UNDERSTANDING UO_2^+ BY MODELING ELECTRONIC AND VIBRATIONAL SPECTROSCOPY

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Spin-orbit configuration interaction (*SO-CI*) continues to be a valuable electronic structure tool in understanding the electronic states of small actinide containing molecules.[1] Recent interest has a variation of a familiar actinide molecule, UO_2^+. The additional electron would appear to be a simple alteration or perturbation to an understood system, but experimentally it presents some questions for theory to investigate. Principal questions involve characterization of the lowest electronic states in UO_2^+ involves occupation of the either the $5f_\phi$ or the $5f_\delta$ non-bonding orbitals and some simple excitation generates a multitude of electronic states. Use of self-consistent field with improved virtual orbital calculations (*SCF*) will again be the foundation of the *SO-CISD* determination of the potential energy surfaces (*PES*) of the ground and low lying excited states of the UO_2^+ molecule. *PES* evaluation will occur along the internal coordinates of r_{UO} and $\theta_{\angle OUO}$, and will be variationally fit to determine bound vibrational levels present within the ground and low-lying excited states. Vibrational and electronic energy levels should help clarify and describe new and interesting spectra and other properties.

[1]Gibson, J. K.; Haire, R. G.; Marcalo, J.; de Matos, A. P.; Mrozik, M. K.; Pitzer, R. M.; Bursten, B. E. *Organomet.* **2007**, *26*(16), 3947–3956.