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亚甲基硅烯与乙烯环加成反应机理的理论研究

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摘要 用二阶微扰和密度泛函理论研究了单重态亚甲基硅烯与乙烯环加成反应的机理,采用MP2/6-31G*和B3LYP/6-31G*方法分别计算了势能面上各驻点的构型参数、振动频率,利用CCSD(T)//MP2/6-31G*和CCSD(T)//B3LYP/6-31G*分别计算了各构型的能量。结果表明,

单重态亚甲基硅烯与乙烯环加成反应的主反应途径为: 两反应物首先生成了一富能络合物INT,

它是一无势垒的放热反应, 放出的能量为13.3 kJ·mol⁻¹。然后该络合物通过过渡态TS2.1

异构化为了四元环活性产物P2.1, 其势垒为32.0 kJ·mol⁻¹。

关键词 [亚甲基硅烯,环加成反应,势能面,二阶微扰和密度泛函理论](#)

分类号

Theoretical Study on the Mechanism of the Cycloaddition Reaction between Methylidenesilene and Ethylene

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Abstract The mechanism of a cycloaddition reaction between singlet methylidenesilene and ethylene has been investigated with MP2/6-31G* and B3LYP/6-31G* methods, including geometry optimization and vibrational analysis for the involved stationary points on the potential energy surface. Energies of the involved conformers were calculated by CCSD(T)//MP2/6-31G* and CCSD(T)//B3LYP/6-31G* methods, respectively. The results show that the dominant reaction pathway of the cycloaddition reaction is that a complex intermediate is firstly formed between the two reactants through a barrier-free exothermic reaction of 13.3 kJ/mol, and the complex is then isomerized to a four-membered ring product P2.1 via a transition state TS2.1 with a barrier of 32.0 kJ/mol.

Key words [methylidenesilene](#) [cycloaddition reaction](#) [potential energy surface](#) [second-order Moller-Plesset perturbation and density functional theory](#)

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