THE ELECTRONIC SPECTRUM AND MOLECULAR STRUCTURE OF HAsO, THE ARSENIC ANALOG OF HNO

ROBERT A. GRIMMINGER, DENNIS J. CLOUTHIER, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA*.

The previously unknown, closed shell transient species HAsO has been observed in the 525 - 665 nm region by laser-induced fluorescence (LIF) spectroscopy. HAsO and its deuterated isotopologue were produced in a pulsed discharge jet using a precursor mixture of AsH_3 and CO_2 in high pressure argon. Vibrational analysis of low-resolution LIF and single vibronic level (SVL) emission spectra has established the ν_2 and ν_3 vibrational frequencies in both states. High resolution spectra of the 0_0^0 bands of both HAsO and DAsO have been recorded and rotationally analyzed, proving that the observed electronic transition is $\tilde{A}^1\mathrm{A}'' - \tilde{X}^1\mathrm{A}'$. Effective molecular structures for the ground and excited states have been determined from the rotational constants of the two isotopologues. The HAsO angle decreases upon electronic excitation in contradiction to the geometry change predicted using Walsh's angular orbital correlation diagrams. Reasons for this anomalous behavior will be discussed.