

IONIZATION MEASUREMENT AND SPECTROSCOPY OF ThS AND ThS⁺

J. H. BARTLETT, M. C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322.*

Gas-phase thorium sulfide has been produced via laser ablation of thorium in a jet-cooled expansion of 0.1% H₂S/He carrier gas. Electronic spectra have been recorded for the first time by laser-induced fluorescence (LIF) over the region 17500-23650 cm⁻¹. Resonance-enhanced multiphoton ionization (REMPI) was used in conjunction with a Wiley-McLaren time-of-flight mass spectrometer to confirm LIF assignments of seven rotationally-resolved bands belonging to ThS. Dispersing fluorescence from the [22.13]¹Π-X¹Σ_g transition revealed a vibrational progression of the ground electronic state of ThS, for which the vibrational constants were $\omega_e = 520.0(7)$ cm⁻¹ and $\omega_e\chi_e = 11.0(9)$ cm⁻¹. An accurate value for the ionization potential of ThS as well as term energies of ThS⁺ up to v⁺ = 7 in the ²Σ⁺ ground state and v⁺ = 3 in the ²Δ_{3/2} first excited state have been obtained using two-photon pulsed-field ionization zero kinetic energy photoelectron spectroscopy (PFI-ZEKE). Vibrational constants for these states have also been determined. High-level electronic structure calculations performed for ThS and ThS⁺ gave term energies and molecular parameters that are in excellent agreement with the experimental results. The change in bond characteristics upon ionization of ThS is found to be consistent with that observed for HfO, HfS, and ThO.