

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Magnetic and Orbital Excitations in $\text{Sr}_3\text{CuIrO}_6$ ¹ J.P. HILL, X. LIU, M. DEAN, W. YIN, A. TSVELIK, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, NY 11973, J. KIM, D. CASA, M.H. UPTON, APS, Argonne National Laboratory, Illinois 60439, USA, H. GRETARSSON, Y.-J. KIM, Dept. of Physics, University of Toronto, Canada M5S 1A7, T. QI, G. CAO, Dept. of Physics and Astronomy, U. Kentucky, Kentucky 40506., L. HOZOI, V. KATUKURI, J. V.D. BRINK, Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — We report resonant inelastic x-ray scattering studies of the one-dimensional $\text{Sr}_3\text{CuIrO}_6$ at the Ir L_3 edge, with $\Delta E=40$ meV. At high energies, we find peaks at 0.6 eV, 0.9 eV, 3 eV, 4 eV and 6 eV. These peaks are non-dispersive, well-defined excitations. On the basis of quantum chemistry calculations, we are able to identify the first two as excitations within the t_{2g} manifold and the next two as between the t_{2g} and e_g manifolds, together with charge transfer excitations from the O $2p$ to the Ir $5d$. The 6 eV feature is another $t_{2g} - e_g$ excitation. From these we are able to determine both the spin-orbit and non-cubic crystal field splittings. We find that they are of comparable strength. In addition, magnetic excitations are observed, corresponding to excitations of the $j_{1/2}$ isospin. We find these are highly dispersive along the chain direction with a bandwidth of 20 meV and a gap of 30 meV. These results allow a complete modeling of the spin and orbital degrees of freedom in this model compound and we conclude an atomic, spin-orbit coupled description works well.

¹Work performed at BNL was supported by US DOE, Office of Science, DMSE under contract no. DE-AC02-98CH10886.

John Hill
Condensed Matter Physics and Materials Science,
Brookhaven National Laboratory, NY 11973

Date submitted: 28 Nov 2011

Electronic form version 1.4