AN EXPERIMENTAL AND QUANTUM CHEMICAL STUDY OF THE ELECTRONIC SPECTRUM OF THE HBCl FREE RADICAL

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The chloroborane (HBCl) free radical has a complex electronic spectrum in the visible that involves a transition from a bent ground state to a linear excited state, both of which are the Renner-Teller components of what would be a $^2\Pi$ state at linearity. We have used the synchronous-scan LIF and single vibronic level emission techniques to untangle the many overlapping vibronic bands and assign upper state K quantum numbers for jet-cooled HBCl and DBCl. The radicals were produced in a pulsed electric discharge jet using a precursor mixture of boron trichloride (BCl_3) and hydrogen or deuterium in high-pressure argon. As an important aid to understanding the data, the ground and excited state high level $ab\,initio$ potential energy surfaces (PES) have been calculated and the vibrational levels obtained variationally. The calculated ground state levels are in excellent agreement with the emission data validating the quality of the PES. Aside from an approximately 100 cm^{-1} shift in the upper state electronic term value, the calculated excited state vibrational energy levels and isotope shifts match the LIF data very well, allowing the observed bands to be assigned with confidence.