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单重态**CCl2**与**O3**反应机理的理论研究

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摘要 用量子化学从头算方法,研究了单重态CCl2与O3反应的机理。在HF/6-31G(d)水平上用梯度解析技术全参数优化上述反应的反应物、中间体、过渡态和产物构型,MP2/6-31G(d)//HF/6-31G(d)方法计算能量。给出了有关化合物的结构数据。结果表明:CCl2与O3首先生成富能中间体CCl2O3,然后中间体裂解生成CCl2O和O2。该反应为强放热反应,放出的热量为516.88kJ.mol^-^1[MP2/6-31G(d)//HF/6-31G(d)]。通过内禀反应坐标(IRC)计算,获得了沿反应途径的势能剖面。

关键词 氯化碳 臭氧 反应机理 单重态 从头计算法

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A theoretical study of the mechanism of the reaction between CCl2 and O3

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Abstract The mechanism of the reaction of the singlet CCl2 with O3 has been studied by using ab initio method at 6-31G(d) level. The geometries of the reactants, intermediate, transition state and products of the reaction have been optimized with the gradient technique. The single point energy calculations of the species have been performed by MP2/6-31G(d) method. The relative structure data of the reactants, intermediate, transition state and products are given. The mechanism proposed here is that the reactant molecules combine with each other first to form an energy-enriched intermediate, followed by decomposition of the intermediate to give CCl2O and O2. The reaction is exothermic by 516.88kJ.mol^-^1 [MP2/6-31G(d)//HF/6-31G(d)]. The potential energy profile along reaction path has been obtained through IRC calculations.

Key words OZONE REACTION MECHANISM SINGLET AB INITIO CALCULATION

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