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研究简报

硅炔氢加成生成甲硅烷基硅烯的量子化学研究

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摘要 利用量子化学从头算和密度泛函理论(DFT), 研究了硅炔和氢气分子加成生成甲硅烷基硅烯的反应机理. 在B3LYP/6-311G**水平上, 全参数优化了反应通道上各驻点(反应物、过渡态和产物)的几何构型, 计算出了它们的振动频率和零点振动能(ZPVE), 并对它们进行了振动分析, 以确定过渡态的真实性. 各物质总能量由QCISD(T)/6-311G**// B3LYP/6-311G**给出, 并对能量进行了零点能校正. 计算表明, 硅炔与氢分子加成反应可生成稳定的甲硅烷基硅烯. 热力学与动力学计算表明, 反应过程是一个放热、熵减少而自发趋势和反应程度较大的反应.

关键词 硅炔 加成反应 密度泛函 过渡态 反应通道

分类号

Quantum Chemistry Research for the Silicyl Alkene Produced by Addition Reaction of Disilyne with Hydrogen

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Abstract The mechanism of the addition reaction of disilyne and hydrogen has been studied by using *ab initio* calculation of quantum chemistry and density functional theory. All of the structures of the stationary points on the reaction channels such as reactants, transition states and products have been optimized at B3LYP/6-311G** level; the vibration frequencies and zero-point vibration energy have been also calculated and analyzed to determine the reality of the transition states. The total energies of the matters were given by the method QCISD(T)/6-311G**//B3LYP/6-311G** and corrected with zero-point energies. The computa-tion indicated that the stable silicyl alkene is produced by the addition reaction of silicon alkyne and hydro-gen. Thermodynamics and dynamics computation indicated that the reaction process is exothermic, has an entropy reduction and spontaneous tendency, and the extent of reaction is large.

Key words disilyne addition reaction density function transition state reaction channel

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