

## SPIN-ORBIT COUPLING EFFECTS ON THE ELECTRONIC PROPERTIES OF $U(\eta^7\text{-C}_7\text{H}_7)_2^-$ ANION

JUN LI and BRUCE E. BURSTEN, *Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.*

The ground state and the low-lying excited states have been determined for the title compound using density functional theory (DFT) with inclusion of scalar (mass-velocity and Darwin) and spin-orbit relativistic effects. Geometry optimization of the  $U(\eta^7\text{-C}_7\text{H}_7)_2^-$  anion with the inclusion of only the scalar relativistic effects leads to a structure that is in good accord with experiment, indicating that spin-orbit effects are not very important for determining the geometry and hence the vibrational frequencies of the ground state. As expected, the spin-orbit effects are indeed significant for the energy levels, ionization energies, and electronic transition energies involving uranium d- and f-relevant orbitals. With inclusion of spin-orbit coupling, the ground state of the  $U(\eta^7\text{-C}_7\text{H}_7)_2^-$  anion is  $E_{13/2}$  with  $(f\sigma + f\pi)^1$  configuration, which is followed by excited states of  $E_{9/2} (f\phi) \ll E_{11/2} (f\pi) < E_{13/2} (f\sigma + f\pi) < E_{7/2} (f\phi) \ll E_{1/2} (d\sigma) \ll E_{11/2} (f\delta) < E_{9/2} (f\delta)$  in the double-group representations. This state ordering is exactly the same as deduced from an electron spin resonance experiment. The ionization energies, electronic transition energies, magnetic moment, and ground state vibrational frequencies have been predicted for further experimental comparison.