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用**DVR**方法研究**Ar-HF**和**Ar-DF**的振转光谱

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摘要 本文用离散变量表示(DVR)方法研究了Ar-HF和Ar-DF体系的振转光谱。对这两个体系的已观测到的振转能级, 用DVR方法得到的计算值与实验结果十分吻合, 误差一般小于0.1cm^-^1, 最大偏差为0.24cm^-^1对Ar-HF的(1113)态。该研究结果与Hutson等用耦合孔道法得到的计算结果基本一致, 但对(3210)振动能级和对(3002)-(3110)态的能级分裂值, 本文计算结果更接近观测值。

关键词 氩 氟化氢 振动态 势能面 国家教委高等学校博士学科点专项科研基金 离散变量表示

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Studies of the rovibrational energy levels of Ar-HF and Ar-DF molecules by using DVR method

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Abstract The rovibrational energy levels of van der Waals complexes Ar-HF and Ar-DF have been obtained by using a numerical calculation based on the discrete variable representation (DVR) method. These calculated energy levels are in good agreement with the observed levels. The higher-order angular anisotropy and the vibrational depdndence of the intermolecular potential energy surface have been investigated by comparision between the calculated and observed values. The isotopic shift rule of the van der Waals stretching and bending vibrational frequency of Ar-DF relative to Ar-HF system has been obtained from DVR calculation of these sysem. The blue shift effects of the van der Waals vibrational frequencies with v appears when HF stretch vibrational excitation is increased.

Key words ARGON HYDROGEN FLUORIDE VIBRATIONAL STATE POTENTIAL ENERGY SURFACES

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