C-甲基硝酮与硝基乙烯**1,3-**偶极环加成反应及其溶剂效应的理论研究

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摘要 用密度泛函B3LYP方法研究了硝基乙烯与C-甲基硝酮的1,3-偶极环加成反应， 并利用自洽反应场方法(SCRF)计算了环己烷与乙腈这两种溶剂分别对反应所产生的 影响。该反应进行时反应物的接近有四种方式，对气相情况下和上述两种溶剂中的 反应物、四种可能产物及其相应过渡态和反应前期复合物构型分别进行了优化并计算了振动频率。四个反应均为放热反应，且均具有很低的反应势垒，四种产物均容易生成。但在气相反应和以环己烷为溶剂的情况下，生成的产物中endo-4型产物略占优势；而在乙腈溶剂中得到endo-5型略占优势的产物。

关键词 环加成反应 溶剂效应 硝酮 自洽场 硝基化合物 环己烷 乙烯

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Theoretical Studies on the 1,3-Dipolar Cycloaddition of C- Methylnitrone with Nitroethylene and Solvent Effect

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Abstract The 1,3-dipolar cycloaddition reaction of C-methylnitrone with nitroethylene was studied using DFT at the B3LYP/6-31G~* level. Self- consistent reaction field (SCRF) method was used to consider the solvent effect of cyclohexane and acetonitrile. In such reaction the reactants have four approaching modes. The structures and frequencies of reactants, intermediates, transition states and products in different circumstances were optimized and calculated. In any circumstances the four reactions are all exothermic reactions with lower energy barriers, so the four products are produced easily. By calculation it is found that in gas phase and cyclohexane solvent, the energy barrier of endo-4 is the lowest one, while in acetonitrile solvent, the energy barrier of endo-5 is the lowest.

Key words CYCLOADDITION REACTION SOLVENT EFFECT NITRONE SELF-CONSISTENT FIELD NITRO COMPOUNDS CYCLOHEXANE ETHYLENE

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