化学学报 2005 63 (8): 703-710 ISSN: 0567-7351 CN: 31-1320/06

研究论文

CH_3与NO反应机理的理论研究

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收稿日期 2004-4-30 修回日期 2005-1-1 网络版发布日期 接受日期

摘要 采用密度泛函B3LYP/6-311G**和高级电子相关耦合簇CCSD(T)/6-311G**方法计算研究了CH_3与NO反应机理, 全参数优化了反应势能面上各驻点的几何构型, 用内禀反应坐标(IRC)计算和频率分析方法, 对过渡态进行了验证. 研究结果表明: CH_3与NO是一多通道多步骤的复杂反应, 可以分别在单重态和三重态势能面上进行. 经过缔合, 氢转移和离解等复杂过程, 最终得到8种产物(**P1**～**P8**).

关键词 反应机理 CH_3 NO 密度泛函

分类号

Theoretical Study on the Reaction of CH_3 with NO

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Abstract The reaction between methyl radicals and nitric oxide has been studied by using the B3LYP/6-311G** and the high-level electron-correlation CCSD(T)/6-311G** levels. The geometries of reactants, the transition states and the products were completely optimized. All the transition states are verified by the vibrational analysis and the internal reaction coordinate (IRC) calculations. The results show that the reaction is of multi-channel and multi-step. It may proceed on singlet and triplet potential energy surface (PES). Eight products, **P1**～**P8**, are obtained via the complex reaction channels, *i.e.* association, H-shift and dissociation.

Key words reaction mechanism methyl radical nitric oxide density functional theory

DOI:

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