

H₂O(HOD) + Cl → HCl(DCl) + OH(OD)反应动态学的理论研究

曹晓燕, 李宗和, 刘若庄

北京师范大学化学系

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摘要 用从头算方法, 获得了H₂O + Cl → HCl + OH(R1), HOD + Cl → DCl + OH(R2), HOD + Cl → HCl + OD(R3)反应的内禀反应坐标(IRC)。根据传统过渡态、变分过渡态理论及相应的隧道效应校正, 计算了反应的速率常数。对已有实验速率常数值的R1反应, 我们计算的结果和实验一致。根据Truhlar的振动选态公式, 分别讨论了激发HOD中OH, OD振动模式对反应速率的影响, 得到激发HOD中的OH振动模式将有利于产物OD + HCl生成, 和实验的结论相一致。

关键词 [氯](#) [重水](#) [从头算法](#) [反应速度常数](#) [过渡态理论](#)

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Theoretical studies on reaction dynamics of H₂O(HOD) + Cl → HCl(DCl) + OH(OD)

CAO XIAOYAN, LI ZONGHE, LIU RUOZHUANG

Abstract Based on ab initio methods with gradient technique, the intrinsic reaction coordinate (IRC) of the reactions H₂O + Cl → HCl + OH(R1), HOD + Cl → DCl + OH(R2) and HOD + Cl → HCl + OD(R3) are traced by using numerical method. The theoretical rate constants for the R1-R3 reactions are calculated by the conventional transition-state theory, variational transition-state theory and semiclassical vibrationally adiabatic transmission coefficients. The calculated rate constants for the R1 reaction are in good agreement with the experimental results. The state-selected reaction rate constants for the R2, R3 reactions are also calculated. It is concluded that the excitation of reactant HOD (n_{OH}=1) is beneficial to the production of product HCl + OD. Their result agrees with experiment.

Key words [CHLORINE](#) [HEAVY WATER](#) [AB INITIO CALCULATION](#) [REACTION RATE CONSTANT](#) [TRANSITION STATE THEORY](#)

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