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CH自由基和NO~2反应研究: I. 反应的热力学计算

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摘要 探讨了CH自由基与NO~2反应的可能路径,通过计算确定了反应物,产物和稳定中间体的电子状态和平衡构型,并运用Gaussian-3方法和MRCISD方法对可能的反应路径进行了热力学计算。在多数情况下与实验值符合较好。对于个别与理论计算差别较大的实验值进行了评述。

关键词 热力学计算 焓 氧化氮 二氧化氮 烃 自由基反应

分类号 0642

An ab initio study on the reaction of CH and NO~2: I. Thermodynamics of the reaction

Zhu Kake,Gan Zhengting,Su Kehe,Wang Yubin,Wen Zhenyi

Abstract The possible products and intermediates of the title reaction were studied theoretically by means of the Gaussian-3 model calculation. The stationery structures and the electronic states of the reactants, products and intermediates were found. Their energies were detected. The thermodynamics of possible reactions are discussed. The calculated results were in good agreement with the recent experimental ones. Some of the extraordinary values were also studied by MRCISD method, and finally the discrepancies were discussed.

Key words THERMODYNAMIC CALCULATIONS ENTHALPY NITROGEN OXIDE HYDROCARBONS FREE RADICAL REACTION

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