化学学报 2000 58 (5): 519-523 ISSN: 1001-604X CN: 31-1547/O6

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CH自由基和**NO~2**反应研究**: II.**反应的动力学计算

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 采用MP2(FULL)/6-31G(d)方法从动力学计算上探讨了CH自由基与NO~2反应的可能途径,找到了反应物,
中间体及产物之间的能量通道和过渡态,报道了它们的构型、
电子态及能量。并通过频率分析和IRC方法对所有的过渡态进行了验证。在此基础上求出了各步反应的活化能。在以前热力学研究的基础上,
对于可能的反应通道进一步作了动力学分析,找到了反应主产物通道的分支比,与实验得到的分支比基本吻合。

关键词 氧化氮 二氧化氮 烃 自由基反应 反应动力学 活化能 过渡态

分类号 0643

An ab initio study on the reaction of CH and NO~2: II. Mechanism of the reaction

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Abstract The reaction of methylidyne radical with molecule NO~2 was studied theoretically by using MP2(FULL)/6-31G(d) and QCISD(T)/6-31G(d). The reaction paths were found both for the formation of intermediates and the dissociation of some intermediates to form the products. The energies and structures of important intermediates and transition states were reported for the first time. The reaction path was followed from the transition state both to the reactant and the product direction by using the intrinsic reaction coordinate (IRC) method. By thermodynamic and mechanic analysis, the main reaction path channel was detected, the main products were found, and branching ratio was calculated, which was in good agreement with the experimental results.

Key words NITROGEN OXIDE HYDROCARBONS FREE RADICAL REACTION REACTION KINETICS ACTIVATION ENERGY TRANSITION STATE

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