

SPECTROSCOPIC STUDY OF ThCl^+ BY TWO-PHOTON IONIZATION

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Despite the irreplaceable role experimental data plays for evaluating the performance of computational predictions, diatomic actinide species have not received much spectroscopic attention. As an early actinide element, thorium-containing species are ideal candidates for these types of studies. The electronic structure is expected to be relatively simple compared to later actinides, and therefore allows straightforward assessment of calculations. Here, we have studied ThCl^+ for the first time via resonant two-photon ionization of jet-cooled ThCl produced by laser ablation of the metal reacted with dilute Cl_2 . Laser-induced Fluorescence (LIF) spectra have been recorded for the neutral molecule from $16000 - 23500 \text{ cm}^{-1}$ in search of a suitable intermediate state for subsequent two-photon ionization experiments. Monochromator dispersion of the fluorescence has recovered the ground state vibration and anharmonic constants of ThCl . Resonant Two-Photon Ionization (R2PI) within a time-of-flight mass spectrometer was used to confirm ThCl production, and Pulsed Field Ionization Zero Kinetic Energy photoelectron spectroscopy (PFI-ZEKE) has been performed to identify the ionization energy as well as several of the low-lying states of the ThCl^+ molecule. These constants have been predicted at the CASPT2 and CCSD(T) levels of theory, and a discussion of the calculations' performance will be presented alongside the recorded spectra.