THEORETICAL AND EXPERIMENTAL STUDY OF THE IR SPECTRUM OF THE BrHI AND BrDI ANIONS

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A new potential energy surface and dipole moment surface were constructed for $BrHI^-$ by a 3-D spline interpolation of ab initio data at the MRCI/aVQZ level of theory and basis set, with ECP's for the halogens. "Exact" vibrational calculations were performed on this potential energy surface for $BrH(D)I^-$ using two very different codes. The asymmetric stretch and bending modes are found to be strongly coupled, and are shown to be in close 1:2 Fermi resonance. This is verified by a simple de-perturbation of the wavefunctions. The IR transition probabilities were also obtained by integrating dipole moment matrix elements over both vibrational and rotational coordinates. Excellent agreement was found with the recently measured IR spectrum of $BrH(D)I^-$ using the Ar-messenger technique by Neumark and co-workers.