

Iridium double perovskite Sr₂YIrO₆: A combined structural and specific heat study

Corredor L., Aslan-Cansever G., Sturza M., Manna K., Maljuk A., Gass S., Dey T., Wolter A., Kataeva O., Zimmermann A., Geyer M., Blum C., Wurmehl S., Büchner B.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2017 American Physical Society. Recently, the iridate double perovskite Sr₂YIrO₆ has attracted considerable attention due to the report of unexpected magnetism in this Ir⁵⁺ (5d⁴) material, in which according to the Jeff model, a nonmagnetic ground state is expected. However, in recent works on polycrystalline samples of the series Ba_{2-x}Sr_xYIrO₆ no indication of magnetic transitions have been found. We present a structural, magnetic, and thermodynamic characterization of Sr₂YIrO₆ single crystals, with emphasis on the temperature and magnetic field dependence of the specific heat. As determined by x-ray diffraction, the Sr₂YIrO₆ single crystals have a cubic structure, with space group Fm $\bar{3}$ m. In agreement with the expected nonmagnetic ground state of Ir⁵⁺ (5d⁴) in Sr₂YIrO₆, no magnetic transition is observed down to 430 mK. Moreover, our results suggest that the low-temperature anomaly observed in the specific heat is not related to the onset of long-range magnetic order. Instead, it is identified as a Schottky anomaly caused by paramagnetic impurities present in the sample, of the order of $n \sim 0.5(2)\%$. These impurities lead to non-negligible spin correlations, which nonetheless, are not associated with long-range magnetic ordering.

<http://dx.doi.org/10.1103/PhysRevB.95.064418>

References

- [1] J. G. Rau, E. Kin-Ho Lee, and Hae-Young Kee, *Annu. Rev. Condens. Matter Phys.* 7, 195 (2016). 1947-5454 10.1146/annurev-conmatphys-031115-011319
- [2] W. Witczak-Krempa, G. Chen, Y. Baek Kim, and L. Balents, *Annu. Rev. Condens. Matter Phys.* 5, 57 (2014). 1947-5454 10.1146/annurev-conmatphys-020911-125138
- [3] A. Nag, *Phys. Rev. Lett.* 116, 097205 (2016). PRLTAO 0031-9007 10.1103/PhysRevLett.116.097205
- [4] S. Chikara, O. Korneta, W. P. Crummett, L. E. DeLong, P. Schlottmann, and G. Cao, *Phys. Rev. B* 80, 140407 (R) (2009). PRBMDO 1098-0121 10.1103/PhysRevB.80.140407
- [5] M. Ge, T. F. Qi, O. B. Korneta, D. E. De Long, P. Schlottmann, W. P. Crummett, and G. Cao, *Phys. Rev. B* 84, 100402 (R) (2011). PRBMDO 1098-0121 10.1103/PhysRevB.84.100402
- [6] Y. Chen and H. Y. Kee, *Phys. Rev. B* 90, 195145 (2014). PRBMDO 1098-0121 10.1103/PhysRevB.90.195145
- [7] G. Jackeli and G. Khaliullin, *Phys. Rev. Lett.* 102, 017205 (2009). PRLTAO 0031-9007 10.1103/PhysRevLett.102.017205
- [8] D. Pesin and L. Balents, *Nat. Phys.* 6, 376 (2010). 1745-2473 10.1038/nphys1606
- [9] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, *Phys. Rev. B* 83, 205101 (2011). PRBMDO 1098-0121 10.1103/PhysRevB.83.205101
- [10] W. Witczak-Krempa and Y. B. Kim, *Phys. Rev. B* 85, 045124 (2012). PRBMDO 1098-0121 10.1103/PhysRevB.85.045124

- [11] A. A. Burkov and L. Balents, *Phys. Rev. Lett.* 107, 127205 (2011). PRLTAO 0031-9007 10.1103/PhysRevLett.107.127205
- [12] W. Witczak-Krempa, T. P. Choy, and Y. B. Kim, *Phys. Rev. B* 82, 165122 (2010). PRBMDO 1098-0121 10.1103/PhysRevB.82.165122
- [13] M. Kargarian, J. Wen, and G. A. Fiete, *Phys. Rev. B* 83, 165112 (2011). PRBMDO 1098-0121 10.1103/PhysRevB.83.165112
- [14] X. Wan, A. Vishwanath, and S. Y. Savrasov, *Phys. Rev. Lett.* 108, 146601 (2012). PRLTAO 0031-9007 10.1103/PhysRevLett.108.146601
- [15] A. Go, W. Witczak-Krempa, G. S. Jeon, K. Park, and Y. B. Kim, *Phys. Rev. Lett.* 109, 066401 (2012). PRLTAO 0031-9007 10.1103/PhysRevLett.109.066401
- [16] N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements* (Elsevier-Butterworth-Heinemann, Amsterdam, 2012).
- [17] G. Chen, R. Pereira, and L. Balents, *Phys. Rev. B* 82, 174440 (2010). PRBMDO 1098-0121 10.1103/PhysRevB.82.174440
- [18] B. J. Kim, *Phys. Rev. Lett.* 101, 076402 (2008). PRLTAO 0031-9007 10.1103/PhysRevLett.101.076402
- [19] M. Wakeshima, D. Harada, and Y. J. Hinatsu, *J. Alloys Compd.* 287, 130 (1999). JALCEU 0925-8388 10.1016/S0925-8388(99)00057-2
- [20] G. Cao, T. F. Qi, L. Li, J. Terzic, S. J. Yuan, L. E. DeLong, G. Murthy, and R. K. Kaul, *Phys. Rev. Lett.* 112, 056402 (2014). PRLTAO 0031-9007 10.1103/PhysRevLett.112.056402
- [21] S. Bhowal, S. Baidya, I. Dasgupta, and T. Saha-Dasgupta, *Phys. Rev. B* 92, 121113 (R) (2015). PRBMDO 1098-0121 10.1103/PhysRevB.92.121113
- [22] K. Pajskr, P. Novák, V. Pokorný, J. Kolorenč, R. Arita, and J. Kuneš, *Phys. Rev. B* 93, 035129 (2016). 2469-9950 10.1103/PhysRevB.93.035129
- [23] B. Ranjbar, E. Reynolds, P. Kayser, and B. J. Kennedy, *Inorg. Chem.* 54, 10468 (2015). INOCAJ 0020-1669 10.1021/acs.inorgchem.5b01905
- [24] B. F. Phelan, E. M. Seibel, D. Badoe, Jr., W. Xie, and R. J. Cava, *Solid State Commun.* 236, 37 (2016). SSCOA4 0038-1098 10.1016/j.ssc.2016.03.017
- [25] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.95.064418> for anisotropic displacement parameters and selected bond lengths and angles.
- [26] Bruker, computer code apex2 Software Suite for Crystallographic Programs, Bruker AXS Inc., Madison, WI, 2009.
- [27] Bruker, computer code Area Detector Control and Integration Software, Version 5.x. In smart and saint, Bruker AXS Inc., Madison, WI, 1996.
- [28] G. M. Sheldrick, *Acta Crystallogr. Sect. A* 64, 112 (2008). ACACEQ 0108-7673 10.1107/S0108767307043930
- [29] G. M. Sheldrick, computer code cell now, program for unit cell determination, University of Göttingen, Germany, 2005 and Bruker AXS Inc., Madison, WI, 2005.
- [30] G. M. Sheldrick, computer code twinabs, Bruker AXS scaling for twinned crystals, Version 2007/3, and sadabs, University of Göttingen, Germany, 2007 and Bruker AXS Inc, Madison WI, 2007.
- [31] A. L. Spek, *Acta Crystallogr. Sect. D* 65, 148 (2009). ABCRE6 0907-4449 10.1107/S090744490804362X
- [32] A.-C. Dippel, H.-P. Liermann, J. T. Delitz, P. Walter, H. Schulte-Schrepping, O. H. Seeck, and H. Franz, *J. Synchrotron Radiat.* 22, 675 (2015). 1600-5775 10.1107/S1600577515002222
- [33] H. M. Rietveld, *J. Appl. Crystallogr.* 2, 65 (1969). JACGAR 0021-8898 10.1107/S0021889869006558
- [34] T. Roisnel and J. Rodríguez-Carvajal, *Mater. Sci. Forum* 378-381, 118 (2001). 10.4028/www.scientific.net/MSF.378-381.118
- [35] T. Dey, *Phys. Rev. B* 93, 014434 (2016). 2469-9950 10.1103/PhysRevB.93.014434
- [36] M. Bremholm, S. E. Dutton, P. W. Stephens, and R. J. Cava, *J. Solid State Chem.* 184, 601 (2011). JSSCBI 0022-4596 10.1016/j.jssc.2011.01.028
- [37] Note that the tiny humps in the 5-T curve are due to technical artifacts which are arising from the combination of the large number of data points and negligible changes in the susceptibility in the shown temperature regime.
- [38] P. Kayser, M. J. Martínez-Lope, J. A. Alonso, M. Retuerto, M. Croft, A. Ignatov, and M. T. Fernández-Díaz, *Inorg. Chem.* 52, 11013 (2013). INOCAJ 0020-1669 10.1021/ic401161d
- [39] A Brillouin function with (Equation presented) also allows to fit the data. However, this fit leads to unphysical (Equation presented) values.
- [40] Y. Du, Z. X. Cheng, S. X. Dou, X. L. Wang, H. Y. Zhao, and H. Kimura, *Appl. Phys. Lett.* 97, 122502 (2010). APPLAB 0003-6951 10.1063/1.3490221
- [41] C. G. F. Blum, *J. Cryst. Growth* 421, 39 (2015). JCRGAE 0022-0248 10.1016/j.jcrysgro.2015.04.004

[42] Y. Cai, Y. Li, and J. Cheng, in *Perovskite Materials-Synthesis, Characterisation, Properties, and Applications* (InTech, Rijeka, 2016).