

PROBING THE ELECTRONIC STRUCTURE OF UO^+ WITH HIGH-RESOLUTION PHOTOELECTRON SPECTROSCOPY

VASILY GONCHAROV AND MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322.*

The pulsed field ionization - zero kinetic energy photoelectron (PFI-ZEKE) technique has been used to observe the low-lying energy levels of UO^+ . Rotationally resolved photoelectron spectra were recorded for the ground state and the first 9 electronically excited states. Extensive vibrational progressions were observed. For all observed vibronic states of UO^+ , Ω^+ assignments were unambiguously determined from observations of the first rotational lines in PFI-ZEKE photoelectron spectra. Accurate values of term energies, vibrational frequencies and anharmonicity constants for the observed low-lying energy levels of UO^+ along with the accurate values for the ionization energies of UO and U will be reported.

The pattern of observed low-lying electronic states indicates that they originate from the $\text{U}^{3+} [5f^3] \text{O}^{2-}$ configuration, where the Uranium ion-centered interactions between $5f$ electrons are significantly stronger than interactions with the intra-molecular electric field. The latter lifts the spatial degeneracy of the U^{3+} ion-core states, but the total angular momentum quantum numbers remain reasonably well defined.

The comparison between the experimental data and the results of theoretical predictions for the electronic structure of UO^+ will be also presented.