ELECTRONIC STRUCTURE AND SPECTROSCOPY OF OThF

ARIANNA RODRIGUEZ, JIARUI YAN, JIANDE HAN, MICHAEL HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA, USA*.

Electronic spectra of gas-phase polyatomic actinide species such as UO_2[a] and UF_2 have yielded electronic spectra where the rotational structure cannot be resolved at a resolution of 0.06 cm^{-1}. The molecules are predicted to be linear, so the lack of resolvable rotational structure appears to be a consequence of high electronic state densities. To probe this notion we have examined OThF, where the electronic complexity is reduced as there is only one unpaired electron in the metal-centered orbitals. Gas phase OThF has been generated by laser ablating Th metal in the presence of trace amounts of SF_6 and O_2. Six prominent vibronic bands were observed in the range 27700-28900 cm^{-1}. These bands were detected using both REMPI and LIF techniques. An additional intense band was observed at 22430 cm^{-1}. TD-DFT calculations indicate that OThF is a bent molecule in the ground and low-lying electronically excited states. Attempts to obtain rotationally resolved data and computational studies of OThF are in progress.

[a]Han, J.; Goncharov, V.; Kaledin, L. A.; Komissarov, A. V.; Heaven, M. C., Electronic spectroscopy and ionization potential of UO_2 in the gas phase. *Journal of Chemical Physics* **2004**, *120*, 5155-5163.