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J_{eff} =1/2 Mott spin-orbit insulating state close to the cubic limit in Ca_4IrO_6[1] S. CALDER, G.-X. CAO, S. OKAMOTO, Oak Ridge National Lab, J.W. KIM, Argonne National Laboratory, V.R. COOPER, Z. GAI, B.C. SALES, M.D. LUMSDEN, D. MANDRUS, A.D. CHRISTIANSON, Oak Ridge National Lab — The J_{eff} =1/2 Mott spin-orbit insulating state is manifested in systems with large cubic crystal field splitting and spin-orbit coupling that are comparable to the on-site Coulomb interaction, U. 5d transition metal oxides host parameters in this regime and recently strong evidence for this state in Sr_2IrO_4, and additional iridates, has been presented. All the candidates, however, have distorted octahedra, such as the elongation along the c-axis in Sr_2IrO_4, and consequently a non-cubic local crystal field environment. Consequently the materials form a mixed J_{eff} =1/2,3/2 ground state. The lack of a material with an unmixed J_{eff} =1/2 has impacted the development and testing of robust models of this novel insulating and magnetic state. We present neutron diffraction, resonant x-ray scattering and DFT calculations that not only reveal Ca_4IrO_6 is a new candidate J_{eff} =1/2 material with long-range magnetic order, but furthermore resides close to the required cubic limit. Both our experimental and theoretical investigation indicate Ca_4IrO_6 is uniquely positioned to act as a canonical system to investigate of the J_{eff} =1/2 state.

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