

MAR17-2016-020003

Abstract for an Invited Paper  
for the MAR17 Meeting of  
the American Physical Society

### **The Consequences of Spin-Orbit Coupling on the $5d^3$ Electronic Configuration**

A. D. CHRISTIANSON, Oak Ridge National Laboratory

The impact of spin-orbit coupling on collective properties of matter is of considerable interest. The most intensively investigated materials in this regard are Iridium-based transition metal oxides which exhibit a host of interesting ground states that originate from a  $5d^5$   $J_{\text{eff}} = 1/2$  electronic configuration. Moving beyond the  $J_{\text{eff}} = 1/2$  paradigm to other electronic configurations where spin-orbit coupling plays a prominent role is a key objective of ongoing research. Here we focus on several Osmium-based transition metal oxides such as  $\text{NaOsO}_3$ ,  $\text{Cd}_2\text{Os}_2\text{O}_7$ ,  $\text{Ca}_3\text{LiOsO}_6$ ,  $\text{Sr}_2\text{ScOsO}_6$ ,  $\text{Ba}_2\text{YOsO}_6$ , and  $\text{Sr}_2\text{FeOsO}_6$ , which are nominally in the  $5d^3$  electronic configuration. Within the LS coupling picture and a strong octahedral crystal field, the  $5d^3$  configuration is expected to be an orbital singlet and spin-orbit effects should be minimal. Nevertheless, our neutron and x-ray scattering investigations of these materials as well as investigations by other groups show dramatic effects of spin-orbit coupling including reduced moment magnetic order, enhanced spin-phonon coupling, and large spin gaps. In particular, the anisotropy induced by spin-orbit coupling tips the balance of the frustrated interactions and drives the selection of particular magnetic ground states. To understand the mechanism driving the spin-orbit effects, we have explored the ground state  $t_{2g}$  manifold with resonant inelastic x-ray scattering and observe a spectrum inexplicable by an LS coupling picture. On the other hand, an intermediate coupling approach reveals that the ground state wave function is a  $J=3/2$  configuration which answers the question of how strong spin-orbit coupling effects arise in  $5d^3$  systems.