SPECTROSCOPIC AND $AB\ INITIO$ STUDIES OF THE HBF FREE RADICAL

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Subsequent to our spectroscopic detection of the HBX (X = F, Cl, Br) free radicals,[a] we have studied the electronic spectrum of the jet-cooled HBF free radical in detail. The $\tilde{A}^2A' - \tilde{X}^2A''$ band system in the 600 - 700 nm region is assigned as the transition between two Renner-Teller components of a $^2\Pi$ state in which the radical is bent in the ground state and linear in the excited state. High resolution studies of HBF and DBF have allowed us to resolve the spin and asymmetry splittings in the spectra and combination differences have been used to obtain the ground state molecular structure. As an aid to understanding the complex vibrational structure in the spectrum, ground and excited state potential energy surfaces (PESs) have been calculated using high-level $ab\ initio$ methods. The vibronic energy levels were obtained from the PESs by variational methods and were used to assign the vibrational quantum numbers of the observed bands of H(D)^{11}BF and H(D)^{10}BF. Single vibronic level emission spectra have also been recorded to establish the ground state vibrational frequencies.

[a] S-G. He, F. X. Sunahori and D. J. Clouthier *J. A. C. S.* **127** (10814), 2005.