

## ELECTRONIC STATES OF ACTINYL IONS

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Actinyl ions,  $\text{MO}_2^{2+}$ , and the corresponding  $\text{MO}_2^+$  ions, where M is an actinide metal, are characterized by very strong bonds to the two oxygens. These axial bonds involve the metal  $\sigma$  and  $\pi$  orbitals to moderate-to-strong extents, thus raising the corresponding antibonding orbitals to high energy. Thus the low-lying (approximately degenerate) metal orbitals are  $5f\delta$  and  $5f\phi$ . The ground states and low-lying excited states of these ions can be described systematically as weak-field states based on this reduced space of  $5f$  orbitals. Higher excited states are equally well characterized as excitations from the bonding  $\sigma_u$  MO into this space. The general order of strengths of interactions is

axial field > electron repulsion between open-shell electrons > spin-orbit > equatorial field

The coupling, although intermediate, is closest to  $\Lambda$ -S, implying the utility of Hund's Rules.