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AB INITIO CALCULATIONS OF ANHARMONIC VIBRATIONAL SPECTROSCOPY FOR HYDROGEN FLUORIDE (HF)_N (N=3,4) AND MIXED HYDROGEN FLUORIDE/WATER (HF)_N(H₂O)_N (N=1,2)



Ab Initio Calculations of Anharmonic Vibrational Spectroscopy for Hydrogen Fluoride (HF)_N (N=3,4) and Mixed Hydrogen Fluoride/Water (HF)_N(H₂O)_N (N=1,2) Clusters
NASA Technical Reports Server (NTRS), et al., Galina M. Ghaban

Bibliogov, United States, 2013. Paperback. Book Condition: New. 246 x 189 mm. Language: English. Brand New Book ***** Print on Demand *****.Anharmonic vibrational frequencies and intensities are computed for hydrogen fluoride clusters (HF)_n with n=3,4 and mixed clusters of hydrogen fluoride with water (HF)_n(H₂O)_n where n=1,2. For the (HF)₄(H₂O)₄ complex, the vibrational spectra are calculated at the harmonic level, and anharmonic effects are estimated. Potential energy surfaces for these systems are obtained at the MP2/TZP level of electronic structure...

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