Physical Review B 2016 vol.93 N1

Ba2YIrO6: A cubic double perovskite material with Ir5+ ions

Dey T., Maljuk A., Efremov D., Kataeva O., Gass S., Blum C., Steckel F., Gruner D., Ritschel T., Wolter A., Geck J., Hess C., Koepernik K., Van Den Brink J., Wurmehl S., Büchner B.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2016 American Physical Society.Materials with a 5d4 electronic configuration are generally considered to have a nonmagnetic ground state (J=0). Interestingly, Sr2YIrO6 (Ir5+ having 5d4 electronic configuration) was recently reported to exhibit long-range magnetic order at low temperature and the distorted IrO6 octahedra were discussed to cause the magnetism in this material. Hence, a comparison of structurally distorted Sr2YIrO6 with cubic Ba2YIrO6 may shed light on the source of magnetism in such Ir5+ materials with 5d4 configuration. Besides, Ir5+ materials having 5d4 are also interesting in the context of recently predicted excitonic types of magnetism. Here we report a single-crystal-based analysis of the structural, magnetic, and thermodynamic properties of Ba2YIrO6. We observe that in Ba2YIrO6 for temperatures down to 0.4 K, long-range magnetic order is absent but at the same time correlated magnetic moments are present. We show that these moments are absent in fully relativistic ab initio band-structure calculations; hence, their origin is presently unclear.

http://dx.doi.org/10.1103/PhysRevB.93.014434