

亚烷基卡宾与甲醛环加成反应机理的理论研究

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**摘要** 用二阶微扰理论研究了单重态亚烷基卡宾与甲醛发生的三种环加成反应的机理,采用MP2/6-31G~\*方法计算了势能面上各驻点的构型参数、振动频率和能量。根据能量数据可以预言环加成反应(1)的a途径将是单重态亚烷基卡宾与甲醛环加成反应的主要反应通道,该反应由两步组成:(I)

亚烷基卡宾与甲醛生成了一富能中间体(INT1a),是一无势垒的放热反应,(II)

中间体异构化为产物亚烷基环乙烷,其势垒为24.1 kJ·mol<sup>-1</sup>(MP2/6-31G~\*)。

**关键词** [碳烯](#) [环加成反应](#) [势能面](#) [微扰化](#) [甲醛](#) [反应机理](#)

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## Theoretical Study on the Mechanism of the Cycloaddition reaction between Alkylidene carbene and Formaldehyde

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**Abstract** The mechanisms of three cycloaddition reactions of singlet alkylidene carbene and formaldehyde have been studied by using second-order Moller-Plesset perturbation theory. The geometrical parameters, harmonic vibrational frequencies and energies of stationary points on the potential energy surface are calculated by MP2/6-31G~\* method. According to the data of energy, we predict that path a of the cycloaddition reaction (1) would be the major reactive channel of the cycloaddition reactions of singlet alkylidene carbene with formaldehyde, which proceeds in two steps: (I) Alkylidene carbene and formaldehyde form an energy-rich intermediate, through an exothermal reaction with no energy barrier, and (II) the intermediate isomerizes to the product alkylideneoxirane. The energy barrier for the latter step is 24.1 kJ·mol<sup>-1</sup> at MP2/6-31G~\* level.

**Key words** [CARBENE](#) [CYCLOADDITION REACTION](#) [POTENTIAL ENERGY SURFACES](#) [perturbation theory](#) [FORMALDEHYDE](#) [REACTION MECHANISM](#)

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