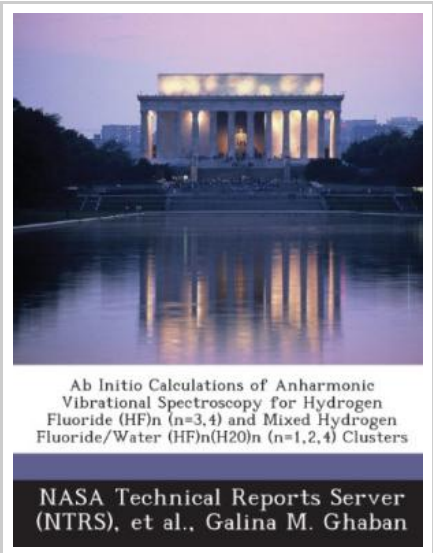

AB Initio Calculations of Anharmonic Vibrational Spectroscopy for Hydrogen Fluoride (Hf)N (N=3,4) and Mixed Hydrogen Fluoride/Water (Hf)N(h20)N (N=1,2

By 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 theory. Vibrational states are calculated from the potential surface points using the correlation-corrected vibrational self-consistent field (CC-VSCF) method. The method accounts for the anharmonicities and couplings between all vibrational modes and provides fairly accurate anharmonic vibrational spectra that can be directly compared with experimental results without a need for empirical scaling. For (HF)n, good agreement is found with experimental data. This agreement shows that the MP2 potential surfaces for these systems are reasonably reliable. The accuracy is best for the stiff intramolecular modes, which indicates the validity of MP2 in describing coupling between intramolecular and intermolecular degrees of freedom. For (HF)n(H2O)n experimental results are unavailable. The computed intramolecular frequencies show a strong dependence on cluster size. Intensity features are

Reviews

This book is definitely not straightforward to get started on studying but extremely exciting to read. It is really simplistic but shocks in the 50 percent of the ebook. Once you begin to read the book, it is extremely difficult to leave it before concluding.

-- ***Ally Reichel***

This publication is amazing. It is definitely basic but shocks in the fifty percent of your publication. You wont feel monotony at anytime of your own time (that's what catalogues are for concerning if you question me).

-- ***Prof. Kirk Cruickshank DDS***