研究论文

CH$_2$＝CHCl与O(^{3}P)反应的理论研究

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摘要　用量子化学密度泛函理论和QCISD (Quadratic configuration interaction calculation)方法, 对O(^{3}P)与CH$_2$CHCl的反应进行了理论研究. 在UB3LYP/6-311＋＋G(d,p), UB3LYP/6-31＋＋G(3df, 3pd)计算水平上, 优化了反应物、产物、中间体和过渡态的几何构型, 并在UQCISD(T)/6-311＋＋G(2df,2pd)水平上计算了单点能量. 为了确证过渡态的真实性, 在UB3LYP/6-311＋＋G(3df,3pd)水平上进行了内禀坐标(IRC)计算和频率分析, 并确定了反应机理. 研究结果表明, 反应主要产物为CH$_2$CHO和Cl.

关键词　CH$_2$＝CHCl　O(^{3}P)　反应机理密度泛函理论　密度泛函理论

分类号

Theoretical Study on Reaction between O(^{3}P) and CH$_2$＝CHCl

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Abstract By means of the density functional theory and QCISD (Quadratic configuration interaction calculation) methods, the reaction between O(^{3}P) and CH$_2$＝CHCl has been studied. The geometries for the reactants, products, intermediates and transition states have been completely optimized at UB3LYP/6-311＋＋G(d,p), UB3LYP/6-311＋＋G(3df,3pd) computational levels. All the transition states have been verified by the vibrational analysis and the internal reaction coordinate calculations. The mechanism of the reaction has been confirmed. In view of energies, the channel of forming the products CH$_2$＝CHO＋Cl is more favorable than the other channels.

Key words CH$_2$＝CHCl　O(^{3}P)　reaction mechanism　density functional theory

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