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三维H+H~2(v, j)→H~2(v', j')+H反应中复合态生成及产物转动 态分布的量子 散射理论研究

吕文彩,蔡政亭,邓从豪

山东大学理论化学研究室.济南(250100)

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摘要 用排列通道线性组合-散射波函数(LCAC-SW,linearcombinationofarrangementchannels-scatteringwavefunction)量子反应散射方法计算了H+H~2(v,j)→H~2(v',j')+H三维态-态反应几率,分析了反应体系的复合态生成(或能量共振结构),并由产物的转动态分布解释了能量共振的起源来自于平动态-内态之间的干涉效应。

关键词 氢 复合态 量子散射理论 转动态

分类号 0641

A quantum scattering theoretical study on the compound-state formation and the rotational-state distribution of the product for the three-dimensional state-to-state H+H~2(v, j)→H~2(v', j')+H reaction

Lu Wencai,Cai Zhengting,Deng Conghao

Shandong Univ, Theoret Chem Lab.Jinan(250100)

Abstract This paper reports the three-dimensional state-to-state reaction probabilities for the H+H~2(v, j)→H~2(v', j')+H system calculated by LCAC-SW (linear combination of arrangement channels-scattering wavefunction) approach. The compound-state formation (or energy resonance structure) of this system is analyzed. The results of the rotational-state distribution for the product of this reaction show that the energy resonance is due to the interference effect between the translational motion of the system and the internal state of the reactant.

Key words HYDROGEN ROTATIONAL STATE

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