H7+H2O2 4.76E+04 2.5 16494.0

311. C3H8+HO2=iC3H7+H2O2 9.64E+03 2.6 13910.0

312. C3H8+CH3=nC3H7+CH4 9.04E-01 3.6 7154.0

313. C3H8+CH3=iC3H7+CH4 1.51E+00 3.5 5481.0

314. C3H8+CH2OH=nC3H7+CH3OH 1.99E+02 3.0 3976.0

315. C3H8+CH3O=nC3H7+CH3OH 4.34E+11 0.0 6458.0

316. C3H8+CH2SING=nC3H7+CH3 9.04E-01 3.6 7154.0

317. C3H8+C2H3=nC3H7+C2H4 6.03E+02 3.3 10502.0

318. C3H8+C2H=nC3H7+C2H2 3.61E+12 0.0 0.0

319. C3H8+C2H5=nC3H7+C2H6 9.04E-02 3.6 9141.0

320. C3H8+HCO=nC3H7+CH2O 2.05E+05 2.5 18431.0

321. C3H8+iC3H7=nC3H7+C3H8 8.40E-03 4.2 8716.0

322. C3H8+CH3CO=nC3H7+CH3CHO 4.22E+04 2.6 17658.0

323. C3H8+CH2=nC3H7+CH3 9.03E-01 3.6 7154.0

324. C3H8+CH2OH=iC3H7+CH3OH 6.03E+01 3.0 11989.0

325. C3H8+CH3O=iC3H7+CH3OH 1.45E+11 0.0 4571.0

326. C3H8+CH2SING=iC3H7+CH3 1.51E+00 3.5 7472.0

327. C3H8+C2H3=iC3H7+C2H4 1.02E+03 3.1 8829.0

328. C3H8+C2H=iC3H7+C2H2 1.21E+12 0.0 0.0

329. C3H8+C2H5=iC3H7+C2H6 1.21E+00 3.5 7468.0

330. C3H8+HCO=iC3H7+CH2O 1.08E+07 1.9 17006.0

331. C3H8+CH3CO=iC3H7+CH3CHO 5.30E+06 2.0 16241.0

332. C3H8+CH2=iC3H7+CH3 1.51E+00 3.5 7472.0

333. nC3H7+H=C3H6+H2 1.81E+12 0.0 0.0

334. nC3H7+H(+M)=C3H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+59 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

335. nC3H7+H=C2H5+CH3 3.40E+18 -1.3 5386.0

336. nC3H7+O=C2H5+CH2O 9.60E+13 0.0 0.0

337. nC3H7+O2=C3H6+HO2 9.04E+10 0.0 0.0

338. nC3H7+HO2=C2H5+OH+CH2O 2.41E+13 0.0 0.0

339. nC3H7+OH=C3H6+H2O 2.41E+13 0.0 0.0

340. nC3H7+CH3=CH4+C3H6 1.14E+13 -0.3 0.0

341. nC3H7+C2H5=C3H6+C2H6 1.45E+12 0.0 0.0

342. nC3H7+C2H5=C3H8+C2H4 1.15E+12 0.0 0.0

343. nC3H7+C2H3=C3H8+C2H2 1.21E+12 0.0 0.0

344. nC3H7+C2H2=AC3H5+C2H4 7.23E+11 0.0 9004.0

345. nC3H7+C2H=C3H3+C2H5 1.21E+13 0.0 0.0

346. nC3H7+C2H=C3H6+C2H2 6.03E+12 0.0 0.0

347. nC3H7+iC3H7=C3H8+C3H6 5.13E+13 -0.3 0.0

348. nC3H7+HCO=CO+C3H8 6.03E+13 0.0 0.0

349. nC3H7+CH3O=C3H8+CH2O 2.41E+13 0.0 0.0

350. nC3H7+CH2SING=C2H5+C2H4 2.58E+13 0.0 0.0

351. nC3H7+CH2SING=C3H6+CH3 1.03E+13 0.0 0.0

352. nC3H7+CH2=C2H4+C2H5 1.81E+13 0.0 0.0

353. nC3H7+CH2=C3H6+CH3 1.81E+12 0.0 0.0

354. nC3H7+CH2OH=C3H6+CH3OH 4.82E+11 0.0 0.0

355. iC3H7=CH3+C2H4 1.00E+14 0.0 45000.0

356. iC3H7+H=C3H6+H2 3.61E+12 0.0 0.0

357. iC3H7+H(+M)=C3H8(+M) 2.40E+13 0.0 0.0

Low pressure limit: 0.17000E+59 -0.12080E+02 0.11264E+05

TROE centering: 0.64900E+00 0.12131E+04 0.12131E+04 0.13370E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

358. iC3H7+H=CH3+C2H5 5.90E+23 -2.8 10009.0

359. iC3H7+O=CH3CHO+CH3 9.60E+13 0.0 0.0

360. iC3H7+O2=C3H6+HO2 1.26E+11 0.0 0.0

361. iC3H7+HO2=CH3CHO+OH+CH3 2.41E+13 0.0 0.0

362. iC3H7+OH=C3H6+H2O 2.41E+13 0.0 0.0

363. iC3H7+CH3=CH4+C3H6 2.19E+14 -0.7 0.0

364. iC3H7+C2H5=C3H6+C2H6 2.30E+13 -0.3 0.0

365. iC3H7+C2H5=C3H8+C2H4 1.84E+13 -0.3 0.0

366. iC3H7+C2H3=C2H4+C3H6 1.52E+14 -0.7 0.0

367. iC3H7+C2H3=C3H8+C2H2 1.52E+14 -0.7 0.0

368. iC3H7+C2H2=CH3+iiiC4H6 2.77E+10 0.0 6504.0

369. iC3H7+C2H=C3H6+C2H2 3.60E+12 0.0 0.0

370. iC3H7+iC3H7=C3H8+C3H6 2.11E+14 -0.7 0.0

371. iC3H7+HCO=CO+C3H8 1.20E+14 0.0 0.0

372. iC3H7+CH3O=C3H8+CH2O 1.21E+13 0.0 0.0

373. iC3H7+CH2SING=C3H6+CH3 1.04E+13 0.0 0.0

374. iC3H7+CH2=C3H6+CH3 3.01E+13 0.0 0.0

375. iC3H7+CH2OH=C3H6+CH3OH 2.89E+12 0.0 0.0

376. iC3H7+CH2OH=C3H8+CH2O 2.35E+12 0.0 0.0

377. CH3+C2H3(+M)=C3H6(+M) 2.50E+13 0.0 0.0

Low pressure limit: 0.42700E+59 -0.11940E+02 0.97700E+04

TROE centering: 0.17500E+00 0.13410E+04 0.60000E+05 0.10140E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

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     CO2             Enhanced by    2.000E+00
     C2H2            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
378. C3H6+H=H2+AC3H5                                 1.70E+05    2.5     2492.0
379. C3H6+H=C2H4+CH3                                 8.80E+16   -1.1     6461.0
380. C3H6+H=SC3H5+H2                                 7.81E+05    2.5    12285.0
381. C3H6+H(+M)=nC3H7(+M)                            1.33E+13    0.0     3260.7
     Low pressure limit:  0.62600E+39 -0.66600E+01  0.70000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.13100E+04  0.48097E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
382. C3H6+H(+M)=iC3H7(+M)                            1.33E+13    0.0     1559.8
     Low pressure limit:  0.87000E+43 -0.75000E+01  0.47218E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.64540E+03  0.68443E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
383. C3H6+H=TC3H5+H2                                 3.90E+05    2.5     5821.0
384. C3H6=H2+AC3H4                                   4.00E+13    0.0    80000.0
385. C3H6=CH4+C2H2                                   3.50E+12    0.0    70000.0
386. C3H6+O=C2H5+HCO                                 3.50E+07    1.6     -972.0
387. C3H6+O=AC3H5+OH                                 1.75E+11    0.7     5884.0
388. C3H6+O=SC3H5+OH                                 1.21E+11    0.7     8960.0
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389. C3H6+O=TC3H5+OH 6.03E+10 0.7 7633.0

390. C3H6+O=CH3+H+CH2CO 1.20E+08 1.6 327.0

391. C3H6+OH=AC3H5+H2O 3.12E+06 2.0 -298.0

392. C3H6+OH=SC3H5+H2O 2.14E+06 2.0 2778.0

393. C3H6+OH=TC3H5+H2O 1.11E+06 2.0 1451.0

394. C3H6+HO2=AC3H5+H2O2 9.63E+03 2.6 13910.0

395. C3H6+O2=AC3H5+HO2 6.03E+13 0.0 47590.0

396. C3H6+CH3=AC3H5+CH4 2.20E+00 3.5 5675.0

397. C3H6+CH3=TC3H5+CH4 8.40E-01 3.5 11660.0

398. C3H6+C2H5=AC3H5+C2H6 2.23E+00 3.5 6637.0

399. C3H6+C2H2=AC3H5+C2H3 4.04E+13 0.0 46818.0

400. C3H6+C2H3=AC3H5+C2H4 2.21E+00 3.5 4682.0

401. C3H6+C2H3=SC3H5+C2H4 1.35E+00 3.5 10842.0

402. C3H6+C2H3=TC3H5+C2H4 8.40E-01 3.5 9670.0

403. C3H6+C2H3=iiiC4H6+CH3 7.23E+11 0.0 5008.0

404. C3H6+C2H4=AC3H5+C2H5 5.78E+13 0.0 51584.0

405. C3H6+C2H4=nC3H7+C2H3 6.03E+13 0.0 75446.0

406. C3H6+CH2OH=AC3H5+CH3OH 6.03E+01 3.0 12000.0

407. C3H6+nC3H7=AC3H5+C3H8 2.23E+00 3.5 6637.0

408. C3H6+nC3H7=IC4H8+C2H5 2.23E+00 3.5 -2000.0

409. C3H6+iC3H7=C3H8+AC3H5 6.62E-02 4.0 8066.0

410. C3H6+C3H6=AC3H5+nC3H7 2.53E+14 0.0 55179.0

411. C3H6+C3H6=AC3H5+iC3H7 4.88E+13 0.0 52309.0

412. CH3+C2H3=AC3H5+H 1.50E+24 -2.8 18618.0

413. CH3+C2H3=SC3H5+H 3.20E+35 -7.8 13300.0

414. CH3+C2H3=TC3H5+H 4.99E+22 -4.4 18850.0

415. AC3H5+H(+M)=C3H6(+M) 2.00E+14 0.0 0.0

Low pressure limit: 0.13300E+61 -0.12000E+02 0.59678E+04

TROE centering: 0.20000E-01 0.10970E+04 0.10967E+05 0.68600E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

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     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
416. AC3H5+H=AC3H4+H2                                 1.80E+13    0.0        0.0
417. TC3H5+H=AC3H4+H2                                 3.30E+12    0.0        0.0
418. SC3H5+H=AC3H4+H2                                 3.30E+12    0.0        0.0
419. AC3H5+O=C2H3CHO+H                                6.00E+13    0.0        0.0
420. AC3H5+O=C2H3+CH2O                                1.80E+14    0.0        0.0
421. SC3H5+O=CH2CO+CH3                                1.81E+14    0.0        0.0
422. TC3H5+O=H+HCCO+CH3                               1.81E+14    0.0        0.0
423. AC3H5+OH=C2H3CHO+H+H                             5.30E+37   -6.7    29306.0
424. AC3H5+OH=AC3H4+H2O                               6.00E+12    0.0        0.0
425. AC3H5+O2=AC3H4+HO2                               4.99E+15   -1.4    22428.0
426. AC3H5+O2=CH2O+CH3CO                              1.19E+15   -1.0    20128.0
427. AC3H5+O2=OH+C2H3CHO                              1.82E+13   -0.4    22859.0
428. SC3H5+O2=CH3CHO+HCO                              4.34E+12    0.0        0.0
429. TC3H5+O2=CH3CHO+HCO                              4.34E+12    0.0        0.0
430. AC3H5+HO2=C2H3+CH2O+OH                           6.60E+12    0.0        0.0
431. AC3H5+CH3=AC3H4+CH4                              3.00E+12   -0.3     -131.0
432. AC3H5+CH3(+M)=IC4H8(+M)                          1.00E+14   -0.3     -262.0
     Low pressure limit:  0.35100E+61 -0.12970E+02  0.60000E+04
     TROE centering:      0.89600E+00  0.60000E+05  0.16060E+04  0.61180E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
433. SC3H5+CH3=AC3H4+CH4                              1.00E+11    0.0        0.0
434. TC3H5+CH3=AC3H4+CH4                              1.00E+11    0.0        0.0
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435.	AC3H5+C2H3=AC3H4+C2H4	1.00E+12	0.0	0.0
436.	SC3H5+C2H3=AC3H4+C2H4	1.00E+11	0.0	0.0
437.	TC3H5+C2H3=AC3H4+C2H4	1.00E+11	0.0	0.0
438.	AC3H5+CH2O=C3H6+HCO	1.26E+08	1.9	18191.0
439.	AC3H5+HCO=C3H6+CO	6.00E+13	0.0	0.0
440.	AC3H5+AC3H5=AC3H4+C3H6	8.43E+10	0.0	-262.0
441.	AC3H5+CH2=iiiC4H6+H	3.00E+13	0.0	0.0
442.	AC3H5+nC3H7=AC3H4+C3H8	7.23E+11	0.0	-131.0
443.	AC3H5+iC3H7=AC3H4+C3H8	4.58E+12	-0.3	-131.0
444.	AC3H5=TC3H5	3.90E+59	-15.4	75400.0
445.	AC3H5=SC3H5	1.30E+55	-14.5	73800.0
446.	TC3H5=SC3H5	1.60E+44	-12.2	52200.0
447.	AC3H4=PC3H4	6.03E+53	-12.2	84276.0
448.	AC3H4+H=AC3H5	1.24E+52	-12.0	17839.0
	Declared duplicate reaction...			
449.	AC3H4+H=AC3H5	6.92E+36	-8.2	7462.0
	Declared duplicate reaction...			
450.	AC3H4+H=TC3H5	1.55E+53	-13.1	14472.0
	Declared duplicate reaction...			
451.	AC3H4+H=TC3H5	9.88E+44	-11.2	8212.0
	Declared duplicate reaction...			
452.	PC3H4+H=TC3H5	3.17E+52	-12.7	14226.0
	Declared duplicate reaction...			
453.	PC3H4+H=TC3H5	2.59E+45	-11.2	8046.0
	Declared duplicate reaction...			
454.	PC3H4+H=SC3H5	3.38E+49	-12.8	14072.0
	Declared duplicate reaction...			
455.	PC3H4+H=SC3H5	2.98E+43	-11.4	8736.0
	Declared duplicate reaction...			
456.	AC3H4+H=PC3H4+H	1.48E+13	0.3	4103.0
457.	AC3H4+H=CH3+C2H2	2.72E+09	1.2	6834.0
458.	PC3H4+H=CH3+C2H2	3.89E+10	1.0	4114.0

459.	C2H2+CH3=SC3H5	-6.81E+48	-12.3	16642.0
	Declared duplicate reaction...			
460.	C2H2+CH3=SC3H5	1.52E+44	-10.7	15256.0
	Declared duplicate reaction...			
461.	C2H2+CH3=TC3H5	6.80E+20	-4.2	18000.0
462.	C2H2+CH3=AC3H5	8.20E+53	-13.3	33200.0
463.	AC3H4+H=C3H3+H2	6.60E+03	3.1	5522.0
464.	AC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
465.	PC3H4+H=C3H3+H2	3.57E+04	2.8	4821.0
466.	AC3H4+O=C2H4+CO	2.00E+07	1.8	1000.0
467.	AC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
468.	AC3H4+CH3=C3H3+CH4	1.30E+12	0.0	7700.0
469.	PC3H4+O=HCCO+CH3	7.30E+12	0.0	2250.0
470.	PC3H4+O=C2H4+CO	1.00E+13	0.0	2250.0
471.	PC3H4+O=C3H3+OH	3.44E+04	2.2	4830.0
472.	PC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
473.	PC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
474.	PC3H4+CH3=C3H3+CH4	1.80E+12	0.0	7700.0
475.	C3H3+H=PC3H4	3.63E+36	-7.4	6039.0
476.	C3H3+H=AC3H4	3.39E+36	-7.4	6337.0
477.	C3H3+CH3=iiC4H6	3.61E+13	0.0	0.0
478.	C2H3+C2H3=iiiC4H6	7.00E+57	-13.8	17629.0
479.	C3H3+H=C3H2+H2	2.14E+05	2.5	7453.0
480.	C3H3+O=>C2H2+HCO	1.38E+14	0.0	0.0
481.	C3H3+O=C2H3+CO	4.62E+13	0.0	0.0
482.	C3H3+O=C2H+CH2O	4.62E+13	0.0	0.0
483.	C3H3+O=>C2H2+CO+H	4.62E+13	0.0	0.0
484.	C3H3+OH=C3H2+H2O	2.00E+13	0.0	8000.0
485.	C3H3+HCO=AC3H4+CO	2.50E+13	0.0	0.0
486.	C3H3+HCO=PC3H4+CO	2.50E+13	0.0	0.0
487.	C3H3+CH=iC4H3+H	5.00E+13	0.0	0.0
488.	C3H3+CH2=C4H4+H	5.00E+13	0.0	0.0

489.	C3H3+O2=CH2CO+HCO	1.70E+05	1.7	1500.0
490.	C3H3+HCCO=C4H4+CO	2.50E+13	0.0	0.0
491.	C3H3+HO2=OH+CO+C2H3	8.00E+11	0.0	0.0
492.	C3H3+HO2=AC3H4+O2	3.00E+11	0.0	0.0
493.	C3H3+HO2=PC3H4+O2	2.50E+12	0.0	0.0
494.	C3H2+O2=H+CO+HCCO	2.00E+12	0.0	1000.0
495.	C3H2+O=C2H2+CO	6.80E+13	0.0	0.0
496.	C3H2+OH=C2H2+HCO	6.80E+13	0.0	0.0
497.	C3H2+H=C3H3	1.10E+40	-8.0	84700.0
498.	C3H2+CH=C4H2+H	5.00E+13	0.0	0.0
499.	C3H2+CH2=nC4H3+H	5.00E+13	0.0	0.0
500.	C3H2+CH3=C4H4+H	5.00E+12	0.0	0.0
501.	C3H2+HCCO=nC4H3+CO	1.00E+13	0.0	0.0
502.	C2H3CO+M=>C2H3+CO+M	8.51E+15	0.0	23000.0
503.	C2H3+CO+M=>C2H3CO+M	1.58E+11	0.0	6000.0
504.	C2H3CHO+HO2=>C2H3CH2O+O2	1.29E+11	0.0	32000.0
505.	C2H3CH2O=>C2H3CHO+H	1.00E+14	0.0	19000.0
506.	C2H3CHO+H=>C2H3CH2O	1.00E+08	0.0	10000.0
507.	C2H3CHO+OH=>C2H3CO+H2O	1.00E+13	0.0	0.0
508.	C2H3CO+H2O=>C2H3CHO+OH	1.91E+13	0.0	36620.0
509.	C2H3CHO+H=>C2H3CO+H2	3.98E+13	0.0	4200.0
510.	C2H3CO+H2=>C2H3CHO+H	1.78E+13	0.0	23670.0
511.	C2H3CHO+O=>C2H3CO+OH	5.01E+12	0.0	1790.0
512.	C2H3CO+OH=>C2H3CHO+O	1.00E+12	0.0	19160.0
513.	C2H3CHO+HO2=>C2H3CO+H2O2	1.70E+12	0.0	10700.0
514.	C2H3CO+H2O2=>C2H3CHO+HO2	1.00E+12	0.0	14100.0
515.	C2H3CHO+CH3=>C2H3CO+CH4	1.74E+12	0.0	8440.0
516.	C2H3CO+CH4=>C2H3CHO+CH3	1.51E+13	0.0	28000.0
517.	C2H3CH2O+O2=>C2H3CHO+HO2	1.74E+11	0.0	1750.0
518.	C2H3CH2O=>CH2O+C2H3	1.00E+14	0.0	21600.0
519.	CH2O+C2H3=>C2H3CH2O	1.00E+11	0.0	0.0
520.	C4H+H2=C4H2+H	2.00E+13	0.0	5000.0

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521. C4H+O2=CO+CO+C2H                                 1.20E+12    0.0        0.0
522. C4H2+OH=H2O+C4H                                  9.15E+09    1.0    21746.0
523. H2C4O+OH=C2H2+CO+HCO                             1.00E+13    0.0        0.0
524. iC4H3+O=H2C4O+H                                  2.00E+13    0.0        0.0
525. C4H2+OH=H+H2C4O                                  1.63E+15   -1.1     2549.0
526. C4H2+OH=CO+C3H3                                  1.69E+28   -4.6    20140.0
527. C4H2+H=nC4H3                                     1.44E+63  -15.7    24018.0
     Declared duplicate reaction...
528. C4H2+H=nC4H3                                     4.16E+32   -6.5     9726.1
     Declared duplicate reaction...
529. C4H2+H(+M)=iC4H3(+M)                             4.31E+10    1.2     1752.9
     Low pressure limit:  0.23000E+46 -0.80950E+01  0.25066E+04
     TROE centering:      0.74800E-01  0.10000E-49 -0.42159E+04  0.10000E+51
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
530. C4H2+O=C3H2+CO                                   2.70E+13    0.0     1720.0
531. C4H2+C2H=C6H2+H                                  9.60E+13    0.0        0.0
532. C4H2+C2H=C6H3                                    1.10E+30   -6.3     2790.0
533. nC4H3=iC4H3                                      3.70E+61  -15.8    54890.0
534. nC4H3+H=iC4H3+H                                  2.40E+11    0.8     2410.0
535. nC4H3+H=C2H2+H2CC                                1.60E+19   -1.6     2220.0
536. nC4H3+H=C4H4                                     1.10E+42   -9.7     7000.0
537. nC4H3+H=C4H2+H2                                  3.00E+13    0.0        0.0
538. nC4H3+OH=C4H2+H2O                                2.00E+12    0.0        0.0
539. nC4H3+C2H2=l-C6H4+H                              3.70E+16   -1.2    11100.0
540. nC4H3+C2H2=A1                                    2.30E+68  -17.6    24400.0
541. nC4H3+C2H2=c-C6H4+H                              1.90E+36   -7.2    17900.0
542. iC4H3+H=C2H2+H2CC                                2.40E+19   -1.6     2800.0
543. iC4H3+H=C4H4                                     4.20E+44  -10.3     7890.0
544. iC4H3+H=C4H2+H2                                  5.00E+13    0.0        0.0
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545.	iC4H3+OH=C4H2+H2O	4.00E+12	0.0	0.0
546.	iC4H3+O2=HCCO+CH2CO	7.86E+16	-1.8	0.0
547.	C4H4+H=n-C4H5	4.20E+50	-12.3	12500.0
548.	C4H4+H=i-C4H5	9.60E+52	-12.8	14300.0
549.	C4H4+H=nC4H3+H2	6.65E+05	2.5	12240.0
550.	C4H4+H=iC4H3+H2	3.33E+05	2.5	9240.0
551.	C4H4+OH=nC4H3+H2O	3.10E+07	2.0	3430.0
552.	C4H4+OH=iC4H3+H2O	1.55E+07	2.0	430.0
553.	C4H4+O=C3H3+HCO	6.00E+08	1.4	-860.0
554.	C4H4+C2H=l-C6H4+H	1.20E+13	0.0	0.0
555.	n-C4H5=i-C4H5	1.30E+62	-16.4	49600.0
556.	n-C4H5+H=i-C4H5+H	1.00E+36	-6.3	17486.0
557.	n-C4H5+H=C4H4+H2	1.50E+13	0.0	0.0
558.	n-C4H5+OH=C4H4+H2O	2.00E+12	0.0	0.0
559.	n-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
560.	n-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
561.	n-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
562.	n-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
563.	n-C4H5+O2=HCO+C2H3CHO	9.20E+16	-1.4	1010.0
564.	i-C4H5+H=C4H4+H2	3.00E+13	0.0	0.0
565.	i-C4H5+H=C3H3+CH3	1.00E+14	0.0	0.0
566.	i-C4H5+OH=C4H4+H2O	4.00E+12	0.0	0.0
567.	i-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
568.	i-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
569.	i-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
570.	i-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
571.	i-C4H5+O2=CH2CO+CH2CHO	2.16E+10	0.0	2500.0
572.	n-C4H5+C5H6=iiiC4H6+C5H5	6.00E+12	0.0	0.0
573.	i-C4H5+C5H6=iiiC4H6+C5H5	6.00E+12	0.0	0.0
574.	iiiC4H6=i-C4H5+H	8.20E+51	-10.9	118409.0
575.	iiiC4H6=n-C4H5+H	3.50E+61	-13.9	129677.0
576.	iiiC4H6=C4H4+H2	2.50E+15	0.0	94700.0

577.	iiiC4H6+H=n-C4H5+H2	3.00E+07	2.0	13000.0
578.	iiiC4H6+H=i-C4H5+H2	3.00E+07	2.0	6000.0
579.	C2H4+C2H3=iiiC4H6+H	7.40E+14	-0.7	8420.0
580.	iiiC4H6+H=PC3H4+CH3	2.00E+12	0.0	7000.0
581.	iiiC4H6+H=AC3H4+CH3	2.00E+12	0.0	7000.0
582.	iiiC4H6+O=n-C4H5+OH	7.50E+06	1.9	3740.0
583.	iiiC4H6+O=i-C4H5+OH	7.50E+06	1.9	3740.0
584.	iiiC4H6+O=HCO+AC3H5	6.02E+08	1.4	-858.0
585.	iiiC4H6+OH=CH3CHO+C2H3	6.30E+12	0.0	-874.0
586.	iiiC4H6+OH=AC3H5+CH2O	6.30E+12	0.0	-874.0
587.	iiiC4H6+OH=n-C4H5+H2O	2.00E+07	2.0	5000.0
588.	iiiC4H6+OH=i-C4H5+H2O	2.00E+07	2.0	2000.0
589.	iiiC4H6+CH3=n-C4H5+CH4	2.00E+14	0.0	22800.0
590.	iiiC4H6+CH3=i-C4H5+CH4	1.00E+14	0.0	19800.0
591.	iiiC4H6+C2H3=n-C4H5+C2H4	5.00E+13	0.0	22800.0
592.	iiiC4H6+C2H3=i-C4H5+C2H4	2.50E+13	0.0	19800.0
593.	iiiC4H6+C3H3=n-C4H5+AC3H4	1.00E+13	0.0	22500.0
594.	iiiC4H6+C3H3=i-C4H5+AC3H4	5.00E+12	0.0	19500.0
595.	iiiC4H6+AC3H5=n-C4H5+C3H6	1.00E+13	0.0	22500.0
596.	iiiC4H6+AC3H5=i-C4H5+C3H6	5.00E+12	0.0	19500.0
597.	iiC4H6=i-C4H5+H	4.20E+15	0.0	92600.0
598.	iiC4H6+H=iiiC4H6+H	2.00E+13	0.0	4000.0
599.	iiC4H6+H=i-C4H5+H2	1.70E+05	2.5	2490.0
600.	iiC4H6+H=AC3H4+CH3	2.00E+13	0.0	2000.0
601.	iiC4H6+H=PC3H4+CH3	2.00E+13	0.0	2000.0
602.	iiC4H6+CH3=i-C4H5+CH4	7.00E+13	0.0	18500.0
603.	iiC4H6+O=CH2CO+C2H4	1.20E+08	1.6	327.0
604.	iiC4H6+O=i-C4H5+OH	1.80E+11	0.7	5880.0
605.	iiC4H6+OH=i-C4H5+H2O	3.10E+06	2.0	-298.0
606.	iiC4H6=iiiC4H6	3.00E+13	0.0	65000.0
607.	IC4H8+H=C2H4+C2H5	1.60E+22	-2.4	11180.0
608.	IC4H8+H=C3H6+CH3	3.20E+22	-2.4	11180.0

609. IC4H8+H=C4H7+H2 6.50E+05 2.5 6756.0

610. IC4H8+O=nC3H7+HCO 3.30E+08 1.4 -402.0

611. IC4H8+O=C4H7+OH 1.50E+13 0.0 5760.0

Declared duplicate reaction...

612. IC4H8+O=C4H7+OH 2.60E+13 0.0 4470.0

Declared duplicate reaction...

613. IC4H8+OH=C4H7+H2O 7.00E+02 2.7 527.0

614. IC4H8+O2=C4H7+HO2 2.00E+13 0.0 50930.0

615. IC4H8+HO2=C4H7+H2O2 1.00E+12 0.0 14340.0

616. IC4H8+CH3=C4H7+CH4 4.50E-01 3.6 7153.0

617. C4H7=iiiC4H6+H 1.27E+24 -4.8 23777.0

618. C4H7+H(+M)=IC4H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+49 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

619. C4H7+H=CH3+AC3H5 2.00E+21 -2.0 11000.0

620. C4H7+H=iiiC4H6+H2 1.80E+12 0.0 0.0

621. C4H7+O2=iiiC4H6+HO2 1.00E+11 0.0 0.0

622. C4H7+HCO=IC4H8+CO 6.00E+13 0.0 0.0

623. C4H7+CH3=iiiC4H6+CH4 1.10E+13 0.0 0.0

624. C2H4+C2H3=C4H7 1.23E+35 -7.8 9930.0

625. IC4H8+H(+M)=nC4H9(+M) 1.33E+13 0.0 3260.7

Low pressure limit: 0.62600E+39 -0.66600E+01 0.70000E+04

TROE centering: 0.10000E+01 0.10000E+04 0.13100E+04 0.48097E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

	CH4	Enhanced by	2.000E+00		
	CO	Enhanced by	1.500E+00		
	CO2	Enhanced by	2.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	7.000E-01		
626.	C2H4+C2H5=nC4H9		1.50E+11	0.0	7300.0
627.	nC4H9+H=IC4H8+H2		1.80E+12	0.0	0.0
628.	nC4H9+O=nC3H7+CH2O		9.60E+13	0.0	0.0
629.	nC4H9+OH=IC4H8+H2O		2.40E+13	0.0	0.0
630.	nC4H9+O2=IC4H8+HO2		2.70E+11	0.0	0.0
631.	nC4H9+HO2=nC3H7+OH+CH2O		2.40E+13	0.0	0.0
632.	nC4H9+CH3=IC4H8+CH4		1.10E+13	0.0	0.0
633.	CH+C4H2=C5H2+H		1.00E+14	0.0	0.0
634.	H2CCCCCH+H=C5H2+H2		1.00E+13	0.0	0.0
635.	HCCCHCCH+H=C5H2+H2		1.00E+13	0.0	0.0
636.	H2CCCCCH+CH3=C5H2+CH4		3.00E+12	0.0	5000.0
637.	HCCCHCCH+CH3=C5H2+CH4		3.00E+12	0.0	5000.0
638.	C3H3+C2H=H2CCCCCH+H		1.00E+13	0.0	0.0
639.	CH2+C4H2=H2CCCCCH+H		1.30E+13	0.0	4326.0
640.	CH2SING+C4H2=H2CCCCCH+H		2.54E+16	-0.9	0.0
641.	HCCCHCCH+H=H2CCCCCH+H		1.00E+13	0.0	0.0
642.	H2CCCCCH+CH3=FC6H6		1.00E+11	0.0	0.0
643.	H2CCCCCH+CH3=A1+H		1.00E+11	0.0	0.0
644.	H2CCCCCH+CH3=A		5.00E+10	0.0	0.0
645.	C3H2+C2H2=HCCCHCCH+H		5.00E+12	0.0	5000.0
646.	C3H3+C2H=HCCCHCCH+H		3.00E+13	0.0	0.0
647.	CH2SING+C4H2=HCCCHCCH+H		2.54E+16	-0.9	0.0
648.	C3H3+C3H3=HCCCHCCH+CH3		5.00E+11	0.0	0.0
649.	HCCCHCCH+CH3=FC6H6		1.00E+11	0.0	0.0
650.	HCCCHCCH+CH3=A1+H		1.00E+11	0.0	0.0
651.	iC4H3+CH3=l-C5H5+H		3.00E+13	0.0	0.0
652.	C5H5=l-C5H5		4.09E+47	-10.4	54874.0

653.	C3H3+C2H2=l-C5H5	5.62E+32	-7.3	6758.0
654.	C5H5+H=C5H6	2.71E+63	-14.8	21050.0
655.	C5H5=C3H3+C2H2	2.79E+79	-18.3	130834.0
656.	C5H5+O=n-C4H5+CO	7.27E+13	-0.3	470.0
657.	C5H5+O=C5H5O	1.84E+03	1.0	-6960.0
658.	C5H5+O=C5H4O+H	6.71E+13	0.0	40.0
659.	C5H5+HO2=C5H5O+OH	3.00E+13	0.0	0.0
660.	C5H5O=n-C4H5+CO	2.51E+11	0.0	43900.0
661.	C5H5O=C5H4O+H	2.90E+32	-6.5	21220.0
662.	C5H5O=i-C4H5+CO	1.10E+79	-19.6	66250.0
663.	C5H5+OH=iiiC4H6+CO	1.20E+14	0.0	4500.0
664.	C5H5+OH=C5H4OH+H	2.15E+30	-4.6	25050.0
665.	C5H4O+H=C5H4OH	1.10E+69	-16.0	37130.0
666.	C5H4OH+O2=C5H4O+HO2	3.00E+13	0.0	5000.0
667.	C5H4O+H=n-C4H5+CO	2.10E+61	-13.3	40810.0
668.	C5H4O+O=C4H4+CO2	1.00E+13	0.0	2000.0
669.	C5H4O=2C2H2+CO	1.10E+47	-9.6	99500.0
670.	C5H6+H=C5H5+H2	2.80E+13	0.0	2259.0
671.	C5H6+H=AC3H5+C2H2	6.60E+14	0.0	12345.0
672.	C5H6+OH=C5H5+H2O	3.08E+06	2.0	0.0
673.	C5H6+O=C5H5+OH	4.77E+04	2.7	1106.0
674.	C5H6+O2=C5H5+HO2	4.00E+13	0.0	37150.0
675.	C5H6+HO2=C5H5+H2O2	1.10E+04	2.6	12900.0
676.	C5H6+CH3=C5H5+CH4	1.80E-01	4.0	0.0
677.	C5H6+C2H3=C5H5+C2H4	1.20E-01	4.0	0.0
678.	C5H6+A1=C5H5+A	1.00E-01	4.0	0.0
679.	C5H6=CH2CHCHCCH2	1.35E+15	0.0	80450.0
680.	CH2CHCHCCH2=PC3H4+C2H2	2.88E+13	0.0	66550.0
681.	C5H6=C2H2+AC3H4	3.80E+17	0.0	104000.0
682.	C5H6=CH2CHCH2CCH	8.50E+14	0.0	90540.0
683.	CH2CHCH2CCH=C2H2+AC3H4	3.55E+13	0.0	63360.0
684.	C6H2+H=C6H3	4.30E+45	-10.2	13250.0

685. C6H3+H=C4H2+C2H2 2.40E+19 -1.6 2800.0

686. C6H3+H=l-C6H4 4.20E+44 -10.3 7890.0

687. C6H3+H=C6H2+H2 3.00E+13 0.0 0.0

688. C6H3+OH=C6H2+H2O 5.00E+12 0.0 0.0

689. C6H3+O2=>CO+C3H2+HCCO 5.00E+11 0.0 0.0

690. l-C6H4+H=n-C6H5 3.30E+44 -10.0 18800.0

691. l-C6H4+H=A1 3.60E+77 -20.1 28100.0

692. A1(+M)=c-C6H4+H(+M) 4.30E+12 0.6 77313.0

Low pressure limit: 0.10000E+85 -0.18866E+02 0.90064E+05

TROE centering: 0.90200E+00 0.69600E+03 0.35800E+03 0.38560E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

693. A1+H=c-C6H4+H2 2.00E+11 1.1 24500.0

694. l-C6H4+H=C6H3+H2 6.65E+06 2.5 9240.0

695. l-C6H4+OH=C6H3+H2O 3.10E+06 2.0 430.0

696. n-C6H5=A1 1.30E+62 -15.9 35800.0

697. n-C6H5=c-C6H4+H 2.70E+65 -15.9 59700.0

698. n-C6H5+H=i-C6H5+H 2.40E+11 0.8 2410.0

699. n-C6H5+H=l-C6H6 1.10E+42 -9.7 7000.0

700. i-C6H5+H=l-C6H6 4.20E+44 -10.3 7890.0

701. n-C6H5+H=l-C6H4+H2 1.50E+13 0.0 0.0

702. i-C6H5+H=l-C6H4+H2 3.00E+13 0.0 0.0

703. n-C6H5+OH=l-C6H4+H2O 2.50E+12 0.0 0.0

704. i-C6H5+OH=l-C6H4+H2O 5.00E+12 0.0 0.0

705. n-C6H5+O2=>C4H4+HCO+CO 4.16E+10 0.0 2500.0

706. i-C6H5+O2=>CH2CO+CH2CO+C2H 7.86E+16 -1.8 0.0

707. nC4H3+C2H2=n-C6H5 6.00E+33 -7.4 13700.0

708. l-C6H6+H+M=n-C6H7+M 2.90E+17 -0.5 1000.0

H2 Enhanced by 2.000E+00

	H2O	Enhanced by	6.000E+00		
	CO	Enhanced by	1.500E+00		
	CO2	Enhanced by	2.000E+00		
	CH4	Enhanced by	2.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	7.000E-01		
709.	l-C6H6+H+M=CYC6H7+M			1.70E+28 -4.7	2800.0
	H2	Enhanced by	2.000E+00		
	H2O	Enhanced by	6.000E+00		
	CO	Enhanced by	1.500E+00		
	CO2	Enhanced by	2.000E+00		
	CH4	Enhanced by	2.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	7.000E-01		
710.	l-C6H6+H=n-C6H5+H2			6.65E+05 2.5	12240.0
711.	l-C6H6+H=i-C6H5+H2			3.33E+05 2.5	9240.0
712.	l-C6H6+OH=n-C6H5+H2O			6.20E+06 2.0	3430.0
713.	l-C6H6+OH=i-C6H5+H2O			3.10E+06 2.0	430.0
714.	n-C6H7=CYC6H7			4.10E+24 -7.1	3900.0
715.	n-C6H7=A+H			8.40E+21 -4.2	11300.0
716.	n-C6H7+H=i-C6H7+H			4.00E+41 -8.1	19200.0
717.	i-C6H7+H=C6H8			1.20E+60 -13.9	21000.0
718.	n-C6H7+H=C6H8			8.70E+69 -17.0	24000.0
719.	n-C6H7+H=l-C6H6+H2			1.50E+13 0.0	0.0
720.	i-C6H7+H=l-C6H6+H2			3.00E+13 0.0	0.0
721.	n-C6H7+OH=l-C6H6+H2O			2.50E+12 0.0	0.0
722.	i-C6H7+OH=l-C6H6+H2O			5.00E+12 0.0	0.0
723.	n-C6H7+O2=>iiiC4H6+CO+HCO			4.16E+10 0.0	2500.0
724.	i-C6H7+O2=>CH2CO+CH2CO+C2H3			7.86E+16 -1.8	0.0
725.	C6H8+H=n-C6H7+H2			1.33E+06 2.5	12240.0
726.	C6H8+H=i-C6H7+H2			6.65E+05 2.5	9240.0
727.	C6H8+OH=n-C6H7+H2O			6.20E+06 2.0	3430.0

728.	C6H8+OH=i-C6H7+H2O	3.10E+06	2.0	430.0
729.	A1+O=C5H5+CO	9.00E+13	0.0	0.0
730.	CH2SING+A=A1+CH3	1.70E+14	0.0	0.0
731.	C3H3+C3H3=C4H5C2H	6.48E+68	-16.7	2872.0
	Declared duplicate reaction...			
732.	C3H3+C3H3=C4H5C2H	1.54E+36	-7.8	5580.0
	Declared duplicate reaction...			
733.	C3H3+C3H3=FC6H6	7.25E+65	-16.0	25035.0
	Declared duplicate reaction...			
734.	C3H3+C3H3=FC6H6	4.19E+39	-9.0	6098.0
	Declared duplicate reaction...			
735.	C3H3+C3H3=A	1.64E+66	-15.9	27529.0
	Declared duplicate reaction...			
736.	C3H3+C3H3=A	1.20E+35	-7.4	5058.0
	Declared duplicate reaction...			
737.	C3H3+C3H3=A1+H	2.02E+33	-6.0	15940.0
738.	C3H3+AC3H5=FC6H6+H+H	3.26E+29	-5.4	3390.0
739.	nC4H3+C2H3=A	2.87E+14	0.0	817.0
740.	n-C4H5+C2H3=A+H2	2.80E-07	5.6	-1890.0
741.	n-C4H5+C2H3=CY13C6H8	5.50E+15	-1.7	1470.0
742.	iiiC4H6+C2H3=CY13C6H8+H	2.28E+12	-0.2	9920.0
743.	n-C4H5+C2H2=A+H	2.94E+16	-1.1	9257.0
744.	n-C4H5+C2H2=l-C6H6+H	1.14E+09	1.4	17338.0
745.	n-C4H5+C2H2=FC6H6+H	1.52E+15	-0.8	8762.0
746.	C2H2+n-C4H5=CYC6H7	2.85E+48	-12.3	15693.4
	Declared duplicate reaction...			
747.	C2H2+n-C4H5=CYC6H7	3.49E-06	4.0	-5112.0
	Declared duplicate reaction...			
748.	i-C4H5+C2H2=A+H	1.47E+23	-3.3	24907.0
749.	i-C4H5+C2H2=FC6H6+H	1.01E+34	-5.9	28786.0
750.	i-C4H5+C2H2=C4H5C2H+H	5.70E+18	-1.4	30351.0
751.	C2H2+i-C4H5=CYC6H7	1.14E+31	-9.2	19403.0

	Declared duplicate reaction...			
752.	C2H2+i-C4H5=CYC6H7	4.34E+39	-9.1	19210.0
	Declared duplicate reaction...			
753.	C5H5+CH3=FC6H6+H2	9.26E+01	2.2	8811.4
754.	FC6H6=A	5.62E+81	-19.4	121500.0
755.	FC6H6=A1+H	2.57E+97	-23.2	153470.0
756.	FC6H6+H=A+H	3.00E+12	0.5	2000.0
757.	CY13C6H8=A+H2	4.39E+37	-7.3	71949.0
758.	CY13C6H8=CYC6H7+H	2.42E+59	-13.3	96147.0
759.	CYC6H7=A+H	2.64E+59	-14.3	44929.0
760.	A=A1+H	1.35+108	-25.8	181750.0
761.	A+H=A1+H2	2.50E+14	0.0	16000.0
762.	A+OH=A1+H2O	1.63E+08	1.4	1450.0
763.	A+O2=A1+HO2	6.30E+13	0.0	60000.0
764.	A+O=A1+OH	2.00E+13	0.0	14704.0
765.	hexene1+H=hex1yl	2.92E+41	-9.3	9784.0
	Declared duplicate reaction...			
766.	hexene1+H=hex1yl	1.24E+62	-15.6	22448.0
	Declared duplicate reaction...			
767.	hexene1+H=hex2yl	1.68E+63	-15.8	21543.0
	Declared duplicate reaction...			
768.	hexene1+H=hex2yl	3.53E+47	-11.0	11174.0
	Declared duplicate reaction...			
769.	hex1yl=hex2yl	2.00E+11	0.0	11100.0
770.	hex1yl=hex3yl	2.00E+11	0.0	18100.0
771.	hex2yl+O2=>CH3CHO+IC4H8+OH	2.10E+11	0.0	6858.0
772.	hex2yl+HO2=>CH3CHO+nC4H9+OH	1.00E+13	0.0	0.0
773.	hex2yl+OH=hexene1+H2O	3.64E+13	0.0	0.0
774.	hex2yl+O=CH3CHO+nC4H9	1.61E+13	0.0	0.0
775.	hex3yl=IC4H8+C2H5	6.00E+13	0.0	29700.0
776.	hex2yl=C3H6+nC3H7	5.00E+13	0.0	28700.0
777.	hex1yl=C2H4+nC4H9	1.00E+13	0.0	28700.0

778. hex1yl+H=hexene1+H2	1.81E+12	0.0	0.0
779. hex2yl+O2=hexene1+HO2	3.00E+12	0.0	4500.0
780. hex1yl+O2=hexene1+HO2	2.00E+12	0.0	2000.0
781. hex1yl+OH=hexene1+H2O	2.43E+13	0.0	0.0
782. hex1yl+CH3=hexene1+CH4	1.00E+12	0.0	0.0
783. hex1yl+C2H5=hexene1+C2H6	1.00E+12	0.0	0.0
784. hex1yl+C2H3=hexene1+C2H4	1.00E+12	0.0	0.0
785. hex1yl+AC3H5=hexene1+C3H6	1.00E+12	0.0	0.0
786. hex2yl+CH3=hexene1+CH4	1.00E+12	0.0	0.0
787. hex2yl+C2H5=hexene1+C2H6	1.00E+12	0.0	0.0
788. hex2yl+C2H3=hexene1+C2H4	1.00E+12	0.0	0.0
789. hex2yl+AC3H5=hexene1+C3H6	1.00E+12	0.0	0.0
790. hexene1=AC3H5+nC3H7	1.08E+80	-19.3	95177.0
791. hexene1=C4H7+C2H5	2.71E+80	-19.3	107015.0
792. C2H3+nC4H9=hexene1	1.00E+13	0.0	0.0
793. hexene1+O2=C6H11-13+HO2	4.00E+12	0.0	40000.0
794. hexene1+O2=C6H11-15+HO2	2.80E+13	0.0	48300.0
795. hexene1+O2=C6H11-14+HO2	2.80E+13	0.0	48300.0
796. hexene1+O2=C6H11+HO2	2.10E+13	0.0	51300.0
797. hexene1+HO2=C6H11-14+H2O2	6.80E+12	0.0	17000.0
798. hexene1+HO2=C6H11-15+H2O2	6.80E+12	0.0	17000.0
799. hexene1+HO2=C6H11+H2O2	5.60E+12	0.0	19400.0
800. hexene1+HO2=C6H11-13+H2O2	1.00E+11	0.0	17060.0
801. hexene1+O=C6H11+OH	4.20E+02	3.5	3092.0
802. hexene1+O=C6H11-15+OH	2.25E+03	3.3	1653.0
803. hexene1+O=C6H11-14+OH	2.25E+03	3.3	1653.0
804. hexene1+O=C6H11-13+OH	4.00E+13	0.0	4000.0
805. hexene1+H=C6H11+H2	2.80E+07	2.0	7700.0
806. hexene1+H=C6H11-15+H2	9.10E+06	0.0	5000.0
807. hexene1+H=C6H11-14+H2	9.10E+06	0.0	5000.0
808. hexene1+H=C6H11-13+H2	6.55E+12	0.0	4445.0
809. hexene1+OH=C6H11+H2O	2.85E+05	2.3	236.0

810.	hexene1+OH=C6H11-15+H2O	6.35E+06	2.0	-500.0
811.	hexene1+OH=C6H11-14+H2O	6.35E+06	2.0	-500.0
812.	hexene1+OH=C6H11-13+H2O	6.00E+13	0.0	1230.0
813.	hexene1+CH3=C6H11+CH4	1.47E+12	0.0	11722.0
814.	hexene1+CH3=C6H11-15+CH4	6.60E+11	0.0	10120.0
815.	hexene1+CH3=C6H11-14+CH4	6.60E+11	0.0	10120.0
816.	hexene1+CH3=C6H11-13+CH4	2.00E+11	0.0	6800.0
817.	hexene1+C2H3=C6H11-13+C2H4	2.00E+11	0.0	6800.0
818.	hexene1+C2H3=C6H11-14+C2H4	6.60E+12	0.0	10120.0
819.	hexene1+C2H3=C6H11-15+C2H4	6.60E+12	0.0	10120.0
820.	hexene1+C2H3=C6H11+C2H4	2.94E+12	0.0	11722.0
821.	C6H11-13+H=hexene1	1.00E+13	0.0	0.0
822.	hexene1+nC3H7=C6H11-13+C3H8	1.00E+11	0.0	8300.0
823.	C6H11-13+HO2=>nC3H7+C2H3CHO+OH	1.00E+12	0.0	8000.0
824.	C6H11=C6H11-12	1.00E+11	0.0	20320.0
825.	C6H11-12=C6H11-15	2.00E+11	0.0	18100.0
826.	C6H11-12=nC3H7+AC3H4	1.00E+12	0.0	33000.0
827.	C6H11-14=C2H3+IC4H8	4.00E+13	0.0	35500.0
828.	C6H11-15=AC3H5+C3H6	4.00E+13	0.0	35500.0
829.	C6H11=C4H7+C2H4	8.13E+51	-12.2	41926.0
830.	C6H11=C6H11-13	1.42E+80	-21.3	41217.0
831.	C6H11=C2H5+iiiC4H6	5.41E+78	-19.9	59833.0
832.	C6H11-13=C4H7+C2H4	8.18E+84	-21.4	72373.0
833.	C6H11-13=C2H5+iiiC4H6	8.36E+68	-16.6	62898.0
834.	CYC6H9=CY13C6H8+H	1.62E+57	-13.0	66036.0
835.	CYC6H9=C6H9	5.36E+50	-11.9	48276.0
836.	CYC6H9=n-C4H5+C2H4	2.77E+73	-17.3	89006.0
837.	CYC6H9=C6H8+H	4.44E+73	-17.3	89006.0
838.	C6H9=CY13C6H8+H	3.21E+52	-12.5	41221.0
839.	C6H9=n-C4H5+C2H4	2.45E+52	-12.1	51404.0
840.	C6H9=C6H8+H	3.92E+52	-12.1	51404.0
841.	CYC6H9+O2=CY13C6H8+HO2	1.60E+12	0.0	15160.0

842.	CYC6H9+HO2=CY13C6H8+H2O2	1.00E+12	0.0	0.0
843.	CYC6H9+OH=CY13C6H8+H2O	6.02E+12	0.0	0.0
844.	CYC6H9+O=CY13C6H8+OH	1.80E+13	0.0	0.0
845.	CYC6H9+H=CY13C6H8+H2	3.16E+13	0.0	0.0
846.	CYC6H9+CH3=CY13C6H8+CH4	8.00E+12	0.0	0.0
847.	CYC6H9+HCO=CY13C6H8+CH2O	4.00E+12	0.0	0.0
848.	CY13C6H8+O2=CYC6H7+HO2	8.31E+11	0.0	24858.0
849.	CY13C6H8+HO2=CYC6H7+H2O2	4.00E+12	0.0	17057.0
850.	CY13C6H8+OH=CYC6H7+H2O	6.00E+06	2.0	-1520.0
851.	CY13C6H8+O=CYC6H7+OH	1.40E+13	0.0	-795.0
852.	CY13C6H8+H=CYC6H7+H2	1.10E+05	2.5	-1900.0
853.	CY13C6H8+CH3=CYC6H7+CH4	1.23E+11	0.0	5201.0
854.	CY13C6H8+C2H3=CYC6H7+C2H4	1.23E+11	0.0	5201.0
855.	CY13C6H8+HCO=CYC6H7+CH2O	1.23E+11	0.0	5201.0
856.	CY13C6H8+C2H2=A+C2H4	3.10E+10	0.0	27200.0
857.	CYC6H7+O2=A+HO2	1.00E+12	0.0	0.0
858.	CYC6H7+HO2=A+H2O2	1.00E+12	0.0	0.0
859.	CYC6H7+HO2=C5H6+HCO+OH	4.50E+12	0.0	0.0
860.	CYC6H7+OH=A+H2O	6.02E+12	0.0	0.0
861.	CYC6H7+O=A+OH	1.80E+13	0.0	0.0
862.	CYC6H7+O=C5H6+HCO	8.26E+13	0.0	0.0
863.	CYC6H7+H=A+H2	3.16E+13	0.0	0.0
864.	CYC6H7+CH3=A+CH4	8.00E+12	0.0	0.0
865.	CYC6H7+HCO=A+CH2O	4.00E+12	0.0	0.0
866.	C6H11+H=C6H10+H2	1.80E+12	0.0	0.0
867.	C6H11+O2=C6H10+HO2	1.00E+11	0.0	0.0
868.	C6H11+CH3=C6H10+CH4	1.10E+13	0.0	0.0
869.	C6H11+O=C6H10+OH	4.82E+13	0.0	0.0
870.	C6H11+OH=C6H10+H2O	2.41E+13	0.0	0.0
871.	C6H10+H=C4H7+C2H4	1.46E+30	-4.3	21647.0
872.	C6H10+O=CH2CO+C4H7+H	1.20E+08	1.6	327.0
873.	C6H9+O2=C6H8+HO2	1.60E+12	0.0	5000.0

874.	C6H9+H=C6H8+H2	1.80E+12	0.0	0.0
875.	C6H9+CH3=C6H8+CH4	1.10E+13	0.0	0.0
876.	C6H9+O=C6H8+OH	4.82E+13	0.0	0.0
877.	C6H9+OH=C6H8+H2O	2.41E+13	0.0	0.0
878.	C6H8+O=CH2CO+n-C4H5+H	1.20E+08	1.6	327.0
879.	THP+H=THP-2-yl+H2	2.50E+14	0.0	11020.0
880.	THP+CH3=THP-2-yl+CH4	2.60E+14	0.0	16255.0
881.	THP+H=THP-3-yl+H2	2.24E+14	0.0	10964.0
882.	THP+CH3=THP-3-yl+CH4	1.14E+14	0.0	17294.0
883.	THP+H=THP-4-yl+H2	1.06E+14	0.0	9950.0
884.	THP+CH3=THP-4-yl+CH4	5.36E+13	0.0	16599.0
885.	THP+C2H3=THP-2-yl+C2H4	2.60E+14	0.0	16255.0
886.	THP+HCO=THP-2-yl+CH2O	2.60E+14	0.0	16255.0
887.	THP+CH3CO=THP-2-yl+CH3CHO	2.60E+14	0.0	16255.0
888.	THP+C2H3=THP-3-yl+C2H4	1.14E+14	0.0	17294.0
889.	THP+HCO=THP-3-yl+CH2O	1.14E+14	0.0	17294.0
890.	THP+CH3CO=THP-3-yl+CH3CHO	1.14E+14	0.0	17294.0
891.	THP+C2H3=THP-4-yl+C2H4	5.36E+13	0.0	16599.0
892.	THP+HCO=THP-4-yl+CH2O	5.36E+13	0.0	16599.0
893.	THP+CH3CO=THP-4-yl+CH3CHO	5.36E+13	0.0	16599.0
894.	THP+O2=THP-2-yl+HO2	2.50E+13	0.0	49000.0
895.	THP+O2=THP-3-yl+HO2	2.50E+13	0.0	49000.0
896.	THP+O2=THP-4-yl+HO2	1.25E+13	0.0	49000.0
897.	THP+HO2=THP-2-yl+H2O2	4.00E+12	0.0	17057.0
898.	THP+HO2=THP-3-yl+H2O2	4.00E+12	0.0	17057.0
899.	THP+HO2=THP-4-yl+H2O2	2.00E+12	0.0	17057.0
900.	THP+OH=THP-2-yl+H2O	7.50E+06	2.0	-765.0
901.	THP+OH=THP-3-yl+H2O	7.50E+06	2.0	-765.0
902.	THP+OH=THP-4-yl+H2O	3.75E+06	2.0	-765.0
903.	THP+O=THP-2-yl+OH	8.67E+05	2.6	2563.0
904.	THP+O=THP-3-yl+OH	8.67E+05	2.6	2563.0
905.	THP+O=THP-4-yl+OH	4.33E+05	2.6	2563.0

906. THP+M=THP-2-yl+H+M	1.00E+16	0.0	95000.0
907. THP+M=THP-3-yl+H+M	1.00E+16	0.0	95000.0
908. THP+M=THP-4-yl+H+M	5.00E+15	0.0	95000.0
909. THP-2-yl=THP-2-ene+H	1.46E+44	-10.4	41739.0
910. THP-3-yl=THP-2-ene+H	1.88E+44	-10.4	41489.0
911. THP-3-yl=THP-3-ene+H	1.88E+41	-10.4	41489.0
912. THP-4-yl=THP-3-ene+H	2.82E+41	-10.3	41451.0
913. THP-2-yl+O2=THP-2-ene+HO2	1.20E+11	0.0	0.0
914. THP-3-yl+O2=THP-2-ene+HO2	1.20E+11	0.0	0.0
915. THP-3-yl+O2=THP-3-ene+HO2	1.20E+11	0.0	0.0
916. THP-4-yl+O2=THP-3-ene+HO2	2.40E+11	0.0	0.0
917. THP-2-yl+HO2=THP-2-ene+H2O2	1.00E+12	0.0	2000.0
918. THP-3-yl+HO2=THP-2-ene+H2O2	1.00E+12	0.0	2000.0
919. THP-3-yl+HO2=THP-3-ene+H2O2	1.00E+12	0.0	2000.0
920. THP-4-yl+HO2=THP-3-ene+H2O2	2.00E+12	0.0	2000.0
921. THP-2-yl+OH=THP-2-ene+H2O	2.40E+13	0.0	0.0
922. THP-3-yl+OH=THP-2-ene+H2O	2.40E+13	0.0	0.0
923. THP-3-yl+OH=THP-3-ene+H2O	2.40E+13	0.0	0.0
924. THP-4-yl+OH=THP-3-ene+H2O	4.80E+13	0.0	0.0
925. THP-2-yl+O=THP-2-ene+OH	4.82E+13	0.0	0.0
926. THP-3-yl+O=THP-2-ene+OH	4.82E+13	0.0	0.0
927. THP-3-yl+O=THP-3-ene+OH	4.82E+13	0.0	0.0
928. THP-4-yl+O=THP-3-ene+OH	9.64E+13	0.0	0.0
929. THP-2-yl+H=THP-2-ene+H2	1.00E+11	0.0	0.0
930. THP-3-yl+H=THP-2-ene+H2	1.00E+11	0.0	0.0
931. THP-3-yl+H=THP-3-ene+H2	1.00E+11	0.0	0.0
932. THP-4-yl+H=THP-3-ene+H2	2.00E+11	0.0	0.0
933. THP-2-yl+CH3=THP-2-ene+CH4	2.00E+12	0.0	0.0
934. THP-3-yl+CH3=THP-2-ene+CH4	2.00E+12	0.0	0.0
935. THP-3-yl+CH3=THP-3-ene+CH4	2.00E+12	0.0	0.0
936. THP-4-yl+CH3=THP-3-ene+CH4	4.00E+12	0.0	0.0
937. THP-2-yl+HCO=THP-2-ene+CH2O	2.00E+12	0.0	0.0

938.	THP-3-yl+HCO=THP-2-ene+CH2O	2.00E+12	0.0	0.0
939.	THP-3-yl+HCO=THP-3-ene+CH2O	2.00E+12	0.0	0.0
940.	THP-4-yl+HCO=THP-3-ene+CH2O	4.00E+12	0.0	0.0
941.	THP-2-yl=OCHCH2CH2CH2CH2	8.77E+70	-18.4	42566.0
942.	THP-2-yl=CH2CHOCH2CH2CH2	6.04E+59	-14.9	38989.0
943.	THP-3-yl=CH2CHCH2OCH2CH2	5.28E+61	-15.6	39307.0
944.	THP-3-yl=CH2CHCH2CH2CH2O	2.41E+61	-15.4	39233.0
945.	THP-4-yl=CH2CHCH2CH2OCH2	7.83E+60	-15.2	38996.0
946.	THP-2-ene=THP-234-enyl+H	2.99E+53	-11.5	95520.0
947.	THP-3-ene=THP-234-enyl+H	2.99E+53	-11.5	95520.0
948.	THP-3-ene=THP-345-enyl+H	2.99E+53	-11.5	95520.0
949.	THP-2-ene+O2=THP-234-enyl+HO2	3.60E+13	0.0	34800.0
950.	THP-3-ene+O2=THP-234-enyl+HO2	3.60E+13	0.0	34800.0
951.	THP-3-ene+O2=THP-345-enyl+HO2	3.60E+13	0.0	34800.0
952.	THP-2-ene+HO2=THP-234-enyl+H2O2	1.00E+11	0.0	17060.0
953.	THP-3-ene+HO2=THP-234-enyl+H2O2	1.00E+11	0.0	17060.0
954.	THP-3-ene+HO2=THP-345-enyl+H2O2	1.00E+11	0.0	17060.0
955.	THP-2-ene+OH=THP-234-enyl+H2O	3.00E+13	0.0	300.0
956.	THP-3-ene+OH=THP-234-enyl+H2O	3.00E+13	0.0	300.0
957.	THP-3-ene+OH=THP-345-enyl+H2O	3.00E+13	0.0	300.0
958.	THP-2-ene+O=THP-234-enyl+OH	3.10E+12	0.0	4445.0
959.	THP-3-ene+O=THP-234-enyl+OH	3.10E+12	0.0	4445.0
960.	THP-3-ene+O=THP-345-enyl+OH	3.10E+12	0.0	4445.0
961.	THP-2-ene+H=THP-234-enyl+H2	3.10E+12	0.0	4445.0
962.	THP-3-ene+H=THP-234-enyl+H2	3.10E+12	0.0	4445.0
963.	THP-3-ene+H=THP-345-enyl+H2	3.10E+12	0.0	4445.0
964.	THP-2-ene+CH3=THP-234-enyl+CH4	8.25E+10	0.0	4118.0
965.	THP-3-ene+CH3=THP-234-enyl+CH4	8.25E+10	0.0	4118.0
966.	THP-3-ene+CH3=THP-345-enyl+CH4	8.25E+10	0.0	4118.0
967.	THP-2-ene+HCO=THP-234-enyl+CH2O	8.25E+10	0.0	4118.0
968.	THP-3-ene+HCO=THP-234-enyl+CH2O	8.25E+10	0.0	4118.0
969.	THP-3-ene+HCO=THP-345-enyl+CH2O	8.25E+10	0.0	4118.0

970.	THP-234-enyl=CH2CHCHCHOCH2	2.68E+50	-11.9	48276.0
971.	THP-234-enyl=OCHCHCHCH2CH2	2.68E+50	-11.9	48276.0
972.	THP-345-enyl=CH2CHCHCHCH2O	2.68E+50	-11.9	48276.0
973.	THP-234-enyl=THP-2-4-ene+H	1.62E+57	-13.0	66036.0
974.	THP-345-enyl=THP-2-4-ene+H	1.62E+57	-13.0	66036.0
975.	THP-234-enyl+O2=THP-2-4-ene+HO2	1.60E+12	0.0	15160.0
976.	THP-345-enyl+O2=THP-2-4-ene+HO2	1.60E+12	0.0	15160.0
977.	THP-234-enyl+HO2=THP-2-4-ene+H2O2	1.00E+12	0.0	0.0
978.	THP-345-enyl+HO2=THP-2-4-ene+H2O2	1.00E+12	0.0	0.0
979.	THP-234-enyl+OH=THP-2-4-ene+H2O	6.02E+12	0.0	0.0
980.	THP-345-enyl+OH=THP-2-4-ene+H2O	6.02E+12	0.0	0.0
981.	THP-234-enyl+O=THP-2-4-ene+OH	1.80E+13	0.0	0.0
982.	THP-345-enyl+O=THP-2-4-ene+OH	1.80E+13	0.0	0.0
983.	THP-234-enyl+H=THP-2-4-ene+H2	3.16E+13	0.0	0.0
984.	THP-345-enyl+H=THP-2-4-ene+H2	3.16E+13	0.0	0.0
985.	THP-234-enyl+CH3=THP-2-4-ene+CH4	8.00E+12	0.0	0.0
986.	THP-345-enyl+CH3=THP-2-4-ene+CH4	8.00E+12	0.0	0.0
987.	THP-234-enyl+HCO=THP-2-4-ene+CH2O	4.00E+12	0.0	0.0
988.	THP-345-enyl+HCO=THP-2-4-ene+CH2O	4.00E+12	0.0	0.0
989.	THP-2-4-ene+O2=THP-5yl+HO2	4.16E+11	0.0	24858.0
990.	THP-2-4-ene+HO2=THP-5yl+H2O2	2.00E+12	0.0	17057.0
991.	THP-2-4-ene+OH=THP-5yl+H2O	3.00E+06	2.0	-1520.0
992.	THP-2-4-ene+O=THP-5yl+OH	7.00E+12	0.0	-795.0
993.	THP-2-4-ene+H=THP-5yl+H2	5.50E+04	2.5	-1900.0
994.	THP-2-4-ene+CH3=THP-5yl+CH4	6.15E+10	0.0	5201.0
995.	THP-2-4-ene+C2H3=THP-5yl+C2H4	6.15E+10	0.0	5201.0
996.	THP-2-4-ene+HCO=THP-5yl+CH2O	6.15E+10	0.0	5201.0
997.	OCHCH2CH2CH2CH2=C2H4+C3H5O	6.31E+48	-11.4	37253.0
998.	CH2CHOCH2CH2CH2=C2H4+CH2CHOCH2	7.06E+48	-11.4	37190.0
999.	CH2CHCH2OCH2CH2=C2H4+C2H3CH2O	8.26E+48	-11.4	37100.0
1000.	CH2CHCH2CH2OCH2=CH2O+C4H7	1.67E+49	-11.6	36676.0
1001.	CH2CHCH2CH2CH2O=CH2O+C4H7	1.69E+48	-11.2	37272.0

1002.	OCHCH2CH2CH2CH2=OCHCH2CH2CHCH2+H	1.15E+52	-12.3	49620.0
1003.	CH2CHOCH2CH2CH2=CH2CHOCH2CHCH2+H	1.16E+52	-12.3	49506.0
1004.	CH2CHCH2OCH2CH2=CH2CHOCH2CHCH2+H	1.17E+52	-12.3	49343.0
1005.	CH2CHCH2CH2CH2O=OCHCH2CH2CHCH2+H	1.21E+52	-12.3	48579.0
1006.	OCHCH2CH2CH2CH2+H=OCHCH2CH2CHCH2+H2	1.80E+12	0.0	0.0
1007.	OCHCH2CH2CH2CH2+O2=OCHCH2CH2CHCH2+HO2	1.00E+11	0.0	0.0
1008.	OCHCH2CH2CH2CH2+CH3=OCHCH2CH2CHCH2+CH4	1.10E+13	0.0	0.0
1009.	OCHCH2CH2CH2CH2+O=OCHCH2CH2CHCH2+OH	4.82E+13	0.0	0.0
1010.	OCHCH2CH2CH2CH2+OH=OCHCH2CH2CHCH2+H2O	2.41E+13	0.0	0.0
1011.	CH2CHOCH2CH2CH2+H=CH2CHOCH2CHCH2+H2	1.80E+12	0.0	0.0
1012.	CH2CHOCH2CH2CH2+O2=CH2CHOCH2CHCH2+HO2	1.00E+11	0.0	0.0
1013.	CH2CHOCH2CH2CH2+CH3=CH2CHOCH2CHCH2+CH4	1.10E+13	0.0	0.0
1014.	CH2CHOCH2CH2CH2+O=CH2CHOCH2CHCH2+OH	4.82E+13	0.0	0.0
1015.	CH2CHOCH2CH2CH2+OH=CH2CHOCH2CHCH2+H2O	2.41E+13	0.0	0.0
1016.	CH2CHCH2OCH2CH2+H=CH2CHOCH2CHCH2+H2	1.80E+12	0.0	0.0
1017.	CH2CHCH2OCH2CH2+O2=CH2CHOCH2CHCH2+HO2	1.00E+11	0.0	0.0
1018.	CH2CHCH2OCH2CH2+CH3=CH2CHOCH2CHCH2+CH4	1.10E+13	0.0	0.0
1019.	CH2CHCH2OCH2CH2+O=CH2CHOCH2CHCH2+OH	4.82E+13	0.0	0.0
1020.	CH2CHCH2OCH2CH2+OH=CH2CHOCH2CHCH2+H2O	2.41E+13	0.0	0.0
1021.	CH2CHCH2CH2CH2O+H=OCHCH2CH2CHCH2+H2	1.80E+12	0.0	0.0
1022.	CH2CHCH2CH2CH2O+O2=OCHCH2CH2CHCH2+HO2	1.00E+11	0.0	0.0
1023.	CH2CHCH2CH2CH2O+CH3=OCHCH2CH2CHCH2+CH4	1.10E+13	0.0	0.0
1024.	CH2CHCH2CH2CH2O+O=OCHCH2CH2CHCH2+OH	4.82E+13	0.0	0.0
1025.	CH2CHCH2CH2CH2O+OH=OCHCH2CH2CHCH2+H2O	2.41E+13	0.0	0.0
1026.	CH2CHOCH2CHCH2=CH2CHO+AC3H5	2.00E+15	0.0	5680.0
1027.	OCHCH2CH2CHCH2=CH2CHO+AC3H5	2.00E+15	0.0	5680.0
1028.	CH2O+n-C4H5=CH2CHCHCHOCH2	1.00E+11	0.0	0.0
1029.	CH2O+n-C4H5=CH2CHCHCHCH2O	1.00E+11	0.0	0.0
1030.	C2H4+C2H2+HCO=OCHCHCHCH2CH2	1.00E+11	0.0	0.0
1031.	C3H5O=C2H3CHO+H	1.27E+24	-4.8	23777.0
1032.	C3H5O+H=C2H3CHO+H2	1.80E+12	0.0	0.0
1033.	C3H5O+O2=C2H3CHO+HO2	1.00E+11	0.0	0.0

1034. C3H5O+CH3=C2H3CHO+CH4	1.10E+13	0.0	0.0
1035. C2H4+HCO=C3H5O	1.23E+35	-7.8	9930.0
1036. CH2O+C2H3=CH2CHOCH2	1.23E+35	-7.8	9930.0
1037. OCHCHCHCH2CH2=OCHCHCHCHCH2+H	3.92E+52	-12.1	51404.0
1038. OCHCHCHCH2CH2+O2=OCHCHCHCHCH2+HO2	1.60E+12	0.0	0.0
1039. OCHCHCHCH2CH2+H=OCHCHCHCHCH2+H2	1.80E+12	0.0	0.0
1040. OCHCHCHCH2CH2+CH3=OCHCHCHCHCH2+CH4	1.10E+13	0.0	0.0
1041. OCHCHCHCH2CH2+O=OCHCHCHCHCH2+OH	4.82E+13	0.0	0.0
1042. OCHCHCHCH2CH2+OH=OCHCHCHCHCH2+H2O	2.41E+13	0.0	0.0
1043. THP=CH2O+IC4H8	8.25E+15	0.0	83000.0
1044. THP=C2H4+C3H6O	1.65E+16	0.0	83000.0
1045. THP=C3H6+CH3CHO	1.65E+16	0.0	83000.0
1046. C3H6O=HCO+C2H5	1.00E+13	0.0	57200.0

UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX F

MORPHOLINE REACTION SET

The following is the reaction set for H/N/O combustion described in Chapters 7 and 8. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	HE	C	O	N	AR
1	H	G	0	1.01E+00	200	3500	1	0	0	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0	0	0
3	C	G	0	1.20E+01	200	3500	0	0	1	0	0	0
4	O	G	0	1.60E+01	200	3500	0	0	0	1	0	0
5	O2	G	0	3.20E+01	200	3500	0	0	0	2	0	0
6	OH	G	0	1.70E+01	200	6000	1	0	0	1	0	0
7	H2O	G	0	1.80E+01	200	3500	2	0	0	1	0	0
8	HO2	G	0	3.30E+01	200	3500	1	0	0	2	0	0
9	H2O2	G	0	3.40E+01	200	3500	2	0	0	2	0	0
10	CH	G	0	1.30E+01	200	6000	1	0	1	0	0	0
11	CH2	G	0	1.40E+01	200	6000	2	0	1	0	0	0
12	CH2SING	G	0	1.40E+01	200	6000	2	0	1	0	0	0
13	CH3	G	0	1.50E+01	200	6000	3	0	1	0	0	0
14	CH4	G	0	1.60E+01	200	3500	4	0	1	0	0	0
15	C2	G	0	2.40E+01	200	6000	0	0	2	0	0	0
16	CO	G	0	2.80E+01	200	3500	0	0	1	1	0	0
17	HCO	G	0	2.90E+01	200	3500	1	0	1	1	0	0
18	CH2O	G	0	3.00E+01	200	3500	2	0	1	1	0	0
19	CH2OH	G	0	3.10E+01	200	6000	3	0	1	1	0	0
20	CH3O	G	0	3.10E+01	200	6000	3	0	1	1	0	0
21	CH3OH	G	0	3.20E+01	200	3500	4	0	1	1	0	0
22	C2H	G	0	2.50E+01	200	3500	1	0	2	0	0	0
23	C2H2	G	0	2.60E+01	200	3500	2	0	2	0	0	0

24	H2CC	G	0	2.60E+01	200	6000	2	0	2	0	0	0
25	C2H3	G	0	2.70E+01	200	5000	3	0	2	0	0	0
26	C2H4	G	0	2.81E+01	200	3500	4	0	2	0	0	0
27	C2H5	G	0	2.91E+01	200	3500	5	0	2	0	0	0
28	C2H6	G	0	3.01E+01	200	3500	6	0	2	0	0	0
29	C3H2	G	0	3.80E+01	300	5000	2	0	3	0	0	0
30	C3H3	G	0	3.91E+01	200	6000	3	0	3	0	0	0
31	AR	G	0	3.99E+01	300	5000	0	0	0	0	0	1
32	AC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
33	PC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
34	C2O	G	0	4.00E+01	300	4000	0	0	2	1	0	0
35	HCCO	G	0	4.10E+01	300	4000	1	0	2	1	0	0
36	AC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
37	TC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
38	SC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
39	CH2CO	G	0	4.20E+01	200	3500	2	0	2	1	0	0
40	C3H6	G	0	4.21E+01	300	5000	6	0	3	0	0	0
41	CH3CO	G	0	4.30E+01	200	6000	3	0	2	1	0	0
42	CH2CHO	G	0	4.30E+01	300	5000	3	0	2	1	0	0
43	nC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
44	iC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
45	C2H4O	G	0	4.41E+01	300	5000	4	0	2	1	0	0
46	CH3CHO	G	0	4.41E+01	200	6000	4	0	2	1	0	0
47	C3H8	G	0	4.41E+01	300	3000	8	0	3	0	0	0
48	CO2	G	0	4.40E+01	200	3500	0	0	1	2	0	0
49	OCHO	G	0	4.50E+01	300	5000	1	0	1	2	0	0
50	C2H5O	G	0	4.51E+01	200	6000	5	0	2	1	0	0
51	CH3CHOH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
52	C2H4OH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
53	CH3OCH2	G	0	4.51E+01	300	5000	5	0	2	1	0	0
54	CH3OCH3	G	0	4.61E+01	270	3000	6	0	2	1	0	0

55	C2H5OH	G	0	4.61E+01	200	6000	6	0	2	1	0	0
56	CH3OCO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
57	CH3OCHO	G	0	6.01E+01	300	5000	4	0	2	2	0	0
58	CH3OCH2O	G	0	6.11E+01	300	5000	5	0	2	2	0	0
59	HOC2H4O2	G	0	7.71E+01	300	5000	5	0	2	3	0	0
60	C4H	G	0	4.91E+01	300	3000	1	0	4	0	0	0
61	C2H5OO	G	0	6.11E+01	300	5000	5	0	2	2	0	0
62	C2H3CO	G	0	5.51E+01	200	6000	3	0	3	1	0	0
63	C2H3CHO	G	0	5.61E+01	298	3000	4	0	3	1	0	0
64	C2H3CH2O	G	0	5.71E+01	300	3000	5	0	3	1	0	0
65	C4H2	G	0	5.01E+01	300	3000	2	0	4	0	0	0
66	iC4H3	G	0	5.11E+01	200	5000	3	0	4	0	0	0
67	nC4H3	G	0	5.11E+01	300	4000	3	0	4	0	0	0
68	C4H4	G	0	5.21E+01	300	3000	4	0	4	0	0	0
69	n-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
70	i-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
71	iiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
72	iiiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
73	C4H7	G	0	5.51E+01	300	3000	7	0	4	0	0	0
74	IC4H8	G	0	5.61E+01	300	5000	8	0	4	0	0	0
75	nC4H9	G	0	5.71E+01	200	6000	9	0	4	0	0	0
76	OCHCHO	G	0	5.80E+01	300	3000	2	0	2	2	0	0
77	C2H3OO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
78	C5H2	G	0	6.21E+01	200	5000	2	0	5	0	0	0
79	H2CCCCCH	G	0	6.31E+01	200	5000	3	0	5	0	0	0
80	HCCCHCCH	G	0	6.31E+01	200	5000	3	0	5	0	0	0
81	C5H5	G	0	6.51E+01	300	5000	5	0	5	0	0	0
82	l-C5H5	G	0	6.51E+01	300	5000	5	0	5	0	0	0
83	H2C4O	G	0	6.61E+01	300	4000	2	0	4	1	0	0
84	C5H6	G	0	6.61E+01	300	5000	6	0	5	0	0	0
85	CH2CHCH2CCH	G	0	6.61E+01	300	5000	6	0	5	0	0	0

86	CH2CHCHCCH2	G	0	6.61E+01	300	5000	6	0	5	0	0	0
87	C6H2	G	0	7.41E+01	300	3000	2	0	6	0	0	0
88	C6H3	G	0	7.51E+01	300	3000	3	0	6	0	0	0
89	l-C6H4	G	0	7.61E+01	300	3000	4	0	6	0	0	0
90	c-C6H4	G	0	7.61E+01	300	3000	4	0	6	0	0	0
91	n-C6H5	G	0	7.71E+01	300	3000	5	0	6	0	0	0
92	i-C6H5	G	0	7.71E+01	300	3000	5	0	6	0	0	0
93	A1	G	0	7.71E+01	300	3000	5	0	6	0	0	0
94	A	G	0	7.81E+01	300	3000	6	0	6	0	0	0
95	FC6H6	G	0	7.81E+01	200	6000	6	0	6	0	0	0
96	l-C6H6	G	0	7.81E+01	300	3000	6	0	6	0	0	0
97	C4H5C2H	G	0	7.81E+01	200	5000	6	0	6	0	0	0
98	CYC6H7	G	0	7.91E+01	200	6000	7	0	6	0	0	0
99	n-C6H7	G	0	7.91E+01	300	3000	7	0	6	0	0	0
100	i-C6H7	G	0	7.91E+01	300	3000	7	0	6	0	0	0
101	C5H4O	G	0	8.01E+01	300	5000	4	0	5	1	0	0
102	C6H8	G	0	8.01E+01	300	3000	8	0	6	0	0	0
103	CY13C6H8	G	0	8.01E+01	200	6000	8	0	6	0	0	0
104	C5H5O	G	0	8.11E+01	300	5000	5	0	5	1	0	0
105	C5H4OH	G	0	8.11E+01	300	5000	5	0	5	1	0	0
106	C6H9	G	0	8.11E+01	298	3000	9	0	6	0	0	0
107	CYC6H9	G	0	8.11E+01	298	3000	9	0	6	0	0	0
108	CYC6H10	G	0	8.21E+01	200	6000	10	0	6	0	0	0
109	C6H10	G	0	8.21E+01	298	3000	10	0	6	0	0	0
110	CYC6H11	G	0	8.32E+01	298	5000	11	0	6	0	0	0
111	C6H11-12	G	0	8.32E+01	300	5000	11	0	6	0	0	0
112	C6H11-13	G	0	8.32E+01	300	5000	11	0	6	0	0	0
113	C6H11-14	G	0	8.32E+01	300	5000	11	0	6	0	0	0
114	C6H11-15	G	0	8.32E+01	300	5000	11	0	6	0	0	0
115	C6H11	G	0	8.32E+01	298	3000	11	0	6	0	0	0
116	CYC6H12	G	0	8.42E+01	200	5000	12	0	6	0	0	0

117	hexene1	G	0	8.42E+01	200	6000	12	0	6	0	0	0
118	hex1yl	G	0	8.52E+01	200	6000	13	0	6	0	0	0
119	hex2yl	G	0	8.52E+01	200	6000	13	0	6	0	0	0
120	hex3yl	G	0	8.52E+01	300	5000	13	0	6	0	0	0
121	N	G	0	1.40E+01	300	5000	0	0	0	0	1	0
122	NH	G	0	1.50E+01	200	6000	1	0	0	0	1	0
123	NH2	G	0	1.60E+01	300	5000	2	0	0	0	1	0
124	NH3	G	0	1.70E+01	300	5000	3	0	0	0	1	0
125	N2	G	0	2.80E+01	200	6000	0	0	0	0	2	0
126	NNH	G	0	2.90E+01	200	6000	1	0	0	0	2	0
127	N2H2	G	0	3.00E+01	300	5000	2	0	0	0	2	0
128	H2NN	G	0	3.00E+01	300	5000	2	0	0	0	2	0
129	N2H3	G	0	3.10E+01	300	5000	3	0	0	0	2	0
130	N2H4	G	0	3.20E+01	300	5000	4	0	0	0	2	0
131	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0
132	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
133	HON	G	0	3.10E+01	300	5000	1	0	0	1	1	0
134	HNOH	G	0	3.20E+01	200	6000	2	0	0	1	1	0
135	NH2O	G	0	3.20E+01	300	4000	2	0	0	1	1	0
136	NH2OH	G	0	3.30E+01	300	5000	3	0	0	1	1	0
137	HNNNH2	G	0	4.50E+01	300	5000	3	0	0	0	3	0
138	N2O	G	0	4.40E+01	300	5000	0	0	0	1	2	0
139	HNNO	G	0	4.50E+01	300	5000	1	0	0	1	2	0
140	NH2NO	G	0	4.60E+01	200	6000	2	0	0	1	2	0
141	NHNHO	G	0	4.60E+01	300	5000	2	0	0	1	2	0
142	NH2NHO	G	0	4.70E+01	300	5000	3	0	0	1	2	0
143	NO2	G	0	4.60E+01	200	6000	0	0	0	2	1	0
144	HONO	G	0	4.70E+01	200	6000	1	0	0	2	1	0
145	HNO2	G	0	4.70E+01	300	4000	1	0	0	2	1	0
146	HNOO	G	0	4.70E+01	300	5000	1	0	0	2	1	0
147	HONHO	G	0	4.80E+01	300	5000	2	0	0	2	1	0

148	NH2NO2	G	0	6.20E+01	200	6000	2	0	0	2	2	0
149	NO3	G	0	6.20E+01	200	6000	0	0	0	3	1	0
150	HNO3	G	0	6.30E+01	200	6000	1	0	0	3	1	0
151	N2O4	G	0	9.20E+01	200	6000	0	0	0	4	2	0
152	HE	G	0	4.00E+00	200	6000	0	1	0	0	0	0
153	CN	G	0	2.60E+01	200	6000	0	0	1	0	1	0
154	HCN	G	0	2.70E+01	300	4000	1	0	1	0	1	0
155	HNC	G	0	2.70E+01	300	5000	1	0	1	0	1	0
156	CHNH	G	0	2.80E+01	300	4000	2	0	1	0	1	0
157	NCH2	G	0	2.80E+01	300	4000	2	0	1	0	1	0
158	CH2NH	G	0	2.90E+01	300	5000	3	0	1	0	1	0
159	CH3N	G	0	2.90E+01	200	5000	3	0	1	0	1	0
160	CH3NH	G	0	3.01E+01	300	5000	4	0	1	0	1	0
161	CH2NH2	G	0	3.01E+01	300	5000	4	0	1	0	1	0
162	CH3NH2	G	0	3.11E+01	300	5000	5	0	1	0	1	0
163	NCN	G	0	4.00E+01	300	4000	0	0	1	0	2	0
164	CHCNH	G	0	4.00E+01	298	3000	2	0	2	0	1	0
165	CH2CN	G	0	4.00E+01	200	6000	2	0	2	0	1	0
166	HCNN	G	0	4.10E+01	300	5000	1	0	1	0	2	0
167	CH2CNH	G	0	4.11E+01	200	5000	3	0	2	0	1	0
168	CH2CHN	G	0	4.11E+01	298	3000	3	0	2	0	1	0
169	CH2CHN(S)	G	0	4.11E+01	298	3000	3	0	2	0	1	0
170	CHCNH2	G	0	4.11E+01	298	3000	3	0	2	0	1	0
171	CH3CN	G	0	4.11E+01	200	6000	3	0	2	0	1	0
172	c-C2H3N	G	0	4.11E+01	298	3000	3	0	2	0	1	0
173	CH2NN	G	0	4.20E+01	200	6000	2	0	1	0	2	0
174	NCO	G	0	4.20E+01	300	5000	0	0	1	1	1	0
175	CH3NCH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
176	CH3CHN	G	0	4.21E+01	298	3000	4	0	2	0	1	0
177	CH3CNH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
178	CH2CNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0

179	CHCHNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
180	CH2NCH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
181	CH2CHNH	G	0	4.21E+01	200	5000	4	0	2	0	1	0
182	CH3CHNH	G	0	4.31E+01	298	3000	5	0	2	0	1	0
183	CH3NCH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
184	CH2CHNH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
185	CH3CH2NH	G	0	4.41E+01	298	3000	6	0	2	0	1	0
186	CH3CHNH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
187	CH2CH2NH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
188	CH3CH2NH2	G	0	4.51E+01	298	3000	7	0	2	0	1	0
189	HCNO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
190	HNCO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
191	HOCN	G	0	4.30E+01	300	5000	1	0	1	1	1	0
192	CH3NN	G	0	4.30E+01	200	6000	3	0	1	0	2	0
193	H2NCO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
194	CH3NNH	G	0	4.41E+01	200	6000	4	0	1	0	2	0
195	H2NCHO	G	0	4.50E+01	200	6000	3	0	1	1	1	0
196	CH2NNH2	G	0	4.41E+01	200	5000	4	0	1	0	2	0
197	CH3NCH3	G	0	4.41E+01	298	3000	6	0	2	0	1	0
198	CH3NHCH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
199	CH2NO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
200	HOCO	G	0	4.50E+01	300	4000	1	0	1	2	0	0
201	CH3NO	G	0	4.50E+01	300	4000	3	0	1	1	1	0
202	CH3NHCH3	G	0	4.51E+01	298	3000	7	0	2	0	1	0
203	NCCN	G	0	5.20E+01	300	5000	0	0	2	0	2	0
204	CHCHNCH2	G	0	5.41E+01	200	5000	4	0	3	0	1	0
205	CH2CHNCH2	G	0	5.51E+01	200	5000	5	0	3	0	1	0
206	NCNO	G	0	5.60E+01	300	4000	0	0	1	1	2	0
207	NCHCHO	G	0	5.60E+01	200	5000	2	0	2	1	1	0
208	CH2NHCHCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
209	CH2CH2NCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0

210	NHCH2CHO	G	0	5.81E+01	200	5000	4	0	2	1	1	0
211	OCH2CHNH	G	0	5.81E+01	200	5000	4	0	2	1	1	0
212	CH3NNCH3	G	0	5.81E+01	300	4000	6	0	2	0	2	0
213	H2CNO2	G	0	6.00E+01	300	4000	2	0	1	2	1	0
214	CH3NO2	G	0	6.10E+01	300	4000	3	0	1	2	1	0
215	CH3ONO	G	0	6.10E+01	300	4000	3	0	1	2	1	0
216	CH3ONO2	G	0	7.70E+01	300	4000	3	0	1	3	1	0
217	cyCHOCHCHNCH	G	0	8.21E+01	200	5000	4	0	4	1	1	0
218	cyOCHCHNCHCH2	G	0	8.31E+01	200	5000	5	0	4	1	1	0
219	cyNCH2CH2OCHCH	G	0	8.41E+01	200	5000	6	0	4	1	1	0
220	CH2CH2NCHCHO	G	0	8.41E+01	200	5000	6	0	4	1	1	0
221	CH2OCHCHNCH2	G	0	8.41E+01	200	5000	6	0	4	1	1	0
222	CH2CHOCH2CHNH	G	0	8.51E+01	200	5000	7	0	4	1	1	0
223	OCHCH2NHCHCH2	G	0	8.51E+01	200	5000	7	0	4	1	1	0
224	cyOCHCHNHCH2CH2	G	0	8.51E+01	200	5000	7	0	4	1	1	0
225	cyOCH2CHNCH2CH2	G	0	8.51E+01	200	5000	7	0	4	1	1	0
226	NHCH2CH2OCHCH2	G	0	8.61E+01	200	5000	8	0	4	1	1	0
227	CH2CH2NHCH2CHO	G	0	8.61E+01	200	5000	8	0	4	1	1	0
228	OCH2CH2NHCHCH2	G	0	8.61E+01	200	5000	8	0	4	1	1	0
229	CH2CH2OCH2CHNH	G	0	8.61E+01	200	5000	8	0	4	1	1	0
230	CH2OCH2CH2NCH2	G	0	8.61E+01	200	5000	8	0	4	1	1	0
231	cyOrthoMorphyl	G	0	8.61E+01	200	5000	8	0	4	1	1	0
232	cyMetaMorphyl	G	0	8.61E+01	200	5000	8	0	4	1	1	0
233	cyParaMorphyl	G	0	8.61E+01	200	5000	8	0	4	1	1	0
234	cyMorph	G	0	8.71E+01	200	5000	9	0	4	1	1	0
235	CH2CHOCH2	G	0	5.71E+01	298	3000	5	0	3	1	0	0
236	CH3CH2NHCH2CHO	G	0	8.71E+01	200	5000	9	0	4	1	1	0
237	NH2CH2CH2OCHCH2	G	0	8.71E+01	200	5000	9	0	4	1	1	0
238	CH3CH2OCH2CHNH	G	0	8.71E+01	200	5000	9	0	4	1	1	0
239	OHCH2CH2NHCHCH2	G	0	8.71E+01	200	5000	9	0	4	1	1	0
240	CH3OCH2CH2NCH2	G	0	8.71E+01	200	5000	9	0	4	1	1	0

241	CH2CHOH	G	0	4.41E+01	200	5000	4	0	2	1	0	0
242	cyOrthoOOMorphyl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
243	cyMetaOOMorphyl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
244	cyParaOOMorphyl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
245	cyOrtho*Morph3yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
246	cyOrtho*Morph4yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
247	cyOrtho*Morph5yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
248	cyOrtho*Morph6yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
249	cyMeta*Morph2yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
250	cyMeta*Morph4yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
251	cyMeta*Morph5yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
252	cyMeta*Morph6yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
253	cyPara*Morph2yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
254	cyPara*Morph3yl	G	0	1.18E+02	200	5000	8	0	4	3	1	0
255	CH2CH2OCH*CHNH	G	0	1.18E+02	200	5000	8	0	4	3	1	0
256	CH2CH2NHCH*CHO	G	0	1.18E+02	200	5000	8	0	4	3	1	0
257	CH2OCH2CH*NCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
258	OCH2CH2N*CHCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
259	OCH2CH2NHCHCH*	G	0	1.18E+02	200	5000	8	0	4	3	1	0
260	NHCH2CH2OCHCH*	G	0	1.18E+02	200	5000	8	0	4	3	1	0
261	CH2OCH2CH2NCH*	G	0	1.18E+02	200	5000	8	0	4	3	1	0
262	CH2CH2OCH2CHN*	G	0	1.18E+02	200	5000	8	0	4	3	1	0
263	CH2OCH*CH2NCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
264	NHCH2CH*OCHCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
265	OCH2CH*NHCHCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
266	CH2CH2N*CH2CHO	G	0	1.18E+02	200	5000	8	0	4	3	1	0
267	CH*OCH2CH2NCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
268	CH*CH2NHCH2CHO	G	0	1.18E+02	200	5000	8	0	4	3	1	0
269	CH*CH2OCH2CHNH	G	0	1.18E+02	200	5000	8	0	4	3	1	0
270	N*CH2CH2OCHCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
271	CH2CH*OCH2CHNH	G	0	1.18E+02	200	5000	8	0	4	3	1	0

272	OCH*CH2NHCHCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
273	CH2CH*NHCH2CHO	G	0	1.18E+02	200	5000	8	0	4	3	1	0
274	NHCH*CH2OCHCH2	G	0	1.18E+02	200	5000	8	0	4	3	1	0
275	OCH*CHNH	G	0	9.01E+01	200	5000	4	0	2	3	1	0
276	NHCH*CHO	G	0	9.01E+01	200	5000	4	0	2	3	1	0
277	CH2CH*NCH2	G	0	8.81E+01	200	5000	6	0	3	2	1	0
278	CH2NHCHCH*	G	0	8.81E+01	200	5000	6	0	3	2	1	0
279	CH2OCHCH*	G	0	8.91E+01	200	5000	5	0	3	3	0	0
280	CH2CH2NCH*	G	0	8.81E+01	200	5000	6	0	3	2	1	0
281	OCH2CHN*	G	0	9.01E+01	200	5000	4	0	2	3	1	0
282	CH*CH2NCH2	G	0	8.81E+01	200	5000	6	0	3	2	1	0
283	CH*OCHCH2	G	0	8.91E+01	200	5000	5	0	3	3	0	0
284	CH*NHCHCH2	G	0	8.81E+01	200	5000	6	0	3	2	1	0
285	N*CH2CHO	G	0	9.01E+01	200	5000	4	0	2	3	1	0
286	OCHOOH	G	0	6.20E+01	200	5000	2	0	1	3	0	0
287	CH2NOOH	G	0	6.10E+01	200	5000	3	0	1	2	1	0
288	NHCHOOH	G	0	6.10E+01	200	5000	3	0	1	2	1	0
289	NCHOOH	G	0	6.00E+01	200	5000	2	0	1	2	1	0
290	CHNOOH	G	0	6.00E+01	200	5000	2	0	1	2	1	0
291	NHCHCHO	G	0	5.71E+01	200	5000	3	0	2	1	1	0
292	CH2CHOOH	G	0	6.01E+01	300	5000	4	0	2	2	0	0
293	CHCHOOH	G	0	5.90E+01	300	5000	3	0	2	2	0	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. 2O+M=O2+M			6.16E+15	-0.5	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			

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 2. 2O+AR=O2+AR                                    1.89E+13    0.0    -1790.0
 3. O+H+M=OH+M                                     4.71E+18   -1.0        0.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    7.500E-01
 4. H2+M=2H+M                                      4.58E+19   -1.4   104380.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    0.000E+00
 5. H2+AR=2H+AR                                    5.84E+18   -1.1   104380.0
 6. H+OH+M=H2O+M                                   2.21E+22   -2.0        0.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    0.000E+00
 7. H+OH+AR=H2O+AR                                 8.41E+21   -2.0        0.0
 8. H2O2(+M)=2OH(+M)                               2.95E+14    0.0    48400.0
    Low pressure limit:  0.12000E+18  0.00000E+00  0.45500E+05
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    1.600E-01
 9. H2O+O=OH+OH                                    2.97E+06    2.0    13400.0
10. O+H2=H+OH                                      5.08E+04    2.7     6290.0
11. OH+H2=H+H2O                                    2.16E+08    1.5     3430.0
12. H+O2(+M)=HO2(+M)                               1.48E+12    0.6        0.0
    Low pressure limit:  0.35000E+17 -0.41000E+00 -0.11200E+04
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    5.000E-02
13. H+O2=O+OH                                      4.49E+08    1.3    16191.0
    Declared duplicate reaction...
14. H+O2=O+OH                                      2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
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15. O+HO2=OH+O2                                   3.25E+13    0.0        0.0
16. H+HO2=O2+H2                                   1.66E+13    0.0      820.0
17. H+HO2=2OH                                     7.08E+13    0.0      300.0
18. OH+HO2=O2+H2O                                 4.64E+13    0.0     -500.0
19. 2HO2=O2+H2O2                                  1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
20. 2HO2=O2+H2O2                                  4.20E+14    0.0    11980.0
    Declared duplicate reaction...
21. O+H2O2=OH+HO2                                 9.55E+06    2.0     3970.0
22. H+H2O2=HO2+H2                                 4.82E+13    0.0     7950.0
23. H+H2O2=OH+H2O                                 2.41E+13    0.0     3970.0
24. OH+H2O2=HO2+H2O                               1.00E+12    0.0        0.0
    Declared duplicate reaction...
25. OH+H2O2=HO2+H2O                               5.80E+14    0.0     9560.0
    Declared duplicate reaction...
26. O+CO(+M)=CO2(+M)                              1.80E+10    0.0     2385.0
    Low pressure limit:  0.60200E+15  0.00000E+00  0.30000E+04
    H2              Enhanced by    2.000E+00
    O2              Enhanced by    6.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    3.500E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    5.000E-01
27. O2+CO=O+CO2                                   2.50E+12    0.0    47800.0
28. H2+CO(+M)=CH2O(+M)                            4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
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    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
29. OH+CO=H+CO2                                    4.10E+04    2.1    -1578.0
30. HO2+CO=OH+CO2                                  1.50E+14    0.0    23600.0
31. O+HCO=OH+CO                                    3.00E+13    0.0        0.0
32. O+HCO=H+CO2                                    3.00E+13    0.0        0.0
33. H+HCO(+M)=CH2O(+M)                             1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
34. H+HCO=H2+CO                                    7.30E+13    0.0        0.0
35. OH+HCO=H2O+CO                                  3.00E+13    0.0        0.0
36. HCO+M=H+CO+M                                   1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
37. HCO+O2=HO2+CO                                  4.22E+12    0.0        0.0
38. HCO+HO2=CO2+OH+H                               3.00E+13    0.0        0.0
39. O+CH2O=OH+HCO                                  1.81E+13    0.0     3078.0
40. O2+CH2O=HO2+HCO                                2.05E+13    0.0    38920.0
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41. H+CH2O=HCO+H2 5.18E+07 1.7 1834.0

42. H+CH2O(+M)=CH2OH(+M) 5.40E+11 0.5 3600.0

Low pressure limit: 0.12700E+33 -0.48200E+01 0.65300E+04

TROE centering: 0.71870E+00 0.10300E+03 0.12910E+04 0.41600E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

43. H+CH2O(+M)=CH3O(+M) 5.40E+11 0.5 2600.0

Low pressure limit: 0.22000E+31 -0.48000E+01 0.55600E+04

TROE centering: 0.75800E+00 0.94000E+02 0.15550E+04 0.42000E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

44. OH+CH2O=HCO+H2O 3.43E+09 1.2 -447.0

45. HO2+CH2O=HCO+H2O2 1.47E+13 0.0 15200.0

46. O+CH2OH=OH+CH2O 4.20E+13 0.0 0.0

47. H+CH2OH=H2+CH2O 6.00E+12 0.0 0.0

48. H+CH2OH=OH+CH3 9.63E+13 0.0 0.0

49. OH+CH2OH=H2O+CH2O 2.40E+13 0.0 0.0

50. CH2OH+O2=HO2+CH2O 2.41E+14 0.0 5017.0

Declared duplicate reaction...

51. CH2OH+O2=HO2+CH2O 1.51E+15 -1.0 0.0

Declared duplicate reaction...

52. CH2OH+HO2=CH2O+H2O2 1.20E+13 0.0 0.0

53. CH2OH+HCO=CH3OH+CO 1.20E+14 0.0 0.0

54. CH2OH+HCO=CH2O+CH2O 1.80E+14 0.0 0.0

55.	2CH2OH=CH3OH+CH2O	3.00E+12	0.0	0.0
56.	CH2OH+CH3O=CH3OH+CH2O	2.40E+13	0.0	0.0
57.	O+CH3O=OH+CH2O	6.00E+12	0.0	0.0
58.	H+CH3O=H2+CH2O	2.00E+13	0.0	0.0
59.	H+CH3O=OH+CH3	3.20E+13	0.0	0.0
60.	OH+CH3O=H2O+CH2O	1.80E+13	0.0	0.0
61.	CH3O+O2=HO2+CH2O	9.03E+13	0.0	11980.0
	Declared duplicate reaction...			
62.	CH3O+O2=HO2+CH2O	2.20E+10	0.0	1748.0
	Declared duplicate reaction...			
63.	CH3O+HO2=CH2O+H2O2	3.00E+11	0.0	0.0
64.	CH3O+CO=CH3+CO2	1.57E+13	0.0	11800.0
65.	CH3O+HCO=CH3OH+CO	9.00E+13	0.0	0.0
66.	2CH3O=CH3OH+CH2O	6.00E+13	0.0	0.0
67.	O+CH3OH=OH+CH2OH	3.88E+05	2.5	3080.0
68.	H+CH3OH=CH2OH+H2	1.44E+13	0.0	6095.0
69.	H+CH3OH=CH3O+H2	3.60E+12	0.0	6095.0
70.	OH+CH3OH=CH2OH+H2O	7.10E+06	1.8	-596.0
71.	OH+CH3OH=CH3O+H2O	1.00E+06	2.1	496.5
72.	CH3+CH3OH=CH2OH+CH4	3.19E+01	3.2	7172.0
73.	O2+CH3OH=CH2OH+HO2	2.05E+13	0.0	44900.0
74.	HCO+CH3OH=CH2OH+CH2O	9.63E+03	2.9	13110.0
75.	HO2+CH3OH=CH2OH+H2O2	3.98E+13	0.0	19400.0
76.	CH3O+CH3OH=CH2OH+CH3OH	3.00E+11	0.0	4060.0
77.	CH3OH(+M)=CH3+OH(+M)	1.90E+16	0.0	91730.0
	Low pressure limit: 0.29500E+45 -0.73500E+01 0.95460E+05			
	TROE centering: 0.41400E+00 0.27900E+03 0.54590E+04			
	H2 Enhanced by 2.000E+00			
	H2O Enhanced by 6.000E+00			
	CH4 Enhanced by 2.000E+00			
	CO Enhanced by 1.500E+00			
	CO2 Enhanced by 2.000E+00			

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    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
78. CH3OH(+M)=CH2OH+H(+M)                          2.69E+16   -0.1    98940.0
    Low pressure limit:  0.23400E+41 -0.63300E+01  0.10310E+06
    TROE centering:      0.77300E+00  0.69300E+03  0.53330E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
79. O+CH4=OH+CH3                                   1.02E+09    1.5     8600.0
80. H+CH4=CH3+H2                                   6.60E+08    1.6    10840.0
81. OH+CH4=CH3+H2O                                 1.00E+08    1.6     3120.0
82. CH+CH4=H+C2H4                                  6.00E+13    0.0        0.0
83. CH2SING+CH4=2CH3                               1.60E+13    0.0     -570.0
84. CH2+CH4=2CH3                                   2.46E+06    2.0     8270.0
85. O+CH3=H+CH2O                                   5.06E+13    0.0        0.0
86. O+CH3=H+H2+CO                                  3.37E+13    0.0        0.0
87. H+CH3(+M)=CH4(+M)                              1.39E+16   -0.5      536.0
    Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
    TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
88. OH+CH3=CH2+H2O                                 5.60E+07    1.6     5420.0
89. OH+CH3=CH2SING+H2O                             6.44E+17   -1.3     1417.0
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 90. HO2+CH3=O2+CH4                                  1.00E+12    0.0        0.0
 91. HO2+CH3=OH+CH3O                                 2.00E+13    0.0        0.0
 92. CH+CH3=H+C2H3                                   3.00E+13    0.0        0.0
 93. CH2SING+CH3=H+C2H4                              1.20E+13    0.0     -570.0
 94. CH3+O2=O+CH3O                                   3.56E+13    0.0    30480.0
 95. CH3+O2=OH+CH2O                                  2.31E+12    0.0    20315.0
 96. CH3+H2O2=HO2+CH4                                2.45E+04    2.5     5180.0
 97. 2CH3(+M)=C2H6(+M)                               6.77E+16   -1.2      654.0
     Low pressure limit:  0.34000E+42 -0.70300E+01  0.27630E+04
     TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
 98. 2CH3=H+C2H5                                     6.84E+12    0.1    10600.0
 99. CH3+HCO=CH4+CO                                  1.21E+14    0.0        0.0
100. CH3+CH2O=HCO+CH4                                3.32E+03    2.8     5860.0
101. CH2+CH3=H+C2H4                                  4.00E+13    0.0        0.0
102. O+CH2=H+HCO                                     8.00E+13    0.0        0.0
103. O+CH2SING=H2+CO                                 1.50E+13    0.0        0.0
104. O+CH2SING=H+HCO                                 1.50E+13    0.0        0.0
105. H+CH2(+M)=CH3(+M)                               6.00E+14    0.0        0.0
     Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
     TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
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     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
106. H+CH2SING=CH+H2                                3.00E+13    0.0        0.0
107. OH+CH2=H+CH2O                                  2.00E+13    0.0        0.0
108. OH+CH2=CH+H2O                                  1.13E+07    2.0     3000.0
109. OH+CH2SING=H+CH2O                              3.00E+13    0.0        0.0
110. HO2+CH2=OH+CH2O                                2.00E+13    0.0        0.0
111. CH+CH2=H+C2H2                                  4.00E+13    0.0        0.0
112. CH2+O2=OH+H+CO                                 5.00E+12    0.0     1500.0
113. CH2+O2=CO2+2H                                  5.80E+12    0.0     1500.0
114. CH2+O2=O+CH2O                                  2.40E+12    0.0     1500.0
115. CH2+H2=H+CH3                                   5.00E+05    2.0     7230.0
116. 2CH2=H2+C2H2                                   1.60E+15    0.0    11944.0
117. 2CH2=H+H+C2H2                                  2.00E+14    0.0    10989.0
118. CH2SING+CO=CH2+CO                              9.00E+12    0.0        0.0
119. CH2SING+AR=CH2+AR                              9.00E+12    0.0      600.0
120. CH2SING+CO2=CH2+CO2                            7.00E+12    0.0        0.0
121. CH2SING+CO2=CO+CH2O                            1.40E+13    0.0        0.0
122. CH2+CO(+M)=CH2CO(+M)                           8.10E+11    0.5     4510.0
     Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
123. CH2SING+O2=H+OH+CO                             2.80E+13    0.0        0.0
124. CH2SING+O2=CO+H2O                              1.20E+13    0.0        0.0
125. CH2SING+H2=CH3+H                               7.00E+13    0.0        0.0
126. CH2SING+H2O(+M)=CH3OH(+M)                      4.82E+17   -1.2     1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
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     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
127. CH2SING+H2O=CH2+H2O                              3.00E+13    0.0        0.0
128. CH2SING+H2O=H2+CH2O                              6.82E+10    0.2     -935.0
129. O+CH=H+CO                                        5.70E+13    0.0        0.0
130. OH+CH=H+HCO                                      3.00E+13    0.0        0.0
131. CH+O2=O+HCO                                      6.71E+13    0.0        0.0
132. CH+H2=H+CH2                                      1.08E+14    0.0     3110.0
133. CH+H2O=H+CH2O                                    5.71E+12    0.0     -755.0
134. CH+CO(+M)=HCCO(+M)                               5.00E+13    0.0        0.0
     Low pressure limit:  0.26900E+29 -0.37400E+01  0.19360E+04
     TROE centering:      0.57570E+00  0.23700E+03  0.16520E+04  0.50690E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
135. CH+CO2=HCO+CO                                    1.90E+14    0.0    15792.0
136. CH+CH2O=H+CH2CO                                  9.46E+13    0.0     -515.0
137. CH+HCCO=CO+C2H2                                  5.00E+13    0.0        0.0
138. O+C2H6=OH+C2H5                                   3.00E+07    2.0     5115.0
139. H+C2H6=C2H5+H2                                   5.40E+02    3.5     5210.0
140. OH+C2H6=C2H5+H2O                                 7.26E+06    2.0      864.0
141. CH3+C2H6=C2H5+CH4                                5.50E-01    4.0     8300.0
142. CH2SING+C2H6=CH3+C2H5                            4.00E+13    0.0     -550.0
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143. C2H6+O2=C2H5+HO2                                 4.04E+13    0.0    50872.0
144. C2H6+CH2OH=CH3OH+C2H5                            1.99E+02    3.0    13976.0
145. C2H6+CH3O=CH3OH+C2H5                             2.41E+11    0.0     7094.0
146. C2H6+C2H=C2H2+C2H5                               3.61E+12    0.0        0.0
147. C2H6+C2H3=C2H4+C2H5                              6.01E+02    3.3    10502.0
148. C2H6+CH3CO=CH3CHO+C2H5                           1.81E+04    2.8    17527.0
149. C2H6+HCO=CH2O+C2H5                               4.70E+04    2.7    18235.0
150. O+C2H5=CH3+CH2O                                  2.24E+13    0.0        0.0
151. O+C2H5=H+CH3CHO                                  1.10E+14    0.0        0.0
152. H+C2H5=H2+C2H4                                   2.00E+12    0.0        0.0
153. H+C2H5(+M)=C2H6(+M)                              5.21E+17   -1.0     1580.0
     Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
     TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
154. C2H5+O2=HO2+C2H4                                 1.92E+07    1.0    -2035.0
155. C2H5+HO2=C2H5O+OH                                3.00E+13    0.0        0.0
156. C2H5+HO2=C2H4+H2O2                               3.01E+11    0.0        0.0
157. C2H5+OH=C2H4+H2O                                 2.41E+13    0.0        0.0
158. C2H5+CH3=CH4+C2H4                                1.13E+12   -0.5        0.0
159. CH3+C2H5(+M)=C3H8(+M)                            9.60E+14   -0.5        0.0
     Low pressure limit:  0.68000E+62 -0.13420E+02  0.60000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.14339E+04  0.53288E+04
160. C2H5+CH2OH=C2H4+CH3OH                            2.41E+12    0.0        0.0
161. C2H5+CH2OH=C2H6+CH2O                             2.41E+12    0.0        0.0
162. C2H5+CH3O=C2H6+CH2O                              2.41E+13    0.0        0.0
163. C2H5+C2H=C2H2+C2H4                               1.81E+12    0.0        0.0
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164. CH2+C2H5=C2H4+CH3                                 1.81E+13    0.0        0.0
165. CH2SING+C2H5=C2H4+CH3                             9.00E+12    0.0        0.0
166. C2H5+CH2SING=C3H6+H                               9.00E+12    0.0        0.0
167. C2H5+H2O2=C2H6+HO2                                8.73E+09    0.0      974.0
168. H+C2H4(+M)=C2H5(+M)                               1.37E+09    1.5     1355.0
     Low pressure limit:  0.20260E+40 -0.66420E+01  0.57690E+04
     TROE centering:     -0.56900E+00  0.29900E+03 -0.91470E+04  0.15240E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
169. H+C2H4=C2H3+H2                                    1.12E+07    2.1    13366.0
170. OH+C2H4=C2H3+H2O                                  1.31E-01    4.2     -860.0
171. OH+C2H4=CH3+CH2O                                  3.19E+01    2.7    -1172.0
172. OH+C2H4=CH3CHO+H                                  8.73E-05    4.6     -618.0
173. CH3+C2H4=C2H3+CH4                                 2.27E+05    2.0     9200.0
174. CH3+C2H4(+M)<=>nC3H7(+M)                          2.55E+06    1.6     5700.0
     Low pressure limit:  0.30000E+64 -0.14600E+02  0.18170E+05
     TROE centering:      0.18940E+00  0.27700E+03  0.87480E+04  0.78910E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
175. C2H4(+M)=H2+C2H2(+M)                              8.00E+12    0.4    88770.0
     Low pressure limit:  0.15800E+52 -0.93000E+01  0.97800E+05
     TROE centering:      0.73450E+00  0.18000E+03  0.10350E+04  0.54170E+04
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     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
176. C2H4+CH2SING=AC3H5+H                          4.53E+13    0.0     -556.0
177. C2H4+HO2=C2H4O+OH                             6.03E+09    0.0     7949.0
178. C2H4+O=H+CH2CHO                               7.33E+07    1.6     1260.0
179. C2H4+O=CH3+HCO                                1.13E+08    1.6     1020.0
180. C2H4+O=C2H3+OH                                2.15E+06    2.5    11900.0
181. C2H4+O2=C2H3+HO2                              4.22E+13    0.0    60800.0
182. C2H4+CO=C2H3+HCO                              1.51E+14    0.0    90616.0
183. C2H4+C2H=C4H4+H                               1.21E+13    0.0        0.0
184. C2H4+C2H2=C2H3+C2H3                           2.41E+13    0.0    68360.0
185. C2H4+C2H4=C2H5+C2H3                           4.82E+14    0.0    71539.0
186. H+C2H3(+M)=C2H4(+M)                           6.08E+12    0.3      280.0
     Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
187. H+C2H2(+M)=C2H3(+M)                           1.71E+10    1.3     2709.0
     Low pressure limit:  0.63480E+32 -0.46639E+01  0.37800E+04
     TROE centering:      0.00000E+00  0.78784E+05 -0.10210E+05  0.10000E-29
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
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     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
188. H+C2H3=H2+C2H2                                  9.64E+13    0.0        0.0
189. OH+C2H3=H2O+C2H2                                5.00E+12    0.0        0.0
190. C2H3+O2=C2H2+HO2                                1.34E+06    1.6     -383.0
     Declared duplicate reaction...
191. C2H3+O2=C2H2+HO2                                1.37E+02    3.4     3663.0
     Declared duplicate reaction...
192. C2H3+O2=HCO+CH2O                                9.33E+13   -0.7      268.7
193. C2H3+O2=H+CO+CH2O                               2.19E+14   -0.7      268.7
194. C2H3+O2=CH2CHO+O                                7.52E+08    1.0     -137.4
195. C2H3+HO2=OH+CH2CO+H                             3.01E+13    0.0        0.0
196. C2H3+CH3=C2H2+CH4                               3.92E+11    0.0        0.0
197. C2H3+O=CH2CO+H                                  1.00E+14    0.0        0.0
198. C2H3OO+H=CH2CHO+OH                              1.00E+14    0.0        0.0
199. C2H3OO+CH2=CH2CHO+CH2O                          2.00E+13    0.0        0.0
200. C2H3OO+OH=CH2CHO+HO2                            2.00E+13    0.0        0.0
201. C2H3OO+O=CH2CHO+O2                              2.00E+13    0.0        0.0
202. C2H3+CH2OH=C2H4+CH2O                            3.01E+13    0.0        0.0
203. C2H3+CH3O=C2H4+CH2O                             2.41E+13    0.0        0.0
204. C2H3+CH3OH=C2H4+CH3O                            1.44E+01    3.1     6935.0
205. C2H3+CH3OH=C2H4+CH2OH                           3.19E+01    3.2     7172.0
206. C2H3+CO=C2H3CO                                  1.51E+11    0.0     4809.0
207. C2H3+C2H=C4H4                                   1.00E+14    0.0        0.0
208. C2H3+C2H=C2H2+C2H2                              9.64E+11    0.0        0.0
209. C2H3+CH3CO=C2H3CO+CH3                           1.81E+13    0.0        0.0
210. C2H5+C2H3=AC3H5+CH3                             8.00E+25   -3.5    11775.0
211. C2H3+C2H5(+M)=IC4H8(+M)                         1.50E+13    0.0        0.0
     Low pressure limit:  0.15500E+57 -0.11790E+02  0.89845E+04
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     TROE centering:      0.19800E+00  0.22779E+04  0.60000E+05  0.57232E+04
212. C2H3+C2H5=C2H2+C2H6                              4.82E+11    0.0        0.0
213. C2H3+CH2SING=C2H2+CH3                            1.81E+13    0.0        0.0
214. C2H3+CH2=C2H2+CH3                                1.81E+13    0.0        0.0
215. C2H3+H2O2=C2H4+HO2                               1.21E+10    0.0     -596.0
216. C2H3+CH2O=C2H4+HCO                               5.43E+03    2.8     5862.0
217. C2H3+CH2=AC3H4+H                                 3.00E+13    0.0        0.0
218. C2H3+C2H3=i-C4H5+H                               1.50E+30   -5.0    13000.0
219. C2H3+C2H3=n-C4H5+H                               1.10E+24   -3.3    12400.0
220. H2CC+C2H2(+M)=C4H4(+M)                           3.50E+05    2.1    -2400.0
     Low pressure limit:  0.14000E+61 -0.12599E+02  0.74170E+04
     TROE centering:      0.98000E+00  0.56000E+02  0.58000E+03  0.41640E+04
     H2              Enhanced by    2.000E+00
     CH4             Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     C2H2            Enhanced by    3.000E+00
     CO              Enhanced by    1.500E+00
     C2H4            Enhanced by    3.000E+00
     C2H6            Enhanced by    3.000E+00
     CO2             Enhanced by    2.000E+00
221. C2H2(+M)=H2CC(+M)                                8.00E+14   -0.5    50750.0
     Low pressure limit:  0.24500E+16 -0.64000E+00  0.49700E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H4            Enhanced by    2.500E+00
222. H2CC+C2H4=iiiC4H6                                1.00E+12    0.0        0.0
223. H2CC+O2=CH2+CO2                                  1.00E+13    0.0        0.0
224. H2CC+H=C2H2+H                                    1.00E+14    0.0        0.0
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225. H2CC+OH=CH2CO+H 2.00E+13 0.0 0.0

226. C2H2+O=C2H+OH 4.60E+19 -1.4 28950.0

227. C2H2+O=CH2+CO 2.35E+08 1.4 2204.5

228. C2H2+O=HCCO+H 9.40E+08 1.4 2204.5

229. OH+C2H2=C2H+H2O 2.63E+06 2.1 17060.0

230. OH+C2H2=H+CH2CO 1.52E+04 2.3 -292.0

231. OH+C2H2=CH3+CO 4.37E+06 1.4 227.0

232. C2H2+CH=C3H2+H 1.10E+13 0.0 0.0

233. C2H2+CH2=C3H3+H 1.20E+13 0.0 6620.0

234. C2H2+CH3=C2H+CH4 1.81E+11 0.0 17289.0

235. C2H2+O2=2HCO 1.00E+12 0.0 28000.0

236. C2H2+CH2OH=C2H3+CH2O 7.23E+11 0.0 9004.0

237. C2H2+CO=C2H+HCO 4.82E+14 0.0 106713.0

238. C2H2+C2H=C4H2+H 3.00E+13 0.0 0.0

239. C2H2+C2H(+M)=nC4H3(+M) 8.30E+10 0.9 -363.0

Low pressure limit: 0.12400E+32 -0.47200E+01 0.18710E+04

TROE centering: 0.10000E+01 0.10000E+03 0.56130E+04 0.13387E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

C2H2 Enhanced by 2.500E+00

C2H4 Enhanced by 2.500E+00

240. C2H2+C2H(+M)=iC4H3(+M) 8.30E+10 0.9 -363.0

Low pressure limit: 0.12400E+32 -0.47200E+01 0.18710E+04

TROE centering: 0.10000E+01 0.10000E+03 0.56130E+04 0.13387E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

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     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
241. C2H2+CH2SING=C3H3+H                          3.42E+15   -0.6     -230.7
242. C2H2+CH2SING=CH2+C2H2                        8.55E+14   -0.6     -230.7
243. HCCO+C2H2=C3H3+CO                            1.00E+11    0.0     3000.0
244. C2H2+C2H3=n-C4H5                             1.10E+32   -7.3     6200.0
245. C2H2+C2H3=i-C4H5                             2.10E+36   -8.8     9100.0
246. C2H3+C2H2=C4H4+H                             5.00E+14   -0.7     6700.0
247. O+C2H=CH+CO                                  1.00E+13    0.0        0.0
248. H+C2H(+M)=C2H2(+M)                           1.00E+17   -1.0        0.0
     Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
     TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
249. OH+C2H=H+HCCO                                2.00E+13    0.0        0.0
250. C2H+O2=HCO+CO                                1.00E+13    0.0     -775.0
251. C2H+H2=H+C2H2                                5.68E+10    0.9     1993.0
252. C2H+HO2=HCCO+OH                              1.81E+13    0.0        0.0
253. C2H+CH3=C3H3+H                               2.41E+13    0.0        0.0
254. C2H+O2=HCCO+O                                6.03E+11    0.0        0.0
255. C2H+CH2OH=C2H2+CH2O                          3.61E+13    0.0        0.0
256. C2H+CH2OH=C3H3+OH                            1.21E+13    0.0        0.0
257. C2H+CH3OH=C2H2+CH2OH                         6.03E+12    0.0        0.0
258. C2H+CH3O=CH2O+C2H2                           2.41E+13    0.0        0.0
259. C2H+CH3OH=C2H2+CH3O                          1.21E+12    0.0        0.0
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260.	C2H+CH2=CH+C2H2	1.81E+13	0.0	0.0
261.	C2H+CH2SING=C2H2+CH	1.81E+13	0.0	0.0
262.	O+HCCO=H+2CO	1.00E+14	0.0	0.0
263.	H+HCCO=CH2SING+CO	5.00E+13	0.0	0.0
264.	CH2+HCCO=C2H3+CO	3.00E+13	0.0	0.0
265.	HCCO+O2=CO2+CO+H	4.78E+12	-0.1	1150.0
266.	HCCO+O2=CO+CO+OH	1.91E+11	0.0	1023.0
267.	HCCO+O2=O+CO+HCO	2.18E+02	2.7	3541.0
268.	2HCCO=2CO+C2H2	1.00E+13	0.0	0.0
269.	HCCO+CH3=C2H4+CO	5.00E+13	0.0	0.0
270.	O+CH2CO=OH+HCCO	1.00E+13	0.0	8000.0
271.	O+CH2CO=CH2+CO2	1.75E+12	0.0	1350.0
272.	H+CH2CO=HCCO+H2	5.00E+13	0.0	8000.0
273.	CH2CO+H=CH3+CO	7.77E+08	1.4	2780.0
274.	CH2CHO=H+CH2CO	2.48E+27	-5.2	44304.0
275.	CH2CHO=CH3+CO	1.54E+31	-6.3	42478.0
276.	OH+CH2CO=HCCO+H2O	7.50E+12	0.0	2000.0
277.	CH2CO+OH=CH2OH+CO	1.00E+13	0.0	0.0
278.	CH3CO=CH3+CO	2.40E+15	-2.0	14805.0
279.	CH2CHO+H=CH3CHO	6.40E+35	-7.6	5215.0
280.	CH2CHO+H=CH3+HCO	4.99E+14	-0.3	912.0
281.	CH2CHO+O=CH2O+HCO	5.00E+13	0.0	0.0
282.	CH2CHO+OH=H2O+CH2CO	1.20E+13	0.0	0.0
283.	CH2CHO+OH=HCO+CH2OH	3.01E+13	0.0	0.0
284.	CH2CHO+O2=CH2CO+HO2	1.57E+11	0.0	0.0
285.	CH3CHO=CH3+HCO	9.59E+14	0.0	74180.0
286.	CH3CHO+O2=CH3CO+HO2	2.00E+13	0.5	42200.0
287.	CH3CHO+H=CH2CHO+H2	4.10E+09	1.2	2405.0
288.	CH3CHO+OH=CH3CO+H2O	2.35E+10	0.7	-1113.0
289.	CH3CHO+O=CH2CHO+OH	5.85E+12	0.0	1808.0
290.	CH3CHO+HO2=CH3CO+H2O2	1.70E+12	0.0	10700.0
291.	CH3CHO+CH3=CH3CO+CH4	1.70E+12	0.0	8440.0

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292. CH3CHO+HCO=CH3CO+CH2O                          7.80E+13    0.0     8440.0
293. C2H5+O2(+M)=C2H5OO(+M)                         2.02E+10    1.0      -63.6
     Low pressure limit:  0.84900E+30 -0.42900E+01  0.22000E+03
     TROE centering:      0.10300E+00  0.60100E+03  0.10000E-09
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
294. C2H5OO(+M)=C2H4+HO2(+M)                        7.14E+04    2.3    27955.0
     Low pressure limit:  0.83100E+22 -0.65100E+00  0.22890E+05
     TROE centering:      0.00000E+00  0.10600E+03  0.10600E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
295. C2H5OO+HO2=C2H5O+OH+O2                         1.75E+10    0.0    -3275.0
296. C2H5O=CH3+CH2O                                 1.00E+15    0.0    21523.0
297. C2H5O=CH3CHO+H                                 2.00E+14    0.0    23215.0
298. C2H5O+O2=CH3CHO+HO2                            6.03E+10    0.0     1643.0
299. C2H4O+O2=CH2CHO+HO2                            4.00E+13    0.0    61500.0
300. C2H4O+H=CH2CHO+H2                              2.00E+13    0.0     8300.0
301. C2H4O+H=C2H3+H2O                               5.00E+09    0.0     5000.0
302. C2H4O+H=C2H4+OH                                9.51E+10    0.0     5000.0
303. C2H4O+OH=CH2CHO+H2O                            4.79E+13    0.0     5955.0
304. C2H4O+O=CH2CHO+OH                              1.91E+12    0.0     5250.0
305. C2H4O+HO2=CH2CHO+H2O2                          4.00E+12    0.0    17000.0
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306. C2H4O=CH3CHO	6.00E+13	0.0	57167.0
307. C2H4O=CH3+HCO	4.90E+13	0.0	57167.0
308. C2H4O=CH4+CO	1.21E+13	0.0	57167.0
309. C3H8+H=nC3H7+H2	1.30E+06	2.5	6756.0
310. C3H8+H=iC3H7+H2	1.30E+06	2.4	4471.0
311. C3H8+O=nC3H7+OH	1.90E+05	2.7	3716.0
312. C3H8+O=iC3H7+OH	4.76E+04	2.7	2106.0
313. C3H8+OH=iC3H7+H2O	1.40E+03	2.8	-310.0
314. C3H8+OH=nC3H7+H2O	1.37E+03	2.7	580.0
315. C3H8+O2=nC3H7+HO2	3.97E+13	0.0	50872.0
316. C3H8+O2=iC3H7+HO2	3.97E+13	0.0	47693.0
317. C3H8+HO2=nC3H7+H2O2	4.76E+04	2.5	16494.0
318. C3H8+HO2=iC3H7+H2O2	9.64E+03	2.6	13910.0
319. C3H8+CH3=nC3H7+CH4	9.04E-01	3.6	7154.0
320. C3H8+CH3=iC3H7+CH4	1.51E+00	3.5	5481.0
321. C3H8+CH2OH=nC3H7+CH3OH	1.99E+02	3.0	3976.0
322. C3H8+CH3O=nC3H7+CH3OH	4.34E+11	0.0	6458.0
323. C3H8+CH2SING=nC3H7+CH3	9.04E-01	3.6	7154.0
324. C3H8+C2H3=nC3H7+C2H4	6.03E+02	3.3	10502.0
325. C3H8+C2H=nC3H7+C2H2	3.61E+12	0.0	0.0
326. C3H8+C2H5=nC3H7+C2H6	9.04E-02	3.6	9141.0
327. C3H8+HCO=nC3H7+CH2O	2.05E+05	2.5	18431.0
328. C3H8+iC3H7=nC3H7+C3H8	8.40E-03	4.2	8716.0
329. C3H8+CH3CO=nC3H7+CH3CHO	4.22E+04	2.6	17658.0
330. C3H8+CH2=nC3H7+CH3	9.03E-01	3.6	7154.0
331. C3H8+CH2OH=iC3H7+CH3OH	6.03E+01	3.0	11989.0
332. C3H8+CH3O=iC3H7+CH3OH	1.45E+11	0.0	4571.0
333. C3H8+CH2SING=iC3H7+CH3	1.51E+00	3.5	7472.0
334. C3H8+C2H3=iC3H7+C2H4	1.02E+03	3.1	8829.0
335. C3H8+C2H=iC3H7+C2H2	1.21E+12	0.0	0.0
336. C3H8+C2H5=iC3H7+C2H6	1.21E+00	3.5	7468.0
337. C3H8+HCO=iC3H7+CH2O	1.08E+07	1.9	17006.0

338. C3H8+CH3CO=iC3H7+CH3CHO 5.30E+06 2.0 16241.0

339. C3H8+CH2=iC3H7+CH3 1.51E+00 3.5 7472.0

340. nC3H7+H=C3H6+H2 1.81E+12 0.0 0.0

341. nC3H7+H(+M)=C3H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+59 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

342. nC3H7+H=C2H5+CH3 3.40E+18 -1.3 5386.0

343. nC3H7+O=C2H5+CH2O 9.60E+13 0.0 0.0

344. nC3H7+O2=C3H6+HO2 9.04E+10 0.0 0.0

345. nC3H7+HO2=C2H5+OH+CH2O 2.41E+13 0.0 0.0

346. nC3H7+OH=C3H6+H2O 2.41E+13 0.0 0.0

347. nC3H7+CH3=CH4+C3H6 1.14E+13 -0.3 0.0

348. nC3H7+C2H5=C3H6+C2H6 1.45E+12 0.0 0.0

349. nC3H7+C2H5=C3H8+C2H4 1.15E+12 0.0 0.0

350. nC3H7+C2H3=C3H8+C2H2 1.21E+12 0.0 0.0

351. nC3H7+C2H2=AC3H5+C2H4 7.23E+11 0.0 9004.0

352. nC3H7+C2H=C3H3+C2H5 1.21E+13 0.0 0.0

353. nC3H7+C2H=C3H6+C2H2 6.03E+12 0.0 0.0

354. nC3H7+iC3H7=C3H8+C3H6 5.13E+13 -0.3 0.0

355. nC3H7+HCO=CO+C3H8 6.03E+13 0.0 0.0

356. nC3H7+CH3O=C3H8+CH2O 2.41E+13 0.0 0.0

357. nC3H7+CH2SING=C2H5+C2H4 2.58E+13 0.0 0.0

358. nC3H7+CH2SING=C3H6+CH3 1.03E+13 0.0 0.0

359. nC3H7+CH2=C2H4+C2H5 1.81E+13 0.0 0.0

360. nC3H7+CH2=C3H6+CH3 1.81E+12 0.0 0.0

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361. nC3H7+CH2OH=C3H6+CH3OH                          4.82E+11    0.0        0.0
362. iC3H7=CH3+C2H4                                  1.00E+14    0.0    45000.0
363. iC3H7+H=C3H6+H2                                 3.61E+12    0.0        0.0
364. iC3H7+H(+M)=C3H8(+M)                            2.40E+13    0.0        0.0
     Low pressure limit:  0.17000E+59 -0.12080E+02  0.11264E+05
     TROE centering:      0.64900E+00  0.12131E+04  0.12131E+04  0.13370E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
365. iC3H7+H=CH3+C2H5                                5.90E+23   -2.8    10009.0
366. iC3H7+O=CH3CHO+CH3                              9.60E+13    0.0        0.0
367. iC3H7+O2=C3H6+HO2                               1.26E+11    0.0        0.0
368. iC3H7+HO2=CH3CHO+OH+CH3                         2.41E+13    0.0        0.0
369. iC3H7+OH=C3H6+H2O                               2.41E+13    0.0        0.0
370. iC3H7+CH3=CH4+C3H6                              2.19E+14   -0.7        0.0
371. iC3H7+C2H5=C3H6+C2H6                            2.30E+13   -0.3        0.0
372. iC3H7+C2H5=C3H8+C2H4                            1.84E+13   -0.3        0.0
373. iC3H7+C2H3=C2H4+C3H6                            1.52E+14   -0.7        0.0
374. iC3H7+C2H3=C3H8+C2H2                            1.52E+14   -0.7        0.0
375. iC3H7+C2H2=CH3+iiiC4H6                          2.77E+10    0.0     6504.0
376. iC3H7+C2H=C3H6+C2H2                             3.60E+12    0.0        0.0
377. iC3H7+iC3H7=C3H8+C3H6                           2.11E+14   -0.7        0.0
378. iC3H7+HCO=CO+C3H8                               1.20E+14    0.0        0.0
379. iC3H7+CH3O=C3H8+CH2O                            1.21E+13    0.0        0.0
380. iC3H7+CH2SING=C3H6+CH3                          1.04E+13    0.0        0.0
381. iC3H7+CH2=C3H6+CH3                              3.01E+13    0.0        0.0
382. iC3H7+CH2OH=C3H6+CH3OH                          2.89E+12    0.0        0.0
383. iC3H7+CH2OH=C3H8+CH2O                           2.35E+12    0.0        0.0
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384. CH3+C2H3(+M)=C3H6(+M)                          2.50E+13    0.0        0.0
     Low pressure limit:  0.42700E+59 -0.11940E+02  0.97700E+04
     TROE centering:      0.17500E+00  0.13410E+04  0.60000E+05  0.10140E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H2            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
385. C3H6+H=H2+AC3H5                                1.70E+05    2.5     2492.0
386. C3H6+H=C2H4+CH3                                8.80E+16   -1.1     6461.0
387. C3H6+H=SC3H5+H2                                7.81E+05    2.5    12285.0
388. C3H6+H(+M)=nC3H7(+M)                           1.33E+13    0.0     3260.7
     Low pressure limit:  0.62600E+39 -0.66600E+01  0.70000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.13100E+04  0.48097E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
389. C3H6+H(+M)=iC3H7(+M)                           1.33E+13    0.0     1559.8
     Low pressure limit:  0.87000E+43 -0.75000E+01  0.47218E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.64540E+03  0.68443E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
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AR Enhanced by 7.000E-01

390.	C3H6+H=TC3H5+H2	3.90E+05	2.5	5821.0
391.	C3H6=H2+AC3H4	4.00E+13	0.0	80000.0
392.	C3H6=CH4+C2H2	3.50E+12	0.0	70000.0
393.	C3H6+O=C2H5+HCO	3.50E+07	1.6	-972.0
394.	C3H6+O=AC3H5+OH	1.75E+11	0.7	5884.0
395.	C3H6+O=SC3H5+OH	1.21E+11	0.7	8960.0
396.	C3H6+O=TC3H5+OH	6.03E+10	0.7	7633.0
397.	C3H6+O=CH3+H+CH2CO	1.20E+08	1.6	327.0
398.	C3H6+OH=AC3H5+H2O	3.12E+06	2.0	-298.0
399.	C3H6+OH=SC3H5+H2O	2.14E+06	2.0	2778.0
400.	C3H6+OH=TC3H5+H2O	1.11E+06	2.0	1451.0
401.	C3H6+HO2=AC3H5+H2O2	9.63E+03	2.6	13910.0
402.	C3H6+O2=AC3H5+HO2	6.03E+13	0.0	47590.0
403.	C3H6+CH3=AC3H5+CH4	2.20E+00	3.5	5675.0
404.	C3H6+CH3=TC3H5+CH4	8.40E-01	3.5	11660.0
405.	C3H6+C2H5=AC3H5+C2H6	2.23E+00	3.5	6637.0
406.	C3H6+C2H2=AC3H5+C2H3	4.04E+13	0.0	46818.0
407.	C3H6+C2H3=AC3H5+C2H4	2.21E+00	3.5	4682.0
408.	C3H6+C2H3=SC3H5+C2H4	1.35E+00	3.5	10842.0
409.	C3H6+C2H3=TC3H5+C2H4	8.40E-01	3.5	9670.0
410.	C3H6+C2H3=iiiC4H6+CH3	7.23E+11	0.0	5008.0
411.	C3H6+C2H4=AC3H5+C2H5	5.78E+13	0.0	51584.0
412.	C3H6+C2H4=nC3H7+C2H3	6.03E+13	0.0	75446.0
413.	C3H6+CH2OH=AC3H5+CH3OH	6.03E+01	3.0	12000.0
414.	C3H6+nC3H7=AC3H5+C3H8	2.23E+00	3.5	6637.0
415.	C3H6+nC3H7=IC4H8+C2H5	2.23E+00	3.5	-2000.0
416.	C3H6+iC3H7=C3H8+AC3H5	6.62E-02	4.0	8066.0
417.	C3H6+C3H6=AC3H5+nC3H7	2.53E+14	0.0	55179.0
418.	C3H6+C3H6=AC3H5+iC3H7	4.88E+13	0.0	52309.0
419.	CH3+C2H3=AC3H5+H	1.50E+24	-2.8	18618.0
420.	CH3+C2H3=SC3H5+H	3.20E+35	-7.8	13300.0

421. CH3+C2H3=TC3H5+H 4.99E+22 -4.4 18850.0

422. AC3H5+H(+M)=C3H6(+M) 2.00E+14 0.0 0.0

Low pressure limit: 0.13300E+61 -0.12000E+02 0.59678E+04

TROE centering: 0.20000E-01 0.10970E+04 0.10967E+05 0.68600E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

423. AC3H5+H=AC3H4+H2 1.80E+13 0.0 0.0

424. TC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

425. SC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

426. AC3H5+O=C2H3CHO+H 6.00E+13 0.0 0.0

427. AC3H5+O=C2H3+CH2O 1.80E+14 0.0 0.0

428. SC3H5+O=CH2CO+CH3 1.81E+14 0.0 0.0

429. TC3H5+O=H+HCCO+CH3 1.81E+14 0.0 0.0

430. AC3H5+OH=C2H3CHO+H+H 5.30E+37 -6.7 29306.0

431. AC3H5+OH=AC3H4+H2O 6.00E+12 0.0 0.0

432. AC3H5+O2=AC3H4+HO2 4.99E+15 -1.4 22428.0

433. AC3H5+O2=CH2O+CH3CO 1.19E+15 -1.0 20128.0

434. AC3H5+O2=OH+C2H3CHO 1.82E+13 -0.4 22859.0

435. SC3H5+O2=CH3CHO+HCO 4.34E+12 0.0 0.0

436. TC3H5+O2=CH3CHO+HCO 4.34E+12 0.0 0.0

437. AC3H5+HO2=C2H3+CH2O+OH 6.60E+12 0.0 0.0

438. AC3H5+CH3=AC3H4+CH4 3.00E+12 -0.3 -131.0

439. AC3H5+CH3(+M)=IC4H8(+M) 1.00E+14 -0.3 -262.0

Low pressure limit: 0.35100E+61 -0.12970E+02 0.60000E+04

TROE centering: 0.89600E+00 0.60000E+05 0.16060E+04 0.61180E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

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     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
440. SC3H5+CH3=AC3H4+CH4                          1.00E+11    0.0        0.0
441. TC3H5+CH3=AC3H4+CH4                          1.00E+11    0.0        0.0
442. AC3H5+C2H3=AC3H4+C2H4                        1.00E+12    0.0        0.0
443. SC3H5+C2H3=AC3H4+C2H4                        1.00E+11    0.0        0.0
444. TC3H5+C2H3=AC3H4+C2H4                        1.00E+11    0.0        0.0
445. AC3H5+CH2O=C3H6+HCO                          1.26E+08    1.9    18191.0
446. AC3H5+HCO=C3H6+CO                            6.00E+13    0.0        0.0
447. AC3H5+AC3H5=AC3H4+C3H6                       8.43E+10    0.0     -262.0
448. AC3H5+CH2=iiiC4H6+H                          3.00E+13    0.0        0.0
449. AC3H5+nC3H7=AC3H4+C3H8                       7.23E+11    0.0     -131.0
450. AC3H5+iC3H7=AC3H4+C3H8                       4.58E+12   -0.3     -131.0
451. AC3H5=TC3H5                                  3.90E+59  -15.4    75400.0
452. AC3H5=SC3H5                                  1.30E+55  -14.5    73800.0
453. TC3H5=SC3H5                                  1.60E+44  -12.2    52200.0
454. AC3H4=PC3H4                                  6.03E+53  -12.2    84276.0
455. AC3H4+H=AC3H5                                1.24E+52  -12.0    17839.0
     Declared duplicate reaction...
456. AC3H4+H=AC3H5                                6.92E+36   -8.2     7462.0
     Declared duplicate reaction...
457. AC3H4+H=TC3H5                                1.55E+53  -13.1    14472.0
     Declared duplicate reaction...
458. AC3H4+H=TC3H5                                9.88E+44  -11.2     8212.0
     Declared duplicate reaction...
459. PC3H4+H=TC3H5                                3.17E+52  -12.7    14226.0
     Declared duplicate reaction...
460. PC3H4+H=TC3H5                                2.59E+45  -11.2     8046.0
     Declared duplicate reaction...
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461.	PC3H4+H=SC3H5	3.38E+49	-12.8	14072.0
	Declared duplicate reaction...			
462.	PC3H4+H=SC3H5	2.98E+43	-11.4	8736.0
	Declared duplicate reaction...			
463.	AC3H4+H=PC3H4+H	1.48E+13	0.3	4103.0
464.	AC3H4+H=CH3+C2H2	2.72E+09	1.2	6834.0
465.	PC3H4+H=CH3+C2H2	3.89E+10	1.0	4114.0
466.	C2H2+CH3=SC3H5	-6.81E+48	-12.3	16642.0
	Declared duplicate reaction...			
467.	C2H2+CH3=SC3H5	1.52E+44	-10.7	15256.0
	Declared duplicate reaction...			
468.	C2H2+CH3=TC3H5	6.80E+20	-4.2	18000.0
469.	C2H2+CH3=AC3H5	8.20E+53	-13.3	33200.0
470.	AC3H4+H=C3H3+H2	6.60E+03	3.1	5522.0
471.	AC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
472.	PC3H4+H=C3H3+H2	3.57E+04	2.8	4821.0
473.	AC3H4+O=C2H4+CO	2.00E+07	1.8	1000.0
474.	AC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
475.	AC3H4+CH3=C3H3+CH4	1.30E+12	0.0	7700.0
476.	PC3H4+O=HCCO+CH3	7.30E+12	0.0	2250.0
477.	PC3H4+O=C2H4+CO	1.00E+13	0.0	2250.0
478.	PC3H4+O=C3H3+OH	3.44E+04	2.2	4830.0
479.	PC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
480.	PC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
481.	PC3H4+CH3=C3H3+CH4	1.80E+12	0.0	7700.0
482.	C3H3+H=PC3H4	3.63E+36	-7.4	6039.0
483.	C3H3+H=AC3H4	3.39E+36	-7.4	6337.0
484.	C3H3+CH3=iiC4H6	3.61E+13	0.0	0.0
485.	C2H3+C2H3=iiiC4H6	7.00E+57	-13.8	17629.0
486.	C3H3+H=C3H2+H2	2.14E+05	2.5	7453.0
487.	C3H3+O=>C2H2+HCO	1.38E+14	0.0	0.0
488.	C3H3+O=C2H3+CO	4.62E+13	0.0	0.0

489.	C3H3+O=C2H+CH2O	4.62E+13	0.0	0.0
490.	C3H3+O=>C2H2+CO+H	4.62E+13	0.0	0.0
491.	C3H3+OH=C3H2+H2O	2.00E+13	0.0	8000.0
492.	C3H3+HCO=AC3H4+CO	2.50E+13	0.0	0.0
493.	C3H3+HCO=PC3H4+CO	2.50E+13	0.0	0.0
494.	C3H3+CH=iC4H3+H	5.00E+13	0.0	0.0
495.	C3H3+CH2=C4H4+H	5.00E+13	0.0	0.0
496.	C3H3+O2=CH2CO+HCO	1.70E+05	1.7	1500.0
497.	C3H3+HCCO=C4H4+CO	2.50E+13	0.0	0.0
498.	C3H3+HO2=OH+CO+C2H3	8.00E+11	0.0	0.0
499.	C3H3+HO2=AC3H4+O2	3.00E+11	0.0	0.0
500.	C3H3+HO2=PC3H4+O2	2.50E+12	0.0	0.0
501.	C3H2+O2=H+CO+HCCO	2.00E+12	0.0	1000.0
502.	C3H2+O=C2H2+CO	6.80E+13	0.0	0.0
503.	C3H2+OH=C2H2+HCO	6.80E+13	0.0	0.0
504.	C3H2+H=C3H3	1.10E+40	-8.0	84700.0
505.	C3H2+CH=C4H2+H	5.00E+13	0.0	0.0
506.	C3H2+CH2=nC4H3+H	5.00E+13	0.0	0.0
507.	C3H2+CH3=C4H4+H	5.00E+12	0.0	0.0
508.	C3H2+HCCO=nC4H3+CO	1.00E+13	0.0	0.0
509.	C2H3CO+M=>C2H3+CO+M	8.51E+15	0.0	23000.0
510.	C2H3+CO+M=>C2H3CO+M	1.58E+11	0.0	6000.0
511.	C2H3CHO+HO2=>C2H3CH2O+O2	1.29E+11	0.0	32000.0
512.	C2H3CH2O=>C2H3CHO+H	1.00E+14	0.0	19000.0
513.	C2H3CHO+H=>C2H3CH2O	1.00E+08	0.0	10000.0
514.	C2H3CHO+OH=>C2H3CO+H2O	1.00E+13	0.0	0.0
515.	C2H3CO+H2O=>C2H3CHO+OH	1.91E+13	0.0	36620.0
516.	C2H3CHO+H=>C2H3CO+H2	3.98E+13	0.0	4200.0
517.	C2H3CO+H2=>C2H3CHO+H	1.78E+13	0.0	23670.0
518.	C2H3CHO+O=>C2H3CO+OH	5.01E+12	0.0	1790.0
519.	C2H3CO+OH=>C2H3CHO+O	1.00E+12	0.0	19160.0
520.	C2H3CHO+HO2=>C2H3CO+H2O2	1.70E+12	0.0	10700.0

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521. C2H3CO+H2O2=>C2H3CHO+HO2                          1.00E+12    0.0    14100.0
522. C2H3CHO+CH3=>C2H3CO+CH4                           1.74E+12    0.0     8440.0
523. C2H3CO+CH4=>C2H3CHO+CH3                           1.51E+13    0.0    28000.0
524. C2H3CH2O+O2=>C2H3CHO+HO2                          1.74E+11    0.0     1750.0
525. C2H3CH2O=>CH2O+C2H3                               1.00E+14    0.0    21600.0
526. CH2O+C2H3=>C2H3CH2O                               1.00E+11    0.0        0.0
527. C4H+H2=C4H2+H                                     2.00E+13    0.0     5000.0
528. C4H+O2=CO+CO+C2H                                  1.20E+12    0.0        0.0
529. C4H2+OH=H2O+C4H                                   9.15E+09    1.0    21746.0
530. H2C4O+OH=C2H2+CO+HCO                              1.00E+13    0.0        0.0
531. iC4H3+O=H2C4O+H                                   2.00E+13    0.0        0.0
532. C4H2+OH=H+H2C4O                                   1.63E+15   -1.1     2549.0
533. C4H2+OH=CO+C3H3                                   1.69E+28   -4.6    20140.0
534. C4H2+H=nC4H3                                      1.44E+63  -15.7    24018.0
     Declared duplicate reaction...
535. C4H2+H=nC4H3                                      4.16E+32   -6.5     9726.1
     Declared duplicate reaction...
536. C4H2+H(+M)=iC4H3(+M)                              4.31E+10    1.2     1752.9
     Low pressure limit:  0.23000E+46 -0.80950E+01  0.25066E+04
     TROE centering:      0.74800E-01  0.10000E-49 -0.42159E+04  0.10000E+51
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
537. C4H2+O=C3H2+CO                                    2.70E+13    0.0     1720.0
538. C4H2+C2H=C6H2+H                                   9.60E+13    0.0        0.0
539. C4H2+C2H=C6H3                                     1.10E+30   -6.3     2790.0
540. nC4H3=iC4H3                                       3.70E+61  -15.8    54890.0
541. nC4H3+H=iC4H3+H                                   2.40E+11    0.8     2410.0
542. nC4H3+H=C2H2+H2CC                                 1.60E+19   -1.6     2220.0
543. nC4H3+H=C4H4                                      1.10E+42   -9.7     7000.0
544. nC4H3+H=C4H2+H2                                   3.00E+13    0.0        0.0
```

545.	nC4H3+OH=C4H2+H2O	2.00E+12	0.0	0.0
546.	nC4H3+C2H2=l-C6H4+H	3.70E+16	-1.2	11100.0
547.	nC4H3+C2H2=A1	2.30E+68	-17.6	24400.0
548.	nC4H3+C2H2=c-C6H4+H	1.90E+36	-7.2	17900.0
549.	iC4H3+H=C2H2+H2CC	2.40E+19	-1.6	2800.0
550.	iC4H3+H=C4H4	4.20E+44	-10.3	7890.0
551.	iC4H3+H=C4H2+H2	5.00E+13	0.0	0.0
552.	iC4H3+OH=C4H2+H2O	4.00E+12	0.0	0.0
553.	iC4H3+O2=HCCO+CH2CO	7.86E+16	-1.8	0.0
554.	C4H4+H=n-C4H5	4.20E+50	-12.3	12500.0
555.	C4H4+H=i-C4H5	9.60E+52	-12.8	14300.0
556.	C4H4+H=nC4H3+H2	6.65E+05	2.5	12240.0
557.	C4H4+H=iC4H3+H2	3.33E+05	2.5	9240.0
558.	C4H4+OH=nC4H3+H2O	3.10E+07	2.0	3430.0
559.	C4H4+OH=iC4H3+H2O	1.55E+07	2.0	430.0
560.	C4H4+O=C3H3+HCO	6.00E+08	1.4	-860.0
561.	C4H4+C2H=l-C6H4+H	1.20E+13	0.0	0.0
562.	n-C4H5=i-C4H5	1.30E+62	-16.4	49600.0
563.	n-C4H5+H=i-C4H5+H	1.00E+36	-6.3	17486.0
564.	n-C4H5+H=C4H4+H2	1.50E+13	0.0	0.0
565.	n-C4H5+OH=C4H4+H2O	2.00E+12	0.0	0.0
566.	n-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
567.	n-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
568.	n-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
569.	n-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
570.	n-C4H5+O2=HCO+C2H3CHO	9.20E+16	-1.4	1010.0
571.	i-C4H5+H=C4H4+H2	3.00E+13	0.0	0.0
572.	i-C4H5+H=C3H3+CH3	1.00E+14	0.0	0.0
573.	i-C4H5+OH=C4H4+H2O	4.00E+12	0.0	0.0
574.	i-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
575.	i-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
576.	i-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0

577.	i-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
578.	i-C4H5+O2=CH2CO+CH2CHO	2.16E+10	0.0	2500.0
579.	n-C4H5+C5H6=iiiC4H6+C5H5	6.00E+12	0.0	0.0
580.	i-C4H5+C5H6=iiiC4H6+C5H5	6.00E+12	0.0	0.0
581.	iiiC4H6=i-C4H5+H	8.20E+51	-10.9	118409.0
582.	iiiC4H6=n-C4H5+H	3.50E+61	-13.9	129677.0
583.	iiiC4H6=C4H4+H2	2.50E+15	0.0	94700.0
584.	iiiC4H6+H=n-C4H5+H2	3.00E+07	2.0	13000.0
585.	iiiC4H6+H=i-C4H5+H2	3.00E+07	2.0	6000.0
586.	C2H4+C2H3=iiiC4H6+H	7.40E+14	-0.7	8420.0
587.	iiiC4H6+H=PC3H4+CH3	2.00E+12	0.0	7000.0
588.	iiiC4H6+H=AC3H4+CH3	2.00E+12	0.0	7000.0
589.	iiiC4H6+O=n-C4H5+OH	7.50E+06	1.9	3740.0
590.	iiiC4H6+O=i-C4H5+OH	7.50E+06	1.9	3740.0
591.	iiiC4H6+O=HCO+AC3H5	6.02E+08	1.4	-858.0
592.	iiiC4H6+OH=CH3CHO+C2H3	6.30E+12	0.0	-874.0
593.	iiiC4H6+OH=AC3H5+CH2O	6.30E+12	0.0	-874.0
594.	iiiC4H6+OH=n-C4H5+H2O	2.00E+07	2.0	5000.0
595.	iiiC4H6+OH=i-C4H5+H2O	2.00E+07	2.0	2000.0
596.	iiiC4H6+CH3=n-C4H5+CH4	2.00E+14	0.0	22800.0
597.	iiiC4H6+CH3=i-C4H5+CH4	1.00E+14	0.0	19800.0
598.	iiiC4H6+C2H3=n-C4H5+C2H4	5.00E+13	0.0	22800.0
599.	iiiC4H6+C2H3=i-C4H5+C2H4	2.50E+13	0.0	19800.0
600.	iiiC4H6+C3H3=n-C4H5+AC3H4	1.00E+13	0.0	22500.0
601.	iiiC4H6+C3H3=i-C4H5+AC3H4	5.00E+12	0.0	19500.0
602.	iiiC4H6+AC3H5=n-C4H5+C3H6	1.00E+13	0.0	22500.0
603.	iiiC4H6+AC3H5=i-C4H5+C3H6	5.00E+12	0.0	19500.0
604.	iiiC4H6+C2H3=A+H2+H	5.62E+11	0.0	3240.0
605.	iiC4H6=i-C4H5+H	4.20E+15	0.0	92600.0
606.	iiC4H6+H=iiiC4H6+H	2.00E+13	0.0	4000.0
607.	iiC4H6+H=i-C4H5+H2	1.70E+05	2.5	2490.0
608.	iiC4H6+H=AC3H4+CH3	2.00E+13	0.0	2000.0

609. iiC4H6+H=PC3H4+CH3 2.00E+13 0.0 2000.0

610. iiC4H6+CH3=i-C4H5+CH4 7.00E+13 0.0 18500.0

611. iiC4H6+O=CH2CO+C2H4 1.20E+08 1.6 327.0

612. iiC4H6+O=i-C4H5+OH 1.80E+11 0.7 5880.0

613. iiC4H6+OH=i-C4H5+H2O 3.10E+06 2.0 -298.0

614. iiC4H6=iiiC4H6 3.00E+13 0.0 65000.0

615. IC4H8+H=C2H4+C2H5 1.60E+22 -2.4 11180.0

616. IC4H8+H=C3H6+CH3 3.20E+22 -2.4 11180.0

617. IC4H8+H=C4H7+H2 6.50E+05 2.5 6756.0

618. IC4H8+O=nC3H7+HCO 3.30E+08 1.4 -402.0

619. IC4H8+O=C4H7+OH 1.50E+13 0.0 5760.0

Declared duplicate reaction...

620. IC4H8+O=C4H7+OH 2.60E+13 0.0 4470.0

Declared duplicate reaction...

621. IC4H8+OH=C4H7+H2O 7.00E+02 2.7 527.0

622. IC4H8+O2=C4H7+HO2 2.00E+13 0.0 50930.0

623. IC4H8+HO2=C4H7+H2O2 1.00E+12 0.0 14340.0

624. IC4H8+CH3=C4H7+CH4 4.50E-01 3.6 7153.0

625. C4H7=iiiC4H6+H 1.27E+24 -4.8 23777.0

626. C4H7+H(+M)=IC4H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+49 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

627. C4H7+H=CH3+AC3H5 2.00E+21 -2.0 11000.0

628. C4H7+H=iiiC4H6+H2 1.80E+12 0.0 0.0

629. C4H7+O2=iiiC4H6+HO2 1.00E+11 0.0 0.0

630. C4H7+HCO=IC4H8+CO 6.00E+13 0.0 0.0

631. C4H7+CH3=iiiC4H6+CH4 1.10E+13 0.0 0.0

632. C2H4+C2H3=C4H7 1.23E+35 -7.8 9930.0

633. IC4H8+H(+M)=nC4H9(+M) 1.33E+13 0.0 3260.7

Low pressure limit: 0.62600E+39 -0.66600E+01 0.70000E+04

TROE centering: 0.10000E+01 0.10000E+04 0.13100E+04 0.48097E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

634. C2H4+C2H5=nC4H9 1.50E+11 0.0 7300.0

635. nC4H9+H=IC4H8+H2 1.80E+12 0.0 0.0

636. nC4H9+O=nC3H7+CH2O 9.60E+13 0.0 0.0

637. nC4H9+OH=IC4H8+H2O 2.40E+13 0.0 0.0

638. nC4H9+O2=IC4H8+HO2 2.70E+11 0.0 0.0

639. nC4H9+HO2=nC3H7+OH+CH2O 2.40E+13 0.0 0.0

640. nC4H9+CH3=IC4H8+CH4 1.10E+13 0.0 0.0

641. CH+C4H2=C5H2+H 1.00E+14 0.0 0.0

642. H2CCCCCH+H=C5H2+H2 1.00E+13 0.0 0.0

643. HCCCHCCH+H=C5H2+H2 1.00E+13 0.0 0.0

644. H2CCCCCH+CH3=C5H2+CH4 3.00E+12 0.0 5000.0

645. HCCCHCCH+CH3=C5H2+CH4 3.00E+12 0.0 5000.0

646. C3H3+C2H=H2CCCCCH+H 1.00E+13 0.0 0.0

647. CH2+C4H2=H2CCCCCH+H 1.30E+13 0.0 4326.0

648. CH2SING+C4H2=H2CCCCCH+H 2.54E+16 -0.9 0.0

649. HCCCHCCH+H=H2CCCCCH+H 1.00E+13 0.0 0.0

650. H2CCCCCH+CH3=FC6H6 1.00E+11 0.0 0.0

651. H2CCCCCH+CH3=A1+H 1.00E+11 0.0 0.0

652. H2CCCCCH+CH3=A 5.00E+10 0.0 0.0

653. C3H2+C2H2=HCCCHCCH+H	5.00E+12	0.0	5000.0
654. C3H3+C2H=HCCCHCCH+H	3.00E+13	0.0	0.0
655. CH2SING+C4H2=HCCCHCCH+H	2.54E+16	-0.9	0.0
656. C3H3+C3H3=HCCCHCCH+CH3	5.00E+11	0.0	0.0
657. HCCCHCCH+CH3=FC6H6	1.00E+11	0.0	0.0
658. HCCCHCCH+CH3=A1+H	1.00E+11	0.0	0.0
659. iC4H3+CH3=l-C5H5+H	3.00E+13	0.0	0.0
660. C5H5=l-C5H5	4.09E+47	-10.4	54874.0
661. C3H3+C2H2=l-C5H5	5.62E+32	-7.3	6758.0
662. C5H5+H=C5H6	2.71E+63	-14.8	21050.0
663. C5H5=C3H3+C2H2	2.79E+79	-18.3	130834.0
664. C5H5+O=n-C4H5+CO	7.27E+13	-0.3	470.0
665. C5H5+O=C5H5O	1.84E+03	1.0	-6960.0
666. C5H5+O=C5H4O+H	6.71E+13	0.0	40.0
667. C5H5+HO2=C5H5O+OH	3.00E+13	0.0	0.0
668. C5H5O=n-C4H5+CO	2.51E+11	0.0	43900.0
669. C5H5O=C5H4O+H	2.90E+32	-6.5	21220.0
670. C5H5O=i-C4H5+CO	1.10E+79	-19.6	66250.0
671. C5H5+OH=iiiC4H6+CO	1.20E+14	0.0	4500.0
672. C5H5+OH=C5H4OH+H	2.15E+30	-4.6	25050.0
673. C5H4O+H=C5H4OH	1.10E+69	-16.0	37130.0
674. C5H4OH+O2=C5H4O+HO2	3.00E+13	0.0	5000.0
675. C5H4O+H=n-C4H5+CO	2.10E+61	-13.3	40810.0
676. C5H4O+O=C4H4+CO2	1.00E+13	0.0	2000.0
677. C5H4O=2C2H2+CO	1.10E+47	-9.6	99500.0
678. C5H6+H=C5H5+H2	2.80E+13	0.0	2259.0
679. C5H6+H=AC3H5+C2H2	6.60E+14	0.0	12345.0
680. C5H6+OH=C5H5+H2O	3.08E+06	2.0	0.0
681. C5H6+O=C5H5+OH	4.77E+04	2.7	1106.0
682. C5H6+O2=C5H5+HO2	4.00E+13	0.0	37150.0
683. C5H6+HO2=C5H5+H2O2	1.10E+04	2.6	12900.0
684. C5H6+CH3=C5H5+CH4	1.80E-01	4.0	0.0

685. C5H6+C2H3=C5H5+C2H4 1.20E-01 4.0 0.0

686. C5H6+A1=C5H5+A 1.00E-01 4.0 0.0

687. C5H6=CH2CHCHCCH2 1.35E+15 0.0 80450.0

688. CH2CHCHCCH2=PC3H4+C2H2 2.88E+13 0.0 66550.0

689. C5H6=C2H2+AC3H4 3.80E+17 0.0 104000.0

690. C5H6=CH2CHCH2CCH 8.50E+14 0.0 90540.0

691. CH2CHCH2CCH=C2H2+AC3H4 3.55E+13 0.0 63360.0

692. C6H2+H=C6H3 4.30E+45 -10.2 13250.0

693. C6H3+H=C4H2+C2H2 2.40E+19 -1.6 2800.0

694. C6H3+H=l-C6H4 4.20E+44 -10.3 7890.0

695. C6H3+H=C6H2+H2 3.00E+13 0.0 0.0

696. C6H3+OH=C6H2+H2O 5.00E+12 0.0 0.0

697. C6H3+O2=>CO+C3H2+HCCO 5.00E+11 0.0 0.0

698. l-C6H4+H=n-C6H5 3.30E+44 -10.0 18800.0

699. l-C6H4+H=A1 3.60E+77 -20.1 28100.0

700. A1(+M)=c-C6H4+H(+M) 4.30E+12 0.6 77313.0

Low pressure limit: 0.10000E+85 -0.18866E+02 0.90064E+05

TROE centering: 0.90200E+00 0.69600E+03 0.35800E+03 0.38560E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

701. A1+H=c-C6H4+H2 2.00E+11 1.1 24500.0

702. l-C6H4+H=C6H3+H2 6.65E+06 2.5 9240.0

703. l-C6H4+OH=C6H3+H2O 3.10E+06 2.0 430.0

704. n-C6H5=A1 1.30E+62 -15.9 35800.0

705. n-C6H5=c-C6H4+H 2.70E+65 -15.9 59700.0

706. n-C6H5+H=i-C6H5+H 2.40E+11 0.8 2410.0

707. n-C6H5+H=l-C6H6 1.10E+42 -9.7 7000.0

708. i-C6H5+H=l-C6H6 4.20E+44 -10.3 7890.0

709. n-C6H5+H=l-C6H4+H2 1.50E+13 0.0 0.0

710.	i-C6H5+H=l-C6H4+H2			3.00E+13	0.0	0.0
711.	n-C6H5+OH=l-C6H4+H2O			2.50E+12	0.0	0.0
712.	i-C6H5+OH=l-C6H4+H2O			5.00E+12	0.0	0.0
713.	n-C6H5+O2=>C4H4+HCO+CO			4.16E+10	0.0	2500.0
714.	i-C6H5+O2=>CH2CO+CH2CO+C2H			7.86E+16	-1.8	0.0
715.	nC4H3+C2H2=n-C6H5			6.00E+33	-7.4	13700.0
716.	l-C6H6+H+M=n-C6H7+M			2.90E+17	-0.5	1000.0
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	CH4	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	7.000E-01			
717.	l-C6H6+H+M=CYC6H7+M			1.70E+28	-4.7	2800.0
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	CH4	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	7.000E-01			
718.	l-C6H6+H=n-C6H5+H2			6.65E+05	2.5	12240.0
719.	l-C6H6+H=i-C6H5+H2			3.33E+05	2.5	9240.0
720.	l-C6H6+OH=n-C6H5+H2O			6.20E+06	2.0	3430.0
721.	l-C6H6+OH=i-C6H5+H2O			3.10E+06	2.0	430.0
722.	n-C6H7=CYC6H7			4.10E+24	-7.1	3900.0
723.	n-C6H7=A+H			8.40E+21	-4.2	11300.0
724.	n-C6H7+H=i-C6H7+H			4.00E+41	-8.1	19200.0
725.	i-C6H7+H=C6H8			1.20E+60	-13.9	21000.0
726.	n-C6H7+H=C6H8			8.70E+69	-17.0	24000.0
727.	n-C6H7+H=l-C6H6+H2			1.50E+13	0.0	0.0

728.	i-C6H7+H=l-C6H6+H2	3.00E+13	0.0	0.0
729.	n-C6H7+OH=l-C6H6+H2O	2.50E+12	0.0	0.0
730.	i-C6H7+OH=l-C6H6+H2O	5.00E+12	0.0	0.0
731.	n-C6H7+O2=>iiiC4H6+CO+HCO	4.16E+10	0.0	2500.0
732.	i-C6H7+O2=>CH2CO+CH2CO+C2H3	7.86E+16	-1.8	0.0
733.	C6H8+H=n-C6H7+H2	1.33E+06	2.5	12240.0
734.	C6H8+H=i-C6H7+H2	6.65E+05	2.5	9240.0
735.	C6H8+OH=n-C6H7+H2O	6.20E+06	2.0	3430.0
736.	C6H8+OH=i-C6H7+H2O	3.10E+06	2.0	430.0
737.	A1+O=C5H5+CO	9.00E+13	0.0	0.0
738.	CH2SING+A=A1+CH3	1.70E+14	0.0	0.0
739.	C3H3+C3H3=C4H5C2H	6.48E+68	-16.7	2872.0
	Declared duplicate reaction...			
740.	C3H3+C3H3=C4H5C2H	1.54E+36	-7.8	5580.0
	Declared duplicate reaction...			
741.	C3H3+C3H3=FC6H6	7.25E+65	-16.0	25035.0
	Declared duplicate reaction...			
742.	C3H3+C3H3=FC6H6	4.19E+39	-9.0	6098.0
	Declared duplicate reaction...			
743.	C3H3+C3H3=A	1.64E+66	-15.9	27529.0
	Declared duplicate reaction...			
744.	C3H3+C3H3=A	1.20E+35	-7.4	5058.0
	Declared duplicate reaction...			
745.	C3H3+C3H3=A1+H	2.02E+33	-6.0	15940.0
746.	C3H3+AC3H5=FC6H6+H+H	3.26E+29	-5.4	3390.0
747.	nC4H3+C2H3=A	2.87E+14	0.0	817.0
748.	n-C4H5+C2H3=A+H2	2.80E-07	5.6	-1890.0
749.	n-C4H5+C2H3=CY13C6H8	5.50E+15	-1.7	1470.0
750.	iiiC4H6+C2H3=CY13C6H8+H	2.28E+12	-0.2	9920.0
751.	n-C4H5+C2H2=A+H	2.94E+16	-1.1	9257.0
752.	n-C4H5+C2H2=l-C6H6+H	1.14E+09	1.4	17338.0
753.	n-C4H5+C2H2=FC6H6+H	1.52E+15	-0.8	8762.0

754.	C2H2+n-C4H5=CYC6H7	2.85E+48	-12.3	15693.4
	Declared duplicate reaction...			
755.	C2H2+n-C4H5=CYC6H7	3.49E-06	4.0	-5112.0
	Declared duplicate reaction...			
756.	i-C4H5+C2H2=A+H	1.47E+23	-3.3	24907.0
757.	i-C4H5+C2H2=FC6H6+H	1.01E+34	-5.9	28786.0
758.	i-C4H5+C2H2=C4H5C2H+H	5.70E+18	-1.4	30351.0
759.	C2H2+i-C4H5=CYC6H7	1.14E+31	-9.2	19403.0
	Declared duplicate reaction...			
760.	C2H2+i-C4H5=CYC6H7	4.34E+39	-9.1	19210.0
	Declared duplicate reaction...			
761.	C5H5+CH3=FC6H6+H2	9.26E+01	2.2	8811.4
762.	FC6H6=A	5.62E+81	-19.4	121500.0
763.	FC6H6=A1+H	2.57E+97	-23.2	153470.0
764.	FC6H6+H=A+H	3.00E+12	0.5	2000.0
765.	CY13C6H8=A+H2	4.39E+37	-7.3	71949.0
766.	CY13C6H8=CYC6H7+H	2.42E+59	-13.3	96147.0
767.	CYC6H7=A+H	2.64E+59	-14.3	44929.0
768.	A=A1+H	1.35+108	-25.8	181750.0
769.	A+H=A1+H2	2.50E+14	0.0	16000.0
770.	A+OH=A1+H2O	1.63E+08	1.4	1450.0
771.	A+O2=A1+HO2	6.30E+13	0.0	60000.0
772.	A+O=A1+OH	2.00E+13	0.0	14704.0
773.	hexene1+H=hex1yl	2.92E+41	-9.3	9784.0
	Declared duplicate reaction...			
774.	hexene1+H=hex1yl	1.24E+62	-15.6	22448.0
	Declared duplicate reaction...			
775.	hexene1+H=hex2yl	1.68E+63	-15.8	21543.0
	Declared duplicate reaction...			
776.	hexene1+H=hex2yl	3.53E+47	-11.0	11174.0
	Declared duplicate reaction...			
777.	hex1yl=hex2yl	2.00E+11	0.0	11100.0

778.	hex1yl=hex3yl	2.00E+11	0.0	18100.0
779.	hex2yl+O2=>CH3CHO+IC4H8+OH	2.10E+11	0.0	6858.0
780.	hex2yl+HO2=>CH3CHO+nC4H9+OH	1.00E+13	0.0	0.0
781.	hex2yl+OH=hexene1+H2O	3.64E+13	0.0	0.0
782.	hex2yl+O=CH3CHO+nC4H9	1.61E+13	0.0	0.0
783.	hex3yl=IC4H8+C2H5	6.00E+13	0.0	29700.0
784.	hex2yl=C3H6+nC3H7	5.00E+13	0.0	28700.0
785.	hex1yl=C2H4+nC4H9	1.00E+13	0.0	28700.0
786.	hex1yl+H=hexene1+H2	1.81E+12	0.0	0.0
787.	hex2yl+O2=hexene1+HO2	3.00E+12	0.0	4500.0
788.	hex1yl+O2=hexene1+HO2	2.00E+12	0.0	2000.0
789.	hex1yl+OH=hexene1+H2O	2.43E+13	0.0	0.0
790.	hex1yl+CH3=hexene1+CH4	1.00E+12	0.0	0.0
791.	hex1yl+C2H5=hexene1+C2H6	1.00E+12	0.0	0.0
792.	hex1yl+C2H3=hexene1+C2H4	1.00E+12	0.0	0.0
793.	hex1yl+AC3H5=hexene1+C3H6	1.00E+12	0.0	0.0
794.	hex2yl+CH3=hexene1+CH4	1.00E+12	0.0	0.0
795.	hex2yl+C2H5=hexene1+C2H6	1.00E+12	0.0	0.0
796.	hex2yl+C2H3=hexene1+C2H4	1.00E+12	0.0	0.0
797.	hex2yl+AC3H5=hexene1+C3H6	1.00E+12	0.0	0.0
798.	hexene1=AC3H5+nC3H7	1.08E+80	-19.3	95177.0
799.	hexene1=C4H7+C2H5	2.71E+80	-19.3	107015.0
800.	C2H3+nC4H9=hexene1	1.00E+13	0.0	0.0
801.	hexene1+O2=C6H11-13+HO2	4.00E+12	0.0	40000.0
802.	hexene1+O2=C6H11-15+HO2	2.80E+13	0.0	48300.0
803.	hexene1+O2=C6H11-14+HO2	2.80E+13	0.0	48300.0
804.	hexene1+O2=C6H11+HO2	2.10E+13	0.0	51300.0
805.	hexene1+HO2=C6H11-14+H2O2	6.80E+12	0.0	17000.0
806.	hexene1+HO2=C6H11-15+H2O2	6.80E+12	0.0	17000.0
807.	hexene1+HO2=C6H11+H2O2	5.60E+12	0.0	19400.0
808.	hexene1+HO2=C6H11-13+H2O2	1.00E+11	0.0	17060.0
809.	hexene1+O=C6H11+OH	4.20E+02	3.5	3092.0

810.	hexene1+O=C6H11-15+OH	2.25E+03	3.3	1653.0
811.	hexene1+O=C6H11-14+OH	2.25E+03	3.3	1653.0
812.	hexene1+O=C6H11-13+OH	4.00E+13	0.0	4000.0
813.	hexene1+H=C6H11+H2	2.80E+07	2.0	7700.0
814.	hexene1+H=C6H11-15+H2	9.10E+06	0.0	5000.0
815.	hexene1+H=C6H11-14+H2	9.10E+06	0.0	5000.0
816.	hexene1+H=C6H11-13+H2	6.55E+12	0.0	4445.0
817.	hexene1+OH=C6H11+H2O	2.85E+05	2.3	236.0
818.	hexene1+OH=C6H11-15+H2O	6.35E+06	2.0	-500.0
819.	hexene1+OH=C6H11-14+H2O	6.35E+06	2.0	-500.0
820.	hexene1+OH=C6H11-13+H2O	6.00E+13	0.0	1230.0
821.	hexene1+CH3=C6H11+CH4	1.47E+12	0.0	11722.0
822.	hexene1+CH3=C6H11-15+CH4	6.60E+11	0.0	10120.0
823.	hexene1+CH3=C6H11-14+CH4	6.60E+11	0.0	10120.0
824.	hexene1+CH3=C6H11-13+CH4	2.00E+11	0.0	6800.0
825.	hexene1+C2H3=C6H11-13+C2H4	2.00E+11	0.0	6800.0
826.	hexene1+C2H3=C6H11-14+C2H4	6.60E+12	0.0	10120.0
827.	hexene1+C2H3=C6H11-15+C2H4	6.60E+12	0.0	10120.0
828.	hexene1+C2H3=C6H11+C2H4	2.94E+12	0.0	11722.0
829.	C6H11-13+H=hexene1	1.00E+13	0.0	0.0
830.	hexene1+nC3H7=C6H11-13+C3H8	1.00E+11	0.0	8300.0
831.	C6H11-13+HO2=>nC3H7+C2H3CHO+OH	1.00E+12	0.0	8000.0
832.	C6H11=C6H11-12	1.00E+11	0.0	20320.0
833.	C6H11-12=C6H11-15	2.00E+11	0.0	18100.0
834.	C6H11-12=nC3H7+AC3H4	1.00E+12	0.0	33000.0
835.	C6H11-14=C2H3+IC4H8	4.00E+13	0.0	35500.0
836.	C6H11-15=AC3H5+C3H6	4.00E+13	0.0	35500.0
837.	CYC6H12=hexene1	5.88+157	-40.2	180653.2
838.	CYC6H12+M=CYC6H11+H+M	3.00E+16	0.0	95000.0
839.	CYC6H12+O2=CYC6H11+HO2	7.50E+13	0.0	49000.0
840.	CYC6H12+HO2=CYC6H11+H2O2	1.20E+13	0.0	17057.0
841.	CYC6H12+O=CYC6H11+OH	2.60E+06	2.6	2563.0

842. CYC6H12+H=CYC6H11+H2	6.00E+14	0.0	8373.0
843. CYC6H12+CH3=CYC6H11+CH4	1.35E+12	0.0	9540.0
844. CYC6H12+C2H3=CYC6H11+C2H4	1.35E+12	0.0	9540.0
845. CYC6H12+C2H5=CYC6H11+C2H6	1.35E+12	0.0	9540.0
846. CYC6H12+AC3H5=CYC6H11+C3H6	1.35E+12	0.0	9540.0
847. CYC6H12+SC3H5=CYC6H11+C3H6	1.35E+12	0.0	9540.0
848. CYC6H12+TC3H5=CYC6H11+C3H6	1.35E+12	0.0	9540.0
849. CYC6H12+CH3O=CYC6H11+CH3OH	4.32E+11	0.0	4473.0
850. CYC6H12+HCO=CYC6H11+CH2O	1.35E+12	0.0	9540.0
851. CYC6H11=C6H11	1.26E+92	-24.4	54251.0
852. CYC6H11=C6H11-13	3.40E+97	-25.6	64287.0
853. CYC6H11=CYC6H10+H	3.93E+56	-13.8	48532.0
854. CYC6H11=C4H7+C2H4	4.11E+70	-17.1	63299.0
855. CYC6H11=iiiC4H6+C2H5	1.95E+89	-22.5	77468.0
856. C6H11=C4H7+C2H4	8.13E+51	-12.2	41926.0
857. C6H11=CYC6H10+H	1.39E+59	-15.1	40495.0
858. C6H11=C6H11-13	1.42E+80	-21.3	41217.0
859. C6H11=C2H5+iiiC4H6	5.41E+78	-19.9	59833.0
860. C6H11-13=C4H7+C2H4	8.18E+84	-21.4	72373.0
861. C6H11-13=CYC6H10+H	7.01E+83	-21.8	67519.0
862. C6H11-13=C2H5+iiiC4H6	8.36E+68	-16.6	62898.0
863. CYC6H11+O2=CYC6H10+HO2	2.40E+11	0.0	0.0
864. CYC6H11+HO2=CYC6H10+H2O2	2.00E+12	0.0	2000.0
865. CYC6H11+OH=CYC6H10+H2O	4.80E+13	0.0	0.0
866. CYC6H11+O=CYC6H10+OH	9.64E+13	0.0	0.0
867. CYC6H11+H=CYC6H10+H2	2.00E+11	0.0	0.0
868. CYC6H11+CH3=CYC6H10+CH4	4.00E+12	0.0	0.0
869. CYC6H11+HCO=CYC6H10+CH2O	4.00E+12	0.0	0.0
870. CYC6H10=iiiC4H6+C2H4	1.01E+44	-8.7	78963.0
871. CYC6H10=CY13C6H8+H2	2.26E+38	-7.4	70907.0
872. CYC6H10=CYC6H9+H	5.98E+53	-11.5	95520.0
873. CYC6H10+O2=CYC6H9+HO2	7.20E+13	0.0	34800.0

874.	CYC6H10+HO2=CYC6H9+H2O2	2.00E+11	0.0	17060.0
875.	CYC6H10+OH=CYC6H9+H2O	6.00E+13	0.0	300.0
876.	CYC6H10+O=CYC6H9+OH	6.20E+12	0.0	4445.0
877.	CYC6H10+H=CYC6H9+H2	6.20E+12	0.0	4445.0
878.	CYC6H10+CH3=CYC6H9+CH4	1.65E+11	0.0	4118.0
879.	CYC6H10+HCO=CYC6H9+CH2O	1.65E+11	0.0	4118.0
880.	CYC6H9=CY13C6H8+H	1.62E+57	-13.0	66036.0
881.	CYC6H9=C6H9	5.36E+50	-11.9	48276.0
882.	CYC6H9=n-C4H5+C2H4	2.77E+73	-17.3	89006.0
883.	CYC6H9=C6H8+H	4.44E+73	-17.3	89006.0
884.	C6H9=CY13C6H8+H	3.21E+52	-12.5	41221.0
885.	C6H9=n-C4H5+C2H4	2.45E+52	-12.1	51404.0
886.	C6H9=C6H8+H	3.92E+52	-12.1	51404.0
887.	CYC6H9+O2=CY13C6H8+HO2	1.60E+12	0.0	15160.0
888.	CYC6H9+HO2=CY13C6H8+H2O2	1.00E+12	0.0	0.0
889.	CYC6H9+OH=CY13C6H8+H2O	6.02E+12	0.0	0.0
890.	CYC6H9+O=CY13C6H8+OH	1.80E+13	0.0	0.0
891.	CYC6H9+H=CY13C6H8+H2	3.16E+13	0.0	0.0
892.	CYC6H9+CH3=CY13C6H8+CH4	8.00E+12	0.0	0.0
893.	CYC6H9+HCO=CY13C6H8+CH2O	4.00E+12	0.0	0.0
894.	CY13C6H8+O2=CYC6H7+HO2	8.31E+11	0.0	24858.0
895.	CY13C6H8+HO2=CYC6H7+H2O2	4.00E+12	0.0	17057.0
896.	CY13C6H8+OH=CYC6H7+H2O	6.00E+06	2.0	-1520.0
897.	CY13C6H8+O=CYC6H7+OH	1.40E+13	0.0	-795.0
898.	CY13C6H8+H=CYC6H7+H2	1.10E+05	2.5	-1900.0
899.	CY13C6H8+CH3=CYC6H7+CH4	1.23E+11	0.0	5201.0
900.	CY13C6H8+C2H3=CYC6H7+C2H4	1.23E+11	0.0	5201.0
901.	CY13C6H8+HCO=CYC6H7+CH2O	1.23E+11	0.0	5201.0
902.	CY13C6H8+C2H2=A+C2H4	3.10E+10	0.0	27200.0
903.	CYC6H7+O2=A+HO2	1.00E+12	0.0	0.0
904.	CYC6H7+HO2=A+H2O2	1.00E+12	0.0	0.0
905.	CYC6H7+HO2=C5H6+HCO+OH	4.50E+12	0.0	0.0

906.	CYC6H7+OH=A+H2O	6.02E+12	0.0	0.0
907.	CYC6H7+O=A+OH	1.80E+13	0.0	0.0
908.	CYC6H7+O=C5H6+HCO	8.26E+13	0.0	0.0
909.	CYC6H7+H=A+H2	3.16E+13	0.0	0.0
910.	CYC6H7+CH3=A+CH4	8.00E+12	0.0	0.0
911.	CYC6H7+HCO=A+CH2O	4.00E+12	0.0	0.0
912.	C6H11+H=C6H10+H2	1.80E+12	0.0	0.0
913.	C6H11+O2=C6H10+HO2	1.00E+11	0.0	0.0
914.	C6H11+CH3=C6H10+CH4	1.10E+13	0.0	0.0
915.	C6H11+O=C6H10+OH	4.82E+13	0.0	0.0
916.	C6H11+OH=C6H10+H2O	2.41E+13	0.0	0.0
917.	C6H10+H=C4H7+C2H4	1.46E+30	-4.3	21647.0
918.	C6H10+O=CH2CO+C4H7+H	1.20E+08	1.6	327.0
919.	C6H9+O2=C6H8+HO2	1.60E+12	0.0	5000.0
920.	C6H9+H=C6H8+H2	1.80E+12	0.0	0.0
921.	C6H9+CH3=C6H8+CH4	1.10E+13	0.0	0.0
922.	C6H9+O=C6H8+OH	4.82E+13	0.0	0.0
923.	C6H9+OH=C6H8+H2O	2.41E+13	0.0	0.0
924.	C6H8+O=CH2CO+n-C4H5+H	1.20E+08	1.6	327.0
925.	C2H5OH=CH3+CH2OH	1.26E+51	-10.6	100869.0
926.	C2H5OH=C2H4+H2O	8.80E+25	-3.7	70799.0
927.	C2H5OH+OH=C2H4OH+H2O	1.81E+11	0.4	716.5
928.	C2H5OH+OH=CH3CHOH+H2O	3.09E+10	0.5	-379.8
929.	C2H5OH+OH=C2H5O+H2O	1.05E+10	0.8	716.9
930.	C2H5OH+H=C2H4OH+H2	1.90E+07	1.8	5098.0
931.	C2H5OH+H=CH3CHOH+H2	2.58E+07	1.6	2827.0
932.	C2H5OH+H=C2H5O+H2	1.50E+07	1.6	3038.0
933.	C2H5OH+O=C2H4OH+OH	9.41E+07	1.7	5459.0
934.	C2H5OH+O=CH3CHOH+OH	1.88E+07	1.9	1824.0
935.	C2H5OH+O=C2H5O+OH	1.58E+07	2.0	4448.0
936.	C2H5OH+CH3=C2H4OH+CH4	2.19E+02	3.2	9622.0
937.	C2H5OH+CH3=CH3CHOH+CH4	7.28E+02	3.0	7948.0

938.	C2H5OH+CH3=C2H5O+CH4	1.45E+02	3.0	7649.0
939.	C2H5OH+HO2=CH3CHOH+H2O2	8.20E+03	2.5	10750.0
940.	C2H5OH+HO2=C2H4OH+H2O2	2.43E+04	2.5	15750.0
941.	C2H5OH+HO2=C2H5O+H2O2	3.80E+12	0.0	24000.0
942.	C2H5O+M=CH3CHO+H+M	5.60E+34	-5.9	25274.0
943.	C2H5O+M=CH3+CH2O+M	5.35E+37	-7.0	23800.0
944.	C2H5O+CO=C2H5+CO2	4.68E+02	3.2	5380.0
945.	C2H5O+H=CH3+CH2OH	3.00E+13	0.0	0.0
946.	C2H5O+H=C2H4+H2O	3.00E+13	0.0	0.0
947.	C2H5O+OH=CH3CHO+H2O	1.00E+13	0.0	0.0
948.	CH3CHOH+O2=CH3CHO+HO2	4.82E+13	0.0	5017.0
	Declared duplicate reaction...			
949.	CH3CHOH+O2=CH3CHO+HO2	8.43E+14	-1.2	0.0
	Declared duplicate reaction...			
950.	CH3CHOH+O=CH3CHO+OH	1.00E+14	0.0	0.0
951.	CH3CHOH+H=C2H4+H2O	3.00E+13	0.0	0.0
952.	CH3CHOH+H=CH3+CH2OH	3.00E+13	0.0	0.0
953.	CH3CHOH+HO2=CH3CHO+OH+OH	4.00E+13	0.0	0.0
954.	CH3CHOH+OH=CH3CHO+H2O	5.00E+12	0.0	0.0
955.	CH3CHOH+M=CH3CHO+H+M	1.00E+14	0.0	25000.0
956.	C2H4+OH=C2H4OH	2.41E+11	0.0	-2385.0
957.	C2H4OH+O2=HOC2H4O2	1.00E+12	0.0	-1100.0
958.	HOC2H4O2=CH2O+CH2O+OH	1.80E+11	0.0	24500.0
959.	CH3OCH3=CH3+CH3O	1.88E+49	-10.4	93453.5
960.	CH3OCH3+OH=CH3OCH2+H2O	6.71E+06	2.0	-629.9
961.	CH3OCH3+H=CH3OCH2+H2	2.97E+07	2.0	4033.6
962.	CH3OCH3+O=CH3OCH2+OH	1.86E-03	5.3	-109.0
963.	CH3OCH3+HO2=CH3OCH2+H2O2	1.68E+13	0.0	17690.0
964.	CH3OCH3+CH3=CH3OCH2+CH4	3.86E-08	6.2	2513.9
965.	CH3OCH3+O2=CH3OCH2+HO2	4.10E+13	0.0	44910.0
966.	CH3OCH3+CH3O=CH3OCH2+CH3OH	6.02E+11	0.0	4074.0
967.	CH3OCH2=CH2O+CH3	1.60E+13	0.0	25500.0

968.	CH3OCH2+CH3O=CH3OCH3+CH2O	2.41E+13	0.0	0.0
969.	CH3OCH2+CH2O=CH3OCH3+HCO	5.49E+03	2.8	5862.0
970.	CH3OCH2+O2=>CH2O+CH2O+OH	5.02E+23	-3.8	3100.0
971.	CH3OCH2+HO2=CH3OCH2O+OH	9.00E+12	0.0	0.0
972.	CH3OCH2O=CH3OCHO+H	1.74E+16	-0.7	11720.0
973.	CH3OCHO=CH3+OCHO	1.39E+18	-1.0	79140.0
974.	CH3OCHO+O2=CH3OCO+HO2	1.00E+13	0.0	49700.0
975.	CH3OCHO+OH=CH3OCO+H2O	2.34E+07	1.6	-35.0
976.	CH3OCHO+HO2=CH3OCO+H2O2	1.22E+12	0.0	17000.0
977.	CH3OCHO+O=CH3OCO+OH	2.35E+05	2.5	2230.0
978.	CH3OCHO+H=CH3OCO+H2	4.55E+06	2.0	5000.0
979.	CH3OCHO+CH3=CH3OCO+CH4	7.55E-01	3.5	5481.0
980.	CH3OCHO+CH3O=CH3OCO+CH3OH	5.48E+11	0.0	5000.0
981.	CH3OCO=CH3O+CO	7.45E+12	-1.8	17150.0
982.	CH3OCO=CH3+CO2	1.51E+12	-1.8	13820.0
983.	OCHO+M=H+CO2+M	2.44E+15	-0.5	26500.0
984.	NH+M=N+H+M	2.65E+14	0.0	75500.0
985.	NH+H=N+H2	3.20E+13	0.0	325.0
986.	NH+O=N+OH	1.70E+08	1.5	3368.0
987.	NH+OH=N+H2O	1.60E+07	1.7	-576.0
988.	NH2+M=NH+H+M	3.16E+23	-2.0	91400.0
989.	NH2+H=NH+H2	4.00E+13	0.0	3650.0
990.	NH2+O=NH+OH	7.00E+12	0.0	0.0
	Declared duplicate reaction...			
991.	NH2+O=NH+OH	8.60E-01	4.0	1673.0
	Declared duplicate reaction...			
992.	NH2+OH=NH+H2O	3.30E+06	1.9	-217.0
993.	NH2+O2=NH+HO2	1.00E+14	0.0	49997.0
994.	NH+NH=NH2+N	5.70E-01	3.9	342.0
995.	NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
996.	NH3+M=NH+H2+M	6.30E+14	0.0	93390.0
997.	NH3+H=NH2+H2	6.36E+05	2.4	10171.0

998.	NH3+O=NH2+OH			2.80E+02	3.3	4471.0
999.	NH3+OH=NH2+H2O			2.00E+06	2.0	566.0
1000.	NH2+HO2=NH3+O2			9.20E+05	1.9	-1152.0
1001.	NH3+HO2=NH2+H2O2			3.00E+11	0.0	22000.0
1002.	NH2+NH=NH3+N			9.60E+03	2.5	107.0
1003.	NH2+NH2=NH3+NH			5.60E+00	3.5	552.0
1004.	N2+M=N+N+M			1.00E+28	-3.3	225000.0
1005.	NH+N=N2+H			3.00E+13	0.0	0.0
1006.	NH+NH=N2+H+H			2.50E+13	0.0	0.0
1007.	NH2+N=N2+H+H			7.10E+13	0.0	0.0
1008.	NH+NH=N2+H2			1.00E+08	1.0	0.0
1009.	NNH=N2+H			1.00E+09	0.0	0.0
1010.	NNH+H=N2+H2			1.00E+14	0.0	0.0
1011.	NH+NH=NNH+H			5.10E+13	0.0	0.0
1012.	NNH+O=N2+OH			1.20E+13	0.1	-217.0
1013.	NNH+OH=N2+H2O			5.00E+13	0.0	0.0
1014.	NNH+O2=N2+HO2			5.60E+14	-0.4	-13.0
1015.	NNH+O2=N2+H+O2			5.00E+13	0.0	0.0
1016.	NNH+HO2=N2+H2O2			1.40E+04	2.7	-1599.0
1017.	NNH+N=NH+N2			3.00E+13	0.0	2000.0
1018.	NNH+NH=N2+NH2			5.00E+13	0.0	0.0
1019.	NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
1020.	N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
	H2O	Enhanced by	1.500E+01			
	O2	Enhanced by	2.000E+00			
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
1021.	N2H2+M=NH+NH+M			3.16E+16	0.0	99400.0
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
1022.	NH2+NH=N2H2+H			4.30E+14	-0.3	-77.0
1023.	N2H2+H=NNH+H2			8.50E+04	2.6	230.0

1024.	NH2+NH2=N2H2+H2	1.70E+08	1.6	11783.0
1025.	N2H2+O=NNH+OH	3.30E+08	1.5	496.0
1026.	N2H2+OH=NNH+H2O	5.90E+01	3.4	1360.0
1027.	N2H2+N=NNH+NH	1.00E+06	2.0	0.0
1028.	N2H2+NH=NNH+NH2	1.00E+13	0.0	6000.0
1029.	N2H2+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
1030.	NNH+NNH=N2H2+N2	1.00E+13	0.0	4000.0
1031.	H2NN=NNH+H	3.40E+26	-4.8	46228.0
1032.	N2H2=H2NN	2.00E+41	-9.4	68413.0
1033.	H2NN+H=N2H2+H	7.00E+13	0.0	0.0
1034.	H2NN+H=NNH+H2	4.80E+08	1.5	-894.0
1035.	NH2+NH2=H2NN+H2	7.20E+04	1.9	8802.0
1036.	H2NN+O=OH+NNH	3.30E+08	1.5	-894.0
1037.	H2NN+OH=NNH+H2O	2.40E+06	2.0	-1192.0
1038.	H2NN+HO2=NNH+H2O2	2.90E+04	2.7	-1599.0
1039.	H2NN+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
1040.	N2H3=N2H2+H	3.60E+47	-10.4	68970.0
1041.	N2H3+M=NH2+NH+M	5.00E+16	0.0	60000.0
1042.	NH2+NH2=N2H3+H	1.20E+12	0.0	10078.0
1043.	N2H3+H=N2H2+H2	2.40E+08	1.5	0.0
1044.	N2H3+H=NH+NH3	1.00E+11	0.0	0.0
1045.	NH3+NH2=N2H3+H2	1.00E+11	0.5	21600.0
1046.	N2H3+O=N2H2+OH	1.70E+08	1.5	-645.0
1047.	N2H3+OH=N2H2+H2O	1.20E+06	2.0	-1192.0
1048.	N2H3+OH=H2NN+H2O	3.00E+13	0.0	0.0
1049.	N2H3+HO2=N2H2+H2O2	1.40E+04	2.7	-1600.0
1050.	N2H3+N=N2H2+NH	1.00E+06	2.0	0.0
1051.	N2H3+NH=N2H2+NH2	2.00E+13	0.0	0.0
1052.	N2H3+NH2=N2H2+NH3	9.20E+05	1.9	-1152.0
1053.	N2H3+NH2=H2NN+NH3	3.00E+13	0.0	0.0
1054.	N2H3+NNH=N2H2+N2H2	1.00E+13	0.0	4000.0
1055.	N2H3+N2H3=NH3+NH3+N2	3.00E+12	0.0	0.0

1056.	NH2+NH2(+M)=N2H4(+M)		5.60E+14	-0.4	66.0
	Low pressure limit: 0.16000E+35 -0.54900E+01 0.19870E+04				
	TROE centering: 0.31000E+00 0.10000E-29 0.10000E+31 0.10000E+31				
1057.	N2H4+M=N2H3+H+M		1.00E+15	0.0	63600.0
	N2	Enhanced by 2.400E+00			
	NH3	Enhanced by 3.000E+00			
	N2H4	Enhanced by 4.000E+00			
1058.	N2H4=H2NN+H2		5.30E+39	-8.3	69267.0
1059.	N2H4+H=N2H3+H2		7.00E+12	0.0	2500.0
1060.	N2H4+H=NH2+NH3		2.40E+09	0.0	3100.0
1061.	N2H4+O=N2H3+OH		6.70E+08	1.5	2850.0
1062.	N2H4+O=N2H2+H2O		4.40E+11	0.0	-1270.0
1063.	N2H4+OH=N2H3+H2O		4.00E+13	0.0	0.0
1064.	N2H3+HO2=N2H4+O2		9.20E+05	1.9	2125.0
1065.	N2H4+N=N2H3+NH		1.00E+10	1.0	2000.0
1066.	N2H4+NH=NH2+N2H3		1.00E+09	1.5	2000.0
1067.	N2H4+NH2=N2H3+NH3		3.90E+12	0.0	1500.0
1068.	N2H3+N2H2=N2H4+NNH		1.00E+13	0.0	6000.0
1069.	N2H3+N2H3=N2H4+N2H2		1.20E+13	0.0	0.0
1070.	NO+M=N+O+M		1.40E+15	0.0	148430.0
	N2	Enhanced by 1.000E+00			
	H2	Enhanced by 2.200E+00			
	H2O	Enhanced by 6.700E+00			
	CO2	Enhanced by 3.000E+00			
	N2O	Enhanced by 2.200E+00			
1071.	N+OH=NO+H		3.80E+13	0.0	0.0
1072.	NH+O=NO+H		9.20E+13	0.0	0.0
1073.	NH2+O=NO+H2		5.00E+12	0.0	0.0
1074.	NH+OH=NO+H2		2.00E+13	0.0	0.0
1075.	NO+O=O2+N		1.81E+09	1.0	38725.0
1076.	NH+O2=NO+OH		1.30E+06	1.5	100.0
1077.	N+NO=N2+O		3.30E+12	0.3	0.0

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1078. NH+NO=N2+OH                                      2.20E+13   -0.2        0.0
1079. NNH+O=NH+NO                                      5.20E+11    0.4     -409.0
1080. NH2+NO=N2+H2O                                    2.80E+20   -2.7     1258.0
1081. NH2+NO=NNH+OH                                    2.29E+10    0.4     -814.0
1082. N2H2+O=NH2+NO                                    1.00E+13    0.0        0.0
1083. H2NN+O=NH2+NO                                    7.00E+13    0.0        0.0
1084. H2NN+OH=>NH2+NO+H                                2.00E+12    0.0        0.0
1085. N2H3+O=>NH2+NO+H                                 3.00E+13    0.0        0.0
1086. H2NN+HO2=>NH2+NO+OH                              9.00E+12    0.0        0.0
1087. NO+H(+M)=HNO(+M)                                 1.50E+15   -0.4        0.0
      Low pressure limit:  0.24000E+15  0.20600E+00 -0.15500E+04
      TROE centering:      0.82000E+00  0.10000E-29  0.10000E+31  0.10000E+31
      N2              Enhanced by    1.600E+00
1088. HNO+H=H2+NO                                      4.50E+11    0.7      655.0
1089. NH+OH=HNO+H                                      3.20E+14   -0.4      -46.0
1090. NH2+O=HNO+H                                      6.63E+14   -0.5        0.0
1091. NH+H2O=HNO+H2                                    2.00E+13    0.0    13850.0
1092. HNO+O=OH+NO                                      1.81E+13    0.0        0.0
1093. NH+O2=HNO+O                                      4.60E+05    2.0     6494.0
1094. HNO+OH=NO+H2O                                    3.60E+13    0.0        0.0
1095. NH2+O2=HNO+OH                                    2.90E-02    3.8    18185.0
1096. NH2+HO2=HNO+H2O                                  5.68E+15   -1.1      707.0
1097. HNO+O2=NO+HO2                                    2.00E+13    0.0    15887.0
1098. NH2+HNO=NH3+NO                                   3.60E+06    1.6    -1250.0
1099. N2H3+O=NH2+HNO                                   3.00E+13    0.0        0.0
1100. N2H3+OH=NH3+HNO                                  1.00E+12    0.0    15000.0
1101. NNH+NO=N2+HNO                                    5.00E+13    0.0        0.0
1102. H+NO+N2=HNO+N2                                   4.00E+20   -1.8        0.0
1103. HON+M=NO+H+M                                     5.10E+19   -1.7    16045.0
      AR              Enhanced by    7.000E-01
      H2O             Enhanced by    7.000E+00
      CO2             Enhanced by    2.000E+00
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1104. HON+H=HNO+H                                   2.00E+13    0.0        0.0
1105. HON+H=OH+NH                                   2.00E+13    0.0        0.0
1106. HON+O=OH+NO                                   7.00E+13    0.0        0.0
1107. HNOH+M=H+HNO+M                                2.00E+24   -2.8    58901.0
1108. HNOH+H=NH2+OH                                 4.00E+13    0.0        0.0
1109. HNOH+H=HNO+H2                                 4.80E+08    1.5      377.0
1110. HNOH+O=HNO+OH                                 7.00E+13    0.0        0.0
      Declared duplicate reaction...
1111. HNOH+O=HNO+OH                                 3.30E+08    1.5     -357.0
      Declared duplicate reaction...
1112. HNOH+OH=HNO+H2O                               2.40E+06    2.0    -1192.0
1113. HNOH+O2=HNO+HO2                               3.00E+12    0.0    25000.0
1114. HNOH+HO2=HNO+H2O2                             2.90E+04    2.7    -1599.0
1115. HNOH+NH2=N2H3+OH                              1.00E+01    3.5     -467.0
1116. HNOH+NH2=H2NN+H2O                             8.80E+16   -1.1     1113.0
1117. HNOH+NH2=HNO+NH3                              1.80E+06    1.9    -1152.0
1118. NH2O+M=HNO+H+M                                2.80E+24   -2.8    64915.0
      H2O             Enhanced by    1.000E+01
1119. NH2O+M=HNOH+M                                 1.10E+29   -4.0    44000.0
      H2O             Enhanced by    1.000E+01
1120. NH2O+H=NH2+OH                                 5.00E+13    0.0        0.0
1121. NH2O+H=HNO+H2                                 3.00E+07    2.0     2000.0
1122. NH2O+O=HNO+OH                                 3.00E+07    2.0     2000.0
1123. NH2+O2=NH2O+O                                 2.50E+11    0.5    29570.0
1124. NH2O+OH=HNO+H2O                               2.00E+07    2.0     1000.0
1125. NH2+HO2=NH2O+OH                               5.00E+13    0.0        0.0
1126. NH2O+O2=HNO+HO2                               3.00E+12    0.0    25000.0
1127. NH2O+HO2=HNO+H2O2                             2.90E+04    2.7    -1599.0
1128. NH2O+NH2=HNO+NH3                              3.00E+12    0.0     1000.0
1129. NH2O+NO=HNO+HNO                               2.00E+04    2.0    13000.0
1130. NH2OH(+M)=NH2+OH(+M)                          1.40E+20   -1.3    64080.0
      Low pressure limit:  0.54000E+38 -0.59600E+01  0.66783E+05
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      TROE centering:      0.31000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1131. NH2OH+H=HNOH+H2                                 4.80E+08    1.5     6246.0
1132. NH2OH+H=NH2O+H2                                 2.40E+08    1.5     5064.0
1133. NH2OH+O=HNOH+OH                                 3.30E+08    1.5     3863.0
1134. NH2OH+O=NH2O+OH                                 1.70E+08    1.5     3009.0
1135. NH2OH+OH=HNOH+H2O                               1.50E+04    2.6    -3537.0
1136. NH2OH+OH=NH2O+H2O                               1.50E+05    2.3    -1296.0
1137. NH2O+HO2=O2+NH2OH                               2.90E+04    2.7    -1599.0
1138. HNOH+HO2=NH2OH+O2                               2.90E+04    2.7    -1599.0
1139. NH2OH+HO2=HNOH+H2O2                             2.90E+04    2.7     9552.0
1140. NH2OH+HO2=NH2O+H2O2                             1.40E+04    2.7     6414.0
1141. N2H4+O=NH2OH+NH                                 2.90E+11    0.0    -1270.0
1142. NH2OH+NH=HNOH+NH2                               2.90E-03    4.4     1564.0
1143. NH2OH+NH=NH2O+NH2                               1.50E-03    4.6     2424.0
1144. NH2OH+NH2=HNOH+NH3                              1.10E-01    4.0      -97.0
1145. NH2OH+NH2=NH2O+NH3                              9.50E+00    3.4    -1013.0
1146. H2NN+NH2=HNNNH2+H                               7.90E+06    1.9    -1331.0
1147. N2O(+M)=N2+O(+M)                                1.30E+12    0.0    62570.0
      Low pressure limit:  0.40000E+15  0.00000E+00  0.56600E+05
      N2              Enhanced by    1.700E+00
      O2              Enhanced by    1.400E+00
      CO2             Enhanced by    3.000E+00
      H2O             Enhanced by    1.200E+01
1148. N2O+H=N2+OH                                     3.30E+10    0.0     4729.0
      Declared duplicate reaction...
1149. N2O+H=N2+OH                                     4.40E+14    0.0    19254.0
      Declared duplicate reaction...
1150. NH+NO=N2O+H                                     2.90E+14   -0.4        0.0
      Declared duplicate reaction...
1151. NH+NO=N2O+H                                    -2.20E+13   -0.2        0.0
      Declared duplicate reaction...
1152. NNH+O=N2O+H                                     1.00E+14    0.0        0.0
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1153.	NH2+NO=H2+N2O	1.00E+13	0.0	33700.0
1154.	NO+NO=N2O+O	3.61E+12	0.0	65335.0
	Declared duplicate reaction...			
1155.	N2O+O=NO+NO	6.62E+13	0.0	26611.0
	Declared duplicate reaction...			
1156.	N2O+O=O2+N2	1.02E+14	0.0	28001.0
1157.	N2O+OH=HNO+NO	1.20E-04	4.3	25080.0
1158.	N2O+OH=N2+HO2	1.00E+14	0.0	30000.0
1159.	NNH+O2=N2O+OH	2.90E+11	-0.3	149.0
1160.	HNO+HNO=N2O+H2O	9.00E+08	0.0	3100.0
1161.	NH+N2O=N2+HNO	2.00E+12	0.0	6000.0
1162.	N2H2+NO=N2O+NH2	3.00E+10	0.0	0.0
1163.	HNNO+M=H+N2O+M	2.20E+15	0.0	21600.0
1164.	HNNO+M=N2+OH+M	1.00E+15	0.0	25600.0
1165.	HNNO+H=H2+N2O	2.00E+13	0.0	0.0
1166.	NH2+NO=HNNO+H	8.00E+13	0.0	28000.0
1167.	NNH+HO2=HNNO+OH	2.40E+13	0.0	1698.0
1168.	HNNO+NO=N2O+HNO	1.00E+12	0.0	0.0
1169.	NH2+NO=NH2NO	3.50E+31	-6.8	3724.0
1170.	NH2NO=N2+H2O	3.10E+34	-7.1	36262.0
1171.	NH2NO+H=HNNO+H2	4.80E+08	1.5	7407.0
1172.	N2H3+O=NH2NO+H	3.00E+13	0.0	0.0
1173.	H2NN+OH=NH2NO+H	2.00E+12	0.0	0.0
1174.	NH2NO+O=HNNO+OH	3.30E+08	1.5	4697.0
1175.	NH2NO+OH=HNNO+H2O	2.40E+06	2.0	-70.0
1176.	H2NN+HO2=NH2NO+OH	6.60E+05	1.9	7050.0
1177.	NH2NO+HO2=HNNO+H2O2	2.90E+04	2.7	12620.0
1178.	NH2NO+NH2=HNNO+NH3	1.80E+06	1.9	4538.0
1179.	NH2NHO=NH2+HNO	2.40E+40	-8.7	41584.0
1180.	NH2NHO+H=NHNHO+H2	4.80E+08	1.5	-894.0
1181.	NH2NHO+O=NHNHO+OH	3.30E+08	1.5	-894.0
1182.	NH2NHO+OH=NHNHO+H2O	2.40E+06	2.0	-1192.0

1183. N2H3+HO2=NH2NHO+OH 3.00E+13 0.0 0.0

1184. NH2NHO+HO2=NHNHO+H2O2 2.90E+04 2.7 -1599.0

1185. NH2NHO+NH2=NHNHO+NH3 1.80E+06 1.9 -1152.0

1186. NO2(+M)=NO+O(+M) 7.60E+18 -1.3 73245.0

Low pressure limit: 0.24700E+29 -0.33700E+01 0.74756E+05

TROE centering: 0.10000E+00 0.29510E+03 0.97270E+03 0.49816E+04

N2O Enhanced by 1.500E+00

H2O Enhanced by 4.400E+00

N2 Enhanced by 1.000E+00

CO2 Enhanced by 2.300E+00

Declared duplicate reaction...

1187. NO+O(+M)=NO2(+M) 1.30E+15 -0.8 0.0

Low pressure limit: 0.47100E+25 -0.28700E+01 0.15510E+04

TROE centering: 0.10000E+00 0.29510E+03 0.97270E+03 0.46816E+04

Declared duplicate reaction...

1188. NO2+H=NO+OH 1.30E+14 0.0 357.0

1189. NH+O2=H+NO2 2.30E+10 0.0 2482.0

1190. NO2+O=O2+NO 3.91E+12 0.0 -238.0

1191. NO2+OH=HO2+NO 1.81E+13 0.0 6673.0

1192. HON+O2=NO2+OH 1.00E+12 0.0 4968.0

1193. NO2+N=N2O+O 3.49E+12 0.0 -437.0

1194. NH+NO2=N2O+OH 4.10E+12 0.0 0.0

1195. NH+NO2=HNO+NO 5.90E+12 0.0 0.0

1196. NH2+NO2=N2O+H2O 3.00E+14 -0.8 242.0

1197. NH2+NO2=NH2O+NO 1.30E+15 -0.8 242.0

1198. H2NN+O2=NH2+NO2 1.50E+12 0.0 5958.0

1199. HNNO+NO=NNH+NO2 3.20E+12 0.0 270.0

1200. N2O+NO=NO2+N2 5.30E+05 2.2 46280.0

1201. NO+NO+NO=N2O+NO2 1.07E+10 0.0 26800.0

1202. HNO+NO+NO=HNNO+NO2 1.70E+11 0.0 2100.0

1203. NO2+NO2=NO+NO+O2 1.63E+12 0.0 26108.0

1204. HONO(+M)=OH+NO(+M) 1.20E+19 -1.2 49667.0

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      Low pressure limit:  0.30100E+31 -0.38000E+01  0.50322E+05
      TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
      Declared duplicate reaction...
1205. NO+OH(+M)=HONO(+M)                              1.99E+12   -0.1     -721.0
      Low pressure limit:  0.50800E+24 -0.25100E+01 -0.68000E+02
      TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
      Declared duplicate reaction...
1206. NO2+H2=HONO+H                                   1.30E+04    2.8    29770.0
1207. HONO+H=H2O+NO                                   8.10E+06    1.9     3843.0
1208. HONO+H=OH+HNO                                   5.60E+10    0.9     4965.0
1209. HON+OH=HONO+H                                   4.00E+13    0.0        0.0
1210. HONO+O=OH+NO2                                   1.20E+13    0.0     5958.0
1211. HON+O2=HONO+O                                   1.00E+12    0.0     4965.0
1212. HONO+OH=H2O+NO2                                 1.26E+10    1.0      135.0
1213. NO2+HO2=HONO+O2                                 6.30E+08    1.2     5000.0
1214. NH+HONO=NH2+NO2                                 1.00E+13    0.0        0.0
1215. NH2+HONO=NH3+NO2                                7.10E+01    3.0    -4940.0
1216. HNNO+NO=N2+HONO                                 2.60E+11    0.0      810.0
1217. HNO+NO2=HONO+NO                                 4.40E+04    2.6     4040.0
1218. NH2O+NO2=HONO+HNO                               6.00E+11    0.0     2000.0
1219. HNOH+NO2=HONO+HNO                               6.00E+11    0.0     2000.0
1220. HNNO+NO2=N2O+HONO                               1.00E+12    0.0        0.0
1221. HONO+HONO=NO+NO2+H2O                            3.50E-01    3.6    12140.0
1222. HNO2(+M)=HONO(+M)                               2.50E+14    0.0    32300.0
      Low pressure limit:  0.31000E+19  0.00000E+00  0.31500E+05
      TROE centering:      0.11490E+01  0.10000E-29  0.31250E+04  0.10000E+31
1223. NO2+H2=HNO2+H                                   2.40E+00    3.7    32400.0
1224. HNO2+O=OH+NO2                                   1.70E+08    1.5     2363.0
1225. HNO2+OH=H2O+NO2                                 1.20E+06    2.0     -794.0
1226. NO2+HO2=HNO2+O2                                 1.90E+01    3.3     4983.0
1227. HNO2+NH2=NO2+NH3                                9.20E+05    1.9      874.0
1228. HNO+NO2=HNO2+NO                                 6.02E+11    0.0     1986.0
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1229. NH+O2=HNOO                                      3.70E+24   -5.0     2294.0
1230. NH+O2+M=HNOO+M                                  3.00E+26   -4.0     2274.0
1231. HNOO+M=OH+NO+M                                  1.50E+36   -6.2    31119.0
1232. HNOH+HO2=HONHO+OH                               4.00E+13    0.0        0.0
1233. NH2+NO2=NH2NO2                                  3.50E+31   -6.8     3726.0
1234. NO2+O(+M)=NO3(+M)                               1.32E+13    0.0        0.0
      Low pressure limit:  0.14900E+29 -0.40800E+01  0.24660E+04
      TROE centering:      0.32600E+00  0.50000E+03  0.62049E+04  0.26060E+04
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      N2              Enhanced by    1.000E+00
      HNO3            Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
      NO3             Enhanced by    5.000E+00
1235. NO3+H=NO2+OH                                    6.00E+13    0.0        0.0
1236. NO3+O=NO2+O2                                    1.00E+13    0.0        0.0
1237. NO3+OH=NO2+HO2                                  1.40E+13    0.0        0.0
1238. NO3+HO2=NO2+O2+OH                               1.50E+12    0.0        0.0
1239. NO3+NH=HNO+NO2                                  1.50E+13    0.0        0.0
1240. NO3+NH2=NH2O+NO2                                9.00E+05    0.0      100.0
1241. HNNO+NO2=NNH+NO3                                1.00E+13    0.0        0.0
1242. NO2+NO2=NO3+NO                                  9.60E+09    0.7    20900.0
1243. NO3+NO2=NO+NO2+O2                               5.00E+10    0.0     2940.0
1244. NO3+NO3=NO2+NO2+O2                              5.12E+11    0.0     4870.0
1245. NO2+OH(+M)=HNO3(+M)                             2.41E+13    0.0        0.0
      Low pressure limit:  0.64200E+33 -0.54900E+01  0.23490E+04
      TROE centering:      0.40000E+00  0.45070E+03  0.15840E+04
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      N2              Enhanced by    1.000E+00
      HNO3            Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
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      NO3             Enhanced by    5.000E+00
1246. HNO3+H=NO3+H2                                 5.60E+08    1.5    16400.0
1247. HNO3+H=H2O+NO2                                6.10E+01    3.3     6285.0
1248. HNO3+H=OH+HONO                                3.80E+05    2.3     6976.0
1249. HNO3+H=HNO2+OH                                6.00E+13    0.0     7000.0
1250. HNO3+O=OH+NO3                                 1.80E+07    0.0        0.0
1251. HNO3+OH=H2O+NO3                               9.00E+10    0.0        0.0
1252. HNO3+OH(+M)=H2O+NO3(+M)                       2.47E+08    0.0    -2860.0
      Low pressure limit:  0.68900E+15  0.00000E+00 -0.14400E+04
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      HNO3            Enhanced by    5.000E+00
      NO3             Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
1253. NO3+H2O2=HNO3+HO2                             1.00E+12    0.0     8500.0
1254. NO3+NH=HNO3+N                                 1.00E+12    0.0     5000.0
1255. NO3+NH2=HNO3+NH                               1.00E+12    0.0    10000.0
1256. HNO3+NH=HNOH+NO2                              1.50E+13    0.0     6000.0
1257. HNO3+NH2=NO3+NH3                              9.00E+05    2.0     7300.0
1258. HNO3+NH2=NH2O+HNO2                            3.00E+12    0.0     9000.0
1259. HNO3+NH3=NH2O+H2O+NO                          2.32E+01    3.5    44930.0
1260. NH3+HNO3=H2O+NH2NO2                           8.00E-01    3.5    43100.0
1261. HONO+NO2=HNO3+NO                              2.00E+11    0.0    32700.0
1262. HONO+NO3=HNO3+NO2                             1.00E+12    0.0     6000.0
1263. HNO2+NO3=HNO3+NO2                             1.00E+12    0.0     5000.0
1264. N2O4(+M)=NO2+NO2(+M)                          4.05E+18   -1.1    12840.0
      Low pressure limit:  0.19600E+29 -0.38000E+01  0.12840E+05
1265. N2O4+H2O=HONO+HNO3                            2.52E+14    0.0    11586.0
1266. NH+CH3=CH4+N                                  8.20E+05    1.9     5848.0
1267. C2H5+N=C2H4+NH                                4.30E+13    0.0        0.0
1268. CH3+NH2=CH4+NH                                2.80E+06    1.9     9205.0
1269. CH3+NH2=CH2+NH3                               1.60E+06    1.9     7566.0
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1270.	CH2SING+NH3=CH3+NH2	1.00E+14	0.0	0.0
1271.	CH4+NH2=CH3+NH3	1.50E+03	3.0	9940.0
1272.	C2H+NH3=C2H2+NH2	7.20E+12	0.0	-735.0
1273.	C2H4+NH2=C2H3+NH3	5.30E+12	0.0	10274.0
1274.	C2H6+NH2=C2H5+NH3	4.50E+01	3.5	5600.0
1275.	NNH+CH3<=>CH4+N2	2.50E+13	0.0	0.0
1276.	N2H2+CH3=NNH+CH4	1.60E+06	1.9	2969.0
1277.	H2NN+CH3=CH4+NNH	1.60E+06	1.9	129.0
1278.	N2H3+CH3=N2H2+CH4	8.20E+05	1.9	1817.0
1279.	N2H3+CH3=H2NN+CH4	3.00E+13	0.0	0.0
1280.	N2H4+CH3=N2H3+CH4	3.30E+06	1.9	5322.0
1281.	CH2SING+NO=CH2+NO	1.00E+14	0.0	0.0
1282.	C+NO<=>CO+N	2.90E+13	0.0	0.0
1283.	CH+NO=HCO+N	6.80E+12	0.0	0.0
1284.	CH+NO=CO+NH	9.10E+12	0.0	0.0
1285.	CH2+NO=NH2+CO	2.30E+16	-1.4	1331.0
1286.	C2+NO=C2O+N	2.30E+13	0.0	8640.0
1287.	N+CO2<=>NO+CO	3.00E+12	0.0	11300.0
1288.	NH+CO2<=>HNO+CO	1.00E+13	0.0	14350.0
1289.	HNO+CH3=NO+CH4	8.20E+05	1.9	480.0
1290.	C2H3+NO=C2H2+HNO	1.00E+12	0.0	1000.0
1291.	HCO+NO=HNO+CO	7.23E+12	0.0	0.0
1292.	HCO+HNO=CH2O+NO	6.00E+11	0.0	2000.0
1293.	CH3O+NO=HNO+CH2O	7.50E+12	0.0	2017.0
	Declared duplicate reaction...			
1294.	CH3O+NO=HNO+CH2O	2.50E+18	-2.6	0.0
	Declared duplicate reaction...			
1295.	CH2OH+NO=CH2O+HNO	1.30E+12	0.0	0.0
1296.	CH3O+HNO=NO+CH3OH	3.20E+13	0.0	0.0
1297.	CH2OH+HNO=NO+CH3OH	3.00E+13	0.0	0.0
1298.	CH2CHO+NO=HNO+CH2CO	1.00E+12	0.0	8600.0
1299.	NH2O+CH3=CH3O+NH2	2.00E+13	0.0	0.0

1300.	NH2O+CH3=CH4+HNO	1.60E+06	1.9	2959.0
1301.	HNOH+CH3=CH4+HNO	1.60E+06	1.9	2095.0
1302.	NH2OH+CH3=HNOH+CH4	1.60E+06	1.9	6345.0
1303.	NH2OH+CH3=NH2O+CH4	8.20E+05	1.9	5491.0
1304.	CH+NO2=HCO+NO	1.01E+14	0.0	0.0
1305.	CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
1306.	NO2+CH3=NO+CH3O	1.40E+13	0.0	0.0
1307.	C2H3+NO2=NO+CH2CHO	7.70E+14	-0.6	0.0
1308.	C2H5+NO2=NO+C2H5O	4.00E+13	-0.2	0.0
1309.	CO+NO2=NO+CO2	9.04E+13	0.0	33780.0
1310.	HCO+NO2=CO+NO+OH	1.20E+23	-3.3	2355.0
1311.	HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
1312.	CH3CO+NO2=>CH3+CO2+NO	1.50E+13	0.0	0.0
1313.	CH4+NO2=HONO+CH3	6.50E+14	0.0	45800.0
1314.	C2H4+NO2=HONO+C2H3	6.50E+14	0.0	41400.0
1315.	C2H6+NO2=HONO+C2H5	6.50E+14	0.0	41400.0
1316.	HOCO+NO=CO+HONO	1.50E+12	0.0	0.0
1317.	HCO+NO2=CO+HONO	1.24E+23	-3.3	2355.0
1318.	CH2O+NO2=HCO+HONO	8.02E+02	2.8	13730.0
1319.	CH3O+NO2=CH2O+HONO	6.00E+12	0.0	2285.0
1320.	CH2OH+NO2=HONO+CH2O	5.00E+12	0.0	0.0
1321.	CH3OH+NO2=HONO+CH2OH	1.50E+02	3.3	20035.0
1322.	CH2CHO+NO2=CH2CO+HONO	8.90E+12	0.0	-159.0
1323.	CH3CHO+NO2=HONO+CH2CHO	1.30E+12	0.0	3700.0
1324.	CH4+NO2=HNO2+CH3	6.00E+14	0.0	37600.0
1325.	C2H4+NO2=HNO2+C2H3	6.00E+14	0.0	33200.0
1326.	C2H6+NO2=HNO2+C2H5	6.00E+14	0.0	33200.0
1327.	CH2O+NO2=HNO2+HCO	1.10E-01	4.2	19850.0
1328.	CH3OH+NO2=HNO2+CH2OH	2.40E+03	2.9	27470.0
1329.	CH2SING+N2O=CH2O+N2	3.80E+13	0.0	0.0
1330.	CO+N2O=N2+CO2	2.70E+11	0.0	20237.0
1331.	NH2NO+CH3=HNNO+CH4	1.60E+06	1.9	7179.0

1332.	NH2NHO+CH3=NHNHO+CH4		1.60E+06	1.9	377.0
1333.	CN+M=C+N+M		2.50E+14	0.0	141100.0
	N2	Enhanced by 1.500E+00			
	CO2	Enhanced by 2.400E+00			
1334.	CH+N=CN+H		1.70E+14	-0.1	0.0
1335.	CN+O=CO+N		1.90E+12	0.5	723.0
1336.	NO+C=CN+O		1.10E+13	0.0	0.0
1337.	CH+NO=OH+CN		3.30E+12	0.0	0.0
1338.	CN+O2=NO+CO		2.80E+17	-2.0	0.0
1339.	CN+N=C+N2		1.80E+14	0.0	0.0
1340.	CN+NO=N2+CO		3.90E+11	0.0	27820.0
1341.	C+N2O=CN+NO		4.80E+12	0.0	0.0
1342.	CN+NO2=CO+N2O		4.90E+14	-0.8	344.0
1343.	CN+NO2=N2+CO2		3.70E+14	-0.8	344.0
1344.	C2+N2=CN+CN		1.50E+13	0.0	41730.0
1345.	HCN(+M)=H+CN(+M)		8.30E+17	-0.9	123800.0
	Low pressure limit:	0.35700E+27 -0.26000E+01 0.12490E+06			
	TROE centering:	0.73420E+00 0.11201E+04 0.10000E+06			
	N2O	Enhanced by 5.000E+00			
	H2O	Enhanced by 5.000E+00			
	N2	Enhanced by 1.000E+00			
	CO2	Enhanced by 1.600E+00			
	H2	Enhanced by 2.000E+00			
	CH4	Enhanced by 2.000E+00			
	CO	Enhanced by 1.500E+00			
	C2H6	Enhanced by 3.000E+00			
	AR	Enhanced by 7.000E-01			
1346.	CH2+N=HCN+H		5.00E+13	0.0	0.0
1347.	CN+H2=HCN+H		3.60E+08	1.6	2999.0
1348.	CH+NH=HCN+H		3.00E+13	0.0	0.0
1349.	CH3+N=HCN+H2		3.70E+12	0.1	-89.0
1350.	C2H3+N=HCN+CH2		2.00E+13	0.0	0.0

1351. CH4+CN=CH3+HCN	8.60E+05	2.3	-32.0
1352. C3H3+N=HCN+C2H2	1.00E+13	0.0	0.0
1353. C2H6+CN=C2H5+HCN	1.20E+08	1.8	-994.0
1354. CH+N2=HCN+N	4.40E+12	0.0	21964.0
1355. CH2+N2=HCN+NH	1.00E+13	0.0	73954.0
1356. CH2SING+N2<=>NH+HCN	1.00E+11	0.0	65000.0
1357. CN+NH3=HCN+NH2	9.20E+12	0.0	-357.0
1358. HCN+N2=H+CN+N2	3.60E+26	-2.6	124890.0
1359. HCN+O=NH+CO	3.50E+03	2.6	4980.0
1360. HCN+O=CN+OH	4.20E+10	0.4	20663.0
1361. HCN+OH=CN+H2O	3.90E+06	1.8	10287.0
1362. OH+HCN=NH2+CO	7.83E-04	4.0	4000.0
1363. HCN+O2=CN+HO2	3.00E+13	0.0	75100.0
1364. HCCO+N=HCN+CO	5.00E+13	0.0	0.0
1365. CH2O+CN=HCO+HCN	1.70E+03	2.7	-1427.0
1366. CH+NO=HCN+O	5.30E+13	0.0	0.0
1367. CH2+NO=HCN+OH	2.90E+14	-0.7	755.0
1368. CH2SING+NO<=>OH+HCN	2.90E+14	-0.7	760.0
1369. CH3+NO=HCN+H2O	4.90E+08	0.5	12392.0
1370. C2H+NO=HCN+CO	6.00E+13	0.0	570.0
1371. C2H3+NO=HCN+CH2O	7.00E+21	-3.4	1025.0
1372. HCCO+NO=HCN+CO2	3.70E+14	-0.8	-90.0
1373. CN+HNO=HCN+NO	1.80E+13	0.0	0.0
1374. CN+HONO=HCN+NO2	1.20E+13	0.0	0.0
1375. CH+N2O=HCN+NO	1.90E+13	0.0	-511.0
1376. HCN=HNC	1.50E+23	-4.2	49428.0
1377. HCN+M=HNC+M	1.60E+26	-3.2	54600.0
AR Enhanced by 7.000E-01			
H2O Enhanced by 7.000E+00			
CO2 Enhanced by 2.000E+00			
Warning...superceding enhancement factor for AR			
AR Enhanced by 7.000E-01			

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      Warning...superceding enhancement factor for H2O
      H2O             Enhanced by    7.000E+00
      Warning...superceding enhancement factor for CO2
      CO2             Enhanced by    2.000E+00
      Warning...superceding enhancement factor for AR
      AR              Enhanced by    7.000E-01
      Warning...superceding enhancement factor for H2O
      H2O             Enhanced by    7.000E+00
      Warning...superceding enhancement factor for CO2
      CO2             Enhanced by    2.000E+00
1378. HNC+H=HCN+H                                    7.80E+13    0.0     3600.0
1379. O+HNC=NH+CO                                    4.60E+12    0.0     2184.0
1380. HNC+OH=CN+H2O                                  1.50E+12    0.0     7680.0
1381. HNC+O2=NH+CO2                                  1.60E+19   -2.2     1777.0
1382. H+HCN(+M)<=>NCH2(+M)                           3.30E+13    0.0        0.0
      Low pressure limit:  0.14000E+27 -0.34000E+01  0.19000E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
      AR              Enhanced by    7.000E-01
      N2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
1383. CH+NH3=NCH2+H+H                                4.40E+13    0.0     -630.0
1384. NCH2+H=HCN+H2                                  2.40E+08    1.5     -894.0
1385. CH3+N=NCH2+H                                   6.10E+14   -0.3      288.0
1386. CH+NH2=NCH2+H                                  3.00E+13    0.0        0.0
1387. CH3+NH=NCH2+H2                                 3.50E+13    0.0      290.0
1388. NCH2+CH3=HCN+CH4                               8.10E+05    1.9    -1112.0
1389. C2H5+N=CH3+NCH2                                2.30E+13    0.0        0.0
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1390.	NCH2+N=HCN+NH	7.20E+13	0.0	400.0
1391.	NCH2+N=N2+CH2	6.00E+13	0.0	397.0
1392.	NCH2+NH=HCN+NH2	1.70E+08	1.5	-894.0
1393.	NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0
1394.	CH2+NO=NCH2+O	8.10E+07	1.4	4111.0
1395.	NCH2+O=HCN+OH	1.70E+08	1.5	-894.0
1396.	CH3+NO=NCH2+OH	1.50E-01	3.5	3950.0
1397.	NCH2+OH=HCN+H2O	1.50E+19	-2.2	2166.0
	Declared duplicate reaction...			
1398.	NCH2+OH=HCN+H2O	1.20E+06	2.0	-1192.0
	Declared duplicate reaction...			
1399.	NCH2+O2=CH2O+NO	3.00E+12	0.0	5958.0
1400.	NCH2+O2=HCN+HO2	2.70E+04	2.0	17300.0
1401.	NCH2+HO2=HCN+H2O2	1.40E+04	2.7	-1609.0
1402.	NCH2+NO=HCN+HNO	1.00E+07	2.0	4400.0
1403.	CHNH=HCN+H	6.10E+28	-5.7	24257.0
1404.	CH3+N=CHNH+H	1.20E+11	0.5	-367.0
1405.	CHNH+H=NCH2+H	2.00E+13	0.0	0.0
1406.	CHNH+H=HCN+H2	2.40E+08	1.5	-894.0
1407.	CHNH+O=HCN+OH	1.70E+08	1.5	-894.0
1408.	CHNH+OH=HCN+H2O	1.20E+06	2.0	-1192.0
1409.	CHNH+CH3=HCN+CH4	8.20E+05	1.9	-1112.0
1410.	CH2NH+M=HCN+H2+M	1.00E+14	0.0	10000.0
1411.	NH+CH3=CH2NH+H	4.00E+13	0.0	0.0
1412.	CH2NH+H=NCH2+H2	2.40E+08	1.5	7318.0
1413.	CH2NH+H=CHNH+H2	3.00E+08	1.5	6126.0
1414.	CH+NH3=CH2NH+H	4.40E+13	0.0	-630.0
1415.	CH2SING+NH2=CH2NH+H	3.00E+13	0.0	0.0
1416.	CH2SING+NH3=CH2NH+H+H	1.00E+14	0.0	0.0
1417.	CH3+NH2<=>CH2NH+H2	2.40E+06	1.2	17369.0
1418.	CH2NH+O=NCH2+OH	1.70E+08	1.5	4627.0
1419.	CH2NH+O=CHNH+OH	2.20E+08	1.5	5402.0

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1420. CH2NH+O=CH2O+NH                                 1.70E+06    2.1        0.0
1421. CH2NH+OH=NCH2+H2O                               1.20E+06    2.0      -89.0
1422. CH2NH+OH=CHNH+H2O                               2.40E+06    2.0      457.0
1423. CH2NH+OH=CH2O+NH2                               1.80E+05    2.0    14800.0
1424. NCH2+HO2=CH2NH+O2                               1.40E+04    2.7    -1609.0
1425. CH2NH+CH3=NCH2+CH4                              8.20E+05    1.9     7119.0
1426. CH2NH+CH3=CHNH+CH4                              5.30E+05    1.9     9681.0
1427. CH2NH+NH2=NCH2+NH3                              9.20E+05    1.9     4438.0
1428. CH2NH+NH2=CHNH+NH3                              1.80E+06    1.9     6087.0
1429. CH3N(+AR)<=>CH2NH(+AR)                          1.83E+13    0.2    43980.0
      Low pressure limit:  0.22300E+29 -0.44500E+01  0.46000E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
1430. CH3N(+AR)<=>NCH2+H(+AR)                         7.40E+11    0.9    35470.0
      Low pressure limit:  0.18700E+31 -0.45200E+01  0.37950E+05
      TROE centering:      0.74900E+00  0.21800E+03  0.10000E+02  0.26000E+09
1431. CH3NH=CH2NH+H                                   1.30E+42   -9.2    41316.0
      Declared duplicate reaction...
1432. CH3NH(+AR)<=>CH2NH+H(+AR)                       7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      Declared duplicate reaction...
1433. CH3NH+M=CH3+NH+M                                1.00E+14    0.0    18000.0
1434. CH3+NH2<=>CH3NH+H                               9.08E+13   -0.4    15714.0
1435. CH3NH+H=CH2NH+H2                                7.20E+08    1.5     -894.0
1436. CH3NH+O=CH2NH+OH                                5.00E+08    1.5     -894.0
1437. CH3NH+O=CH3O+NH                                 6.00E+13    0.0        0.0
1438. CH3NH+OH=CH2NH+H2O                              3.60E+06    2.0    -1192.0
1439. CH3NH+OH=CH4+HNO                                6.00E+12    0.0        0.0
1440. HNOH+CH3=CH3NH+OH                               2.00E+13    0.0        0.0
1441. CH3NH+O2=CH2NH+HO2                              1.00E+07    2.0     6300.0
1442. CH3NH+O2=CH3O+HNO                               6.00E+12    0.0     4000.0
1443. CH3NH+CH3=CH2NH+CH4                             2.40E+06    1.9    -1112.0
1444. CH2NH2=CH2NH+H                                  2.40E+48  -10.8    52010.0
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      Declared duplicate reaction...
1445. CH2NH2(+AR)<=>CH2NH+H(+AR)                      7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
      Declared duplicate reaction...
1446. CH3+NH2<=>CH2NH2+H                              5.15E+14   -0.6    10155.0
1447. CH2NH2+H=CH2NH+H2                               4.80E+08    1.5     -894.0
1448. CH2NH2+O=CH2O+NH2                               7.00E+13    0.0        0.0
1449. CH2NH2+O=CH2NH+OH                               3.30E+08    1.5     -894.0
1450. CH2NH2+OH=CH2OH+NH2                             4.00E+13    0.0        0.0
1451. CH2NH2+OH=CH2NH+H2O                             2.40E+06    2.0    -1192.0
1452. CH2NH2+O2=CH2NH+HO2                             1.00E+22   -3.1     6752.0
1453. CH2NH2+O2=NH2+CH2O+O                            6.00E+18   -1.6    30175.0
1454. CH2NH2+CH3=C2H5+NH2                             2.00E+13    0.0     2701.0
1455. CH2NH2+CH3=CH2NH+CH4                            1.60E+06    1.9     -626.0
1456. CH3+NH2<=>CH3NH2                                1.03E+33   -6.3     5750.0
1457. CH3+NH2(+M)=CH3NH2(+M)                          7.20E+12    0.4        0.0
      Low pressure limit:  0.22000E+31 -0.38500E+01  0.00000E+00
1458. CH3NH2(+AR)<=>CH2NH+H2(+AR)                     9.99E+08    1.2   102880.0
      Low pressure limit:  0.24600E+31 -0.47500E+01  0.10700E+06
      TROE centering:      0.82000E+00  0.15459E+03  0.10000E+01  0.40100E+06
1459. CH3NH2+M=CH2NH+H2+M                             2.40E+13    0.0   107260.0
1460. CH3NH2(+AR)<=>CH2NH2+H(+AR)                     3.93E+15   -0.1    93820.0
      Low pressure limit:  0.68200E+41 -0.70100E+01  0.98400E+05
      TROE centering:      0.00000E+00  0.23101E+03  0.10000E+01  0.40100E+06
1461. CH3NH2(+AR)<=>CH3NH+H(+AR)                      1.44E+16   -0.3   100940.0
      Low pressure limit:  0.11400E+39 -0.63500E+01  0.10500E+06
      TROE centering:      0.67000E+00  0.16967E+03  0.10000E+01  0.40100E+06
1462. CH3NH2+H=CH2NH2+H2                              5.60E+08    1.5     5461.0
1463. CH3NH2+H=CH3NH+H2                               4.80E+08    1.5     9701.0
1464. CH3NH2+O=CH2NH2+OH                              4.00E+08    1.5     5193.0
1465. CH3NH2+O=CH3NH+OH                               3.30E+08    1.5     6345.0
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1466.	CH3NH2+OH=CH2NH2+H2O	3.60E+06	2.0	238.0
1467.	CH3NH2+OH=CH3NH+H2O	2.40E+06	2.0	447.0
1468.	CH3NH2+CH3=CH2NH2+CH4	1.50E+06	1.9	9163.0
1469.	CH3NH2+CH3=CH3NH+CH4	1.60E+06	1.9	8837.0
1470.	CH3NH2+NH2=CH2NH2+NH3	2.80E+06	1.9	5491.0
1471.	CH3NH2+NH2=CH3NH+NH3	1.80E+06	1.9	7139.0
1472.	CH3NCH=CH3+HCN	8.10E+15	-2.4	14942.0
1473.	CH3NCH+H=CH2NCH2+H	2.00E+13	0.0	0.0
1474.	CH2NCH2=CH3NCH	1.30E+45	-10.1	66111.0
1475.	CH2NCH2+H=CH3+NCH2	3.00E+13	0.0	0.0
1476.	CH2NCH2+O=CH2O+NCH2	3.00E+13	0.0	0.0
1477.	CH2NCH2+OH=CH2OH+NCH2	2.00E+13	0.0	0.0
1478.	CH2NCH2+H=CH3NCH2	5.80E+13	0.2	-125.0
1479.	CH3NCH2+H=CH2NCH2+H2	5.60E+08	1.5	5464.0
1480.	CH3NCH2+H=CH3NCH+H2	3.00E+08	1.5	6130.0
1481.	CH3NCH2+O=CH2NCH2+OH	4.00E+08	1.5	5196.0
1482.	CH3NCH2+O=CH3NCH+OH	2.20E+08	1.5	5404.0
1483.	CH3NCH2+OH=CH2NCH2+H2O	8.00E+12	0.0	0.0
1484.	CH3NCH2+OH=CH3NCH+H2O	2.40E+06	2.0	457.0
1485.	CH3NCH2+CH3=CH2NCH2+CH4	1.50E+06	1.9	9170.0
1486.	CH3NCH2+CH3=CH3NCH+CH4	5.30E+05	1.9	9687.0
1487.	CH3NCH2+NH2=CH2NCH2+NH3	2.80E+06	1.9	5494.0
1488.	CH3NCH2+NH2=CH3NCH+NH3	1.80E+06	1.9	6090.0
1489.	CH3NCH3=CH3NCH2+H	1.60E+15	-7.5	38425.0
1490.	CH3NCH3+H=CH3NCH2+H2	3.20E+12	0.0	0.0
1491.	CH3NCH3+OH=CH3NCH2+H2O	2.40E+13	0.0	0.0
1492.	CH3NCH3+CH3=CH3NCH2+CH4	6.00E+12	0.0	0.0
1493.	CH3NHCH2=CH3+CH2NH	9.80E+43	-10.3	37459.0
1494.	CH3NHCH2=CH3NCH2+H	5.90E+44	-10.3	46803.0
1495.	CH3NHCH2+H=CH3NCH2+H2	4.80E+08	1.5	-894.0
1496.	CH3NHCH2+O=CH2O+CH3NH	7.00E+13	0.0	0.0
1497.	CH3NHCH2+O=CH3NCH2+OH	3.30E+08	1.5	-894.0

1498. CH3NHCH2+OH=CH2OH+CH3NH 4.00E+13 0.0 0.0

1499. CH3NHCH2+OH=CH3NCH2+H2O 2.40E+06 2.0 -1192.0

1500. CH3NHCH2+CH3=C2H5+CH3NH 2.00E+13 0.0 2702.0

1501. CH3NHCH2+CH3=CH3NCH2+CH4 1.60E+06 1.9 -626.0

1502. CH3NHCH2+H(+M)=CH3NHCH3(+M) 5.20E+17 -1.0 1580.0

Low pressure limit: 0.19900E+42 -0.70800E+01 0.66850E+04

TROE centering: 0.84220E+00 0.12500E+03 0.22190E+04 0.68820E+04

1503. CH3NCH3+H=CH3NHCH3 1.00E+12 0.0 0.0

1504. CH3NHCH3+H=CH3NHCH2+H2 5.60E+08 1.5 5464.0

1505. CH3NHCH3+H=CH3NCH3+H2 4.80E+08 1.5 9706.0

1506. CH3NHCH3+O=CH3NHCH2+OH 6.10E+12 0.0 556.0

1507. CH3NHCH3+O=CH3NCH3+OH 3.00E+12 0.0 556.0

1508. CH3NHCH3+OH=CH3NHCH2+H2O 2.00E+13 0.0 0.0

1509. CH3NHCH3+OH=CH3NCH3+H2O 1.90E+13 0.0 0.0

1510. CH3NHCH3+CH3=CH3NHCH2+CH4 1.50E+06 1.9 9170.0

1511. CH3NHCH3+CH3=CH3NCH3+CH4 1.60E+06 1.9 8842.0

1512. CH3NHCH3+NH2=CH3NHCH2+NH3 2.80E+06 1.9 5494.0

1513. CH3NHCH3+NH2=CH3NCH3+NH3 1.80E+06 1.9 7143.0

1514. CHCNH+H=CH2+HNC 1.50E+14 0.0 0.0

1515. CHCNH+O=H+CO+HNC 1.00E+14 0.0 0.0

1516. CHCNH+OH=HCO+CHNH 1.00E+13 0.0 0.0

1517. CHCNH+O2=HNC+CO+OH 1.60E+11 0.0 1020.0

1518. CHCNH+O2=HNC+HCO+O 2.20E+02 2.7 3540.0

1519. CH2SING+HCN=CH2CN+H 1.80E+14 0.0 0.0

1520. CH3+CN=CH2CN+H 1.00E+14 0.0 0.0

1521. CH2CN+O=CH2O+CN 1.00E+14 0.0 0.0

1522. CH2OH+CN=CH2CN+OH 5.00E+13 0.0 0.0

1523. CH3CN=CH2CN+H 7.90E+14 0.0 94940.0

1524. CH3CN+H=HCN+CH3 4.40E+10 0.8 6800.0

1525. CH3CN+H=HNC+CH3 2.80E+15 -0.3 20030.0

1526. CH3CN+H=CH2CN+H2 6.00E+04 3.0 8522.0

1527. CH3CN+O=CH2CN+OH 4.70E+08 1.2 14360.0

1528.	CH3CN+OH=CH2CN+H2O	2.00E+07	2.0	2000.0
1529.	CH3CN+CH3=CH2CN+CH4	5.00E+12	0.0	7000.0
1530.	CH3CN+CN=CH2CN+HCN	5.00E+13	0.0	2000.0
1531.	c-C2H3N=CH3CN	4.70E+13	0.0	41500.0
1532.	c-C2H3N+H=CH2NCH2	9.80E+09	1.2	1969.0
1533.	c-C2H3N+H=CH2CHNH	1.10E+10	1.2	2422.0
1534.	c-C2H3N+O=>NCH2+HCO	1.00E+13	0.0	0.0
1535.	c-C2H3N+O=>C2H3+NO	1.00E+13	0.0	0.0
1536.	c-C2H3N+OH=>NCH2+CH2O	5.00E+12	0.0	0.0
1537.	CH2CHN(S)+M=CH2CHN+M	1.00E+13	0.0	0.0
	H Enhanced by 0.000E+00			
1538.	CH2CHN(S)+H=CH2CHN+H	1.00E+14	0.0	0.0
1539.	CH2CHN(S)+H=CH3+HCN	3.00E+13	0.0	0.0
1540.	CH2CHN(S)=c-C2H3N	3.00E+13	0.0	4000.0
1541.	CH2CHN(S)=CH3CN	3.00E+13	0.0	8000.0
1542.	CH2CHN(S)+O=>HCO+HCN+H	3.00E+13	0.0	0.0
1543.	CH2CHN(S)+OH=>CH2O+HCN+H	3.00E+13	0.0	0.0
1544.	CH2CNH=CH3CN	2.50E+13	0.0	70300.0
1545.	CH2CNH+H=CH3CN+H	3.00E+13	0.0	0.0
1546.	CH2CNH+H=CH3+HNC	3.30E+10	0.9	2840.0
1547.	CH2CNH+H=CHCNH+H2	3.00E+07	2.0	10000.0
1548.	CH2CNH+H=CH2CN+H2	2.40E+08	1.5	7322.0
1549.	CH2CNH+O=CH2+HNCO	1.80E+12	0.0	1350.0
1550.	CH2CNH+O=CHCNH+OH	2.00E+07	2.0	10000.0
1551.	CH2CNH+O=CH2CN+OH	1.70E+08	1.5	4630.0
1552.	CH2CNH+OH=CH2OH+HNC	1.00E+12	0.0	-1013.0
1553.	CH2CNH+OH=CHCNH+H2O	1.00E+07	2.0	3000.0
1554.	CH2CNH+OH=CH2CN+H2O	1.20E+06	2.0	-89.0
1555.	CH2CNH+CH3=CH2CN+CH4	8.20E+05	1.9	7123.0
1556.	CH2CNH+NH2=CH2CN+NH3	9.20E+05	1.9	4441.0
1557.	CH2CHN+H=CH3+HCN	1.00E+13	0.0	0.0
1558.	CH2CHN+O=CH2O+HCN	5.00E+13	0.0	0.0

1559.	CHCNH2+H=CHCNH+H2	4.80E+08	1.5	9706.0
1560.	CHCNH2+O=CHCNH+OH	3.30E+08	1.5	6348.0
1561.	CHCNH2+O=HCCO+NH2	1.40E+07	2.0	1900.0
1562.	CHCNH2+OH=CHCNH+H2O	2.00E+12	0.0	0.0
1563.	CHCNH2+CH3=CHCNH+CH4	1.60E+06	1.9	8842.0
1564.	CHCNH2+NH2=CHCNH+NH3	1.80E+06	1.9	7143.0
1565.	CH3+HCN=CH3CHN	1.00E+12	0.0	9900.0
1566.	CH3CHN+H=CH3CN+H2	2.40E+08	1.5	-894.0
1567.	CH3CHN+H=CH2CHN+H2	9.00E+13	0.0	15100.0
1568.	CH2CHN(S)+H2=CH3CHN+H	7.20E+13	0.0	0.0
1569.	CH3CHN+O=CH3CN+OH	1.70E+08	1.5	-894.0
1570.	CH3CHN+OH=CH3CN+H2O	1.20E+06	2.0	-1192.0
1571.	CH3CHN+OH=CH2CHN+H2O	1.10E+03	3.0	2780.0
1572.	CH3CHN+OH=CH2CHN(S)+H2O	4.40E+13	-0.3	-727.0
1573.	CH3CHN+NH2=CH3CN+NH3	9.20E+05	1.9	-1152.0
1574.	CH3CNH=CH3+HNC	6.50E+18	-2.5	33000.0
1575.	CH3CNH=CH3CN+H	7.70E+25	-5.2	24000.0
1576.	CH3CNH+H=CH3+CHNH	2.10E+13	0.0	0.0
1577.	CH3CNH+H=CH2CNH+H2	1.20E+13	0.0	0.0
1578.	CH3CNH+H=CH3CN+H2	2.40E+08	1.5	-894.0
1579.	CH3CNH+O=CH2CNH+OH	5.30E+13	0.0	0.0
1580.	CH3CNH+O=CH3CN+OH	1.70E+08	1.5	-894.0
1581.	CH3CNH+OH=CH2CNH+H2O	1.20E+13	0.0	0.0
1582.	CH3CNH+OH=CH3CN+H2O	1.20E+06	2.0	-1192.0
1583.	CH3CNH+O2=CH2O+CO+NH2	1.90E+12	0.0	0.0
1584.	CH3CNH+CH3=CH2CNH+CH4	5.30E+13	0.0	0.0
1585.	CH3CNH+CH3=CH3CN+CH4	8.20E+05	1.9	-1113.0
1586.	CH2CHNH+H=CH3+CHNH	1.00E+14	0.0	0.0
1587.	CH2CHNH+H=CH3CNH+H	3.00E+13	0.0	0.0
1588.	CH2CHNH+H=CH2CNH+H2	2.00E+13	0.0	0.0
1589.	CH2CHNH+O=CH2CNH+OH	2.00E+13	0.0	0.0
1590.	CH2CHNH+OH=CH2CNH+H2O	2.00E+13	0.0	0.0

1591. CH2CHNH+OH=CH2OH+CHNH 1.00E+13 0.0 0.0

1592. CH2CHNH+O2=CH2O+CO+NH2 5.70E+17 -1.8 11067.0

1593. CHCNH2+H(+M)=CH2CNH2(+M) 1.70E+10 1.3 2709.0

Low pressure limit: 0.63000E+32 -0.46640E+01 0.37800E+04

TROE centering: 0.78780E+00 -0.10212E+05 0.10000E+31

H2 Enhanced by 2.000E+00

CO Enhanced by 2.000E+00

CO2 Enhanced by 3.000E+00

H2O Enhanced by 5.000E+00

1594. CH2CNH2+H=CHCNH2+H2 4.50E+13 0.0 0.0

1595. CH2CNH2+O=CH2CO+NH2 3.00E+13 0.0 0.0

1596. CH2CNH2+OH=CHCNH2+H2O 2.00E+13 0.0 0.0

1597. CH2CNH2+O2=OCHCHO+NH2 4.00E+12 0.0 0.0

1598. CH2CNH2+CH3=CHCNH2+CH4 2.00E+13 0.0 0.0

1599. NH2+C2H2=CHCHNH2 7.80E-18 8.3 7430.0

1600. CHCNH2+H(+M)=CHCHNH2(+M) 1.70E+10 1.3 2709.0

Low pressure limit: 0.63000E+32 -0.46640E+01 0.37800E+04

TROE centering: 0.78780E+00 -0.10212E+05 0.10000E+31

H2 Enhanced by 2.000E+00

CO Enhanced by 2.000E+00

CO2 Enhanced by 3.000E+00

H2O Enhanced by 5.000E+00

1601. CHCHNH2+H=CHCNH2+H2 4.50E+13 0.0 0.0

1602. CHCHNH2+OH=CHCNH2+H2O 2.00E+13 0.0 0.0

1603. CHCHNH2+O2=OCHCHO+NH2 4.00E+12 0.0 0.0

1604. CHCHNH2+CH3=CHCNH2+CH4 2.00E+13 0.0 0.0

1605. CH2CHNH+H=CH3CHNH 5.80E+13 0.2 -125.0

1606. CH3+CHNH=CH3CHNH 1.80E+13 0.0 0.0

1607. CH3CHNH+H=CH3CNH+H2 4.70E+13 -0.3 3000.0

1608. CH3CHNH+H=CH2CHNH+H2 1.90E+12 0.4 5359.0

1609. CH3CHNH+H=CH3CHN+H2 2.40E+08 1.5 7322.0

1610. CH3CHNH+O=CH3CNH+OH 1.80E+18 -1.9 2975.0

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1611. CH3CHNH+O=CH2CHNH+OH                          3.70E+13   -0.2     3556.0
1612. CH3CHNH+O=CH3CHN+OH                           1.70E+08    1.5     4630.0
1613. CH3CHNH+OH=CH3CNH+H2O                         2.40E+11    0.3    -1000.0
1614. CH3CHNH+OH=CH2CHNH+H2O                        3.00E+13   -0.6      800.0
1615. CH3CHNH+OH=CH3CHN+H2O                         1.20E+06    2.0      -89.0
1616. CH3CHNH+CH3=CH3CNH+CH4                        3.90E-07    5.8     2200.0
1617. CH3CHNH+CH3=CH2CHNH+CH4                       2.50E+01    3.1     5727.0
1618. CH3CHNH+CH3=CH3CHN+CH4                        8.20E+05    1.9     7123.0
1619. CH3CHNH+NH2=CH3CHN+NH3                        9.20E+05    1.9     4441.0
1620. CHCHNH2+H(+M)=CH2CHNH2(+M)                    3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1621. CH2CNH2+H(+M)=CH2CHNH2(+M)                    3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1622. CH3CHNH=CH2CHNH2                              5.00E+18   -2.5    67995.0
1623. CH2CHNH2+H=CHCHNH2+H2                         2.40E+02    3.6    11266.0
1624. CH2CHNH2+H=CH2CNH2+H2                         2.40E+02    3.6    11266.0
1625. CH2CHNH2+H=CH2CHNH+H2                         4.80E+08    1.5     9700.0
1626. CH3CHNH+H=CH2CHNH2+H                          3.00E+13    0.0        0.0
1627. CH2CHNH2+O=CH2CHNH+OH                         3.30E+08    1.5     6348.0
1628. CH2CHNH2+OH=CHCHNH2+H2O                       1.30E-01    4.2     -860.0
1629. CH2CHNH2+OH=CH2CNH2+H2O                       1.30E-01    4.2     -860.0
1630. CH2CHNH2+OH=CH2CHNH+H2O                       2.40E+06    2.0      447.0
1631. CH2CHNH2+CH3=CHCHNH2+CH4                      6.00E+07    1.6    16630.0
1632. CH2CHNH2+CH3=CH2CNH2+CH4                      6.00E+07    1.6    16630.0
1633. CH2CHNH2+CH3=CH2CHNH+CH4                      1.60E+06    1.9     8842.0
1634. CH2CHNH2+NH2=CHCHNH2+NH3                      5.30E+12    0.0    10274.0
1635. CH2CHNH2+NH2=CH2CNH2+NH3                      5.30E+12    0.0    10274.0
1636. CH2CHNH2+NH2=CH2CHNH+NH3                      1.80E+06    1.9     7143.0
1637. CH3CH2NH=CH2NH+CH3                            1.90E+10    0.0    23500.0
1638. CH3CH2NH=CH3CHNH+H                            1.60E+36   -7.9    36342.0
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1639. CH3CH2NH+H=CH3+CH2NH2                           1.40E+12    0.7      346.0
1640. CH3CH2NH+H=CH3CHNH+H2                           7.20E+08    1.5     -894.0
1641. CH3CH2NH+O=CH3CHNH+OH                           5.00E+08    1.5     -894.0
1642. CH3CH2NH+OH=CH3CHNH+H2O                         3.60E+06    2.0    -1192.0
1643. CH3CH2NH+CH3=CH3CHNH+CH4                        2.40E+06    1.9    -1113.0
1644. CH2CHNH2+H(+M)=CH3CHNH2(+M)                     1.40E+09    1.5     1355.0
      Low pressure limit:  0.20000E+40 -0.66420E+01  0.57690E+04
      TROE centering:     -0.56900E+00  0.29900E+03  0.91470E+04  0.15240E+03
1645. CH3CHNH2=CH3CHNH+H                              1.10E+45  -10.2    47817.0
1646. CH3CHNH2+H=CH2CHNH2+H2                          4.90E+08    1.7      588.0
1647. CH3CHNH2+H=CH3+CH2NH2                           8.40E+16   -0.9     2903.0
1648. CH3CHNH2+H=C2H4+NH3                             4.70E+21   -3.0     2845.0
1649. CH3CHNH2+H=C2H5+NH2                             2.00E+13    0.0        0.0
1650. CH3CHNH2+O=CH2CHNH2+OH                          2.50E+13    0.0        0.0
1651. CH3CHNH2+OH=CH2CHNH2+H2O                        2.40E+13    0.0        0.0
1652. CH3CHNH2+O2=CH2CHNH2+HO2                        6.70E+20   -3.0     2504.0
1653. CH3CHNH2+CH3=CH2CHNH2+CH4                       1.80E+13    0.0     -769.0
1654. C2H4+NH2=CH2CH2NH2                              1.20E+11    0.0     3955.0
1655. CH2CH2NH2+H=CH2CHNH2+H2                         1.80E+12    0.0        0.0
1656. CH2CH2NH2+O=CH2O+CH2NH2                         9.60E+13    0.0        0.0
1657. CH2CH2NH2+OH=CH2CHNH2+H2O                       2.40E+13    0.0        0.0
1658. CH2CH2NH2+HO2=>CH2O+OH+CH2NH2                   2.40E+13    0.0        0.0
1659. CH2CH2NH2+O2=CH2CHNH2+HO2                       3.70E+16   -1.6     3418.0
1660. CH2CH2NH2+CH3=CH2CHNH2+CH4                      1.20E+13   -0.3        0.0
1661. CH3CH2NH2=C2H4+NH3                              6.20E+67  -15.9    99348.0
1662. C2H5+NH2(+M)=CH3CH2NH2(+M)                      7.20E+12    0.4        0.0
      Low pressure limit:  0.22000E+31 -0.38500E+01  0.00000E+00
1663. CH3CHNH2+H=CH3CH2NH2                            1.70E+13    0.2        0.0
1664. CH2CH2NH2+H=CH3CH2NH2                           5.40E+13    0.2        0.0
1665. CH3CH2NH2+H=CH2CH2NH2+H2                        1.20E+07    1.8     5100.0
1666. CH3CH2NH2+H=CH3CHNH2+H2                         2.60E+07    1.6     2830.0
1667. CH3CH2NH2+H=CH3CH2NH+H2                         4.80E+08    1.5     9700.0
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1668.	CH3CH2NH2+O=CH2CH2NH2+OH	9.40E+07	1.7	5460.0
1669.	CH3CH2NH2+O=CH3CHNH2+OH	6.80E+12	0.0	1275.0
1670.	CH3CH2NH2+O=CH3CH2NH+OH	3.30E+08	1.5	6348.0
1671.	CH3CH2NH2+OH=CH2CH2NH2+H2O	1.60E+12	0.0	1300.0
1672.	CH3CH2NH2+OH=CH3CHNH2+H2O	1.40E+13	0.0	0.0
1673.	CH3CH2NH2+OH=CH3CH2NH+H2O	2.40E+06	2.0	447.0
1674.	CH3CH2NH2+HO2=CH2CH2NH2+H2O2	1.20E+04	2.5	15750.0
1675.	CH3CH2NH2+HO2=CH3CHNH2+H2O2	8.20E+03	2.5	10750.0
1676.	CH3CH2NH2+CH3=CH2CH2NH2+CH4	2.20E+02	3.2	9620.0
1677.	CH3CH2NH2+CH3=CH3CHNH2+CH4	7.30E+02	3.0	7950.0
1678.	CH3CH2NH2+CH3=CH3CH2NH+CH4	1.60E+06	1.9	8842.0
1679.	CH3CH2NH2+NH2=CH2CH2NH2+NH3	2.20E+02	3.2	9620.0
1680.	CH3CH2NH2+NH2=CH3CHNH2+NH3	7.30E+02	3.0	7950.0
1681.	CH3CH2NH2+NH2=CH3CH2NH+NH3	1.80E+06	1.9	7140.0
1682.	CH2CH2NH2+HCO=CH3CH2NH2+CO	6.00E+13	0.0	0.0
1683.	CH3CHNH2+HCO=CH3CH2NH2+CO	1.20E+14	0.0	0.0
1684.	CH+N2=NCN+H	3.70E+07	1.4	20723.0
1685.	H+NCN=HCN+N	1.89E+14	0.0	8425.0
1686.	NCN+O=CN+NO	1.00E+14	0.0	0.0
1687.	NCN+OH=HCN+NO	5.00E+13	0.0	0.0
1688.	NCN+N=CN+N2	2.00E+13	0.0	0.0
1689.	CN+N2O=NCN+NO	3.80E+03	2.6	3700.0
1690.	CH+N2=HCNN	3.60E+28	-5.8	2621.0
1691.	HCNN+H<=>CH2+N2	1.00E+14	0.0	0.0
1692.	HCNN+O<=>CO+H+N2	2.20E+13	0.0	0.0
1693.	HCNN+O<=>HCN+NO	2.00E+12	0.0	0.0
1694.	HCNN+OH<=>H+HCO+N2	1.20E+13	0.0	0.0
1695.	HCNN+O2=H+CO2+N2	4.00E+12	0.0	0.0
1696.	HCNN+O2=HCO+N2O	4.00E+12	0.0	0.0
1697.	HCNN+O2<=>O+HCO+N2	1.20E+13	0.0	0.0
1698.	CH2+N2=CH2NN	1.60E+32	-7.1	19958.0
1699.	CH3NN+M=CH3+N2+M	1.00E+11	0.0	5900.0

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1700. CH3NNH(+AR)<=>CH3+NNH(+AR)                      3.30E+16   -0.1    55000.0
      Low pressure limit:  0.18800E+32 -0.45500E+01  0.57500E+05
      TROE centering:      0.97000E+00  0.25059E+03  0.10000E+01  0.40100E+06
1701. NCCN+M=CN+CN+M                                  1.10E+34   -4.3   130079.0
      N2              Enhanced by    1.500E+00
      O2              Enhanced by    1.500E+00
      H2              Enhanced by    1.500E+00
      H2O             Enhanced by    1.000E+01
      CO2             Enhanced by    3.000E+00
1702. CN+HCN=NCCN+H                                   1.50E+07    1.7     1529.0
1703. HNC+CN=NCCN+H                                   1.00E+13    0.0        0.0
1704. CH3NNCH3=CH3NN+CH3                              6.92E+15    0.0    50875.0
1705. CH3NNCH3=C2H6+N2                                2.00E+11    0.0    33000.0
1706. NCO+M=N+CO+M                                    2.20E+14    0.0    54050.0
      N2              Enhanced by    1.500E+00
      Warning...superceding enhancement factor for N2
      N2              Enhanced by    1.500E+00
1707. CN+OH=NCO+H                                     4.00E+13    0.0        0.0
1708. CH+NO=H+NCO                                     2.00E+13    0.0        0.0
1709. HCN+O=NCO+H                                     1.40E+04    2.6     4980.0
1710. HNC+O=H+NCO                                     1.60E+01    3.1     -224.0
1711. NCO+H=NH+CO                                     5.20E+13    0.0        0.0
1712. CN+O2=NCO+O                                     7.20E+12    0.0     -417.0
      Declared duplicate reaction...
1713. CN+O2=NCO+O                                    -2.80E+17   -2.0        0.0
      Declared duplicate reaction...
1714. NCO+O=NO+CO                                     2.00E+15   -0.5        0.0
1715. NCO+O=N+CO2                                     8.00E+12    0.0     2502.0
1716. NCO+OH=HON+CO                                   5.30E+12   -0.1     5124.0
1717. NCO+OH=H+CO+NO                                  8.30E+12   -0.1    18032.0
1718. NCO+O2=NO+CO2                                   2.00E+12    0.0    20000.0
1719. CH3CN+O=CH3+NCO                                 6.00E+09    1.8     8130.0
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1720.	CH3NCH+O=>CH3+NCO+H	7.00E+13	0.0	0.0
1721.	C2H2+NCO=HCCO+HCN	1.40E+12	0.0	1815.0
1722.	CN+CO2=NCO+CO	3.67E+06	2.2	26900.0
1723.	C2O+NO=CO+NCO	1.00E+14	0.0	670.0
1724.	C2O+NO2=CO2+NCO	5.10E+13	0.0	125.0
1725.	NCO+N=N2+CO	2.00E+13	0.0	0.0
1726.	CN+NO=NCO+N	9.60E+13	0.0	42100.0
1727.	CN+NO2=NCO+NO	5.30E+15	-0.8	344.0
1728.	NCO+NO=N2+CO2	1.50E+21	-2.7	1824.0
1729.	NCO+NO=N2O+CO	4.00E+19	-2.2	1743.0
1730.	NCN+O2=NO+NCO	4.40E+09	0.5	24580.0
1731.	N2O+NCO=CO+N2+NO	9.00E+13	0.0	27800.0
1732.	NCO+NO2=CO2+N2O	3.00E+12	0.0	-707.0
1733.	NCO+NO2=CO+NO+NO	2.10E+11	0.0	-874.0
1734.	NCCN+O=NCO+CN	4.60E+12	0.0	8877.0
1735.	CN+NCO=NCN+CO	1.80E+13	0.0	0.0
1736.	NCO+NCO=CO+CO+N2	1.80E+13	0.0	0.0
1737.	HCNO=HCN+O	4.20E+31	-6.1	61175.0
1738.	CH2+NO=HCNO+H	3.80E+13	-0.4	576.0
1739.	CH2SING+NO<=>H+HCNO	3.80E+13	-0.4	580.0
1740.	NCH2+O=HCNO+H	2.00E+13	0.0	0.0
1741.	HCNO+H=HCN+OH	7.20E+10	0.8	8612.0
1742.	HCNO+H=NH2+CO	1.70E+14	-0.8	2889.0
1743.	HCNO+O=HCO+NO	6.30E+13	0.0	0.0
1744.	HCNO+O=NCO+OH	7.00E+12	0.0	0.0
1745.	HCNO+OH=HCO+HNO	4.50E+12	0.0	0.0
1746.	HCNO+OH=CH2O+NO	1.00E+12	0.0	0.0
1747.	HCNO+OH=NO+CO+H2	6.50E+12	0.0	0.0
1748.	HCNO+OH=NCO+H2O	3.50E+12	0.0	0.0
1749.	HCNO+OH=NCO+H+OH	4.50E+12	0.0	0.0
1750.	NO+HCCO=HCNO+CO	4.60E+13	0.0	695.0
1751.	HCCO+NO2=HCNO+CO2	1.60E+13	0.0	0.0

1752.	HCNO+CN=HCN+NCO	6.00E+13	0.0	0.0
1753.	HNCO(+M)=NH+CO(+M)	6.00E+13	0.0	99800.0
	Low pressure limit: 0.21700E+29 -0.31000E+01 0.10190E+06			
	TROE centering: 0.46650E+00 0.10000E+04 0.10000E+07			
	N2O Enhanced by 5.000E+00			
	H2O Enhanced by 5.000E+00			
	N2 Enhanced by 1.000E+00			
	CO2 Enhanced by 1.600E+00			
1754.	HNCO+M=H+NCO+M	1.00E+17	0.0	112000.0
1755.	HCNO+H<=>H+HNCO	2.10E+15	-0.7	2850.0
1756.	CH2+NO=HNCO+H	3.10E+17	-1.4	1271.0
1757.	CH2SING+NO<=>H+HNCO	3.10E+17	-1.4	1270.0
1758.	OH+HCN=HNCO+H	1.98E-03	4.0	1000.0
1759.	OH+HNC=HNCO+H	2.80E+13	0.0	3694.0
1760.	CHNH+O=HNCO+H	7.00E+13	0.0	0.0
1761.	HNCO+H=NCO+H2	9.00E+07	1.7	13900.0
1762.	HNCO+H=NH2+CO	3.60E+04	2.5	2343.0
1763.	HNC+O2=HNCO+O	1.50E+12	0.0	4111.0
1764.	HNCO+O=HNO+CO	1.49E+08	1.6	44010.0
1765.	HNCO+O=CO2+NH	9.80E+07	1.4	8524.0
1766.	HNCO+O=NCO+OH	2.20E+06	2.1	11430.0
1767.	HNCO+OH=NH2+CO2	6.30E+10	-0.1	11637.0
1768.	HNCO+OH=NCO+H2O	3.60E+07	1.5	3594.0
1769.	HNCO+O2=HNO+CO2	1.00E+12	0.0	35000.0
1770.	NCO+HO2=HNCO+O2	2.00E+13	0.0	0.0
1771.	HNCO+HO2=NCO+H2O2	3.00E+11	0.0	23700.0
1772.	NCO+CH4=HNCO+CH3	9.80E+12	0.0	8122.0
1773.	CH3CNH+O=CH3+HNCO	1.60E+14	0.0	0.0
1774.	CH2CNH+OH=CH3+HNCO	6.70E+11	0.0	-1013.0
1775.	C2H6+NCO=C2H5+HNCO	1.50E-09	6.9	-2910.0
1776.	NCO+HCO=HNCO+CO	3.60E+13	0.0	0.0
1777.	CH2O+NCO=HNCO+HCO	6.00E+12	0.0	0.0

1778.	CHCNH+O2=HNCO+HCO	4.90E+12	-0.1	1150.0
1779.	CH2CHN+O2=CH2O+HNCO	1.00E+12	0.0	0.0
1780.	HNCO+N=NH+NCO	2.32E+19	0.0	52500.0
1781.	HNCO+NH=NH2+NCO	3.00E+13	0.0	23700.0
1782.	NCO+NH3=HNCO+NH2	2.80E+04	2.5	983.0
1783.	NCO+HNO=HNCO+NO	1.80E+13	0.0	0.0
1784.	HNC+NO2=HNCO+NO	1.00E+12	0.0	32000.0
1785.	NCO+HONO=HNCO+NO2	3.60E+12	0.0	0.0
1786.	HNCO+NO2=HNNO+CO2	2.50E+12	0.0	26000.0
1787.	CN+HNCO=HCN+NCO	1.00E+13	0.0	0.0
1788.	HCN+OH=HOCN+H	5.90E+04	2.4	12500.0
1789.	HCNO+H=HOCN+H	1.40E+11	-0.2	2482.0
1790.	HOCN+H=HNCO+H	3.10E+08	0.8	1916.0
1791.	HOCN+H=NH2+CO	1.20E+08	0.6	2075.0
1792.	HOCN+H=H2+NCO	2.40E+08	1.5	6613.0
1793.	HOCN+O=OH+NCO	1.70E+08	1.5	4131.0
1794.	HOCN+OH=H2O+NCO	1.20E+06	2.0	-248.0
1795.	HOCN+CH3=CH4+NCO	8.20E+05	1.9	6613.0
1796.	CH3+HOCN=CH3CN+OH	5.00E+12	0.0	2000.0
1797.	HOCN+NH2=NCO+NH3	9.20E+05	1.9	3644.0
1798.	NCCN+OH=HOCN+CN	2.00E+12	0.0	18985.0
1799.	CH2NO=HNCO+H	2.30E+42	-9.1	53807.0
1800.	CH2NO+H=CH3+NO	4.00E+13	0.0	0.0
1801.	CH2NO+H=HCNO+H2	4.80E+08	1.5	-894.0
1802.	CH2NO+O=CH2O+NO	7.00E+13	0.0	0.0
1803.	CH2NO+O=HCNO+OH	3.30E+08	1.5	-894.0
1804.	NCH2+HO2=CH2NO+OH	3.00E+13	0.0	0.0
1805.	CH2NO+OH=CH2OH+NO	4.00E+13	0.0	0.0
1806.	CH2NO+OH=HCNO+H2O	2.40E+06	2.0	-1192.0
1807.	CH2NO+O2=CH2O+NO2	1.20E+15	-1.0	20117.0
1808.	CH2NO+CH3=C2H5+NO	3.00E+13	0.0	0.0
1809.	CH2NO+CH3=HCNO+CH4	1.60E+06	1.9	-1112.0

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1810. CH2NO+NH2=CH2NH2+NO                          3.00E+13    0.0        0.0
1811. CH2NO+NH2=HCNO+NH3                           1.80E+06    1.9    -1152.0
1812. H2NCO(+M)=CO+NH2(+M)                         5.90E+12    0.0    25000.0
      Low pressure limit:  0.10000E+15  0.00000E+00  0.21700E+05
1813. H2NCO+H=HNCO+H2                              3.00E+13    0.0        0.0
1814. H2NCO+O=HNCO+OH                              3.00E+13    0.0        0.0
1815. H2NCO+OH=HNCO+H2O                            3.00E+13    0.0        0.0
1816. CH2CHNH2+O=CH3+H2NCO                         3.90E+12    0.0     1494.0
      Declared duplicate reaction...
1817. CH2CHNH2+O=CH3+H2NCO                         6.20E+13    0.0     6855.0
      Declared duplicate reaction...
1818. CH3+NO(+M)=CH3NO(+M)                         9.00E+12    0.0      192.0
      Low pressure limit:  0.25000E+17  0.00000E+00 -0.28410E+04
      TROE centering:      0.50000E+01  0.10000E-29  0.12000E+03  0.10000E+31
1819. CH3+NO=CH3NO                                 1.00E+37   -8.4     5223.0
1820. CH3NO+H=CH2NO+H2                             4.40E+08    1.5      377.0
1821. CH3NO+H=CH3+HNO                              1.80E+13    0.0     2780.0
1822. CH3NO+O=CH2NO+OH                             3.30E+08    1.5     3614.0
1823. CH3NO+O=CH3+NO2                              1.70E+06    2.1        0.0
1824. CH3NO+OH=CH2NO+H2O                           3.60E+06    2.0    -1192.0
1825. CH3NO+OH=CH3+HONO                            2.50E+12    0.0      993.0
1826. CH3NO+CH3=CH2NO+CH4                          7.90E+05    1.9     5412.0
1827. CH3NCH3+O=CH3NO+CH3                          5.00E+13    0.0        0.0
1828. CH3NCH3+O2=CH3NO+CH3O                        1.00E+09    1.0     6000.0
1829. CH3NO+NH2=CH2NO+NH3                          2.80E+06    1.9     1072.0
1830. H2NCHO(+M)=CO+NH3(+M)                        1.00E+14    0.0    75514.0
      Low pressure limit:  0.83000E+15  0.00000E+00  0.49084E+05
1831. H2NCHO+M=HCO+NH2+M                           1.40E+16    0.0    72900.0
1832. H2NCHO+M=H2NCO+H+M                           4.60E+15    0.0    64200.0
1833. H2NCHO+H=H2NCO+H2                            1.30E+13    0.0     6955.0
1834. H2NCHO+H=HCO+NH3                             1.00E+13    0.0    19100.0
1835. H2NCHO+O=H2NCO+OH                            4.00E+08    1.5     5196.0
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1836. CH3CHNH2+O=CH3+H2NCHO                           4.00E+13    0.0        0.0
1837. H2NCHO+OH=H2NCO+H2O                             8.00E+12    0.0        0.0
1838. CH3CHNH2+HO2=>CH3+OH+H2NCHO                     2.40E+13    0.0        0.0
1839. H2NCHO+CH3=H2NCO+CH4                            7.00E+05    2.0     9000.0
1840. H2NCHO+NH2=H2NCO+NH3                            2.00E+06    2.0     5000.0
1841. H2CNO2=CH2O+NO                                  1.00E+13    0.0    36000.0
1842. CH3O+NO(+M)=CH3ONO(+M)                          6.60E+14   -0.6        0.0
      Low pressure limit:  0.27000E+28 -0.35000E+01  0.00000E+00
1843. CH3NO2(+M)=CH3+NO2(+M)                          1.80E+16    0.0    58500.0
      Low pressure limit:  0.13000E+18  0.00000E+00  0.42000E+05
      TROE centering:      0.18320E+00  0.10000E+02  0.10000E+07
1844. CH3NO2+H=CH3+HONO                               3.30E+12    0.0     3730.0
1845. CH3NO2+H=CH3NO+OH                               1.40E+12    0.0     3730.0
1846. CH3NO2+H=H2CNO2+H2                              5.40E+02    3.5     5200.0
1847. CH3NO2+O=H2CNO2+OH                              1.50E+13    0.0     5350.0
1848. CH3NO2+OH=H2CNO2+H2O                            5.00E+05    2.0     1000.0
1849. CH3NO2+OH=CH3OH+NO2                             2.00E+10    0.0    -1000.0
1850. CH3NO2+CH2=H2CNO2+CH3                           6.50E+12    0.0     7900.0
1851. CH3NO2+CH2SING=H2CNO2+CH3                       1.20E+14    0.0        0.0
1852. CH3NO2+CH3=H2CNO2+CH4                           5.50E-01    4.0     8300.0
1853. CN+NO(+M)=NCNO(+M)                              3.98E+13    0.0        0.0
      Low pressure limit:  0.15600E+37 -0.62000E+01  0.48780E+04
      TROE centering:      0.65080E+00  0.10000E+02  0.10000E+07
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    2.000E+00
1854. CH3O+NO2(+M)=CH3ONO2(+M)                        1.20E+13    0.0        0.0
      Low pressure limit:  0.14000E+31 -0.45000E+01  0.00000E+00
1855. cyMorph+M=cyOrthoMorphyl+H+M                    1.00E+16    0.0    95000.0
1856. cyMorph+M=cyMetaMorphyl+H+M                     1.00E+16    0.0    95000.0
1857. cyMorph+M=cyParaMorphyl+H+M                     2.50E+15    0.0    95000.0
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1858.	cyMorph+HO2=cyOrthoMorphyl+H2O2	4.19E+13	0.0	8530.0
1859.	cyMorph+HO2=cyMetaMorphyl+H2O2	3.49E+13	0.0	7810.0
1860.	cyMorph+HO2=cyParaMorphyl+H2O2	4.09E+12	0.0	6520.0
1861.	cyMorph+OH=cyOrthoMorphyl+H2O	6.36E+07	1.7	-236.0
1862.	cyMorph+OH=cyMetaMorphyl+H2O	6.36E+07	1.7	-236.0
1863.	cyMorph+OH=cyParaMorphyl+H2O	1.59E+07	1.7	-236.0
1864.	cyMorph+O=cyOrthoMorphyl+OH	7.70E+15	0.0	10800.0
1865.	cyMorph+O=cyMetaMorphyl+OH	6.42E+15	0.0	9880.0
1866.	cyMorph+O=cyParaMorphyl+OH	7.52E+14	0.0	8240.0
1867.	cyMorph+H=cyOrthoMorphyl+H2	2.09E+15	0.0	15000.0
1868.	cyMorph+H=cyMetaMorphyl+H2	1.74E+15	0.0	13800.0
1869.	cyMorph+H=cyParaMorphyl+H2	2.04E+14	0.0	11500.0
1870.	cyMorph+CH3=cyOrthoMorphyl+CH4	4.71E+12	0.0	17600.0
1871.	cyMorph+CH3=cyMetaMorphyl+CH4	3.92E+12	0.0	16100.0
1872.	cyMorph+CH3=cyParaMorphyl+CH4	4.60E+11	0.0	13400.0
1873.	cyMorph+C2H3=cyOrthoMorphyl+C2H4	4.71E+12	0.0	14300.0
1874.	cyMorph+C2H3=cyMetaMorphyl+C2H4	3.92E+12	0.0	13100.0
1875.	cyMorph+C2H3=cyParaMorphyl+C2H4	4.60E+11	0.0	10900.0
1876.	cyMorph+C2H5=cyOrthoMorphyl+C2H6	4.71E+12	0.0	14300.0
1877.	cyMorph+C2H5=cyMetaMorphyl+C2H6	3.92E+12	0.0	13100.0
1878.	cyMorph+C2H5=cyParaMorphyl+C2H6	4.60E+11	0.0	10900.0
1879.	cyMorph+AC3H5=cyOrthoMorphyl+C3H6	4.71E+12	0.0	14300.0
1880.	cyMorph+AC3H5=cyMetaMorphyl+C3H6	3.92E+12	0.0	13100.0
1881.	cyMorph+AC3H5=cyParaMorphyl+C3H6	4.60E+11	0.0	10900.0
1882.	cyMorph+SC3H5=cyOrthoMorphyl+C3H6	4.71E+12	0.0	14300.0
1883.	cyMorph+SC3H5=cyMetaMorphyl+C3H6	3.92E+12	0.0	13100.0
1884.	cyMorph+SC3H5=cyParaMorphyl+C3H6	4.60E+11	0.0	10900.0
1885.	cyMorph+TC3H5=cyOrthoMorphyl+C3H6	4.71E+12	0.0	14300.0
1886.	cyMorph+TC3H5=cyMetaMorphyl+C3H6	3.92E+12	0.0	13100.0
1887.	cyMorph+TC3H5=cyParaMorphyl+C3H6	4.60E+11	0.0	10900.0
1888.	cyMorph+HCO=cyOrthoMorphyl+CH2O	4.71E+12	0.0	7770.0
1889.	cyMorph+HCO=cyMetaMorphyl+CH2O	3.92E+12	0.0	7120.0

1890.	cyMorph+HCO=cyParaMorphyl+CH2O	4.60E+11	0.0	5940.0
1891.	cyOrthoMorphyl=NHCH2CH2OCHCH2	2.00E+13	0.0	27700.0
1892.	cyOrthoMorphyl=CH2CH2NHCH2CHO	2.00E+13	0.0	27700.0
1893.	cyMetaMorphyl=OCH2CH2NHCHCH2	2.00E+13	0.0	27700.0
1894.	cyMetaMorphyl=CH2CH2OCH2CHNH	2.00E+13	0.0	27700.0
1895.	cyParaMorphyl=CH2OCH2CH2NCH2	4.00E+13	0.0	27700.0
1896.	NHCH2CH2OCHCH2=CH2NH+CH2CHOCH2	2.00E+13	0.0	28700.0
1897.	CH2CH2NHCH2CHO=C2H4+NHCH2CHO	2.00E+13	0.0	28700.0
1898.	OCH2CH2NHCHCH2=CH2O+CH2NHCHCH2	2.00E+13	0.0	28700.0
1899.	CH2CH2OCH2CHNH=C2H4+OCH2CHNH	2.00E+13	0.0	28700.0
1900.	CH2OCH2CH2NCH2=CH2O+CH2CH2NCH2	2.00E+13	0.0	28700.0
1901.	CH2CHOCH2=CH2O+C2H3	1.00E+11	0.0	37000.0
1902.	NHCH2CHO=CH2NH+HCO	1.00E+11	0.0	37000.0
1903.	CH2NHCHCH2=CH2NH+C2H3	1.00E+11	0.0	37000.0
1904.	OCH2CHNH=CH2O+CHNH	1.00E+11	0.0	37000.0
1905.	CH2CH2NCH2=C2H4+NCH2	1.00E+11	0.0	37000.0
1906.	NHCH2CH2OCHCH2=CH2CHOCH2CHNH+H	3.20E+13	0.0	38000.0
1907.	NHCH2CH2OCHCH2+H=CH2CHOCH2CHNH+H2	1.80E+12	0.0	0.0
1908.	NHCH2CH2OCHCH2+O2=CH2CHOCH2CHNH+HO2	1.00E+11	0.0	0.0
1909.	NHCH2CH2OCHCH2+CH3=CH2CHOCH2CHNH+CH4	1.10E+13	0.0	0.0
1910.	NHCH2CH2OCHCH2+O=CH2CHOCH2CHNH+OH	4.82E+13	0.0	0.0
1911.	NHCH2CH2OCHCH2+OH=CH2CHOCH2CHNH+H2O	2.41E+13	0.0	0.0
1912.	CH2CH2NHCH2CHO=OCHCH2NHCHCH2+H	3.20E+13	0.0	38000.0
1913.	CH2CH2NHCH2CHO+H=OCHCH2NHCHCH2+H2	1.80E+12	0.0	0.0
1914.	CH2CH2NHCH2CHO+O2=OCHCH2NHCHCH2+HO2	1.00E+11	0.0	0.0
1915.	CH2CH2NHCH2CHO+CH3=OCHCH2NHCHCH2+CH4	1.10E+13	0.0	0.0
1916.	CH2CH2NHCH2CHO+O=OCHCH2NHCHCH2+OH	4.82E+13	0.0	0.0
1917.	CH2CH2NHCH2CHO+OH=OCHCH2NHCHCH2+H2O	2.41E+13	0.0	0.0
1918.	OCH2CH2NHCHCH2=OCHCH2NHCHCH2+H	3.20E+13	0.0	38000.0
1919.	OCH2CH2NHCHCH2+H=OCHCH2NHCHCH2+H2	1.80E+12	0.0	0.0
1920.	OCH2CH2NHCHCH2+O2=OCHCH2NHCHCH2+HO2	1.00E+11	0.0	0.0
1921.	OCH2CH2NHCHCH2+CH3=OCHCH2NHCHCH2+CH4	1.10E+13	0.0	0.0

1922.	OCH2CH2NHCHCH2+O=OCHCH2NHCHCH2+OH	4.82E+13	0.0	0.0
1923.	OCH2CH2NHCHCH2+OH=OCHCH2NHCHCH2+H2O	2.41E+13	0.0	0.0
1924.	CH2CH2OCH2CHNH=CH2CHOCH2CHNH+H	3.20E+13	0.0	38000.0
1925.	CH2CH2OCH2CHNH+H=CH2CHOCH2CHNH+H2	1.80E+12	0.0	0.0
1926.	CH2CH2OCH2CHNH+O2=CH2CHOCH2CHNH+HO2	1.00E+11	0.0	0.0
1927.	CH2CH2OCH2CHNH+CH3=CH2CHOCH2CHNH+CH4	1.10E+13	0.0	0.0
1928.	CH2CH2OCH2CHNH+O=CH2CHOCH2CHNH+OH	4.82E+13	0.0	0.0
1929.	CH2CH2OCH2CHNH+OH=CH2CHOCH2CHNH+H2O	2.41E+13	0.0	0.0
1930.	CH2CHNH+O2=CH2CNH+HO2	1.57E+11	0.0	0.0
1931.	cyOrthoMorphyl=cyOCHCHNHCH2CH2+H	1.26E+13	0.0	35613.0
1932.	cyOrthoMorphyl+O2=cyOCHCHNHCH2CH2+HO2	1.60E+12	0.0	5000.0
1933.	cyOrthoMorphyl+HO2=cyOCHCHNHCH2CH2+H2O2	1.00E+12	0.0	2000.0
1934.	cyOrthoMorphyl+OH=cyOCHCHNHCH2CH2+H2O	2.40E+13	0.0	0.0
1935.	cyOrthoMorphyl+O=cyOCHCHNHCH2CH2+OH	4.82E+13	0.0	0.0
1936.	cyOrthoMorphyl+H=cyOCHCHNHCH2CH2+H2	1.00E+11	0.0	0.0
1937.	cyOrthoMorphyl+CH3=cyOCHCHNHCH2CH2+CH4	2.00E+12	0.0	0.0
1938.	cyOrthoMorphyl+HCO=cyOCHCHNHCH2CH2+CH2O	2.00E+12	0.0	0.0
1939.	cyMetaMorphyl=cyOCHCHNHCH2CH2+H	1.26E+13	0.0	35613.0
1940.	cyMetaMorphyl+O2=cyOCHCHNHCH2CH2+HO2	1.60E+12	0.0	5000.0
1941.	cyMetaMorphyl+HO2=cyOCHCHNHCH2CH2+H2O2	1.00E+12	0.0	2000.0
1942.	cyMetaMorphyl+OH=cyOCHCHNHCH2CH2+H2O	2.40E+13	0.0	0.0
1943.	cyMetaMorphyl+O=cyOCHCHNHCH2CH2+OH	4.82E+13	0.0	0.0
1944.	cyMetaMorphyl+H=cyOCHCHNHCH2CH2+H2	1.00E+11	0.0	0.0
1945.	cyMetaMorphyl+CH3=cyOCHCHNHCH2CH2+CH4	2.00E+12	0.0	0.0
1946.	cyMetaMorphyl+HCO=cyOCHCHNHCH2CH2+CH2O	2.00E+12	0.0	0.0
1947.	cyMetaMorphyl=cyOCH2CHNCH2CH2+H	6.30E+12	0.0	35613.0
1948.	cyMetaMorphyl+O2=cyOCH2CHNCH2CH2+HO2	8.00E+11	0.0	5000.0
1949.	cyMetaMorphyl+HO2=cyOCH2CHNCH2CH2+H2O2	5.00E+11	0.0	2000.0
1950.	cyMetaMorphyl+OH=cyOCH2CHNCH2CH2+H2O	1.20E+13	0.0	0.0
1951.	cyMetaMorphyl+O=cyOCH2CHNCH2CH2+OH	2.41E+13	0.0	0.0
1952.	cyMetaMorphyl+H=cyOCH2CHNCH2CH2+H2	5.00E+10	0.0	0.0
1953.	cyMetaMorphyl+CH3=cyOCH2CHNCH2CH2+CH4	1.00E+12	0.0	0.0

1954.	cyMetaMorphyl+HCO=cyOCH2CHNCH2CH2+CH2O	1.00E+12	0.0	0.0
1955.	cyParaMorphyl=cyOCH2CHNCH2CH2+H	1.26E+13	0.0	35613.0
1956.	cyParaMorphyl+O2=cyOCH2CHNCH2CH2+HO2	1.60E+12	0.0	5000.0
1957.	cyParaMorphyl+HO2=cyOCH2CHNCH2CH2+H2O2	1.00E+12	0.0	2000.0
1958.	cyParaMorphyl+OH=cyOCH2CHNCH2CH2+H2O	2.40E+13	0.0	0.0
1959.	cyParaMorphyl+O=cyOCH2CHNCH2CH2+OH	4.82E+13	0.0	0.0
1960.	cyParaMorphyl+H=cyOCH2CHNCH2CH2+H2	1.00E+11	0.0	0.0
1961.	cyParaMorphyl+CH3=cyOCH2CHNCH2CH2+CH4	2.00E+12	0.0	0.0
1962.	cyParaMorphyl+HCO=cyOCH2CHNCH2CH2+CH2O	2.00E+12	0.0	0.0
1963.	cyOCHCHNHCH2CH2=cyNCH2CH2OCHCH+H	1.25E+15	0.0	81700.0
1964.	cyOCHCHNHCH2CH2+O2=cyNCH2CH2OCHCH+HO2	1.80E+13	0.0	34800.0
1965.	cyOCHCHNHCH2CH2+HO2=cyNCH2CH2OCHCH+H2O2	5.00E+10	0.0	17060.0
1966.	cyOCHCHNHCH2CH2+OH=cyNCH2CH2OCHCH+H2O	1.50E+13	0.0	300.0
1967.	cyOCHCHNHCH2CH2+O=cyNCH2CH2OCHCH+OH	1.55E+12	0.0	4445.0
1968.	cyOCHCHNHCH2CH2+H=cyNCH2CH2OCHCH+H2	1.55E+12	0.0	4445.0
1969.	cyOCHCHNHCH2CH2+CH3=cyNCH2CH2OCHCH+CH4	4.13E+10	0.0	4118.0
1970.	cyOCHCHNHCH2CH2+C2H3=cyNCH2CH2OCHCH+C2H4	4.13E+10	0.0	4118.0
1971.	cyOCHCHNHCH2CH2+C2H5=cyNCH2CH2OCHCH+C2H6	4.13E+10	0.0	4118.0
1972.	cyOCHCHNHCH2CH2+AC3H5=cyNCH2CH2OCHCH+C3H6	4.13E+10	0.0	4118.0
1973.	cyOCHCHNHCH2CH2+SC3H5=cyNCH2CH2OCHCH+C3H6	4.13E+10	0.0	4118.0
1974.	cyOCHCHNHCH2CH2+TC3H5=cyNCH2CH2OCHCH+C3H6	4.13E+10	0.0	4118.0
1975.	cyOCHCHNHCH2CH2+HCO=cyNCH2CH2OCHCH+CH2O	4.13E+10	0.0	4118.0
1976.	cyOCHCHNHCH2CH2+CH3O=cyNCH2CH2OCHCH+CH3OH	4.13E+10	0.0	4118.0
1977.	cyOCH2CHNCH2CH2=cyNCH2CH2OCHCH+H	2.50E+15	0.0	81700.0
1978.	cyOCH2CHNCH2CH2+O2=cyNCH2CH2OCHCH+HO2	3.60E+13	0.0	34800.0
1979.	cyOCH2CHNCH2CH2+HO2=cyNCH2CH2OCHCH+H2O2	1.00E+11	0.0	17060.0
1980.	cyOCH2CHNCH2CH2+OH=cyNCH2CH2OCHCH+H2O	3.00E+13	0.0	300.0
1981.	cyOCH2CHNCH2CH2+O=cyNCH2CH2OCHCH+OH	3.10E+12	0.0	4445.0
1982.	cyOCH2CHNCH2CH2+H=cyNCH2CH2OCHCH+H2	3.10E+12	0.0	4445.0
1983.	cyOCH2CHNCH2CH2+CH3=cyNCH2CH2OCHCH+CH4	8.25E+10	0.0	4118.0
1984.	cyOCH2CHNCH2CH2+C2H3=cyNCH2CH2OCHCH+C2H4	8.25E+10	0.0	4118.0
1985.	cyOCH2CHNCH2CH2+C2H5=cyNCH2CH2OCHCH+C2H6	8.25E+10	0.0	4118.0

1986.	cyOCH2CHNCH2CH2+AC3H5=cyNCH2CH2OCHCH+C3H6	8.25E+10	0.0	4118.0
1987.	cyOCH2CHNCH2CH2+SC3H5=cyNCH2CH2OCHCH+C3H6	8.25E+10	0.0	4118.0
1988.	cyOCH2CHNCH2CH2+TC3H5=cyNCH2CH2OCHCH+C3H6	8.25E+10	0.0	4118.0
1989.	cyOCH2CHNCH2CH2+HCO=cyNCH2CH2OCHCH+CH2O	8.25E+10	0.0	4118.0
1990.	cyOCH2CHNCH2CH2+CH3O=cyNCH2CH2OCHCH+CH3OH	8.25E+10	0.0	4118.0
1991.	cyNCH2CH2OCHCH=CH2CH2NCHCHO	6.50E+12	0.0	35900.0
1992.	cyNCH2CH2OCHCH=CH2OCHCHNCH2	6.50E+12	0.0	35900.0
1993.	cyNCH2CH2OCHCH=cyOCHCHNCHCH2+H	6.00E+13	0.0	49300.0
1994.	cyNCH2CH2OCHCH+O2=cyOCHCHNCHCH2+HO2	8.00E+11	0.0	15160.0
1995.	cyNCH2CH2OCHCH+HO2=cyOCHCHNCHCH2+H2O2	5.00E+11	0.0	0.0
1996.	cyNCH2CH2OCHCH+OH=cyOCHCHNCHCH2+H2O	3.01E+12	0.0	0.0
1997.	cyNCH2CH2OCHCH+O=cyOCHCHNCHCH2+OH	9.00E+12	0.0	0.0
1998.	cyNCH2CH2OCHCH+H=cyOCHCHNCHCH2+H2	1.58E+13	0.0	0.0
1999.	cyNCH2CH2OCHCH+CH3=cyOCHCHNCHCH2+CH4	4.00E+12	0.0	0.0
2000.	cyNCH2CH2OCHCH+C2H3=cyOCHCHNCHCH2+C2H4	2.00E+12	0.0	0.0
2001.	cyNCH2CH2OCHCH+C2H5=cyOCHCHNCHCH2+C2H6	2.00E+12	0.0	0.0
2002.	cyNCH2CH2OCHCH+AC3H5=cyOCHCHNCHCH2+C3H6	2.00E+12	0.0	0.0
2003.	cyNCH2CH2OCHCH+SC3H5=cyOCHCHNCHCH2+C3H6	2.00E+12	0.0	0.0
2004.	cyNCH2CH2OCHCH+TC3H5=cyOCHCHNCHCH2+C3H6	2.00E+12	0.0	0.0
2005.	cyNCH2CH2OCHCH+HCO=cyOCHCHNCHCH2+CH2O	2.00E+12	0.0	0.0
2006.	cyNCH2CH2OCHCH+CH3O=cyOCHCHNCHCH2+CH3OH	2.00E+12	0.0	0.0
2007.	cyOCHCHNCHCH2=cyCHOCHCHNCH+H	1.30E+14	0.0	77100.0
2008.	cyOCHCHNCHCH2+O2=cyCHOCHCHNCH+HO2	4.15E+11	0.0	24858.0
2009.	cyOCHCHNCHCH2+HO2=cyCHOCHCHNCH+H2O2	2.00E+12	0.0	17057.0
2010.	cyOCHCHNCHCH2+OH=cyCHOCHCHNCH+H2O	3.00E+06	2.0	-1520.0
2011.	cyOCHCHNCHCH2+O=cyCHOCHCHNCH+OH	7.00E+12	0.0	-795.0
2012.	cyOCHCHNCHCH2+H=cyCHOCHCHNCH+H2	5.50E+04	2.5	-1900.0
2013.	cyOCHCHNCHCH2+CH3=cyCHOCHCHNCH+CH4	6.15E+10	0.0	5201.0
2014.	cyOCHCHNCHCH2+C2H3=cyCHOCHCHNCH+C2H4	6.15E+10	0.0	5201.0
2015.	cyOCHCHNCHCH2+C2H5=cyCHOCHCHNCH+C2H6	6.15E+10	0.0	5201.0
2016.	cyOCHCHNCHCH2+AC3H5=cyCHOCHCHNCH+C3H6	6.15E+10	0.0	5201.0
2017.	cyOCHCHNCHCH2+HCO=cyCHOCHCHNCH+CH2O	6.15E+10	0.0	5201.0

2018.	cyOCHCHNCHCH2+CH3O=cyCHOCHCHNCH+CH3OH	6.15E+10	0.0	5201.0
2019.	CH2CH2NCH2+H=CH2CHNCH2+H2	1.80E+12	0.0	0.0
2020.	CH2CH2NCH2+O2=CH2CHNCH2+HO2	1.00E+11	0.0	0.0
2021.	CH2CH2NCH2+CH3=CH2CHNCH2+CH4	1.10E+13	0.0	0.0
2022.	CH2CHOCH2CHNH=CH2CHNH+CH2CHO	2.00E+15	0.0	56800.0
2023.	OCHCH2NHCHCH2=CH2CHNH+CH2CHO	2.00E+15	0.0	56800.0
2024.	CH2CH2NCHCHO=C2H4+NCHCHO	2.00E+13	0.0	35500.0
2025.	CH2OCHCHNCH2=CH2O+CHCHNCH2	2.00E+13	0.0	35500.0
2026.	NCHCHO=HCN+HCO	1.00E+14	0.0	43900.0
2027.	CHCHNCH2=C2H2+NCH2	1.00E+14	0.0	43900.0
2028.	cyMorph=C2H4OH+CH2CHNH	1.77E+55	-12.7	78800.0
2029.	cyMorph=CH2CH2NH2+CH2CHO	1.77E+55	-12.7	78800.0
2030.	cyMorph=CH3CH2NH+CH2CHO	2.23E+55	-12.7	78400.0
2031.	cyMorph=CH2CHNH+C2H5O	2.23E+55	-12.7	78400.0
2032.	cyOrthoMorphyl=HCO+C2H4+CH2NH	3.16E+15	-2.0	23000.0
2033.	cyMetaMorphyl=CH2O+C2H4+CHNH	3.16E+15	-2.0	23000.0
2034.	cyParaMorphyl=NCH2+C2H4+CH2O	1.05E+15	-2.0	23000.0
2035.	cyOrthoMorphyl=CH3CH2NH+CH2CO	7.84E+08	0.0	23000.0
2036.	cyMetaMorphyl=CH2CNH+C2H5O	7.84E+08	0.0	23000.0
2037.	cyMorph=CH3CH2NHCH2CHO	6.40E+65	-15.3	88293.0
2038.	cyMorph=NH2CH2CH2OCHCH2	6.23E+63	-14.8	85767.0
2039.	cyMorph=CH3CH2OCH2CHNH	6.40E+65	-15.3	88293.0
2040.	cyMorph=OHCH2CH2NHCHCH2	6.23E+63	-14.8	85767.0
2041.	cyMorph=CH3OCH2CH2NCH2	3.36E+15	0.4	82760.0
2042.	CH3CH2NHCH2CHO=CH3CH2NH+CH2CHO	1.46E+27	-3.0	78550.0
2043.	NH2CH2CH2OCHCH2=CH2CH2NH2+CH2CHO	1.46E+27	-3.0	78550.0
2044.	CH3CH2OCH2CHNH=C2H5O+CH2CHNH	1.46E+27	-3.0	78550.0
2045.	OHCH2CH2NHCHCH2=C2H4OH+CH2CHNH	1.46E+27	-3.0	78550.0
2046.	CH3OCH2CH2NCH2=CH3OCH2+CH2NCH2	1.46E+27	-3.0	78550.0
2047.	CH3CH2NHCH2CHO=CH3CHNH+CH2CHOH	3.98E+12	0.0	57392.0
2048.	NH2CH2CH2OCHCH2=CH2CHNH+CH3CHOH	3.98E+12	0.0	57392.0
2049.	CH3CH2OCH2CHNH=CH3CHO+CH2CHNH2	3.98E+12	0.0	57392.0

2050.	OHCH2CH2NHCHCH2=CH2CHOH+CH3CHNH	3.98E+12	0.0	57392.0
2051.	CH2CHOH=CH3CHO	2.54E+12	0.0	56460.0
2052.	CH2CHOH+H2O=CH3CHO+H2O	5.21E+09	0.0	25520.0
2053.	cyOrthoMorphyl+O2=cyOrthoOOMorphyl	3.00E+12	0.0	0.0
2054.	cyMetaMorphyl+O2=cyMetaOOMorphyl	3.00E+12	0.0	0.0
2055.	cyParaMorphyl+O2=cyParaOOMorphyl	3.00E+12	0.0	0.0
2056.	cyOrthoOOMorphyl=cyOCHCHNHCH2CH2+HO2	1.92E+12	0.0	29000.0
2057.	cyMetaOOMorphyl=cyOCHCHNHCH2CH2+HO2	1.92E+12	0.0	29000.0
2058.	cyMetaOOMorphyl=cyOCH2CHNCH2CH2+HO2	9.62E+11	0.0	29000.0
2059.	cyParaOOMorphyl=cyOCH2CHNCH2CH2+HO2	3.85E+12	0.0	29000.0
2060.	cyOrthoOOMorphyl=cyOrtho*Morph3yl	2.47E+11	0.0	31000.0
2061.	cyMetaOOMorphyl=cyMeta*Morph2yl	2.47E+11	0.0	31000.0
2062.	cyMetaOOMorphyl=cyMeta*Morph4yl	1.24E+11	0.0	31000.0
2063.	cyParaOOMorphyl=cyPara*Morph3yl	4.94E+11	0.0	31000.0
2064.	cyOrthoOOMorphyl=cyOrtho*Morph6yl	9.30E+10	0.0	24077.0
2065.	cyOrthoOOMorphyl=cyOrtho*Morph4yl	4.65E+10	0.0	24077.0
2066.	cyMetaOOMorphyl=cyMeta*Morph5yl	9.30E+10	0.0	24077.0
2067.	cyParaOOMorphyl=cyPara*Morph2yl	1.86E+11	0.0	24077.0
2068.	cyOrthoOOMorphyl=cyOrtho*Morph5yl	1.08E+10	0.0	24356.0
2069.	cyMetaOOMorphyl=cyMeta*Morph6yl	1.08E+10	0.0	24356.0
2070.	CH2CH2OCH*CHNH=cyOrtho*Morph3yl	2.00E+08	0.9	5900.0
2071.	CH2CH2NHCH*CHO=cyMeta*Morph2yl	2.00E+08	0.9	5900.0
2072.	CH2OCH2CH*NCH2=cyMeta*Morph4yl	2.00E+08	0.9	5900.0
2073.	OCH2CH2N*CHCH2=cyPara*Morph3yl	2.00E+08	0.9	5900.0
2074.	OCH2CH2NHCHCH*=cyOrtho*Morph3yl	1.00E+08	0.9	5900.0
2075.	NHCH2CH2OCHCH*=cyMeta*Morph2yl	1.00E+08	0.9	5900.0
2076.	CH2OCH2CH2NCH*=cyMeta*Morph4yl	1.00E+08	0.9	5900.0
2077.	CH2CH2OCH2CHN*=cyPara*Morph3yl	1.00E+08	0.9	5900.0
2078.	CH2OCH*CH2NCH2=cyOrtho*Morph4yl	2.00E+08	0.9	5900.0
2079.	NHCH2CH*OCHCH2=cyOrtho*Morph6yl	2.00E+08	0.9	5900.0
2080.	OCH2CH*NHCHCH2=cyMeta*Morph5yl	2.00E+08	0.9	5900.0
2081.	CH2CH2N*CH2CHO=cyPara*Morph2yl	2.00E+08	0.9	5900.0

2082. CH*OCH2CH2NCH2=cyOrtho*Morph4yl	5.00E+07	0.9	5900.0
2083. CH*CH2NHCH2CHO=cyOrtho*Morph6yl	5.00E+07	0.9	5900.0
2084. CH*CH2OCH2CHNH=cyMeta*Morph5yl	5.00E+07	0.9	5900.0
2085. N*CH2CH2OCHCH2=cyPara*Morph2yl	5.00E+07	0.9	5900.0
2086. CH2CH*OCH2CHNH=cyOrtho*Morph5yl	1.00E+08	0.9	5900.0
2087. OCH*CH2NHCHCH2=cyOrtho*Morph5yl	1.00E+08	0.9	5900.0
2088. CH2CH*NHCH2CHO=cyMeta*Morph6yl	1.00E+08	0.9	5900.0
2089. NHCH*CH2OCHCH2=cyMeta*Morph6yl	1.00E+08	0.9	5900.0
2090. OCH*CHNH+C2H4=CH2CH2OCH*CHNH	1.32E+04	2.5	6130.0
2091. NHCH*CHO+C2H4=CH2CH2NHCH*CHO	1.32E+04	2.5	6130.0
2092. CH2CH*NCH2+CH2O=CH2OCH2CH*NCH2	1.32E+04	2.5	6130.0
2093. CH2NHCHCH*+CH2O=OCH2CH2NHCHCH*	1.32E+04	2.5	6130.0
2094. CH2OCHCH*+CH2NH=NHCH2CH2OCHCH*	1.32E+04	2.5	6130.0
2095. CH2CH2NCH*+CH2O=CH2OCH2CH2NCH*	1.32E+04	2.5	6130.0
2096. OCH2CHN*+C2H4=CH2CH2OCH2CHN*	1.32E+04	2.5	6130.0
2097. CH*CH2NCH2+CH2O=CH2OCH*CH2NCH2	1.32E+04	2.5	6130.0
2098. CH*OCHCH2+CH2NH=NHCH2CH*OCHCH2	1.32E+04	2.5	6130.0
2099. CH*NHCHCH2+CH2O=OCH2CH*NHCHCH2	1.32E+04	2.5	6130.0
2100. N*CH2CHO+C2H4=CH2CH2N*CH2CHO	1.32E+04	2.5	6130.0
2101. OCHOOH+CH2CH2NCH2=CH*OCH2CH2NCH2	1.32E+04	2.5	6130.0
2102. CH2CHOOH+NHCH2CHO=CH*CH2NHCH2CHO	1.32E+04	2.5	6130.0
2103. CH2CHOOH+OCH2CHNH=CH*CH2OCH2CHNH	1.32E+04	2.5	6130.0
2104. CH2NOOH+CH2CHOCH2=N*CH2CH2OCHCH2	1.32E+04	2.5	6130.0
2105. CH2CHOOH+OCH2CHNH=CH2CH*OCH2CHNH	1.89E+03	2.7	6850.0
2106. OCHOOH+CH2NHCHCH2=OCH*CH2NHCHCH2	1.89E+03	2.7	6850.0
2107. CH2CHOOH+NHCH2CHO=CH2CH*NHCH2CHO	1.89E+03	2.7	6850.0
2108. NHCHOOH+CH2CHOCH2=NHCH*CH2OCHCH2	1.89E+03	2.7	6850.0
2109. CH2CHOCH2CHNH+HO2=CH2CH*OCH2CHNH	2.00E+11	0.0	12500.0
2110. CH2CHOCH2CHNH+HO2=NHCH*CH2OCHCH2	2.00E+11	0.0	12500.0
2111. OCHCH2NHCHCH2+HO2=OCH*CH2NHCHCH2	2.00E+11	0.0	12500.0
2112. OCHCH2NHCHCH2+HO2=CH2CH*NHCH2CHO	2.00E+11	0.0	12500.0
2113. NHCHCHO+HO2=OCH*CHNH	2.00E+11	0.0	7600.0

2114.	NHCHCHO+HO2=NHCH*CHO	2.00E+11	0.0	7600.0
2115.	CH2CHNCH2+HO2=CH2CH*NCH2	2.00E+11	0.0	7600.0
2116.	CH2CHNCH2+HO2+CH2O=OCH2CH2N*CHCH2	2.00E+11	0.0	7600.0
2117.	CHCHOOH+CH2NH=CH2NHCHCH*	2.00E+11	0.0	2010.0
2118.	CHCHOOH+CH2O=CH2OCHCH*	2.00E+11	0.0	2010.0
2119.	NCHOOH+C2H4=CH2CH2NCH*	2.00E+11	0.0	2010.0
2120.	CHNOOH+CH2O=OCH2CHN*	2.00E+11	0.0	2010.0
2121.	NCH2+CH2CHOOH=CH*CH2NCH2	1.32E+04	2.5	6130.0
2122.	C2H3+OCHOOH=CH*OCHCH2	1.32E+04	2.5	6130.0
2123.	C2H3+NHCHOOH=CH*NHCHCH2	1.32E+04	2.5	6130.0
2124.	HCO+CH2NOOH=N*CH2CHO	1.32E+04	2.5	6130.0
2125.	CH2NOOH+OH=CHNOOH+H2O	1.80E+06	2.0	-1133.0
2126.	NHCHOOH+OH=NCHOOH+H2O	9.00E+05	2.0	-1133.0
2127.	CH2NOOH+H=CHNOOH+H2	1.15E+06	2.5	4124.0
2128.	NHCHOOH+H=NCHOOH+H2	5.75E+05	2.5	4124.0
2129.	CH2NOOH+CH3=CHNOOH+CH4	5.42E+04	2.3	7287.0
2130.	NHCHOOH+CH3=NCHOOH+CH4	2.71E+04	2.3	7287.0
2131.	CH2NOOH+HO2=CHNOOH+H2O2	1.12E+13	0.0	17686.0
2132.	NHCHOOH+HO2=NCHOOH+H2O2	5.60E+12	0.0	17686.0
2133.	HCN+HO2=CHNOOH	2.00E+11	0.0	12500.0
2134.	HCN+HO2=NCHOOH	2.00E+11	0.0	12500.0
2135.	HCO+HO2=OCHOOH	2.00E+11	0.0	12500.0
2136.	CH2CHOOH+OH=CHCHOOH+H2O	1.80E+06	2.0	-1133.0
2137.	CH2CHOOH+H=CHCHOOH+H2	1.15E+06	2.5	4124.0
2138.	CH2CHOOH+CH3=CHCHOOH+CH4	5.42E+04	2.3	7287.0
2139.	CH2CHOOH+HO2=CHCHOOH+H2O2	1.12E+13	0.0	17686.0
2140.	C2H2+HO2=CHCHOOH	2.00E+11	0.0	12500.0
2141.	CHNH+HCO=NHCHCHO	7.00E+57	-13.8	17629.0
2142.	NCHCHO+HCO=NHCHCHO+CO	5.00E+12	0.0	0.0
2143.	NCHCHO+H2O2=NHCHCHO+HO2	1.21E+10	0.0	-596.0
2144.	NCHCHO+HO2=NHCHCHO+O2	6.00E+11	0.0	0.0
2145.	NHCHCHO=NCHCHO+H	3.50E+61	-13.9	129677.0

2146.	NHCHCHO+H=NCHCHO+H2	3.00E+07	2.0	13000.0
2147.	CH2NH+HCO=NHCHCHO+H	7.40E+14	-0.7	8420.0
2148.	CH2O+CHNH=NHCHCHO+H	7.40E+14	-0.7	8420.0
2149.	NHCHCHO+O=NCHCHO+OH	7.50E+06	1.9	3740.0
2150.	NHCHCHO+OH=NCHCHO+H2O	2.00E+07	2.0	5000.0
2151.	NHCHCHO+CH3=NCHCHO+CH4	2.00E+14	0.0	22800.0
2152.	NHCHCHO+C2H3=NCHCHO+C2H4	5.00E+13	0.0	22800.0
2153.	NHCHCHO+C3H3=NCHCHO+AC3H4	1.00E+13	0.0	22500.0
2154.	NHCHCHO+AC3H5=NCHCHO+C3H6	1.00E+13	0.0	22500.0
2155.	NHCH2CHO=NHCHCHO+H	1.27E+24	-4.8	23777.0
2156.	OCH2CHNH=NHCHCHO+H	1.27E+24	-4.8	23777.0
2157.	NHCH2CHO+H=NHCHCHO+H2	1.80E+12	0.0	0.0
2158.	OCH2CHNH+H=NHCHCHO+H2	1.80E+12	0.0	0.0
2159.	NHCH2CHO+O2=NHCHCHO+HO2	1.00E+11	0.0	0.0
2160.	OCH2CHNH+O2=NHCHCHO+HO2	1.00E+11	0.0	0.0
2161.	NHCH2CHO+CH3=NHCHCHO+CH4	1.10E+13	0.0	0.0
2162.	OCH2CHNH+CH3=NHCHCHO+CH4	1.10E+13	0.0	0.0

UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX G

MMH/RFNA FULL REACTION SET

The following is the full reaction set for MMH/RFNA combustion described in Chapter 10 and used in Chapter 11. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	HE	C	O	N	AR
1	H	G	0	1.008E+00	200	3500	1	0	0	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0	0	0
3	C	G	0	1.20E+01	200	3500	0	0	1	0	0	0
4	O	G	0	1.60E+01	200	3500	0	0	0	1	0	0
5	O2	G	0	3.20E+01	200	3500	0	0	0	2	0	0
6	OH	G	0	1.70E+01	200	6000	1	0	0	1	0	0
7	H2O	G	0	1.80E+01	200	3500	2	0	0	1	0	0
8	HO2	G	0	3.30E+01	200	3500	1	0	0	2	0	0
9	H2O2	G	0	3.40E+01	200	3500	2	0	0	2	0	0
10	CH	G	0	1.30E+01	200	6000	1	0	1	0	0	0
11	CH2	G	0	1.40E+01	200	6000	2	0	1	0	0	0
12	CH2SING	G	0	1.40E+01	200	6000	2	0	1	0	0	0
13	CH3	G	0	1.50E+01	200	6000	3	0	1	0	0	0
14	CH4	G	0	1.60E+01	200	3500	4	0	1	0	0	0
15	C2	G	0	2.40E+01	200	6000	0	0	2	0	0	0
16	CO	G	0	2.80E+01	200	3500	0	0	1	1	0	0
17	HCO	G	0	2.90E+01	200	3500	1	0	1	1	0	0
18	CH2O	G	0	3.00E+01	200	3500	2	0	1	1	0	0
19	CH2OH	G	0	3.10E+01	200	6000	3	0	1	1	0	0
20	CH3O	G	0	3.10E+01	200	6000	3	0	1	1	0	0
21	CH3OH	G	0	3.20E+01	200	3500	4	0	1	1	0	0
22	C2H	G	0	2.50E+01	200	3500	1	0	2	0	0	0
23	C2H2	G	0	2.60E+01	200	3500	2	0	2	0	0	0

24	H2CC	G	0	2.60E+01	200	6000	2	0	2	0	0	0
25	C2H3	G	0	2.70E+01	200	5000	3	0	2	0	0	0
26	C2H4	G	0	2.81E+01	200	3500	4	0	2	0	0	0
27	C2H5	G	0	2.91E+01	200	3500	5	0	2	0	0	0
28	C2H6	G	0	3.01E+01	200	3500	6	0	2	0	0	0
29	C3H2	G	0	3.80E+01	300	5000	2	0	3	0	0	0
30	C3H3	G	0	3.91E+01	200	6000	3	0	3	0	0	0
31	AR	G	0	3.99E+01	300	5000	0	0	0	0	0	1
32	AC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
33	PC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
34	C2O	G	0	4.00E+01	300	4000	0	0	2	1	0	0
35	HCCO	G	0	4.10E+01	300	4000	1	0	2	1	0	0
36	AC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
37	TC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
38	SC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
39	CH2CO	G	0	4.20E+01	200	3500	2	0	2	1	0	0
40	C3H6	G	0	4.21E+01	300	5000	6	0	3	0	0	0
41	CH3CO	G	0	4.30E+01	200	6000	3	0	2	1	0	0
42	CH2CHO	G	0	4.30E+01	300	5000	3	0	2	1	0	0
43	nC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
44	iC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
45	C2H4O	G	0	4.41E+01	300	5000	4	0	2	1	0	0
46	CH3CHO	G	0	4.41E+01	200	6000	4	0	2	1	0	0
47	C3H8	G	0	4.41E+01	300	3000	8	0	3	0	0	0
48	CO2	G	0	4.40E+01	200	3500	0	0	1	2	0	0
49	OCHO	G	0	4.50E+01	300	5000	1	0	1	2	0	0
50	C2H5O	G	0	4.51E+01	200	6000	5	0	2	1	0	0
51	CH3CHOH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
52	C2H4OH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
53	CH3OCH2	G	0	4.51E+01	300	5000	5	0	2	1	0	0
54	CH3OCH3	G	0	4.61E+01	270	3000	6	0	2	1	0	0

55	C2H5OH	G	0	4.61E+01	200	6000	6	0	2	1	0	0
56	CH3OCO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
57	CH3OCHO	G	0	6.01E+01	300	5000	4	0	2	2	0	0
58	CH3OCH2O	G	0	6.11E+01	300	5000	5	0	2	2	0	0
59	HOC2H4O2	G	0	7.71E+01	300	5000	5	0	2	3	0	0
60	C4H	G	0	4.91E+01	300	3000	1	0	4	0	0	0
61	C2H5OO	G	0	6.11E+01	300	5000	5	0	2	2	0	0
62	C2H3CO	G	0	5.51E+01	200	6000	3	0	3	1	0	0
63	C2H3CHO	G	0	5.61E+01	298	3000	4	0	3	1	0	0
64	C2H3CH2O	G	0	5.71E+01	300	3000	5	0	3	1	0	0
65	C4H2	G	0	5.01E+01	300	3000	2	0	4	0	0	0
66	iC4H3	G	0	5.11E+01	200	5000	3	0	4	0	0	0
67	nC4H3	G	0	5.11E+01	300	4000	3	0	4	0	0	0
68	C4H4	G	0	5.21E+01	300	3000	4	0	4	0	0	0
69	n-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
70	i-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
71	iiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
72	iiiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
73	C4H7	G	0	5.51E+01	300	3000	7	0	4	0	0	0
74	IC4H8	G	0	5.61E+01	300	5000	8	0	4	0	0	0
75	nC4H9	G	0	5.71E+01	200	6000	9	0	4	0	0	0
76	OCHCHO	G	0	5.80E+01	300	3000	2	0	2	2	0	0
77	C2H3OO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
78	N	G	0	1.40E+01	300	5000	0	0	0	0	1	0
79	NH	G	0	1.50E+01	200	6000	1	0	0	0	1	0
80	NH2	G	0	1.60E+01	300	5000	2	0	0	0	1	0
81	NH3	G	0	1.70E+01	300	5000	3	0	0	0	1	0
82	N2	G	0	2.80E+01	200	6000	0	0	0	0	2	0
83	NNH	G	0	2.90E+01	200	6000	1	0	0	0	2	0
84	N2H2	G	0	3.00E+01	300	5000	2	0	0	0	2	0
85	H2NN	G	0	3.00E+01	300	5000	2	0	0	0	2	0

86	N2H3	G	0	3.10E+01	300	5000	3	0	0	0	2	0
87	N2H4	G	0	3.20E+01	300	5000	4	0	0	0	2	0
88	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0
89	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
90	HON	G	0	3.10E+01	300	5000	1	0	0	1	1	0
91	HNOH	G	0	3.20E+01	200	6000	2	0	0	1	1	0
92	NH2O	G	0	3.20E+01	300	4000	2	0	0	1	1	0
93	NH2OH	G	0	3.30E+01	300	5000	3	0	0	1	1	0
94	HNNNH2	G	0	4.50E+01	300	5000	3	0	0	0	3	0
95	N2O	G	0	4.40E+01	300	5000	0	0	0	1	2	0
96	HNNO	G	0	4.50E+01	300	5000	1	0	0	1	2	0
97	NH2NO	G	0	4.60E+01	200	6000	2	0	0	1	2	0
98	NHNHO	G	0	4.60E+01	300	5000	2	0	0	1	2	0
99	NH2NHO	G	0	4.70E+01	300	5000	3	0	0	1	2	0
100	NO2	G	0	4.60E+01	200	6000	0	0	0	2	1	0
101	HONO	G	0	4.70E+01	200	6000	1	0	0	2	1	0
102	HNO2	G	0	4.70E+01	300	4000	1	0	0	2	1	0
103	HNOO	G	0	4.70E+01	300	5000	1	0	0	2	1	0
104	HONHO	G	0	4.80E+01	300	5000	2	0	0	2	1	0
105	NH2NO2	G	0	6.20E+01	200	6000	2	0	0	2	2	0
106	NO3	G	0	6.20E+01	200	6000	0	0	0	3	1	0
107	HNO3	G	0	6.30E+01	200	6000	1	0	0	3	1	0
108	N2O4	G	0	9.20E+01	200	6000	0	0	0	4	2	0
109	HE	G	0	4.00E+00	200	6000	0	1	0	0	0	0
110	CN	G	0	2.60E+01	200	6000	0	0	1	0	1	0
111	HCN	G	0	2.70E+01	300	4000	1	0	1	0	1	0
112	HNC	G	0	2.70E+01	300	5000	1	0	1	0	1	0
113	CHNH	G	0	2.80E+01	300	4000	2	0	1	0	1	0
114	NCH2	G	0	2.80E+01	300	4000	2	0	1	0	1	0
115	CH2NH	G	0	2.90E+01	300	5000	3	0	1	0	1	0
116	CH3N	G	0	2.90E+01	200	5000	3	0	1	0	1	0

117	CH3NH	G	0	3.01E+01	300	5000	4	0	1	0	1	0
118	CH2NH2	G	0	3.01E+01	300	5000	4	0	1	0	1	0
119	CH3NH2	G	0	3.11E+01	300	5000	5	0	1	0	1	0
120	NCN	G	0	4.00E+01	300	4000	0	0	1	0	2	0
121	CHCNH	G	0	4.00E+01	298	3000	2	0	2	0	1	0
122	CH2CN	G	0	4.00E+01	200	6000	2	0	2	0	1	0
123	HCNN	G	0	4.10E+01	300	5000	1	0	1	0	2	0
124	CH2CNH	G	0	4.11E+01	200	5000	3	0	2	0	1	0
125	CH2CHN	G	0	4.11E+01	298	3000	3	0	2	0	1	0
126	CH2CHN(S)	G	0	4.11E+01	298	3000	3	0	2	0	1	0
127	CHCNH2	G	0	4.11E+01	298	3000	3	0	2	0	1	0
128	CH3CN	G	0	4.11E+01	200	6000	3	0	2	0	1	0
129	c-C2H3N	G	0	4.11E+01	298	3000	3	0	2	0	1	0
130	CH2NN	G	0	4.20E+01	200	6000	2	0	1	0	2	0
131	NCO	G	0	4.20E+01	300	5000	0	0	1	1	1	0
132	CH3NCH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
133	CH3CHN	G	0	4.21E+01	298	3000	4	0	2	0	1	0
134	CH3CNH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
135	CH2CNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
136	CHCHNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
137	CH2NCH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
138	CH2CHNH	G	0	4.21E+01	200	5000	4	0	2	0	1	0
139	CH3CHNH	G	0	4.31E+01	298	3000	5	0	2	0	1	0
140	CH3NCH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
141	CH2CHNH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
142	CH3CH2NH	G	0	4.41E+01	298	3000	6	0	2	0	1	0
143	CH3CHNH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
144	CH2CH2NH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
145	CH3CH2NH2	G	0	4.51E+01	298	3000	7	0	2	0	1	0
146	CH3NHNH2	G	0	4.61E+01	298	6000	6	0	1	0	2	0
147	CH2NHNH2	G	0	4.51E+01	200	5000	5	0	1	0	2	0

148	CH3NNH2	G	0	4.51E+01	200	6000	5	0	1	0	2	0
149	CH3NHNH	G	0	4.51E+01	200	5000	5	0	1	0	2	0
150	CH3NN	G	0	4.30E+01	200	6000	3	0	1	0	2	0
151	CH2NNH2	G	0	4.41E+01	200	5000	4	0	1	0	2	0
152	HCNO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
153	HNCO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
154	HOCN	G	0	4.30E+01	300	5000	1	0	1	1	1	0
155	H2NCO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
156	CH3NNH	G	0	4.41E+01	200	6000	4	0	1	0	2	0
157	H2NCHO	G	0	4.50E+01	200	6000	3	0	1	1	1	0
158	CH3NCH3	G	0	4.41E+01	298	3000	6	0	2	0	1	0
159	CH3NHCH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
160	CH2NO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
161	HOCO	G	0	4.50E+01	300	4000	1	0	1	2	0	0
162	CH3NO	G	0	4.50E+01	300	4000	3	0	1	1	1	0
163	CH3NHCH3	G	0	4.51E+01	298	3000	7	0	2	0	1	0
164	NCCN	G	0	5.20E+01	300	5000	0	0	2	0	2	0
165	CHCHNCH2	G	0	5.41E+01	200	5000	4	0	3	0	1	0
166	CH2CHNCH2	G	0	5.51E+01	200	5000	5	0	3	0	1	0
167	NCNO	G	0	5.60E+01	300	4000	0	0	1	1	2	0
168	NCHCHO	G	0	5.60E+01	200	5000	2	0	2	1	1	0
169	CH2NHCHCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
170	CH2CH2NCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
171	NHCH2CHO	G	0	5.81E+01	200	5000	4	0	2	1	1	0
172	OCH2CHNH	G	0	5.81E+01	200	5000	4	0	2	1	1	0
173	CH3NNCH3	G	0	5.81E+01	300	4000	6	0	2	0	2	0
174	H2CNO2	G	0	6.00E+01	300	4000	2	0	1	2	1	0
175	CH3NO2	G	0	6.10E+01	300	4000	3	0	1	2	1	0
176	CH3ONO	G	0	6.10E+01	300	4000	3	0	1	2	1	0
177	CH3ONO2	G	0	7.70E+01	300	4000	3	0	1	3	1	0

(k = A T**b exp(-E/RT))

	REACTIONS CONSIDERED			A	b	E
1.	2O+M=O2+M			6.16E+15	-0.5	0.0
	H2O	Enhanced by	1.200E+01			
	H2	Enhanced by	2.500E+00			
	AR	Enhanced by	0.000E+00			
2.	2O+AR=O2+AR			1.89E+13	0.0	-1790.0
3.	O+H+M=OH+M			4.71E+18	-1.0	0.0
	H2O	Enhanced by	1.200E+01			
	H2	Enhanced by	2.500E+00			
	AR	Enhanced by	7.500E-01			
4.	H2+M=2H+M			4.58E+19	-1.4	104380.0
	H2O	Enhanced by	1.200E+01			
	H2	Enhanced by	2.500E+00			
	AR	Enhanced by	0.000E+00			
5.	H2+AR=2H+AR			5.84E+18	-1.1	104380.0
6.	H+OH+M=H2O+M			2.21E+22	-2.0	0.0
	H2O	Enhanced by	1.200E+01			
	H2	Enhanced by	2.500E+00			
	AR	Enhanced by	0.000E+00			
7.	H+OH+AR=H2O+AR			8.41E+21	-2.0	0.0
8.	H2O2(+M)=2OH(+M)			2.95E+14	0.0	48400.0
	Low pressure limit:	0.12000E+18	0.00000E+00	0.45500E+05		
	H2O	Enhanced by	1.200E+01			
	H2	Enhanced by	2.500E+00			
	AR	Enhanced by	1.600E-01			
9.	H2O+O=OH+OH			2.97E+06	2.0	13400.0
10.	O+H2=H+OH			5.08E+04	2.7	6290.0
11.	OH+H2=H+H2O			2.16E+08	1.5	3430.0
12.	H+O2(+M)=HO2(+M)			1.48E+12	0.6	0.0

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    Low pressure limit:  0.35000E+17 -0.41000E+00 -0.11200E+04
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    5.000E-02
13. H+O2=O+OH                                     4.49E+08    1.3    16191.0
    Declared duplicate reaction...
14. H+O2=O+OH                                     2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
15. O+HO2=OH+O2                                   3.25E+13    0.0        0.0
16. H+HO2=O2+H2                                   1.66E+13    0.0      820.0
17. H+HO2=2OH                                     7.08E+13    0.0      300.0
18. OH+HO2=O2+H2O                                 4.64E+13    0.0     -500.0
19. 2HO2=O2+H2O2                                  1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
20. 2HO2=O2+H2O2                                  4.20E+14    0.0    11980.0
    Declared duplicate reaction...
21. O+H2O2=OH+HO2                                 9.55E+06    2.0     3970.0
22. H+H2O2=HO2+H2                                 4.82E+13    0.0     7950.0
23. H+H2O2=OH+H2O                                 2.41E+13    0.0     3970.0
24. OH+H2O2=HO2+H2O                               1.00E+12    0.0        0.0
    Declared duplicate reaction...
25. OH+H2O2=HO2+H2O                               5.80E+14    0.0     9560.0
    Declared duplicate reaction...
26. O+CO(+M)=CO2(+M)                              1.80E+10    0.0     2385.0
    Low pressure limit:  0.60200E+15  0.00000E+00  0.30000E+04
    H2              Enhanced by    2.000E+00
    O2              Enhanced by    6.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    3.500E+00
    C2H6            Enhanced by    3.000E+00
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    AR              Enhanced by    5.000E-01
27. O2+CO=O+CO2                                   2.50E+12    0.0    47800.0
28. H2+CO(+M)=CH2O(+M)                            4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
29. OH+CO=H+CO2                                   4.10E+04    2.1    -1578.0
30. HO2+CO=OH+CO2                                 1.50E+14    0.0    23600.0
31. O+HCO=OH+CO                                   3.00E+13    0.0        0.0
32. O+HCO=H+CO2                                   3.00E+13    0.0        0.0
33. H+HCO(+M)=CH2O(+M)                            1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
34. H+HCO=H2+CO                                   7.30E+13    0.0        0.0
35. OH+HCO=H2O+CO                                 3.00E+13    0.0        0.0
36. HCO+M=H+CO+M                                  1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
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    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
37. HCO+O2=HO2+CO                                 4.22E+12    0.0        0.0
38. HCO+HO2=CO2+OH+H                              3.00E+13    0.0        0.0
39. O+CH2O=OH+HCO                                 1.81E+13    0.0     3078.0
40. O2+CH2O=HO2+HCO                               2.05E+13    0.0    38920.0
41. H+CH2O=HCO+H2                                 5.18E+07    1.7     1834.0
42. H+CH2O(+M)=CH2OH(+M)                          5.40E+11    0.5     3600.0
    Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
    TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
43. H+CH2O(+M)=CH3O(+M)                           5.40E+11    0.5     2600.0
    Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
    TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
44. OH+CH2O=HCO+H2O                               3.43E+09    1.2     -447.0
45. HO2+CH2O=HCO+H2O2                             1.47E+13    0.0    15200.0
46. O+CH2OH=OH+CH2O                               4.20E+13    0.0        0.0
47. H+CH2OH=H2+CH2O                               6.00E+12    0.0        0.0
48. H+CH2OH=OH+CH3                                9.63E+13    0.0        0.0
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49.	OH+CH2OH=H2O+CH2O	2.40E+13	0.0	0.0
50.	CH2OH+O2=HO2+CH2O	2.41E+14	0.0	5017.0
	Declared duplicate reaction...			
51.	CH2OH+O2=HO2+CH2O	1.51E+15	-1.0	0.0
	Declared duplicate reaction...			
52.	CH2OH+HO2=CH2O+H2O2	1.20E+13	0.0	0.0
53.	CH2OH+HCO=CH3OH+CO	1.20E+14	0.0	0.0
54.	CH2OH+HCO=CH2O+CH2O	1.80E+14	0.0	0.0
55.	2CH2OH=CH3OH+CH2O	3.00E+12	0.0	0.0
56.	CH2OH+CH3O=CH3OH+CH2O	2.40E+13	0.0	0.0
57.	O+CH3O=OH+CH2O	6.00E+12	0.0	0.0
58.	H+CH3O=H2+CH2O	2.00E+13	0.0	0.0
59.	H+CH3O=OH+CH3	3.20E+13	0.0	0.0
60.	OH+CH3O=H2O+CH2O	1.80E+13	0.0	0.0
61.	CH3O+O2=HO2+CH2O	9.03E+13	0.0	11980.0
	Declared duplicate reaction...			
62.	CH3O+O2=HO2+CH2O	2.20E+10	0.0	1748.0
	Declared duplicate reaction...			
63.	CH3O+HO2=CH2O+H2O2	3.00E+11	0.0	0.0
64.	CH3O+CO=CH3+CO2	1.57E+13	0.0	11800.0
65.	CH3O+HCO=CH3OH+CO	9.00E+13	0.0	0.0
66.	2CH3O=CH3OH+CH2O	6.00E+13	0.0	0.0
67.	O+CH3OH=OH+CH2OH	3.88E+05	2.5	3080.0
68.	H+CH3OH=CH2OH+H2	1.44E+13	0.0	6095.0
69.	H+CH3OH=CH3O+H2	3.60E+12	0.0	6095.0
70.	OH+CH3OH=CH2OH+H2O	7.10E+06	1.8	-596.0
71.	OH+CH3OH=CH3O+H2O	1.00E+06	2.1	496.5
72.	CH3+CH3OH=CH2OH+CH4	3.19E+01	3.2	7172.0
73.	O2+CH3OH=CH2OH+HO2	2.05E+13	0.0	44900.0
74.	HCO+CH3OH=CH2OH+CH2O	9.63E+03	2.9	13110.0
75.	HO2+CH3OH=CH2OH+H2O2	3.98E+13	0.0	19400.0
76.	CH3O+CH3OH=CH2OH+CH3OH	3.00E+11	0.0	4060.0

77. CH3OH(+M)=CH3+OH(+M) 1.90E+16 0.0 91730.0

Low pressure limit: 0.29500E+45 -0.73500E+01 0.95460E+05

TROE centering: 0.41400E+00 0.27900E+03 0.54590E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

78. CH3OH(+M)=CH2OH+H(+M) 2.69E+16 -0.1 98940.0

Low pressure limit: 0.23400E+41 -0.63300E+01 0.10310E+06

TROE centering: 0.77300E+00 0.69300E+03 0.53330E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

79. O+CH4=OH+CH3 1.02E+09 1.5 8600.0

80. H+CH4=CH3+H2 6.60E+08 1.6 10840.0

81. OH+CH4=CH3+H2O 1.00E+08 1.6 3120.0

82. CH+CH4=H+C2H4 6.00E+13 0.0 0.0

83. CH2SING+CH4=2CH3 1.60E+13 0.0 -570.0

84. CH2+CH4=2CH3 2.46E+06 2.0 8270.0

85. O+CH3=H+CH2O 5.06E+13 0.0 0.0

86. O+CH3=H+H2+CO 3.37E+13 0.0 0.0

87. H+CH3(+M)=CH4(+M) 1.39E+16 -0.5 536.0

Low pressure limit: 0.26200E+34 -0.47600E+01 0.24400E+04

TROE centering: 0.78300E+00 0.74000E+02 0.29410E+04 0.69640E+04

H2 Enhanced by 2.000E+00

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     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
  88. OH+CH3=CH2+H2O                                  5.60E+07    1.6     5420.0
  89. OH+CH3=CH2SING+H2O                              6.44E+17   -1.3     1417.0
  90. HO2+CH3=O2+CH4                                  1.00E+12    0.0        0.0
  91. HO2+CH3=OH+CH3O                                 2.00E+13    0.0        0.0
  92. CH+CH3=H+C2H3                                   3.00E+13    0.0        0.0
  93. CH2SING+CH3=H+C2H4                              1.20E+13    0.0     -570.0
  94. CH3+O2=O+CH3O                                   3.56E+13    0.0    30480.0
  95. CH3+O2=OH+CH2O                                  2.31E+12    0.0    20315.0
  96. CH3+H2O2=HO2+CH4                                2.45E+04    2.5     5180.0
  97. 2CH3(+M)=C2H6(+M)                               6.77E+16   -1.2      654.0
     Low pressure limit:  0.34000E+42 -0.70300E+01  0.27630E+04
     TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
  98. 2CH3=H+C2H5                                     6.84E+12    0.1    10600.0
  99. CH3+HCO=CH4+CO                                  1.21E+14    0.0        0.0
 100. CH3+CH2O=HCO+CH4                                3.32E+03    2.8     5860.0
 101. CH2+CH3=H+C2H4                                  4.00E+13    0.0        0.0
 102. O+CH2=H+HCO                                     8.00E+13    0.0        0.0
 103. O+CH2SING=H2+CO                                 1.50E+13    0.0        0.0
 104. O+CH2SING=H+HCO                                 1.50E+13    0.0        0.0
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105. H+CH2(+M)=CH3(+M)                              6.00E+14    0.0        0.0
     Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
     TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
106. H+CH2SING=CH+H2                               3.00E+13    0.0        0.0
107. OH+CH2=H+CH2O                                 2.00E+13    0.0        0.0
108. OH+CH2=CH+H2O                                 1.13E+07    2.0     3000.0
109. OH+CH2SING=H+CH2O                             3.00E+13    0.0        0.0
110. HO2+CH2=OH+CH2O                               2.00E+13    0.0        0.0
111. CH+CH2=H+C2H2                                 4.00E+13    0.0        0.0
112. CH2+O2=OH+H+CO                                5.00E+12    0.0     1500.0
113. CH2+O2=CO2+2H                                 5.80E+12    0.0     1500.0
114. CH2+O2=O+CH2O                                 2.40E+12    0.0     1500.0
115. CH2+H2=H+CH3                                  5.00E+05    2.0     7230.0
116. 2CH2=H2+C2H2                                  1.60E+15    0.0    11944.0
117. 2CH2=H+H+C2H2                                 2.00E+14    0.0    10989.0
118. CH2SING+CO=CH2+CO                             9.00E+12    0.0        0.0
119. CH2SING+AR=CH2+AR                             9.00E+12    0.0      600.0
120. CH2SING+CO2=CH2+CO2                           7.00E+12    0.0        0.0
121. CH2SING+CO2=CO+CH2O                           1.40E+13    0.0        0.0
122. CH2+CO(+M)=CH2CO(+M)                          8.10E+11    0.5     4510.0
     Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
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     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
123. CH2SING+O2=H+OH+CO                              2.80E+13    0.0        0.0
124. CH2SING+O2=CO+H2O                               1.20E+13    0.0        0.0
125. CH2SING+H2=CH3+H                                7.00E+13    0.0        0.0
126. CH2SING+H2O(+M)=CH3OH(+M)                       4.82E+17   -1.2     1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
127. CH2SING+H2O=CH2+H2O                             3.00E+13    0.0        0.0
128. CH2SING+H2O=H2+CH2O                             6.82E+10    0.2     -935.0
129. O+CH=H+CO                                       5.70E+13    0.0        0.0
130. OH+CH=H+HCO                                     3.00E+13    0.0        0.0
131. CH+O2=O+HCO                                     6.71E+13    0.0        0.0
132. CH+H2=H+CH2                                     1.08E+14    0.0     3110.0
133. CH+H2O=H+CH2O                                   5.71E+12    0.0     -755.0
134. CH+CO(+M)=HCCO(+M)                              5.00E+13    0.0        0.0
     Low pressure limit:  0.26900E+29 -0.37400E+01  0.19360E+04
     TROE centering:      0.57570E+00  0.23700E+03  0.16520E+04  0.50690E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
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135. CH+CO2=HCO+CO                                    1.90E+14    0.0    15792.0
136. CH+CH2O=H+CH2CO                                  9.46E+13    0.0     -515.0
137. CH+HCCO=CO+C2H2                                  5.00E+13    0.0        0.0
138. O+C2H6=OH+C2H5                                   3.00E+07    2.0     5115.0
139. H+C2H6=C2H5+H2                                   5.40E+02    3.5     5210.0
140. OH+C2H6=C2H5+H2O                                 7.26E+06    2.0      864.0
141. CH3+C2H6=C2H5+CH4                                5.50E-01    4.0     8300.0
142. CH2SING+C2H6=CH3+C2H5                            4.00E+13    0.0     -550.0
143. C2H6+O2=C2H5+HO2                                 4.04E+13    0.0    50872.0
144. C2H6+CH2OH=CH3OH+C2H5                            1.99E+02    3.0    13976.0
145. C2H6+CH3O=CH3OH+C2H5                             2.41E+11    0.0     7094.0
146. C2H6+C2H=C2H2+C2H5                               3.61E+12    0.0        0.0
147. C2H6+C2H3=C2H4+C2H5                              6.01E+02    3.3    10502.0
148. C2H6+CH3CO=CH3CHO+C2H5                           1.81E+04    2.8    17527.0
149. C2H6+HCO=CH2O+C2H5                               4.70E+04    2.7    18235.0
150. O+C2H5=CH3+CH2O                                  2.24E+13    0.0        0.0
151. O+C2H5=H+CH3CHO                                  1.10E+14    0.0        0.0
152. H+C2H5=H2+C2H4                                   2.00E+12    0.0        0.0
153. H+C2H5(+M)=C2H6(+M)                              5.21E+17   -1.0     1580.0
     Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
     TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
154. C2H5+O2=HO2+C2H4                                 1.92E+07    1.0    -2035.0
155. C2H5+HO2=C2H5O+OH                                3.00E+13    0.0        0.0
156. C2H5+HO2=C2H4+H2O2                               3.01E+11    0.0        0.0
157. C2H5+OH=C2H4+H2O                                 2.41E+13    0.0        0.0
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158. C2H5+CH3=CH4+C2H4                                1.13E+12   -0.5        0.0
159. CH3+C2H5(+M)=C3H8(+M)                            9.60E+14   -0.5        0.0
     Low pressure limit:  0.68000E+62 -0.13420E+02  0.60000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.14339E+04  0.53288E+04
160. C2H5+CH2OH=C2H4+CH3OH                            2.41E+12    0.0        0.0
161. C2H5+CH2OH=C2H6+CH2O                             2.41E+12    0.0        0.0
162. C2H5+CH3O=C2H6+CH2O                              2.41E+13    0.0        0.0
163. C2H5+C2H=C2H2+C2H4                               1.81E+12    0.0        0.0
164. CH2+C2H5=C2H4+CH3                                1.81E+13    0.0        0.0
165. CH2SING+C2H5=C2H4+CH3                            9.00E+12    0.0        0.0
166. C2H5+CH2SING=C3H6+H                              9.00E+12    0.0        0.0
167. C2H5+H2O2=C2H6+HO2                               8.73E+09    0.0      974.0
168. H+C2H4(+M)=C2H5(+M)                              1.37E+09    1.5     1355.0
     Low pressure limit:  0.20260E+40 -0.66420E+01  0.57690E+04
     TROE centering:     -0.56900E+00  0.29900E+03 -0.91470E+04  0.15240E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
169. H+C2H4=C2H3+H2                                   1.12E+07    2.1    13366.0
170. OH+C2H4=C2H3+H2O                                 1.31E-01    4.2     -860.0
171. OH+C2H4=CH3+CH2O                                 3.19E+01    2.7    -1172.0
172. OH+C2H4=CH3CHO+H                                 8.73E-05    4.6     -618.0
173. CH3+C2H4=C2H3+CH4                                2.27E+05    2.0     9200.0
174. CH3+C2H4(+M)<=>nC3H7(+M)                         2.55E+06    1.6     5700.0
     Low pressure limit:  0.30000E+64 -0.14600E+02  0.18170E+05
     TROE centering:      0.18940E+00  0.27700E+03  0.87480E+04  0.78910E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
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     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
175. C2H4(+M)=H2+C2H2(+M)                          8.00E+12    0.4    88770.0
     Low pressure limit:  0.15800E+52 -0.93000E+01  0.97800E+05
     TROE centering:      0.73450E+00  0.18000E+03  0.10350E+04  0.54170E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
176. C2H4+CH2SING=AC3H5+H                          4.53E+13    0.0     -556.0
177. C2H4+HO2=C2H4O+OH                             6.03E+09    0.0     7949.0
178. C2H4+O=H+CH2CHO                               7.33E+07    1.6     1260.0
179. C2H4+O=CH3+HCO                                1.13E+08    1.6     1020.0
180. C2H4+O=C2H3+OH                                2.15E+06    2.5    11900.0
181. C2H4+O2=C2H3+HO2                              4.22E+13    0.0    60800.0
182. C2H4+CO=C2H3+HCO                              1.51E+14    0.0    90616.0
183. C2H4+C2H=C4H4+H                               1.21E+13    0.0        0.0
184. C2H4+C2H2=C2H3+C2H3                           2.41E+13    0.0    68360.0
185. C2H4+C2H4=C2H5+C2H3                           4.82E+14    0.0    71539.0
186. H+C2H3(+M)=C2H4(+M)                           6.08E+12    0.3      280.0
     Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
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     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
187. H+C2H2(+M)=C2H3(+M)                          1.71E+10    1.3     2709.0
     Low pressure limit:  0.63480E+32 -0.46639E+01  0.37800E+04
     TROE centering:      0.00000E+00  0.78784E+05 -0.10210E+05  0.10000E-29
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
188. H+C2H3=H2+C2H2                               9.64E+13    0.0        0.0
189. OH+C2H3=H2O+C2H2                             5.00E+12    0.0        0.0
190. C2H3+O2=C2H2+HO2                             1.34E+06    1.6     -383.0
     Declared duplicate reaction...
191. C2H3+O2=C2H2+HO2                             1.37E+02    3.4     3663.0
     Declared duplicate reaction...
192. C2H3+O2=HCO+CH2O                             9.33E+13   -0.7      268.7
193. C2H3+O2=H+CO+CH2O                            2.19E+14   -0.7      268.7
194. C2H3+O2=CH2CHO+O                             7.52E+08    1.0     -137.4
195. C2H3+HO2=OH+CH2CO+H                          3.01E+13    0.0        0.0
196. C2H3+CH3=C2H2+CH4                            3.92E+11    0.0        0.0
197. C2H3+O=CH2CO+H                               1.00E+14    0.0        0.0
198. C2H3OO+H=CH2CHO+OH                           1.00E+14    0.0        0.0
199. C2H3OO+CH2=CH2CHO+CH2O                       2.00E+13    0.0        0.0
200. C2H3OO+OH=CH2CHO+HO2                         2.00E+13    0.0        0.0
201. C2H3OO+O=CH2CHO+O2                           2.00E+13    0.0        0.0
202. C2H3+CH2OH=C2H4+CH2O                         3.01E+13    0.0        0.0
203. C2H3+CH3O=C2H4+CH2O                          2.41E+13    0.0        0.0
204. C2H3+CH3OH=C2H4+CH3O                         1.44E+01    3.1     6935.0
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205. C2H3+CH3OH=C2H4+CH2OH                            3.19E+01    3.2     7172.0
206. C2H3+CO=C2H3CO                                   1.51E+11    0.0     4809.0
207. C2H3+C2H=C4H4                                    1.00E+14    0.0        0.0
208. C2H3+C2H=C2H2+C2H2                               9.64E+11    0.0        0.0
209. C2H3+CH3CO=C2H3CO+CH3                            1.81E+13    0.0        0.0
210. C2H5+C2H3=AC3H5+CH3                              8.00E+25   -3.5    11775.0
211. C2H3+C2H5(+M)=IC4H8(+M)                          1.50E+13    0.0        0.0
     Low pressure limit:  0.15500E+57 -0.11790E+02  0.89845E+04
     TROE centering:      0.19800E+00  0.22779E+04  0.60000E+05  0.57232E+04
212. C2H3+C2H5=C2H2+C2H6                              4.82E+11    0.0        0.0
213. C2H3+CH2SING=C2H2+CH3                            1.81E+13    0.0        0.0
214. C2H3+CH2=C2H2+CH3                                1.81E+13    0.0        0.0
215. C2H3+H2O2=C2H4+HO2                               1.21E+10    0.0     -596.0
216. C2H3+CH2O=C2H4+HCO                               5.43E+03    2.8     5862.0
217. C2H3+CH2=AC3H4+H                                 3.00E+13    0.0        0.0
218. C2H3+C2H3=i-C4H5+H                               1.50E+30   -5.0    13000.0
219. C2H3+C2H3=n-C4H5+H                               1.10E+24   -3.3    12400.0
220. H2CC+C2H2(+M)=C4H4(+M)                           3.50E+05    2.1    -2400.0
     Low pressure limit:  0.14000E+61 -0.12599E+02  0.74170E+04
     TROE centering:      0.98000E+00  0.56000E+02  0.58000E+03  0.41640E+04
     H2              Enhanced by    2.000E+00
     CH4             Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     C2H2            Enhanced by    3.000E+00
     CO              Enhanced by    1.500E+00
     C2H4            Enhanced by    3.000E+00
     C2H6            Enhanced by    3.000E+00
     CO2             Enhanced by    2.000E+00
221. C2H2(+M)=H2CC(+M)                                8.00E+14   -0.5    50750.0
     Low pressure limit:  0.24500E+16 -0.64000E+00  0.49700E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
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     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H4            Enhanced by    2.500E+00
222. H2CC+C2H4=iiiC4H6                              1.00E+12    0.0        0.0
223. H2CC+O2=CH2+CO2                                1.00E+13    0.0        0.0
224. H2CC+H=C2H2+H                                  1.00E+14    0.0        0.0
225. H2CC+OH=CH2CO+H                                2.00E+13    0.0        0.0
226. C2H2+O=C2H+OH                                  4.60E+19   -1.4    28950.0
227. C2H2+O=CH2+CO                                  2.35E+08    1.4     2204.5
228. C2H2+O=HCCO+H                                  9.40E+08    1.4     2204.5
229. OH+C2H2=C2H+H2O                                2.63E+06    2.1    17060.0
230. OH+C2H2=H+CH2CO                                1.52E+04    2.3     -292.0
231. OH+C2H2=CH3+CO                                 4.37E+06    1.4      227.0
232. C2H2+CH=C3H2+H                                 1.10E+13    0.0        0.0
233. C2H2+CH2=C3H3+H                                1.20E+13    0.0     6620.0
234. C2H2+CH3=C2H+CH4                               1.81E+11    0.0    17289.0
235. C2H2+O2=2HCO                                   1.00E+12    0.0    28000.0
236. C2H2+CH2OH=C2H3+CH2O                           7.23E+11    0.0     9004.0
237. C2H2+CO=C2H+HCO                                4.82E+14    0.0   106713.0
238. C2H2+C2H=C4H2+H                                3.00E+13    0.0        0.0
239. C2H2+C2H(+M)=nC4H3(+M)                         8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
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     C2H4            Enhanced by    2.500E+00
240. C2H2+C2H(+M)=iC4H3(+M)                          8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
241. C2H2+CH2SING=C3H3+H                             3.42E+15   -0.6     -230.7
242. C2H2+CH2SING=CH2+C2H2                           8.55E+14   -0.6     -230.7
243. HCCO+C2H2=C3H3+CO                               1.00E+11    0.0     3000.0
244. C2H2+C2H3=n-C4H5                                1.10E+32   -7.3     6200.0
245. C2H2+C2H3=i-C4H5                                2.10E+36   -8.8     9100.0
246. C2H3+C2H2=C4H4+H                                5.00E+14   -0.7     6700.0
247. O+C2H=CH+CO                                     1.00E+13    0.0        0.0
248. H+C2H(+M)=C2H2(+M)                              1.00E+17   -1.0        0.0
     Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
     TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
249. OH+C2H=H+HCCO                                   2.00E+13    0.0        0.0
250. C2H+O2=HCO+CO                                   1.00E+13    0.0     -775.0
251. C2H+H2=H+C2H2                                   5.68E+10    0.9     1993.0
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252.	C2H+HO2=HCCO+OH	1.81E+13	0.0	0.0
253.	C2H+CH3=C3H3+H	2.41E+13	0.0	0.0
254.	C2H+O2=HCCO+O	6.03E+11	0.0	0.0
255.	C2H+CH2OH=C2H2+CH2O	3.61E+13	0.0	0.0
256.	C2H+CH2OH=C3H3+OH	1.21E+13	0.0	0.0
257.	C2H+CH3OH=C2H2+CH2OH	6.03E+12	0.0	0.0
258.	C2H+CH3O=CH2O+C2H2	2.41E+13	0.0	0.0
259.	C2H+CH3OH=C2H2+CH3O	1.21E+12	0.0	0.0
260.	C2H+CH2=CH+C2H2	1.81E+13	0.0	0.0
261.	C2H+CH2SING=C2H2+CH	1.81E+13	0.0	0.0
262.	O+HCCO=H+2CO	1.00E+14	0.0	0.0
263.	H+HCCO=CH2SING+CO	5.00E+13	0.0	0.0
264.	CH2+HCCO=C2H3+CO	3.00E+13	0.0	0.0
265.	HCCO+O2=CO2+CO+H	4.78E+12	-0.1	1150.0
266.	HCCO+O2=CO+CO+OH	1.91E+11	0.0	1023.0
267.	HCCO+O2=O+CO+HCO	2.18E+02	2.7	3541.0
268.	2HCCO=2CO+C2H2	1.00E+13	0.0	0.0
269.	HCCO+CH3=C2H4+CO	5.00E+13	0.0	0.0
270.	O+CH2CO=OH+HCCO	1.00E+13	0.0	8000.0
271.	O+CH2CO=CH2+CO2	1.75E+12	0.0	1350.0
272.	H+CH2CO=HCCO+H2	5.00E+13	0.0	8000.0
273.	CH2CO+H=CH3+CO	7.77E+08	1.4	2780.0
274.	CH2CHO=H+CH2CO	2.48E+27	-5.2	44304.0
275.	CH2CHO=CH3+CO	1.54E+31	-6.3	42478.0
276.	OH+CH2CO=HCCO+H2O	7.50E+12	0.0	2000.0
277.	CH2CO+OH=CH2OH+CO	1.00E+13	0.0	0.0
278.	CH3CO=CH3+CO	2.40E+15	-2.0	14805.0
279.	CH2CHO+H=CH3CHO	6.40E+35	-7.6	5215.0
280.	CH2CHO+H=CH3+HCO	4.99E+14	-0.3	912.0
281.	CH2CHO+O=CH2O+HCO	5.00E+13	0.0	0.0
282.	CH2CHO+OH=H2O+CH2CO	1.20E+13	0.0	0.0
283.	CH2CHO+OH=HCO+CH2OH	3.01E+13	0.0	0.0

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284. CH2CHO+O2=CH2CO+HO2                              1.57E+11    0.0        0.0
285. CH3CHO=CH3+HCO                                   9.59E+14    0.0    74180.0
286. CH3CHO+O2=CH3CO+HO2                              2.00E+13    0.5    42200.0
287. CH3CHO+H=CH2CHO+H2                               4.10E+09    1.2     2405.0
288. CH3CHO+OH=CH3CO+H2O                              2.35E+10    0.7    -1113.0
289. CH3CHO+O=CH2CHO+OH                               5.85E+12    0.0     1808.0
290. CH3CHO+HO2=CH3CO+H2O2                            1.70E+12    0.0    10700.0
291. CH3CHO+CH3=CH3CO+CH4                             1.70E+12    0.0     8440.0
292. CH3CHO+HCO=CH3CO+CH2O                            7.80E+13    0.0     8440.0
293. C2H5+O2(+M)=C2H5OO(+M)                           2.02E+10    1.0      -63.6
     Low pressure limit:  0.84900E+30 -0.42900E+01  0.22000E+03
     TROE centering:      0.10300E+00  0.60100E+03  0.10000E-09
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
294. C2H5OO(+M)=C2H4+HO2(+M)                          7.14E+04    2.3    27955.0
     Low pressure limit:  0.83100E+22 -0.65100E+00  0.22890E+05
     TROE centering:      0.00000E+00  0.10600E+03  0.10600E+03
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
295. C2H5OO+HO2=C2H5O+OH+O2                           1.75E+10    0.0    -3275.0
296. C2H5O=CH3+CH2O                                   1.00E+15    0.0    21523.0
297. C2H5O=CH3CHO+H                                   2.00E+14    0.0    23215.0
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298.	C2H5O+O2=CH3CHO+HO2	6.03E+10	0.0	1643.0
299.	C2H4O+O2=CH2CHO+HO2	4.00E+13	0.0	61500.0
300.	C2H4O+H=CH2CHO+H2	2.00E+13	0.0	8300.0
301.	C2H4O+H=C2H3+H2O	5.00E+09	0.0	5000.0
302.	C2H4O+H=C2H4+OH	9.51E+10	0.0	5000.0
303.	C2H4O+OH=CH2CHO+H2O	4.79E+13	0.0	5955.0
304.	C2H4O+O=CH2CHO+OH	1.91E+12	0.0	5250.0
305.	C2H4O+HO2=CH2CHO+H2O2	4.00E+12	0.0	17000.0
306.	C2H4O=CH3CHO	6.00E+13	0.0	57167.0
307.	C2H4O=CH3+HCO	4.90E+13	0.0	57167.0
308.	C2H4O=CH4+CO	1.21E+13	0.0	57167.0
309.	C3H8+H=nC3H7+H2	1.30E+06	2.5	6756.0
310.	C3H8+H=iC3H7+H2	1.30E+06	2.4	4471.0
311.	C3H8+O=nC3H7+OH	1.90E+05	2.7	3716.0
312.	C3H8+O=iC3H7+OH	4.76E+04	2.7	2106.0
313.	C3H8+OH=iC3H7+H2O	1.40E+03	2.8	-310.0
314.	C3H8+OH=nC3H7+H2O	1.37E+03	2.7	580.0
315.	C3H8+O2=nC3H7+HO2	3.97E+13	0.0	50872.0
316.	C3H8+O2=iC3H7+HO2	3.97E+13	0.0	47693.0
317.	C3H8+HO2=nC3H7+H2O2	4.76E+04	2.5	16494.0
318.	C3H8+HO2=iC3H7+H2O2	9.64E+03	2.6	13910.0
319.	C3H8+CH3=nC3H7+CH4	9.04E-01	3.6	7154.0
320.	C3H8+CH3=iC3H7+CH4	1.51E+00	3.5	5481.0
321.	C3H8+CH2OH=nC3H7+CH3OH	1.99E+02	3.0	3976.0
322.	C3H8+CH3O=nC3H7+CH3OH	4.34E+11	0.0	6458.0
323.	C3H8+CH2SING=nC3H7+CH3	9.04E-01	3.6	7154.0
324.	C3H8+C2H3=nC3H7+C2H4	6.03E+02	3.3	10502.0
325.	C3H8+C2H=nC3H7+C2H2	3.61E+12	0.0	0.0
326.	C3H8+C2H5=nC3H7+C2H6	9.04E-02	3.6	9141.0
327.	C3H8+HCO=nC3H7+CH2O	2.05E+05	2.5	18431.0
328.	C3H8+iC3H7=nC3H7+C3H8	8.40E-03	4.2	8716.0
329.	C3H8+CH3CO=nC3H7+CH3CHO	4.22E+04	2.6	17658.0

330. C3H8+CH2=nC3H7+CH3 9.03E-01 3.6 7154.0

331. C3H8+CH2OH=iC3H7+CH3OH 6.03E+01 3.0 11989.0

332. C3H8+CH3O=iC3H7+CH3OH 1.45E+11 0.0 4571.0

333. C3H8+CH2SING=iC3H7+CH3 1.51E+00 3.5 7472.0

334. C3H8+C2H3=iC3H7+C2H4 1.02E+03 3.1 8829.0

335. C3H8+C2H=iC3H7+C2H2 1.21E+12 0.0 0.0

336. C3H8+C2H5=iC3H7+C2H6 1.21E+00 3.5 7468.0

337. C3H8+HCO=iC3H7+CH2O 1.08E+07 1.9 17006.0

338. C3H8+CH3CO=iC3H7+CH3CHO 5.30E+06 2.0 16241.0

339. C3H8+CH2=iC3H7+CH3 1.51E+00 3.5 7472.0

340. nC3H7+H=C3H6+H2 1.81E+12 0.0 0.0

341. nC3H7+H(+M)=C3H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+59 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

342. nC3H7+H=C2H5+CH3 3.40E+18 -1.3 5386.0

343. nC3H7+O=C2H5+CH2O 9.60E+13 0.0 0.0

344. nC3H7+O2=C3H6+HO2 9.04E+10 0.0 0.0

345. nC3H7+HO2=C2H5+OH+CH2O 2.41E+13 0.0 0.0

346. nC3H7+OH=C3H6+H2O 2.41E+13 0.0 0.0

347. nC3H7+CH3=CH4+C3H6 1.14E+13 -0.3 0.0

348. nC3H7+C2H5=C3H6+C2H6 1.45E+12 0.0 0.0

349. nC3H7+C2H5=C3H8+C2H4 1.15E+12 0.0 0.0

350. nC3H7+C2H3=C3H8+C2H2 1.21E+12 0.0 0.0

351. nC3H7+C2H2=AC3H5+C2H4 7.23E+11 0.0 9004.0

352. nC3H7+C2H=C3H3+C2H5 1.21E+13 0.0 0.0

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353. nC3H7+C2H=C3H6+C2H2                              6.03E+12    0.0        0.0
354. nC3H7+iC3H7=C3H8+C3H6                           5.13E+13   -0.3        0.0
355. nC3H7+HCO=CO+C3H8                               6.03E+13    0.0        0.0
356. nC3H7+CH3O=C3H8+CH2O                            2.41E+13    0.0        0.0
357. nC3H7+CH2SING=C2H5+C2H4                         2.58E+13    0.0        0.0
358. nC3H7+CH2SING=C3H6+CH3                          1.03E+13    0.0        0.0
359. nC3H7+CH2=C2H4+C2H5                             1.81E+13    0.0        0.0
360. nC3H7+CH2=C3H6+CH3                              1.81E+12    0.0        0.0
361. nC3H7+CH2OH=C3H6+CH3OH                          4.82E+11    0.0        0.0
362. iC3H7=CH3+C2H4                                  1.00E+14    0.0    45000.0
363. iC3H7+H=C3H6+H2                                 3.61E+12    0.0        0.0
364. iC3H7+H(+M)=C3H8(+M)                            2.40E+13    0.0        0.0
     Low pressure limit:  0.17000E+59 -0.12080E+02  0.11264E+05
     TROE centering:      0.64900E+00  0.12131E+04  0.12131E+04  0.13370E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
365. iC3H7+H=CH3+C2H5                                5.90E+23   -2.8    10009.0
366. iC3H7+O=CH3CHO+CH3                              9.60E+13    0.0        0.0
367. iC3H7+O2=C3H6+HO2                               1.26E+11    0.0        0.0
368. iC3H7+HO2=CH3CHO+OH+CH3                         2.41E+13    0.0        0.0
369. iC3H7+OH=C3H6+H2O                               2.41E+13    0.0        0.0
370. iC3H7+CH3=CH4+C3H6                              2.19E+14   -0.7        0.0
371. iC3H7+C2H5=C3H6+C2H6                            2.30E+13   -0.3        0.0
372. iC3H7+C2H5=C3H8+C2H4                            1.84E+13   -0.3        0.0
373. iC3H7+C2H3=C2H4+C3H6                            1.52E+14   -0.7        0.0
374. iC3H7+C2H3=C3H8+C2H2                            1.52E+14   -0.7        0.0
375. iC3H7+C2H2=CH3+iiiC4H6                          2.77E+10    0.0     6504.0
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376. iC3H7+C2H=C3H6+C2H2                              3.60E+12    0.0        0.0
377. iC3H7+iC3H7=C3H8+C3H6                           2.11E+14   -0.7        0.0
378. iC3H7+HCO=CO+C3H8                               1.20E+14    0.0        0.0
379. iC3H7+CH3O=C3H8+CH2O                            1.21E+13    0.0        0.0
380. iC3H7+CH2SING=C3H6+CH3                          1.04E+13    0.0        0.0
381. iC3H7+CH2=C3H6+CH3                              3.01E+13    0.0        0.0
382. iC3H7+CH2OH=C3H6+CH3OH                          2.89E+12    0.0        0.0
383. iC3H7+CH2OH=C3H8+CH2O                           2.35E+12    0.0        0.0
384. CH3+C2H3(+M)=C3H6(+M)                           2.50E+13    0.0        0.0
     Low pressure limit:  0.42700E+59 -0.11940E+02  0.97700E+04
     TROE centering:      0.17500E+00  0.13410E+04  0.60000E+05  0.10140E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H2            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
385. C3H6+H=H2+AC3H5                                 1.70E+05    2.5     2492.0
386. C3H6+H=C2H4+CH3                                 8.80E+16   -1.1     6461.0
387. C3H6+H=SC3H5+H2                                 7.81E+05    2.5    12285.0
388. C3H6+H(+M)=nC3H7(+M)                            1.33E+13    0.0     3260.7
     Low pressure limit:  0.62600E+39 -0.66600E+01  0.70000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.13100E+04  0.48097E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
389. C3H6+H(+M)=iC3H7(+M)                            1.33E+13    0.0     1559.8
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Low pressure limit: 0.87000E+43 -0.75000E+01 0.47218E+04

TROE centering: 0.10000E+01 0.10000E+04 0.64540E+03 0.68443E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

390.	C3H6+H=TC3H5+H2	3.90E+05	2.5	5821.0
391.	C3H6=H2+AC3H4	4.00E+13	0.0	80000.0
392.	C3H6=CH4+C2H2	3.50E+12	0.0	70000.0
393.	C3H6+O=C2H5+HCO	3.50E+07	1.6	-972.0
394.	C3H6+O=AC3H5+OH	1.75E+11	0.7	5884.0
395.	C3H6+O=SC3H5+OH	1.21E+11	0.7	8960.0
396.	C3H6+O=TC3H5+OH	6.03E+10	0.7	7633.0
397.	C3H6+O=CH3+H+CH2CO	1.20E+08	1.6	327.0
398.	C3H6+OH=AC3H5+H2O	3.12E+06	2.0	-298.0
399.	C3H6+OH=SC3H5+H2O	2.14E+06	2.0	2778.0
400.	C3H6+OH=TC3H5+H2O	1.11E+06	2.0	1451.0
401.	C3H6+HO2=AC3H5+H2O2	9.63E+03	2.6	13910.0
402.	C3H6+O2=AC3H5+HO2	6.03E+13	0.0	47590.0
403.	C3H6+CH3=AC3H5+CH4	2.20E+00	3.5	5675.0
404.	C3H6+CH3=TC3H5+CH4	8.40E-01	3.5	11660.0
405.	C3H6+C2H5=AC3H5+C2H6	2.23E+00	3.5	6637.0
406.	C3H6+C2H2=AC3H5+C2H3	4.04E+13	0.0	46818.0
407.	C3H6+C2H3=AC3H5+C2H4	2.21E+00	3.5	4682.0
408.	C3H6+C2H3=SC3H5+C2H4	1.35E+00	3.5	10842.0
409.	C3H6+C2H3=TC3H5+C2H4	8.40E-01	3.5	9670.0
410.	C3H6+C2H3=iiiC4H6+CH3	7.23E+11	0.0	5008.0
411.	C3H6+C2H4=AC3H5+C2H5	5.78E+13	0.0	51584.0
412.	C3H6+C2H4=nC3H7+C2H3	6.03E+13	0.0	75446.0

413. C3H6+CH2OH=AC3H5+CH3OH 6.03E+01 3.0 12000.0

414. C3H6+nC3H7=AC3H5+C3H8 2.23E+00 3.5 6637.0

415. C3H6+nC3H7=IC4H8+C2H5 2.23E+00 3.5 -2000.0

416. C3H6+iC3H7=C3H8+AC3H5 6.62E-02 4.0 8066.0

417. C3H6+C3H6=AC3H5+nC3H7 2.53E+14 0.0 55179.0

418. C3H6+C3H6=AC3H5+iC3H7 4.88E+13 0.0 52309.0

419. CH3+C2H3=AC3H5+H 1.50E+24 -2.8 18618.0

420. CH3+C2H3=SC3H5+H 3.20E+35 -7.8 13300.0

421. CH3+C2H3=TC3H5+H 4.99E+22 -4.4 18850.0

422. AC3H5+H(+M)=C3H6(+M) 2.00E+14 0.0 0.0

Low pressure limit: 0.13300E+61 -0.12000E+02 0.59678E+04

TROE centering: 0.20000E-01 0.10970E+04 0.10967E+05 0.68600E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

423. AC3H5+H=AC3H4+H2 1.80E+13 0.0 0.0

424. TC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

425. SC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

426. AC3H5+O=C2H3CHO+H 6.00E+13 0.0 0.0

427. AC3H5+O=C2H3+CH2O 1.80E+14 0.0 0.0

428. SC3H5+O=CH2CO+CH3 1.81E+14 0.0 0.0

429. TC3H5+O=H+HCCO+CH3 1.81E+14 0.0 0.0

430. AC3H5+OH=C2H3CHO+H+H 5.30E+37 -6.7 29306.0

431. AC3H5+OH=AC3H4+H2O 6.00E+12 0.0 0.0

432. AC3H5+O2=AC3H4+HO2 4.99E+15 -1.4 22428.0

433. AC3H5+O2=CH2O+CH3CO 1.19E+15 -1.0 20128.0

434. AC3H5+O2=OH+C2H3CHO 1.82E+13 -0.4 22859.0

435. SC3H5+O2=CH3CHO+HCO 4.34E+12 0.0 0.0

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436. TC3H5+O2=CH3CHO+HCO                              4.34E+12    0.0        0.0
437. AC3H5+HO2=C2H3+CH2O+OH                           6.60E+12    0.0        0.0
438. AC3H5+CH3=AC3H4+CH4                              3.00E+12   -0.3     -131.0
439. AC3H5+CH3(+M)=IC4H8(+M)                          1.00E+14   -0.3     -262.0
     Low pressure limit:  0.35100E+61 -0.12970E+02  0.60000E+04
     TROE centering:      0.89600E+00  0.60000E+05  0.16060E+04  0.61180E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
440. SC3H5+CH3=AC3H4+CH4                              1.00E+11    0.0        0.0
441. TC3H5+CH3=AC3H4+CH4                              1.00E+11    0.0        0.0
442. AC3H5+C2H3=AC3H4+C2H4                            1.00E+12    0.0        0.0
443. SC3H5+C2H3=AC3H4+C2H4                            1.00E+11    0.0        0.0
444. TC3H5+C2H3=AC3H4+C2H4                            1.00E+11    0.0        0.0
445. AC3H5+CH2O=C3H6+HCO                              1.26E+08    1.9    18191.0
446. AC3H5+HCO=C3H6+CO                                6.00E+13    0.0        0.0
447. AC3H5+AC3H5=AC3H4+C3H6                           8.43E+10    0.0     -262.0
448. AC3H5+CH2=iiiC4H6+H                              3.00E+13    0.0        0.0
449. AC3H5+nC3H7=AC3H4+C3H8                           7.23E+11    0.0     -131.0
450. AC3H5+iC3H7=AC3H4+C3H8                           4.58E+12   -0.3     -131.0
451. AC3H5=TC3H5                                      3.90E+59  -15.4    75400.0
452. AC3H5=SC3H5                                      1.30E+55  -14.5    73800.0
453. TC3H5=SC3H5                                      1.60E+44  -12.2    52200.0
454. AC3H4=PC3H4                                      6.03E+53  -12.2    84276.0
455. AC3H4+H=AC3H5                                    1.24E+52  -12.0    17839.0
     Declared duplicate reaction...
456. AC3H4+H=AC3H5                                    6.92E+36   -8.2     7462.0
     Declared duplicate reaction...
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457.	AC3H4+H=TC3H5	1.55E+53	-13.1	14472.0
	Declared duplicate reaction...			
458.	AC3H4+H=TC3H5	9.88E+44	-11.2	8212.0
	Declared duplicate reaction...			
459.	PC3H4+H=TC3H5	3.17E+52	-12.7	14226.0
	Declared duplicate reaction...			
460.	PC3H4+H=TC3H5	2.59E+45	-11.2	8046.0
	Declared duplicate reaction...			
461.	PC3H4+H=SC3H5	3.38E+49	-12.8	14072.0
	Declared duplicate reaction...			
462.	PC3H4+H=SC3H5	2.98E+43	-11.4	8736.0
	Declared duplicate reaction...			
463.	AC3H4+H=PC3H4+H	1.48E+13	0.3	4103.0
464.	AC3H4+H=CH3+C2H2	2.72E+09	1.2	6834.0
465.	PC3H4+H=CH3+C2H2	3.89E+10	1.0	4114.0
466.	C2H2+CH3=SC3H5	-6.81E+48	-12.3	16642.0
	Declared duplicate reaction...			
467.	C2H2+CH3=SC3H5	1.52E+44	-10.7	15256.0
	Declared duplicate reaction...			
468.	C2H2+CH3=TC3H5	6.80E+20	-4.2	18000.0
469.	C2H2+CH3=AC3H5	8.20E+53	-13.3	33200.0
470.	AC3H4+H=C3H3+H2	6.60E+03	3.1	5522.0
471.	AC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
472.	PC3H4+H=C3H3+H2	3.57E+04	2.8	4821.0
473.	AC3H4+O=C2H4+CO	2.00E+07	1.8	1000.0
474.	AC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
475.	AC3H4+CH3=C3H3+CH4	1.30E+12	0.0	7700.0
476.	PC3H4+O=HCCO+CH3	7.30E+12	0.0	2250.0
477.	PC3H4+O=C2H4+CO	1.00E+13	0.0	2250.0
478.	PC3H4+O=C3H3+OH	3.44E+04	2.2	4830.0
479.	PC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
480.	PC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0

481.	PC3H4+CH3=C3H3+CH4	1.80E+12	0.0	7700.0
482.	C3H3+H=PC3H4	3.63E+36	-7.4	6039.0
483.	C3H3+H=AC3H4	3.39E+36	-7.4	6337.0
484.	C3H3+CH3=iiC4H6	3.61E+13	0.0	0.0
485.	C2H3+C2H3=iiiC4H6	7.00E+57	-13.8	17629.0
486.	C3H3+H=C3H2+H2	2.14E+05	2.5	7453.0
487.	C3H3+O=>C2H2+HCO	1.38E+14	0.0	0.0
488.	C3H3+O=C2H3+CO	4.62E+13	0.0	0.0
489.	C3H3+O=C2H+CH2O	4.62E+13	0.0	0.0
490.	C3H3+O=>C2H2+CO+H	4.62E+13	0.0	0.0
491.	C3H3+OH=C3H2+H2O	2.00E+13	0.0	8000.0
492.	C3H3+HCO=AC3H4+CO	2.50E+13	0.0	0.0
493.	C3H3+HCO=PC3H4+CO	2.50E+13	0.0	0.0
494.	C3H3+CH=iC4H3+H	5.00E+13	0.0	0.0
495.	C3H3+CH2=C4H4+H	5.00E+13	0.0	0.0
496.	C3H3+O2=CH2CO+HCO	1.70E+05	1.7	1500.0
497.	C3H3+HCCO=C4H4+CO	2.50E+13	0.0	0.0
498.	C3H3+HO2=OH+CO+C2H3	8.00E+11	0.0	0.0
499.	C3H3+HO2=AC3H4+O2	3.00E+11	0.0	0.0
500.	C3H3+HO2=PC3H4+O2	2.50E+12	0.0	0.0
501.	C3H2+O2=H+CO+HCCO	2.00E+12	0.0	1000.0
502.	C3H2+O=C2H2+CO	6.80E+13	0.0	0.0
503.	C3H2+OH=C2H2+HCO	6.80E+13	0.0	0.0
504.	C3H2+H=C3H3	1.10E+40	-8.0	84700.0
505.	C3H2+CH=C4H2+H	5.00E+13	0.0	0.0
506.	C3H2+CH2=nC4H3+H	5.00E+13	0.0	0.0
507.	C3H2+CH3=C4H4+H	5.00E+12	0.0	0.0
508.	C3H2+HCCO=nC4H3+CO	1.00E+13	0.0	0.0
509.	C2H3CO+M=>C2H3+CO+M	8.51E+15	0.0	23000.0
510.	C2H3+CO+M=>C2H3CO+M	1.58E+11	0.0	6000.0
511.	C2H3CHO+HO2=>C2H3CH2O+O2	1.29E+11	0.0	32000.0
512.	C2H3CH2O=>C2H3CHO+H	1.00E+14	0.0	19000.0

513. C2H3CHO+H=>C2H3CH2O 1.00E+08 0.0 10000.0

514. C2H3CHO+OH=>C2H3CO+H2O 1.00E+13 0.0 0.0

515. C2H3CO+H2O=>C2H3CHO+OH 1.91E+13 0.0 36620.0

516. C2H3CHO+H=>C2H3CO+H2 3.98E+13 0.0 4200.0

517. C2H3CO+H2=>C2H3CHO+H 1.78E+13 0.0 23670.0

518. C2H3CHO+O=>C2H3CO+OH 5.01E+12 0.0 1790.0

519. C2H3CO+OH=>C2H3CHO+O 1.00E+12 0.0 19160.0

520. C2H3CHO+HO2=>C2H3CO+H2O2 1.70E+12 0.0 10700.0

521. C2H3CO+H2O2=>C2H3CHO+HO2 1.00E+12 0.0 14100.0

522. C2H3CHO+CH3=>C2H3CO+CH4 1.74E+12 0.0 8440.0

523. C2H3CO+CH4=>C2H3CHO+CH3 1.51E+13 0.0 28000.0

524. C2H3CH2O+O2=>C2H3CHO+HO2 1.74E+11 0.0 1750.0

525. C2H3CH2O=>CH2O+C2H3 1.00E+14 0.0 21600.0

526. CH2O+C2H3=>C2H3CH2O 1.00E+11 0.0 0.0

527. C4H+H2=C4H2+H 2.00E+13 0.0 5000.0

528. C4H+O2=CO+CO+C2H 1.20E+12 0.0 0.0

529. C4H2+OH=H2O+C4H 9.15E+09 1.0 21746.0

530. C4H2+OH=CO+C3H3 1.69E+28 -4.6 20140.0

531. C4H2+H=nC4H3 1.44E+63 -15.7 24018.0

Declared duplicate reaction...

532. C4H2+H=nC4H3 4.16E+32 -6.5 9726.1

Declared duplicate reaction...

533. C4H2+H(+M)=iC4H3(+M) 4.31E+10 1.2 1752.9

Low pressure limit: 0.23000E+46 -0.80950E+01 0.25066E+04

TROE centering: 0.74800E-01 0.10000E-49 -0.42159E+04 0.10000E+51

H2 Enhanced by 2.000E+00

CO Enhanced by 2.000E+00

CO2 Enhanced by 3.000E+00

H2O Enhanced by 5.000E+00

534. C4H2+O=C3H2+CO 2.70E+13 0.0 1720.0

535. nC4H3=iC4H3 3.70E+61 -15.8 54890.0

536. nC4H3+H=iC4H3+H 2.40E+11 0.8 2410.0

537.	nC4H3+H=C2H2+H2CC	1.60E+19	-1.6	2220.0
538.	nC4H3+H=C4H4	1.10E+42	-9.7	7000.0
539.	nC4H3+H=C4H2+H2	3.00E+13	0.0	0.0
540.	nC4H3+OH=C4H2+H2O	2.00E+12	0.0	0.0
541.	iC4H3+H=C2H2+H2CC	2.40E+19	-1.6	2800.0
542.	iC4H3+H=C4H4	4.20E+44	-10.3	7890.0
543.	iC4H3+H=C4H2+H2	5.00E+13	0.0	0.0
544.	iC4H3+OH=C4H2+H2O	4.00E+12	0.0	0.0
545.	iC4H3+O2=HCCO+CH2CO	7.86E+16	-1.8	0.0
546.	C4H4+H=n-C4H5	4.20E+50	-12.3	12500.0
547.	C4H4+H=i-C4H5	9.60E+52	-12.8	14300.0
548.	C4H4+H=nC4H3+H2	6.65E+05	2.5	12240.0
549.	C4H4+H=iC4H3+H2	3.33E+05	2.5	9240.0
550.	C4H4+OH=nC4H3+H2O	3.10E+07	2.0	3430.0
551.	C4H4+OH=iC4H3+H2O	1.55E+07	2.0	430.0
552.	C4H4+O=C3H3+HCO	6.00E+08	1.4	-860.0
553.	n-C4H5=i-C4H5	1.30E+62	-16.4	49600.0
554.	n-C4H5+H=i-C4H5+H	1.00E+36	-6.3	17486.0
555.	n-C4H5+H=C4H4+H2	1.50E+13	0.0	0.0
556.	n-C4H5+OH=C4H4+H2O	2.00E+12	0.0	0.0
557.	n-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
558.	n-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
559.	n-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
560.	n-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
561.	n-C4H5+O2=HCO+C2H3CHO	9.20E+16	-1.4	1010.0
562.	i-C4H5+H=C4H4+H2	3.00E+13	0.0	0.0
563.	i-C4H5+H=C3H3+CH3	1.00E+14	0.0	0.0
564.	i-C4H5+OH=C4H4+H2O	4.00E+12	0.0	0.0
565.	i-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
566.	i-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
567.	i-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
568.	i-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0

569.	i-C4H5+O2=CH2CO+CH2CHO	2.16E+10	0.0	2500.0
570.	iiiC4H6=i-C4H5+H	8.20E+51	-10.9	118409.0
571.	iiiC4H6=n-C4H5+H	3.50E+61	-13.9	129677.0
572.	iiiC4H6=C4H4+H2	2.50E+15	0.0	94700.0
573.	iiiC4H6+H=n-C4H5+H2	3.00E+07	2.0	13000.0
574.	iiiC4H6+H=i-C4H5+H2	3.00E+07	2.0	6000.0
575.	C2H4+C2H3=iiiC4H6+H	7.40E+14	-0.7	8420.0
576.	iiiC4H6+H=PC3H4+CH3	2.00E+12	0.0	7000.0
577.	iiiC4H6+H=AC3H4+CH3	2.00E+12	0.0	7000.0
578.	iiiC4H6+O=n-C4H5+OH	7.50E+06	1.9	3740.0
579.	iiiC4H6+O=i-C4H5+OH	7.50E+06	1.9	3740.0
580.	iiiC4H6+O=HCO+AC3H5	6.02E+08	1.4	-858.0
581.	iiiC4H6+OH=CH3CHO+C2H3	6.30E+12	0.0	-874.0
582.	iiiC4H6+OH=AC3H5+CH2O	6.30E+12	0.0	-874.0
583.	iiiC4H6+OH=n-C4H5+H2O	2.00E+07	2.0	5000.0
584.	iiiC4H6+OH=i-C4H5+H2O	2.00E+07	2.0	2000.0
585.	iiiC4H6+CH3=n-C4H5+CH4	2.00E+14	0.0	22800.0
586.	iiiC4H6+CH3=i-C4H5+CH4	1.00E+14	0.0	19800.0
587.	iiiC4H6+C2H3=n-C4H5+C2H4	5.00E+13	0.0	22800.0
588.	iiiC4H6+C2H3=i-C4H5+C2H4	2.50E+13	0.0	19800.0
589.	iiiC4H6+C3H3=n-C4H5+AC3H4	1.00E+13	0.0	22500.0
590.	iiiC4H6+C3H3=i-C4H5+AC3H4	5.00E+12	0.0	19500.0
591.	iiiC4H6+AC3H5=n-C4H5+C3H6	1.00E+13	0.0	22500.0
592.	iiiC4H6+AC3H5=i-C4H5+C3H6	5.00E+12	0.0	19500.0
593.	iiC4H6=i-C4H5+H	4.20E+15	0.0	92600.0
594.	iiC4H6+H=iiiC4H6+H	2.00E+13	0.0	4000.0
595.	iiC4H6+H=i-C4H5+H2	1.70E+05	2.5	2490.0
596.	iiC4H6+H=AC3H4+CH3	2.00E+13	0.0	2000.0
597.	iiC4H6+H=PC3H4+CH3	2.00E+13	0.0	2000.0
598.	iiC4H6+CH3=i-C4H5+CH4	7.00E+13	0.0	18500.0
599.	iiC4H6+O=CH2CO+C2H4	1.20E+08	1.6	327.0
600.	iiC4H6+O=i-C4H5+OH	1.80E+11	0.7	5880.0

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601. iiC4H6+OH=i-C4H5+H2O                              3.10E+06    2.0     -298.0
602. iiC4H6=iiiC4H6                                    3.00E+13    0.0    65000.0
603. IC4H8+H=C2H4+C2H5                                 1.60E+22   -2.4    11180.0
604. IC4H8+H=C3H6+CH3                                  3.20E+22   -2.4    11180.0
605. IC4H8+H=C4H7+H2                                   6.50E+05    2.5     6756.0
606. IC4H8+O=nC3H7+HCO                                 3.30E+08    1.4     -402.0
607. IC4H8+O=C4H7+OH                                   1.50E+13    0.0     5760.0
     Declared duplicate reaction...
608. IC4H8+O=C4H7+OH                                   2.60E+13    0.0     4470.0
     Declared duplicate reaction...
609. IC4H8+OH=C4H7+H2O                                 7.00E+02    2.7      527.0
610. IC4H8+O2=C4H7+HO2                                 2.00E+13    0.0    50930.0
611. IC4H8+HO2=C4H7+H2O2                               1.00E+12    0.0    14340.0
612. IC4H8+CH3=C4H7+CH4                                4.50E-01    3.6     7153.0
613. C4H7=iiiC4H6+H                                    1.27E+24   -4.8    23777.0
614. C4H7+H(+M)=IC4H8(+M)                              3.60E+13    0.0        0.0
     Low pressure limit:  0.30100E+49 -0.93200E+01  0.58336E+04
     TROE centering:      0.49800E+00  0.13140E+04  0.13140E+04  0.50000E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
615. C4H7+H=CH3+AC3H5                                  2.00E+21   -2.0    11000.0
616. C4H7+H=iiiC4H6+H2                                 1.80E+12    0.0        0.0
617. C4H7+O2=iiiC4H6+HO2                               1.00E+11    0.0        0.0
618. C4H7+HCO=IC4H8+CO                                 6.00E+13    0.0        0.0
619. C4H7+CH3=iiiC4H6+CH4                              1.10E+13    0.0        0.0
620. C2H4+C2H3=C4H7                                    1.23E+35   -7.8     9930.0
621. IC4H8+H(+M)=nC4H9(+M)                             1.33E+13    0.0     3260.7
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Low pressure limit: 0.62600E+39 -0.66600E+01 0.70000E+04

TROE centering: 0.10000E+01 0.10000E+04 0.13100E+04 0.48097E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

622.	C2H4+C2H5=nC4H9	1.50E+11	0.0	7300.0
623.	nC4H9+H=IC4H8+H2	1.80E+12	0.0	0.0
624.	nC4H9+O=nC3H7+CH2O	9.60E+13	0.0	0.0
625.	nC4H9+OH=IC4H8+H2O	2.40E+13	0.0	0.0
626.	nC4H9+O2=IC4H8+HO2	2.70E+11	0.0	0.0
627.	nC4H9+HO2=nC3H7+OH+CH2O	2.40E+13	0.0	0.0
628.	nC4H9+CH3=IC4H8+CH4	1.10E+13	0.0	0.0
629.	C2H5OH=CH3+CH2OH	1.26E+51	-10.6	100869.0
630.	C2H5OH=C2H4+H2O	8.80E+25	-3.7	70799.0
631.	C2H5OH+OH=C2H4OH+H2O	1.81E+11	0.4	716.5
632.	C2H5OH+OH=CH3CHOH+H2O	3.09E+10	0.5	-379.8
633.	C2H5OH+OH=C2H5O+H2O	1.05E+10	0.8	716.9
634.	C2H5OH+H=C2H4OH+H2	1.90E+07	1.8	5098.0
635.	C2H5OH+H=CH3CHOH+H2	2.58E+07	1.6	2827.0
636.	C2H5OH+H=C2H5O+H2	1.50E+07	1.6	3038.0
637.	C2H5OH+O=C2H4OH+OH	9.41E+07	1.7	5459.0
638.	C2H5OH+O=CH3CHOH+OH	1.88E+07	1.9	1824.0
639.	C2H5OH+O=C2H5O+OH	1.58E+07	2.0	4448.0
640.	C2H5OH+CH3=C2H4OH+CH4	2.19E+02	3.2	9622.0
641.	C2H5OH+CH3=CH3CHOH+CH4	7.28E+02	3.0	7948.0
642.	C2H5OH+CH3=C2H5O+CH4	1.45E+02	3.0	7649.0
643.	C2H5OH+HO2=CH3CHOH+H2O2	8.20E+03	2.5	10750.0
644.	C2H5OH+HO2=C2H4OH+H2O2	2.43E+04	2.5	15750.0

645.	C2H5OH+HO2=C2H5O+H2O2	3.80E+12	0.0	24000.0
646.	C2H5O+M=CH3CHO+H+M	5.60E+34	-5.9	25274.0
647.	C2H5O+M=CH3+CH2O+M	5.35E+37	-7.0	23800.0
648.	C2H5O+CO=C2H5+CO2	4.68E+02	3.2	5380.0
649.	C2H5O+H=CH3+CH2OH	3.00E+13	0.0	0.0
650.	C2H5O+H=C2H4+H2O	3.00E+13	0.0	0.0
651.	C2H5O+OH=CH3CHO+H2O	1.00E+13	0.0	0.0
652.	CH3CHOH+O2=CH3CHO+HO2	4.82E+13	0.0	5017.0
	Declared duplicate reaction...			
653.	CH3CHOH+O2=CH3CHO+HO2	8.43E+14	-1.2	0.0
	Declared duplicate reaction...			
654.	CH3CHOH+O=CH3CHO+OH	1.00E+14	0.0	0.0
655.	CH3CHOH+H=C2H4+H2O	3.00E+13	0.0	0.0
656.	CH3CHOH+H=CH3+CH2OH	3.00E+13	0.0	0.0
657.	CH3CHOH+HO2=CH3CHO+OH+OH	4.00E+13	0.0	0.0
658.	CH3CHOH+OH=CH3CHO+H2O	5.00E+12	0.0	0.0
659.	CH3CHOH+M=CH3CHO+H+M	1.00E+14	0.0	25000.0
660.	C2H4+OH=C2H4OH	2.41E+11	0.0	-2385.0
661.	C2H4OH+O2=HOC2H4O2	1.00E+12	0.0	-1100.0
662.	HOC2H4O2=CH2O+CH2O+OH	1.80E+11	0.0	24500.0
663.	CH3OCH3=CH3+CH3O	1.88E+49	-10.4	93453.5
664.	CH3OCH3+OH=CH3OCH2+H2O	6.71E+06	2.0	-629.9
665.	CH3OCH3+H=CH3OCH2+H2	2.97E+07	2.0	4033.6
666.	CH3OCH3+O=CH3OCH2+OH	1.86E-03	5.3	-109.0
667.	CH3OCH3+HO2=CH3OCH2+H2O2	1.68E+13	0.0	17690.0
668.	CH3OCH3+CH3=CH3OCH2+CH4	3.86E-08	6.2	2513.9
669.	CH3OCH3+O2=CH3OCH2+HO2	4.10E+13	0.0	44910.0
670.	CH3OCH3+CH3O=CH3OCH2+CH3OH	6.02E+11	0.0	4074.0
671.	CH3OCH2=CH2O+CH3	1.60E+13	0.0	25500.0
672.	CH3OCH2+CH3O=CH3OCH3+CH2O	2.41E+13	0.0	0.0
673.	CH3OCH2+CH2O=CH3OCH3+HCO	5.49E+03	2.8	5862.0
674.	CH3OCH2+O2=>CH2O+CH2O+OH	5.02E+23	-3.8	3100.0

675.	CH3OCH2+HO2=CH3OCH2O+OH	9.00E+12	0.0	0.0
676.	CH3OCH2O=CH3OCHO+H	1.74E+16	-0.7	11720.0
677.	CH3OCHO=CH3+OCHO	1.39E+18	-1.0	79140.0
678.	CH3OCHO+O2=CH3OCO+HO2	1.00E+13	0.0	49700.0
679.	CH3OCHO+OH=CH3OCO+H2O	2.34E+07	1.6	-35.0
680.	CH3OCHO+HO2=CH3OCO+H2O2	1.22E+12	0.0	17000.0
681.	CH3OCHO+O=CH3OCO+OH	2.35E+05	2.5	2230.0
682.	CH3OCHO+H=CH3OCO+H2	4.55E+06	2.0	5000.0
683.	CH3OCHO+CH3=CH3OCO+CH4	7.55E-01	3.5	5481.0
684.	CH3OCHO+CH3O=CH3OCO+CH3OH	5.48E+11	0.0	5000.0
685.	CH3OCO=CH3O+CO	7.45E+12	-1.8	17150.0
686.	CH3OCO=CH3+CO2	1.51E+12	-1.8	13820.0
687.	OCHO+M=H+CO2+M	2.44E+15	-0.5	26500.0
688.	NH+M=N+H+M	2.65E+14	0.0	75500.0
689.	NH+H=N+H2	3.20E+13	0.0	325.0
690.	NH+O=N+OH	1.70E+08	1.5	3368.0
691.	NH+OH=N+H2O	1.60E+07	1.7	-576.0
692.	NH2+M=NH+H+M	3.16E+23	-2.0	91400.0
693.	NH2+H=NH+H2	4.00E+13	0.0	3650.0
694.	NH2+O=NH+OH	7.00E+12	0.0	0.0
	Declared duplicate reaction...			
695.	NH2+O=NH+OH	8.60E-01	4.0	1673.0
	Declared duplicate reaction...			
696.	NH2+OH=NH+H2O	3.30E+06	1.9	-217.0
697.	NH2+O2=NH+HO2	1.00E+14	0.0	49997.0
698.	NH+NH=NH2+N	5.70E-01	3.9	342.0
699.	NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
700.	NH3+M=NH+H2+M	6.30E+14	0.0	93390.0
701.	NH3+H=NH2+H2	6.36E+05	2.4	10171.0
702.	NH3+O=NH2+OH	2.80E+02	3.3	4471.0
703.	NH3+OH=NH2+H2O	2.00E+06	2.0	566.0
704.	NH2+HO2=NH3+O2	9.20E+05	1.9	-1152.0

705.	NH3+HO2=NH2+H2O2			3.00E+11	0.0	22000.0
706.	NH2+NH=NH3+N			9.60E+03	2.5	107.0
707.	NH2+NH2=NH3+NH			5.60E+00	3.5	552.0
708.	N2+M=N+N+M			1.00E+28	-3.3	225000.0
709.	NH+N=N2+H			3.00E+13	0.0	0.0
710.	NH+NH=N2+H+H			2.50E+13	0.0	0.0
711.	NH2+N=N2+H+H			7.10E+13	0.0	0.0
712.	NH+NH=N2+H2			1.00E+08	1.0	0.0
713.	NNH=N2+H			1.00E+09	0.0	0.0
714.	NNH+H=N2+H2			1.00E+14	0.0	0.0
715.	NH+NH=NNH+H			5.10E+13	0.0	0.0
716.	NNH+O=N2+OH			1.20E+13	0.1	-217.0
717.	NNH+OH=N2+H2O			5.00E+13	0.0	0.0
718.	NNH+O2=N2+HO2			5.60E+14	-0.4	-13.0
719.	NNH+O2=N2+H+O2			5.00E+13	0.0	0.0
720.	NNH+HO2=N2+H2O2			1.40E+04	2.7	-1599.0
721.	NNH+N=NH+N2			3.00E+13	0.0	2000.0
722.	NNH+NH=N2+NH2			5.00E+13	0.0	0.0
723.	NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
724.	N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
	H2O	Enhanced by	1.500E+01			
	O2	Enhanced by	2.000E+00			
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
725.	N2H2+M=NH+NH+M			3.16E+16	0.0	99400.0
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
726.	NH2+NH=N2H2+H			4.30E+14	-0.3	-77.0
727.	N2H2+H=NNH+H2			8.50E+04	2.6	230.0
728.	NH2+NH2=N2H2+H2			1.70E+08	1.6	11783.0
729.	N2H2+O=NNH+OH			3.30E+08	1.5	496.0
730.	N2H2+OH=NNH+H2O			5.90E+01	3.4	1360.0

731.	N2H2+N=NNH+NH	1.00E+06	2.0	0.0
732.	N2H2+NH=NNH+NH2	1.00E+13	0.0	6000.0
733.	N2H2+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
734.	NNH+NNH=N2H2+N2	1.00E+13	0.0	4000.0
735.	H2NN=NNH+H	3.40E+26	-4.8	46228.0
736.	N2H2=H2NN	2.00E+41	-9.4	68413.0
737.	H2NN+H=N2H2+H	7.00E+13	0.0	0.0
738.	H2NN+H=NNH+H2	4.80E+08	1.5	-894.0
739.	NH2+NH2=H2NN+H2	7.20E+04	1.9	8802.0
740.	H2NN+O=OH+NNH	3.30E+08	1.5	-894.0
741.	H2NN+OH=NNH+H2O	2.40E+06	2.0	-1192.0
742.	H2NN+HO2=NNH+H2O2	2.90E+04	2.7	-1599.0
743.	H2NN+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
744.	N2H3=N2H2+H	3.60E+47	-10.4	68970.0
745.	N2H3+M=NH2+NH+M	5.00E+16	0.0	60000.0
746.	NH2+NH2=N2H3+H	1.20E+12	0.0	10078.0
747.	N2H3+H=N2H2+H2	2.40E+08	1.5	0.0
748.	N2H3+H=NH+NH3	1.00E+11	0.0	0.0
749.	NH3+NH2=N2H3+H2	1.00E+11	0.5	21600.0
750.	N2H3+O=N2H2+OH	1.70E+08	1.5	-645.0
751.	N2H3+OH=N2H2+H2O	1.20E+06	2.0	-1192.0
752.	N2H3+OH=H2NN+H2O	3.00E+13	0.0	0.0
753.	N2H3+HO2=N2H2+H2O2	1.40E+04	2.7	-1600.0
754.	N2H3+N=N2H2+NH	1.00E+06	2.0	0.0
755.	N2H3+NH=N2H2+NH2	2.00E+13	0.0	0.0
756.	N2H3+NH2=N2H2+NH3	9.20E+05	1.9	-1152.0
757.	N2H3+NH2=H2NN+NH3	3.00E+13	0.0	0.0
758.	N2H3+NNH=N2H2+N2H2	1.00E+13	0.0	4000.0
759.	N2H3+N2H3=NH3+NH3+N2	3.00E+12	0.0	0.0
760.	NH2+NH2(+M)=N2H4(+M)	5.60E+14	-0.4	66.0
	Low pressure limit: 0.16000E+35 -0.54900E+01 0.19870E+04			
	TROE centering: 0.31000E+00 0.10000E-29 0.10000E+31 0.10000E+31			

761.	N2H4+M=N2H3+H+M			1.00E+15	0.0	63600.0
	N2	Enhanced by	2.400E+00			
	NH3	Enhanced by	3.000E+00			
	N2H4	Enhanced by	4.000E+00			
762.	N2H4=H2NN+H2			5.30E+39	-8.3	69267.0
763.	N2H4+H=N2H3+H2			7.00E+12	0.0	2500.0
764.	N2H4+H=NH2+NH3			2.40E+09	0.0	3100.0
765.	N2H4+O=N2H3+OH			6.70E+08	1.5	2850.0
766.	N2H4+O=N2H2+H2O			4.40E+11	0.0	-1270.0
767.	N2H4+OH=N2H3+H2O			4.00E+13	0.0	0.0
768.	N2H3+HO2=N2H4+O2			9.20E+05	1.9	2125.0
769.	N2H4+N=N2H3+NH			1.00E+10	1.0	2000.0
770.	N2H4+NH=NH2+N2H3			1.00E+09	1.5	2000.0
771.	N2H4+NH2=N2H3+NH3			3.90E+12	0.0	1500.0
772.	N2H3+N2H2=N2H4+NNH			1.00E+13	0.0	6000.0
773.	N2H3+N2H3=N2H4+N2H2			1.20E+13	0.0	0.0
774.	NO+M=N+O+M			1.40E+15	0.0	148430.0
	N2	Enhanced by	1.000E+00			
	H2	Enhanced by	2.200E+00			
	H2O	Enhanced by	6.700E+00			
	CO2	Enhanced by	3.000E+00			
	N2O	Enhanced by	2.200E+00			
775.	N+OH=NO+H			3.80E+13	0.0	0.0
776.	NH+O=NO+H			9.20E+13	0.0	0.0
777.	NH2+O=NO+H2			5.00E+12	0.0	0.0
778.	NH+OH=NO+H2			2.00E+13	0.0	0.0
779.	NO+O=O2+N			1.81E+09	1.0	38725.0
780.	NH+O2=NO+OH			1.30E+06	1.5	100.0
781.	N+NO=N2+O			3.30E+12	0.3	0.0
782.	NH+NO=N2+OH			2.20E+13	-0.2	0.0
783.	NNH+O=NH+NO			5.20E+11	0.4	-409.0
784.	NH2+NO=N2+H2O			2.80E+20	-2.7	1258.0

785. NH2+NO=NNH+OH 2.29E+10 0.4 -814.0

786. N2H2+O=NH2+NO 1.00E+13 0.0 0.0

787. H2NN+O=NH2+NO 7.00E+13 0.0 0.0

788. H2NN+OH=>NH2+NO+H 2.00E+12 0.0 0.0

789. N2H3+O=>NH2+NO+H 3.00E+13 0.0 0.0

790. H2NN+HO2=>NH2+NO+OH 9.00E+12 0.0 0.0

791. NO+H(+M)=HNO(+M) 1.50E+15 -0.4 0.0

Low pressure limit: 0.24000E+15 0.20600E+00 -0.15500E+04

TROE centering: 0.82000E+00 0.10000E-29 0.10000E+31 0.10000E+31

N2 Enhanced by 1.600E+00

792. HNO+H=H2+NO 4.50E+11 0.7 655.0

793. NH+OH=HNO+H 3.20E+14 -0.4 -46.0

794. NH2+O=HNO+H 6.63E+14 -0.5 0.0

795. NH+H2O=HNO+H2 2.00E+13 0.0 13850.0

796. HNO+O=OH+NO 1.81E+13 0.0 0.0

797. NH+O2=HNO+O 4.60E+05 2.0 6494.0

798. HNO+OH=NO+H2O 3.60E+13 0.0 0.0

799. NH2+O2=HNO+OH 2.90E-02 3.8 18185.0

800. NH2+HO2=HNO+H2O 5.68E+15 -1.1 707.0

801. HNO+O2=NO+HO2 2.00E+13 0.0 15887.0

802. NH2+HNO=NH3+NO 3.60E+06 1.6 -1250.0

803. N2H3+O=NH2+HNO 3.00E+13 0.0 0.0

804. N2H3+OH=NH3+HNO 1.00E+12 0.0 15000.0

805. NNH+NO=N2+HNO 5.00E+13 0.0 0.0

806. H+NO+N2=HNO+N2 4.00E+20 -1.8 0.0

807. HON+M=NO+H+M 5.10E+19 -1.7 16045.0

AR Enhanced by 7.000E-01

H2O Enhanced by 7.000E+00

CO2 Enhanced by 2.000E+00

808. HON+H=HNO+H 2.00E+13 0.0 0.0

809. HON+H=OH+NH 2.00E+13 0.0 0.0

810. HON+O=OH+NO 7.00E+13 0.0 0.0

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811. HNOH+M=H+HNO+M                                   2.00E+24   -2.8    58901.0
812. HNOH+H=NH2+OH                                    4.00E+13    0.0        0.0
813. HNOH+H=HNO+H2                                    4.80E+08    1.5      377.0
814. HNOH+O=HNO+OH                                    7.00E+13    0.0        0.0
     Declared duplicate reaction...
815. HNOH+O=HNO+OH                                    3.30E+08    1.5     -357.0
     Declared duplicate reaction...
816. HNOH+OH=HNO+H2O                                  2.40E+06    2.0    -1192.0
817. HNOH+O2=HNO+HO2                                  3.00E+12    0.0    25000.0
818. HNOH+HO2=HNO+H2O2                                2.90E+04    2.7    -1599.0
819. HNOH+NH2=N2H3+OH                                 1.00E+01    3.5     -467.0
820. HNOH+NH2=H2NN+H2O                                8.80E+16   -1.1     1113.0
821. HNOH+NH2=HNO+NH3                                 1.80E+06    1.9    -1152.0
822. NH2O+M=HNO+H+M                                   2.80E+24   -2.8    64915.0
     H2O             Enhanced by    1.000E+01
823. NH2O+M=HNOH+M                                    1.10E+29   -4.0    44000.0
     H2O             Enhanced by    1.000E+01
824. NH2O+H=NH2+OH                                    5.00E+13    0.0        0.0
825. NH2O+H=HNO+H2                                    3.00E+07    2.0     2000.0
826. NH2O+O=HNO+OH                                    3.00E+07    2.0     2000.0
827. NH2+O2=NH2O+O                                    2.50E+11    0.5    29570.0
828. NH2O+OH=HNO+H2O                                  2.00E+07    2.0     1000.0
829. NH2+HO2=NH2O+OH                                  5.00E+13    0.0        0.0
830. NH2O+O2=HNO+HO2                                  3.00E+12    0.0    25000.0
831. NH2O+HO2=HNO+H2O2                                2.90E+04    2.7    -1599.0
832. NH2O+NH2=HNO+NH3                                 3.00E+12    0.0     1000.0
833. NH2O+NO=HNO+HNO                                  2.00E+04    2.0    13000.0
834. NH2OH(+M)=NH2+OH(+M)                             1.40E+20   -1.3    64080.0
     Low pressure limit:  0.54000E+38 -0.59600E+01  0.66783E+05
     TROE centering:      0.31000E+00  0.10000E-29  0.10000E+31  0.10000E+31
835. NH2OH+H=HNOH+H2                                  4.80E+08    1.5     6246.0
836. NH2OH+H=NH2O+H2                                  2.40E+08    1.5     5064.0
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837. NH2OH+O=HNOH+OH                                  3.30E+08    1.5     3863.0
838. NH2OH+O=NH2O+OH                                  1.70E+08    1.5     3009.0
839. NH2OH+OH=HNOH+H2O                                1.50E+04    2.6    -3537.0
840. NH2OH+OH=NH2O+H2O                                1.50E+05    2.3    -1296.0
841. NH2O+HO2=O2+NH2OH                                2.90E+04    2.7    -1599.0
842. HNOH+HO2=NH2OH+O2                                2.90E+04    2.7    -1599.0
843. NH2OH+HO2=HNOH+H2O2                              2.90E+04    2.7     9552.0
844. NH2OH+HO2=NH2O+H2O2                              1.40E+04    2.7     6414.0
845. N2H4+O=NH2OH+NH                                  2.90E+11    0.0    -1270.0
846. NH2OH+NH=HNOH+NH2                                2.90E-03    4.4     1564.0
847. NH2OH+NH=NH2O+NH2                                1.50E-03    4.6     2424.0
848. NH2OH+NH2=HNOH+NH3                               1.10E-01    4.0      -97.0
849. NH2OH+NH2=NH2O+NH3                               9.50E+00    3.4    -1013.0
850. H2NN+NH2=HNNNH2+H                                7.90E+06    1.9    -1331.0
851. N2O(+M)=N2+O(+M)                                 1.30E+12    0.0    62570.0
     Low pressure limit:  0.40000E+15  0.00000E+00  0.56600E+05
     N2              Enhanced by    1.700E+00
     O2              Enhanced by    1.400E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    1.200E+01
852. N2O+H=N2+OH                                      3.30E+10    0.0     4729.0
     Declared duplicate reaction...
853. N2O+H=N2+OH                                      4.40E+14    0.0    19254.0
     Declared duplicate reaction...
854. NH+NO=N2O+H                                      2.90E+14   -0.4        0.0
     Declared duplicate reaction...
855. NH+NO=N2O+H                                     -2.20E+13   -0.2        0.0
     Declared duplicate reaction...
856. NNH+O=N2O+H                                      1.00E+14    0.0        0.0
857. NH2+NO=H2+N2O                                    1.00E+13    0.0    33700.0
858. NO+NO=N2O+O                                      3.61E+12    0.0    65335.0
     Declared duplicate reaction...
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859.	N2O+O=NO+NO	6.62E+13	0.0	26611.0
	Declared duplicate reaction...			
860.	N2O+O=O2+N2	1.02E+14	0.0	28001.0
861.	N2O+OH=HNO+NO	1.20E-04	4.3	25080.0
862.	N2O+OH=N2+HO2	1.00E+14	0.0	30000.0
863.	NNH+O2=N2O+OH	2.90E+11	-0.3	149.0
864.	HNO+HNO=N2O+H2O	9.00E+08	0.0	3100.0
865.	NH+N2O=N2+HNO	2.00E+12	0.0	6000.0
866.	N2H2+NO=N2O+NH2	3.00E+10	0.0	0.0
867.	HNNO+M=H+N2O+M	2.20E+15	0.0	21600.0
868.	HNNO+M=N2+OH+M	1.00E+15	0.0	25600.0
869.	HNNO+H=H2+N2O	2.00E+13	0.0	0.0
870.	NH2+NO=HNNO+H	8.00E+13	0.0	28000.0
871.	NNH+HO2=HNNO+OH	2.40E+13	0.0	1698.0
872.	HNNO+NO=N2O+HNO	1.00E+12	0.0	0.0
873.	NH2+NO=NH2NO	3.50E+31	-6.8	3724.0
874.	NH2NO=N2+H2O	3.10E+34	-7.1	36262.0
875.	NH2NO+H=HNNO+H2	4.80E+08	1.5	7407.0
876.	N2H3+O=NH2NO+H	3.00E+13	0.0	0.0
877.	H2NN+OH=NH2NO+H	2.00E+12	0.0	0.0
878.	NH2NO+O=HNNO+OH	3.30E+08	1.5	4697.0
879.	NH2NO+OH=HNNO+H2O	2.40E+06	2.0	-70.0
880.	H2NN+HO2=NH2NO+OH	6.60E+05	1.9	7050.0
881.	NH2NO+HO2=HNNO+H2O2	2.90E+04	2.7	12620.0
882.	NH2NO+NH2=HNNO+NH3	1.80E+06	1.9	4538.0
883.	NH2NHO=NH2+HNO	2.40E+40	-8.7	41584.0
884.	NH2NHO+H=NHNHO+H2	4.80E+08	1.5	-894.0
885.	NH2NHO+O=NHNHO+OH	3.30E+08	1.5	-894.0
886.	NH2NHO+OH=NHNHO+H2O	2.40E+06	2.0	-1192.0
887.	N2H3+HO2=NH2NHO+OH	3.00E+13	0.0	0.0
888.	NH2NHO+HO2=NHNHO+H2O2	2.90E+04	2.7	-1599.0
889.	NH2NHO+NH2=NHNHO+NH3	1.80E+06	1.9	-1152.0

890. NO2(+M)=NO+O(+M) 7.60E+18 -1.3 73245.0

Low pressure limit: 0.24700E+29 -0.33700E+01 0.74756E+05

TROE centering: 0.10000E+00 0.29510E+03 0.97270E+03 0.49816E+04

N2O Enhanced by 1.500E+00

H2O Enhanced by 4.400E+00

N2 Enhanced by 1.000E+00

CO2 Enhanced by 2.300E+00

Declared duplicate reaction...

891. NO+O(+M)=NO2(+M) 1.30E+15 -0.8 0.0

Low pressure limit: 0.47100E+25 -0.28700E+01 0.15510E+04

TROE centering: 0.10000E+00 0.29510E+03 0.97270E+03 0.46816E+04

Declared duplicate reaction...

892. NO2+H=NO+OH 1.30E+14 0.0 357.0

893. NH+O2=H+NO2 2.30E+10 0.0 2482.0

894. NO2+O=O2+NO 3.91E+12 0.0 -238.0

895. NO2+OH=HO2+NO 1.81E+13 0.0 6673.0

896. HON+O2=NO2+OH 1.00E+12 0.0 4968.0

897. NO2+N=N2O+O 3.49E+12 0.0 -437.0

898. NH+NO2=N2O+OH 4.10E+12 0.0 0.0

899. NH+NO2=HNO+NO 5.90E+12 0.0 0.0

900. NH2+NO2=N2O+H2O 3.00E+14 -0.8 242.0

901. NH2+NO2=NH2O+NO 1.30E+15 -0.8 242.0

902. H2NN+O2=NH2+NO2 1.50E+12 0.0 5958.0

903. HNNO+NO=NNH+NO2 3.20E+12 0.0 270.0

904. N2O+NO=NO2+N2 5.30E+05 2.2 46280.0

905. NO+NO+NO=N2O+NO2 1.07E+10 0.0 26800.0

906. HNO+NO+NO=HNNO+NO2 1.70E+11 0.0 2100.0

907. NO2+NO2=NO+NO+O2 1.63E+12 0.0 26108.0

908. HONO(+M)=OH+NO(+M) 1.20E+19 -1.2 49667.0

Low pressure limit: 0.30100E+31 -0.38000E+01 0.50322E+05

TROE centering: 0.37000E+00 0.11980E+02 0.10000E+06

Declared duplicate reaction...

909. NO+OH(+M)=HONO(+M) 1.99E+12 -0.1 -721.0

Low pressure limit: 0.50800E+24 -0.25100E+01 -0.68000E+02

TROE centering: 0.37000E+00 0.11980E+02 0.10000E+06

Declared duplicate reaction...

910. NO2+H2=HONO+H 1.30E+04 2.8 29770.0

911. HONO+H=H2O+NO 8.10E+06 1.9 3843.0

912. HONO+H=OH+HNO 5.60E+10 0.9 4965.0

913. HON+OH=HONO+H 4.00E+13 0.0 0.0

914. HONO+O=OH+NO2 1.20E+13 0.0 5958.0

915. HON+O2=HONO+O 1.00E+12 0.0 4965.0

916. HONO+OH=H2O+NO2 1.26E+10 1.0 135.0

917. NO2+HO2=HONO+O2 6.30E+08 1.2 5000.0

918. NH+HONO=NH2+NO2 1.00E+13 0.0 0.0

919. NH2+HONO=NH3+NO2 7.10E+01 3.0 -4940.0

920. HNNO+NO=N2+HONO 2.60E+11 0.0 810.0

921. HNO+NO2=HONO+NO 4.40E+04 2.6 4040.0

922. NH2O+NO2=HONO+HNO 6.00E+11 0.0 2000.0

923. HNOH+NO2=HONO+HNO 6.00E+11 0.0 2000.0

924. HNNO+NO2=N2O+HONO 1.00E+12 0.0 0.0

925. HONO+HONO=NO+NO2+H2O 3.50E-01 3.6 12140.0

926. HNO2(+M)=HONO(+M) 2.50E+14 0.0 32300.0

Low pressure limit: 0.31000E+19 0.00000E+00 0.31500E+05

TROE centering: 0.11490E+01 0.10000E-29 0.31250E+04 0.10000E+31

927. NO2+H2=HNO2+H 2.40E+00 3.7 32400.0

928. HNO2+O=OH+NO2 1.70E+08 1.5 2363.0

929. HNO2+OH=H2O+NO2 1.20E+06 2.0 -794.0

930. NO2+HO2=HNO2+O2 1.90E+01 3.3 4983.0

931. HNO2+NH2=NO2+NH3 9.20E+05 1.9 874.0

932. HNO+NO2=HNO2+NO 6.02E+11 0.0 1986.0

933. NH+O2=HNOO 3.70E+24 -5.0 2294.0

934. NH+O2+M=HNOO+M 3.00E+26 -4.0 2274.0

935. HNOO+M=OH+NO+M 1.50E+36 -6.2 31119.0

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936. HNOH+HO2=HONHO+OH                                4.00E+13    0.0        0.0
937. NH2+NO2=NH2NO2                                   3.50E+31   -6.8     3726.0
938. NO2+O(+M)=NO3(+M)                                1.32E+13    0.0        0.0
     Low pressure limit:  0.14900E+29 -0.40800E+01  0.24660E+04
     TROE centering:      0.32600E+00  0.50000E+03  0.62049E+04  0.26060E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     HNO3            Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
     NO3             Enhanced by    5.000E+00
939. NO3+H=NO2+OH                                     6.00E+13    0.0        0.0
940. NO3+O=NO2+O2                                     1.00E+13    0.0        0.0
941. NO3+OH=NO2+HO2                                   1.40E+13    0.0        0.0
942. NO3+HO2=NO2+O2+OH                                1.50E+12    0.0        0.0
943. NO3+NH=HNO+NO2                                   1.50E+13    0.0        0.0
944. NO3+NH2=NH2O+NO2                                 9.00E+05    0.0      100.0
945. HNNO+NO2=NNH+NO3                                 1.00E+13    0.0        0.0
946. NO2+NO2=NO3+NO                                   9.60E+09    0.7    20900.0
947. NO3+NO2=NO+NO2+O2                                5.00E+10    0.0     2940.0
948. NO3+NO3=NO2+NO2+O2                               5.12E+11    0.0     4870.0
949. NO2+OH(+M)=HNO3(+M)                              2.41E+13    0.0        0.0
     Low pressure limit:  0.64200E+33 -0.54900E+01  0.23490E+04
     TROE centering:      0.40000E+00  0.45070E+03  0.15840E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     HNO3            Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
     NO3             Enhanced by    5.000E+00
950. HNO3+H=NO3+H2                                    5.60E+08    1.5    16400.0
951. HNO3+H=H2O+NO2                                   6.10E+01    3.3     6285.0
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952. HNO3+H=OH+HONO 3.80E+05 2.3 6976.0

953. HNO3+H=HNO2+OH 6.00E+13 0.0 7000.0

954. HNO3+O=OH+NO3 1.80E+07 0.0 0.0

955. HNO3+OH=H2O+NO3 9.00E+10 0.0 0.0

956. HNO3+OH(+M)=H2O+NO3(+M) 2.47E+08 0.0 -2860.0

Low pressure limit: 0.68900E+15 0.00000E+00 -0.14400E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

HNO3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

957. NO3+H2O2=HNO3+HO2 1.00E+12 0.0 8500.0

958. NO3+NH=HNO3+N 1.00E+12 0.0 5000.0

959. NO3+NH2=HNO3+NH 1.00E+12 0.0 10000.0

960. HNO3+NH=HNOH+NO2 1.50E+13 0.0 6000.0

961. HNO3+NH2=NO3+NH3 9.00E+05 2.0 7300.0

962. HNO3+NH2=NH2O+HNO2 3.00E+12 0.0 9000.0

963. HNO3+NH3=NH2O+H2O+NO 2.32E+01 3.5 44930.0

964. NH3+HNO3=H2O+NH2NO2 8.00E-01 3.5 43100.0

965. HONO+NO2=HNO3+NO 2.00E+11 0.0 32700.0

966. HONO+NO3=HNO3+NO2 1.00E+12 0.0 6000.0

967. HNO2+NO3=HNO3+NO2 1.00E+12 0.0 5000.0

968. N2O4(+M)=NO2+NO2(+M) 4.05E+18 -1.1 12840.0

Low pressure limit: 0.19600E+29 -0.38000E+01 0.12840E+05

969. N2O4+H2O=HONO+HNO3 2.52E+14 0.0 11586.0

970. NH+CH3=CH4+N 8.20E+05 1.9 5848.0

971. C2H5+N=C2H4+NH 4.30E+13 0.0 0.0

972. CH3+NH2=CH4+NH 2.80E+06 1.9 9205.0

973. CH3+NH2=CH2+NH3 1.60E+06 1.9 7566.0

974. CH2SING+NH3=CH3+NH2 1.00E+14 0.0 0.0

975. CH4+NH2=CH3+NH3 1.50E+03 3.0 9940.0

976. C2H+NH3=C2H2+NH2 7.20E+12 0.0 -735.0

977.	C2H4+NH2=C2H3+NH3	5.30E+12	0.0	10274.0
978.	C2H6+NH2=C2H5+NH3	4.50E+01	3.5	5600.0
979.	NNH+CH3<=>CH4+N2	2.50E+13	0.0	0.0
980.	N2H2+CH3=NNH+CH4	1.60E+06	1.9	2969.0
981.	H2NN+CH3=CH4+NNH	1.60E+06	1.9	129.0
982.	N2H3+CH3=N2H2+CH4	8.20E+05	1.9	1817.0
983.	N2H3+CH3=H2NN+CH4	3.00E+13	0.0	0.0
984.	N2H4+CH3=N2H3+CH4	3.30E+06	1.9	5322.0
985.	CH2SING+NO=CH2+NO	1.00E+14	0.0	0.0
986.	C+NO<=>CO+N	2.90E+13	0.0	0.0
987.	CH+NO=HCO+N	6.80E+12	0.0	0.0
988.	CH+NO=CO+NH	9.10E+12	0.0	0.0
989.	CH2+NO=NH2+CO	2.30E+16	-1.4	1331.0
990.	C2+NO=C2O+N	2.30E+13	0.0	8640.0
991.	N+CO2<=>NO+CO	3.00E+12	0.0	11300.0
992.	NH+CO2<=>HNO+CO	1.00E+13	0.0	14350.0
993.	HNO+CH3=NO+CH4	8.20E+05	1.9	480.0
994.	C2H3+NO=C2H2+HNO	1.00E+12	0.0	1000.0
995.	HCO+NO=HNO+CO	7.23E+12	0.0	0.0
996.	HCO+HNO=CH2O+NO	6.00E+11	0.0	2000.0
997.	CH3O+NO=HNO+CH2O	7.50E+12	0.0	2017.0
	Declared duplicate reaction...			
998.	CH3O+NO=HNO+CH2O	2.50E+18	-2.6	0.0
	Declared duplicate reaction...			
999.	CH2OH+NO=CH2O+HNO	1.30E+12	0.0	0.0
1000.	CH3O+HNO=NO+CH3OH	3.20E+13	0.0	0.0
1001.	CH2OH+HNO=NO+CH3OH	3.00E+13	0.0	0.0
1002.	CH2CHO+NO=HNO+CH2CO	1.00E+12	0.0	8600.0
1003.	NH2O+CH3=CH3O+NH2	2.00E+13	0.0	0.0
1004.	NH2O+CH3=CH4+HNO	1.60E+06	1.9	2959.0
1005.	HNOH+CH3=CH4+HNO	1.60E+06	1.9	2095.0
1006.	NH2OH+CH3=HNOH+CH4	1.60E+06	1.9	6345.0

1007. NH2OH+CH3=NH2O+CH4	8.20E+05	1.9	5491.0
1008. CH+NO2=HCO+NO	1.01E+14	0.0	0.0
1009. CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
1010. NO2+CH3=NO+CH3O	1.40E+13	0.0	0.0
1011. C2H3+NO2=NO+CH2CHO	7.70E+14	-0.6	0.0
1012. C2H5+NO2=NO+C2H5O	4.00E+13	-0.2	0.0
1013. CO+NO2=NO+CO2	9.04E+13	0.0	33780.0
1014. HCO+NO2=CO+NO+OH	1.20E+23	-3.3	2355.0
1015. HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
1016. CH3CO+NO2=>CH3+CO2+NO	1.50E+13	0.0	0.0
1017. CH4+NO2=HONO+CH3	6.50E+14	0.0	45800.0
1018. C2H4+NO2=HONO+C2H3	6.50E+14	0.0	41400.0
1019. C2H6+NO2=HONO+C2H5	6.50E+14	0.0	41400.0
1020. HOCO+NO=CO+HONO	1.50E+12	0.0	0.0
1021. HCO+NO2=CO+HONO	1.24E+23	-3.3	2355.0
1022. CH2O+NO2=HCO+HONO	8.02E+02	2.8	13730.0
1023. CH3O+NO2=CH2O+HONO	6.00E+12	0.0	2285.0
1024. CH2OH+NO2=HONO+CH2O	5.00E+12	0.0	0.0
1025. CH3OH+NO2=HONO+CH2OH	1.50E+02	3.3	20035.0
1026. CH2CHO+NO2=CH2CO+HONO	8.90E+12	0.0	-159.0
1027. CH3CHO+NO2=HONO+CH2CHO	1.30E+12	0.0	3700.0
1028. CH4+NO2=HNO2+CH3	6.00E+14	0.0	37600.0
1029. C2H4+NO2=HNO2+C2H3	6.00E+14	0.0	33200.0
1030. C2H6+NO2=HNO2+C2H5	6.00E+14	0.0	33200.0
1031. CH2O+NO2=HNO2+HCO	1.10E-01	4.2	19850.0
1032. CH3OH+NO2=HNO2+CH2OH	2.40E+03	2.9	27470.0
1033. CH2SING+N2O=CH2O+N2	3.80E+13	0.0	0.0
1034. CO+N2O=N2+CO2	2.70E+11	0.0	20237.0
1035. NH2NO+CH3=HNNO+CH4	1.60E+06	1.9	7179.0
1036. NH2NHO+CH3=NHNHO+CH4	1.60E+06	1.9	377.0
1037. CN+M=C+N+M	2.50E+14	0.0	141100.0
N2 Enhanced by 1.500E+00			

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      CO2             Enhanced by    2.400E+00
1038. CH+N=CN+H                                    1.70E+14   -0.1        0.0
1039. CN+O=CO+N                                    1.90E+12    0.5      723.0
1040. NO+C=CN+O                                    1.10E+13    0.0        0.0
1041. CH+NO=OH+CN                                  3.30E+12    0.0        0.0
1042. CN+O2=NO+CO                                  2.80E+17   -2.0        0.0
1043. CN+N=C+N2                                    1.80E+14    0.0        0.0
1044. CN+NO=N2+CO                                  3.90E+11    0.0    27820.0
1045. C+N2O=CN+NO                                  4.80E+12    0.0        0.0
1046. CN+NO2=CO+N2O                                4.90E+14   -0.8      344.0
1047. CN+NO2=N2+CO2                                3.70E+14   -0.8      344.0
1048. C2+N2=CN+CN                                  1.50E+13    0.0    41730.0
1049. HCN(+M)=H+CN(+M)                             8.30E+17   -0.9   123800.0
      Low pressure limit:  0.35700E+27 -0.26000E+01  0.12490E+06
      TROE centering:      0.73420E+00  0.11201E+04  0.10000E+06
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    1.600E+00
      H2              Enhanced by    2.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      C2H6            Enhanced by    3.000E+00
      AR              Enhanced by    7.000E-01
1050. CH2+N=HCN+H                                  5.00E+13    0.0        0.0
1051. CN+H2=HCN+H                                  3.60E+08    1.6     2999.0
1052. CH+NH=HCN+H                                  3.00E+13    0.0        0.0
1053. CH3+N=HCN+H2                                 3.70E+12    0.1      -89.0
1054. C2H3+N=HCN+CH2                               2.00E+13    0.0        0.0
1055. CH4+CN=CH3+HCN                               8.60E+05    2.3      -32.0
1056. C3H3+N=HCN+C2H2                              1.00E+13    0.0        0.0
1057. C2H6+CN=C2H5+HCN                             1.20E+08    1.8     -994.0
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1058. CH+N2=HCN+N                                     4.40E+12    0.0    21964.0
1059. CH2+N2=HCN+NH                                   1.00E+13    0.0    73954.0
1060. CH2SING+N2<=>NH+HCN                             1.00E+11    0.0    65000.0
1061. CN+NH3=HCN+NH2                                  9.20E+12    0.0     -357.0
1062. HCN+N2=H+CN+N2                                  3.60E+26   -2.6   124890.0
1063. HCN+O=NH+CO                                     3.50E+03    2.6     4980.0
1064. HCN+O=CN+OH                                     4.20E+10    0.4    20663.0
1065. HCN+OH=CN+H2O                                   3.90E+06    1.8    10287.0
1066. OH+HCN=NH2+CO                                   7.83E-04    4.0     4000.0
1067. HCN+O2=CN+HO2                                   3.00E+13    0.0    75100.0
1068. HCCO+N=HCN+CO                                   5.00E+13    0.0        0.0
1069. CH2O+CN=HCO+HCN                                 1.70E+03    2.7    -1427.0
1070. CH+NO=HCN+O                                     5.30E+13    0.0        0.0
1071. CH2+NO=HCN+OH                                   2.90E+14   -0.7      755.0
1072. CH2SING+NO<=>OH+HCN                             2.90E+14   -0.7      760.0
1073. CH3+NO=HCN+H2O                                  4.90E+08    0.5    12392.0
1074. C2H+NO=HCN+CO                                   6.00E+13    0.0      570.0
1075. C2H3+NO=HCN+CH2O                                7.00E+21   -3.4     1025.0
1076. HCCO+NO=HCN+CO2                                 3.70E+14   -0.8      -90.0
1077. CN+HNO=HCN+NO                                   1.80E+13    0.0        0.0
1078. CN+HONO=HCN+NO2                                 1.20E+13    0.0        0.0
1079. CH+N2O=HCN+NO                                   1.90E+13    0.0     -511.0
1080. HCN=HNC                                         1.50E+23   -4.2    49428.0
1081. HCN+M=HNC+M                                     1.60E+26   -3.2    54600.0
      AR              Enhanced by    7.000E-01
      H2O             Enhanced by    7.000E+00
      CO2             Enhanced by    2.000E+00
      Warning...superceding enhancement factor for AR
      AR              Enhanced by    7.000E-01
      Warning...superceding enhancement factor for H2O
      H2O             Enhanced by    7.000E+00
      Warning...superceding enhancement factor for CO2
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      CO2             Enhanced by    2.000E+00
      Warning...superceding enhancement factor for AR
      AR              Enhanced by    7.000E-01
      Warning...superceding enhancement factor for H2O
      H2O             Enhanced by    7.000E+00
      Warning...superceding enhancement factor for CO2
      CO2             Enhanced by    2.000E+00
1082. HNC+H=HCN+H                                   7.80E+13    0.0     3600.0
1083. O+HNC=NH+CO                                   4.60E+12    0.0     2184.0
1084. HNC+OH=CN+H2O                                 1.50E+12    0.0     7680.0
1085. HNC+O2=NH+CO2                                 1.60E+19   -2.2     1777.0
1086. H+HCN(+M)<=>NCH2(+M)                          3.30E+13    0.0        0.0
      Low pressure limit:  0.14000E+27 -0.34000E+01  0.19000E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
      AR              Enhanced by    7.000E-01
      N2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
1087. CH+NH3=NCH2+H+H                               4.40E+13    0.0     -630.0
1088. NCH2+H=HCN+H2                                 2.40E+08    1.5     -894.0
1089. CH3+N=NCH2+H                                  6.10E+14   -0.3      288.0
1090. CH+NH2=NCH2+H                                 3.00E+13    0.0        0.0
1091. CH3+NH=NCH2+H2                                3.50E+13    0.0      290.0
1092. NCH2+CH3=HCN+CH4                              8.10E+05    1.9    -1112.0
1093. C2H5+N=CH3+NCH2                               2.30E+13    0.0        0.0
1094. NCH2+N=HCN+NH                                 7.20E+13    0.0      400.0
1095. NCH2+N=N2+CH2                                 6.00E+13    0.0      397.0
1096. NCH2+NH=HCN+NH2                               1.70E+08    1.5     -894.0
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1097.	NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0
1098.	CH2+NO=NCH2+O	8.10E+07	1.4	4111.0
1099.	NCH2+O=HCN+OH	1.70E+08	1.5	-894.0
1100.	CH3+NO=NCH2+OH	1.50E-01	3.5	3950.0
1101.	NCH2+OH=HCN+H2O	1.50E+19	-2.2	2166.0
	Declared duplicate reaction...			
1102.	NCH2+OH=HCN+H2O	1.20E+06	2.0	-1192.0
	Declared duplicate reaction...			
1103.	NCH2+O2=CH2O+NO	3.00E+12	0.0	5958.0
1104.	NCH2+O2=HCN+HO2	2.70E+04	2.0	17300.0
1105.	NCH2+HO2=HCN+H2O2	1.40E+04	2.7	-1609.0
1106.	NCH2+NO=HCN+HNO	1.00E+07	2.0	4400.0
1107.	CHNH=HCN+H	6.10E+28	-5.7	24257.0
1108.	CH3+N=CHNH+H	1.20E+11	0.5	-367.0
1109.	CHNH+H=NCH2+H	2.00E+13	0.0	0.0
1110.	CHNH+H=HCN+H2	2.40E+08	1.5	-894.0
1111.	CHNH+O=HCN+OH	1.70E+08	1.5	-894.0
1112.	CHNH+OH=HCN+H2O	1.20E+06	2.0	-1192.0
1113.	CHNH+CH3=HCN+CH4	8.20E+05	1.9	-1112.0
1114.	CH2NH+M=HCN+H2+M	1.00E+14	0.0	10000.0
1115.	NH+CH3=CH2NH+H	4.00E+13	0.0	0.0
1116.	CH2NH+H=NCH2+H2	2.40E+08	1.5	7318.0
1117.	CH2NH+H=CHNH+H2	3.00E+08	1.5	6126.0
1118.	CH+NH3=CH2NH+H	4.40E+13	0.0	-630.0
1119.	CH2SING+NH2=CH2NH+H	3.00E+13	0.0	0.0
1120.	CH2SING+NH3=CH2NH+H+H	1.00E+14	0.0	0.0
1121.	CH3+NH2<=>CH2NH+H2	2.40E+06	1.2	17369.0
1122.	CH2NH+O=NCH2+OH	1.70E+08	1.5	4627.0
1123.	CH2NH+O=CHNH+OH	2.20E+08	1.5	5402.0
1124.	CH2NH+O=CH2O+NH	1.70E+06	2.1	0.0
1125.	CH2NH+OH=NCH2+H2O	1.20E+06	2.0	-89.0
1126.	CH2NH+OH=CHNH+H2O	2.40E+06	2.0	457.0

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1127. CH2NH+OH=CH2O+NH2                                1.80E+05    2.0    14800.0
1128. NCH2+HO2=CH2NH+O2                                1.40E+04    2.7    -1609.0
1129. CH2NH+CH3=NCH2+CH4                               8.20E+05    1.9     7119.0
1130. CH2NH+CH3=CHNH+CH4                               5.30E+05    1.9     9681.0
1131. CH2NH+NH2=NCH2+NH3                               9.20E+05    1.9     4438.0
1132. CH2NH+NH2=CHNH+NH3                               1.80E+06    1.9     6087.0
1133. CH3N(+AR)<=>CH2NH(+AR)                           1.83E+13    0.2    43980.0
      Low pressure limit:  0.22300E+29 -0.44500E+01  0.46000E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
1134. CH3N(+AR)<=>NCH2+H(+AR)                          7.40E+11    0.9    35470.0
      Low pressure limit:  0.18700E+31 -0.45200E+01  0.37950E+05
      TROE centering:      0.74900E+00  0.21800E+03  0.10000E+02  0.26000E+09
1135. CH3NH=CH2NH+H                                    1.30E+42   -9.2    41316.0
      Declared duplicate reaction...
1136. CH3NH(+AR)<=>CH2NH+H(+AR)                        7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      Declared duplicate reaction...
1137. CH3NH+M=CH3+NH+M                                 1.00E+14    0.0    18000.0
1138. CH3+NH2<=>CH3NH+H                                9.08E+13   -0.4    15714.0
1139. CH3NH+H=CH2NH+H2                                 7.20E+08    1.5     -894.0
1140. CH3NH+O=CH2NH+OH                                 5.00E+08    1.5     -894.0
1141. CH3NH+O=CH3O+NH                                  6.00E+13    0.0        0.0
1142. CH3NH+OH=CH2NH+H2O                               3.60E+06    2.0    -1192.0
1143. CH3NH+OH=CH4+HNO                                 6.00E+12    0.0        0.0
1144. HNOH+CH3=CH3NH+OH                                2.00E+13    0.0        0.0
1145. CH3NH+O2=CH2NH+HO2                               1.00E+07    2.0     6300.0
1146. CH3NH+O2=CH3O+HNO                                6.00E+12    0.0     4000.0
1147. CH3NH+CH3=CH2NH+CH4                              2.40E+06    1.9    -1112.0
1148. CH2NH2=CH2NH+H                                   2.40E+48  -10.8    52010.0
      Declared duplicate reaction...
1149. CH2NH2(+AR)<=>CH2NH+H(+AR)                       7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
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      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
      Declared duplicate reaction...
1150. CH3+NH2<=>CH2NH2+H                              5.15E+14   -0.6    10155.0
1151. CH2NH2+H=CH2NH+H2                               4.80E+08    1.5     -894.0
1152. CH2NH2+O=CH2O+NH2                               7.00E+13    0.0        0.0
1153. CH2NH2+O=CH2NH+OH                               3.30E+08    1.5     -894.0
1154. CH2NH2+OH=CH2OH+NH2                             4.00E+13    0.0        0.0
1155. CH2NH2+OH=CH2NH+H2O                             2.40E+06    2.0    -1192.0
1156. CH2NH2+O2=CH2NH+HO2                             1.00E+22   -3.1     6752.0
1157. CH2NH2+O2=NH2+CH2O+O                            6.00E+18   -1.6    30175.0
1158. CH2NH2+CH3=C2H5+NH2                             2.00E+13    0.0     2701.0
1159. CH2NH2+CH3=CH2NH+CH4                            1.60E+06    1.9     -626.0
1160. CH3+NH2<=>CH3NH2                                1.03E+33   -6.3     5750.0
1161. CH3+NH2(+M)=CH3NH2(+M)                          7.20E+12    0.4        0.0
      Low pressure limit:  0.22000E+31 -0.38500E+01  0.00000E+00
1162. CH3NH2(+AR)<=>CH2NH+H2(+AR)                     9.99E+08    1.2   102880.0
      Low pressure limit:  0.24600E+31 -0.47500E+01  0.10700E+06
      TROE centering:      0.82000E+00  0.15459E+03  0.10000E+01  0.40100E+06
1163. CH3NH2+M=CH2NH+H2+M                             2.40E+13    0.0   107260.0
1164. CH3NH2(+AR)<=>CH2NH2+H(+AR)                     3.93E+15   -0.1    93820.0
      Low pressure limit:  0.68200E+41 -0.70100E+01  0.98400E+05
      TROE centering:      0.00000E+00  0.23101E+03  0.10000E+01  0.40100E+06
1165. CH3NH2(+AR)<=>CH3NH+H(+AR)                      1.44E+16   -0.3   100940.0
      Low pressure limit:  0.11400E+39 -0.63500E+01  0.10500E+06
      TROE centering:      0.67000E+00  0.16967E+03  0.10000E+01  0.40100E+06
1166. CH3NH2+H=CH2NH2+H2                              5.60E+08    1.5     5461.0
1167. CH3NH2+H=CH3NH+H2                               4.80E+08    1.5     9701.0
1168. CH3NH2+O=CH2NH2+OH                              4.00E+08    1.5     5193.0
1169. CH3NH2+O=CH3NH+OH                               3.30E+08    1.5     6345.0
1170. CH3NH2+OH=CH2NH2+H2O                            3.60E+06    2.0      238.0
1171. CH3NH2+OH=CH3NH+H2O                             2.40E+06    2.0      447.0
1172. CH3NH2+CH3=CH2NH2+CH4                           1.50E+06    1.9     9163.0
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1173. CH3NH2+CH3=CH3NH+CH4	1.60E+06	1.9	8837.0
1174. CH3NH2+NH2=CH2NH2+NH3	2.80E+06	1.9	5491.0
1175. CH3NH2+NH2=CH3NH+NH3	1.80E+06	1.9	7139.0
1176. CH3NCH=CH3+HCN	8.10E+15	-2.4	14942.0
1177. CH3NCH+H=CH2NCH2+H	2.00E+13	0.0	0.0
1178. CH2NCH2=CH3NCH	1.30E+45	-10.1	66111.0
1179. CH2NCH2+H=CH3+NCH2	3.00E+13	0.0	0.0
1180. CH2NCH2+O=CH2O+NCH2	3.00E+13	0.0	0.0
1181. CH2NCH2+OH=CH2OH+NCH2	2.00E+13	0.0	0.0
1182. CH2NCH2+H=CH3NCH2	5.80E+13	0.2	-125.0
1183. CH3NCH2+H=CH2NCH2+H2	5.60E+08	1.5	5464.0
1184. CH3NCH2+H=CH3NCH+H2	3.00E+08	1.5	6130.0
1185. CH3NCH2+O=CH2NCH2+OH	4.00E+08	1.5	5196.0
1186. CH3NCH2+O=CH3NCH+OH	2.20E+08	1.5	5404.0
1187. CH3NCH2+OH=CH2NCH2+H2O	8.00E+12	0.0	0.0
1188. CH3NCH2+OH=CH3NCH+H2O	2.40E+06	2.0	457.0
1189. CH3NCH2+CH3=CH2NCH2+CH4	1.50E+06	1.9	9170.0
1190. CH3NCH2+CH3=CH3NCH+CH4	5.30E+05	1.9	9687.0
1191. CH3NCH2+NH2=CH2NCH2+NH3	2.80E+06	1.9	5494.0
1192. CH3NCH2+NH2=CH3NCH+NH3	1.80E+06	1.9	6090.0
1193. CH3NCH3=CH3NCH2+H	1.60E+15	-7.5	38425.0
1194. CH3NCH3+H=CH3NCH2+H2	3.20E+12	0.0	0.0
1195. CH3NCH3+OH=CH3NCH2+H2O	2.40E+13	0.0	0.0
1196. CH3NCH3+CH3=CH3NCH2+CH4	6.00E+12	0.0	0.0
1197. CH3NHCH2=CH3+CH2NH	9.80E+43	-10.3	37459.0
1198. CH3NHCH2=CH3NCH2+H	5.90E+44	-10.3	46803.0
1199. CH3NHCH2+H=CH3NCH2+H2	4.80E+08	1.5	-894.0
1200. CH3NHCH2+O=CH2O+CH3NH	7.00E+13	0.0	0.0
1201. CH3NHCH2+O=CH3NCH2+OH	3.30E+08	1.5	-894.0
1202. CH3NHCH2+OH=CH2OH+CH3NH	4.00E+13	0.0	0.0
1203. CH3NHCH2+OH=CH3NCH2+H2O	2.40E+06	2.0	-1192.0
1204. CH3NHCH2+CH3=C2H5+CH3NH	2.00E+13	0.0	2702.0

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1205. CH3NHCH2+CH3=CH3NCH2+CH4                        1.60E+06    1.9     -626.0
1206. CH3NHCH2+H(+M)=CH3NHCH3(+M)                     5.20E+17   -1.0     1580.0
      Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
      TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
1207. CH3NCH3+H=CH3NHCH3                              1.00E+12    0.0        0.0
1208. CH3NHCH3+H=CH3NHCH2+H2                          5.60E+08    1.5     5464.0
1209. CH3NHCH3+H=CH3NCH3+H2                           4.80E+08    1.5     9706.0
1210. CH3NHCH3+O=CH3NHCH2+OH                          6.10E+12    0.0      556.0
1211. CH3NHCH3+O=CH3NCH3+OH                           3.00E+12    0.0      556.0
1212. CH3NHCH3+OH=CH3NHCH2+H2O                        2.00E+13    0.0        0.0
1213. CH3NHCH3+OH=CH3NCH3+H2O                         1.90E+13    0.0        0.0
1214. CH3NHCH3+CH3=CH3NHCH2+CH4                       1.50E+06    1.9     9170.0
1215. CH3NHCH3+CH3=CH3NCH3+CH4                        1.60E+06    1.9     8842.0
1216. CH3NHCH3+NH2=CH3NHCH2+NH3                       2.80E+06    1.9     5494.0
1217. CH3NHCH3+NH2=CH3NCH3+NH3                        1.80E+06    1.9     7143.0
1218. CHCNH+H=CH2+HNC                                 1.50E+14    0.0        0.0
1219. CHCNH+O=H+CO+HNC                                1.00E+14    0.0        0.0
1220. CHCNH+OH=HCO+CHNH                               1.00E+13    0.0        0.0
1221. CHCNH+O2=HNC+CO+OH                              1.60E+11    0.0     1020.0
1222. CHCNH+O2=HNC+HCO+O                              2.20E+02    2.7     3540.0
1223. CH2SING+HCN=CH2CN+H                             1.80E+14    0.0        0.0
1224. CH3+CN=CH2CN+H                                  1.00E+14    0.0        0.0
1225. CH2CN+O=CH2O+CN                                 1.00E+14    0.0        0.0
1226. CH2OH+CN=CH2CN+OH                               5.00E+13    0.0        0.0
1227. CH3CN=CH2CN+H                                   7.90E+14    0.0    94940.0
1228. CH3CN+H=HCN+CH3                                 4.40E+10    0.8     6800.0
1229. CH3CN+H=HNC+CH3                                 2.80E+15   -0.3    20030.0
1230. CH3CN+H=CH2CN+H2                                6.00E+04    3.0     8522.0
1231. CH3CN+O=CH2CN+OH                                4.70E+08    1.2    14360.0
1232. CH3CN+OH=CH2CN+H2O                              2.00E+07    2.0     2000.0
1233. CH3CN+CH3=CH2CN+CH4                             5.00E+12    0.0     7000.0
1234. CH3CN+CN=CH2CN+HCN                              5.00E+13    0.0     2000.0
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1235.	c-C2H3N=CH3CN	4.70E+13	0.0	41500.0
1236.	c-C2H3N+H=CH2NCH2	9.80E+09	1.2	1969.0
1237.	c-C2H3N+H=CH2CHNH	1.10E+10	1.2	2422.0
1238.	c-C2H3N+O=>NCH2+HCO	1.00E+13	0.0	0.0
1239.	c-C2H3N+O=>C2H3+NO	1.00E+13	0.0	0.0
1240.	c-C2H3N+OH=>NCH2+CH2O	5.00E+12	0.0	0.0
1241.	CH2CHN(S)+M=CH2CHN+M	1.00E+13	0.0	0.0
	H Enhanced by 0.000E+00			
1242.	CH2CHN(S)+H=CH2CHN+H	1.00E+14	0.0	0.0
1243.	CH2CHN(S)+H=CH3+HCN	3.00E+13	0.0	0.0
1244.	CH2CHN(S)=c-C2H3N	3.00E+13	0.0	4000.0
1245.	CH2CHN(S)=CH3CN	3.00E+13	0.0	8000.0
1246.	CH2CHN(S)+O=>HCO+HCN+H	3.00E+13	0.0	0.0
1247.	CH2CHN(S)+OH=>CH2O+HCN+H	3.00E+13	0.0	0.0
1248.	CH2CNH=CH3CN	2.50E+13	0.0	70300.0
1249.	CH2CNH+H=CH3CN+H	3.00E+13	0.0	0.0
1250.	CH2CNH+H=CH3+HNC	3.30E+10	0.9	2840.0
1251.	CH2CNH+H=CHCNH+H2	3.00E+07	2.0	10000.0
1252.	CH2CNH+H=CH2CN+H2	2.40E+08	1.5	7322.0
1253.	CH2CNH+O=CH2+HNCO	1.80E+12	0.0	1350.0
1254.	CH2CNH+O=CHCNH+OH	2.00E+07	2.0	10000.0
1255.	CH2CNH+O=CH2CN+OH	1.70E+08	1.5	4630.0
1256.	CH2CNH+OH=CH2OH+HNC	1.00E+12	0.0	-1013.0
1257.	CH2CNH+OH=CHCNH+H2O	1.00E+07	2.0	3000.0
1258.	CH2CNH+OH=CH2CN+H2O	1.20E+06	2.0	-89.0
1259.	CH2CNH+CH3=CH2CN+CH4	8.20E+05	1.9	7123.0
1260.	CH2CNH+NH2=CH2CN+NH3	9.20E+05	1.9	4441.0
1261.	CH2CHN+H=CH3+HCN	1.00E+13	0.0	0.0
1262.	CH2CHN+O=CH2O+HCN	5.00E+13	0.0	0.0
1263.	CHCNH2+H=CHCNH+H2	4.80E+08	1.5	9706.0
1264.	CHCNH2+O=CHCNH+OH	3.30E+08	1.5	6348.0
1265.	CHCNH2+O=HCCO+NH2	1.40E+07	2.0	1900.0

1266.	CHCNH2+OH=CHCNH+H2O	2.00E+12	0.0	0.0
1267.	CHCNH2+CH3=CHCNH+CH4	1.60E+06	1.9	8842.0
1268.	CHCNH2+NH2=CHCNH+NH3	1.80E+06	1.9	7143.0
1269.	CH3+HCN=CH3CHN	1.00E+12	0.0	9900.0
1270.	CH3CHN+H=CH3CN+H2	2.40E+08	1.5	-894.0
1271.	CH3CHN+H=CH2CHN+H2	9.00E+13	0.0	15100.0
1272.	CH2CHN(S)+H2=CH3CHN+H	7.20E+13	0.0	0.0
1273.	CH3CHN+O=CH3CN+OH	1.70E+08	1.5	-894.0
1274.	CH3CHN+OH=CH3CN+H2O	1.20E+06	2.0	-1192.0
1275.	CH3CHN+OH=CH2CHN+H2O	1.10E+03	3.0	2780.0
1276.	CH3CHN+OH=CH2CHN(S)+H2O	4.40E+13	-0.3	-727.0
1277.	CH3CHN+NH2=CH3CN+NH3	9.20E+05	1.9	-1152.0
1278.	CH3CNH=CH3+HNC	6.50E+18	-2.5	33000.0
1279.	CH3CNH=CH3CN+H	7.70E+25	-5.2	24000.0
1280.	CH3CNH+H=CH3+CHNH	2.10E+13	0.0	0.0
1281.	CH3CNH+H=CH2CNH+H2	1.20E+13	0.0	0.0
1282.	CH3CNH+H=CH3CN+H2	2.40E+08	1.5	-894.0
1283.	CH3CNH+O=CH2CNH+OH	5.30E+13	0.0	0.0
1284.	CH3CNH+O=CH3CN+OH	1.70E+08	1.5	-894.0
1285.	CH3CNH+OH=CH2CNH+H2O	1.20E+13	0.0	0.0
1286.	CH3CNH+OH=CH3CN+H2O	1.20E+06	2.0	-1192.0
1287.	CH3CNH+O2=CH2O+CO+NH2	1.90E+12	0.0	0.0
1288.	CH3CNH+CH3=CH2CNH+CH4	5.30E+13	0.0	0.0
1289.	CH3CNH+CH3=CH3CN+CH4	8.20E+05	1.9	-1113.0
1290.	CH2CHNH+H=CH3+CHNH	1.00E+14	0.0	0.0
1291.	CH2CHNH+H=CH3CNH+H	3.00E+13	0.0	0.0
1292.	CH2CHNH+H=CH2CNH+H2	2.00E+13	0.0	0.0
1293.	CH2CHNH+O=CH2CNH+OH	2.00E+13	0.0	0.0
1294.	CH2CHNH+OH=CH2CNH+H2O	2.00E+13	0.0	0.0
1295.	CH2CHNH+OH=CH2OH+CHNH	1.00E+13	0.0	0.0
1296.	CH2CHNH+O2=CH2O+CO+NH2	5.70E+17	-1.8	11067.0
1297.	CHCNH2+H(+M)=CH2CNH2(+M)	1.70E+10	1.3	2709.0

Low pressure limit: 0.63000E+32 -0.46640E+01 0.37800E+04

TROE centering: 0.78780E+00 -0.10212E+05 0.10000E+31

H2 Enhanced by 2.000E+00

CO Enhanced by 2.000E+00

CO2 Enhanced by 3.000E+00

H2O Enhanced by 5.000E+00

1298.	CH2CNH2+H=CHCNH2+H2	4.50E+13	0.0	0.0
1299.	CH2CNH2+O=CH2CO+NH2	3.00E+13	0.0	0.0
1300.	CH2CNH2+OH=CHCNH2+H2O	2.00E+13	0.0	0.0
1301.	CH2CNH2+O2=OCHCHO+NH2	4.00E+12	0.0	0.0
1302.	CH2CNH2+CH3=CHCNH2+CH4	2.00E+13	0.0	0.0
1303.	NH2+C2H2=CHCHNH2	7.80E-18	8.3	7430.0
1304.	CHCNH2+H(+M)=CHCHNH2(+M)	1.70E+10	1.3	2709.0

Low pressure limit: 0.63000E+32 -0.46640E+01 0.37800E+04

TROE centering: 0.78780E+00 -0.10212E+05 0.10000E+31

H2 Enhanced by 2.000E+00

CO Enhanced by 2.000E+00

CO2 Enhanced by 3.000E+00

H2O Enhanced by 5.000E+00

1305.	CHCHNH2+H=CHCNH2+H2	4.50E+13	0.0	0.0
1306.	CHCHNH2+OH=CHCNH2+H2O	2.00E+13	0.0	0.0
1307.	CHCHNH2+O2=OCHCHO+NH2	4.00E+12	0.0	0.0
1308.	CHCHNH2+CH3=CHCNH2+CH4	2.00E+13	0.0	0.0
1309.	CH2CHNH+H=CH3CHNH	5.80E+13	0.2	-125.0
1310.	CH3+CHNH=CH3CHNH	1.80E+13	0.0	0.0
1311.	CH3CHNH+H=CH3CNH+H2	4.70E+13	-0.3	3000.0
1312.	CH3CHNH+H=CH2CHNH+H2	1.90E+12	0.4	5359.0
1313.	CH3CHNH+H=CH3CHN+H2	2.40E+08	1.5	7322.0
1314.	CH3CHNH+O=CH3CNH+OH	1.80E+18	-1.9	2975.0
1315.	CH3CHNH+O=CH2CHNH+OH	3.70E+13	-0.2	3556.0
1316.	CH3CHNH+O=CH3CHN+OH	1.70E+08	1.5	4630.0
1317.	CH3CHNH+OH=CH3CNH+H2O	2.40E+11	0.3	-1000.0

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1318. CH3CHNH+OH=CH2CHNH+H2O                          3.00E+13   -0.6      800.0
1319. CH3CHNH+OH=CH3CHN+H2O                           1.20E+06    2.0      -89.0
1320. CH3CHNH+CH3=CH3CNH+CH4                          3.90E-07    5.8     2200.0
1321. CH3CHNH+CH3=CH2CHNH+CH4                         2.50E+01    3.1     5727.0
1322. CH3CHNH+CH3=CH3CHN+CH4                          8.20E+05    1.9     7123.0
1323. CH3CHNH+NH2=CH3CHN+NH3                          9.20E+05    1.9     4441.0
1324. CHCHNH2+H(+M)=CH2CHNH2(+M)                      3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1325. CH2CNH2+H(+M)=CH2CHNH2(+M)                      3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1326. CH3CHNH=CH2CHNH2                                5.00E+18   -2.5    67995.0
1327. CH2CHNH2+H=CHCHNH2+H2                           2.40E+02    3.6    11266.0
1328. CH2CHNH2+H=CH2CNH2+H2                           2.40E+02    3.6    11266.0
1329. CH2CHNH2+H=CH2CHNH+H2                           4.80E+08    1.5     9700.0
1330. CH3CHNH+H=CH2CHNH2+H                            3.00E+13    0.0        0.0
1331. CH2CHNH2+O=CH2CHNH+OH                           3.30E+08    1.5     6348.0
1332. CH2CHNH2+OH=CHCHNH2+H2O                         1.30E-01    4.2     -860.0
1333. CH2CHNH2+OH=CH2CNH2+H2O                         1.30E-01    4.2     -860.0
1334. CH2CHNH2+OH=CH2CHNH+H2O                         2.40E+06    2.0      447.0
1335. CH2CHNH2+CH3=CHCHNH2+CH4                        6.00E+07    1.6    16630.0
1336. CH2CHNH2+CH3=CH2CNH2+CH4                        6.00E+07    1.6    16630.0
1337. CH2CHNH2+CH3=CH2CHNH+CH4                        1.60E+06    1.9     8842.0
1338. CH2CHNH2+NH2=CHCHNH2+NH3                        5.30E+12    0.0    10274.0
1339. CH2CHNH2+NH2=CH2CNH2+NH3                        5.30E+12    0.0    10274.0
1340. CH2CHNH2+NH2=CH2CHNH+NH3                        1.80E+06    1.9     7143.0
1341. CH3CH2NH=CH2NH+CH3                              1.90E+10    0.0    23500.0
1342. CH3CH2NH=CH3CHNH+H                              1.60E+36   -7.9    36342.0
1343. CH3CH2NH+H=CH3+CH2NH2                           1.40E+12    0.7      346.0
1344. CH3CH2NH+H=CH3CHNH+H2                           7.20E+08    1.5     -894.0
1345. CH3CH2NH+O=CH3CHNH+OH                           5.00E+08    1.5     -894.0
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1346. CH3CH2NH+OH=CH3CHNH+H2O                          3.60E+06    2.0    -1192.0
1347. CH3CH2NH+CH3=CH3CHNH+CH4                         2.40E+06    1.9    -1113.0
1348. CH2CHNH2+H(+M)=CH3CHNH2(+M)                      1.40E+09    1.5     1355.0
      Low pressure limit:  0.20000E+40 -0.66420E+01  0.57690E+04
      TROE centering:     -0.56900E+00  0.29900E+03  0.91470E+04  0.15240E+03
1349. CH3CHNH2=CH3CHNH+H                               1.10E+45  -10.2    47817.0
1350. CH3CHNH2+H=CH2CHNH2+H2                           4.90E+08    1.7      588.0
1351. CH3CHNH2+H=CH3+CH2NH2                            8.40E+16   -0.9     2903.0
1352. CH3CHNH2+H=C2H4+NH3                              4.70E+21   -3.0     2845.0
1353. CH3CHNH2+H=C2H5+NH2                              2.00E+13    0.0        0.0
1354. CH3CHNH2+O=CH2CHNH2+OH                           2.50E+13    0.0        0.0
1355. CH3CHNH2+OH=CH2CHNH2+H2O                         2.40E+13    0.0        0.0
1356. CH3CHNH2+O2=CH2CHNH2+HO2                         6.70E+20   -3.0     2504.0
1357. CH3CHNH2+CH3=CH2CHNH2+CH4                        1.80E+13    0.0     -769.0
1358. C2H4+NH2=CH2CH2NH2                               1.20E+11    0.0     3955.0
1359. CH2CH2NH2+H=CH2CHNH2+H2                          1.80E+12    0.0        0.0
1360. CH2CH2NH2+O=CH2O+CH2NH2                          9.60E+13    0.0        0.0
1361. CH2CH2NH2+OH=CH2CHNH2+H2O                        2.40E+13    0.0        0.0
1362. CH2CH2NH2+HO2=>CH2O+OH+CH2NH2                    2.40E+13    0.0        0.0
1363. CH2CH2NH2+O2=CH2CHNH2+HO2                        3.70E+16   -1.6     3418.0
1364. CH2CH2NH2+CH3=CH2CHNH2+CH4                       1.20E+13   -0.3        0.0
1365. CH3CH2NH2=C2H4+NH3                               6.20E+67  -15.9    99348.0
1366. C2H5+NH2(+M)=CH3CH2NH2(+M)                       7.20E+12    0.4        0.0
      Low pressure limit:  0.22000E+31 -0.38500E+01  0.00000E+00
1367. CH3CHNH2+H=CH3CH2NH2                             1.70E+13    0.2        0.0
1368. CH2CH2NH2+H=CH3CH2NH2                            5.40E+13    0.2        0.0
1369. CH3CH2NH2+H=CH2CH2NH2+H2                         1.20E+07    1.8     5100.0
1370. CH3CH2NH2+H=CH3CHNH2+H2                          2.60E+07    1.6     2830.0
1371. CH3CH2NH2+H=CH3CH2NH+H2                          4.80E+08    1.5     9700.0
1372. CH3CH2NH2+O=CH2CH2NH2+OH                         9.40E+07    1.7     5460.0
1373. CH3CH2NH2+O=CH3CHNH2+OH                          6.80E+12    0.0     1275.0
1374. CH3CH2NH2+O=CH3CH2NH+OH                          3.30E+08    1.5     6348.0
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1375.	CH3CH2NH2+OH=CH2CH2NH2+H2O	1.60E+12	0.0	1300.0
1376.	CH3CH2NH2+OH=CH3CHNH2+H2O	1.40E+13	0.0	0.0
1377.	CH3CH2NH2+OH=CH3CH2NH+H2O	2.40E+06	2.0	447.0
1378.	CH3CH2NH2+HO2=CH2CH2NH2+H2O2	1.20E+04	2.5	15750.0
1379.	CH3CH2NH2+HO2=CH3CHNH2+H2O2	8.20E+03	2.5	10750.0
1380.	CH3CH2NH2+CH3=CH2CH2NH2+CH4	2.20E+02	3.2	9620.0
1381.	CH3CH2NH2+CH3=CH3CHNH2+CH4	7.30E+02	3.0	7950.0
1382.	CH3CH2NH2+CH3=CH3CH2NH+CH4	1.60E+06	1.9	8842.0
1383.	CH3CH2NH2+NH2=CH2CH2NH2+NH3	2.20E+02	3.2	9620.0
1384.	CH3CH2NH2+NH2=CH3CHNH2+NH3	7.30E+02	3.0	7950.0
1385.	CH3CH2NH2+NH2=CH3CH2NH+NH3	1.80E+06	1.9	7140.0
1386.	CH2CH2NH2+HCO=CH3CH2NH2+CO	6.00E+13	0.0	0.0
1387.	CH3CHNH2+HCO=CH3CH2NH2+CO	1.20E+14	0.0	0.0
1388.	CH+N2=NCN+H	3.70E+07	1.4	20723.0
1389.	H+NCN=HCN+N	1.89E+14	0.0	8425.0
1390.	NCN+O=CN+NO	1.00E+14	0.0	0.0
1391.	NCN+OH=HCN+NO	5.00E+13	0.0	0.0
1392.	NCN+N=CN+N2	2.00E+13	0.0	0.0
1393.	CN+N2O=NCN+NO	3.80E+03	2.6	3700.0
1394.	CH+N2=HCNN	3.60E+28	-5.8	2621.0
1395.	HCNN+H<=>CH2+N2	1.00E+14	0.0	0.0
1396.	HCNN+O<=>CO+H+N2	2.20E+13	0.0	0.0
1397.	HCNN+O<=>HCN+NO	2.00E+12	0.0	0.0
1398.	HCNN+OH<=>H+HCO+N2	1.20E+13	0.0	0.0
1399.	HCNN+O2=H+CO2+N2	4.00E+12	0.0	0.0
1400.	HCNN+O2=HCO+N2O	4.00E+12	0.0	0.0
1401.	HCNN+O2<=>O+HCO+N2	1.20E+13	0.0	0.0
1402.	CH2+N2=CH2NN	1.60E+32	-7.1	19958.0
1403.	CH3NN+M=CH3+N2+M	1.00E+11	0.0	5900.0
1404.	CH3NNH(+M)<=>CH3+NNH(+M)	3.30E+16	-0.1	55000.0
	Low pressure limit: 0.18800E+32 -0.45500E+01 0.57500E+05			
	TROE centering: 0.97000E+00 0.25059E+03 0.10000E+01 0.40100E+06			

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1405. H2NN+CH3=CH3NNH+H                                8.30E+05    1.9     6494.0
1406. CH3NNH+O=CH3NN+OH                                9.60E+12    0.0        0.0
1407. CH3NNH+OH=CH3NN+H2O                              3.92E+13    0.0        0.0
1408. CH3NN+HO2=CH3NNH+O2                              1.00E+06    2.0        0.0
1409. CH3NNH+HO2=CH3NN+H2O2                            1.00E+11    0.0     1987.0
1410. CH3NNH+CH3=CH4+CH3NN                             7.40E+13    0.0     5210.0
1411. CH3NNH+NH2=NH3+CH3NN                             7.40E+13    0.0     5210.0
1412. CH3NNH+NO2=CH3NN+HONO                            2.20E+11    0.0     5900.0
1413. CH2NNH2+H=NCH2+NH3                               1.76E+08    1.3     8801.1
1414. H2NN+CH3=CH2NNH2+H                               8.30E+05    1.9     6494.0
1415. CH3NNH2(+M)<=>CH3NNH+H(+M)                       1.35E+08    1.7    47280.0
      Low pressure limit:  0.12200E+54 -0.10750E+02  0.53560E+05
1416. CH3NNH2(+M)<=>CH2NNH2+H(+M)                      1.15E+09    1.2    50330.0
      Low pressure limit:  0.17100E+50 -0.99400E+01  0.56000E+05
      TROE centering:      0.00000E+00  0.33100E+03  0.10000E+02  0.47800E+05
1417. CH3NNH2+O=CH3NNH+OH                              1.00E+08    2.0        0.0
1418. CH3NNH2+OH=CH3NNH+H2O                            1.00E+08    2.0        0.0
1419. CH3NNH2+O2=CH3NNH+HO2                            4.00E+12    0.0        0.0
1420. CH3NNH2+HO2=CH3NNH+H2O2                          1.00E+08    2.0        0.0
1421. CH3NNH2+NO2=CH3NNH+HONO                          1.00E+08    2.0        0.0
1422. CH2NHNH2(+M)<=>CH2NH+NH2(+M)                     3.87E+12    0.2    12200.0
      Low pressure limit:  0.16200E+28 -0.39800E+01  0.11800E+05
      TROE centering:      0.86600E+00  0.29800E+03  0.10000E+02  0.28000E+06
1423. CH2NHNH2(+M)<=>CH2NNH2+H(+M)                     5.92E+11    0.3    36300.0
      Low pressure limit:  0.52500E+16 -0.72000E+00  0.34800E+05
      TROE centering:      0.00000E+00  0.49400E+03  0.10000E+02  0.28000E+06
1424. CH3NHNH(+M)<=>CH3+N2H2(+M)                       4.64E+09    1.6    35620.0
      Low pressure limit:  0.34800E+49 -0.97000E+01  0.41200E+05
      TROE centering:      0.00000E+00  0.23300E+03  0.10000E+02  0.30800E+06
1425. CH3NHNH(+M)<=>CH3NNH+H(+M)                       1.40E+07    2.0    44660.0
      Low pressure limit:  0.18200E+37 -0.65600E+01  0.48600E+05
      TROE centering:      0.00000E+00  0.13400E+03  0.10000E+02  0.51000E+05
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1426. CH3NHNH2(+M)<=>CH3NNH2+H(+M)                    4.66E+16   -0.2    77610.0
      Low pressure limit:  0.10900E+50 -0.95600E+01  0.83400E+05
      TROE centering:      0.00000E+00  0.16900E+03  0.13700E+02  0.40000E+05
1427. CH3NHNH2(+M)<=>CH3NHNH+H(+M)                    4.69E+16   -0.2    80120.0
      Low pressure limit:  0.44400E+48 -0.91900E+01  0.85700E+05
      TROE centering:      0.00000E+00  0.14900E+03  0.42800E+02  0.42400E+05
1428. CH3NHNH2(+M)<=>CH2NHNH2+H(+M)                   6.42E+16   -0.2    91800.0
      Low pressure limit:  0.18000E+44 -0.79800E+01  0.96700E+05
      TROE centering:      0.98900E+00  0.10700E+03  0.60700E+02  0.60100E+05
1429. CH3NHNH2(+M)<=>CH3NNH+H2(+M)                    9.70E+08    1.3   107500.0
      Low pressure limit:  0.10500E+69 -0.13840E+02  0.11500E+06
      TROE centering:      0.00000E+00  0.50000E+06  0.10000E+02  0.41700E+05
1430. CH3NHNH2(+M)<=>CH2NNH2+H2(+M)                   2.69E+09    1.2   105430.0
      Low pressure limit:  0.10500E+69 -0.13840E+02  0.11400E+03
      TROE centering:      0.19500E+00  0.47200E+04  0.10000E+01  0.10000E+01
1431. CH3NHNH2(+M)<=>N2H3+CH3(+M)                     3.12E+16   -0.2    65180.0
      Low pressure limit:  0.73400E+62 -0.13010E+02  0.72900E+05
      TROE centering:      0.00000E+00  0.27100E+03  0.10000E+02  0.41700E+05
1432. CH3NHNH2(+M)<=>H2NN+CH4(+M)                     1.36E+09    1.6    67110.0
      Low pressure limit:  0.24700E+52 -0.10400E+02  0.74300E+05
      TROE centering:      0.00000E+00  0.26000E+03  0.10000E+02  0.77500E+05
1433. CH3NHNH2(+M)<=>N2H2+CH4(+M)                     1.61E+10    1.1   108880.0
      Low pressure limit:  0.43820E+64 -0.12620E+02  0.11600E+06
      TROE centering:      0.00000E+00  0.97800E+03  0.10000E+02  0.41700E+05
1434. CH3NHNH2(+M)<=>CH3NH+NH2(+M)                    2.40E+16   -0.1    63790.0
      Low pressure limit:  0.89200E+65 -0.13840E+02  0.71900E+05
1435. CH3NHNH2(+M)<=>CH2NH+NH3(+M)                    3.50E+08    1.4    68330.0
      Low pressure limit:  0.80500E+49 -0.10300E+02  0.75300E+05
      TROE centering:      0.00000E+00  0.24200E+03  0.10000E+02  0.41700E+05
1436. CH3NHNH2(+M)<=>CH3N+NH3(+M)                     4.33E+09    1.2    62170.0
      Low pressure limit:  0.75000E+70 -0.15570E+02  0.71600E+05
      TROE centering:      0.35500E+00  0.29300E+03  0.10000E+02  0.41300E+05
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1437.	CH3NHNH2+H=CH3NNH2+H2	2.08E+07	1.8	4488.1
1438.	CH3NHNH2+H=CH3NHNH+H2	1.68E+09	1.1	7289.0
1439.	CH3NHNH2+H=CH2NHNH2+H2	7.88E+07	1.7	11162.0
1440.	CH3NHNH2+H=CH3NH+NH3	1.37E+09	1.1	5526.4
1441.	CH3NHNH2+O=CH3NNH+H2O	9.60E+12	0.0	0.0
1442.	CH3NHNH2+O=CH3NNH2+OH	9.60E+12	0.0	0.0
1443.	CH3NHNH2+O=CH3NHNH+OH	2.69E+12	0.0	0.0
1444.	CH3NHNH2+O=CH2NHNH2+OH	1.30E+12	0.0	0.0
1445.	CH3NHNH2+OH=CH3NNH2+H2O	3.92E+13	0.0	0.0
1446.	CH3NHNH2+OH=CH3NHNH+H2O	1.10E+13	0.0	0.0
1447.	CH3NHNH2+OH=CH2NHNH2+H2O	5.30E+12	0.0	0.0
1448.	CH3NNH2+HO2=CH3NHNH2+O2	1.00E+06	2.0	0.0
1449.	CH3NHNH2+HO2=CH3NNH2+H2O2	2.70E+11	0.0	1987.0
1450.	CH3NHNH2+HO2=CH3NHNH+H2O2	7.56E+10	0.0	1987.0
1451.	CH3NHNH2+HO2=CH2NHNH2+H2O2	3.65E+10	0.0	1987.0
1452.	CH3NHNH2+CH3=CH4+CH3NNH2	4.79E+01	3.4	3578.3
1453.	CH3NHNH2+CH3=CH3NHNH+CH4	3.21E+02	3.1	5748.1
1454.	CH3NHNH2+CH3=CH2NHNH2+CH4	2.27E+01	3.5	7669.4
1455.	CH3NHNH2+NH=CH3NNH2+NH2	1.45E+02	3.3	4435.5
1456.	CH3NHNH2+NH=CH3NHNH+NH2	6.20E+02	3.1	7062.4
1457.	CH3NHNH2+NH=CH2NHNH2+NH2	3.93E+01	3.6	10910.0
1458.	CH3NHNH2+NH2=CH3NNH2+NH3	1.65E+02	3.0	870.1
1459.	CH3NHNH2+NH2=CH3NHNH+NH3	5.98E+01	3.1	2110.2
1460.	CH3NHNH2+NH2=CH2NHNH2+NH3	1.04E+00	3.6	1894.1
1461.	CH3NHNH2+NO2=CH3NNH2+HONO	2.20E+11	0.0	5900.0
1462.	CH3NHNH2+NO2=CH3NHNH+HONO	7.87E+10	0.0	8839.0
1463.	CH3NHNH2+NO2=CH2NHNH2+HONO	1.39E+09	0.0	9803.0
1464.	CH3NHNH2+NO=CH3NNH2+HNO	1.85E+13	0.0	8524.0
1465.	CH3NHNH2+NO=CH3NHNH+HNO	1.24E+12	0.0	9605.0
1466.	CH3NHNH2+NO=CH2NHNH2+HNO	5.05E+12	0.0	11310.0
1467.	NCCN+M=CN+CN+M	1.10E+34	-4.3	130079.0
	N2 Enhanced by 1.500E+00			

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      O2              Enhanced by    1.500E+00
      H2              Enhanced by    1.500E+00
      H2O             Enhanced by    1.000E+01
      CO2             Enhanced by    3.000E+00
1468. CN+HCN=NCCN+H                                 1.50E+07    1.7     1529.0
1469. HNC+CN=NCCN+H                                 1.00E+13    0.0        0.0
1470. CH3NNCH3=CH3NN+CH3                            6.92E+15    0.0    50875.0
1471. CH3NNCH3=C2H6+N2                              2.00E+11    0.0    33000.0
1472. NCO+M=N+CO+M                                  2.20E+14    0.0    54050.0
      N2              Enhanced by    1.500E+00
      Warning...superceding enhancement factor for N2
      N2              Enhanced by    1.500E+00
1473. CN+OH=NCO+H                                   4.00E+13    0.0        0.0
1474. CH+NO=H+NCO                                   2.00E+13    0.0        0.0
1475. HCN+O=NCO+H                                   1.40E+04    2.6     4980.0
1476. HNC+O=H+NCO                                   1.60E+01    3.1     -224.0
1477. NCO+H=NH+CO                                   5.20E+13    0.0        0.0
1478. CN+O2=NCO+O                                   7.20E+12    0.0     -417.0
      Declared duplicate reaction...
1479. CN+O2=NCO+O                                  -2.80E+17   -2.0        0.0
      Declared duplicate reaction...
1480. NCO+O=NO+CO                                   2.00E+15   -0.5        0.0
1481. NCO+O=N+CO2                                   8.00E+12    0.0     2502.0
1482. NCO+OH=HON+CO                                 5.30E+12   -0.1     5124.0
1483. NCO+OH=H+CO+NO                                8.30E+12   -0.1    18032.0
1484. NCO+O2=NO+CO2                                 2.00E+12    0.0    20000.0
1485. CH3CN+O=CH3+NCO                               6.00E+09    1.8     8130.0
1486. CH3NCH+O=>CH3+NCO+H                           7.00E+13    0.0        0.0
1487. C2H2+NCO=HCCO+HCN                             1.40E+12    0.0     1815.0
1488. CN+CO2=NCO+CO                                 3.67E+06    2.2    26900.0
1489. C2O+NO=CO+NCO                                 1.00E+14    0.0      670.0
1490. C2O+NO2=CO2+NCO                               5.10E+13    0.0      125.0
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1491.	NCO+N=N2+CO	2.00E+13	0.0	0.0
1492.	CN+NO=NCO+N	9.60E+13	0.0	42100.0
1493.	CN+NO2=NCO+NO	5.30E+15	-0.8	344.0
1494.	NCO+NO=N2+CO2	1.50E+21	-2.7	1824.0
1495.	NCO+NO=N2O+CO	4.00E+19	-2.2	1743.0
1496.	NCN+O2=NO+NCO	4.40E+09	0.5	24580.0
1497.	N2O+NCO=CO+N2+NO	9.00E+13	0.0	27800.0
1498.	NCO+NO2=CO2+N2O	3.00E+12	0.0	-707.0
1499.	NCO+NO2=CO+NO+NO	2.10E+11	0.0	-874.0
1500.	NCCN+O=NCO+CN	4.60E+12	0.0	8877.0
1501.	CN+NCO=NCN+CO	1.80E+13	0.0	0.0
1502.	NCO+NCO=CO+CO+N2	1.80E+13	0.0	0.0
1503.	HCNO=HCN+O	4.20E+31	-6.1	61175.0
1504.	CH2+NO=HCNO+H	3.80E+13	-0.4	576.0
1505.	CH2SING+NO<=>H+HCNO	3.80E+13	-0.4	580.0
1506.	NCH2+O=HCNO+H	2.00E+13	0.0	0.0
1507.	HCNO+H=HCN+OH	7.20E+10	0.8	8612.0
1508.	HCNO+H=NH2+CO	1.70E+14	-0.8	2889.0
1509.	HCNO+O=HCO+NO	6.30E+13	0.0	0.0
1510.	HCNO+O=NCO+OH	7.00E+12	0.0	0.0
1511.	HCNO+OH=HCO+HNO	4.50E+12	0.0	0.0
1512.	HCNO+OH=CH2O+NO	1.00E+12	0.0	0.0
1513.	HCNO+OH=NO+CO+H2	6.50E+12	0.0	0.0
1514.	HCNO+OH=NCO+H2O	3.50E+12	0.0	0.0
1515.	HCNO+OH=NCO+H+OH	4.50E+12	0.0	0.0
1516.	NO+HCCO=HCNO+CO	4.60E+13	0.0	695.0
1517.	HCCO+NO2=HCNO+CO2	1.60E+13	0.0	0.0
1518.	HCNO+CN=HCN+NCO	6.00E+13	0.0	0.0
1519.	HNCO(+M)=NH+CO(+M)	6.00E+13	0.0	99800.0
	Low pressure limit: 0.21700E+29 -0.31000E+01 0.10190E+06			
	TROE centering: 0.46650E+00 0.10000E+04 0.10000E+07			
	N2O Enhanced by 5.000E+00			

	H2O	Enhanced by	5.000E+00		
	N2	Enhanced by	1.000E+00		
	CO2	Enhanced by	1.600E+00		
1520.	HNCO+M=H+NCO+M		1.00E+17	0.0	112000.0
1521.	HCNO+H<=>H+HNCO		2.10E+15	-0.7	2850.0
1522.	CH2+NO=HNCO+H		3.10E+17	-1.4	1271.0
1523.	CH2SING+NO<=>H+HNCO		3.10E+17	-1.4	1270.0
1524.	OH+HCN=HNCO+H		1.98E-03	4.0	1000.0
1525.	OH+HNC=HNCO+H		2.80E+13	0.0	3694.0
1526.	CHNH+O=HNCO+H		7.00E+13	0.0	0.0
1527.	HNCO+H=NCO+H2		9.00E+07	1.7	13900.0
1528.	HNCO+H=NH2+CO		3.60E+04	2.5	2343.0
1529.	HNC+O2=HNCO+O		1.50E+12	0.0	4111.0
1530.	HNCO+O=HNO+CO		1.49E+08	1.6	44010.0
1531.	HNCO+O=CO2+NH		9.80E+07	1.4	8524.0
1532.	HNCO+O=NCO+OH		2.20E+06	2.1	11430.0
1533.	HNCO+OH=NH2+CO2		6.30E+10	-0.1	11637.0
1534.	HNCO+OH=NCO+H2O		3.60E+07	1.5	3594.0
1535.	HNCO+O2=HNO+CO2		1.00E+12	0.0	35000.0
1536.	NCO+HO2=HNCO+O2		2.00E+13	0.0	0.0
1537.	HNCO+HO2=NCO+H2O2		3.00E+11	0.0	23700.0
1538.	NCO+CH4=HNCO+CH3		9.80E+12	0.0	8122.0
1539.	CH3CNH+O=CH3+HNCO		1.60E+14	0.0	0.0
1540.	CH2CNH+OH=CH3+HNCO		6.70E+11	0.0	-1013.0
1541.	C2H6+NCO=C2H5+HNCO		1.50E-09	6.9	-2910.0
1542.	NCO+HCO=HNCO+CO		3.60E+13	0.0	0.0
1543.	CH2O+NCO=HNCO+HCO		6.00E+12	0.0	0.0
1544.	CHCNH+O2=HNCO+HCO		4.90E+12	-0.1	1150.0
1545.	CH2CHN+O2=CH2O+HNCO		1.00E+12	0.0	0.0
1546.	HNCO+N=NH+NCO		2.32E+19	0.0	52500.0
1547.	HNCO+NH=NH2+NCO		3.00E+13	0.0	23700.0
1548.	NCO+NH3=HNCO+NH2		2.80E+04	2.5	983.0

1549.	NCO+HNO=HNCO+NO	1.80E+13	0.0	0.0
1550.	HNC+NO2=HNCO+NO	1.00E+12	0.0	32000.0
1551.	NCO+HONO=HNCO+NO2	3.60E+12	0.0	0.0
1552.	HNCO+NO2=HNNO+CO2	2.50E+12	0.0	26000.0
1553.	CN+HNCO=HCN+NCO	1.00E+13	0.0	0.0
1554.	HCN+OH=HOCN+H	5.90E+04	2.4	12500.0
1555.	HCNO+H=HOCN+H	1.40E+11	-0.2	2482.0
1556.	HOCN+H=HNCO+H	3.10E+08	0.8	1916.0
1557.	HOCN+H=NH2+CO	1.20E+08	0.6	2075.0
1558.	HOCN+H=H2+NCO	2.40E+08	1.5	6613.0
1559.	HOCN+O=OH+NCO	1.70E+08	1.5	4131.0
1560.	HOCN+OH=H2O+NCO	1.20E+06	2.0	-248.0
1561.	HOCN+CH3=CH4+NCO	8.20E+05	1.9	6613.0
1562.	CH3+HOCN=CH3CN+OH	5.00E+12	0.0	2000.0
1563.	HOCN+NH2=NCO+NH3	9.20E+05	1.9	3644.0
1564.	NCCN+OH=HOCN+CN	2.00E+12	0.0	18985.0
1565.	CH2NO=HNCO+H	2.30E+42	-9.1	53807.0
1566.	CH2NO+H=CH3+NO	4.00E+13	0.0	0.0
1567.	CH2NO+H=HCNO+H2	4.80E+08	1.5	-894.0
1568.	CH2NO+O=CH2O+NO	7.00E+13	0.0	0.0
1569.	CH2NO+O=HCNO+OH	3.30E+08	1.5	-894.0
1570.	NCH2+HO2=CH2NO+OH	3.00E+13	0.0	0.0
1571.	CH2NO+OH=CH2OH+NO	4.00E+13	0.0	0.0
1572.	CH2NO+OH=HCNO+H2O	2.40E+06	2.0	-1192.0
1573.	CH2NO+O2=CH2O+NO2	1.20E+15	-1.0	20117.0
1574.	CH2NO+CH3=C2H5+NO	3.00E+13	0.0	0.0
1575.	CH2NO+CH3=HCNO+CH4	1.60E+06	1.9	-1112.0
1576.	CH2NO+NH2=CH2NH2+NO	3.00E+13	0.0	0.0
1577.	CH2NO+NH2=HCNO+NH3	1.80E+06	1.9	-1152.0
1578.	H2NCO(+M)=CO+NH2(+M)	5.90E+12	0.0	25000.0
	Low pressure limit: 0.10000E+15 0.00000E+00 0.21700E+05			
1579.	H2NCO+H=HNCO+H2	3.00E+13	0.0	0.0

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1580. H2NCO+O=HNCO+OH                                 3.00E+13    0.0        0.0
1581. H2NCO+OH=HNCO+H2O                               3.00E+13    0.0        0.0
1582. CH2CHNH2+O=CH3+H2NCO                            3.90E+12    0.0     1494.0
      Declared duplicate reaction...
1583. CH2CHNH2+O=CH3+H2NCO                            6.20E+13    0.0     6855.0
      Declared duplicate reaction...
1584. CH3+NO(+M)=CH3NO(+M)                            9.00E+12    0.0      192.0
      Low pressure limit:  0.25000E+17  0.00000E+00 -0.28410E+04
      TROE centering:      0.50000E+01  0.10000E-29  0.12000E+03  0.10000E+31
1585. CH3+NO=CH3NO                                    1.00E+37   -8.4     5223.0
1586. CH3NO+H=CH2NO+H2                                4.40E+08    1.5      377.0
1587. CH3NO+H=CH3+HNO                                 1.80E+13    0.0     2780.0
1588. CH3NO+O=CH2NO+OH                                3.30E+08    1.5     3614.0
1589. CH3NO+O=CH3+NO2                                 1.70E+06    2.1        0.0
1590. CH3NO+OH=CH2NO+H2O                              3.60E+06    2.0    -1192.0
1591. CH3NO+OH=CH3+HONO                               2.50E+12    0.0      993.0
1592. CH3NO+CH3=CH2NO+CH4                             7.90E+05    1.9     5412.0
1593. CH3NCH3+O=CH3NO+CH3                             5.00E+13    0.0        0.0
1594. CH3NCH3+O2=CH3NO+CH3O                           1.00E+09    1.0     6000.0
1595. CH3NO+NH2=CH2NO+NH3                             2.80E+06    1.9     1072.0
1596. H2NCHO(+M)=CO+NH3(+M)                           1.00E+14    0.0    75514.0
      Low pressure limit:  0.83000E+15  0.00000E+00  0.49084E+05
1597. H2NCHO+M=HCO+NH2+M                              1.40E+16    0.0    72900.0
1598. H2NCHO+M=H2NCO+H+M                              4.60E+15    0.0    64200.0
1599. H2NCHO+H=H2NCO+H2                               1.30E+13    0.0     6955.0
1600. H2NCHO+H=HCO+NH3                                1.00E+13    0.0    19100.0
1601. H2NCHO+O=H2NCO+OH                               4.00E+08    1.5     5196.0
1602. CH3CHNH2+O=CH3+H2NCHO                           4.00E+13    0.0        0.0
1603. H2NCHO+OH=H2NCO+H2O                             8.00E+12    0.0        0.0
1604. CH3CHNH2+HO2=>CH3+OH+H2NCHO                     2.40E+13    0.0        0.0
1605. H2NCHO+CH3=H2NCO+CH4                            7.00E+05    2.0     9000.0
1606. H2NCHO+NH2=H2NCO+NH3                            2.00E+06    2.0     5000.0
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1607. H2CNO2=CH2O+NO                                  1.00E+13    0.0    36000.0
1608. CH3O+NO(+M)=CH3ONO(+M)                          6.60E+14   -0.6        0.0
      Low pressure limit:  0.27000E+28 -0.35000E+01  0.00000E+00
1609. CH3NO2(+M)=CH3+NO2(+M)                          1.80E+16    0.0    58500.0
      Low pressure limit:  0.13000E+18  0.00000E+00  0.42000E+05
      TROE centering:      0.18320E+00  0.10000E+02  0.10000E+07
1610. CH3NO2+H=CH3+HONO                               3.30E+12    0.0     3730.0
1611. CH3NO2+H=CH3NO+OH                               1.40E+12    0.0     3730.0
1612. CH3NO2+H=H2CNO2+H2                              5.40E+02    3.5     5200.0
1613. CH3NO2+O=H2CNO2+OH                              1.50E+13    0.0     5350.0
1614. CH3NO2+OH=H2CNO2+H2O                            5.00E+05    2.0     1000.0
1615. CH3NO2+OH=CH3OH+NO2                             2.00E+10    0.0    -1000.0
1616. CH3NO2+CH2=H2CNO2+CH3                           6.50E+12    0.0     7900.0
1617. CH3NO2+CH2SING=H2CNO2+CH3                       1.20E+14    0.0        0.0
1618. CH3NO2+CH3=H2CNO2+CH4                           5.50E-01    4.0     8300.0
1619. CN+NO(+M)=NCNO(+M)                              3.98E+13    0.0        0.0
      Low pressure limit:  0.15600E+37 -0.62000E+01  0.48780E+04
      TROE centering:      0.65080E+00  0.10000E+02  0.10000E+07
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    2.000E+00
1620. CH3O+NO2(+M)=CH3ONO2(+M)                        1.20E+13    0.0        0.0
      Low pressure limit:  0.14000E+31 -0.45000E+01  0.00000E+00
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UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX H

MMH/RFNA REDUCED REACTION SET 1

The following is the reduced reaction set for MMH/RFNA combustion labeled "reduced reaction set 1" described in Chapter 10. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	HE	C	O	N	AR
1	H	G	0	1.01E+00	200	3500	1	0	0	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0	0	0
3	O	G	0	1.60E+01	200	3500	0	0	0	1	0	0
4	O2	G	0	3.20E+01	200	3500	0	0	0	2	0	0
5	OH	G	0	1.70E+01	200	6000	1	0	0	1	0	0
6	H2O	G	0	1.80E+01	200	3500	2	0	0	1	0	0
7	HO2	G	0	3.30E+01	200	3500	1	0	0	2	0	0
8	H2O2	G	0	3.40E+01	200	3500	2	0	0	2	0	0
9	CH	G	0	1.30E+01	200	6000	1	0	1	0	0	0
10	CH2	G	0	1.40E+01	200	6000	2	0	1	0	0	0
11	CH2SING	G	0	1.40E+01	200	6000	2	0	1	0	0	0
12	CH3	G	0	1.50E+01	200	6000	3	0	1	0	0	0
13	CH4	G	0	1.60E+01	200	3500	4	0	1	0	0	0
14	CO	G	0	2.80E+01	200	3500	0	0	1	1	0	0
15	HCO	G	0	2.90E+01	200	3500	1	0	1	1	0	0
16	CH2O	G	0	3.00E+01	200	3500	2	0	1	1	0	0
17	CH2OH	G	0	3.10E+01	200	6000	3	0	1	1	0	0
18	CH3O	G	0	3.10E+01	200	6000	3	0	1	1	0	0
19	CH3OH	G	0	3.20E+01	200	3500	4	0	1	1	0	0
20	C2H	G	0	2.50E+01	200	3500	1	0	2	0	0	0
21	C2H2	G	0	2.60E+01	200	3500	2	0	2	0	0	0
22	C2H3	G	0	2.70E+01	200	5000	3	0	2	0	0	0

23	C2H4	G	0	2.81E+01	200	3500	4	0	2	0	0	0
24	C2H5	G	0	2.91E+01	200	3500	5	0	2	0	0	0
25	C2H6	G	0	3.01E+01	200	3500	6	0	2	0	0	0
26	AR	G	0	3.99E+01	300	5000	0	0	0	0	0	1
27	HCCO	G	0	4.10E+01	300	4000	1	0	2	1	0	0
28	CH2CO	G	0	4.20E+01	200	3500	2	0	2	1	0	0
29	CH3CO	G	0	4.30E+01	200	6000	3	0	2	1	0	0
30	CH2CHO	G	0	4.30E+01	300	5000	3	0	2	1	0	0
31	CH3CHO	G	0	4.41E+01	200	6000	4	0	2	1	0	0
32	CO2	G	0	4.40E+01	200	3500	0	0	1	2	0	0
33	N	G	0	1.40E+01	300	5000	0	0	0	0	1	0
34	NH	G	0	1.50E+01	200	6000	1	0	0	0	1	0
35	NH2	G	0	1.60E+01	300	5000	2	0	0	0	1	0
36	NH3	G	0	1.70E+01	300	5000	3	0	0	0	1	0
37	N2	G	0	2.80E+01	200	6000	0	0	0	0	2	0
38	NNH	G	0	2.90E+01	200	6000	1	0	0	0	2	0
39	N2H2	G	0	3.00E+01	300	5000	2	0	0	0	2	0
40	H2NN	G	0	3.00E+01	300	5000	2	0	0	0	2	0
41	N2H3	G	0	3.10E+01	300	5000	3	0	0	0	2	0
42	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0
43	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
44	HNOH	G	0	3.20E+01	200	6000	2	0	0	1	1	0
45	NH2O	G	0	3.20E+01	300	4000	2	0	0	1	1	0
46	NH2OH	G	0	3.30E+01	300	5000	3	0	0	1	1	0
47	N2O	G	0	4.40E+01	300	5000	0	0	0	1	2	0
48	HNNO	G	0	4.50E+01	300	5000	1	0	0	1	2	0
49	NH2NO	G	0	4.60E+01	200	6000	2	0	0	1	2	0
50	NO2	G	0	4.60E+01	200	6000	0	0	0	2	1	0
51	HONO	G	0	4.70E+01	200	6000	1	0	0	2	1	0
52	HNO2	G	0	4.70E+01	300	4000	1	0	0	2	1	0
53	HONHO	G	0	4.80E+01	300	5000	2	0	0	2	1	0

54	NO3	G	0	6.20E+01	200	6000	0	0	0	3	1	0
55	HNO3	G	0	6.30E+01	200	6000	1	0	0	3	1	0
56	N2O4	G	0	9.20E+01	200	6000	0	0	0	4	2	0
57	HE	G	0	4.00E+00	200	6000	0	1	0	0	0	0
58	CN	G	0	2.60E+01	200	6000	0	0	1	0	1	0
59	HCN	G	0	2.70E+01	300	4000	1	0	1	0	1	0
60	HNC	G	0	2.70E+01	300	5000	1	0	1	0	1	0
61	CHNH	G	0	2.80E+01	300	4000	2	0	1	0	1	0
62	NCH2	G	0	2.80E+01	300	4000	2	0	1	0	1	0
63	CH2NH	G	0	2.90E+01	300	5000	3	0	1	0	1	0
64	CH3N	G	0	2.90E+01	200	5000	3	0	1	0	1	0
65	CH3NH	G	0	3.01E+01	300	5000	4	0	1	0	1	0
66	CH2NH2	G	0	3.01E+01	300	5000	4	0	1	0	1	0
67	CH3NH2	G	0	3.11E+01	300	5000	5	0	1	0	1	0
68	NCN	G	0	4.00E+01	300	4000	0	0	1	0	2	0
69	CH2CN	G	0	4.00E+01	200	6000	2	0	2	0	1	0
70	CH3CN	G	0	4.11E+01	200	6000	3	0	2	0	1	0
71	NCO	G	0	4.20E+01	300	5000	0	0	1	1	1	0
72	CH3NHNH2	G	0	4.61E+01	298	6000	6	0	1	0	2	0
73	CH2NHNH2	G	0	4.51E+01	200	5000	5	0	1	0	2	0
74	CH3NNH2	G	0	4.51E+01	200	6000	5	0	1	0	2	0
75	CH3NHNH	G	0	4.51E+01	200	5000	5	0	1	0	2	0
76	CH3NN	G	0	4.30E+01	200	6000	3	0	1	0	2	0
77	CH2NNH2	G	0	4.41E+01	200	5000	4	0	1	0	2	0
78	HCNO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
79	HNCO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
80	HOCN	G	0	4.30E+01	300	5000	1	0	1	1	1	0
81	CH3NNH	G	0	4.41E+01	200	6000	4	0	1	0	2	0
82	CH2NO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
83	HOCO	G	0	4.50E+01	300	4000	1	0	1	2	0	0
84	CH3NO	G	0	4.50E+01	300	4000	3	0	1	1	1	0

85	CH3NO2	G	0	6.10E+01	300	4000	3	0	1	2	1	0
86	CH3ONO	G	0	6.10E+01	300	4000	3	0	1	2	1	0
87	CH3ONO2	G	0	7.70E+01	300	4000	3	0	1	3	1	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. O+H+M=OH+M			4.71E+18	-1.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	7.500E-01			
2. H2+M=2H+M			4.58E+19	-1.4	104380.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
3. H+OH+M=H2O+M			2.21E+22	-2.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
4. H2O2(+M)=2OH(+M)			2.95E+14	0.0	48400.0
Low pressure limit:	0.12000E+18	0.00000E+00	0.45500E+05		
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	1.600E-01			
5. H2O+O=OH+OH			2.97E+06	2.0	13400.0
6. O+H2=H+OH			5.08E+04	2.7	6290.0
7. OH+H2=H+H2O			2.16E+08	1.5	3430.0
8. H+O2(+M)=HO2(+M)			1.48E+12	0.6	0.0
Low pressure limit:	0.35000E+17	-0.41000E+00	-0.11200E+04		
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			

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    AR              Enhanced by    5.000E-02
 9. H+O2=O+OH                                          4.49E+08    1.3    16191.0
    Declared duplicate reaction...
10. H+O2=O+OH                                          2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
11. O+HO2=OH+O2                                        3.25E+13    0.0        0.0
12. H+HO2=O2+H2                                        1.66E+13    0.0      820.0
13. H+HO2=2OH                                          7.08E+13    0.0      300.0
14. OH+HO2=O2+H2O                                      4.64E+13    0.0     -500.0
15. 2HO2=O2+H2O2                                       1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
16. 2HO2=O2+H2O2                                       4.20E+14    0.0    11980.0
    Declared duplicate reaction...
17. OH+H2O2=HO2+H2O                                    1.00E+12    0.0        0.0
    Declared duplicate reaction...
18. OH+H2O2=HO2+H2O                                    5.80E+14    0.0     9560.0
    Declared duplicate reaction...
19. H2+CO(+M)=CH2O(+M)                                 4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
20. OH+CO=H+CO2                                        4.10E+04    2.1    -1578.0
21. HO2+CO=OH+CO2                                      1.50E+14    0.0    23600.0
22. O+HCO=H+CO2                                        3.00E+13    0.0        0.0
23. H+HCO(+M)=CH2O(+M)                                 1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
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    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
24. H+HCO=H2+CO                                  7.30E+13    0.0        0.0
25. OH+HCO=H2O+CO                                3.00E+13    0.0        0.0
26. HCO+M=H+CO+M                                 1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
27. HCO+O2=HO2+CO                                4.22E+12    0.0        0.0
28. HCO+HO2=CO2+OH+H                             3.00E+13    0.0        0.0
29. H+CH2O=HCO+H2                                5.18E+07    1.7     1834.0
30. H+CH2O(+M)=CH2OH(+M)                         5.40E+11    0.5     3600.0
    Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
    TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
31. H+CH2O(+M)=CH3O(+M)                          5.40E+11    0.5     2600.0
    Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
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TROE centering: 0.75800E+00 0.94000E+02 0.15550E+04 0.42000E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

32.	OH+CH2O=HCO+H2O	3.43E+09	1.2	-447.0
33.	HO2+CH2O=HCO+H2O2	1.47E+13	0.0	15200.0
34.	H+CH2OH=H2+CH2O	6.00E+12	0.0	0.0
35.	H+CH2OH=OH+CH3	9.63E+13	0.0	0.0
36.	OH+CH2OH=H2O+CH2O	2.40E+13	0.0	0.0
37.	CH2OH+O2=HO2+CH2O	2.41E+14	0.0	5017.0
	Declared duplicate reaction...			
38.	CH2OH+O2=HO2+CH2O	1.51E+15	-1.0	0.0
	Declared duplicate reaction...			
39.	CH2OH+HO2=CH2O+H2O2	1.20E+13	0.0	0.0
40.	CH2OH+HCO=CH3OH+CO	1.20E+14	0.0	0.0
41.	CH2OH+HCO=CH2O+CH2O	1.80E+14	0.0	0.0
42.	CH2OH+CH3O=CH3OH+CH2O	2.40E+13	0.0	0.0
43.	H+CH3O=H2+CH2O	2.00E+13	0.0	0.0
44.	H+CH3O=OH+CH3	3.20E+13	0.0	0.0
45.	OH+CH3O=H2O+CH2O	1.80E+13	0.0	0.0
46.	CH3O+O2=HO2+CH2O	9.03E+13	0.0	11980.0
	Declared duplicate reaction...			
47.	CH3O+O2=HO2+CH2O	2.20E+10	0.0	1748.0
	Declared duplicate reaction...			
48.	CH3O+HO2=CH2O+H2O2	3.00E+11	0.0	0.0
49.	CH3O+CO=CH3+CO2	1.57E+13	0.0	11800.0
50.	CH3O+HCO=CH3OH+CO	9.00E+13	0.0	0.0
51.	2CH3O=CH3OH+CH2O	6.00E+13	0.0	0.0
52.	O+CH3OH=OH+CH2OH	3.88E+05	2.5	3080.0

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53. H+CH3OH=CH2OH+H2                                  1.44E+13    0.0     6095.0
54. H+CH3OH=CH3O+H2                                   3.60E+12    0.0     6095.0
55. OH+CH3OH=CH2OH+H2O                                7.10E+06    1.8     -596.0
56. OH+CH3OH=CH3O+H2O                                 1.00E+06    2.1      496.5
57. CH3+CH3OH=CH2OH+CH4                               3.19E+01    3.2     7172.0
58. HCO+CH3OH=CH2OH+CH2O                              9.63E+03    2.9    13110.0
59. HO2+CH3OH=CH2OH+H2O2                              3.98E+13    0.0    19400.0
60. CH3O+CH3OH=CH2OH+CH3OH                            3.00E+11    0.0     4060.0
61. CH3OH(+M)=CH3+OH(+M)                              1.90E+16    0.0    91730.0
    Low pressure limit:  0.29500E+45 -0.73500E+01  0.95460E+05
    TROE centering:      0.41400E+00  0.27900E+03  0.54590E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
62. CH3OH(+M)=CH2OH+H(+M)                             2.69E+16   -0.1    98940.0
    Low pressure limit:  0.23400E+41 -0.63300E+01  0.10310E+06
    TROE centering:      0.77300E+00  0.69300E+03  0.53330E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
63. O+CH4=OH+CH3                                      1.02E+09    1.5     8600.0
64. H+CH4=CH3+H2                                      6.60E+08    1.6    10840.0
65. OH+CH4=CH3+H2O                                    1.00E+08    1.6     3120.0
66. CH+CH4=H+C2H4                                     6.00E+13    0.0        0.0
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67. CH2SING+CH4=2CH3                                  1.60E+13    0.0     -570.0
68. CH2+CH4=2CH3                                      2.46E+06    2.0     8270.0
69. O+CH3=H+CH2O                                      5.06E+13    0.0        0.0
70. O+CH3=H+H2+CO                                     3.37E+13    0.0        0.0
71. H+CH3(+M)=CH4(+M)                                 1.39E+16   -0.5      536.0
    Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
    TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
72. OH+CH3=CH2+H2O                                    5.60E+07    1.6     5420.0
73. OH+CH3=CH2SING+H2O                                6.44E+17   -1.3     1417.0
74. HO2+CH3=O2+CH4                                    1.00E+12    0.0        0.0
75. HO2+CH3=OH+CH3O                                   2.00E+13    0.0        0.0
76. CH+CH3=H+C2H3                                     3.00E+13    0.0        0.0
77. CH2SING+CH3=H+C2H4                                1.20E+13    0.0     -570.0
78. CH3+O2=O+CH3O                                     3.56E+13    0.0    30480.0
79. CH3+O2=OH+CH2O                                    2.31E+12    0.0    20315.0
80. 2CH3(+M)=C2H6(+M)                                 6.77E+16   -1.2      654.0
    Low pressure limit:  0.34000E+42 -0.70300E+01  0.27630E+04
    TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
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 81. 2CH3=H+C2H5                                    6.84E+12    0.1    10600.0
 82. CH3+HCO=CH4+CO                                 1.21E+14    0.0        0.0
 83. CH3+CH2O=HCO+CH4                               3.32E+03    2.8     5860.0
 84. CH2+CH3=H+C2H4                                 4.00E+13    0.0        0.0
 85. O+CH2=H+HCO                                    8.00E+13    0.0        0.0
 86. H+CH2SING=CH+H2                                3.00E+13    0.0        0.0
 87. OH+CH2=H+CH2O                                  2.00E+13    0.0        0.0
 88. OH+CH2=CH+H2O                                  1.13E+07    2.0     3000.0
 89. OH+CH2SING=H+CH2O                              3.00E+13    0.0        0.0
 90. CH2+O2=OH+H+CO                                 5.00E+12    0.0     1500.0
 91. CH2+O2=CO2+2H                                  5.80E+12    0.0     1500.0
 92. CH2+O2=O+CH2O                                  2.40E+12    0.0     1500.0
 93. CH2+H2=H+CH3                                   5.00E+05    2.0     7230.0
 94. 2CH2=H2+C2H2                                   1.60E+15    0.0    11944.0
 95. CH2SING+CO=CH2+CO                              9.00E+12    0.0        0.0
 96. CH2SING+CO2=CH2+CO2                            7.00E+12    0.0        0.0
 97. CH2SING+CO2=CO+CH2O                            1.40E+13    0.0        0.0
 98. CH2+CO(+M)=CH2CO(+M)                           8.10E+11    0.5     4510.0
     Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
 99. CH2SING+O2=H+OH+CO                             2.80E+13    0.0        0.0
100. CH2SING+O2=CO+H2O                              1.20E+13    0.0        0.0
101. CH2SING+H2=CH3+H                               7.00E+13    0.0        0.0
102. CH2SING+H2O(+M)=CH3OH(+M)                      4.82E+17   -1.2     1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
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     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
103. CH2SING+H2O=CH2+H2O                          3.00E+13    0.0        0.0
104. CH2SING+H2O=H2+CH2O                          6.82E+10    0.2     -935.0
105. CH+H2=H+CH2                                  1.08E+14    0.0     3110.0
106. CH+H2O=H+CH2O                                5.71E+12    0.0     -755.0
107. CH+CH2O=H+CH2CO                              9.46E+13    0.0     -515.0
108. O+C2H6=OH+C2H5                               3.00E+07    2.0     5115.0
109. H+C2H6=C2H5+H2                               5.40E+02    3.5     5210.0
110. OH+C2H6=C2H5+H2O                             7.26E+06    2.0      864.0
111. CH3+C2H6=C2H5+CH4                            5.50E-01    4.0     8300.0
112. C2H6+HCO=CH2O+C2H5                           4.70E+04    2.7    18235.0
113. H+C2H5(+M)=C2H6(+M)                          5.21E+17   -1.0     1580.0
     Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
     TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
114. C2H5+OH=C2H4+H2O                             2.41E+13    0.0        0.0
115. C2H5+CH3O=C2H6+CH2O                          2.41E+13    0.0        0.0
116. H+C2H4(+M)=C2H5(+M)                          1.37E+09    1.5     1355.0
     Low pressure limit:  0.20260E+40 -0.66420E+01  0.57690E+04
     TROE centering:     -0.56900E+00  0.29900E+03 -0.91470E+04  0.15240E+03
     H2              Enhanced by    2.000E+00
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     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
117. H+C2H4=C2H3+H2                                  1.12E+07    2.1    13366.0
118. OH+C2H4=C2H3+H2O                                1.31E-01    4.2     -860.0
119. OH+C2H4=CH3CHO+H                                8.73E-05    4.6     -618.0
120. CH3+C2H4=C2H3+CH4                               2.27E+05    2.0     9200.0
121. C2H4(+M)=H2+C2H2(+M)                            8.00E+12    0.4    88770.0
     Low pressure limit:  0.15800E+52 -0.93000E+01  0.97800E+05
     TROE centering:      0.73450E+00  0.18000E+03  0.10350E+04  0.54170E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
122. C2H4+O=H+CH2CHO                                 7.33E+07    1.6     1260.0
123. C2H4+O=CH3+HCO                                  1.13E+08    1.6     1020.0
124. C2H4+O=C2H3+OH                                  2.15E+06    2.5    11900.0
125. H+C2H3(+M)=C2H4(+M)                             6.08E+12    0.3      280.0
     Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
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     AR              Enhanced by    7.000E-01
126. H+C2H2(+M)=C2H3(+M)                              1.71E+10    1.3     2709.0
     Low pressure limit:  0.63480E+32 -0.46639E+01  0.37800E+04
     TROE centering:      0.00000E+00  0.78784E+05 -0.10210E+05  0.10000E-29
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
127. H+C2H3=H2+C2H2                                   9.64E+13    0.0        0.0
128. OH+C2H3=H2O+C2H2                                 5.00E+12    0.0        0.0
129. C2H3+O2=C2H2+HO2                                 1.34E+06    1.6     -383.0
     Declared duplicate reaction...
130. C2H3+O2=C2H2+HO2                                 1.37E+02    3.4     3663.0
     Declared duplicate reaction...
131. C2H3+CH2O=C2H4+HCO                               5.43E+03    2.8     5862.0
132. C2H2+O=C2H+OH                                    4.60E+19   -1.4    28950.0
133. C2H2+O=CH2+CO                                    2.35E+08    1.4     2204.5
134. C2H2+O=HCCO+H                                    9.40E+08    1.4     2204.5
135. OH+C2H2=C2H+H2O                                  2.63E+06    2.1    17060.0
136. OH+C2H2=H+CH2CO                                  1.52E+04    2.3     -292.0
137. OH+C2H2=CH3+CO                                   4.37E+06    1.4      227.0
138. C2H+H2=H+C2H2                                    5.68E+10    0.9     1993.0
139. HCCO+CH3=C2H4+CO                                 5.00E+13    0.0        0.0
140. H+CH2CO=HCCO+H2                                  5.00E+13    0.0     8000.0
141. CH2CO+H=CH3+CO                                   7.77E+08    1.4     2780.0
142. CH2CHO=H+CH2CO                                   2.48E+27   -5.2    44304.0
143. CH2CHO=CH3+CO                                    1.54E+31   -6.3    42478.0
144. OH+CH2CO=HCCO+H2O                                7.50E+12    0.0     2000.0
145. CH2CO+OH=CH2OH+CO                                1.00E+13    0.0        0.0
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146.	CH3CO=CH3+CO		2.40E+15	-2.0	14805.0
147.	CH2CHO+OH=H2O+CH2CO		1.20E+13	0.0	0.0
148.	CH2CHO+OH=HCO+CH2OH		3.01E+13	0.0	0.0
149.	CH3CHO=CH3+HCO		9.59E+14	0.0	74180.0
150.	CH3CHO+H=CH2CHO+H2		4.10E+09	1.2	2405.0
151.	CH3CHO+OH=CH3CO+H2O		2.35E+10	0.7	-1113.0
152.	CH3CHO+HCO=CH3CO+CH2O		7.80E+13	0.0	8440.0
153.	NH+H=N+H2		3.20E+13	0.0	325.0
154.	NH+OH=N+H2O		1.60E+07	1.7	-576.0
155.	NH2+H=NH+H2		4.00E+13	0.0	3650.0
156.	NH2+O=NH+OH		7.00E+12	0.0	0.0
	Declared duplicate reaction...				
157.	NH2+O=NH+OH		8.60E-01	4.0	1673.0
	Declared duplicate reaction...				
158.	NH2+OH=NH+H2O		3.30E+06	1.9	-217.0
159.	NH3+H=NH2+H2		6.36E+05	2.4	10171.0
160.	NH3+O=NH2+OH		2.80E+02	3.3	4471.0
161.	NH3+OH=NH2+H2O		2.00E+06	2.0	566.0
162.	NH2+NH2=NH3+NH		5.60E+00	3.5	552.0
163.	NNH=N2+H		1.00E+09	0.0	0.0
164.	N2H2+M=NNH+H+M		5.00E+16	0.0	50000.0
	H2O	Enhanced by 1.500E+01			
	O2	Enhanced by 2.000E+00			
	N2	Enhanced by 2.000E+00			
	H2	Enhanced by 2.000E+00			
165.	N2H2+H=NNH+H2		8.50E+04	2.6	230.0
166.	NH2+NH2=N2H2+H2		1.70E+08	1.6	11783.0
167.	N2H2+OH=NNH+H2O		5.90E+01	3.4	1360.0
168.	H2NN=NNH+H		3.40E+26	-4.8	46228.0
169.	H2NN+H=N2H2+H		7.00E+13	0.0	0.0
170.	H2NN+H=NNH+H2		4.80E+08	1.5	-894.0
171.	H2NN+OH=NNH+H2O		2.40E+06	2.0	-1192.0

172.	H2NN+HO2=NNH+H2O2	2.90E+04	2.7	-1599.0
173.	N+OH=NO+H	3.80E+13	0.0	0.0
174.	NH+O=NO+H	9.20E+13	0.0	0.0
175.	NH+OH=NO+H2	2.00E+13	0.0	0.0
176.	NO+O=O2+N	1.81E+09	1.0	38725.0
177.	N+NO=N2+O	3.30E+12	0.3	0.0
178.	NH+NO=N2+OH	2.20E+13	-0.2	0.0
179.	NNH+O=NH+NO	5.20E+11	0.4	-409.0
180.	NH2+NO=N2+H2O	2.80E+20	-2.7	1258.0
181.	NH2+NO=NNH+OH	2.29E+10	0.4	-814.0
182.	NO+H(+M)=HNO(+M)	1.50E+15	-0.4	0.0
	Low pressure limit: 0.24000E+15 0.20600E+00 -0.15500E+04			
	TROE centering: 0.82000E+00 0.10000E-29 0.10000E+31 0.10000E+31			
	N2 Enhanced by 1.600E+00			
183.	HNO+H=H2+NO	4.50E+11	0.7	655.0
184.	NH+OH=HNO+H	3.20E+14	-0.4	-46.0
185.	NH+H2O=HNO+H2	2.00E+13	0.0	13850.0
186.	HNO+O=OH+NO	1.81E+13	0.0	0.0
187.	HNO+OH=NO+H2O	3.60E+13	0.0	0.0
188.	HNO+O2=NO+HO2	2.00E+13	0.0	15887.0
189.	NNH+NO=N2+HNO	5.00E+13	0.0	0.0
190.	H+NO+N2=HNO+N2	4.00E+20	-1.8	0.0
191.	HNOH+OH=HNO+H2O	2.40E+06	2.0	-1192.0
192.	HNOH+HO2=HNO+H2O2	2.90E+04	2.7	-1599.0
193.	NH2O+M=HNOH+M	1.10E+29	-4.0	44000.0
	H2O Enhanced by 1.000E+01			
194.	NH2O+H=NH2+OH	5.00E+13	0.0	0.0
195.	NH2O+H=HNO+H2	3.00E+07	2.0	2000.0
196.	NH2O+OH=HNO+H2O	2.00E+07	2.0	1000.0
197.	NH2+HO2=NH2O+OH	5.00E+13	0.0	0.0
198.	NH2O+HO2=HNO+H2O2	2.90E+04	2.7	-1599.0
199.	NH2O+NO=HNO+HNO	2.00E+04	2.0	13000.0

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200. NH2OH+OH=HNOH+H2O                                1.50E+04    2.6    -3537.0
201. NH2OH+OH=NH2O+H2O                                1.50E+05    2.3    -1296.0
202. NH2O+HO2=O2+NH2OH                                2.90E+04    2.7    -1599.0
203. HNOH+HO2=NH2OH+O2                                2.90E+04    2.7    -1599.0
204. N2O(+M)=N2+O(+M)                                 1.30E+12    0.0    62570.0
     Low pressure limit:  0.40000E+15  0.00000E+00  0.56600E+05
     N2              Enhanced by    1.700E+00
     O2              Enhanced by    1.400E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    1.200E+01
205. N2O+H=N2+OH                                      3.30E+10    0.0     4729.0
     Declared duplicate reaction...
206. N2O+H=N2+OH                                      4.40E+14    0.0    19254.0
     Declared duplicate reaction...
207. NH+NO=N2O+H                                      2.90E+14   -0.4        0.0
     Declared duplicate reaction...
208. NH+NO=N2O+H                                     -2.20E+13   -0.2        0.0
     Declared duplicate reaction...
209. NNH+O=N2O+H                                      1.00E+14    0.0        0.0
210. NH2+NO=H2+N2O                                    1.00E+13    0.0    33700.0
211. N2O+OH=HNO+NO                                    1.20E-04    4.3    25080.0
212. N2O+OH=N2+HO2                                    1.00E+14    0.0    30000.0
213. N2H2+NO=N2O+NH2                                  3.00E+10    0.0        0.0
214. HNNO+M=H+N2O+M                                   2.20E+15    0.0    21600.0
215. HNNO+M=N2+OH+M                                   1.00E+15    0.0    25600.0
216. NH2+NO=HNNO+H                                    8.00E+13    0.0    28000.0
217. NH2NO=N2+H2O                                     3.10E+34   -7.1    36262.0
218. H2NN+OH=NH2NO+H                                  2.00E+12    0.0        0.0
219. NO2(+M)=NO+O(+M)                                 7.60E+18   -1.3    73245.0
     Low pressure limit:  0.24700E+29 -0.33700E+01  0.74756E+05
     TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.49816E+04
     N2O             Enhanced by    1.500E+00
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     H2O             Enhanced by    4.400E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    2.300E+00
     Declared duplicate reaction...
220. NO+O(+M)=NO2(+M)                                1.30E+15   -0.8        0.0
     Low pressure limit:  0.47100E+25 -0.28700E+01  0.15510E+04
     TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.46816E+04
     Declared duplicate reaction...
221. NO2+H=NO+OH                                     1.30E+14    0.0      357.0
222. NO2+O=O2+NO                                     3.91E+12    0.0     -238.0
223. NO2+OH=HO2+NO                                   1.81E+13    0.0     6673.0
224. NH+NO2=N2O+OH                                   4.10E+12    0.0        0.0
225. NH+NO2=HNO+NO                                   5.90E+12    0.0        0.0
226. NH2+NO2=N2O+H2O                                 3.00E+14   -0.8      242.0
227. NH2+NO2=NH2O+NO                                 1.30E+15   -0.8      242.0
228. N2O+NO=NO2+N2                                   5.30E+05    2.2    46280.0
229. NO2+NO2=NO+NO+O2                                1.63E+12    0.0    26108.0
230. HONO(+M)=OH+NO(+M)                              1.20E+19   -1.2    49667.0
     Low pressure limit:  0.30100E+31 -0.38000E+01  0.50322E+05
     TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
     Declared duplicate reaction...
231. NO+OH(+M)=HONO(+M)                              1.99E+12   -0.1     -721.0
     Low pressure limit:  0.50800E+24 -0.25100E+01 -0.68000E+02
     TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
     Declared duplicate reaction...
232. NO2+H2=HONO+H                                   1.30E+04    2.8    29770.0
233. HONO+H=H2O+NO                                   8.10E+06    1.9     3843.0
234. HONO+H=OH+HNO                                   5.60E+10    0.9     4965.0
235. HONO+OH=H2O+NO2                                 1.26E+10    1.0      135.0
236. NO2+HO2=HONO+O2                                 6.30E+08    1.2     5000.0
237. NH+HONO=NH2+NO2                                 1.00E+13    0.0        0.0
238. NH2+HONO=NH3+NO2                                7.10E+01    3.0    -4940.0
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239. HNO+NO2=HONO+NO                                  4.40E+04    2.6     4040.0
240. NH2O+NO2=HONO+HNO                                6.00E+11    0.0     2000.0
241. HNOH+NO2=HONO+HNO                                6.00E+11    0.0     2000.0
242. HONO+HONO=NO+NO2+H2O                             3.50E-01    3.6    12140.0
243. HNO2(+M)=HONO(+M)                                2.50E+14    0.0    32300.0
     Low pressure limit:  0.31000E+19  0.00000E+00  0.31500E+05
     TROE centering:      0.11490E+01  0.10000E-29  0.31250E+04  0.10000E+31
244. NO2+H2=HNO2+H                                    2.40E+00    3.7    32400.0
245. HNO2+OH=H2O+NO2                                  1.20E+06    2.0     -794.0
246. NO2+HO2=HNO2+O2                                  1.90E+01    3.3     4983.0
247. HNO+NO2=HNO2+NO                                  6.02E+11    0.0     1986.0
248. HNOH+HO2=HONHO+OH                                4.00E+13    0.0        0.0
249. NO2+O(+M)=NO3(+M)                                1.32E+13    0.0        0.0
     Low pressure limit:  0.14900E+29 -0.40800E+01  0.24660E+04
     TROE centering:      0.32600E+00  0.50000E+03  0.62049E+04  0.26060E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     HNO3            Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
     NO3             Enhanced by    5.000E+00
250. NO2+NO2=NO3+NO                                   9.60E+09    0.7    20900.0
251. NO2+OH(+M)=HNO3(+M)                              2.41E+13    0.0        0.0
     Low pressure limit:  0.64200E+33 -0.54900E+01  0.23490E+04
     TROE centering:      0.40000E+00  0.45070E+03  0.15840E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     HNO3            Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
     NO3             Enhanced by    5.000E+00
252. HONO+NO3=HNO3+NO2                                1.00E+12    0.0     6000.0
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253.	N2O4(+M)=NO2+NO2(+M)	4.05E+18	-1.1	12840.0
	Low pressure limit: 0.19600E+29 -0.38000E+01 0.12840E+05			
254.	N2O4+H2O=HONO+HNO3	2.52E+14	0.0	11586.0
255.	CH3+NH2=CH4+NH	2.80E+06	1.9	9205.0
256.	CH3+NH2=CH2+NH3	1.60E+06	1.9	7566.0
257.	CH2SING+NH3=CH3+NH2	1.00E+14	0.0	0.0
258.	CH4+NH2=CH3+NH3	1.50E+03	3.0	9940.0
259.	N2H3+CH3=H2NN+CH4	3.00E+13	0.0	0.0
260.	CH2SING+NO=CH2+NO	1.00E+14	0.0	0.0
261.	CH+NO=HCO+N	6.80E+12	0.0	0.0
262.	CH+NO=CO+NH	9.10E+12	0.0	0.0
263.	CH2+NO=NH2+CO	2.30E+16	-1.4	1331.0
264.	N+CO2<=>NO+CO	3.00E+12	0.0	11300.0
265.	NH+CO2<=>HNO+CO	1.00E+13	0.0	14350.0
266.	HNO+CH3=NO+CH4	8.20E+05	1.9	480.0
267.	C2H3+NO=C2H2+HNO	1.00E+12	0.0	1000.0
268.	HCO+NO=HNO+CO	7.23E+12	0.0	0.0
269.	CH3O+NO=HNO+CH2O	7.50E+12	0.0	2017.0
	Declared duplicate reaction...			
270.	CH3O+NO=HNO+CH2O	2.50E+18	-2.6	0.0
	Declared duplicate reaction...			
271.	CH2OH+NO=CH2O+HNO	1.30E+12	0.0	0.0
272.	CH3O+HNO=NO+CH3OH	3.20E+13	0.0	0.0
273.	CH2OH+HNO=NO+CH3OH	3.00E+13	0.0	0.0
274.	CH2CHO+NO=HNO+CH2CO	1.00E+12	0.0	8600.0
275.	NH2O+CH3=CH3O+NH2	2.00E+13	0.0	0.0
276.	CH+NO2=HCO+NO	1.01E+14	0.0	0.0
277.	CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
278.	NO2+CH3=NO+CH3O	1.40E+13	0.0	0.0
279.	C2H3+NO2=NO+CH2CHO	7.70E+14	-0.6	0.0
280.	CO+NO2=NO+CO2	9.04E+13	0.0	33780.0
281.	HCO+NO2=CO+NO+OH	1.20E+23	-3.3	2355.0

282. HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
283. CH3CO+NO2=>CH3+CO2+NO	1.50E+13	0.0	0.0
284. CH4+NO2=HONO+CH3	6.50E+14	0.0	45800.0
285. HOCO+NO=CO+HONO	1.50E+12	0.0	0.0
286. HCO+NO2=CO+HONO	1.24E+23	-3.3	2355.0
287. CH2O+NO2=HCO+HONO	8.02E+02	2.8	13730.0
288. CH3O+NO2=CH2O+HONO	6.00E+12	0.0	2285.0
289. CH2OH+NO2=HONO+CH2O	5.00E+12	0.0	0.0
290. CH3OH+NO2=HONO+CH2OH	1.50E+02	3.3	20035.0
291. CH2CHO+NO2=CH2CO+HONO	8.90E+12	0.0	-159.0
292. CH3CHO+NO2=HONO+CH2CHO	1.30E+12	0.0	3700.0
293. CH4+NO2=HNO2+CH3	6.00E+14	0.0	37600.0
294. C2H4+NO2=HNO2+C2H3	6.00E+14	0.0	33200.0
295. C2H6+NO2=HNO2+C2H5	6.00E+14	0.0	33200.0
296. CH2O+NO2=HNO2+HCO	1.10E-01	4.2	19850.0
297. CH3OH+NO2=HNO2+CH2OH	2.40E+03	2.9	27470.0
298. CH2SING+N2O=CH2O+N2	3.80E+13	0.0	0.0
299. CO+N2O=N2+CO2	2.70E+11	0.0	20237.0
300. CN+O=CO+N	1.90E+12	0.5	723.0
301. CH+NO=OH+CN	3.30E+12	0.0	0.0
302. CN+H2=HCN+H	3.60E+08	1.6	2999.0
303. CH4+CN=CH3+HCN	8.60E+05	2.3	-32.0
304. C2H6+CN=C2H5+HCN	1.20E+08	1.8	-994.0
305. HCN+O=NH+CO	3.50E+03	2.6	4980.0
306. HCN+OH=CN+H2O	3.90E+06	1.8	10287.0
307. OH+HCN=NH2+CO	7.83E-04	4.0	4000.0
308. CH+NO=HCN+O	5.30E+13	0.0	0.0
309. CH2+NO=HCN+OH	2.90E+14	-0.7	755.0
310. CH2SING+NO<=>OH+HCN	2.90E+14	-0.7	760.0
311. CH3+NO=HCN+H2O	4.90E+08	0.5	12392.0
312. C2H+NO=HCN+CO	6.00E+13	0.0	570.0
313. HCCO+NO=HCN+CO2	3.70E+14	-0.8	-90.0

314.	HCN=HNC		1.50E+23	-4.2	49428.0
315.	HCN+M=HNC+M		1.60E+26	-3.2	54600.0
	AR	Enhanced by 7.000E-01			
	H2O	Enhanced by 7.000E+00			
	CO2	Enhanced by 2.000E+00			
316.	HNC+H=HCN+H		7.80E+13	0.0	3600.0
317.	O+HNC=NH+CO		4.60E+12	0.0	2184.0
318.	HNC+O2=NH+CO2		1.60E+19	-2.2	1777.0
319.	H+HCN(+M)<=>NCH2(+M)		3.30E+13	0.0	0.0
	Low pressure limit: 0.14000E+27 -0.34000E+01 0.19000E+04				
	H2	Enhanced by 2.000E+00			
	H2O	Enhanced by 6.000E+00			
	CH4	Enhanced by 2.000E+00			
	CO	Enhanced by 1.500E+00			
	CO2	Enhanced by 2.000E+00			
	C2H6	Enhanced by 3.000E+00			
	AR	Enhanced by 7.000E-01			
	N2O	Enhanced by 5.000E+00			
	N2	Enhanced by 1.000E+00			
320.	NCH2+H=HCN+H2		2.40E+08	1.5	-894.0
321.	CH3+N=NCH2+H		6.10E+14	-0.3	288.0
322.	CH3+NH=NCH2+H2		3.50E+13	0.0	290.0
323.	CH2+NO=NCH2+O		8.10E+07	1.4	4111.0
324.	CH3+NO=NCH2+OH		1.50E-01	3.5	3950.0
325.	NCH2+NO=HCN+HNO		1.00E+07	2.0	4400.0
326.	CHNH=HCN+H		6.10E+28	-5.7	24257.0
327.	CHNH+H=NCH2+H		2.00E+13	0.0	0.0
328.	CH2NH+M=HCN+H2+M		1.00E+14	0.0	10000.0
329.	NH+CH3=CH2NH+H		4.00E+13	0.0	0.0
330.	CH2SING+NH3=CH2NH+H+H		1.00E+14	0.0	0.0
331.	CH2NH+OH=CHNH+H2O		2.40E+06	2.0	457.0
332.	CH3NH=CH2NH+H		1.30E+42	-9.2	41316.0

333.	CH3NH(+M)<=>CH2NH+H(+M)	7.91E+11	0.3	36260.0
	Low pressure limit: 0.16400E+40 -0.70200E+01	0.40100E+05		
334.	CH3NH+M=CH3+NH+M	1.00E+14	0.0	18000.0
335.	CH3+NH2<=>CH3NH+H	9.08E+13	-0.4	15714.0
336.	CH3NH+H=CH2NH+H2	7.20E+08	1.5	-894.0
337.	CH3NH+OH=CH2NH+H2O	3.60E+06	2.0	-1192.0
338.	CH3NH+OH=CH4+HNO	6.00E+12	0.0	0.0
339.	HNOH+CH3=CH3NH+OH	2.00E+13	0.0	0.0
340.	CH3NH+O2=CH2NH+HO2	1.00E+07	2.0	6300.0
341.	CH3NH+O2=CH3O+HNO	6.00E+12	0.0	4000.0
342.	CH3NH+CH3=CH2NH+CH4	2.40E+06	1.9	-1112.0
343.	CH2NH2=CH2NH+H	2.40E+48	-10.8	52010.0
344.	CH3+NH2(+M)=CH3NH2(+M)	7.20E+12	0.4	0.0
	Low pressure limit: 0.22000E+31 -0.38500E+01	0.00000E+00		
345.	CH3NH2+OH=CH2NH2+H2O	3.60E+06	2.0	238.0
346.	CH2SING+HCN=CH2CN+H	1.80E+14	0.0	0.0
347.	CH3+CN=CH2CN+H	1.00E+14	0.0	0.0
348.	CH2CN+O=CH2O+CN	1.00E+14	0.0	0.0
349.	CH3CN=CH2CN+H	7.90E+14	0.0	94940.0
350.	CH3CN+H=HCN+CH3	4.40E+10	0.8	6800.0
351.	CH3CN+H=HNC+CH3	2.80E+15	-0.3	20030.0
352.	CH3CN+H=CH2CN+H2	6.00E+04	3.0	8522.0
353.	CH3CN+OH=CH2CN+H2O	2.00E+07	2.0	2000.0
354.	H+NCN=HCN+N	1.89E+14	0.0	8425.0
355.	NCN+OH=HCN+NO	5.00E+13	0.0	0.0
356.	CH3NN+M=CH3+N2+M	1.00E+11	0.0	5900.0
357.	CH3NNH(+M)<=>CH3+NNH(+M)	3.30E+16	-0.1	55000.0
	Low pressure limit: 0.18800E+32 -0.45500E+01	0.57500E+05		
	TROE centering: 0.97000E+00 0.25059E+03	0.10000E+01	0.40100E+06	
358.	H2NN+CH3=CH3NNH+H	8.30E+05	1.9	6494.0
359.	CH3NNH+O=CH3NN+OH	9.60E+12	0.0	0.0
360.	CH3NNH+OH=CH3NN+H2O	3.92E+13	0.0	0.0

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361. CH3NN+HO2=CH3NNH+O2                              1.00E+06    2.0        0.0
362. CH3NNH+HO2=CH3NN+H2O2                            1.00E+11    0.0     1987.0
363. CH3NNH+CH3=CH4+CH3NN                             7.40E+13    0.0     5210.0
364. CH3NNH+NH2=NH3+CH3NN                             7.40E+13    0.0     5210.0
365. CH3NNH+NO2=CH3NN+HONO                            2.20E+11    0.0     5900.0
366. CH2NNH2+H=NCH2+NH3                               1.76E+08    1.3     8801.1
367. H2NN+CH3=CH2NNH2+H                               8.30E+05    1.9     6494.0
368. CH3NNH2(+M)<=>CH3NNH+H(+M)                       1.35E+08    1.7    47280.0
     Low pressure limit:  0.12200E+54 -0.10750E+02  0.53560E+05
369. CH3NNH2(+M)<=>CH2NNH2+H(+M)                      1.15E+09    1.2    50330.0
     Low pressure limit:  0.17100E+50 -0.99400E+01  0.56000E+05
     TROE centering:      0.00000E+00  0.33100E+03  0.10000E+02  0.47800E+05
370. CH3NNH2+O=CH3NNH+OH                              1.00E+08    2.0        0.0
371. CH3NNH2+OH=CH3NNH+H2O                            1.00E+08    2.0        0.0
372. CH3NNH2+O2=CH3NNH+HO2                            4.00E+12    0.0        0.0
373. CH3NNH2+HO2=CH3NNH+H2O2                          1.00E+08    2.0        0.0
374. CH3NNH2+NO2=CH3NNH+HONO                          1.00E+08    2.0        0.0
375. CH2NHNH2(+M)<=>CH2NH+NH2(+M)                     3.87E+12    0.2    12200.0
     Low pressure limit:  0.16200E+28 -0.39800E+01  0.11800E+05
     TROE centering:      0.86600E+00  0.29800E+03  0.10000E+02  0.28000E+06
376. CH2NHNH2(+M)<=>CH2NNH2+H(+M)                     5.92E+11    0.3    36300.0
     Low pressure limit:  0.52500E+16 -0.72000E+00  0.34800E+05
     TROE centering:      0.00000E+00  0.49400E+03  0.10000E+02  0.28000E+06
377. CH3NHNH(+M)<=>CH3+N2H2(+M)                       4.64E+09    1.6    35620.0
     Low pressure limit:  0.34800E+49 -0.97000E+01  0.41200E+05
     TROE centering:      0.00000E+00  0.23300E+03  0.10000E+02  0.30800E+06
378. CH3NHNH(+M)<=>CH3NNH+H(+M)                       1.40E+07    2.0    44660.0
     Low pressure limit:  0.18200E+37 -0.65600E+01  0.48600E+05
     TROE centering:      0.00000E+00  0.13400E+03  0.10000E+02  0.51000E+05
379. CH3NHNH2(+M)<=>CH3NNH2+H(+M)                     4.66E+16   -0.2    77610.0
     Low pressure limit:  0.10900E+50 -0.95600E+01  0.83400E+05
     TROE centering:      0.00000E+00  0.16900E+03  0.13700E+02  0.40000E+05
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380. CH3NHNH2(+M)<=>CH3NHNH+H(+M)                    4.69E+16   -0.2    80120.0
     Low pressure limit:  0.44400E+48 -0.91900E+01  0.85700E+05
     TROE centering:      0.00000E+00  0.14900E+03  0.42800E+02  0.42400E+05
381. CH3NHNH2(+M)<=>CH2NHNH2+H(+M)                   6.42E+16   -0.2    91800.0
     Low pressure limit:  0.18000E+44 -0.79800E+01  0.96700E+05
     TROE centering:      0.98900E+00  0.10700E+03  0.60700E+02  0.60100E+05
382. CH3NHNH2(+M)<=>CH3NNH+H2(+M)                    9.70E+08    1.3   107500.0
     Low pressure limit:  0.10500E+69 -0.13840E+02  0.11500E+06
     TROE centering:      0.00000E+00  0.50000E+06  0.10000E+02  0.41700E+05
383. CH3NHNH2(+M)<=>CH2NNH2+H2(+M)                   2.69E+09    1.2   105430.0
     Low pressure limit:  0.10500E+69 -0.13840E+02  0.11400E+03
     TROE centering:      0.19500E+00  0.47200E+04  0.10000E+01  0.10000E+01
384. CH3NHNH2(+M)<=>N2H3+CH3(+M)                     3.12E+16   -0.2    65180.0
     Low pressure limit:  0.73400E+62 -0.13010E+02  0.72900E+05
     TROE centering:      0.00000E+00  0.27100E+03  0.10000E+02  0.41700E+05
385. CH3NHNH2(+M)<=>H2NN+CH4(+M)                     1.36E+09    1.6    67110.0
     Low pressure limit:  0.24700E+52 -0.10400E+02  0.74300E+05
     TROE centering:      0.00000E+00  0.26000E+03  0.10000E+02  0.77500E+05
386. CH3NHNH2(+M)<=>N2H2+CH4(+M)                     1.61E+10    1.1   108880.0
     Low pressure limit:  0.43820E+64 -0.12620E+02  0.11600E+06
     TROE centering:      0.00000E+00  0.97800E+03  0.10000E+02  0.41700E+05
387. CH3NHNH2(+M)<=>CH3NH+NH2(+M)                    2.40E+16   -0.1    63790.0
     Low pressure limit:  0.89200E+65 -0.13840E+02  0.71900E+05
388. CH3NHNH2(+M)<=>CH2NH+NH3(+M)                    3.50E+08    1.4    68330.0
     Low pressure limit:  0.80500E+49 -0.10300E+02  0.75300E+05
     TROE centering:      0.00000E+00  0.24200E+03  0.10000E+02  0.41700E+05
389. CH3NHNH2(+M)<=>CH3N+NH3(+M)                     4.33E+09    1.2    62170.0
     Low pressure limit:  0.75000E+70 -0.15570E+02  0.71600E+05
     TROE centering:      0.35500E+00  0.29300E+03  0.10000E+02  0.41300E+05
390. CH3NHNH2+H=CH3NNH2+H2                           2.08E+07    1.8     4488.1
391. CH3NHNH2+H=CH3NHNH+H2                           1.68E+09    1.1     7289.0
392. CH3NHNH2+H=CH2NHNH2+H2                          7.88E+07    1.7    11162.0
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393.	CH3NHNH2+H=CH3NH+NH3	1.37E+09	1.1	5526.4
394.	CH3NHNH2+O=CH3NNH+H2O	9.60E+12	0.0	0.0
395.	CH3NHNH2+O=CH3NNH2+OH	9.60E+12	0.0	0.0
396.	CH3NHNH2+O=CH3NHNH+OH	2.69E+12	0.0	0.0
397.	CH3NHNH2+O=CH2NHNH2+OH	1.30E+12	0.0	0.0
398.	CH3NHNH2+OH=CH3NNH2+H2O	3.92E+13	0.0	0.0
399.	CH3NHNH2+OH=CH3NHNH+H2O	1.10E+13	0.0	0.0
400.	CH3NHNH2+OH=CH2NHNH2+H2O	5.30E+12	0.0	0.0
401.	CH3NNH2+HO2=CH3NHNH2+O2	1.00E+06	2.0	0.0
402.	CH3NHNH2+HO2=CH3NNH2+H2O2	2.70E+11	0.0	1987.0
403.	CH3NHNH2+HO2=CH3NHNH+H2O2	7.56E+10	0.0	1987.0
404.	CH3NHNH2+HO2=CH2NHNH2+H2O2	3.65E+10	0.0	1987.0
405.	CH3NHNH2+CH3=CH4+CH3NNH2	4.79E+01	3.4	3578.3
406.	CH3NHNH2+CH3=CH3NHNH+CH4	3.21E+02	3.1	5748.1
407.	CH3NHNH2+CH3=CH2NHNH2+CH4	2.27E+01	3.5	7669.4
408.	CH3NHNH2+NH=CH3NNH2+NH2	1.45E+02	3.3	4435.5
409.	CH3NHNH2+NH=CH3NHNH+NH2	6.20E+02	3.1	7062.4
410.	CH3NHNH2+NH=CH2NHNH2+NH2	3.93E+01	3.6	10910.0
411.	CH3NHNH2+NH2=CH3NNH2+NH3	1.65E+02	3.0	870.1
412.	CH3NHNH2+NH2=CH3NHNH+NH3	5.98E+01	3.1	2110.2
413.	CH3NHNH2+NH2=CH2NHNH2+NH3	1.04E+00	3.6	1894.1
414.	CH3NHNH2+NO2=CH3NNH2+HONO	2.20E+11	0.0	5900.0
415.	CH3NHNH2+NO2=CH3NHNH+HONO	7.87E+10	0.0	8839.0
416.	CH3NHNH2+NO2=CH2NHNH2+HONO	1.39E+09	0.0	9803.0
417.	CH3NHNH2+NO=CH3NNH2+HNO	1.85E+13	0.0	8524.0
418.	CH3NHNH2+NO=CH3NHNH+HNO	1.24E+12	0.0	9605.0
419.	CH3NHNH2+NO=CH2NHNH2+HNO	5.05E+12	0.0	11310.0
420.	CN+OH=NCO+H	4.00E+13	0.0	0.0
421.	CH+NO=H+NCO	2.00E+13	0.0	0.0
422.	HCN+O=NCO+H	1.40E+04	2.6	4980.0
423.	NCO+H=NH+CO	5.20E+13	0.0	0.0
424.	CN+O2=NCO+O	7.20E+12	0.0	-417.0

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     Declared duplicate reaction...
425. CN+O2=NCO+O                                    -2.80E+17   -2.0        0.0
     Declared duplicate reaction...
426. CH3CN+O=CH3+NCO                                 6.00E+09    1.8     8130.0
427. C2H2+NCO=HCCO+HCN                               1.40E+12    0.0     1815.0
428. CN+CO2=NCO+CO                                   3.67E+06    2.2    26900.0
429. CN+NO2=NCO+NO                                   5.30E+15   -0.8      344.0
430. NCO+NO=N2+CO2                                   1.50E+21   -2.7     1824.0
431. NCO+NO=N2O+CO                                   4.00E+19   -2.2     1743.0
432. NCO+NO2=CO2+N2O                                 3.00E+12    0.0     -707.0
433. HCNO=HCN+O                                      4.20E+31   -6.1    61175.0
434. CH2+NO=HCNO+H                                   3.80E+13   -0.4      576.0
435. CH2SING+NO<=>H+HCNO                             3.80E+13   -0.4      580.0
436. NCH2+O=HCNO+H                                   2.00E+13    0.0        0.0
437. HCNO+H=HCN+OH                                   7.20E+10    0.8     8612.0
438. HCNO+O=HCO+NO                                   6.30E+13    0.0        0.0
439. HCNO+O=NCO+OH                                   7.00E+12    0.0        0.0
440. HCNO+OH=HCO+HNO                                 4.50E+12    0.0        0.0
441. HCNO+OH=CH2O+NO                                 1.00E+12    0.0        0.0
442. HCNO+OH=NO+CO+H2                                6.50E+12    0.0        0.0
443. HCNO+OH=NCO+H2O                                 3.50E+12    0.0        0.0
444. HCNO+OH=NCO+H+OH                                4.50E+12    0.0        0.0
445. NO+HCCO=HCNO+CO                                 4.60E+13    0.0      695.0
446. HCNO+CN=HCN+NCO                                 6.00E+13    0.0        0.0
447. HNCO(+M)=NH+CO(+M)                              6.00E+13    0.0    99800.0
     Low pressure limit:  0.21700E+29 -0.31000E+01  0.10190E+06
     TROE centering:      0.46650E+00  0.10000E+04  0.10000E+07
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.600E+00
448. HCNO+H<=>H+HNCO                                 2.10E+15   -0.7     2850.0
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449.	CH2+NO=HNCO+H	3.10E+17	-1.4	1271.0
450.	CH2SING+NO<=>H+HNCO	3.10E+17	-1.4	1270.0
451.	OH+HCN=HNCO+H	1.98E-03	4.0	1000.0
452.	OH+HNC=HNCO+H	2.80E+13	0.0	3694.0
453.	HNCO+H=NCO+H2	9.00E+07	1.7	13900.0
454.	HNCO+H=NH2+CO	3.60E+04	2.5	2343.0
455.	HNC+O2=HNCO+O	1.50E+12	0.0	4111.0
456.	HNCO+O=CO2+NH	9.80E+07	1.4	8524.0
457.	HNCO+O=NCO+OH	2.20E+06	2.1	11430.0
458.	HNCO+OH=NCO+H2O	3.60E+07	1.5	3594.0
459.	NCO+CH4=HNCO+CH3	9.80E+12	0.0	8122.0
460.	C2H6+NCO=C2H5+HNCO	1.50E-09	6.9	-2910.0
461.	CH2O+NCO=HNCO+HCO	6.00E+12	0.0	0.0
462.	HNCO+N=NH+NCO	2.32E+19	0.0	52500.0
463.	NCO+NH3=HNCO+NH2	2.80E+04	2.5	983.0
464.	NCO+HNO=HNCO+NO	1.80E+13	0.0	0.0
465.	CN+HNCO=HCN+NCO	1.00E+13	0.0	0.0
466.	HCN+OH=HOCN+H	5.90E+04	2.4	12500.0
467.	HOCN+H=H2+NCO	2.40E+08	1.5	6613.0
468.	HOCN+OH=H2O+NCO	1.20E+06	2.0	-248.0
469.	CH3+HOCN=CH3CN+OH	5.00E+12	0.0	2000.0
470.	CH2NO=HNCO+H	2.30E+42	-9.1	53807.0
471.	CH2NO+H=CH3+NO	4.00E+13	0.0	0.0
472.	CH2NO+H=HCNO+H2	4.80E+08	1.5	-894.0
473.	CH2NO+OH=CH2OH+NO	4.00E+13	0.0	0.0
474.	CH3+NO=CH3NO	1.00E+37	-8.4	5223.0
475.	CH3NO+OH=CH2NO+H2O	3.60E+06	2.0	-1192.0
476.	CH3NO+OH=CH3+HONO	2.50E+12	0.0	993.0
477.	CH3O+NO(+M)=CH3ONO(+M)	6.60E+14	-0.6	0.0
	Low pressure limit: 0.27000E+28 -0.35000E+01 0.00000E+00			
478.	CH3NO2(+M)=CH3+NO2(+M)	1.80E+16	0.0	58500.0
	Low pressure limit: 0.13000E+18 0.00000E+00 0.42000E+05			

```
     TROE centering:      0.18320E+00  0.10000E+02  0.10000E+07

479. CH3NO2+H=CH3+HONO                                3.30E+12    0.0     3730.0

480. CH3NO2+H=CH3NO+OH                                1.40E+12    0.0     3730.0

481. CH3NO2+OH=CH3OH+NO2                              2.00E+10    0.0    -1000.0

482. CH3O+NO2(+M)=CH3ONO2(+M)                         1.20E+13    0.0        0.0

     Low pressure limit:  0.14000E+31 -0.45000E+01  0.00000E+00
```

UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX I

MMH/RFNA REDUCED REACTION SET 2

The following is the reduced reaction set for MMH/RFNA combustion labeled "reduced reaction set 2" described in Chapter 10. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE		ELEMENT COUNT					
					LOW	HIGH	H	HE	C	O	N	AR
1	H	G	0	1.01E+00	200	3500	1	0	0	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0	0	0
3	O	G	0	1.60E+01	200	3500	0	0	0	1	0	0
4	OH	G	0	1.70E+01	200	6000	1	0	0	1	0	0
5	H2O	G	0	1.80E+01	200	3500	2	0	0	1	0	0
6	HO2	G	0	3.30E+01	200	3500	1	0	0	2	0	0
7	CH2	G	0	1.40E+01	200	6000	2	0	1	0	0	0
8	CH3	G	0	1.50E+01	200	6000	3	0	1	0	0	0
9	CH4	G	0	1.60E+01	200	3500	4	0	1	0	0	0
10	CO	G	0	2.80E+01	200	3500	0	0	1	1	0	0
11	HCO	G	0	2.90E+01	200	3500	1	0	1	1	0	0
12	CH2O	G	0	3.00E+01	200	3500	2	0	1	1	0	0
13	CH3O	G	0	3.10E+01	200	6000	3	0	1	1	0	0
14	CO2	G	0	4.40E+01	200	3500	0	0	1	2	0	0
15	N	G	0	1.40E+01	300	5000	0	0	0	0	1	0
16	NH	G	0	1.50E+01	200	6000	1	0	0	0	1	0
17	NH2	G	0	1.60E+01	300	5000	2	0	0	0	1	0
18	NH3	G	0	1.70E+01	300	5000	3	0	0	0	1	0
19	N2	G	0	2.80E+01	200	6000	0	0	0	0	2	0
20	NNH	G	0	2.90E+01	200	6000	1	0	0	0	2	0
21	N2H2	G	0	3.00E+01	300	5000	2	0	0	0	2	0
22	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0

23	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
24	N2O	G	0	4.40E+01	300	5000	0	0	0	1	2	0
25	NO2	G	0	4.60E+01	200	6000	0	0	0	2	1	0
26	HONO	G	0	4.70E+01	200	6000	1	0	0	2	1	0
27	HNO3	G	0	6.30E+01	200	6000	1	0	0	3	1	0
28	N2O4	G	0	9.20E+01	200	6000	0	0	0	4	2	0
29	CN	G	0	2.60E+01	200	6000	0	0	1	0	1	0
30	HCN	G	0	2.70E+01	300	4000	1	0	1	0	1	0
31	HNC	G	0	2.70E+01	300	5000	1	0	1	0	1	0
32	NCO	G	0	4.20E+01	300	5000	0	0	1	1	1	0
33	CH3NHNH2	G	0	4.61E+01	298	6000	6	0	1	0	2	0
34	CH2NHNH2	G	0	4.51E+01	200	5000	5	0	1	0	2	0
35	CH3NNH2	G	0	4.51E+01	200	6000	5	0	1	0	2	0
36	CH3NHNH	G	0	4.51E+01	200	5000	5	0	1	0	2	0
37	CH3NN	G	0	4.30E+01	200	6000	3	0	1	0	2	0
38	CH2NNH2	G	0	4.41E+01	200	5000	4	0	1	0	2	0
39	HNCO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
40	CH3NNH	G	0	4.41E+01	200	6000	4	0	1	0	2	0
41	CH3ONO2	G	0	7.70E+01	300	4000	3	0	1	3	1	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. O+H+M=OH+M			4.71E+18	-1.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
2. H2+M=2H+M			4.58E+19	-1.4	104380.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
3. H+OH+M=H2O+M			2.21E+22	-2.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			

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 4. H2O+O=OH+OH                                    2.97E+06    2.0    13400.0
 5. O+H2=H+OH                                      5.08E+04    2.7     6290.0
 6. OH+H2=H+H2O                                    2.16E+08    1.5     3430.0
 7. H+HO2=2OH                                      7.08E+13    0.0      300.0
 8. H2+CO(+M)=CH2O(+M)                             4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
 9. OH+CO=H+CO2                                    4.10E+04    2.1    -1578.0
10. HO2+CO=OH+CO2                                  1.50E+14    0.0    23600.0
11. O+HCO=H+CO2                                    3.00E+13    0.0        0.0
12. H+HCO(+M)=CH2O(+M)                             1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
13. H+HCO=H2+CO                                    7.30E+13    0.0        0.0
14. OH+HCO=H2O+CO                                  3.00E+13    0.0        0.0
15. HCO+M=H+CO+M                                   1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
16. HCO+HO2=CO2+OH+H                               3.00E+13    0.0        0.0
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17. H+CH2O=HCO+H2                                 5.18E+07    1.7     1834.0
18. H+CH2O(+M)=CH3O(+M)                           5.40E+11    0.5     2600.0
    Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
    TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
19. OH+CH2O=HCO+H2O                               3.43E+09    1.2     -447.0
20. H+CH3O=H2+CH2O                                2.00E+13    0.0        0.0
21. H+CH3O=OH+CH3                                 3.20E+13    0.0        0.0
22. OH+CH3O=H2O+CH2O                              1.80E+13    0.0        0.0
23. CH3O+CO=CH3+CO2                               1.57E+13    0.0    11800.0
24. O+CH4=OH+CH3                                  1.02E+09    1.5     8600.0
25. H+CH4=CH3+H2                                  6.60E+08    1.6    10840.0
26. OH+CH4=CH3+H2O                                1.00E+08    1.6     3120.0
27. CH2+CH4=2CH3                                  2.46E+06    2.0     8270.0
28. O+CH3=H+CH2O                                  5.06E+13    0.0        0.0
29. O+CH3=H+H2+CO                                 3.37E+13    0.0        0.0
30. H+CH3(+M)=CH4(+M)                             1.39E+16   -0.5      536.0
    Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
    TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
31. OH+CH3=CH2+H2O                                5.60E+07    1.6     5420.0
32. HO2+CH3=OH+CH3O                               2.00E+13    0.0        0.0
33. CH3+HCO=CH4+CO                                1.21E+14    0.0        0.0
34. CH3+CH2O=HCO+CH4                              3.32E+03    2.8     5860.0
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35. O+CH2=H+HCO			8.00E+13	0.0	0.0
36. OH+CH2=H+CH2O			2.00E+13	0.0	0.0
37. CH2+H2=H+CH3			5.00E+05	2.0	7230.0
38. NH+H=N+H2			3.20E+13	0.0	325.0
39. NH+OH=N+H2O			1.60E+07	1.7	-576.0
40. NH2+H=NH+H2			4.00E+13	0.0	3650.0
41. NH2+O=NH+OH			7.00E+12	0.0	0.0
Declared duplicate reaction...					
42. NH2+O=NH+OH			8.60E-01	4.0	1673.0
Declared duplicate reaction...					
43. NH2+OH=NH+H2O			3.30E+06	1.9	-217.0
44. NH3+H=NH2+H2			6.36E+05	2.4	10171.0
45. NH3+O=NH2+OH			2.80E+02	3.3	4471.0
46. NH3+OH=NH2+H2O			2.00E+06	2.0	566.0
47. NH2+NH2=NH3+NH			5.60E+00	3.5	552.0
48. NNH=N2+H			1.00E+09	0.0	0.0
49. N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
H2O	Enhanced by	1.500E+01			
N2	Enhanced by	2.000E+00			
H2	Enhanced by	2.000E+00			
50. N2H2+H=NNH+H2			8.50E+04	2.6	230.0
51. NH2+NH2=N2H2+H2			1.70E+08	1.6	11783.0
52. N2H2+OH=NNH+H2O			5.90E+01	3.4	1360.0
53. N+OH=NO+H			3.80E+13	0.0	0.0
54. NH+O=NO+H			9.20E+13	0.0	0.0
55. NH+OH=NO+H2			2.00E+13	0.0	0.0
56. N+NO=N2+O			3.30E+12	0.3	0.0
57. NH+NO=N2+OH			2.20E+13	-0.2	0.0
58. NNH+O=NH+NO			5.20E+11	0.4	-409.0
59. NH2+NO=N2+H2O			2.80E+20	-2.7	1258.0
60. NH2+NO=NNH+OH			2.29E+10	0.4	-814.0
61. NO+H(+M)=HNO(+M)			1.50E+15	-0.4	0.0

```
    Low pressure limit:  0.24000E+15  0.20600E+00 -0.15500E+04
    TROE centering:      0.82000E+00  0.10000E-29  0.10000E+31  0.10000E+31
    N2              Enhanced by    1.600E+00
62. HNO+H=H2+NO                                   4.50E+11    0.7      655.0
63. NH+OH=HNO+H                                   3.20E+14   -0.4      -46.0
64. NH+H2O=HNO+H2                                 2.00E+13    0.0    13850.0
65. HNO+O=OH+NO                                   1.81E+13    0.0        0.0
66. HNO+OH=NO+H2O                                 3.60E+13    0.0        0.0
67. NNH+NO=N2+HNO                                 5.00E+13    0.0        0.0
68. H+NO+N2=HNO+N2                                4.00E+20   -1.8        0.0
69. N2O(+M)=N2+O(+M)                              1.30E+12    0.0    62570.0
    Low pressure limit:  0.40000E+15  0.00000E+00  0.56600E+05
    N2              Enhanced by    1.700E+00
    CO2             Enhanced by    3.000E+00
    H2O             Enhanced by    1.200E+01
70. N2O+H=N2+OH                                   3.30E+10    0.0     4729.0
    Declared duplicate reaction...
71. N2O+H=N2+OH                                   4.40E+14    0.0    19254.0
    Declared duplicate reaction...
72. NH+NO=N2O+H                                   2.90E+14   -0.4        0.0
    Declared duplicate reaction...
73. NH+NO=N2O+H                                  -2.20E+13   -0.2        0.0
    Declared duplicate reaction...
74. NNH+O=N2O+H                                   1.00E+14    0.0        0.0
75. NH2+NO=H2+N2O                                 1.00E+13    0.0    33700.0
76. N2O+OH=HNO+NO                                 1.20E-04    4.3    25080.0
77. N2O+OH=N2+HO2                                 1.00E+14    0.0    30000.0
78. N2H2+NO=N2O+NH2                               3.00E+10    0.0        0.0
79. NO2(+M)=NO+O(+M)                              7.60E+18   -1.3    73245.0
    Low pressure limit:  0.24700E+29 -0.33700E+01  0.74756E+05
    TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.49816E+04
    N2O             Enhanced by    1.500E+00
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    H2O             Enhanced by    4.400E+00
    N2              Enhanced by    1.000E+00
    CO2             Enhanced by    2.300E+00
    Declared duplicate reaction...
80. NO+O(+M)=NO2(+M)                                1.30E+15   -0.8        0.0
    Low pressure limit:  0.47100E+25 -0.28700E+01  0.15510E+04
    TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.46816E+04
    Declared duplicate reaction...
81. NO2+H=NO+OH                                     1.30E+14    0.0      357.0
82. NO2+OH=HO2+NO                                   1.81E+13    0.0     6673.0
83. NH+NO2=N2O+OH                                   4.10E+12    0.0        0.0
84. NH+NO2=HNO+NO                                   5.90E+12    0.0        0.0
85. NH2+NO2=N2O+H2O                                 3.00E+14   -0.8      242.0
86. N2O+NO=NO2+N2                                   5.30E+05    2.2    46280.0
87. HONO(+M)=OH+NO(+M)                              1.20E+19   -1.2    49667.0
    Low pressure limit:  0.30100E+31 -0.38000E+01  0.50322E+05
    TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
    Declared duplicate reaction...
88. NO+OH(+M)=HONO(+M)                              1.99E+12   -0.1     -721.0
    Low pressure limit:  0.50800E+24 -0.25100E+01 -0.68000E+02
    TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
    Declared duplicate reaction...
89. NO2+H2=HONO+H                                   1.30E+04    2.8    29770.0
90. HONO+H=H2O+NO                                   8.10E+06    1.9     3843.0
91. HONO+H=OH+HNO                                   5.60E+10    0.9     4965.0
92. HONO+OH=H2O+NO2                                 1.26E+10    1.0      135.0
93. NH+HONO=NH2+NO2                                 1.00E+13    0.0        0.0
94. NH2+HONO=NH3+NO2                                7.10E+01    3.0    -4940.0
95. HNO+NO2=HONO+NO                                 4.40E+04    2.6     4040.0
96. HONO+HONO=NO+NO2+H2O                            3.50E-01    3.6    12140.0
97. NO2+OH(+M)=HNO3(+M)                             2.41E+13    0.0        0.0
    Low pressure limit:  0.64200E+33 -0.54900E+01  0.23490E+04
```

TROE centering: 0.40000E+00 0.45070E+03 0.15840E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

N2 Enhanced by 1.000E+00

HNO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

98.	N2O4(+M)=NO2+NO2(+M)	4.05E+18	-1.1	12840.0
	Low pressure limit: 0.19600E+29 -0.38000E+01 0.12840E+05			
99.	CH3+NH2=CH4+NH	2.80E+06	1.9	9205.0
100.	CH3+NH2=CH2+NH3	1.60E+06	1.9	7566.0
101.	CH4+NH2=CH3+NH3	1.50E+03	3.0	9940.0
102.	CH2+NO=NH2+CO	2.30E+16	-1.4	1331.0
103.	N+CO2<=>NO+CO	3.00E+12	0.0	11300.0
104.	NH+CO2<=>HNO+CO	1.00E+13	0.0	14350.0
105.	HNO+CH3=NO+CH4	8.20E+05	1.9	480.0
106.	HCO+NO=HNO+CO	7.23E+12	0.0	0.0
107.	CH3O+NO=HNO+CH2O	7.50E+12	0.0	2017.0
	Declared duplicate reaction...			
108.	CH3O+NO=HNO+CH2O	2.50E+18	-2.6	0.0
	Declared duplicate reaction...			
109.	CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
110.	NO2+CH3=NO+CH3O	1.40E+13	0.0	0.0
111.	CO+NO2=NO+CO2	9.04E+13	0.0	33780.0
112.	HCO+NO2=CO+NO+OH	1.20E+23	-3.3	2355.0
113.	HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
114.	CH4+NO2=HONO+CH3	6.50E+14	0.0	45800.0
115.	HCO+NO2=CO+HONO	1.24E+23	-3.3	2355.0
116.	CH2O+NO2=HCO+HONO	8.02E+02	2.8	13730.0
117.	CH3O+NO2=CH2O+HONO	6.00E+12	0.0	2285.0
118.	CO+N2O=N2+CO2	2.70E+11	0.0	20237.0
119.	CN+O=CO+N	1.90E+12	0.5	723.0
120.	CN+H2=HCN+H	3.60E+08	1.6	2999.0

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121. CH4+CN=CH3+HCN                                    8.60E+05    2.3      -32.0
122. HCN+O=NH+CO                                       3.50E+03    2.6     4980.0
123. HCN+OH=CN+H2O                                     3.90E+06    1.8    10287.0
124. OH+HCN=NH2+CO                                     7.83E-04    4.0     4000.0
125. CH2+NO=HCN+OH                                     2.90E+14   -0.7      755.0
126. CH3+NO=HCN+H2O                                    4.90E+08    0.5    12392.0
127. HCN=HNC                                           1.50E+23   -4.2    49428.0
128. HCN+M=HNC+M                                       1.60E+26   -3.2    54600.0
     H2O             Enhanced by    7.000E+00
     CO2             Enhanced by    2.000E+00
129. HNC+H=HCN+H                                       7.80E+13    0.0     3600.0
130. O+HNC=NH+CO                                       4.60E+12    0.0     2184.0
131. CH3NN+M=CH3+N2+M                                  1.00E+11    0.0     5900.0
132. CH3NNH(+M)<=>CH3+NNH(+M)                          3.30E+16   -0.1    55000.0
     Low pressure limit:  0.18800E+32 -0.45500E+01  0.57500E+05
     TROE centering:      0.97000E+00  0.25059E+03  0.10000E+01  0.40100E+06
133. CH3NNH+O=CH3NN+OH                                 9.60E+12    0.0        0.0
134. CH3NNH+OH=CH3NN+H2O                               3.92E+13    0.0        0.0
135. CH3NNH+CH3=CH4+CH3NN                              7.40E+13    0.0     5210.0
136. CH3NNH+NH2=NH3+CH3NN                              7.40E+13    0.0     5210.0
137. CH3NNH+NO2=CH3NN+HONO                             2.20E+11    0.0     5900.0
138. CH3NNH2(+M)<=>CH3NNH+H(+M)                        1.35E+08    1.7    47280.0
     Low pressure limit:  0.12200E+54 -0.10750E+02  0.53560E+05
139. CH3NNH2(+M)<=>CH2NNH2+H(+M)                       1.15E+09    1.2    50330.0
     Low pressure limit:  0.17100E+50 -0.99400E+01  0.56000E+05
     TROE centering:      0.00000E+00  0.33100E+03  0.10000E+02  0.47800E+05
140. CH3NNH2+O=CH3NNH+OH                               1.00E+08    2.0        0.0
141. CH3NNH2+OH=CH3NNH+H2O                             1.00E+08    2.0        0.0
142. CH3NNH2+NO2=CH3NNH+HONO                           1.00E+08    2.0        0.0
143. CH2NHNH2(+M)<=>CH2NNH2+H(+M)                      5.92E+11    0.3    36300.0
     Low pressure limit:  0.52500E+16 -0.72000E+00  0.34800E+05
     TROE centering:      0.00000E+00  0.49400E+03  0.10000E+02  0.28000E+06
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144. CH3NHNH(+M)<=>CH3+N2H2(+M)                      4.64E+09    1.6    35620.0
     Low pressure limit:  0.34800E+49 -0.97000E+01  0.41200E+05
     TROE centering:      0.00000E+00  0.23300E+03  0.10000E+02  0.30800E+06
145. CH3NHNH(+M)<=>CH3NNH+H(+M)                     1.40E+07    2.0    44660.0
     Low pressure limit:  0.18200E+37 -0.65600E+01  0.48600E+05
     TROE centering:      0.00000E+00  0.13400E+03  0.10000E+02  0.51000E+05
146. CH3NHNH2(+M)<=>CH3NNH2+H(+M)                   4.66E+16   -0.2    77610.0
     Low pressure limit:  0.10900E+50 -0.95600E+01  0.83400E+05
     TROE centering:      0.00000E+00  0.16900E+03  0.13700E+02  0.40000E+05
147. CH3NHNH2(+M)<=>CH3NHNH+H(+M)                   4.69E+16   -0.2    80120.0
     Low pressure limit:  0.44400E+48 -0.91900E+01  0.85700E+05
     TROE centering:      0.00000E+00  0.14900E+03  0.42800E+02  0.42400E+05
148. CH3NHNH2(+M)<=>CH2NHNH2+H(+M)                  6.42E+16   -0.2    91800.0
     Low pressure limit:  0.18000E+44 -0.79800E+01  0.96700E+05
     TROE centering:      0.98900E+00  0.10700E+03  0.60700E+02  0.60100E+05
149. CH3NHNH2(+M)<=>CH3NNH+H2(+M)                   9.70E+08    1.3   107500.0
     Low pressure limit:  0.10500E+69 -0.13840E+02  0.11500E+06
     TROE centering:      0.00000E+00  0.50000E+06  0.10000E+02  0.41700E+05
150. CH3NHNH2(+M)<=>CH2NNH2+H2(+M)                  2.69E+09    1.2   105430.0
     Low pressure limit:  0.10500E+69 -0.13840E+02  0.11400E+03
     TROE centering:      0.19500E+00  0.47200E+04  0.10000E+01  0.10000E+01
151. CH3NHNH2(+M)<=>N2H2+CH4(+M)                    1.61E+10    1.1   108880.0
     Low pressure limit:  0.43820E+64 -0.12620E+02  0.11600E+06
     TROE centering:      0.00000E+00  0.97800E+03  0.10000E+02  0.41700E+05
152. CH3NHNH2+H=CH3NNH2+H2                          2.08E+07    1.8     4488.1
153. CH3NHNH2+H=CH3NHNH+H2                          1.68E+09    1.1     7289.0
154. CH3NHNH2+H=CH2NHNH2+H2                         7.88E+07    1.7    11162.0
155. CH3NHNH2+O=CH3NNH+H2O                          9.60E+12    0.0        0.0
156. CH3NHNH2+O=CH3NNH2+OH                          9.60E+12    0.0        0.0
157. CH3NHNH2+O=CH3NHNH+OH                          2.69E+12    0.0        0.0
158. CH3NHNH2+O=CH2NHNH2+OH                         1.30E+12    0.0        0.0
159. CH3NHNH2+OH=CH3NNH2+H2O                        3.92E+13    0.0        0.0
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160. CH3NHNH2+OH=CH3NHNH+H2O                          1.10E+13    0.0        0.0
161. CH3NHNH2+OH=CH2NHNH2+H2O                         5.30E+12    0.0        0.0
162. CH3NHNH2+CH3=CH4+CH3NNH2                         4.79E+01    3.4     3578.3
163. CH3NHNH2+CH3=CH3NHNH+CH4                         3.21E+02    3.1     5748.1
164. CH3NHNH2+CH3=CH2NHNH2+CH4                        2.27E+01    3.5     7669.4
165. CH3NHNH2+NH=CH3NNH2+NH2                          1.45E+02    3.3     4435.5
166. CH3NHNH2+NH=CH3NHNH+NH2                          6.20E+02    3.1     7062.4
167. CH3NHNH2+NH=CH2NHNH2+NH2                         3.93E+01    3.6    10910.0
168. CH3NHNH2+NH2=CH3NNH2+NH3                         1.65E+02    3.0      870.1
169. CH3NHNH2+NH2=CH3NHNH+NH3                         5.98E+01    3.1     2110.2
170. CH3NHNH2+NH2=CH2NHNH2+NH3                        1.04E+00    3.6     1894.1
171. CH3NHNH2+NO2=CH3NNH2+HONO                        2.20E+11    0.0     5900.0
172. CH3NHNH2+NO2=CH3NHNH+HONO                        7.87E+10    0.0     8839.0
173. CH3NHNH2+NO2=CH2NHNH2+HONO                       1.39E+09    0.0     9803.0
174. CH3NHNH2+NO=CH3NNH2+HNO                          1.85E+13    0.0     8524.0
175. CH3NHNH2+NO=CH3NHNH+HNO                          1.24E+12    0.0     9605.0
176. CH3NHNH2+NO=CH2NHNH2+HNO                         5.05E+12    0.0    11310.0
177. CN+OH=NCO+H                                      4.00E+13    0.0        0.0
178. HCN+O=NCO+H                                      1.40E+04    2.6     4980.0
179. NCO+H=NH+CO                                      5.20E+13    0.0        0.0
180. CN+CO2=NCO+CO                                    3.67E+06    2.2    26900.0
181. CN+NO2=NCO+NO                                    5.30E+15   -0.8      344.0
182. NCO+NO=N2+CO2                                    1.50E+21   -2.7     1824.0
183. NCO+NO=N2O+CO                                    4.00E+19   -2.2     1743.0
184. NCO+NO2=CO2+N2O                                  3.00E+12    0.0     -707.0
185. HNCO(+M)=NH+CO(+M)                               6.00E+13    0.0    99800.0
     Low pressure limit:  0.21700E+29 -0.31000E+01  0.10190E+06
     TROE centering:      0.46650E+00  0.10000E+04  0.10000E+07
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.600E+00
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186. CH2+NO=HNCO+H                                    3.10E+17   -1.4     1271.0
187. OH+HCN=HNCO+H                                    1.98E-03    4.0     1000.0
188. OH+HNC=HNCO+H                                    2.80E+13    0.0     3694.0
189. HNCO+H=NCO+H2                                    9.00E+07    1.7    13900.0
190. HNCO+H=NH2+CO                                    3.60E+04    2.5     2343.0
191. HNCO+O=CO2+NH                                    9.80E+07    1.4     8524.0
192. HNCO+O=NCO+OH                                    2.20E+06    2.1    11430.0
193. HNCO+OH=NCO+H2O                                  3.60E+07    1.5     3594.0
194. NCO+CH4=HNCO+CH3                                 9.80E+12    0.0     8122.0
195. CH2O+NCO=HNCO+HCO                                6.00E+12    0.0        0.0
196. HNCO+N=NH+NCO                                    2.32E+19    0.0    52500.0
197. NCO+NH3=HNCO+NH2                                 2.80E+04    2.5      983.0
198. NCO+HNO=HNCO+NO                                  1.80E+13    0.0        0.0
199. CN+HNCO=HCN+NCO                                  1.00E+13    0.0        0.0
200. CH3O+NO2(+M)=CH3ONO2(+M)                         1.20E+13    0.0        0.0
     Low pressure limit:  0.14000E+31 -0.45000E+01  0.00000E+00
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UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

APPENDIX J

TMEDA/RFNA REACTION SET

The following is the reaction set for TMEDA/RFNA combustion described in Chapter 11. Details on the format may be found in Chapter 4.

	SPECIES CONSIDERED	PHASE	CHARGE	MOLEC. WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	HE	C	O	N	AR
1	H	G	0	1.01E+00	200	3500	1	0	0	0	0	0
2	H2	G	0	2.02E+00	200	3500	2	0	0	0	0	0
3	C	G	0	1.20E+01	200	3500	0	0	1	0	0	0
4	O	G	0	1.60E+01	200	3500	0	0	0	1	0	0
5	O2	G	0	3.20E+01	200	3500	0	0	0	2	0	0
6	OH	G	0	1.70E+01	200	6000	1	0	0	1	0	0
7	H2O	G	0	1.80E+01	200	3500	2	0	0	1	0	0
8	HO2	G	0	3.30E+01	200	3500	1	0	0	2	0	0
9	H2O2	G	0	3.40E+01	200	3500	2	0	0	2	0	0
10	CH	G	0	1.30E+01	200	6000	1	0	1	0	0	0
11	CH2	G	0	1.40E+01	200	6000	2	0	1	0	0	0
12	CH2SING	G	0	1.40E+01	200	6000	2	0	1	0	0	0
13	CH3	G	0	1.50E+01	200	6000	3	0	1	0	0	0
14	CH4	G	0	1.60E+01	200	3500	4	0	1	0	0	0
15	C2	G	0	2.40E+01	200	6000	0	0	2	0	0	0
16	CO	G	0	2.80E+01	200	3500	0	0	1	1	0	0
17	HCO	G	0	2.90E+01	200	3500	1	0	1	1	0	0
18	CH2O	G	0	3.00E+01	200	3500	2	0	1	1	0	0
19	CH2OH	G	0	3.10E+01	200	6000	3	0	1	1	0	0
20	CH3O	G	0	3.10E+01	200	6000	3	0	1	1	0	0
21	CH3OH	G	0	3.20E+01	200	3500	4	0	1	1	0	0
22	C2H	G	0	2.50E+01	200	3500	1	0	2	0	0	0
23	C2H2	G	0	2.60E+01	200	3500	2	0	2	0	0	0

24	H2CC	G	0	2.60E+01	200	6000	2	0	2	0	0	0
25	C2H3	G	0	2.70E+01	200	5000	3	0	2	0	0	0
26	C2H4	G	0	2.81E+01	200	3500	4	0	2	0	0	0
27	C2H5	G	0	2.91E+01	200	3500	5	0	2	0	0	0
28	C2H6	G	0	3.01E+01	200	3500	6	0	2	0	0	0
29	C3H2	G	0	3.80E+01	300	5000	2	0	3	0	0	0
30	C3H3	G	0	3.91E+01	200	6000	3	0	3	0	0	0
31	AR	G	0	3.99E+01	300	5000	0	0	0	0	0	1
32	AC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
33	PC3H4	G	0	4.01E+01	200	6000	4	0	3	0	0	0
34	C2O	G	0	4.00E+01	300	4000	0	0	2	1	0	0
35	HCCO	G	0	4.10E+01	300	4000	1	0	2	1	0	0
36	AC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
37	TC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
38	SC3H5	G	0	4.11E+01	300	3000	5	0	3	0	0	0
39	CH2CO	G	0	4.20E+01	200	3500	2	0	2	1	0	0
40	C3H6	G	0	4.21E+01	300	5000	6	0	3	0	0	0
41	CH3CO	G	0	4.30E+01	200	6000	3	0	2	1	0	0
42	CH2CHO	G	0	4.30E+01	300	5000	3	0	2	1	0	0
43	nC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
44	iC3H7	G	0	4.31E+01	300	3000	7	0	3	0	0	0
45	C2H4O	G	0	4.41E+01	300	5000	4	0	2	1	0	0
46	CH3CHO	G	0	4.41E+01	200	6000	4	0	2	1	0	0
47	C3H8	G	0	4.41E+01	300	3000	8	0	3	0	0	0
48	CO2	G	0	4.40E+01	200	3500	0	0	1	2	0	0
49	OCHO	G	0	4.50E+01	300	5000	1	0	1	2	0	0
50	C2H5O	G	0	4.51E+01	200	6000	5	0	2	1	0	0
51	CH3CHOH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
52	C2H4OH	G	0	4.51E+01	300	5000	5	0	2	1	0	0
53	CH3OCH2	G	0	4.51E+01	300	5000	5	0	2	1	0	0
54	CH3OCH3	G	0	4.61E+01	270	3000	6	0	2	1	0	0

55	C2H5OH	G	0	4.61E+01	200	6000	6	0	2	1	0	0
56	CH3OCO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
57	CH3OCHO	G	0	6.01E+01	300	5000	4	0	2	2	0	0
58	CH3OCH2O	G	0	6.11E+01	300	5000	5	0	2	2	0	0
59	HOC2H4O2	G	0	7.71E+01	300	5000	5	0	2	3	0	0
60	C4H	G	0	4.91E+01	300	3000	1	0	4	0	0	0
61	C2H5OO	G	0	6.11E+01	300	5000	5	0	2	2	0	0
62	C2H3CO	G	0	5.51E+01	200	6000	3	0	3	1	0	0
63	C2H3CHO	G	0	5.61E+01	298	3000	4	0	3	1	0	0
64	C2H3CH2O	G	0	5.71E+01	300	3000	5	0	3	1	0	0
65	C4H2	G	0	5.01E+01	300	3000	2	0	4	0	0	0
66	iC4H3	G	0	5.11E+01	200	5000	3	0	4	0	0	0
67	nC4H3	G	0	5.11E+01	300	4000	3	0	4	0	0	0
68	C4H4	G	0	5.21E+01	300	3000	4	0	4	0	0	0
69	n-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
70	i-C4H5	G	0	5.31E+01	300	4000	5	0	4	0	0	0
71	iiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
72	iiiC4H6	G	0	5.41E+01	300	3000	6	0	4	0	0	0
73	C4H7	G	0	5.51E+01	300	3000	7	0	4	0	0	0
74	IC4H8	G	0	5.61E+01	300	5000	8	0	4	0	0	0
75	nC4H9	G	0	5.71E+01	200	6000	9	0	4	0	0	0
76	OCHCHO	G	0	5.80E+01	300	3000	2	0	2	2	0	0
77	C2H3OO	G	0	5.90E+01	300	5000	3	0	2	2	0	0
78	N	G	0	1.40E+01	300	5000	0	0	0	0	1	0
79	NH	G	0	1.50E+01	200	6000	1	0	0	0	1	0
80	NH2	G	0	1.60E+01	300	5000	2	0	0	0	1	0
81	NH3	G	0	1.70E+01	300	5000	3	0	0	0	1	0
82	N2	G	0	2.80E+01	200	6000	0	0	0	0	2	0
83	NNH	G	0	2.90E+01	200	6000	1	0	0	0	2	0
84	N2H2	G	0	3.00E+01	300	5000	2	0	0	0	2	0
85	H2NN	G	0	3.00E+01	300	5000	2	0	0	0	2	0

86	N2H3	G	0	3.10E+01	300	5000	3	0	0	0	2	0
87	N2H4	G	0	3.20E+01	300	5000	4	0	0	0	2	0
88	NO	G	0	3.00E+01	200	6000	0	0	0	1	1	0
89	HNO	G	0	3.10E+01	200	6000	1	0	0	1	1	0
90	HON	G	0	3.10E+01	300	5000	1	0	0	1	1	0
91	HNOH	G	0	3.20E+01	200	6000	2	0	0	1	1	0
92	NH2O	G	0	3.20E+01	300	4000	2	0	0	1	1	0
93	NH2OH	G	0	3.30E+01	300	5000	3	0	0	1	1	0
94	HNNNH2	G	0	4.50E+01	300	5000	3	0	0	0	3	0
95	N2O	G	0	4.40E+01	300	5000	0	0	0	1	2	0
96	HNNO	G	0	4.50E+01	300	5000	1	0	0	1	2	0
97	NH2NO	G	0	4.60E+01	200	6000	2	0	0	1	2	0
98	NHNHO	G	0	4.60E+01	300	5000	2	0	0	1	2	0
99	NH2NHO	G	0	4.70E+01	300	5000	3	0	0	1	2	0
100	NO2	G	0	4.60E+01	200	6000	0	0	0	2	1	0
101	HONO	G	0	4.70E+01	200	6000	1	0	0	2	1	0
102	HNO2	G	0	4.70E+01	300	4000	1	0	0	2	1	0
103	HNOO	G	0	4.70E+01	300	5000	1	0	0	2	1	0
104	HONHO	G	0	4.80E+01	300	5000	2	0	0	2	1	0
105	NH2NO2	G	0	6.20E+01	200	6000	2	0	0	2	2	0
106	NO3	G	0	6.20E+01	200	6000	0	0	0	3	1	0
107	HNO3	G	0	6.30E+01	200	6000	1	0	0	3	1	0
108	N2O4	G	0	9.20E+01	200	6000	0	0	0	4	2	0
109	HE	G	0	4.00E+00	200	6000	0	1	0	0	0	0
110	CN	G	0	2.60E+01	200	6000	0	0	1	0	1	0
111	HCN	G	0	2.70E+01	300	4000	1	0	1	0	1	0
112	HNC	G	0	2.70E+01	300	5000	1	0	1	0	1	0
113	CHNH	G	0	2.80E+01	300	4000	2	0	1	0	1	0
114	NCH2	G	0	2.80E+01	300	4000	2	0	1	0	1	0
115	CH2NH	G	0	2.90E+01	300	5000	3	0	1	0	1	0
116	CH3N	G	0	2.90E+01	200	5000	3	0	1	0	1	0

117	CH3NH	G	0	3.01E+01	300	5000	4	0	1	0	1	0
118	CH2NH2	G	0	3.01E+01	300	5000	4	0	1	0	1	0
119	CH3NH2	G	0	3.11E+01	300	5000	5	0	1	0	1	0
120	NCN	G	0	4.00E+01	300	4000	0	0	1	0	2	0
121	CHCNH	G	0	4.00E+01	298	3000	2	0	2	0	1	0
122	CH2CN	G	0	4.00E+01	200	6000	2	0	2	0	1	0
123	HCNN	G	0	4.10E+01	300	5000	1	0	1	0	2	0
124	CH2CNH	G	0	4.11E+01	200	5000	3	0	2	0	1	0
125	CH2CHN	G	0	4.11E+01	298	3000	3	0	2	0	1	0
126	CH2CHN(S)	G	0	4.11E+01	298	3000	3	0	2	0	1	0
127	CHCNH2	G	0	4.11E+01	298	3000	3	0	2	0	1	0
128	CH3CN	G	0	4.11E+01	200	6000	3	0	2	0	1	0
129	c-C2H3N	G	0	4.11E+01	298	3000	3	0	2	0	1	0
130	CH2NN	G	0	4.20E+01	200	6000	2	0	1	0	2	0
131	NCO	G	0	4.20E+01	300	5000	0	0	1	1	1	0
132	CH3NCH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
133	CH3CHN	G	0	4.21E+01	298	3000	4	0	2	0	1	0
134	CH3CNH	G	0	4.21E+01	298	3000	4	0	2	0	1	0
135	CH2CNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
136	CHCHNH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
137	CH2NCH2	G	0	4.21E+01	298	3000	4	0	2	0	1	0
138	CH2CHNH	G	0	4.21E+01	200	5000	4	0	2	0	1	0
139	CH3CHNH	G	0	4.31E+01	298	3000	5	0	2	0	1	0
140	CH3NCH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
141	CH2CHNH2	G	0	4.31E+01	298	3000	5	0	2	0	1	0
142	CH3CH2NH	G	0	4.41E+01	298	3000	6	0	2	0	1	0
143	CH3CHNH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
144	CH2CH2NH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
145	CH3CH2NH2	G	0	4.51E+01	298	3000	7	0	2	0	1	0
146	CH3NHNH2	G	0	4.61E+01	298	6000	6	0	1	0	2	0
147	CH2NHNH2	G	0	4.51E+01	200	5000	5	0	1	0	2	0

148	CH3NNH2	G	0	4.51E+01	200	6000	5	0	1	0	2	0
149	CH3NHNH	G	0	4.51E+01	200	5000	5	0	1	0	2	0
150	CH3NN	G	0	4.30E+01	200	6000	3	0	1	0	2	0
151	CH2NNH2	G	0	4.41E+01	200	5000	4	0	1	0	2	0
152	HCNO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
153	HNCO	G	0	4.30E+01	300	5000	1	0	1	1	1	0
154	HOCN	G	0	4.30E+01	300	5000	1	0	1	1	1	0
155	H2NCO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
156	CH3NNH	G	0	4.41E+01	200	6000	4	0	1	0	2	0
157	H2NCHO	G	0	4.50E+01	200	6000	3	0	1	1	1	0
158	CH3NCH3	G	0	4.41E+01	298	3000	6	0	2	0	1	0
159	CH3NHCH2	G	0	4.41E+01	298	3000	6	0	2	0	1	0
160	CH2NO	G	0	4.40E+01	200	6000	2	0	1	1	1	0
161	HOCO	G	0	4.50E+01	300	4000	1	0	1	2	0	0
162	CH3NO	G	0	4.50E+01	300	4000	3	0	1	1	1	0
163	CH3NHCH3	G	0	4.51E+01	298	3000	7	0	2	0	1	0
164	NCCN	G	0	5.20E+01	300	5000	0	0	2	0	2	0
165	CHCHNCH2	G	0	5.41E+01	200	5000	4	0	3	0	1	0
166	CH2CHNCH2	G	0	5.51E+01	200	5000	5	0	3	0	1	0
167	NCNO	G	0	5.60E+01	300	4000	0	0	1	1	2	0
168	NCHCHO	G	0	5.60E+01	200	5000	2	0	2	1	1	0
169	CH2NHCHCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
170	CH2CH2NCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
171	NHCH2CHO	G	0	5.81E+01	200	5000	4	0	2	1	1	0
172	OCH2CHNH	G	0	5.81E+01	200	5000	4	0	2	1	1	0
173	CH3NNCH3	G	0	5.81E+01	300	4000	6	0	2	0	2	0
174	H2CNO2	G	0	6.00E+01	300	4000	2	0	1	2	1	0
175	CH3NO2	G	0	6.10E+01	300	4000	3	0	1	2	1	0
176	CH3ONO	G	0	6.10E+01	300	4000	3	0	1	2	1	0
177	CH3ONO2	G	0	7.70E+01	300	4000	3	0	1	3	1	0
178	TMEDA	G	0	1.16E+02	200	5000	16	0	6	0	2	0

179	TMEDA-1	G	0	1.15E+02	200	5000	15	0	6	0	2	0
180	TMEDA-3	G	0	1.15E+02	200	5000	15	0	6	0	2	0
181	TMEDA-2	G	0	1.01E+02	200	5000	13	0	5	0	2	0
182	N(CH3)2CH2CH2	G	0	7.21E+01	200	5000	10	0	4	0	1	0
183	N(CH3)2CH2	G	0	5.81E+01	200	5000	8	0	3	0	1	0
184	TMEDA-0-5	G	0	1.00E+02	200	5000	12	0	5	0	2	0
185	N(CH3)2CHCH2	G	0	7.11E+01	200	5000	9	0	4	0	1	0
186	TMEDA-0-4	G	0	1.00E+02	200	5000	12	0	5	0	2	0
187	TMEDA-0-3	G	0	1.14E+02	200	5000	14	0	6	0	2	0
188	TMEDA-1-3	G	0	1.13E+02	200	5000	13	0	6	0	2	0
189	TMEDA-1-4	G	0	9.92E+01	200	5000	11	0	5	0	2	0
190	TMEDA-1-5	G	0	9.92E+01	200	5000	11	0	5	0	2	0
191	TMEDA-3-5	G	0	9.92E+01	200	5000	11	0	5	0	2	0
192	N(CH3)2CHCH	G	0	7.01E+01	200	5000	8	0	4	0	1	0
193	N(CH3CH2)CHCH2	G	0	7.01E+01	200	5000	8	0	4	0	1	0
194	N(CH3)2CCH2	G	0	7.01E+01	200	5000	8	0	4	0	1	0
195	N(CH3CH2)CH2CH3	G	0	7.21E+01	200	5000	10	0	4	0	1	0
196	CH2CHNCH3	G	0	5.61E+01	200	5000	6	0	3	0	1	0
197	CH3CHNCH2	G	0	5.61E+01	200	5000	6	0	3	0	1	0
198	CH3CH2NCH2	G	0	5.71E+01	200	5000	7	0	3	0	1	0

(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED			A	b	E
1. 2O+M=O2+M			6.16E+15	-0.5	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			
AR	Enhanced by	0.000E+00			
2. 2O+AR=O2+AR			1.89E+13	0.0	-1790.0
3. O+H+M=OH+M			4.71E+18	-1.0	0.0
H2O	Enhanced by	1.200E+01			
H2	Enhanced by	2.500E+00			

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    AR              Enhanced by    7.500E-01
 4. H2+M=2H+M                                      4.58E+19   -1.4   104380.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    0.000E+00
 5. H2+AR=2H+AR                                    5.84E+18   -1.1   104380.0
 6. H+OH+M=H2O+M                                   2.21E+22   -2.0        0.0
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    0.000E+00
 7. H+OH+AR=H2O+AR                                 8.41E+21   -2.0        0.0
 8. H2O2(+M)=2OH(+M)                               2.95E+14    0.0    48400.0
    Low pressure limit:  0.12000E+18  0.00000E+00  0.45500E+05
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    1.600E-01
 9. H2O+O=OH+OH                                    2.97E+06    2.0    13400.0
10. O+H2=H+OH                                      5.08E+04    2.7     6290.0
11. OH+H2=H+H2O                                    2.16E+08    1.5     3430.0
12. H+O2(+M)=HO2(+M)                               1.48E+12    0.6        0.0
    Low pressure limit:  0.35000E+17 -0.41000E+00 -0.11200E+04
    H2O             Enhanced by    1.200E+01
    H2              Enhanced by    2.500E+00
    AR              Enhanced by    5.000E-02
13. H+O2=O+OH                                      4.49E+08    1.3    16191.0
    Declared duplicate reaction...
14. H+O2=O+OH                                      2.08E+16   -0.7    16191.0
    Declared duplicate reaction...
15. O+HO2=OH+O2                                    3.25E+13    0.0        0.0
16. H+HO2=O2+H2                                    1.66E+13    0.0      820.0
17. H+HO2=2OH                                      7.08E+13    0.0      300.0
18. OH+HO2=O2+H2O                                  4.64E+13    0.0     -500.0
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19. 2HO2=O2+H2O2                                  1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
20. 2HO2=O2+H2O2                                  4.20E+14    0.0    11980.0
    Declared duplicate reaction...
21. O+H2O2=OH+HO2                                 9.55E+06    2.0     3970.0
22. H+H2O2=HO2+H2                                 4.82E+13    0.0     7950.0
23. H+H2O2=OH+H2O                                 2.41E+13    0.0     3970.0
24. OH+H2O2=HO2+H2O                               1.00E+12    0.0        0.0
    Declared duplicate reaction...
25. OH+H2O2=HO2+H2O                               5.80E+14    0.0     9560.0
    Declared duplicate reaction...
26. O+CO(+M)=CO2(+M)                              1.80E+10    0.0     2385.0
    Low pressure limit:  0.60200E+15  0.00000E+00  0.30000E+04
    H2              Enhanced by    2.000E+00
    O2              Enhanced by    6.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    3.500E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    5.000E-01
27. O2+CO=O+CO2                                   2.50E+12    0.0    47800.0
28. H2+CO(+M)=CH2O(+M)                            4.30E+07    1.5    79600.0
    Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
    TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
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29. OH+CO=H+CO2                                       4.10E+04    2.1    -1578.0
30. HO2+CO=OH+CO2                                     1.50E+14    0.0    23600.0
31. O+HCO=OH+CO                                       3.00E+13    0.0        0.0
32. O+HCO=H+CO2                                       3.00E+13    0.0        0.0
33. H+HCO(+M)=CH2O(+M)                                1.09E+12    0.5     -260.0
    Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
    TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
34. H+HCO=H2+CO                                       7.30E+13    0.0        0.0
35. OH+HCO=H2O+CO                                     3.00E+13    0.0        0.0
36. HCO+M=H+CO+M                                      1.87E+17   -1.0    17000.0
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
37. HCO+O2=HO2+CO                                     4.22E+12    0.0        0.0
38. HCO+HO2=CO2+OH+H                                  3.00E+13    0.0        0.0
39. O+CH2O=OH+HCO                                     1.81E+13    0.0     3078.0
40. O2+CH2O=HO2+HCO                                   2.05E+13    0.0    38920.0
41. H+CH2O=HCO+H2                                     5.18E+07    1.7     1834.0
42. H+CH2O(+M)=CH2OH(+M)                              5.40E+11    0.5     3600.0
    Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
    TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
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    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
43. H+CH2O(+M)=CH3O(+M)                            5.40E+11    0.5     2600.0
    Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
    TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
44. OH+CH2O=HCO+H2O                                3.43E+09    1.2     -447.0
45. HO2+CH2O=HCO+H2O2                              1.47E+13    0.0    15200.0
46. O+CH2OH=OH+CH2O                                4.20E+13    0.0        0.0
47. H+CH2OH=H2+CH2O                                6.00E+12    0.0        0.0
48. H+CH2OH=OH+CH3                                 9.63E+13    0.0        0.0
49. OH+CH2OH=H2O+CH2O                              2.40E+13    0.0        0.0
50. CH2OH+O2=HO2+CH2O                              2.41E+14    0.0     5017.0
    Declared duplicate reaction...
51. CH2OH+O2=HO2+CH2O                              1.51E+15   -1.0        0.0
    Declared duplicate reaction...
52. CH2OH+HO2=CH2O+H2O2                            1.20E+13    0.0        0.0
53. CH2OH+HCO=CH3OH+CO                             1.20E+14    0.0        0.0
54. CH2OH+HCO=CH2O+CH2O                            1.80E+14    0.0        0.0
55. 2CH2OH=CH3OH+CH2O                              3.00E+12    0.0        0.0
56. CH2OH+CH3O=CH3OH+CH2O                          2.40E+13    0.0        0.0
57. O+CH3O=OH+CH2O                                 6.00E+12    0.0        0.0
58. H+CH3O=H2+CH2O                                 2.00E+13    0.0        0.0
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59. H+CH3O=OH+CH3                                   3.20E+13    0.0        0.0
60. OH+CH3O=H2O+CH2O                                1.80E+13    0.0        0.0
61. CH3O+O2=HO2+CH2O                                9.03E+13    0.0    11980.0
    Declared duplicate reaction...
62. CH3O+O2=HO2+CH2O                                2.20E+10    0.0     1748.0
    Declared duplicate reaction...
63. CH3O+HO2=CH2O+H2O2                              3.00E+11    0.0        0.0
64. CH3O+CO=CH3+CO2                                 1.57E+13    0.0    11800.0
65. CH3O+HCO=CH3OH+CO                               9.00E+13    0.0        0.0
66. 2CH3O=CH3OH+CH2O                                6.00E+13    0.0        0.0
67. O+CH3OH=OH+CH2OH                                3.88E+05    2.5     3080.0
68. H+CH3OH=CH2OH+H2                                1.44E+13    0.0     6095.0
69. H+CH3OH=CH3O+H2                                 3.60E+12    0.0     6095.0
70. OH+CH3OH=CH2OH+H2O                              7.10E+06    1.8     -596.0
71. OH+CH3OH=CH3O+H2O                               1.00E+06    2.1      496.5
72. CH3+CH3OH=CH2OH+CH4                             3.19E+01    3.2     7172.0
73. O2+CH3OH=CH2OH+HO2                              2.05E+13    0.0    44900.0
74. HCO+CH3OH=CH2OH+CH2O                            9.63E+03    2.9    13110.0
75. HO2+CH3OH=CH2OH+H2O2                            3.98E+13    0.0    19400.0
76. CH3O+CH3OH=CH2OH+CH3OH                          3.00E+11    0.0     4060.0
77. CH3OH(+M)=CH3+OH(+M)                            1.90E+16    0.0    91730.0
    Low pressure limit:  0.29500E+45 -0.73500E+01  0.95460E+05
    TROE centering:      0.41400E+00  0.27900E+03  0.54590E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
78. CH3OH(+M)=CH2OH+H(+M)                           2.69E+16   -0.1    98940.0
    Low pressure limit:  0.23400E+41 -0.63300E+01  0.10310E+06
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    TROE centering:      0.77300E+00  0.69300E+03  0.53330E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
79. O+CH4=OH+CH3                                  1.02E+09    1.5     8600.0
80. H+CH4=CH3+H2                                  6.60E+08    1.6    10840.0
81. OH+CH4=CH3+H2O                                1.00E+08    1.6     3120.0
82. CH+CH4=H+C2H4                                 6.00E+13    0.0        0.0
83. CH2SING+CH4=2CH3                              1.60E+13    0.0     -570.0
84. CH2+CH4=2CH3                                  2.46E+06    2.0     8270.0
85. O+CH3=H+CH2O                                  5.06E+13    0.0        0.0
86. O+CH3=H+H2+CO                                 3.37E+13    0.0        0.0
87. H+CH3(+M)=CH4(+M)                             1.39E+16   -0.5      536.0
    Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
    TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CH4             Enhanced by    2.000E+00
    CO              Enhanced by    1.500E+00
    CO2             Enhanced by    2.000E+00
    C2H6            Enhanced by    3.000E+00
    AR              Enhanced by    7.000E-01
88. OH+CH3=CH2+H2O                                5.60E+07    1.6     5420.0
89. OH+CH3=CH2SING+H2O                            6.44E+17   -1.3     1417.0
90. HO2+CH3=O2+CH4                                1.00E+12    0.0        0.0
91. HO2+CH3=OH+CH3O                               2.00E+13    0.0        0.0
92. CH+CH3=H+C2H3                                 3.00E+13    0.0        0.0
93. CH2SING+CH3=H+C2H4                            1.20E+13    0.0     -570.0
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 94. CH3+O2=O+CH3O                                  3.56E+13    0.0    30480.0
 95. CH3+O2=OH+CH2O                                 2.31E+12    0.0    20315.0
 96. CH3+H2O2=HO2+CH4                               2.45E+04    2.5     5180.0
 97. 2CH3(+M)=C2H6(+M)                              6.77E+16   -1.2      654.0
     Low pressure limit:  0.34000E+42 -0.70300E+01  0.27630E+04
     TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
 98. 2CH3=H+C2H5                                    6.84E+12    0.1    10600.0
 99. CH3+HCO=CH4+CO                                 1.21E+14    0.0        0.0
100. CH3+CH2O=HCO+CH4                               3.32E+03    2.8     5860.0
101. CH2+CH3=H+C2H4                                 4.00E+13    0.0        0.0
102. O+CH2=H+HCO                                    8.00E+13    0.0        0.0
103. O+CH2SING=H2+CO                                1.50E+13    0.0        0.0
104. O+CH2SING=H+HCO                                1.50E+13    0.0        0.0
105. H+CH2(+M)=CH3(+M)                              6.00E+14    0.0        0.0
     Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
     TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
106. H+CH2SING=CH+H2                                3.00E+13    0.0        0.0
107. OH+CH2=H+CH2O                                  2.00E+13    0.0        0.0
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108. OH+CH2=CH+H2O                                  1.13E+07    2.0     3000.0
109. OH+CH2SING=H+CH2O                              3.00E+13    0.0        0.0
110. HO2+CH2=OH+CH2O                                2.00E+13    0.0        0.0
111. CH+CH2=H+C2H2                                  4.00E+13    0.0        0.0
112. CH2+O2=OH+H+CO                                 5.00E+12    0.0     1500.0
113. CH2+O2=CO2+2H                                  5.80E+12    0.0     1500.0
114. CH2+O2=O+CH2O                                  2.40E+12    0.0     1500.0
115. CH2+H2=H+CH3                                   5.00E+05    2.0     7230.0
116. 2CH2=H2+C2H2                                   1.60E+15    0.0    11944.0
117. 2CH2=H+H+C2H2                                  2.00E+14    0.0    10989.0
118. CH2SING+CO=CH2+CO                              9.00E+12    0.0        0.0
119. CH2SING+AR=CH2+AR                              9.00E+12    0.0      600.0
120. CH2SING+CO2=CH2+CO2                            7.00E+12    0.0        0.0
121. CH2SING+CO2=CO+CH2O                            1.40E+13    0.0        0.0
122. CH2+CO(+M)=CH2CO(+M)                           8.10E+11    0.5     4510.0
     Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
123. CH2SING+O2=H+OH+CO                             2.80E+13    0.0        0.0
124. CH2SING+O2=CO+H2O                              1.20E+13    0.0        0.0
125. CH2SING+H2=CH3+H                               7.00E+13    0.0        0.0
126. CH2SING+H2O(+M)=CH3OH(+M)                      4.82E+17   -1.2     1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
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     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
127. CH2SING+H2O=CH2+H2O                          3.00E+13    0.0        0.0
128. CH2SING+H2O=H2+CH2O                          6.82E+10    0.2     -935.0
129. O+CH=H+CO                                    5.70E+13    0.0        0.0
130. OH+CH=H+HCO                                  3.00E+13    0.0        0.0
131. CH+O2=O+HCO                                  6.71E+13    0.0        0.0
132. CH+H2=H+CH2                                  1.08E+14    0.0     3110.0
133. CH+H2O=H+CH2O                                5.71E+12    0.0     -755.0
134. CH+CO(+M)=HCCO(+M)                           5.00E+13    0.0        0.0
     Low pressure limit:  0.26900E+29 -0.37400E+01  0.19360E+04
     TROE centering:      0.57570E+00  0.23700E+03  0.16520E+04  0.50690E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
135. CH+CO2=HCO+CO                                1.90E+14    0.0    15792.0
136. CH+CH2O=H+CH2CO                              9.46E+13    0.0     -515.0
137. CH+HCCO=CO+C2H2                              5.00E+13    0.0        0.0
138. O+C2H6=OH+C2H5                               3.00E+07    2.0     5115.0
139. H+C2H6=C2H5+H2                               5.40E+02    3.5     5210.0
140. OH+C2H6=C2H5+H2O                             7.26E+06    2.0      864.0
141. CH3+C2H6=C2H5+CH4                            5.50E-01    4.0     8300.0
142. CH2SING+C2H6=CH3+C2H5                        4.00E+13    0.0     -550.0
143. C2H6+O2=C2H5+HO2                             4.04E+13    0.0    50872.0
144. C2H6+CH2OH=CH3OH+C2H5                        1.99E+02    3.0    13976.0
145. C2H6+CH3O=CH3OH+C2H5                         2.41E+11    0.0     7094.0
146. C2H6+C2H=C2H2+C2H5                           3.61E+12    0.0        0.0
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147. C2H6+C2H3=C2H4+C2H5                              6.01E+02    3.3    10502.0
148. C2H6+CH3CO=CH3CHO+C2H5                          1.81E+04    2.8    17527.0
149. C2H6+HCO=CH2O+C2H5                              4.70E+04    2.7    18235.0
150. O+C2H5=CH3+CH2O                                 2.24E+13    0.0        0.0
151. O+C2H5=H+CH3CHO                                 1.10E+14    0.0        0.0
152. H+C2H5=H2+C2H4                                  2.00E+12    0.0        0.0
153. H+C2H5(+M)=C2H6(+M)                             5.21E+17   -1.0     1580.0
     Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
     TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
154. C2H5+O2=HO2+C2H4                                1.92E+07    1.0    -2035.0
155. C2H5+HO2=C2H5O+OH                               3.00E+13    0.0        0.0
156. C2H5+HO2=C2H4+H2O2                              3.01E+11    0.0        0.0
157. C2H5+OH=C2H4+H2O                                2.41E+13    0.0        0.0
158. C2H5+CH3=CH4+C2H4                               1.13E+12   -0.5        0.0
159. CH3+C2H5(+M)=C3H8(+M)                           9.60E+14   -0.5        0.0
     Low pressure limit:  0.68000E+62 -0.13420E+02  0.60000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.14339E+04  0.53288E+04
160. C2H5+CH2OH=C2H4+CH3OH                           2.41E+12    0.0        0.0
161. C2H5+CH2OH=C2H6+CH2O                            2.41E+12    0.0        0.0
162. C2H5+CH3O=C2H6+CH2O                             2.41E+13    0.0        0.0
163. C2H5+C2H=C2H2+C2H4                              1.81E+12    0.0        0.0
164. CH2+C2H5=C2H4+CH3                               1.81E+13    0.0        0.0
165. CH2SING+C2H5=C2H4+CH3                           9.00E+12    0.0        0.0
166. C2H5+CH2SING=C3H6+H                             9.00E+12    0.0        0.0
167. C2H5+H2O2=C2H6+HO2                              8.73E+09    0.0      974.0
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168. H+C2H4(+M)=C2H5(+M) 1.37E+09 1.5 1355.0

Low pressure limit: 0.20260E+40 -0.66420E+01 0.57690E+04

TROE centering: -0.56900E+00 0.29900E+03 -0.91470E+04 0.15240E+03

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

169. H+C2H4=C2H3+H2 1.12E+07 2.1 13366.0

170. OH+C2H4=C2H3+H2O 1.31E-01 4.2 -860.0

171. OH+C2H4=CH3+CH2O 3.19E+01 2.7 -1172.0

172. OH+C2H4=CH3CHO+H 8.73E-05 4.6 -618.0

173. CH3+C2H4=C2H3+CH4 2.27E+05 2.0 9200.0

174. CH3+C2H4(+M)<=>nC3H7(+M) 2.55E+06 1.6 5700.0

Low pressure limit: 0.30000E+64 -0.14600E+02 0.18170E+05

TROE centering: 0.18940E+00 0.27700E+03 0.87480E+04 0.78910E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

175. C2H4(+M)=H2+C2H2(+M) 8.00E+12 0.4 88770.0

Low pressure limit: 0.15800E+52 -0.93000E+01 0.97800E+05

TROE centering: 0.73450E+00 0.18000E+03 0.10350E+04 0.54170E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

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     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
176. C2H4+CH2SING=AC3H5+H                          4.53E+13    0.0     -556.0
177. C2H4+HO2=C2H4O+OH                             6.03E+09    0.0     7949.0
178. C2H4+O=H+CH2CHO                               7.33E+07    1.6     1260.0
179. C2H4+O=CH3+HCO                                1.13E+08    1.6     1020.0
180. C2H4+O=C2H3+OH                                2.15E+06    2.5    11900.0
181. C2H4+O2=C2H3+HO2                              4.22E+13    0.0    60800.0
182. C2H4+CO=C2H3+HCO                              1.51E+14    0.0    90616.0
183. C2H4+C2H=C4H4+H                               1.21E+13    0.0        0.0
184. C2H4+C2H2=C2H3+C2H3                           2.41E+13    0.0    68360.0
185. C2H4+C2H4=C2H5+C2H3                           4.82E+14    0.0    71539.0
186. H+C2H3(+M)=C2H4(+M)                           6.08E+12    0.3      280.0
     Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
187. H+C2H2(+M)=C2H3(+M)                           1.71E+10    1.3     2709.0
     Low pressure limit:  0.63480E+32 -0.46639E+01  0.37800E+04
     TROE centering:      0.00000E+00  0.78784E+05 -0.10210E+05  0.10000E-29
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
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	AR Enhanced by 7.000E-01			
188.	H+C2H3=H2+C2H2	9.64E+13	0.0	0.0
189.	OH+C2H3=H2O+C2H2	5.00E+12	0.0	0.0
190.	C2H3+O2=C2H2+HO2	1.34E+06	1.6	-383.0
	Declared duplicate reaction...			
191.	C2H3+O2=C2H2+HO2	1.37E+02	3.4	3663.0
	Declared duplicate reaction...			
192.	C2H3+O2=HCO+CH2O	9.33E+13	-0.7	268.7
193.	C2H3+O2=H+CO+CH2O	2.19E+14	-0.7	268.7
194.	C2H3+O2=CH2CHO+O	7.52E+08	1.0	-137.4
195.	C2H3+HO2=OH+CH2CO+H	3.01E+13	0.0	0.0
196.	C2H3+CH3=C2H2+CH4	3.92E+11	0.0	0.0
197.	C2H3+O=CH2CO+H	1.00E+14	0.0	0.0
198.	C2H3OO+H=CH2CHO+OH	1.00E+14	0.0	0.0
199.	C2H3OO+CH2=CH2CHO+CH2O	2.00E+13	0.0	0.0
200.	C2H3OO+OH=CH2CHO+HO2	2.00E+13	0.0	0.0
201.	C2H3OO+O=CH2CHO+O2	2.00E+13	0.0	0.0
202.	C2H3+CH2OH=C2H4+CH2O	3.01E+13	0.0	0.0
203.	C2H3+CH3O=C2H4+CH2O	2.41E+13	0.0	0.0
204.	C2H3+CH3OH=C2H4+CH3O	1.44E+01	3.1	6935.0
205.	C2H3+CH3OH=C2H4+CH2OH	3.19E+01	3.2	7172.0
206.	C2H3+CO=C2H3CO	1.51E+11	0.0	4809.0
207.	C2H3+C2H=C4H4	1.00E+14	0.0	0.0
208.	C2H3+C2H=C2H2+C2H2	9.64E+11	0.0	0.0
209.	C2H3+CH3CO=C2H3CO+CH3	1.81E+13	0.0	0.0
210.	C2H5+C2H3=AC3H5+CH3	8.00E+25	-3.5	11775.0
211.	C2H3+C2H5(+M)=IC4H8(+M)	1.50E+13	0.0	0.0
	Low pressure limit: 0.15500E+57 -0.11790E+02 0.89845E+04			
	TROE centering: 0.19800E+00 0.22779E+04 0.60000E+05 0.57232E+04			
212.	C2H3+C2H5=C2H2+C2H6	4.82E+11	0.0	0.0
213.	C2H3+CH2SING=C2H2+CH3	1.81E+13	0.0	0.0
214.	C2H3+CH2=C2H2+CH3	1.81E+13	0.0	0.0

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215. C2H3+H2O2=C2H4+HO2                              1.21E+10    0.0     -596.0
216. C2H3+CH2O=C2H4+HCO                              5.43E+03    2.8     5862.0
217. C2H3+CH2=AC3H4+H                                3.00E+13    0.0        0.0
218. C2H3+C2H3=i-C4H5+H                              1.50E+30   -5.0    13000.0
219. C2H3+C2H3=n-C4H5+H                              1.10E+24   -3.3    12400.0
220. H2CC+C2H2(+M)=C4H4(+M)                          3.50E+05    2.1    -2400.0
     Low pressure limit:  0.14000E+61 -0.12599E+02  0.74170E+04
     TROE centering:      0.98000E+00  0.56000E+02  0.58000E+03  0.41640E+04
     H2              Enhanced by    2.000E+00
     CH4             Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     C2H2            Enhanced by    3.000E+00
     CO              Enhanced by    1.500E+00
     C2H4            Enhanced by    3.000E+00
     C2H6            Enhanced by    3.000E+00
     CO2             Enhanced by    2.000E+00
221. C2H2(+M)=H2CC(+M)                               8.00E+14   -0.5    50750.0
     Low pressure limit:  0.24500E+16 -0.64000E+00  0.49700E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H4            Enhanced by    2.500E+00
222. H2CC+C2H4=iiiC4H6                               1.00E+12    0.0        0.0
223. H2CC+O2=CH2+CO2                                 1.00E+13    0.0        0.0
224. H2CC+H=C2H2+H                                   1.00E+14    0.0        0.0
225. H2CC+OH=CH2CO+H                                 2.00E+13    0.0        0.0
226. C2H2+O=C2H+OH                                   4.60E+19   -1.4    28950.0
227. C2H2+O=CH2+CO                                   2.35E+08    1.4     2204.5
228. C2H2+O=HCCO+H                                   9.40E+08    1.4     2204.5
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229. OH+C2H2=C2H+H2O                                  2.63E+06    2.1    17060.0
230. OH+C2H2=H+CH2CO                                  1.52E+04    2.3     -292.0
231. OH+C2H2=CH3+CO                                   4.37E+06    1.4      227.0
232. C2H2+CH=C3H2+H                                   1.10E+13    0.0        0.0
233. C2H2+CH2=C3H3+H                                  1.20E+13    0.0     6620.0
234. C2H2+CH3=C2H+CH4                                 1.81E+11    0.0    17289.0
235. C2H2+O2=2HCO                                     1.00E+12    0.0    28000.0
236. C2H2+CH2OH=C2H3+CH2O                             7.23E+11    0.0     9004.0
237. C2H2+CO=C2H+HCO                                  4.82E+14    0.0   106713.0
238. C2H2+C2H=C4H2+H                                  3.00E+13    0.0        0.0
239. C2H2+C2H(+M)=nC4H3(+M)                           8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
240. C2H2+C2H(+M)=iC4H3(+M)                           8.30E+10    0.9     -363.0
     Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
     TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     C2H2            Enhanced by    2.500E+00
     C2H4            Enhanced by    2.500E+00
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241. C2H2+CH2SING=C3H3+H                              3.42E+15   -0.6     -230.7
242. C2H2+CH2SING=CH2+C2H2                            8.55E+14   -0.6     -230.7
243. HCCO+C2H2=C3H3+CO                                1.00E+11    0.0     3000.0
244. C2H2+C2H3=n-C4H5                                 1.10E+32   -7.3     6200.0
245. C2H2+C2H3=i-C4H5                                 2.10E+36   -8.8     9100.0
246. C2H3+C2H2=C4H4+H                                 5.00E+14   -0.7     6700.0
247. O+C2H=CH+CO                                      1.00E+13    0.0        0.0
248. H+C2H(+M)=C2H2(+M)                               1.00E+17   -1.0        0.0
     Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
     TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
249. OH+C2H=H+HCCO                                    2.00E+13    0.0        0.0
250. C2H+O2=HCO+CO                                    1.00E+13    0.0     -775.0
251. C2H+H2=H+C2H2                                    5.68E+10    0.9     1993.0
252. C2H+HO2=HCCO+OH                                  1.81E+13    0.0        0.0
253. C2H+CH3=C3H3+H                                   2.41E+13    0.0        0.0
254. C2H+O2=HCCO+O                                    6.03E+11    0.0        0.0
255. C2H+CH2OH=C2H2+CH2O                              3.61E+13    0.0        0.0
256. C2H+CH2OH=C3H3+OH                                1.21E+13    0.0        0.0
257. C2H+CH3OH=C2H2+CH2OH                             6.03E+12    0.0        0.0
258. C2H+CH3O=CH2O+C2H2                               2.41E+13    0.0        0.0
259. C2H+CH3OH=C2H2+CH3O                              1.21E+12    0.0        0.0
260. C2H+CH2=CH+C2H2                                  1.81E+13    0.0        0.0
261. C2H+CH2SING=C2H2+CH                              1.81E+13    0.0        0.0
262. O+HCCO=H+2CO                                     1.00E+14    0.0        0.0
263. H+HCCO=CH2SING+CO                                5.00E+13    0.0        0.0
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264.	CH2+HCCO=C2H3+CO	3.00E+13	0.0	0.0
265.	HCCO+O2=CO2+CO+H	4.78E+12	-0.1	1150.0
266.	HCCO+O2=CO+CO+OH	1.91E+11	0.0	1023.0
267.	HCCO+O2=O+CO+HCO	2.18E+02	2.7	3541.0
268.	2HCCO=2CO+C2H2	1.00E+13	0.0	0.0
269.	HCCO+CH3=C2H4+CO	5.00E+13	0.0	0.0
270.	O+CH2CO=OH+HCCO	1.00E+13	0.0	8000.0
271.	O+CH2CO=CH2+CO2	1.75E+12	0.0	1350.0
272.	H+CH2CO=HCCO+H2	5.00E+13	0.0	8000.0
273.	CH2CO+H=CH3+CO	7.77E+08	1.4	2780.0
274.	CH2CHO=H+CH2CO	2.48E+27	-5.2	44304.0
275.	CH2CHO=CH3+CO	1.54E+31	-6.3	42478.0
276.	OH+CH2CO=HCCO+H2O	7.50E+12	0.0	2000.0
277.	CH2CO+OH=CH2OH+CO	1.00E+13	0.0	0.0
278.	CH3CO=CH3+CO	2.40E+15	-2.0	14805.0
279.	CH2CHO+H=CH3CHO	6.40E+35	-7.6	5215.0
280.	CH2CHO+H=CH3+HCO	4.99E+14	-0.3	912.0
281.	CH2CHO+O=CH2O+HCO	5.00E+13	0.0	0.0
282.	CH2CHO+OH=H2O+CH2CO	1.20E+13	0.0	0.0
283.	CH2CHO+OH=HCO+CH2OH	3.01E+13	0.0	0.0
284.	CH2CHO+O2=CH2CO+HO2	1.57E+11	0.0	0.0
285.	CH3CHO=CH3+HCO	9.59E+14	0.0	74180.0
286.	CH3CHO+O2=CH3CO+HO2	2.00E+13	0.5	42200.0
287.	CH3CHO+H=CH2CHO+H2	4.10E+09	1.2	2405.0
288.	CH3CHO+OH=CH3CO+H2O	2.35E+10	0.7	-1113.0
289.	CH3CHO+O=CH2CHO+OH	5.85E+12	0.0	1808.0
290.	CH3CHO+HO2=CH3CO+H2O2	1.70E+12	0.0	10700.0
291.	CH3CHO+CH3=CH3CO+CH4	1.70E+12	0.0	8440.0
292.	CH3CHO+HCO=CH3CO+CH2O	7.80E+13	0.0	8440.0
293.	C2H5+O2(+M)=C2H5OO(+M)	2.02E+10	1.0	-63.6
	Low pressure limit: 0.84900E+30 -0.42900E+01 0.22000E+03			
	TROE centering: 0.10300E+00 0.60100E+03 0.10000E-09			

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

294. C2H5OO(+M)=C2H4+HO2(+M) 7.14E+04 2.3 27955.0

Low pressure limit: 0.83100E+22 -0.65100E+00 0.22890E+05

TROE centering: 0.00000E+00 0.10600E+03 0.10600E+03

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

295. C2H5OO+HO2=C2H5O+OH+O2 1.75E+10 0.0 -3275.0

296. C2H5O=CH3+CH2O 1.00E+15 0.0 21523.0

297. C2H5O=CH3CHO+H 2.00E+14 0.0 23215.0

298. C2H5O+O2=CH3CHO+HO2 6.03E+10 0.0 1643.0

299. C2H4O+O2=CH2CHO+HO2 4.00E+13 0.0 61500.0

300. C2H4O+H=CH2CHO+H2 2.00E+13 0.0 8300.0

301. C2H4O+H=C2H3+H2O 5.00E+09 0.0 5000.0

302. C2H4O+H=C2H4+OH 9.51E+10 0.0 5000.0

303. C2H4O+OH=CH2CHO+H2O 4.79E+13 0.0 5955.0

304. C2H4O+O=CH2CHO+OH 1.91E+12 0.0 5250.0

305. C2H4O+HO2=CH2CHO+H2O2 4.00E+12 0.0 17000.0

306. C2H4O=CH3CHO 6.00E+13 0.0 57167.0

307. C2H4O=CH3+HCO 4.90E+13 0.0 57167.0

308. C2H4O=CH4+CO 1.21E+13 0.0 57167.0

309. C3H8+H=nC3H7+H2 1.30E+06 2.5 6756.0

310.	C3H8+H=iC3H7+H2	1.30E+06	2.4	4471.0
311.	C3H8+O=nC3H7+OH	1.90E+05	2.7	3716.0
312.	C3H8+O=iC3H7+OH	4.76E+04	2.7	2106.0
313.	C3H8+OH=iC3H7+H2O	1.40E+03	2.8	-310.0
314.	C3H8+OH=nC3H7+H2O	1.37E+03	2.7	580.0
315.	C3H8+O2=nC3H7+HO2	3.97E+13	0.0	50872.0
316.	C3H8+O2=iC3H7+HO2	3.97E+13	0.0	47693.0
317.	C3H8+HO2=nC3H7+H2O2	4.76E+04	2.5	16494.0
318.	C3H8+HO2=iC3H7+H2O2	9.64E+03	2.6	13910.0
319.	C3H8+CH3=nC3H7+CH4	9.04E-01	3.6	7154.0
320.	C3H8+CH3=iC3H7+CH4	1.51E+00	3.5	5481.0
321.	C3H8+CH2OH=nC3H7+CH3OH	1.99E+02	3.0	3976.0
322.	C3H8+CH3O=nC3H7+CH3OH	4.34E+11	0.0	6458.0
323.	C3H8+CH2SING=nC3H7+CH3	9.04E-01	3.6	7154.0
324.	C3H8+C2H3=nC3H7+C2H4	6.03E+02	3.3	10502.0
325.	C3H8+C2H=nC3H7+C2H2	3.61E+12	0.0	0.0
326.	C3H8+C2H5=nC3H7+C2H6	9.04E-02	3.6	9141.0
327.	C3H8+HCO=nC3H7+CH2O	2.05E+05	2.5	18431.0
328.	C3H8+iC3H7=nC3H7+C3H8	8.40E-03	4.2	8716.0
329.	C3H8+CH3CO=nC3H7+CH3CHO	4.22E+04	2.6	17658.0
330.	C3H8+CH2=nC3H7+CH3	9.03E-01	3.6	7154.0
331.	C3H8+CH2OH=iC3H7+CH3OH	6.03E+01	3.0	11989.0
332.	C3H8+CH3O=iC3H7+CH3OH	1.45E+11	0.0	4571.0
333.	C3H8+CH2SING=iC3H7+CH3	1.51E+00	3.5	7472.0
334.	C3H8+C2H3=iC3H7+C2H4	1.02E+03	3.1	8829.0
335.	C3H8+C2H=iC3H7+C2H2	1.21E+12	0.0	0.0
336.	C3H8+C2H5=iC3H7+C2H6	1.21E+00	3.5	7468.0
337.	C3H8+HCO=iC3H7+CH2O	1.08E+07	1.9	17006.0
338.	C3H8+CH3CO=iC3H7+CH3CHO	5.30E+06	2.0	16241.0
339.	C3H8+CH2=iC3H7+CH3	1.51E+00	3.5	7472.0
340.	nC3H7+H=C3H6+H2	1.81E+12	0.0	0.0
341.	nC3H7+H(+M)=C3H8(+M)	3.60E+13	0.0	0.0

Low pressure limit: 0.30100E+59 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

342.	nC3H7+H=C2H5+CH3	3.40E+18	-1.3	5386.0
343.	nC3H7+O=C2H5+CH2O	9.60E+13	0.0	0.0
344.	nC3H7+O2=C3H6+HO2	9.04E+10	0.0	0.0
345.	nC3H7+HO2=C2H5+OH+CH2O	2.41E+13	0.0	0.0
346.	nC3H7+OH=C3H6+H2O	2.41E+13	0.0	0.0
347.	nC3H7+CH3=CH4+C3H6	1.14E+13	-0.3	0.0
348.	nC3H7+C2H5=C3H6+C2H6	1.45E+12	0.0	0.0
349.	nC3H7+C2H5=C3H8+C2H4	1.15E+12	0.0	0.0
350.	nC3H7+C2H3=C3H8+C2H2	1.21E+12	0.0	0.0
351.	nC3H7+C2H2=AC3H5+C2H4	7.23E+11	0.0	9004.0
352.	nC3H7+C2H=C3H3+C2H5	1.21E+13	0.0	0.0
353.	nC3H7+C2H=C3H6+C2H2	6.03E+12	0.0	0.0
354.	nC3H7+iC3H7=C3H8+C3H6	5.13E+13	-0.3	0.0
355.	nC3H7+HCO=CO+C3H8	6.03E+13	0.0	0.0
356.	nC3H7+CH3O=C3H8+CH2O	2.41E+13	0.0	0.0
357.	nC3H7+CH2SING=C2H5+C2H4	2.58E+13	0.0	0.0
358.	nC3H7+CH2SING=C3H6+CH3	1.03E+13	0.0	0.0
359.	nC3H7+CH2=C2H4+C2H5	1.81E+13	0.0	0.0
360.	nC3H7+CH2=C3H6+CH3	1.81E+12	0.0	0.0
361.	nC3H7+CH2OH=C3H6+CH3OH	4.82E+11	0.0	0.0
362.	iC3H7=CH3+C2H4	1.00E+14	0.0	45000.0
363.	iC3H7+H=C3H6+H2	3.61E+12	0.0	0.0
364.	iC3H7+H(+M)=C3H8(+M)	2.40E+13	0.0	0.0

Low pressure limit: 0.17000E+59 -0.12080E+02 0.11264E+05

TROE centering: 0.64900E+00 0.12131E+04 0.12131E+04 0.13370E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

365. iC3H7+H=CH3+C2H5 5.90E+23 -2.8 10009.0

366. iC3H7+O=CH3CHO+CH3 9.60E+13 0.0 0.0

367. iC3H7+O2=C3H6+HO2 1.26E+11 0.0 0.0

368. iC3H7+HO2=CH3CHO+OH+CH3 2.41E+13 0.0 0.0

369. iC3H7+OH=C3H6+H2O 2.41E+13 0.0 0.0

370. iC3H7+CH3=CH4+C3H6 2.19E+14 -0.7 0.0

371. iC3H7+C2H5=C3H6+C2H6 2.30E+13 -0.3 0.0

372. iC3H7+C2H5=C3H8+C2H4 1.84E+13 -0.3 0.0

373. iC3H7+C2H3=C2H4+C3H6 1.52E+14 -0.7 0.0

374. iC3H7+C2H3=C3H8+C2H2 1.52E+14 -0.7 0.0

375. iC3H7+C2H2=CH3+iiiC4H6 2.77E+10 0.0 6504.0

376. iC3H7+C2H=C3H6+C2H2 3.60E+12 0.0 0.0

377. iC3H7+iC3H7=C3H8+C3H6 2.11E+14 -0.7 0.0

378. iC3H7+HCO=CO+C3H8 1.20E+14 0.0 0.0

379. iC3H7+CH3O=C3H8+CH2O 1.21E+13 0.0 0.0

380. iC3H7+CH2SING=C3H6+CH3 1.04E+13 0.0 0.0

381. iC3H7+CH2=C3H6+CH3 3.01E+13 0.0 0.0

382. iC3H7+CH2OH=C3H6+CH3OH 2.89E+12 0.0 0.0

383. iC3H7+CH2OH=C3H8+CH2O 2.35E+12 0.0 0.0

384. CH3+C2H3(+M)=C3H6(+M) 2.50E+13 0.0 0.0

Low pressure limit: 0.42700E+59 -0.11940E+02 0.97700E+04

TROE centering: 0.17500E+00 0.13410E+04 0.60000E+05 0.10140E+05

H2 Enhanced by 2.000E+00

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     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H2            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
385. C3H6+H=H2+AC3H5                                 1.70E+05    2.5     2492.0
386. C3H6+H=C2H4+CH3                                 8.80E+16   -1.1     6461.0
387. C3H6+H=SC3H5+H2                                 7.81E+05    2.5    12285.0
388. C3H6+H(+M)=nC3H7(+M)                            1.33E+13    0.0     3260.7
     Low pressure limit:  0.62600E+39 -0.66600E+01  0.70000E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.13100E+04  0.48097E+05
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
389. C3H6+H(+M)=iC3H7(+M)                            1.33E+13    0.0     1559.8
     Low pressure limit:  0.87000E+43 -0.75000E+01  0.47218E+04
     TROE centering:      0.10000E+01  0.10000E+04  0.64540E+03  0.68443E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
390. C3H6+H=TC3H5+H2                                 3.90E+05    2.5     5821.0
391. C3H6=H2+AC3H4                                   4.00E+13    0.0    80000.0
392. C3H6=CH4+C2H2                                   3.50E+12    0.0    70000.0
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393. C3H6+O=C2H5+HCO	3.50E+07	1.6	-972.0
394. C3H6+O=AC3H5+OH	1.75E+11	0.7	5884.0
395. C3H6+O=SC3H5+OH	1.21E+11	0.7	8960.0
396. C3H6+O=TC3H5+OH	6.03E+10	0.7	7633.0
397. C3H6+O=CH3+H+CH2CO	1.20E+08	1.6	327.0
398. C3H6+OH=AC3H5+H2O	3.12E+06	2.0	-298.0
399. C3H6+OH=SC3H5+H2O	2.14E+06	2.0	2778.0
400. C3H6+OH=TC3H5+H2O	1.11E+06	2.0	1451.0
401. C3H6+HO2=AC3H5+H2O2	9.63E+03	2.6	13910.0
402. C3H6+O2=AC3H5+HO2	6.03E+13	0.0	47590.0
403. C3H6+CH3=AC3H5+CH4	2.20E+00	3.5	5675.0
404. C3H6+CH3=TC3H5+CH4	8.40E-01	3.5	11660.0
405. C3H6+C2H5=AC3H5+C2H6	2.23E+00	3.5	6637.0
406. C3H6+C2H2=AC3H5+C2H3	4.04E+13	0.0	46818.0
407. C3H6+C2H3=AC3H5+C2H4	2.21E+00	3.5	4682.0
408. C3H6+C2H3=SC3H5+C2H4	1.35E+00	3.5	10842.0
409. C3H6+C2H3=TC3H5+C2H4	8.40E-01	3.5	9670.0
410. C3H6+C2H3=iiiC4H6+CH3	7.23E+11	0.0	5008.0
411. C3H6+C2H4=AC3H5+C2H5	5.78E+13	0.0	51584.0
412. C3H6+C2H4=nC3H7+C2H3	6.03E+13	0.0	75446.0
413. C3H6+CH2OH=AC3H5+CH3OH	6.03E+01	3.0	12000.0
414. C3H6+nC3H7=AC3H5+C3H8	2.23E+00	3.5	6637.0
415. C3H6+nC3H7=IC4H8+C2H5	2.23E+00	3.5	-2000.0
416. C3H6+iC3H7=C3H8+AC3H5	6.62E-02	4.0	8066.0
417. C3H6+C3H6=AC3H5+nC3H7	2.53E+14	0.0	55179.0
418. C3H6+C3H6=AC3H5+iC3H7	4.88E+13	0.0	52309.0
419. CH3+C2H3=AC3H5+H	1.50E+24	-2.8	18618.0
420. CH3+C2H3=SC3H5+H	3.20E+35	-7.8	13300.0
421. CH3+C2H3=TC3H5+H	4.99E+22	-4.4	18850.0
422. AC3H5+H(+M)=C3H6(+M)	2.00E+14	0.0	0.0
Low pressure limit: 0.13300E+61 -0.12000E+02 0.59678E+04			
TROE centering: 0.20000E-01 0.10970E+04 0.10967E+05 0.68600E+04			

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

423. AC3H5+H=AC3H4+H2 1.80E+13 0.0 0.0

424. TC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

425. SC3H5+H=AC3H4+H2 3.30E+12 0.0 0.0

426. AC3H5+O=C2H3CHO+H 6.00E+13 0.0 0.0

427. AC3H5+O=C2H3+CH2O 1.80E+14 0.0 0.0

428. SC3H5+O=CH2CO+CH3 1.81E+14 0.0 0.0

429. TC3H5+O=H+HCCO+CH3 1.81E+14 0.0 0.0

430. AC3H5+OH=C2H3CHO+H+H 5.30E+37 -6.7 29306.0

431. AC3H5+OH=AC3H4+H2O 6.00E+12 0.0 0.0

432. AC3H5+O2=AC3H4+HO2 4.99E+15 -1.4 22428.0

433. AC3H5+O2=CH2O+CH3CO 1.19E+15 -1.0 20128.0

434. AC3H5+O2=OH+C2H3CHO 1.82E+13 -0.4 22859.0

435. SC3H5+O2=CH3CHO+HCO 4.34E+12 0.0 0.0

436. TC3H5+O2=CH3CHO+HCO 4.34E+12 0.0 0.0

437. AC3H5+HO2=C2H3+CH2O+OH 6.60E+12 0.0 0.0

438. AC3H5+CH3=AC3H4+CH4 3.00E+12 -0.3 -131.0

439. AC3H5+CH3(+M)=IC4H8(+M) 1.00E+14 -0.3 -262.0

Low pressure limit: 0.35100E+61 -0.12970E+02 0.60000E+04

TROE centering: 0.89600E+00 0.60000E+05 0.16060E+04 0.61180E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01				
440. SC3H5+CH3=AC3H4+CH4	1.00E+11	0.0	0.0	
441. TC3H5+CH3=AC3H4+CH4	1.00E+11	0.0	0.0	
442. AC3H5+C2H3=AC3H4+C2H4	1.00E+12	0.0	0.0	
443. SC3H5+C2H3=AC3H4+C2H4	1.00E+11	0.0	0.0	
444. TC3H5+C2H3=AC3H4+C2H4	1.00E+11	0.0	0.0	
445. AC3H5+CH2O=C3H6+HCO	1.26E+08	1.9	18191.0	
446. AC3H5+HCO=C3H6+CO	6.00E+13	0.0	0.0	
447. AC3H5+AC3H5=AC3H4+C3H6	8.43E+10	0.0	-262.0	
448. AC3H5+CH2=iiiC4H6+H	3.00E+13	0.0	0.0	
449. AC3H5+nC3H7=AC3H4+C3H8	7.23E+11	0.0	-131.0	
450. AC3H5+iC3H7=AC3H4+C3H8	4.58E+12	-0.3	-131.0	
451. AC3H5=TC3H5	3.90E+59	-15.4	75400.0	
452. AC3H5=SC3H5	1.30E+55	-14.5	73800.0	
453. TC3H5=SC3H5	1.60E+44	-12.2	52200.0	
454. AC3H4=PC3H4	6.03E+53	-12.2	84276.0	
455. AC3H4+H=AC3H5	1.24E+52	-12.0	17839.0	
Declared duplicate reaction...				
456. AC3H4+H=AC3H5	6.92E+36	-8.2	7462.0	
Declared duplicate reaction...				
457. AC3H4+H=TC3H5	1.55E+53	-13.1	14472.0	
Declared duplicate reaction...				
458. AC3H4+H=TC3H5	9.88E+44	-11.2	8212.0	
Declared duplicate reaction...				
459. PC3H4+H=TC3H5	3.17E+52	-12.7	14226.0	
Declared duplicate reaction...				
460. PC3H4+H=TC3H5	2.59E+45	-11.2	8046.0	
Declared duplicate reaction...				
461. PC3H4+H=SC3H5	3.38E+49	-12.8	14072.0	
Declared duplicate reaction...				
462. PC3H4+H=SC3H5	2.98E+43	-11.4	8736.0	
Declared duplicate reaction...				

463.	AC3H4+H=PC3H4+H	1.48E+13	0.3	4103.0
464.	AC3H4+H=CH3+C2H2	2.72E+09	1.2	6834.0
465.	PC3H4+H=CH3+C2H2	3.89E+10	1.0	4114.0
466.	C2H2+CH3=SC3H5	-6.81E+48	-12.3	16642.0
	Declared duplicate reaction...			
467.	C2H2+CH3=SC3H5	1.52E+44	-10.7	15256.0
	Declared duplicate reaction...			
468.	C2H2+CH3=TC3H5	6.80E+20	-4.2	18000.0
469.	C2H2+CH3=AC3H5	8.20E+53	-13.3	33200.0
470.	AC3H4+H=C3H3+H2	6.60E+03	3.1	5522.0
471.	AC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
472.	PC3H4+H=C3H3+H2	3.57E+04	2.8	4821.0
473.	AC3H4+O=C2H4+CO	2.00E+07	1.8	1000.0
474.	AC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
475.	AC3H4+CH3=C3H3+CH4	1.30E+12	0.0	7700.0
476.	PC3H4+O=HCCO+CH3	7.30E+12	0.0	2250.0
477.	PC3H4+O=C2H4+CO	1.00E+13	0.0	2250.0
478.	PC3H4+O=C3H3+OH	3.44E+04	2.2	4830.0
479.	PC3H4+OH=C3H3+H2O	1.00E+07	2.0	1000.0
480.	PC3H4+C2H=C3H3+C2H2	1.00E+13	0.0	0.0
481.	PC3H4+CH3=C3H3+CH4	1.80E+12	0.0	7700.0
482.	C3H3+H=PC3H4	3.63E+36	-7.4	6039.0
483.	C3H3+H=AC3H4	3.39E+36	-7.4	6337.0
484.	C3H3+CH3=iiC4H6	3.61E+13	0.0	0.0
485.	C2H3+C2H3=iiiC4H6	7.00E+57	-13.8	17629.0
486.	C3H3+H=C3H2+H2	2.14E+05	2.5	7453.0
487.	C3H3+O=>C2H2+HCO	1.38E+14	0.0	0.0
488.	C3H3+O=C2H3+CO	4.62E+13	0.0	0.0
489.	C3H3+O=C2H+CH2O	4.62E+13	0.0	0.0
490.	C3H3+O=>C2H2+CO+H	4.62E+13	0.0	0.0
491.	C3H3+OH=C3H2+H2O	2.00E+13	0.0	8000.0
492.	C3H3+HCO=AC3H4+CO	2.50E+13	0.0	0.0

493.	C3H3+HCO=PC3H4+CO	2.50E+13	0.0	0.0
494.	C3H3+CH=iC4H3+H	5.00E+13	0.0	0.0
495.	C3H3+CH2=C4H4+H	5.00E+13	0.0	0.0
496.	C3H3+O2=CH2CO+HCO	1.70E+05	1.7	1500.0
497.	C3H3+HCCO=C4H4+CO	2.50E+13	0.0	0.0
498.	C3H3+HO2=OH+CO+C2H3	8.00E+11	0.0	0.0
499.	C3H3+HO2=AC3H4+O2	3.00E+11	0.0	0.0
500.	C3H3+HO2=PC3H4+O2	2.50E+12	0.0	0.0
501.	C3H2+O2=H+CO+HCCO	2.00E+12	0.0	1000.0
502.	C3H2+O=C2H2+CO	6.80E+13	0.0	0.0
503.	C3H2+OH=C2H2+HCO	6.80E+13	0.0	0.0
504.	C3H2+H=C3H3	1.10E+40	-8.0	84700.0
505.	C3H2+CH=C4H2+H	5.00E+13	0.0	0.0
506.	C3H2+CH2=nC4H3+H	5.00E+13	0.0	0.0
507.	C3H2+CH3=C4H4+H	5.00E+12	0.0	0.0
508.	C3H2+HCCO=nC4H3+CO	1.00E+13	0.0	0.0
509.	C2H3CO+M=>C2H3+CO+M	8.51E+15	0.0	23000.0
510.	C2H3+CO+M=>C2H3CO+M	1.58E+11	0.0	6000.0
511.	C2H3CHO+HO2=>C2H3CH2O+O2	1.29E+11	0.0	32000.0
512.	C2H3CH2O=>C2H3CHO+H	1.00E+14	0.0	19000.0
513.	C2H3CHO+H=>C2H3CH2O	1.00E+08	0.0	10000.0
514.	C2H3CHO+OH=>C2H3CO+H2O	1.00E+13	0.0	0.0
515.	C2H3CO+H2O=>C2H3CHO+OH	1.91E+13	0.0	36620.0
516.	C2H3CHO+H=>C2H3CO+H2	3.98E+13	0.0	4200.0
517.	C2H3CO+H2=>C2H3CHO+H	1.78E+13	0.0	23670.0
518.	C2H3CHO+O=>C2H3CO+OH	5.01E+12	0.0	1790.0
519.	C2H3CO+OH=>C2H3CHO+O	1.00E+12	0.0	19160.0
520.	C2H3CHO+HO2=>C2H3CO+H2O2	1.70E+12	0.0	10700.0
521.	C2H3CO+H2O2=>C2H3CHO+HO2	1.00E+12	0.0	14100.0
522.	C2H3CHO+CH3=>C2H3CO+CH4	1.74E+12	0.0	8440.0
523.	C2H3CO+CH4=>C2H3CHO+CH3	1.51E+13	0.0	28000.0
524.	C2H3CH2O+O2=>C2H3CHO+HO2	1.74E+11	0.0	1750.0

525. C2H3CH2O=>CH2O+C2H3 1.00E+14 0.0 21600.0

526. CH2O+C2H3=>C2H3CH2O 1.00E+11 0.0 0.0

527. C4H+H2=C4H2+H 2.00E+13 0.0 5000.0

528. C4H+O2=CO+CO+C2H 1.20E+12 0.0 0.0

529. C4H2+OH=H2O+C4H 9.15E+09 1.0 21746.0

530. C4H2+OH=CO+C3H3 1.69E+28 -4.6 20140.0

531. C4H2+H=nC4H3 1.44E+63 -15.7 24018.0

Declared duplicate reaction...

532. C4H2+H=nC4H3 4.16E+32 -6.5 9726.1

Declared duplicate reaction...

533. C4H2+H(+M)=iC4H3(+M) 4.31E+10 1.2 1752.9

Low pressure limit: 0.23000E+46 -0.80950E+01 0.25066E+04

TROE centering: 0.74800E-01 0.10000E-49 -0.42159E+04 0.10000E+51

H2 Enhanced by 2.000E+00

CO Enhanced by 2.000E+00

CO2 Enhanced by 3.000E+00

H2O Enhanced by 5.000E+00

534. C4H2+O=C3H2+CO 2.70E+13 0.0 1720.0

535. nC4H3=iC4H3 3.70E+61 -15.8 54890.0

536. nC4H3+H=iC4H3+H 2.40E+11 0.8 2410.0

537. nC4H3+H=C2H2+H2CC 1.60E+19 -1.6 2220.0

538. nC4H3+H=C4H4 1.10E+42 -9.7 7000.0

539. nC4H3+H=C4H2+H2 3.00E+13 0.0 0.0

540. nC4H3+OH=C4H2+H2O 2.00E+12 0.0 0.0

541. iC4H3+H=C2H2+H2CC 2.40E+19 -1.6 2800.0

542. iC4H3+H=C4H4 4.20E+44 -10.3 7890.0

543. iC4H3+H=C4H2+H2 5.00E+13 0.0 0.0

544. iC4H3+OH=C4H2+H2O 4.00E+12 0.0 0.0

545. iC4H3+O2=HCCO+CH2CO 7.86E+16 -1.8 0.0

546. C4H4+H=n-C4H5 4.20E+50 -12.3 12500.0

547. C4H4+H=i-C4H5 9.60E+52 -12.8 14300.0

548. C4H4+H=nC4H3+H2 6.65E+05 2.5 12240.0

549.	C4H4+H=iC4H3+H2	3.33E+05	2.5	9240.0
550.	C4H4+OH=nC4H3+H2O	3.10E+07	2.0	3430.0
551.	C4H4+OH=iC4H3+H2O	1.55E+07	2.0	430.0
552.	C4H4+O=C3H3+HCO	6.00E+08	1.4	-860.0
553.	n-C4H5=i-C4H5	1.30E+62	-16.4	49600.0
554.	n-C4H5+H=i-C4H5+H	1.00E+36	-6.3	17486.0
555.	n-C4H5+H=C4H4+H2	1.50E+13	0.0	0.0
556.	n-C4H5+OH=C4H4+H2O	2.00E+12	0.0	0.0
557.	n-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
558.	n-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
559.	n-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
560.	n-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
561.	n-C4H5+O2=HCO+C2H3CHO	9.20E+16	-1.4	1010.0
562.	i-C4H5+H=C4H4+H2	3.00E+13	0.0	0.0
563.	i-C4H5+H=C3H3+CH3	1.00E+14	0.0	0.0
564.	i-C4H5+OH=C4H4+H2O	4.00E+12	0.0	0.0
565.	i-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.0	0.0
566.	i-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.0	0.0
567.	i-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.0	0.0
568.	i-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.0	-596.0
569.	i-C4H5+O2=CH2CO+CH2CHO	2.16E+10	0.0	2500.0
570.	iiiC4H6=i-C4H5+H	8.20E+51	-10.9	118409.0
571.	iiiC4H6=n-C4H5+H	3.50E+61	-13.9	129677.0
572.	iiiC4H6=C4H4+H2	2.50E+15	0.0	94700.0
573.	iiiC4H6+H=n-C4H5+H2	3.00E+07	2.0	13000.0
574.	iiiC4H6+H=i-C4H5+H2	3.00E+07	2.0	6000.0
575.	C2H4+C2H3=iiiC4H6+H	7.40E+14	-0.7	8420.0
576.	iiiC4H6+H=PC3H4+CH3	2.00E+12	0.0	7000.0
577.	iiiC4H6+H=AC3H4+CH3	2.00E+12	0.0	7000.0
578.	iiiC4H6+O=n-C4H5+OH	7.50E+06	1.9	3740.0
579.	iiiC4H6+O=i-C4H5+OH	7.50E+06	1.9	3740.0
580.	iiiC4H6+O=HCO+AC3H5	6.02E+08	1.4	-858.0

581.	iiiC4H6+OH=CH3CHO+C2H3	6.30E+12	0.0	-874.0
582.	iiiC4H6+OH=AC3H5+CH2O	6.30E+12	0.0	-874.0
583.	iiiC4H6+OH=n-C4H5+H2O	2.00E+07	2.0	5000.0
584.	iiiC4H6+OH=i-C4H5+H2O	2.00E+07	2.0	2000.0
585.	iiiC4H6+CH3=n-C4H5+CH4	2.00E+14	0.0	22800.0
586.	iiiC4H6+CH3=i-C4H5+CH4	1.00E+14	0.0	19800.0
587.	iiiC4H6+C2H3=n-C4H5+C2H4	5.00E+13	0.0	22800.0
588.	iiiC4H6+C2H3=i-C4H5+C2H4	2.50E+13	0.0	19800.0
589.	iiiC4H6+C3H3=n-C4H5+AC3H4	1.00E+13	0.0	22500.0
590.	iiiC4H6+C3H3=i-C4H5+AC3H4	5.00E+12	0.0	19500.0
591.	iiiC4H6+AC3H5=n-C4H5+C3H6	1.00E+13	0.0	22500.0
592.	iiiC4H6+AC3H5=i-C4H5+C3H6	5.00E+12	0.0	19500.0
593.	iiC4H6=i-C4H5+H	4.20E+15	0.0	92600.0
594.	iiC4H6+H=iiiC4H6+H	2.00E+13	0.0	4000.0
595.	iiC4H6+H=i-C4H5+H2	1.70E+05	2.5	2490.0
596.	iiC4H6+H=AC3H4+CH3	2.00E+13	0.0	2000.0
597.	iiC4H6+H=PC3H4+CH3	2.00E+13	0.0	2000.0
598.	iiC4H6+CH3=i-C4H5+CH4	7.00E+13	0.0	18500.0
599.	iiC4H6+O=CH2CO+C2H4	1.20E+08	1.6	327.0
600.	iiC4H6+O=i-C4H5+OH	1.80E+11	0.7	5880.0
601.	iiC4H6+OH=i-C4H5+H2O	3.10E+06	2.0	-298.0
602.	iiC4H6=iiiC4H6	3.00E+13	0.0	65000.0
603.	IC4H8+H=C2H4+C2H5	1.60E+22	-2.4	11180.0
604.	IC4H8+H=C3H6+CH3	3.20E+22	-2.4	11180.0
605.	IC4H8+H=C4H7+H2	6.50E+05	2.5	6756.0
606.	IC4H8+O=nC3H7+HCO	3.30E+08	1.4	-402.0
607.	IC4H8+O=C4H7+OH	1.50E+13	0.0	5760.0
	Declared duplicate reaction...			
608.	IC4H8+O=C4H7+OH	2.60E+13	0.0	4470.0
	Declared duplicate reaction...			
609.	IC4H8+OH=C4H7+H2O	7.00E+02	2.7	527.0
610.	IC4H8+O2=C4H7+HO2	2.00E+13	0.0	50930.0

611. IC4H8+HO2=C4H7+H2O2 1.00E+12 0.0 14340.0

612. IC4H8+CH3=C4H7+CH4 4.50E-01 3.6 7153.0

613. C4H7=iiiC4H6+H 1.27E+24 -4.8 23777.0

614. C4H7+H(+M)=IC4H8(+M) 3.60E+13 0.0 0.0

Low pressure limit: 0.30100E+49 -0.93200E+01 0.58336E+04

TROE centering: 0.49800E+00 0.13140E+04 0.13140E+04 0.50000E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

615. C4H7+H=CH3+AC3H5 2.00E+21 -2.0 11000.0

616. C4H7+H=iiiC4H6+H2 1.80E+12 0.0 0.0

617. C4H7+O2=iiiC4H6+HO2 1.00E+11 0.0 0.0

618. C4H7+HCO=IC4H8+CO 6.00E+13 0.0 0.0

619. C4H7+CH3=iiiC4H6+CH4 1.10E+13 0.0 0.0

620. C2H4+C2H3=C4H7 1.23E+35 -7.8 9930.0

621. IC4H8+H(+M)=nC4H9(+M) 1.33E+13 0.0 3260.7

Low pressure limit: 0.62600E+39 -0.66600E+01 0.70000E+04

TROE centering: 0.10000E+01 0.10000E+04 0.13100E+04 0.48097E+05

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

622. C2H4+C2H5=nC4H9 1.50E+11 0.0 7300.0

623. nC4H9+H=IC4H8+H2 1.80E+12 0.0 0.0

624. nC4H9+O=nC3H7+CH2O 9.60E+13 0.0 0.0

625. nC4H9+OH=IC4H8+H2O	2.40E+13	0.0	0.0
626. nC4H9+O2=IC4H8+HO2	2.70E+11	0.0	0.0
627. nC4H9+HO2=nC3H7+OH+CH2O	2.40E+13	0.0	0.0
628. nC4H9+CH3=IC4H8+CH4	1.10E+13	0.0	0.0
629. C2H5OH=CH3+CH2OH	1.26E+51	-10.6	100869.0
630. C2H5OH=C2H4+H2O	8.80E+25	-3.7	70799.0
631. C2H5OH+OH=C2H4OH+H2O	1.81E+11	0.4	716.5
632. C2H5OH+OH=CH3CHOH+H2O	3.09E+10	0.5	-379.8
633. C2H5OH+OH=C2H5O+H2O	1.05E+10	0.8	716.9
634. C2H5OH+H=C2H4OH+H2	1.90E+07	1.8	5098.0
635. C2H5OH+H=CH3CHOH+H2	2.58E+07	1.6	2827.0
636. C2H5OH+H=C2H5O+H2	1.50E+07	1.6	3038.0
637. C2H5OH+O=C2H4OH+OH	9.41E+07	1.7	5459.0
638. C2H5OH+O=CH3CHOH+OH	1.88E+07	1.9	1824.0
639. C2H5OH+O=C2H5O+OH	1.58E+07	2.0	4448.0
640. C2H5OH+CH3=C2H4OH+CH4	2.19E+02	3.2	9622.0
641. C2H5OH+CH3=CH3CHOH+CH4	7.28E+02	3.0	7948.0
642. C2H5OH+CH3=C2H5O+CH4	1.45E+02	3.0	7649.0
643. C2H5OH+HO2=CH3CHOH+H2O2	8.20E+03	2.5	10750.0
644. C2H5OH+HO2=C2H4OH+H2O2	2.43E+04	2.5	15750.0
645. C2H5OH+HO2=C2H5O+H2O2	3.80E+12	0.0	24000.0
646. C2H5O+M=CH3CHO+H+M	5.60E+34	-5.9	25274.0
647. C2H5O+M=CH3+CH2O+M	5.35E+37	-7.0	23800.0
648. C2H5O+CO=C2H5+CO2	4.68E+02	3.2	5380.0
649. C2H5O+H=CH3+CH2OH	3.00E+13	0.0	0.0
650. C2H5O+H=C2H4+H2O	3.00E+13	0.0	0.0
651. C2H5O+OH=CH3CHO+H2O	1.00E+13	0.0	0.0
652. CH3CHOH+O2=CH3CHO+HO2	4.82E+13	0.0	5017.0
Declared duplicate reaction...			
653. CH3CHOH+O2=CH3CHO+HO2	8.43E+14	-1.2	0.0
Declared duplicate reaction...			
654. CH3CHOH+O=CH3CHO+OH	1.00E+14	0.0	0.0

655.	CH3CHOH+H=C2H4+H2O	3.00E+13	0.0	0.0
656.	CH3CHOH+H=CH3+CH2OH	3.00E+13	0.0	0.0
657.	CH3CHOH+HO2=CH3CHO+OH+OH	4.00E+13	0.0	0.0
658.	CH3CHOH+OH=CH3CHO+H2O	5.00E+12	0.0	0.0
659.	CH3CHOH+M=CH3CHO+H+M	1.00E+14	0.0	25000.0
660.	C2H4+OH=C2H4OH	2.41E+11	0.0	-2385.0
661.	C2H4OH+O2=HOC2H4O2	1.00E+12	0.0	-1100.0
662.	HOC2H4O2=CH2O+CH2O+OH	1.80E+11	0.0	24500.0
663.	CH3OCH3=CH3+CH3O	1.88E+49	-10.4	93453.5
664.	CH3OCH3+OH=CH3OCH2+H2O	6.71E+06	2.0	-629.9
665.	CH3OCH3+H=CH3OCH2+H2	2.97E+07	2.0	4033.6
666.	CH3OCH3+O=CH3OCH2+OH	1.86E-03	5.3	-109.0
667.	CH3OCH3+HO2=CH3OCH2+H2O2	1.68E+13	0.0	17690.0
668.	CH3OCH3+CH3=CH3OCH2+CH4	3.86E-08	6.2	2513.9
669.	CH3OCH3+O2=CH3OCH2+HO2	4.10E+13	0.0	44910.0
670.	CH3OCH3+CH3O=CH3OCH2+CH3OH	6.02E+11	0.0	4074.0
671.	CH3OCH2=CH2O+CH3	1.60E+13	0.0	25500.0
672.	CH3OCH2+CH3O=CH3OCH3+CH2O	2.41E+13	0.0	0.0
673.	CH3OCH2+CH2O=CH3OCH3+HCO	5.49E+03	2.8	5862.0
674.	CH3OCH2+O2=>CH2O+CH2O+OH	5.02E+23	-3.8	3100.0
675.	CH3OCH2+HO2=CH3OCH2O+OH	9.00E+12	0.0	0.0
676.	CH3OCH2O=CH3OCHO+H	1.74E+16	-0.7	11720.0
677.	CH3OCHO=CH3+OCHO	1.39E+18	-1.0	79140.0
678.	CH3OCHO+O2=CH3OCO+HO2	1.00E+13	0.0	49700.0
679.	CH3OCHO+OH=CH3OCO+H2O	2.34E+07	1.6	-35.0
680.	CH3OCHO+HO2=CH3OCO+H2O2	1.22E+12	0.0	17000.0
681.	CH3OCHO+O=CH3OCO+OH	2.35E+05	2.5	2230.0
682.	CH3OCHO+H=CH3OCO+H2	4.55E+06	2.0	5000.0
683.	CH3OCHO+CH3=CH3OCO+CH4	7.55E-01	3.5	5481.0
684.	CH3OCHO+CH3O=CH3OCO+CH3OH	5.48E+11	0.0	5000.0
685.	CH3OCO=CH3O+CO	7.45E+12	-1.8	17150.0
686.	CH3OCO=CH3+CO2	1.51E+12	-1.8	13820.0

687.	OCHO+M=H+CO2+M	2.44E+15	-0.5	26500.0
688.	NH+M=N+H+M	2.65E+14	0.0	75500.0
689.	NH+H=N+H2	3.20E+13	0.0	325.0
690.	NH+O=N+OH	1.70E+08	1.5	3368.0
691.	NH+OH=N+H2O	1.60E+07	1.7	-576.0
692.	NH2+M=NH+H+M	3.16E+23	-2.0	91400.0
693.	NH2+H=NH+H2	4.00E+13	0.0	3650.0
694.	NH2+O=NH+OH	7.00E+12	0.0	0.0
	Declared duplicate reaction...			
695.	NH2+O=NH+OH	8.60E-01	4.0	1673.0
	Declared duplicate reaction...			
696.	NH2+OH=NH+H2O	3.30E+06	1.9	-217.0
697.	NH2+O2=NH+HO2	1.00E+14	0.0	49997.0
698.	NH+NH=NH2+N	5.70E-01	3.9	342.0
699.	NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
700.	NH3+M=NH+H2+M	6.30E+14	0.0	93390.0
701.	NH3+H=NH2+H2	6.36E+05	2.4	10171.0
702.	NH3+O=NH2+OH	2.80E+02	3.3	4471.0
703.	NH3+OH=NH2+H2O	2.00E+06	2.0	566.0
704.	NH2+HO2=NH3+O2	9.20E+05	1.9	-1152.0
705.	NH3+HO2=NH2+H2O2	3.00E+11	0.0	22000.0
706.	NH2+NH=NH3+N	9.60E+03	2.5	107.0
707.	NH2+NH2=NH3+NH	5.60E+00	3.5	552.0
708.	N2+M=N+N+M	1.00E+28	-3.3	225000.0
709.	NH+N=N2+H	3.00E+13	0.0	0.0
710.	NH+NH=N2+H+H	2.50E+13	0.0	0.0
711.	NH2+N=N2+H+H	7.10E+13	0.0	0.0
712.	NH+NH=N2+H2	1.00E+08	1.0	0.0
713.	NNH=N2+H	1.00E+09	0.0	0.0
714.	NNH+H=N2+H2	1.00E+14	0.0	0.0
715.	NH+NH=NNH+H	5.10E+13	0.0	0.0
716.	NNH+O=N2+OH	1.20E+13	0.1	-217.0

717.	NNH+OH=N2+H2O			5.00E+13	0.0	0.0
718.	NNH+O2=N2+HO2			5.60E+14	-0.4	-13.0
719.	NNH+O2=N2+H+O2			5.00E+13	0.0	0.0
720.	NNH+HO2=N2+H2O2			1.40E+04	2.7	-1599.0
721.	NNH+N=NH+N2			3.00E+13	0.0	2000.0
722.	NNH+NH=N2+NH2			5.00E+13	0.0	0.0
723.	NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
724.	N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
	H2O	Enhanced by	1.500E+01			
	O2	Enhanced by	2.000E+00			
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
725.	N2H2+M=NH+NH+M			3.16E+16	0.0	99400.0
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
726.	NH2+NH=N2H2+H			4.30E+14	-0.3	-77.0
727.	N2H2+H=NNH+H2			8.50E+04	2.6	230.0
728.	NH2+NH2=N2H2+H2			1.70E+08	1.6	11783.0
729.	N2H2+O=NNH+OH			3.30E+08	1.5	496.0
730.	N2H2+OH=NNH+H2O			5.90E+01	3.4	1360.0
731.	N2H2+N=NNH+NH			1.00E+06	2.0	0.0
732.	N2H2+NH=NNH+NH2			1.00E+13	0.0	6000.0
733.	N2H2+NH2=NH3+NNH			1.80E+06	1.9	-1152.0
734.	NNH+NNH=N2H2+N2			1.00E+13	0.0	4000.0
735.	H2NN=NNH+H			3.40E+26	-4.8	46228.0
736.	N2H2=H2NN			2.00E+41	-9.4	68413.0
737.	H2NN+H=N2H2+H			7.00E+13	0.0	0.0
738.	H2NN+H=NNH+H2			4.80E+08	1.5	-894.0
739.	NH2+NH2=H2NN+H2			7.20E+04	1.9	8802.0
740.	H2NN+O=OH+NNH			3.30E+08	1.5	-894.0
741.	H2NN+OH=NNH+H2O			2.40E+06	2.0	-1192.0
742.	H2NN+HO2=NNH+H2O2			2.90E+04	2.7	-1599.0

743. H2NN+NH2=NH3+NNH 1.80E+06 1.9 -1152.0

744. N2H3=N2H2+H 3.60E+47 -10.4 68970.0

745. N2H3+M=NH2+NH+M 5.00E+16 0.0 60000.0

746. NH2+NH2=N2H3+H 1.20E+12 0.0 10078.0

747. N2H3+H=N2H2+H2 2.40E+08 1.5 0.0

748. N2H3+H=NH+NH3 1.00E+11 0.0 0.0

749. NH3+NH2=N2H3+H2 1.00E+11 0.5 21600.0

750. N2H3+O=N2H2+OH 1.70E+08 1.5 -645.0

751. N2H3+OH=N2H2+H2O 1.20E+06 2.0 -1192.0

752. N2H3+OH=H2NN+H2O 3.00E+13 0.0 0.0

753. N2H3+HO2=N2H2+H2O2 1.40E+04 2.7 -1600.0

754. N2H3+N=N2H2+NH 1.00E+06 2.0 0.0

755. N2H3+NH=N2H2+NH2 2.00E+13 0.0 0.0

756. N2H3+NH2=N2H2+NH3 9.20E+05 1.9 -1152.0

757. N2H3+NH2=H2NN+NH3 3.00E+13 0.0 0.0

758. N2H3+NNH=N2H2+N2H2 1.00E+13 0.0 4000.0

759. N2H3+N2H3=NH3+NH3+N2 3.00E+12 0.0 0.0

760. NH2+NH2(+M)=N2H4(+M) 5.60E+14 -0.4 66.0

Low pressure limit: 0.16000E+35 -0.54900E+01 0.19870E+04

TROE centering: 0.31000E+00 0.10000E-29 0.10000E+31 0.10000E+31

761. N2H4+M=N2H3+H+M 1.00E+15 0.0 63600.0

N2 Enhanced by 2.400E+00

NH3 Enhanced by 3.000E+00

N2H4 Enhanced by 4.000E+00

762. N2H4=H2NN+H2 5.30E+39 -8.3 69267.0

763. N2H4+H=N2H3+H2 7.00E+12 0.0 2500.0

764. N2H4+H=NH2+NH3 2.40E+09 0.0 3100.0

765. N2H4+O=N2H3+OH 6.70E+08 1.5 2850.0

766. N2H4+O=N2H2+H2O 4.40E+11 0.0 -1270.0

767. N2H4+OH=N2H3+H2O 4.00E+13 0.0 0.0

768. N2H3+HO2=N2H4+O2 9.20E+05 1.9 2125.0

769. N2H4+N=N2H3+NH 1.00E+10 1.0 2000.0

770.	N2H4+NH=NH2+N2H3		1.00E+09	1.5	2000.0
771.	N2H4+NH2=N2H3+NH3		3.90E+12	0.0	1500.0
772.	N2H3+N2H2=N2H4+NNH		1.00E+13	0.0	6000.0
773.	N2H3+N2H3=N2H4+N2H2		1.20E+13	0.0	0.0
774.	NO+M=N+O+M		1.40E+15	0.0	148430.0
	N2	Enhanced by 1.000E+00			
	H2	Enhanced by 2.200E+00			
	H2O	Enhanced by 6.700E+00			
	CO2	Enhanced by 3.000E+00			
	N2O	Enhanced by 2.200E+00			
775.	N+OH=NO+H		3.80E+13	0.0	0.0
776.	NH+O=NO+H		9.20E+13	0.0	0.0
777.	NH2+O=NO+H2		5.00E+12	0.0	0.0
778.	NH+OH=NO+H2		2.00E+13	0.0	0.0
779.	NO+O=O2+N		1.81E+09	1.0	38725.0
780.	NH+O2=NO+OH		1.30E+06	1.5	100.0
781.	N+NO=N2+O		3.30E+12	0.3	0.0
782.	NH+NO=N2+OH		2.20E+13	-0.2	0.0
783.	NNH+O=NH+NO		5.20E+11	0.4	-409.0
784.	NH2+NO=N2+H2O		2.80E+20	-2.7	1258.0
785.	NH2+NO=NNH+OH		2.29E+10	0.4	-814.0
786.	N2H2+O=NH2+NO		1.00E+13	0.0	0.0
787.	H2NN+O=NH2+NO		7.00E+13	0.0	0.0
788.	H2NN+OH=>NH2+NO+H		2.00E+12	0.0	0.0
789.	N2H3+O=>NH2+NO+H		3.00E+13	0.0	0.0
790.	H2NN+HO2=>NH2+NO+OH		9.00E+12	0.0	0.0
791.	NO+H(+M)=HNO(+M)		1.50E+15	-0.4	0.0
	Low pressure limit: 0.24000E+15 0.20600E+00 -0.15500E+04				
	TROE centering: 0.82000E+00 0.10000E-29 0.10000E+31 0.10000E+31				
	N2	Enhanced by 1.600E+00			
792.	HNO+H=H2+NO		4.50E+11	0.7	655.0
793.	NH+OH=HNO+H		3.20E+14	-0.4	-46.0

794.	NH2+O=HNO+H			6.63E+14	-0.5	0.0
795.	NH+H2O=HNO+H2			2.00E+13	0.0	13850.0
796.	HNO+O=OH+NO			1.81E+13	0.0	0.0
797.	NH+O2=HNO+O			4.60E+05	2.0	6494.0
798.	HNO+OH=NO+H2O			3.60E+13	0.0	0.0
799.	NH2+O2=HNO+OH			2.90E-02	3.8	18185.0
800.	NH2+HO2=HNO+H2O			5.68E+15	-1.1	707.0
801.	HNO+O2=NO+HO2			2.00E+13	0.0	15887.0
802.	NH2+HNO=NH3+NO			3.60E+06	1.6	-1250.0
803.	N2H3+O=NH2+HNO			3.00E+13	0.0	0.0
804.	N2H3+OH=NH3+HNO			1.00E+12	0.0	15000.0
805.	NNH+NO=N2+HNO			5.00E+13	0.0	0.0
806.	H+NO+N2=HNO+N2			4.00E+20	-1.8	0.0
807.	HON+M=NO+H+M			5.10E+19	-1.7	16045.0
	AR	Enhanced by	7.000E-01			
	H2O	Enhanced by	7.000E+00			
	CO2	Enhanced by	2.000E+00			
808.	HON+H=HNO+H			2.00E+13	0.0	0.0
809.	HON+H=OH+NH			2.00E+13	0.0	0.0
810.	HON+O=OH+NO			7.00E+13	0.0	0.0
811.	HNOH+M=H+HNO+M			2.00E+24	-2.8	58901.0
812.	HNOH+H=NH2+OH			4.00E+13	0.0	0.0
813.	HNOH+H=HNO+H2			4.80E+08	1.5	377.0
814.	HNOH+O=HNO+OH			7.00E+13	0.0	0.0
	Declared duplicate reaction...					
815.	HNOH+O=HNO+OH			3.30E+08	1.5	-357.0
	Declared duplicate reaction...					
816.	HNOH+OH=HNO+H2O			2.40E+06	2.0	-1192.0
817.	HNOH+O2=HNO+HO2			3.00E+12	0.0	25000.0
818.	HNOH+HO2=HNO+H2O2			2.90E+04	2.7	-1599.0
819.	HNOH+NH2=N2H3+OH			1.00E+01	3.5	-467.0
820.	HNOH+NH2=H2NN+H2O			8.80E+16	-1.1	1113.0

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821. HNOH+NH2=HNO+NH3                                 1.80E+06    1.9    -1152.0
822. NH2O+M=HNO+H+M                                   2.80E+24   -2.8    64915.0
     H2O             Enhanced by    1.000E+01
823. NH2O+M=HNOH+M                                    1.10E+29   -4.0    44000.0
     H2O             Enhanced by    1.000E+01
824. NH2O+H=NH2+OH                                    5.00E+13    0.0        0.0
825. NH2O+H=HNO+H2                                    3.00E+07    2.0     2000.0
826. NH2O+O=HNO+OH                                    3.00E+07    2.0     2000.0
827. NH2+O2=NH2O+O                                    2.50E+11    0.5    29570.0
828. NH2O+OH=HNO+H2O                                  2.00E+07    2.0     1000.0
829. NH2+HO2=NH2O+OH                                  5.00E+13    0.0        0.0
830. NH2O+O2=HNO+HO2                                  3.00E+12    0.0    25000.0
831. NH2O+HO2=HNO+H2O2                                2.90E+04    2.7    -1599.0
832. NH2O+NH2=HNO+NH3                                 3.00E+12    0.0     1000.0
833. NH2O+NO=HNO+HNO                                  2.00E+04    2.0    13000.0
834. NH2OH(+M)=NH2+OH(+M)                             1.40E+20   -1.3    64080.0
     Low pressure limit:  0.54000E+38 -0.59600E+01  0.66783E+05
     TROE centering:      0.31000E+00  0.10000E-29  0.10000E+31  0.10000E+31
835. NH2OH+H=HNOH+H2                                  4.80E+08    1.5     6246.0
836. NH2OH+H=NH2O+H2                                  2.40E+08    1.5     5064.0
837. NH2OH+O=HNOH+OH                                  3.30E+08    1.5     3863.0
838. NH2OH+O=NH2O+OH                                  1.70E+08    1.5     3009.0
839. NH2OH+OH=HNOH+H2O                                1.50E+04    2.6    -3537.0
840. NH2OH+OH=NH2O+H2O                                1.50E+05    2.3    -1296.0
841. NH2O+HO2=O2+NH2OH                                2.90E+04    2.7    -1599.0
842. HNOH+HO2=NH2OH+O2                                2.90E+04    2.7    -1599.0
843. NH2OH+HO2=HNOH+H2O2                              2.90E+04    2.7     9552.0
844. NH2OH+HO2=NH2O+H2O2                              1.40E+04    2.7     6414.0
845. N2H4+O=NH2OH+NH                                  2.90E+11    0.0    -1270.0
846. NH2OH+NH=HNOH+NH2                                2.90E-03    4.4     1564.0
847. NH2OH+NH=NH2O+NH2                                1.50E-03    4.6     2424.0
848. NH2OH+NH2=HNOH+NH3                               1.10E-01    4.0      -97.0
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849. NH2OH+NH2=NH2O+NH3	9.50E+00	3.4	-1013.0
850. H2NN+NH2=HNNNH2+H	7.90E+06	1.9	-1331.0
851. N2O(+M)=N2+O(+M)	1.30E+12	0.0	62570.0
Low pressure limit: 0.40000E+15 0.00000E+00 0.56600E+05			
N2 Enhanced by 1.700E+00			
O2 Enhanced by 1.400E+00			
CO2 Enhanced by 3.000E+00			
H2O Enhanced by 1.200E+01			
852. N2O+H=N2+OH	3.30E+10	0.0	4729.0
Declared duplicate reaction...			
853. N2O+H=N2+OH	4.40E+14	0.0	19254.0
Declared duplicate reaction...			
854. NH+NO=N2O+H	2.90E+14	-0.4	0.0
Declared duplicate reaction...			
855. NH+NO=N2O+H	-2.20E+13	-0.2	0.0
Declared duplicate reaction...			
856. NNH+O=N2O+H	1.00E+14	0.0	0.0
857. NH2+NO=H2+N2O	1.00E+13	0.0	33700.0
858. NO+NO=N2O+O	3.61E+12	0.0	65335.0
Declared duplicate reaction...			
859. N2O+O=NO+NO	6.62E+13	0.0	26611.0
Declared duplicate reaction...			
860. N2O+O=O2+N2	1.02E+14	0.0	28001.0
861. N2O+OH=HNO+NO	1.20E-04	4.3	25080.0
862. N2O+OH=N2+HO2	1.00E+14	0.0	30000.0
863. NNH+O2=N2O+OH	2.90E+11	-0.3	149.0
864. HNO+HNO=N2O+H2O	9.00E+08	0.0	3100.0
865. NH+N2O=N2+HNO	2.00E+12	0.0	6000.0
866. N2H2+NO=N2O+NH2	3.00E+10	0.0	0.0
867. HNNO+M=H+N2O+M	2.20E+15	0.0	21600.0
868. HNNO+M=N2+OH+M	1.00E+15	0.0	25600.0
869. HNNO+H=H2+N2O	2.00E+13	0.0	0.0

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870. NH2+NO=HNNO+H                                    8.00E+13    0.0    28000.0
871. NNH+HO2=HNNO+OH                                  2.40E+13    0.0     1698.0
872. HNNO+NO=N2O+HNO                                  1.00E+12    0.0        0.0
873. NH2+NO=NH2NO                                     3.50E+31   -6.8     3724.0
874. NH2NO=N2+H2O                                     3.10E+34   -7.1    36262.0
875. NH2NO+H=HNNO+H2                                  4.80E+08    1.5     7407.0
876. N2H3+O=NH2NO+H                                   3.00E+13    0.0        0.0
877. H2NN+OH=NH2NO+H                                  2.00E+12    0.0        0.0
878. NH2NO+O=HNNO+OH                                  3.30E+08    1.5     4697.0
879. NH2NO+OH=HNNO+H2O                                2.40E+06    2.0      -70.0
880. H2NN+HO2=NH2NO+OH                                6.60E+05    1.9     7050.0
881. NH2NO+HO2=HNNO+H2O2                              2.90E+04    2.7    12620.0
882. NH2NO+NH2=HNNO+NH3                               1.80E+06    1.9     4538.0
883. NH2NHO=NH2+HNO                                   2.40E+40   -8.7    41584.0
884. NH2NHO+H=NHNHO+H2                                4.80E+08    1.5     -894.0
885. NH2NHO+O=NHNHO+OH                                3.30E+08    1.5     -894.0
886. NH2NHO+OH=NHNHO+H2O                              2.40E+06    2.0    -1192.0
887. N2H3+HO2=NH2NHO+OH                               3.00E+13    0.0        0.0
888. NH2NHO+HO2=NHNHO+H2O2                            2.90E+04    2.7    -1599.0
889. NH2NHO+NH2=NHNHO+NH3                             1.80E+06    1.9    -1152.0
890. NO2(+M)=NO+O(+M)                                 7.60E+18   -1.3    73245.0
     Low pressure limit:  0.24700E+29 -0.33700E+01  0.74756E+05
     TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.49816E+04
     N2O             Enhanced by    1.500E+00
     H2O             Enhanced by    4.400E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    2.300E+00
     Declared duplicate reaction...
891. NO+O(+M)=NO2(+M)                                 1.30E+15   -0.8        0.0
     Low pressure limit:  0.47100E+25 -0.28700E+01  0.15510E+04
     TROE centering:      0.10000E+00  0.29510E+03  0.97270E+03  0.46816E+04
     Declared duplicate reaction...
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892. NO2+H=NO+OH                                    1.30E+14    0.0      357.0
893. NH+O2=H+NO2                                    2.30E+10    0.0     2482.0
894. NO2+O=O2+NO                                    3.91E+12    0.0     -238.0
895. NO2+OH=HO2+NO                                  1.81E+13    0.0     6673.0
896. HON+O2=NO2+OH                                  1.00E+12    0.0     4968.0
897. NO2+N=N2O+O                                    3.49E+12    0.0     -437.0
898. NH+NO2=N2O+OH                                  4.10E+12    0.0        0.0
899. NH+NO2=HNO+NO                                  5.90E+12    0.0        0.0
900. NH2+NO2=N2O+H2O                                3.00E+14   -0.8      242.0
901. NH2+NO2=NH2O+NO                                1.30E+15   -0.8      242.0
902. H2NN+O2=NH2+NO2                                1.50E+12    0.0     5958.0
903. HNNO+NO=NNH+NO2                                3.20E+12    0.0      270.0
904. N2O+NO=NO2+N2                                  5.30E+05    2.2    46280.0
905. NO+NO+NO=N2O+NO2                               1.07E+10    0.0    26800.0
906. HNO+NO+NO=HNNO+NO2                             1.70E+11    0.0     2100.0
907. NO2+NO2=NO+NO+O2                               1.63E+12    0.0    26108.0
908. HONO(+M)=OH+NO(+M)                             1.20E+19   -1.2    49667.0
     Low pressure limit:  0.30100E+31 -0.38000E+01  0.50322E+05
     TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
     Declared duplicate reaction...
909. NO+OH(+M)=HONO(+M)                             1.99E+12   -0.1     -721.0
     Low pressure limit:  0.50800E+24 -0.25100E+01 -0.68000E+02
     TROE centering:      0.37000E+00  0.11980E+02  0.10000E+06
     Declared duplicate reaction...
910. NO2+H2=HONO+H                                  1.30E+04    2.8    29770.0
911. HONO+H=H2O+NO                                  8.10E+06    1.9     3843.0
912. HONO+H=OH+HNO                                  5.60E+10    0.9     4965.0
913. HON+OH=HONO+H                                  4.00E+13    0.0        0.0
914. HONO+O=OH+NO2                                  1.20E+13    0.0     5958.0
915. HON+O2=HONO+O                                  1.00E+12    0.0     4965.0
916. HONO+OH=H2O+NO2                                1.26E+10    1.0      135.0
917. NO2+HO2=HONO+O2                                6.30E+08    1.2     5000.0
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918. NH+HONO=NH2+NO2                                  1.00E+13    0.0        0.0
919. NH2+HONO=NH3+NO2                                 7.10E+01    3.0    -4940.0
920. HNNO+NO=N2+HONO                                  2.60E+11    0.0      810.0
921. HNO+NO2=HONO+NO                                  4.40E+04    2.6     4040.0
922. NH2O+NO2=HONO+HNO                                6.00E+11    0.0     2000.0
923. HNOH+NO2=HONO+HNO                                6.00E+11    0.0     2000.0
924. HNNO+NO2=N2O+HONO                                1.00E+12    0.0        0.0
925. HONO+HONO=NO+NO2+H2O                             3.50E-01    3.6    12140.0
926. HNO2(+M)=HONO(+M)                                2.50E+14    0.0    32300.0
     Low pressure limit:  0.31000E+19  0.00000E+00  0.31500E+05
     TROE centering:      0.11490E+01  0.10000E-29  0.31250E+04  0.10000E+31
927. NO2+H2=HNO2+H                                    2.40E+00    3.7    32400.0
928. HNO2+O=OH+NO2                                    1.70E+08    1.5     2363.0
929. HNO2+OH=H2O+NO2                                  1.20E+06    2.0     -794.0
930. NO2+HO2=HNO2+O2                                  1.90E+01    3.3     4983.0
931. HNO2+NH2=NO2+NH3                                 9.20E+05    1.9      874.0
932. HNO+NO2=HNO2+NO                                  6.02E+11    0.0     1986.0
933. NH+O2=HNOO                                       3.70E+24   -5.0     2294.0
934. NH+O2+M=HNOO+M                                   3.00E+26   -4.0     2274.0
935. HNOO+M=OH+NO+M                                   1.50E+36   -6.2    31119.0
936. HNOH+HO2=HONHO+OH                                4.00E+13    0.0        0.0
937. NH2+NO2=NH2NO2                                   3.50E+31   -6.8     3726.0
938. NO2+O(+M)=NO3(+M)                                1.32E+13    0.0        0.0
     Low pressure limit:  0.14900E+29 -0.40800E+01  0.24660E+04
     TROE centering:      0.32600E+00  0.50000E+03  0.62049E+04  0.26060E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     HNO3            Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
     NO3             Enhanced by    5.000E+00
939. NO3+H=NO2+OH                                     6.00E+13    0.0        0.0
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940. NO3+O=NO2+O2 1.00E+13 0.0 0.0

941. NO3+OH=NO2+HO2 1.40E+13 0.0 0.0

942. NO3+HO2=NO2+O2+OH 1.50E+12 0.0 0.0

943. NO3+NH=HNO+NO2 1.50E+13 0.0 0.0

944. NO3+NH2=NH2O+NO2 9.00E+05 0.0 100.0

945. HNNO+NO2=NNH+NO3 1.00E+13 0.0 0.0

946. NO2+NO2=NO3+NO 9.60E+09 0.7 20900.0

947. NO3+NO2=NO+NO2+O2 5.00E+10 0.0 2940.0

948. NO3+NO3=NO2+NO2+O2 5.12E+11 0.0 4870.0

949. NO2+OH(+M)=HNO3(+M) 2.41E+13 0.0 0.0

Low pressure limit: 0.64200E+33 -0.54900E+01 0.23490E+04

TROE centering: 0.40000E+00 0.45070E+03 0.15840E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

N2 Enhanced by 1.000E+00

HNO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

950. HNO3+H=NO3+H2 5.60E+08 1.5 16400.0

951. HNO3+H=H2O+NO2 6.10E+01 3.3 6285.0

952. HNO3+H=OH+HONO 3.80E+05 2.3 6976.0

953. HNO3+H=HNO2+OH 6.00E+13 0.0 7000.0

954. HNO3+O=OH+NO3 1.80E+07 0.0 0.0

955. HNO3+OH=H2O+NO3 9.00E+10 0.0 0.0

956. HNO3+OH(+M)=H2O+NO3(+M) 2.47E+08 0.0 -2860.0

Low pressure limit: 0.68900E+15 0.00000E+00 -0.14400E+04

N2O Enhanced by 5.000E+00

H2O Enhanced by 9.000E+00

HNO3 Enhanced by 5.000E+00

NO3 Enhanced by 5.000E+00

NH3 Enhanced by 5.000E+00

957. NO3+H2O2=HNO3+HO2 1.00E+12 0.0 8500.0

958.	NO3+NH=HNO3+N	1.00E+12	0.0	5000.0
959.	NO3+NH2=HNO3+NH	1.00E+12	0.0	10000.0
960.	HNO3+NH=HNOH+NO2	1.50E+13	0.0	6000.0
961.	HNO3+NH2=NO3+NH3	9.00E+05	2.0	7300.0
962.	HNO3+NH2=NH2O+HNO2	3.00E+12	0.0	9000.0
963.	HNO3+NH3=NH2O+H2O+NO	2.32E+01	3.5	44930.0
964.	NH3+HNO3=H2O+NH2NO2	8.00E-01	3.5	43100.0
965.	HONO+NO2=HNO3+NO	2.00E+11	0.0	32700.0
966.	HONO+NO3=HNO3+NO2	1.00E+12	0.0	6000.0
967.	HNO2+NO3=HNO3+NO2	1.00E+12	0.0	5000.0
968.	N2O4(+M)=NO2+NO2(+M)	4.05E+18	-1.1	12840.0
	Low pressure limit: 0.19600E+29 -0.38000E+01 0.12840E+05			
969.	N2O4+H2O=HONO+HNO3	2.52E+14	0.0	11586.0
970.	NH+CH3=CH4+N	8.20E+05	1.9	5848.0
971.	C2H5+N=C2H4+NH	4.30E+13	0.0	0.0
972.	CH3+NH2=CH4+NH	2.80E+06	1.9	9205.0
973.	CH3+NH2=CH2+NH3	1.60E+06	1.9	7566.0
974.	CH2SING+NH3=CH3+NH2	1.00E+14	0.0	0.0
975.	CH4+NH2=CH3+NH3	1.50E+03	3.0	9940.0
976.	C2H+NH3=C2H2+NH2	7.20E+12	0.0	-735.0
977.	C2H4+NH2=C2H3+NH3	5.30E+12	0.0	10274.0
978.	C2H6+NH2=C2H5+NH3	4.50E+01	3.5	5600.0
979.	NNH+CH3<=>CH4+N2	2.50E+13	0.0	0.0
980.	N2H2+CH3=NNH+CH4	1.60E+06	1.9	2969.0
981.	H2NN+CH3=CH4+NNH	1.60E+06	1.9	129.0
982.	N2H3+CH3=N2H2+CH4	8.20E+05	1.9	1817.0
983.	N2H3+CH3=H2NN+CH4	3.00E+13	0.0	0.0
984.	N2H4+CH3=N2H3+CH4	3.30E+06	1.9	5322.0
985.	CH2SING+NO=CH2+NO	1.00E+14	0.0	0.0
986.	C+NO<=>CO+N	2.90E+13	0.0	0.0
987.	CH+NO=HCO+N	6.80E+12	0.0	0.0
988.	CH+NO=CO+NH	9.10E+12	0.0	0.0

989.	CH2+NO=NH2+CO	2.30E+16	-1.4	1331.0
990.	C2+NO=C2O+N	2.30E+13	0.0	8640.0
991.	N+CO2<=>NO+CO	3.00E+12	0.0	11300.0
992.	NH+CO2<=>HNO+CO	1.00E+13	0.0	14350.0
993.	HNO+CH3=NO+CH4	8.20E+05	1.9	480.0
994.	C2H3+NO=C2H2+HNO	1.00E+12	0.0	1000.0
995.	HCO+NO=HNO+CO	7.23E+12	0.0	0.0
996.	HCO+HNO=CH2O+NO	6.00E+11	0.0	2000.0
997.	CH3O+NO=HNO+CH2O	7.50E+12	0.0	2017.0
	Declared duplicate reaction...			
998.	CH3O+NO=HNO+CH2O	2.50E+18	-2.6	0.0
	Declared duplicate reaction...			
999.	CH2OH+NO=CH2O+HNO	1.30E+12	0.0	0.0
1000.	CH3O+HNO=NO+CH3OH	3.20E+13	0.0	0.0
1001.	CH2OH+HNO=NO+CH3OH	3.00E+13	0.0	0.0
1002.	CH2CHO+NO=HNO+CH2CO	1.00E+12	0.0	8600.0
1003.	NH2O+CH3=CH3O+NH2	2.00E+13	0.0	0.0
1004.	NH2O+CH3=CH4+HNO	1.60E+06	1.9	2959.0
1005.	HNOH+CH3=CH4+HNO	1.60E+06	1.9	2095.0
1006.	NH2OH+CH3=HNOH+CH4	1.60E+06	1.9	6345.0
1007.	NH2OH+CH3=NH2O+CH4	8.20E+05	1.9	5491.0
1008.	CH+NO2=HCO+NO	1.01E+14	0.0	0.0
1009.	CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
1010.	NO2+CH3=NO+CH3O	1.40E+13	0.0	0.0
1011.	C2H3+NO2=NO+CH2CHO	7.70E+14	-0.6	0.0
1012.	C2H5+NO2=NO+C2H5O	4.00E+13	-0.2	0.0
1013.	CO+NO2=NO+CO2	9.04E+13	0.0	33780.0
1014.	HCO+NO2=CO+NO+OH	1.20E+23	-3.3	2355.0
1015.	HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
1016.	CH3CO+NO2=>CH3+CO2+NO	1.50E+13	0.0	0.0
1017.	CH4+NO2=HONO+CH3	6.50E+14	0.0	45800.0
1018.	C2H4+NO2=HONO+C2H3	6.50E+14	0.0	41400.0

1019.	C2H6+NO2=HONO+C2H5		6.50E+14	0.0	41400.0
1020.	HOCO+NO=CO+HONO		1.50E+12	0.0	0.0
1021.	HCO+NO2=CO+HONO		1.24E+23	-3.3	2355.0
1022.	CH2O+NO2=HCO+HONO		8.02E+02	2.8	13730.0
1023.	CH3O+NO2=CH2O+HONO		6.00E+12	0.0	2285.0
1024.	CH2OH+NO2=HONO+CH2O		5.00E+12	0.0	0.0
1025.	CH3OH+NO2=HONO+CH2OH		1.50E+02	3.3	20035.0
1026.	CH2CHO+NO2=CH2CO+HONO		8.90E+12	0.0	-159.0
1027.	CH3CHO+NO2=HONO+CH2CHO		1.30E+12	0.0	3700.0
1028.	CH4+NO2=HNO2+CH3		6.00E+14	0.0	37600.0
1029.	C2H4+NO2=HNO2+C2H3		6.00E+14	0.0	33200.0
1030.	C2H6+NO2=HNO2+C2H5		6.00E+14	0.0	33200.0
1031.	CH2O+NO2=HNO2+HCO		1.10E-01	4.2	19850.0
1032.	CH3OH+NO2=HNO2+CH2OH		2.40E+03	2.9	27470.0
1033.	CH2SING+N2O=CH2O+N2		3.80E+13	0.0	0.0
1034.	CO+N2O=N2+CO2		2.70E+11	0.0	20237.0
1035.	NH2NO+CH3=HNNO+CH4		1.60E+06	1.9	7179.0
1036.	NH2NHO+CH3=NHNHO+CH4		1.60E+06	1.9	377.0
1037.	CN+M=C+N+M		2.50E+14	0.0	141100.0
	N2	Enhanced by 1.500E+00			
	CO2	Enhanced by 2.400E+00			
1038.	CH+N=CN+H		1.70E+14	-0.1	0.0
1039.	CN+O=CO+N		1.90E+12	0.5	723.0
1040.	NO+C=CN+O		1.10E+13	0.0	0.0
1041.	CH+NO=OH+CN		3.30E+12	0.0	0.0
1042.	CN+O2=NO+CO		2.80E+17	-2.0	0.0
1043.	CN+N=C+N2		1.80E+14	0.0	0.0
1044.	CN+NO=N2+CO		3.90E+11	0.0	27820.0
1045.	C+N2O=CN+NO		4.80E+12	0.0	0.0
1046.	CN+NO2=CO+N2O		4.90E+14	-0.8	344.0
1047.	CN+NO2=N2+CO2		3.70E+14	-0.8	344.0
1048.	C2+N2=CN+CN		1.50E+13	0.0	41730.0

1049. HCN(+M)=H+CN(+M) 8.30E+17 -0.9 123800.0

Low pressure limit: 0.35700E+27 -0.26000E+01 0.12490E+06

TROE centering: 0.73420E+00 0.11201E+04 0.10000E+06

N2O Enhanced by 5.000E+00

H2O Enhanced by 5.000E+00

N2 Enhanced by 1.000E+00

CO2 Enhanced by 1.600E+00

H2 Enhanced by 2.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

1050. CH2+N=HCN+H 5.00E+13 0.0 0.0

1051. CN+H2=HCN+H 3.60E+08 1.6 2999.0

1052. CH+NH=HCN+H 3.00E+13 0.0 0.0

1053. CH3+N=HCN+H2 3.70E+12 0.1 -89.0

1054. C2H3+N=HCN+CH2 2.00E+13 0.0 0.0

1055. CH4+CN=CH3+HCN 8.60E+05 2.3 -32.0

1056. C3H3+N=HCN+C2H2 1.00E+13 0.0 0.0

1057. C2H6+CN=C2H5+HCN 1.20E+08 1.8 -994.0

1058. CH+N2=HCN+N 4.40E+12 0.0 21964.0

1059. CH2+N2=HCN+NH 1.00E+13 0.0 73954.0

1060. CH2SING+N2<=>NH+HCN 1.00E+11 0.0 65000.0

1061. CN+NH3=HCN+NH2 9.20E+12 0.0 -357.0

1062. HCN+N2=H+CN+N2 3.60E+26 -2.6 124890.0

1063. HCN+O=NH+CO 3.50E+03 2.6 4980.0

1064. HCN+O=CN+OH 4.20E+10 0.4 20663.0

1065. HCN+OH=CN+H2O 3.90E+06 1.8 10287.0

1066. OH+HCN=NH2+CO 7.83E-04 4.0 4000.0

1067. HCN+O2=CN+HO2 3.00E+13 0.0 75100.0

1068. HCCO+N=HCN+CO 5.00E+13 0.0 0.0

1069. CH2O+CN=HCO+HCN 1.70E+03 2.7 -1427.0

1070. CH+NO=HCN+O	5.30E+13	0.0	0.0
1071. CH2+NO=HCN+OH	2.90E+14	-0.7	755.0
1072. CH2SING+NO<=>OH+HCN	2.90E+14	-0.7	760.0
1073. CH3+NO=HCN+H2O	4.90E+08	0.5	12392.0
1074. C2H+NO=HCN+CO	6.00E+13	0.0	570.0
1075. C2H3+NO=HCN+CH2O	7.00E+21	-3.4	1025.0
1076. HCCO+NO=HCN+CO2	3.70E+14	-0.8	-90.0
1077. CN+HNO=HCN+NO	1.80E+13	0.0	0.0
1078. CN+HONO=HCN+NO2	1.20E+13	0.0	0.0
1079. CH+N2O=HCN+NO	1.90E+13	0.0	-511.0
1080. HCN=HNC	1.50E+23	-4.2	49428.0
1081. HCN+M=HNC+M	1.60E+26	-3.2	54600.0

AR Enhanced by 7.000E-01

H2O Enhanced by 7.000E+00

CO2 Enhanced by 2.000E+00

Warning...superceding enhancement factor for AR

AR Enhanced by 7.000E-01

Warning...superceding enhancement factor for H2O

H2O Enhanced by 7.000E+00

Warning...superceding enhancement factor for CO2

CO2 Enhanced by 2.000E+00

Warning...superceding enhancement factor for AR

AR Enhanced by 7.000E-01

Warning...superceding enhancement factor for H2O

H2O Enhanced by 7.000E+00

Warning...superceding enhancement factor for CO2

CO2 Enhanced by 2.000E+00

1082. HNC+H=HCN+H	7.80E+13	0.0	3600.0
1083. O+HNC=NH+CO	4.60E+12	0.0	2184.0
1084. HNC+OH=CN+H2O	1.50E+12	0.0	7680.0
1085. HNC+O2=NH+CO2	1.60E+19	-2.2	1777.0
1086. H+HCN(+M)<=>NCH2(+M)	3.30E+13	0.0	0.0

Low pressure limit: 0.14000E+27 -0.34000E+01 0.19000E+04

H2 Enhanced by 2.000E+00

H2O Enhanced by 6.000E+00

CH4 Enhanced by 2.000E+00

CO Enhanced by 1.500E+00

CO2 Enhanced by 2.000E+00

C2H6 Enhanced by 3.000E+00

AR Enhanced by 7.000E-01

N2O Enhanced by 5.000E+00

N2 Enhanced by 1.000E+00

1087.	CH+NH3=NCH2+H+H	4.40E+13	0.0	-630.0
1088.	NCH2+H=HCN+H2	2.40E+08	1.5	-894.0
1089.	CH3+N=NCH2+H	6.10E+14	-0.3	288.0
1090.	CH+NH2=NCH2+H	3.00E+13	0.0	0.0
1091.	CH3+NH=NCH2+H2	3.50E+13	0.0	290.0
1092.	NCH2+CH3=HCN+CH4	8.10E+05	1.9	-1112.0
1093.	C2H5+N=CH3+NCH2	2.30E+13	0.0	0.0
1094.	NCH2+N=HCN+NH	7.20E+13	0.0	400.0
1095.	NCH2+N=N2+CH2	6.00E+13	0.0	397.0
1096.	NCH2+NH=HCN+NH2	1.70E+08	1.5	-894.0
1097.	NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0
1098.	CH2+NO=NCH2+O	8.10E+07	1.4	4111.0
1099.	NCH2+O=HCN+OH	1.70E+08	1.5	-894.0
1100.	CH3+NO=NCH2+OH	1.50E-01	3.5	3950.0
1101.	NCH2+OH=HCN+H2O	1.50E+19	-2.2	2166.0
	Declared duplicate reaction...			
1102.	NCH2+OH=HCN+H2O	1.20E+06	2.0	-1192.0
	Declared duplicate reaction...			
1103.	NCH2+O2=CH2O+NO	3.00E+12	0.0	5958.0
1104.	NCH2+O2=HCN+HO2	2.70E+04	2.0	17300.0
1105.	NCH2+HO2=HCN+H2O2	1.40E+04	2.7	-1609.0
1106.	NCH2+NO=HCN+HNO	1.00E+07	2.0	4400.0

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1107. CHNH=HCN+H                                        6.10E+28   -5.7    24257.0
1108. CH3+N=CHNH+H                                      1.20E+11    0.5     -367.0
1109. CHNH+H=NCH2+H                                     2.00E+13    0.0        0.0
1110. CHNH+H=HCN+H2                                     2.40E+08    1.5     -894.0
1111. CHNH+O=HCN+OH                                     1.70E+08    1.5     -894.0
1112. CHNH+OH=HCN+H2O                                   1.20E+06    2.0    -1192.0
1113. CHNH+CH3=HCN+CH4                                  8.20E+05    1.9    -1112.0
1114. CH2NH+M=HCN+H2+M                                  1.00E+14    0.0    10000.0
1115. NH+CH3=CH2NH+H                                    4.00E+13    0.0        0.0
1116. CH2NH+H=NCH2+H2                                   2.40E+08    1.5     7318.0
1117. CH2NH+H=CHNH+H2                                   3.00E+08    1.5     6126.0
1118. CH+NH3=CH2NH+H                                    4.40E+13    0.0     -630.0
1119. CH2SING+NH2=CH2NH+H                               3.00E+13    0.0        0.0
1120. CH2SING+NH3=CH2NH+H+H                             1.00E+14    0.0        0.0
1121. CH3+NH2<=>CH2NH+H2                                2.40E+06    1.2    17369.0
1122. CH2NH+O=NCH2+OH                                   1.70E+08    1.5     4627.0
1123. CH2NH+O=CHNH+OH                                   2.20E+08    1.5     5402.0
1124. CH2NH+O=CH2O+NH                                   1.70E+06    2.1        0.0
1125. CH2NH+OH=NCH2+H2O                                 1.20E+06    2.0      -89.0
1126. CH2NH+OH=CHNH+H2O                                 2.40E+06    2.0      457.0
1127. CH2NH+OH=CH2O+NH2                                 1.80E+05    2.0    14800.0
1128. NCH2+HO2=CH2NH+O2                                 1.40E+04    2.7    -1609.0
1129. CH2NH+CH3=NCH2+CH4                                8.20E+05    1.9     7119.0
1130. CH2NH+CH3=CHNH+CH4                                5.30E+05    1.9     9681.0
1131. CH2NH+NH2=NCH2+NH3                                9.20E+05    1.9     4438.0
1132. CH2NH+NH2=CHNH+NH3                                1.80E+06    1.9     6087.0
1133. CH3N(+AR)<=>CH2NH(+AR)                            1.83E+13    0.2    43980.0
      Low pressure limit:  0.22300E+29 -0.44500E+01  0.46000E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
1134. CH3N(+AR)<=>NCH2+H(+AR)                           7.40E+11    0.9    35470.0
      Low pressure limit:  0.18700E+31 -0.45200E+01  0.37950E+05
      TROE centering:      0.74900E+00  0.21800E+03  0.10000E+02  0.26000E+09
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1135. CH3NH=CH2NH+H                                   1.30E+42   -9.2    41316.0
      Declared duplicate reaction...
1136. CH3NH(+AR)<=>CH2NH+H(+AR)                       7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      Declared duplicate reaction...
1137. CH3NH+M=CH3+NH+M                                1.00E+14    0.0    18000.0
1138. CH3+NH2<=>CH3NH+H                               9.08E+13   -0.4    15714.0
1139. CH3NH+H=CH2NH+H2                                7.20E+08    1.5     -894.0
1140. CH3NH+O=CH2NH+OH                                5.00E+08    1.5     -894.0
1141. CH3NH+O=CH3O+NH                                 6.00E+13    0.0        0.0
1142. CH3NH+OH=CH2NH+H2O                              3.60E+06    2.0    -1192.0
1143. CH3NH+OH=CH4+HNO                                6.00E+12    0.0        0.0
1144. HNOH+CH3=CH3NH+OH                               2.00E+13    0.0        0.0
1145. CH3NH+O2=CH2NH+HO2                              1.00E+07    2.0     6300.0
1146. CH3NH+O2=CH3O+HNO                               6.00E+12    0.0     4000.0
1147. CH3NH+CH3=CH2NH+CH4                             2.40E+06    1.9    -1112.0
1148. CH2NH2=CH2NH+H                                  2.40E+48  -10.8    52010.0
      Declared duplicate reaction...
1149. CH2NH2(+AR)<=>CH2NH+H(+AR)                      7.91E+11    0.3    36260.0
      Low pressure limit:  0.16400E+40 -0.70200E+01  0.40100E+05
      TROE centering:      0.10000E+01  0.91100E+06  0.10000E+02  0.26000E+09
      Declared duplicate reaction...
1150. CH3+NH2<=>CH2NH2+H                              5.15E+14   -0.6    10155.0
1151. CH2NH2+H=CH2NH+H2                               4.80E+08    1.5     -894.0
1152. CH2NH2+O=CH2O+NH2                               7.00E+13    0.0        0.0
1153. CH2NH2+O=CH2NH+OH                               3.30E+08    1.5     -894.0
1154. CH2NH2+OH=CH2OH+NH2                             4.00E+13    0.0        0.0
1155. CH2NH2+OH=CH2NH+H2O                             2.40E+06    2.0    -1192.0
1156. CH2NH2+O2=CH2NH+HO2                             1.00E+22   -3.1     6752.0
1157. CH2NH2+O2=NH2+CH2O+O                            6.00E+18   -1.6    30175.0
1158. CH2NH2+CH3=C2H5+NH2                             2.00E+13    0.0     2701.0
1159. CH2NH2+CH3=CH2NH+CH4                            1.60E+06    1.9     -626.0
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1160. CH3+NH2<=>CH3NH2                                1.03E+33   -6.3     5750.0
1161. CH3+NH2(+M)=CH3NH2(+M)                          7.20E+12    0.4        0.0
      Low pressure limit:  0.22000E+31 -0.38500E+01  0.00000E+00
1162. CH3NH2(+AR)<=>CH2NH+H2(+AR)                     9.99E+08    1.2   102880.0
      Low pressure limit:  0.24600E+31 -0.47500E+01  0.10700E+06
      TROE centering:      0.82000E+00  0.15459E+03  0.10000E+01  0.40100E+06
1163. CH3NH2+M=CH2NH+H2+M                             2.40E+13    0.0   107260.0
1164. CH3NH2(+AR)<=>CH2NH2+H(+AR)                     3.93E+15   -0.1    93820.0
      Low pressure limit:  0.68200E+41 -0.70100E+01  0.98400E+05
      TROE centering:      0.00000E+00  0.23101E+03  0.10000E+01  0.40100E+06
1165. CH3NH2(+AR)<=>CH3NH+H(+AR)                      1.44E+16   -0.3   100940.0
      Low pressure limit:  0.11400E+39 -0.63500E+01  0.10500E+06
      TROE centering:      0.67000E+00  0.16967E+03  0.10000E+01  0.40100E+06
1166. CH3NH2+H=CH2NH2+H2                              5.60E+08    1.5     5461.0
1167. CH3NH2+H=CH3NH+H2                               4.80E+08    1.5     9701.0
1168. CH3NH2+O=CH2NH2+OH                              4.00E+08    1.5     5193.0
1169. CH3NH2+O=CH3NH+OH                               3.30E+08    1.5     6345.0
1170. CH3NH2+OH=CH2NH2+H2O                            3.60E+06    2.0      238.0
1171. CH3NH2+OH=CH3NH+H2O                             2.40E+06    2.0      447.0
1172. CH3NH2+CH3=CH2NH2+CH4                           1.50E+06    1.9     9163.0
1173. CH3NH2+CH3=CH3NH+CH4                            1.60E+06    1.9     8837.0
1174. CH3NH2+NH2=CH2NH2+NH3                           2.80E+06    1.9     5491.0
1175. CH3NH2+NH2=CH3NH+NH3                            1.80E+06    1.9     7139.0
1176. CH3NCH=CH3+HCN                                  8.10E+15   -2.4    14942.0
1177. CH3NCH+H=CH2NCH2+H                              2.00E+13    0.0        0.0
1178. CH2NCH2=CH3NCH                                  1.30E+45  -10.1    66111.0
1179. CH2NCH2+H=CH3+NCH2                              3.00E+13    0.0        0.0
1180. CH2NCH2+O=CH2O+NCH2                             3.00E+13    0.0        0.0
1181. CH2NCH2+OH=CH2OH+NCH2                           2.00E+13    0.0        0.0
1182. CH2NCH2+H=CH3NCH2                               5.80E+13    0.2     -125.0
1183. CH3NCH2+H=CH2NCH2+H2                            5.60E+08    1.5     5464.0
1184. CH3NCH2+H=CH3NCH+H2                             3.00E+08    1.5     6130.0
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1185. CH3NCH2+O=CH2NCH2+OH 4.00E+08 1.5 5196.0

1186. CH3NCH2+O=CH3NCH+OH 2.20E+08 1.5 5404.0

1187. CH3NCH2+OH=CH2NCH2+H2O 8.00E+12 0.0 0.0

1188. CH3NCH2+OH=CH3NCH+H2O 2.40E+06 2.0 457.0

1189. CH3NCH2+CH3=CH2NCH2+CH4 1.50E+06 1.9 9170.0

1190. CH3NCH2+CH3=CH3NCH+CH4 5.30E+05 1.9 9687.0

1191. CH3NCH2+NH2=CH2NCH2+NH3 2.80E+06 1.9 5494.0

1192. CH3NCH2+NH2=CH3NCH+NH3 1.80E+06 1.9 6090.0

1193. CH3NCH3=CH3NCH2+H 1.60E+15 -7.5 38425.0

1194. CH3NCH3+H=CH3NCH2+H2 3.20E+12 0.0 0.0

1195. CH3NCH3+OH=CH3NCH2+H2O 2.40E+13 0.0 0.0

1196. CH3NCH3+CH3=CH3NCH2+CH4 6.00E+12 0.0 0.0

1197. CH3NHCH2=CH3+CH2NH 9.80E+43 -10.3 37459.0

1198. CH3NHCH2=CH3NCH2+H 5.90E+44 -10.3 46803.0

1199. CH3NHCH2+H=CH3NCH2+H2 4.80E+08 1.5 -894.0

1200. CH3NHCH2+O=CH2O+CH3NH 7.00E+13 0.0 0.0

1201. CH3NHCH2+O=CH3NCH2+OH 3.30E+08 1.5 -894.0

1202. CH3NHCH2+OH=CH2OH+CH3NH 4.00E+13 0.0 0.0

1203. CH3NHCH2+OH=CH3NCH2+H2O 2.40E+06 2.0 -1192.0

1204. CH3NHCH2+CH3=C2H5+CH3NH 2.00E+13 0.0 2702.0

1205. CH3NHCH2+CH3=CH3NCH2+CH4 1.60E+06 1.9 -626.0

1206. CH3NHCH2+H(+M)=CH3NHCH3(+M) 5.20E+17 -1.0 1580.0

Low pressure limit: 0.19900E+42 -0.70800E+01 0.66850E+04

TROE centering: 0.84220E+00 0.12500E+03 0.22190E+04 0.68820E+04

1207. CH3NCH3+H=CH3NHCH3 1.00E+12 0.0 0.0

1208. CH3NHCH3+H=CH3NHCH2+H2 5.60E+08 1.5 5464.0

1209. CH3NHCH3+H=CH3NCH3+H2 4.80E+08 1.5 9706.0

1210. CH3NHCH3+O=CH3NHCH2+OH 6.10E+12 0.0 556.0

1211. CH3NHCH3+O=CH3NCH3+OH 3.00E+12 0.0 556.0

1212. CH3NHCH3+OH=CH3NHCH2+H2O 2.00E+13 0.0 0.0

1213. CH3NHCH3+OH=CH3NCH3+H2O 1.90E+13 0.0 0.0

1214. CH3NHCH3+CH3=CH3NHCH2+CH4 1.50E+06 1.9 9170.0

1215.	CH3NHCH3+CH3=CH3NCH3+CH4	1.60E+06	1.9	8842.0
1216.	CH3NHCH3+NH2=CH3NHCH2+NH3	2.80E+06	1.9	5494.0
1217.	CH3NHCH3+NH2=CH3NCH3+NH3	1.80E+06	1.9	7143.0
1218.	CHCNH+H=CH2+HNC	1.50E+14	0.0	0.0
1219.	CHCNH+O=H+CO+HNC	1.00E+14	0.0	0.0
1220.	CHCNH+OH=HCO+CHNH	1.00E+13	0.0	0.0
1221.	CHCNH+O2=HNC+CO+OH	1.60E+11	0.0	1020.0
1222.	CHCNH+O2=HNC+HCO+O	2.20E+02	2.7	3540.0
1223.	CH2SING+HCN=CH2CN+H	1.80E+14	0.0	0.0
1224.	CH3+CN=CH2CN+H	1.00E+14	0.0	0.0
1225.	CH2CN+O=CH2O+CN	1.00E+14	0.0	0.0
1226.	CH2OH+CN=CH2CN+OH	5.00E+13	0.0	0.0
1227.	CH3CN=CH2CN+H	7.90E+14	0.0	94940.0
1228.	CH3CN+H=HCN+CH3	4.40E+10	0.8	6800.0
1229.	CH3CN+H=HNC+CH3	2.80E+15	-0.3	20030.0
1230.	CH3CN+H=CH2CN+H2	6.00E+04	3.0	8522.0
1231.	CH3CN+O=CH2CN+OH	4.70E+08	1.2	14360.0
1232.	CH3CN+OH=CH2CN+H2O	2.00E+07	2.0	2000.0
1233.	CH3CN+CH3=CH2CN+CH4	5.00E+12	0.0	7000.0
1234.	CH3CN+CN=CH2CN+HCN	5.00E+13	0.0	2000.0
1235.	c-C2H3N=CH3CN	4.70E+13	0.0	41500.0
1236.	c-C2H3N+H=CH2NCH2	9.80E+09	1.2	1969.0
1237.	c-C2H3N+H=CH2CHNH	1.10E+10	1.2	2422.0
1238.	c-C2H3N+O=>NCH2+HCO	1.00E+13	0.0	0.0
1239.	c-C2H3N+O=>C2H3+NO	1.00E+13	0.0	0.0
1240.	c-C2H3N+OH=>NCH2+CH2O	5.00E+12	0.0	0.0
1241.	CH2CHN(S)+M=CH2CHN+M	1.00E+13	0.0	0.0
	H Enhanced by 0.000E+00			
1242.	CH2CHN(S)+H=CH2CHN+H	1.00E+14	0.0	0.0
1243.	CH2CHN(S)+H=CH3+HCN	3.00E+13	0.0	0.0
1244.	CH2CHN(S)=c-C2H3N	3.00E+13	0.0	4000.0
1245.	CH2CHN(S)=CH3CN	3.00E+13	0.0	8000.0

1246.	CH2CHN(S)+O=>HCO+HCN+H	3.00E+13	0.0	0.0
1247.	CH2CHN(S)+OH=>CH2O+HCN+H	3.00E+13	0.0	0.0
1248.	CH2CNH=CH3CN	2.50E+13	0.0	70300.0
1249.	CH2CNH+H=CH3CN+H	3.00E+13	0.0	0.0
1250.	CH2CNH+H=CH3+HNC	3.30E+10	0.9	2840.0
1251.	CH2CNH+H=CHCNH+H2	3.00E+07	2.0	10000.0
1252.	CH2CNH+H=CH2CN+H2	2.40E+08	1.5	7322.0
1253.	CH2CNH+O=CH2+HNCO	1.80E+12	0.0	1350.0
1254.	CH2CNH+O=CHCNH+OH	2.00E+07	2.0	10000.0
1255.	CH2CNH+O=CH2CN+OH	1.70E+08	1.5	4630.0
1256.	CH2CNH+OH=CH2OH+HNC	1.00E+12	0.0	-1013.0
1257.	CH2CNH+OH=CHCNH+H2O	1.00E+07	2.0	3000.0
1258.	CH2CNH+OH=CH2CN+H2O	1.20E+06	2.0	-89.0
1259.	CH2CNH+CH3=CH2CN+CH4	8.20E+05	1.9	7123.0
1260.	CH2CNH+NH2=CH2CN+NH3	9.20E+05	1.9	4441.0
1261.	CH2CHN+H=CH3+HCN	1.00E+13	0.0	0.0
1262.	CH2CHN+O=CH2O+HCN	5.00E+13	0.0	0.0
1263.	CHCNH2+H=CHCNH+H2	4.80E+08	1.5	9706.0
1264.	CHCNH2+O=CHCNH+OH	3.30E+08	1.5	6348.0
1265.	CHCNH2+O=HCCO+NH2	1.40E+07	2.0	1900.0
1266.	CHCNH2+OH=CHCNH+H2O	2.00E+12	0.0	0.0
1267.	CHCNH2+CH3=CHCNH+CH4	1.60E+06	1.9	8842.0
1268.	CHCNH2+NH2=CHCNH+NH3	1.80E+06	1.9	7143.0
1269.	CH3+HCN=CH3CHN	1.00E+12	0.0	9900.0
1270.	CH3CHN+H=CH3CN+H2	2.40E+08	1.5	-894.0
1271.	CH3CHN+H=CH2CHN+H2	9.00E+13	0.0	15100.0
1272.	CH2CHN(S)+H2=CH3CHN+H	7.20E+13	0.0	0.0
1273.	CH3CHN+O=CH3CN+OH	1.70E+08	1.5	-894.0
1274.	CH3CHN+OH=CH3CN+H2O	1.20E+06	2.0	-1192.0
1275.	CH3CHN+OH=CH2CHN+H2O	1.10E+03	3.0	2780.0
1276.	CH3CHN+OH=CH2CHN(S)+H2O	4.40E+13	-0.3	-727.0
1277.	CH3CHN+NH2=CH3CN+NH3	9.20E+05	1.9	-1152.0

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1278. CH3CNH=CH3+HNC                                  6.50E+18   -2.5    33000.0
1279. CH3CNH=CH3CN+H                                  7.70E+25   -5.2    24000.0
1280. CH3CNH+H=CH3+CHNH                               2.10E+13    0.0        0.0
1281. CH3CNH+H=CH2CNH+H2                              1.20E+13    0.0        0.0
1282. CH3CNH+H=CH3CN+H2                               2.40E+08    1.5     -894.0
1283. CH3CNH+O=CH2CNH+OH                              5.30E+13    0.0        0.0
1284. CH3CNH+O=CH3CN+OH                               1.70E+08    1.5     -894.0
1285. CH3CNH+OH=CH2CNH+H2O                            1.20E+13    0.0        0.0
1286. CH3CNH+OH=CH3CN+H2O                             1.20E+06    2.0    -1192.0
1287. CH3CNH+O2=CH2O+CO+NH2                           1.90E+12    0.0        0.0
1288. CH3CNH+CH3=CH2CNH+CH4                           5.30E+13    0.0        0.0
1289. CH3CNH+CH3=CH3CN+CH4                            8.20E+05    1.9    -1113.0
1290. CH2CHNH+H=CH3+CHNH                              1.00E+14    0.0        0.0
1291. CH2CHNH+H=CH3CNH+H                              3.00E+13    0.0        0.0
1292. CH2CHNH+H=CH2CNH+H2                             2.00E+13    0.0        0.0
1293. CH2CHNH+O=CH2CNH+OH                             2.00E+13    0.0        0.0
1294. CH2CHNH+OH=CH2CNH+H2O                           2.00E+13    0.0        0.0
1295. CH2CHNH+OH=CH2OH+CHNH                           1.00E+13    0.0        0.0
1296. CH2CHNH+O2=CH2O+CO+NH2                          5.70E+17   -1.8    11067.0
1297. CHCNH2+H(+M)=CH2CNH2(+M)                        1.70E+10    1.3     2709.0
      Low pressure limit:  0.63000E+32 -0.46640E+01  0.37800E+04
      TROE centering:      0.78780E+00 -0.10212E+05  0.10000E+31
      H2              Enhanced by    2.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
      H2O             Enhanced by    5.000E+00
1298. CH2CNH2+H=CHCNH2+H2                             4.50E+13    0.0        0.0
1299. CH2CNH2+O=CH2CO+NH2                             3.00E+13    0.0        0.0
1300. CH2CNH2+OH=CHCNH2+H2O                           2.00E+13    0.0        0.0
1301. CH2CNH2+O2=OCHCHO+NH2                           4.00E+12    0.0        0.0
1302. CH2CNH2+CH3=CHCNH2+CH4                          2.00E+13    0.0        0.0
1303. NH2+C2H2=CHCHNH2                                7.80E-18    8.3     7430.0
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1304. CHCNH2+H(+M)=CHCHNH2(+M)                          1.70E+10    1.3     2709.0
      Low pressure limit:  0.63000E+32 -0.46640E+01  0.37800E+04
      TROE centering:      0.78780E+00 -0.10212E+05  0.10000E+31
      H2              Enhanced by    2.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
      H2O             Enhanced by    5.000E+00
1305. CHCHNH2+H=CHCNH2+H2                              4.50E+13    0.0        0.0
1306. CHCHNH2+OH=CHCNH2+H2O                            2.00E+13    0.0        0.0
1307. CHCHNH2+O2=OCHCHO+NH2                            4.00E+12    0.0        0.0
1308. CHCHNH2+CH3=CHCNH2+CH4                           2.00E+13    0.0        0.0
1309. CH2CHNH+H=CH3CHNH                                5.80E+13    0.2     -125.0
1310. CH3+CHNH=CH3CHNH                                 1.80E+13    0.0        0.0
1311. CH3CHNH+H=CH3CNH+H2                              4.70E+13   -0.3     3000.0
1312. CH3CHNH+H=CH2CHNH+H2                             1.90E+12    0.4     5359.0
1313. CH3CHNH+H=CH3CHN+H2                              2.40E+08    1.5     7322.0
1314. CH3CHNH+O=CH3CNH+OH                              1.80E+18   -1.9     2975.0
1315. CH3CHNH+O=CH2CHNH+OH                             3.70E+13   -0.2     3556.0
1316. CH3CHNH+O=CH3CHN+OH                              1.70E+08    1.5     4630.0
1317. CH3CHNH+OH=CH3CNH+H2O                            2.40E+11    0.3    -1000.0
1318. CH3CHNH+OH=CH2CHNH+H2O                           3.00E+13   -0.6      800.0
1319. CH3CHNH+OH=CH3CHN+H2O                            1.20E+06    2.0      -89.0
1320. CH3CHNH+CH3=CH3CNH+CH4                           3.90E-07    5.8     2200.0
1321. CH3CHNH+CH3=CH2CHNH+CH4                          2.50E+01    3.1     5727.0
1322. CH3CHNH+CH3=CH3CHN+CH4                           8.20E+05    1.9     7123.0
1323. CH3CHNH+NH2=CH3CHN+NH3                           9.20E+05    1.9     4441.0
1324. CHCHNH2+H(+M)=CH2CHNH2(+M)                       3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
1325. CH2CNH2+H(+M)=CH2CHNH2(+M)                       3.90E+13    0.2        0.0
      Low pressure limit:  0.21000E+25 -0.13000E+01  0.00000E+00
      TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31  0.10000E+31
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1326. CH3CHNH=CH2CHNH2                                5.00E+18   -2.5    67995.0
1327. CH2CHNH2+H=CHCHNH2+H2                           2.40E+02    3.6    11266.0
1328. CH2CHNH2+H=CH2CNH2+H2                           2.40E+02    3.6    11266.0
1329. CH2CHNH2+H=CH2CHNH+H2                           4.80E+08    1.5     9700.0
1330. CH3CHNH+H=CH2CHNH2+H                            3.00E+13    0.0        0.0
1331. CH2CHNH2+O=CH2CHNH+OH                           3.30E+08    1.5     6348.0
1332. CH2CHNH2+OH=CHCHNH2+H2O                         1.30E-01    4.2     -860.0
1333. CH2CHNH2+OH=CH2CNH2+H2O                         1.30E-01    4.2     -860.0
1334. CH2CHNH2+OH=CH2CHNH+H2O                         2.40E+06    2.0      447.0
1335. CH2CHNH2+CH3=CHCHNH2+CH4                        6.00E+07    1.6    16630.0
1336. CH2CHNH2+CH3=CH2CNH2+CH4                        6.00E+07    1.6    16630.0
1337. CH2CHNH2+CH3=CH2CHNH+CH4                        1.60E+06    1.9     8842.0
1338. CH2CHNH2+NH2=CHCHNH2+NH3                        5.30E+12    0.0    10274.0
1339. CH2CHNH2+NH2=CH2CNH2+NH3                        5.30E+12    0.0    10274.0
1340. CH2CHNH2+NH2=CH2CHNH+NH3                        1.80E+06    1.9     7143.0
1341. CH3CH2NH=CH2NH+CH3                              1.90E+10    0.0    23500.0
1342. CH3CH2NH=CH3CHNH+H                              1.60E+36   -7.9    36342.0
1343. CH3CH2NH+H=CH3+CH2NH2                           1.40E+12    0.7      346.0
1344. CH3CH2NH+H=CH3CHNH+H2                           7.20E+08    1.5     -894.0
1345. CH3CH2NH+O=CH3CHNH+OH                           5.00E+08    1.5     -894.0
1346. CH3CH2NH+OH=CH3CHNH+H2O                         3.60E+06    2.0    -1192.0
1347. CH3CH2NH+CH3=CH3CHNH+CH4                        2.40E+06    1.9    -1113.0
1348. CH2CHNH2+H(+M)=CH3CHNH2(+M)                     1.40E+09    1.5     1355.0
      Low pressure limit:  0.20000E+40 -0.66420E+01  0.57690E+04
      TROE centering:     -0.56900E+00  0.29900E+03  0.91470E+04  0.15240E+03
1349. CH3CHNH2=CH3CHNH+H                              1.10E+45  -10.2    47817.0
1350. CH3CHNH2+H=CH2CHNH2+H2                          4.90E+08    1.7      588.0
1351. CH3CHNH2+H=CH3+CH2NH2                           8.40E+16   -0.9     2903.0
1352. CH3CHNH2+H=C2H4+NH3                             4.70E+21   -3.0     2845.0
1353. CH3CHNH2+H=C2H5+NH2                             2.00E+13    0.0        0.0
1354. CH3CHNH2+O=CH2CHNH2+OH                          2.50E+13    0.0        0.0
1355. CH3CHNH2+OH=CH2CHNH2+H2O                        2.40E+13    0.0        0.0
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1356.	CH3CHNH2+O2=CH2CHNH2+HO2	6.70E+20	-3.0	2504.0
1357.	CH3CHNH2+CH3=CH2CHNH2+CH4	1.80E+13	0.0	-769.0
1358.	C2H4+NH2=CH2CH2NH2	1.20E+11	0.0	3955.0
1359.	CH2CH2NH2+H=CH2CHNH2+H2	1.80E+12	0.0	0.0
1360.	CH2CH2NH2+O=CH2O+CH2NH2	9.60E+13	0.0	0.0
1361.	CH2CH2NH2+OH=CH2CHNH2+H2O	2.40E+13	0.0	0.0
1362.	CH2CH2NH2+HO2=>CH2O+OH+CH2NH2	2.40E+13	0.0	0.0
1363.	CH2CH2NH2+O2=CH2CHNH2+HO2	3.70E+16	-1.6	3418.0
1364.	CH2CH2NH2+CH3=CH2CHNH2+CH4	1.20E+13	-0.3	0.0
1365.	CH3CH2NH2=C2H4+NH3	6.20E+67	-15.9	99348.0
1366.	C2H5+NH2(+M)=CH3CH2NH2(+M)	7.20E+12	0.4	0.0
	Low pressure limit: 0.22000E+31 -0.38500E+01	0.00000E+00		
1367.	CH3CHNH2+H=CH3CH2NH2	1.70E+13	0.2	0.0
1368.	CH2CH2NH2+H=CH3CH2NH2	5.40E+13	0.2	0.0
1369.	CH3CH2NH2+H=CH2CH2NH2+H2	1.20E+07	1.8	5100.0
1370.	CH3CH2NH2+H=CH3CHNH2+H2	2.60E+07	1.6	2830.0
1371.	CH3CH2NH2+H=CH3CH2NH+H2	4.80E+08	1.5	9700.0
1372.	CH3CH2NH2+O=CH2CH2NH2+OH	9.40E+07	1.7	5460.0
1373.	CH3CH2NH2+O=CH3CHNH2+OH	6.80E+12	0.0	1275.0
1374.	CH3CH2NH2+O=CH3CH2NH+OH	3.30E+08	1.5	6348.0
1375.	CH3CH2NH2+OH=CH2CH2NH2+H2O	1.60E+12	0.0	1300.0
1376.	CH3CH2NH2+OH=CH3CHNH2+H2O	1.40E+13	0.0	0.0
1377.	CH3CH2NH2+OH=CH3CH2NH+H2O	2.40E+06	2.0	447.0
1378.	CH3CH2NH2+HO2=CH2CH2NH2+H2O2	1.20E+04	2.5	15750.0
1379.	CH3CH2NH2+HO2=CH3CHNH2+H2O2	8.20E+03	2.5	10750.0
1380.	CH3CH2NH2+CH3=CH2CH2NH2+CH4	2.20E+02	3.2	9620.0
1381.	CH3CH2NH2+CH3=CH3CHNH2+CH4	7.30E+02	3.0	7950.0
1382.	CH3CH2NH2+CH3=CH3CH2NH+CH4	1.60E+06	1.9	8842.0
1383.	CH3CH2NH2+NH2=CH2CH2NH2+NH3	2.20E+02	3.2	9620.0
1384.	CH3CH2NH2+NH2=CH3CHNH2+NH3	7.30E+02	3.0	7950.0
1385.	CH3CH2NH2+NH2=CH3CH2NH+NH3	1.80E+06	1.9	7140.0
1386.	CH2CH2NH2+HCO=CH3CH2NH2+CO	6.00E+13	0.0	0.0

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1387. CH3CHNH2+HCO=CH3CH2NH2+CO                       1.20E+14    0.0        0.0
1388. CH+N2=NCN+H                                     3.70E+07    1.4    20723.0
1389. H+NCN=HCN+N                                     1.89E+14    0.0     8425.0
1390. NCN+O=CN+NO                                     1.00E+14    0.0        0.0
1391. NCN+OH=HCN+NO                                   5.00E+13    0.0        0.0
1392. NCN+N=CN+N2                                     2.00E+13    0.0        0.0
1393. CN+N2O=NCN+NO                                   3.80E+03    2.6     3700.0
1394. CH+N2=HCNN                                      3.60E+28   -5.8     2621.0
1395. HCNN+H<=>CH2+N2                                 1.00E+14    0.0        0.0
1396. HCNN+O<=>CO+H+N2                                2.20E+13    0.0        0.0
1397. HCNN+O<=>HCN+NO                                 2.00E+12    0.0        0.0
1398. HCNN+OH<=>H+HCO+N2                              1.20E+13    0.0        0.0
1399. HCNN+O2=H+CO2+N2                                4.00E+12    0.0        0.0
1400. HCNN+O2=HCO+N2O                                 4.00E+12    0.0        0.0
1401. HCNN+O2<=>O+HCO+N2                              1.20E+13    0.0        0.0
1402. CH2+N2=CH2NN                                    1.60E+32   -7.1    19958.0
1403. CH3NN+M=CH3+N2+M                                1.00E+11    0.0     5900.0
1404. CH3NNH(+M)<=>CH3+NNH(+M)                        3.30E+16   -0.1    55000.0
      Low pressure limit:  0.18800E+32 -0.45500E+01  0.57500E+05
      TROE centering:      0.97000E+00  0.25059E+03  0.10000E+01  0.40100E+06
1405. H2NN+CH3=CH3NNH+H                               8.30E+05    1.9     6494.0
1406. CH3NNH+O=CH3NN+OH                               9.60E+12    0.0        0.0
1407. CH3NNH+OH=CH3NN+H2O                             3.92E+13    0.0        0.0
1408. CH3NN+HO2=CH3NNH+O2                             1.00E+06    2.0        0.0
1409. CH3NNH+HO2=CH3NN+H2O2                           1.00E+11    0.0     1987.0
1410. CH3NNH+CH3=CH4+CH3NN                            7.40E+13    0.0     5210.0
1411. CH3NNH+NH2=NH3+CH3NN                            7.40E+13    0.0     5210.0
1412. CH3NNH+NO2=CH3NN+HONO                           2.20E+11    0.0     5900.0
1413. CH2NNH2+H=NCH2+NH3                              1.76E+08    1.3     8801.1
1414. H2NN+CH3=CH2NNH2+H                              8.30E+05    1.9     6494.0
1415. CH3NNH2(+M)<=>CH3NNH+H(+M)                      1.35E+08    1.7    47280.0
      Low pressure limit:  0.12200E+54 -0.10750E+02  0.53560E+05
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1416. CH3NNH2(+M)<=>CH2NNH2+H(+M)                    1.15E+09    1.2    50330.0
      Low pressure limit:  0.17100E+50 -0.99400E+01  0.56000E+05
      TROE centering:      0.00000E+00  0.33100E+03  0.10000E+02  0.47800E+05
1417. CH3NNH2+O=CH3NNH+OH                           1.00E+08    2.0        0.0
1418. CH3NNH2+OH=CH3NNH+H2O                         1.00E+08    2.0        0.0
1419. CH3NNH2+O2=CH3NNH+HO2                         4.00E+12    0.0        0.0
1420. CH3NNH2+HO2=CH3NNH+H2O2                       1.00E+08    2.0        0.0
1421. CH3NNH2+NO2=CH3NNH+HONO                       1.00E+08    2.0        0.0
1422. CH2NHNH2(+M)<=>CH2NH+NH2(+M)                  3.87E+12    0.2    12200.0
      Low pressure limit:  0.16200E+28 -0.39800E+01  0.11800E+05
      TROE centering:      0.86600E+00  0.29800E+03  0.10000E+02  0.28000E+06
1423. CH2NHNH2(+M)<=>CH2NNH2+H(+M)                   5.92E+11    0.3    36300.0
      Low pressure limit:  0.52500E+16 -0.72000E+00  0.34800E+05
      TROE centering:      0.00000E+00  0.49400E+03  0.10000E+02  0.28000E+06
1424. CH3NHNH(+M)<=>CH3+N2H2(+M)                     4.64E+09    1.6    35620.0
      Low pressure limit:  0.34800E+49 -0.97000E+01  0.41200E+05
      TROE centering:      0.00000E+00  0.23300E+03  0.10000E+02  0.30800E+06
1425. CH3NHNH(+M)<=>CH3NNH+H(+M)                     1.40E+07    2.0    44660.0
      Low pressure limit:  0.18200E+37 -0.65600E+01  0.48600E+05
      TROE centering:      0.00000E+00  0.13400E+03  0.10000E+02  0.51000E+05
1426. CH3NHNH2(+M)<=>CH3NNH2+H(+M)                   4.66E+16   -0.2    77610.0
      Low pressure limit:  0.10900E+50 -0.95600E+01  0.83400E+05
      TROE centering:      0.00000E+00  0.16900E+03  0.13700E+02  0.40000E+05
1427. CH3NHNH2(+M)<=>CH3NHNH+H(+M)                   4.69E+16   -0.2    80120.0
      Low pressure limit:  0.44400E+48 -0.91900E+01  0.85700E+05
      TROE centering:      0.00000E+00  0.14900E+03  0.42800E+02  0.42400E+05
1428. CH3NHNH2(+M)<=>CH2NHNH2+H(+M)                  6.42E+16   -0.2    91800.0
      Low pressure limit:  0.18000E+44 -0.79800E+01  0.96700E+05
      TROE centering:      0.98900E+00  0.10700E+03  0.60700E+02  0.60100E+05
1429. CH3NHNH2(+M)<=>CH3NNH+H2(+M)                   9.70E+08    1.3   107500.0
      Low pressure limit:  0.10500E+69 -0.13840E+02  0.11500E+06
      TROE centering:      0.00000E+00  0.50000E+06  0.10000E+02  0.41700E+05
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1430. CH3NHNH2(+M)<=>CH2NNH2+H2(+M)                  2.69E+09    1.2   105430.0
      Low pressure limit:  0.10500E+69 -0.13840E+02  0.11400E+03
      TROE centering:      0.19500E+00  0.47200E+04  0.10000E+01  0.10000E+01
1431. CH3NHNH2(+M)<=>N2H3+CH3(+M)                    3.12E+16   -0.2    65180.0
      Low pressure limit:  0.73400E+62 -0.13010E+02  0.72900E+05
      TROE centering:      0.00000E+00  0.27100E+03  0.10000E+02  0.41700E+05
1432. CH3NHNH2(+M)<=>H2NN+CH4(+M)                    1.36E+09    1.6    67110.0
      Low pressure limit:  0.24700E+52 -0.10400E+02  0.74300E+05
      TROE centering:      0.00000E+00  0.26000E+03  0.10000E+02  0.77500E+05
1433. CH3NHNH2(+M)<=>N2H2+CH4(+M)                    1.61E+10    1.1   108880.0
      Low pressure limit:  0.43820E+64 -0.12620E+02  0.11600E+06
      TROE centering:      0.00000E+00  0.97800E+03  0.10000E+02  0.41700E+05
1434. CH3NHNH2(+M)<=>CH3NH+NH2(+M)                   2.40E+16   -0.1    63790.0
      Low pressure limit:  0.89200E+65 -0.13840E+02  0.71900E+05
1435. CH3NHNH2(+M)<=>CH2NH+NH3(+M)                   3.50E+08    1.4    68330.0
      Low pressure limit:  0.80500E+49 -0.10300E+02  0.75300E+05
      TROE centering:      0.00000E+00  0.24200E+03  0.10000E+02  0.41700E+05
1436. CH3NHNH2(+M)<=>CH3N+NH3(+M)                    4.33E+09    1.2    62170.0
      Low pressure limit:  0.75000E+70 -0.15570E+02  0.71600E+05
      TROE centering:      0.35500E+00  0.29300E+03  0.10000E+02  0.41300E+05
1437. CH3NHNH2+H=CH3NNH2+H2                          2.08E+07    1.8     4488.1
1438. CH3NHNH2+H=CH3NHNH+H2                          1.68E+09    1.1     7289.0
1439. CH3NHNH2+H=CH2NHNH2+H2                         7.88E+07    1.7    11162.0
1440. CH3NHNH2+H=CH3NH+NH3                           1.37E+09    1.1     5526.4
1441. CH3NHNH2+O=CH3NNH+H2O                          9.60E+12    0.0        0.0
1442. CH3NHNH2+O=CH3NNH2+OH                          9.60E+12    0.0        0.0
1443. CH3NHNH2+O=CH3NHNH+OH                          2.69E+12    0.0        0.0
1444. CH3NHNH2+O=CH2NHNH2+OH                         1.30E+12    0.0        0.0
1445. CH3NHNH2+OH=CH3NNH2+H2O                        3.92E+13    0.0        0.0
1446. CH3NHNH2+OH=CH3NHNH+H2O                        1.10E+13    0.0        0.0
1447. CH3NHNH2+OH=CH2NHNH2+H2O                       5.30E+12    0.0        0.0
1448. CH3NNH2+HO2=CH3NHNH2+O2                        1.00E+06    2.0        0.0
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1449.	CH3NHNH2+HO2=CH3NNH2+H2O2	2.70E+11	0.0	1987.0
1450.	CH3NHNH2+HO2=CH3NHNH+H2O2	7.56E+10	0.0	1987.0
1451.	CH3NHNH2+HO2=CH2NHNH2+H2O2	3.65E+10	0.0	1987.0
1452.	CH3NHNH2+CH3=CH4+CH3NNH2	4.79E+01	3.4	3578.3
1453.	CH3NHNH2+CH3=CH3NHNH+CH4	3.21E+02	3.1	5748.1
1454.	CH3NHNH2+CH3=CH2NHNH2+CH4	2.27E+01	3.5	7669.4
1455.	CH3NHNH2+NH=CH3NNH2+NH2	1.45E+02	3.3	4435.5
1456.	CH3NHNH2+NH=CH3NHNH+NH2	6.20E+02	3.1	7062.4
1457.	CH3NHNH2+NH=CH2NHNH2+NH2	3.93E+01	3.6	10910.0
1458.	CH3NHNH2+NH2=CH3NNH2+NH3	1.65E+02	3.0	870.1
1459.	CH3NHNH2+NH2=CH3NHNH+NH3	5.98E+01	3.1	2110.2
1460.	CH3NHNH2+NH2=CH2NHNH2+NH3	1.04E+00	3.6	1894.1
1461.	CH3NHNH2+NO2=CH3NNH2+HONO	2.20E+11	0.0	5900.0
1462.	CH3NHNH2+NO2=CH3NHNH+HONO	7.87E+10	0.0	8839.0
1463.	CH3NHNH2+NO2=CH2NHNH2+HONO	1.39E+09	0.0	9803.0
1464.	CH3NHNH2+NO=CH3NNH2+HNO	1.85E+13	0.0	8524.0
1465.	CH3NHNH2+NO=CH3NHNH+HNO	1.24E+12	0.0	9605.0
1466.	CH3NHNH2+NO=CH2NHNH2+HNO	5.05E+12	0.0	11310.0
1467.	NCCN+M=CN+CN+M	1.10E+34	-4.3	130079.0
	N2 Enhanced by 1.500E+00			
	O2 Enhanced by 1.500E+00			
	H2 Enhanced by 1.500E+00			
	H2O Enhanced by 1.000E+01			
	CO2 Enhanced by 3.000E+00			
1468.	CN+HCN=NCCN+H	1.50E+07	1.7	1529.0
1469.	HNC+CN=NCCN+H	1.00E+13	0.0	0.0
1470.	CH3NNCH3=CH3NN+CH3	6.92E+15	0.0	50875.0
1471.	CH3NNCH3=C2H6+N2	2.00E+11	0.0	33000.0
1472.	NCO+M=N+CO+M	2.20E+14	0.0	54050.0
	N2 Enhanced by 1.500E+00			
	Warning...superceding enhancement factor for N2			
	N2 Enhanced by 1.500E+00			

1473.	CN+OH=NCO+H	4.00E+13	0.0	0.0
1474.	CH+NO=H+NCO	2.00E+13	0.0	0.0
1475.	HCN+O=NCO+H	1.40E+04	2.6	4980.0
1476.	HNC+O=H+NCO	1.60E+01	3.1	-224.0
1477.	NCO+H=NH+CO	5.20E+13	0.0	0.0
1478.	CN+O2=NCO+O	7.20E+12	0.0	-417.0
	Declared duplicate reaction...			
1479.	CN+O2=NCO+O	-2.80E+17	-2.0	0.0
	Declared duplicate reaction...			
1480.	NCO+O=NO+CO	2.00E+15	-0.5	0.0
1481.	NCO+O=N+CO2	8.00E+12	0.0	2502.0
1482.	NCO+OH=HON+CO	5.30E+12	-0.1	5124.0
1483.	NCO+OH=H+CO+NO	8.30E+12	-0.1	18032.0
1484.	NCO+O2=NO+CO2	2.00E+12	0.0	20000.0
1485.	CH3CN+O=CH3+NCO	6.00E+09	1.8	8130.0
1486.	CH3NCH+O=>CH3+NCO+H	7.00E+13	0.0	0.0
1487.	C2H2+NCO=HCCO+HCN	1.40E+12	0.0	1815.0
1488.	CN+CO2=NCO+CO	3.67E+06	2.2	26900.0
1489.	C2O+NO=CO+NCO	1.00E+14	0.0	670.0
1490.	C2O+NO2=CO2+NCO	5.10E+13	0.0	125.0
1491.	NCO+N=N2+CO	2.00E+13	0.0	0.0
1492.	CN+NO=NCO+N	9.60E+13	0.0	42100.0
1493.	CN+NO2=NCO+NO	5.30E+15	-0.8	344.0
1494.	NCO+NO=N2+CO2	1.50E+21	-2.7	1824.0
1495.	NCO+NO=N2O+CO	4.00E+19	-2.2	1743.0
1496.	NCN+O2=NO+NCO	4.40E+09	0.5	24580.0
1497.	N2O+NCO=CO+N2+NO	9.00E+13	0.0	27800.0
1498.	NCO+NO2=CO2+N2O	3.00E+12	0.0	-707.0
1499.	NCO+NO2=CO+NO+NO	2.10E+11	0.0	-874.0
1500.	NCCN+O=NCO+CN	4.60E+12	0.0	8877.0
1501.	CN+NCO=NCN+CO	1.80E+13	0.0	0.0
1502.	NCO+NCO=CO+CO+N2	1.80E+13	0.0	0.0

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1503. HCNO=HCN+O                                        4.20E+31   -6.1    61175.0
1504. CH2+NO=HCNO+H                                     3.80E+13   -0.4      576.0
1505. CH2SING+NO<=>H+HCNO                               3.80E+13   -0.4      580.0
1506. NCH2+O=HCNO+H                                     2.00E+13    0.0        0.0
1507. HCNO+H=HCN+OH                                     7.20E+10    0.8     8612.0
1508. HCNO+H=NH2+CO                                     1.70E+14   -0.8     2889.0
1509. HCNO+O=HCO+NO                                     6.30E+13    0.0        0.0
1510. HCNO+O=NCO+OH                                     7.00E+12    0.0        0.0
1511. HCNO+OH=HCO+HNO                                   4.50E+12    0.0        0.0
1512. HCNO+OH=CH2O+NO                                   1.00E+12    0.0        0.0
1513. HCNO+OH=NO+CO+H2                                  6.50E+12    0.0        0.0
1514. HCNO+OH=NCO+H2O                                   3.50E+12    0.0        0.0
1515. HCNO+OH=NCO+H+OH                                  4.50E+12    0.0        0.0
1516. NO+HCCO=HCNO+CO                                   4.60E+13    0.0      695.0
1517. HCCO+NO2=HCNO+CO2                                 1.60E+13    0.0        0.0
1518. HCNO+CN=HCN+NCO                                   6.00E+13    0.0        0.0
1519. HNCO(+M)=NH+CO(+M)                                6.00E+13    0.0    99800.0
      Low pressure limit:  0.21700E+29 -0.31000E+01  0.10190E+06
      TROE centering:      0.46650E+00  0.10000E+04  0.10000E+07
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    5.000E+00
      N2              Enhanced by    1.000E+00
      CO2             Enhanced by    1.600E+00
1520. HNCO+M=H+NCO+M                                    1.00E+17    0.0   112000.0
1521. HCNO+H<=>H+HNCO                                   2.10E+15   -0.7     2850.0
1522. CH2+NO=HNCO+H                                     3.10E+17   -1.4     1271.0
1523. CH2SING+NO<=>H+HNCO                               3.10E+17   -1.4     1270.0
1524. OH+HCN=HNCO+H                                     1.98E-03    4.0     1000.0
1525. OH+HNC=HNCO+H                                     2.80E+13    0.0     3694.0
1526. CHNH+O=HNCO+H                                     7.00E+13    0.0        0.0
1527. HNCO+H=NCO+H2                                     9.00E+07    1.7    13900.0
1528. HNCO+H=NH2+CO                                     3.60E+04    2.5     2343.0
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1529.	HNC+O2=HNCO+O	1.50E+12	0.0	4111.0
1530.	HNCO+O=HNO+CO	1.49E+08	1.6	44010.0
1531.	HNCO+O=CO2+NH	9.80E+07	1.4	8524.0
1532.	HNCO+O=NCO+OH	2.20E+06	2.1	11430.0
1533.	HNCO+OH=NH2+CO2	6.30E+10	-0.1	11637.0
1534.	HNCO+OH=NCO+H2O	3.60E+07	1.5	3594.0
1535.	HNCO+O2=HNO+CO2	1.00E+12	0.0	35000.0
1536.	NCO+HO2=HNCO+O2	2.00E+13	0.0	0.0
1537.	HNCO+HO2=NCO+H2O2	3.00E+11	0.0	23700.0
1538.	NCO+CH4=HNCO+CH3	9.80E+12	0.0	8122.0
1539.	CH3CNH+O=CH3+HNCO	1.60E+14	0.0	0.0
1540.	CH2CNH+OH=CH3+HNCO	6.70E+11	0.0	-1013.0
1541.	C2H6+NCO=C2H5+HNCO	1.50E-09	6.9	-2910.0
1542.	NCO+HCO=HNCO+CO	3.60E+13	0.0	0.0
1543.	CH2O+NCO=HNCO+HCO	6.00E+12	0.0	0.0
1544.	CHCNH+O2=HNCO+HCO	4.90E+12	-0.1	1150.0
1545.	CH2CHN+O2=CH2O+HNCO	1.00E+12	0.0	0.0
1546.	HNCO+N=NH+NCO	2.32E+19	0.0	52500.0
1547.	HNCO+NH=NH2+NCO	3.00E+13	0.0	23700.0
1548.	NCO+NH3=HNCO+NH2	2.80E+04	2.5	983.0
1549.	NCO+HNO=HNCO+NO	1.80E+13	0.0	0.0
1550.	HNC+NO2=HNCO+NO	1.00E+12	0.0	32000.0
1551.	NCO+HONO=HNCO+NO2	3.60E+12	0.0	0.0
1552.	HNCO+NO2=HNNO+CO2	2.50E+12	0.0	26000.0
1553.	CN+HNCO=HCN+NCO	1.00E+13	0.0	0.0
1554.	HCN+OH=HOCN+H	5.90E+04	2.4	12500.0
1555.	HCNO+H=HOCN+H	1.40E+11	-0.2	2482.0
1556.	HOCN+H=HNCO+H	3.10E+08	0.8	1916.0
1557.	HOCN+H=NH2+CO	1.20E+08	0.6	2075.0
1558.	HOCN+H=H2+NCO	2.40E+08	1.5	6613.0
1559.	HOCN+O=OH+NCO	1.70E+08	1.5	4131.0
1560.	HOCN+OH=H2O+NCO	1.20E+06	2.0	-248.0

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1561. HOCN+CH3=CH4+NCO                                8.20E+05    1.9     6613.0
1562. CH3+HOCN=CH3CN+OH                               5.00E+12    0.0     2000.0
1563. HOCN+NH2=NCO+NH3                                9.20E+05    1.9     3644.0
1564. NCCN+OH=HOCN+CN                                 2.00E+12    0.0    18985.0
1565. CH2NO=HNCO+H                                    2.30E+42   -9.1    53807.0
1566. CH2NO+H=CH3+NO                                  4.00E+13    0.0        0.0
1567. CH2NO+H=HCNO+H2                                 4.80E+08    1.5     -894.0
1568. CH2NO+O=CH2O+NO                                 7.00E+13    0.0        0.0
1569. CH2NO+O=HCNO+OH                                 3.30E+08    1.5     -894.0
1570. NCH2+HO2=CH2NO+OH                               3.00E+13    0.0        0.0
1571. CH2NO+OH=CH2OH+NO                               4.00E+13    0.0        0.0
1572. CH2NO+OH=HCNO+H2O                               2.40E+06    2.0    -1192.0
1573. CH2NO+O2=CH2O+NO2                               1.20E+15   -1.0    20117.0
1574. CH2NO+CH3=C2H5+NO                               3.00E+13    0.0        0.0
1575. CH2NO+CH3=HCNO+CH4                              1.60E+06    1.9    -1112.0
1576. CH2NO+NH2=CH2NH2+NO                             3.00E+13    0.0        0.0
1577. CH2NO+NH2=HCNO+NH3                              1.80E+06    1.9    -1152.0
1578. H2NCO(+M)=CO+NH2(+M)                            5.90E+12    0.0    25000.0
      Low pressure limit:  0.10000E+15  0.00000E+00  0.21700E+05
1579. H2NCO+H=HNCO+H2                                 3.00E+13    0.0        0.0
1580. H2NCO+O=HNCO+OH                                 3.00E+13    0.0        0.0
1581. H2NCO+OH=HNCO+H2O                               3.00E+13    0.0        0.0
1582. CH2CHNH2+O=CH3+H2NCO                            3.90E+12    0.0     1494.0
      Declared duplicate reaction...
1583. CH2CHNH2+O=CH3+H2NCO                            6.20E+13    0.0     6855.0
      Declared duplicate reaction...
1584. CH3+NO(+M)=CH3NO(+M)                            9.00E+12    0.0      192.0
      Low pressure limit:  0.25000E+17  0.00000E+00 -0.28410E+04
      TROE centering:      0.50000E+01  0.10000E-29  0.12000E+03  0.10000E+31
1585. CH3+NO=CH3NO                                    1.00E+37   -8.4     5223.0
1586. CH3NO+H=CH2NO+H2                                4.40E+08    1.5      377.0
1587. CH3NO+H=CH3+HNO                                 1.80E+13    0.0     2780.0
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1588. CH3NO+O=CH2NO+OH                                3.30E+08    1.5     3614.0
1589. CH3NO+O=CH3+NO2                                 1.70E+06    2.1        0.0
1590. CH3NO+OH=CH2NO+H2O                              3.60E+06    2.0    -1192.0
1591. CH3NO+OH=CH3+HONO                               2.50E+12    0.0      993.0
1592. CH3NO+CH3=CH2NO+CH4                             7.90E+05    1.9     5412.0
1593. CH3NCH3+O=CH3NO+CH3                             5.00E+13    0.0        0.0
1594. CH3NCH3+O2=CH3NO+CH3O                           1.00E+09    1.0     6000.0
1595. CH3NO+NH2=CH2NO+NH3                             2.80E+06    1.9     1072.0
1596. H2NCHO(+M)=CO+NH3(+M)                           1.00E+14    0.0    75514.0
      Low pressure limit:  0.83000E+15  0.00000E+00  0.49084E+05
1597. H2NCHO+M=HCO+NH2+M                              1.40E+16    0.0    72900.0
1598. H2NCHO+M=H2NCO+H+M                              4.60E+15    0.0    64200.0
1599. H2NCHO+H=H2NCO+H2                               1.30E+13    0.0     6955.0
1600. H2NCHO+H=HCO+NH3                                1.00E+13    0.0    19100.0
1601. H2NCHO+O=H2NCO+OH                               4.00E+08    1.5     5196.0
1602. CH3CHNH2+O=CH3+H2NCHO                           4.00E+13    0.0        0.0
1603. H2NCHO+OH=H2NCO+H2O                             8.00E+12    0.0        0.0
1604. CH3CHNH2+HO2=>CH3+OH+H2NCHO                     2.40E+13    0.0        0.0
1605. H2NCHO+CH3=H2NCO+CH4                            7.00E+05    2.0     9000.0
1606. H2NCHO+NH2=H2NCO+NH3                            2.00E+06    2.0     5000.0
1607. H2CNO2=CH2O+NO                                  1.00E+13    0.0    36000.0
1608. CH3O+NO(+M)=CH3ONO(+M)                          6.60E+14   -0.6        0.0
      Low pressure limit:  0.27000E+28 -0.35000E+01  0.00000E+00
1609. CH3NO2(+M)=CH3+NO2(+M)                          1.80E+16    0.0    58500.0
      Low pressure limit:  0.13000E+18  0.00000E+00  0.42000E+05
      TROE centering:      0.18320E+00  0.10000E+02  0.10000E+07
1610. CH3NO2+H=CH3+HONO                               3.30E+12    0.0     3730.0
1611. CH3NO2+H=CH3NO+OH                               1.40E+12    0.0     3730.0
1612. CH3NO2+H=H2CNO2+H2                              5.40E+02    3.5     5200.0
1613. CH3NO2+O=H2CNO2+OH                              1.50E+13    0.0     5350.0
1614. CH3NO2+OH=H2CNO2+H2O                            5.00E+05    2.0     1000.0
1615. CH3NO2+OH=CH3OH+NO2                             2.00E+10    0.0    -1000.0
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1616. CH3NO2+CH2=H2CNO2+CH3 6.50E+12 0.0 7900.0

1617. CH3NO2+CH2SING=H2CNO2+CH3 1.20E+14 0.0 0.0

1618. CH3NO2+CH3=H2CNO2+CH4 5.50E-01 4.0 8300.0

1619. CN+NO(+M)=NCNO(+M) 3.98E+13 0.0 0.0

Low pressure limit: 0.15600E+37 -0.62000E+01 0.48780E+04

TROE centering: 0.65080E+00 0.10000E+02 0.10000E+07

N2O Enhanced by 5.000E+00

H2O Enhanced by 5.000E+00

N2 Enhanced by 1.000E+00

CO2 Enhanced by 2.000E+00

1620. CH3O+NO2(+M)=CH3ONO2(+M) 1.20E+13 0.0 0.0

Low pressure limit: 0.14000E+31 -0.45000E+01 0.00000E+00

1621. TMEDA-1+H=TMEDA 1.00E+14 0.0 0.0

1622. TMEDA-3+H=TMEDA 1.00E+14 0.0 0.0

1623. CH3+TMEDA-2=TMEDA 2.00E+13 0.0 0.0

1624. CH3NCH3+N(CH3)2CH2CH2=TMEDA 1.60E+13 0.0 0.0

1625. N(CH3)2CH2+N(CH3)2CH2=TMEDA 8.00E+12 0.0 0.0

1626. TMEDA+H=TMEDA-1+H2 2.66E+06 2.5 6756.0

1627. TMEDA+H=TMEDA-3+H2 2.60E+06 2.4 4471.0

1628. TMEDA+O=TMEDA-1+OH 3.92E+06 2.4 4750.0

1629. TMEDA+O=TMEDA-3+OH 1.10E+06 2.5 2830.0

1630. TMEDA+OH=TMEDA-1+H2O 2.11E+10 1.0 1590.0

1631. TMEDA+OH=TMEDA-3+H2O 9.36E+07 1.6 -35.0

1632. TMEDA+CH3=TMEDA-1+CH4 1.81E+00 3.6 7154.0

1633. TMEDA+CH3=TMEDA-3+CH4 3.02E+00 3.5 5481.0

1634. TMEDA+HO2=TMEDA-1+H2O2 8.16E+01 3.6 17160.0

1635. TMEDA+HO2=TMEDA-3+H2O2 1.29E+02 3.4 13720.0

1636. TMEDA+CH3O=TMEDA-1+CH3OH 8.68E+11 0.0 6548.0

1637. TMEDA+CH3O=TMEDA-3+CH3OH 2.90E+11 0.0 4571.0

1638. TMEDA+O2=TMEDA-1+HO2 1.20E+14 0.0 52290.0

1639. TMEDA+O2=TMEDA-3+HO2 4.00E+13 0.0 49640.0

1640. TMEDA+C2H5=TMEDA-1+C2H6 2.00E+11 0.0 13400.0

1641.	TMEDA+C2H5=TMEDA-3+C2H6	1.00E+11	0.0	10400.0
1642.	TMEDA+C2H3=TMEDA-1+C2H4	2.00E+12	0.0	18000.0
1643.	TMEDA+C2H3=TMEDA-3+C2H4	8.00E+11	0.0	16800.0
1644.	TMEDA-1=CH3NCH2+N(CH3)2CH2CH2	3.68E+15	-0.6	31359.0
1645.	TMEDA-1=CH3+TMEDA-0-5	9.55E+14	-0.6	30592.0
1646.	TMEDA-3=CH3NCH3+N(CH3)2CHCH2	6.98E+12	0.2	24963.0
1647.	TMEDA-3=CH3+TMEDA-0-4	1.77E+13	0.1	30542.0
1648.	H+TMEDA-0-3=TMEDA-3	2.50E+11	0.5	2620.0
1649.	TMEDA-1=TMEDA-3	6.92E+00	3.2	16558.0
1650.	TMEDA-0-3+OH=TMEDA-1-3+H2O	6.56E+08	1.6	-35.0
1651.	TMEDA-0-4+OH=TMEDA-1-4+H2O	6.56E+08	1.6	-35.0
1652.	TMEDA-0-5+OH=TMEDA-1-5+H2O	6.56E+08	1.6	-35.0
1653.	TMEDA-0-5+OH=TMEDA-3-5+H2O	3.28E+08	1.6	-35.0
1654.	TMEDA-0-3+HO2=TMEDA-1-3+H2O2	8.84E+02	3.4	13720.0
1655.	TMEDA-0-4+HO2=TMEDA-1-4+H2O2	8.84E+02	3.4	13720.0
1656.	TMEDA-0-5+HO2=TMEDA-1-5+H2O2	8.84E+02	3.4	13720.0
1657.	TMEDA-0-5+HO2=TMEDA-3-5+H2O2	4.42E+02	3.4	13720.0
1658.	TMEDA-0-3+H=TMEDA-1-3+H2	1.82E+07	2.4	4471.0
1659.	TMEDA-0-4+H=TMEDA-1-4+H2	1.82E+07	2.4	4471.0
1660.	TMEDA-0-5+H=TMEDA-1-5+H2	1.82E+07	2.4	4471.0
1661.	TMEDA-0-5+H=TMEDA-3-5+H2	9.10E+06	2.4	4471.0
1662.	TMEDA-0-3+CH3=TMEDA-1-3+CH4	2.12E+01	3.5	5481.0
1663.	TMEDA-0-4+CH3=TMEDA-1-4+CH4	2.12E+01	3.5	5481.0
1664.	TMEDA-0-5+CH3=TMEDA-1-5+CH4	2.12E+01	3.5	5481.0
1665.	TMEDA-0-5+CH3=TMEDA-3-5+CH4	1.06E+01	3.5	5481.0
1666.	TMEDA-0-3+O=TMEDA-1-3+OH	7.72E+06	2.5	2830.0
1667.	TMEDA-0-4+O=TMEDA-1-4+OH	7.72E+06	2.5	2830.0
1668.	TMEDA-0-5+O=TMEDA-1-5+OH	7.72E+06	2.5	2830.0
1669.	TMEDA-0-5+O=TMEDA-3-5+OH	3.86E+06	2.5	2830.0
1670.	TMEDA-1-3=CH3NCH2+N(CH3)2CHCH	2.50E+13	0.0	30000.0
	Declared duplicate reaction...			
1671.	CH3NCH2+N(CH3)2CHCH=TMEDA-1-3	1.00E+11	0.0	9600.0

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      Declared duplicate reaction...
1672. TMEDA-1-4=CH3NCH2+CH2CHNCH3                2.50E+13    0.0    30000.0
      Declared duplicate reaction...
1673. CH3NCH2+CH2CHNCH3=TMEDA-1-4                1.00E+11    0.0     9600.0
      Declared duplicate reaction...
1674. TMEDA-1-5=CH3NCH2+CH2CH2NCH2               2.50E+13    0.0    30000.0
      Declared duplicate reaction...
1675. CH3NCH2+CH2CH2NCH2=TMEDA-1-5               1.00E+11    0.0     9600.0
      Declared duplicate reaction...
1676. TMEDA-3-5=N(CH3)2CHCH2+NCH2                2.50E+13    0.0    35000.0
      Declared duplicate reaction...
1677. N(CH3)2CHCH2+NCH2=TMEDA-3-5                1.00E+11    0.0     9600.0
      Declared duplicate reaction...
1678. TMEDA-0-4=CH3NCH3+CH2CHNCH3                2.50E+16    0.0    71000.0
      Declared duplicate reaction...
1679. CH3NCH3+CH2CHNCH3=TMEDA-0-4                1.00E+13    0.0        0.0
      Declared duplicate reaction...
1680. TMEDA-0-5=N(CH3)2CH2+CH2NCH2               2.50E+16    0.0    71000.0
      Declared duplicate reaction...
1681. N(CH3)2CH2+CH2NCH2=TMEDA-0-5               1.00E+13    0.0        0.0
      Declared duplicate reaction...
1682. N(CH3CH2)CH2CH3=N(CH3)2CH2CH2              3.00E+11    0.0    21100.0
      Declared duplicate reaction...
1683. N(CH3)2CH2CH2=N(CH3CH2)CH2CH3              3.00E+11    0.0    21100.0
      Declared duplicate reaction...
1684. N(CH3)2CH2CH2=C2H4+CH3NCH3                 1.14E+15   -0.4    27010.0
      Declared duplicate reaction...
1685. C2H4+CH3NCH3=N(CH3)2CH2CH2                 3.30E+11    0.0     7200.0
      Declared duplicate reaction...
1686. N(CH3)2CH2CH2=H+N(CH3)2CHCH2               2.20E+16   -0.9    37480.0
      Declared duplicate reaction...
1687. H+N(CH3)2CHCH2=N(CH3)2CH2CH2               1.00E+13    0.0     2900.0
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Declared duplicate reaction...

1688. N(CH3)2CHCH2+OH=H2O+N(CH3CH2)CHCH2 1.00E+12 0.0 1230.0

Declared duplicate reaction...

1689. H2O+N(CH3CH2)CHCH2=N(CH3)2CHCH2+OH 5.00E+12 0.0 26500.0

Declared duplicate reaction...

1690. N(CH3)2CHCH2+OH=H2O+N(CH3)2CCH2 1.00E+12 0.0 1230.0

Declared duplicate reaction...

1691. H2O+N(CH3)2CCH2=N(CH3)2CHCH2+OH 5.00E+12 0.0 26500.0

Declared duplicate reaction...

1692. N(CH3)2CHCH2+OH=H2O+N(CH3)2CHCH 1.00E+12 0.0 1230.0

Declared duplicate reaction...

1693. H2O+N(CH3)2CHCH=N(CH3)2CHCH2+OH 5.00E+12 0.0 26500.0

Declared duplicate reaction...

1694. N(CH3)2CHCH2+H=H2+N(CH3CH2)CHCH2 1.00E+12 0.0 3800.0

Declared duplicate reaction...

1695. H2+N(CH3CH2)CHCH2=N(CH3)2CHCH2+H 1.00E+12 0.0 25000.0

Declared duplicate reaction...

1696. N(CH3)2CHCH2+H=H2+N(CH3)2CCH2 1.00E+12 0.0 3800.0

Declared duplicate reaction...

1697. H2+N(CH3)2CCH2=N(CH3)2CHCH2+H 1.00E+12 0.0 25000.0

Declared duplicate reaction...

1698. N(CH3)2CHCH2+H=H2+N(CH3)2CHCH 1.00E+12 0.0 3800.0

Declared duplicate reaction...

1699. H2+N(CH3)2CHCH=N(CH3)2CHCH2+H 1.00E+12 0.0 25000.0

Declared duplicate reaction...

1700. N(CH3)2CHCH2+CH3=CH4+N(CH3CH2)CHCH2 5.00E+11 0.0 7300.0

Declared duplicate reaction...

1701. CH4+N(CH3CH2)CHCH2=N(CH3)2CHCH2+CH3 6.00E+11 0.0 25000.0

Declared duplicate reaction...

1702. N(CH3)2CHCH2+CH3=CH4+N(CH3)2CCH2 5.00E+11 0.0 7300.0

Declared duplicate reaction...

1703. CH4+N(CH3)2CCH2=N(CH3)2CHCH2+CH3 6.00E+11 0.0 25000.0

```
      Declared duplicate reaction...
1704. N(CH3)2CHCH2+CH3=CH4+N(CH3)2CHCH              5.00E+11    0.0     7300.0
      Declared duplicate reaction...
1705. CH4+N(CH3)2CHCH=N(CH3)2CHCH2+CH3             6.00E+11    0.0    25000.0
      Declared duplicate reaction...
1706. N(CH3)2CHCH2=CH3+CH2CHNCH3                   2.50E+16    0.0    71000.0
      Declared duplicate reaction...
1707. CH3+CH2CHNCH3=N(CH3)2CHCH2                   1.00E+13    0.0        0.0
      Declared duplicate reaction...
1708. N(CH3CH2)CHCH2=CH3+CH2CHNCH2                 9.55E+14   -0.6    30592.0
1709. N(CH3CH2)CHCH2=C2H3+CH3NCH2                  3.68E+15   -0.6    31359.0
1710. C2H2+CH3NCH3(+M)=N(CH3)2CHCH(+M)             8.30E+10    0.9     -363.0
      Low pressure limit:  0.12400E+32 -0.47200E+01  0.18710E+04
      TROE centering:      0.10000E+01  0.10000E+03  0.56130E+04  0.13387E+05
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
      C2H2            Enhanced by    2.500E+00
      C2H4            Enhanced by    2.500E+00
1711. N(CH3CH2)CH2CH3=CH3CH2NCH2+CH3               1.09E+16   -0.9    29800.0
      Declared duplicate reaction...
1712. CH3+CH3CH2NCH2=N(CH3CH2)CH2CH3               1.50E+11    0.0     9200.0
      Declared duplicate reaction...
1713. N(CH3CH2)CH2CH3=CH3NCH2+C2H5                 1.03E+18   -1.2    31440.0
      Declared duplicate reaction...
1714. CH3NCH2+C2H5=N(CH3CH2)CH2CH3                 1.50E+11    0.0    10600.0
      Declared duplicate reaction...
1715. N(CH3)2CH2=CH3+CH3NCH2                       9.50E+11    0.8    30700.0
      Declared duplicate reaction...
```

1716.	CH3+CH3NCH2=N(CH3)2CH2	1.89E+03	2.7	6850.0
	Declared duplicate reaction...			
1717.	CH2CH2NCH2=CH2CHNCH2+H	3.00E+13	0.0	35000.0
1718.	CH2CH2NCH2=C2H4+NCH2	8.77E+12	-0.2	36260.0
	Declared duplicate reaction...			
1719.	C2H4+NCH2=CH2CH2NCH2	2.00E+11	0.0	7800.0
	Declared duplicate reaction...			
1720.	CH2CHNCH3=CH2CHNCH2+H	1.20E+14	0.0	49300.0
	Declared duplicate reaction...			
1721.	CH2CHNCH2+H=CH2CHNCH3	4.00E+13	0.0	1300.0
	Declared duplicate reaction...			
1722.	CH2CHNCH3+O2=HO2+CH2CHNCH2	1.00E+09	0.0	0.0
	Declared duplicate reaction...			
1723.	CH2CHNCH2+HO2=O2+CH2CHNCH3	1.00E+11	0.0	17000.0
	Declared duplicate reaction...			
1724.	CH2CHNCH3+H=H2+CH2CHNCH2	3.16E+13	0.0	0.0
	Declared duplicate reaction...			
1725.	CH2CHNCH2+H2=H+CH2CHNCH3	1.07E+13	0.0	56810.0
	Declared duplicate reaction...			
1726.	CH2CHNCH3+C2H5=C2H6+CH2CHNCH2	3.98E+12	0.0	0.0
	Declared duplicate reaction...			
1727.	CH2CHNCH2+C2H6=C2H5+CH2CHNCH3	3.21E+12	0.0	49840.0
	Declared duplicate reaction...			
1728.	CH2CHNCH3+C2H3=C2H4+CH2CHNCH2	3.98E+12	0.0	0.0
	Declared duplicate reaction...			
1729.	CH2CHNCH2+C2H4=C2H3+CH2CHNCH3	1.16E+13	0.0	57710.0
	Declared duplicate reaction...			
1730.	CH2CHNCH2=C2H3+NCH2	4.03E+19	-1.0	98150.0
	Declared duplicate reaction...			
1731.	C2H3+NCH2=CH2CHNCH2	1.26E+13	0.0	0.0
	Declared duplicate reaction...			
1732.	CH3CH2NCH2=H+CH3CHNCH2	3.72E+14	-0.1	85200.0

	Declared duplicate reaction...			
1733.	CH3CHNCH2+H=CH3CH2NCH2	5.00E+13	0.0	0.0
	Declared duplicate reaction...			
1734.	CH3CH2NCH2+H=H2+CH2CH2NCH2	6.65E+05	2.5	6756.0
	Declared duplicate reaction...			
1735.	CH2CH2NCH2+H2=H+CH3CH2NCH2	3.04E+04	2.5	11030.0
	Declared duplicate reaction...			
1736.	CH3CH2NCH2+OH=H2O+CH2CH2NCH2	5.27E+09	1.0	1586.0
	Declared duplicate reaction...			
1737.	CH2CH2NCH2+H2O=OH+CH3CH2NCH2	1.04E+09	1.0	21010.0
	Declared duplicate reaction...			
1738.	CH3CH2NCH2+CH3=CH4+CH2CH2NCH2	4.52E-01	3.6	7154.0
	Declared duplicate reaction...			
1739.	CH2CH2NCH2+CH4=CH3+CH3CH2NCH2	5.40E-01	3.6	11910.0
	Declared duplicate reaction...			
1740.	CH3CH2NCH2+HO2=H2O2+CH2CH2NCH2	2.38E+03	2.5	16490.0
	Declared duplicate reaction...			
1741.	CH2CH2NCH2+H2O2=HO2+CH3CH2NCH2	2.80E+03	2.2	4460.0
	Declared duplicate reaction...			
1742.	CH3CH2NCH2+HO2=H2O2+CH3CHNCH2	4.82E+03	2.5	10530.0
	Declared duplicate reaction...			
1743.	CH3CHNCH2+H2O2=HO2+CH3CH2NCH2	1.59E+06	2.0	14350.0
	Declared duplicate reaction...			
1744.	CH3CH2NCH2+CH3=CH4+CH3CHNCH2	3.69E+00	3.3	4002.0
	Declared duplicate reaction...			
1745.	CH3CHNCH2+CH4=CH3+CH3CH2NCH2	1.23E+03	3.0	24610.0
	Declared duplicate reaction...			
1746.	CH3CH2NCH2+OH=H2O+CH3CHNCH2	2.76E+04	2.6	-1919.0
	Declared duplicate reaction...			
1747.	CH3CHNCH2+H2O=OH+CH3CH2NCH2	1.53E+06	2.4	33360.0
	Declared duplicate reaction...			
1748.	CH3CH2NCH2+O2=HO2+CH3CHNCH2	2.00E+13	0.0	37190.0

```
      Declared duplicate reaction...
1749. CH3CHNCH2+HO2=O2+CH3CH2NCH2                4.65E+12    0.1     -168.0
      Declared duplicate reaction...
1750. CH3CH2NCH2+H=H2+CH3CHNCH2                  3.38E+05    2.4      207.0
      Declared duplicate reaction...
1751. CH3CHNCH2+H2=H+CH3CH2NCH2                  4.32E+06    2.1    20330.0
      Declared duplicate reaction...
1752. CH3CH2NCH2=CH3+CH2NCH2                     5.08E+19   -1.3    76510.0
      Declared duplicate reaction...
1753. CH3+CH2NCH2=CH3CH2NCH2                     1.35E+13    0.0        0.0
      Declared duplicate reaction...
1754. CH3CH2NCH2=NCH2+C2H5                       2.88E+23   -2.0   101600.0
      Declared duplicate reaction...
1755. NCH2+C2H5=CH3CH2NCH2                       9.00E+12    0.0        0.0
      Declared duplicate reaction...
1756. CH3CHNCH2=H+CH2CHNCH2                      1.20E+14    0.0    49300.0
      Declared duplicate reaction...
1757. H+CH2CHNCH2=CH3CHNCH2                      4.00E+13    0.0     1300.0
      Declared duplicate reaction...
1758. H+TMEDA-0-4=TMEDA-2                        2.50E+11    0.5     2620.0
1759. H+TMEDA-0-5=TMEDA-2                        2.50E+11    0.5     2620.0
1760. TMEDA-2=CH3NCH2+N(CH3)2CH2                 1.06E+13    0.1    27125.0
```

UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

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