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三维含时量子散射研究**H + CIH**体系

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摘要 用三维含时量子散射理论模拟了H+CIH体系在BW2,mBW2,G3势能面上的动力学行为，其计算结果表明，振动量子态对反应几率影响很大；势能面的地形对转动量子态如何影响反应几率起重要作用；反应几率表现出“黄金规则”，此外，BW2,mBW2势能面上的反应几率几乎相同，而G3势能面上的反应几率较前者低，大概由于G3的势垒高的缘故。

关键词 含时量子散射 三维 势能面 动力学 反应几率

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Three dimensional (3D) and time-dependent (TD) quantum dynamics study of the H + CIH system

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Abstract Dynamic behavior of system HCl + H on BW2, and G3 potential energy surfaces (PESs) has been simulated, using 3D and TD quantum scattering theory. The calculated results show that vibrational state of HCl influences its reaction probabilities greatly, the feature of PESs plays considerable role for how rotational state affecting its reaction probabilities, and the reaction probabilities appear 'Gold Rule' . In addition, the reaction has almost the same properties on BW2 and mBW2 PESs. However, the reaction probabilities on G3 PES are lower than on BW2, mBW2 because its barrier is higher.

Key words THREE-DIMENSIONAL POTENTIAL ENERGY SURFACES DYNAMICS

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