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FULL PAPERS

亚烷基锡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烷基锡烯与乙烯环加成反应的机理,采用MP2/3-21G*和B3LYP/3-21G*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)//MP2/3-21G* 和CCSD(T)//B3LYP/3-21G*分别计算了各构型的能量。结果表明，
单重态亚烷基锡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中间体，
它是一无势垒的放热反应，放出的能量为39.7 kJ•mol^{-1}。然后该中间体通过过渡态$TS_{2.1}$
异构化为了四元环活性产物$P_{2.1}$，其势垒为66.8 kJ•mol^{-1}。

关键词 亚烷基锡烯, 环加成反应, CCSD(T)//MP2/3-21G* ,CCSD(T)//B3LYP/3-21G* 方法, 势能面
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A Theoretical Study on the Mechanism of the Cycloaddition Reaction between Alkylidenestannylene and Ethylene

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Abstract The mechanism of a cycloaddition reaction between singlet alkylidenestannylene and ethylene has been investigated with MP2/3-21G* and B3LYP/3-21G* methods, including geometry optimization and vibrational analysis for the involved stationary points on the potential energy surface. Energies for the involved conformations were calculated by CCSD(T)//MP2/3-21G* and CCSD(T)//B3LYP/3-21G* methods, respectively. The results show that the dominant reaction pathway of the cycloaddition is that an intermediate (INT) is firstly formed between the two reactants through a barrier-free exothermic reaction of 39.7 kJ/mol, and the intermediate then isomerizes to a four-membered ring product ($P_{2.1}$) via a transition state $TS_{2.1}$with a barrier of 66.8 kJ/mol.

Key words alkylidenestannylene cycloaddition reaction CCSD(T)//MP2/3-21G* and CCSD(T)//B3LYP/3-21G* methods potential energy surface

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