

# Searching for Magnetic Order in the Pyrochlore Iridate $\text{Y}_2\text{Ir}_2\text{O}_7$

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The pyrochlore iridates  $\text{A}_2\text{Ir}_2\text{O}_7$  ( $\text{A} = \text{Y}$  or Lanthanide) have recently attracted considerable scientific interest due to their potential for novel spin-orbit-induced physics and tuneable electronic correlations. These compounds display a crystal structure that consists of two interpenetrating networks of corner-sharing tetrahedra, one of which contains octahedrally coordinated  $\text{Ir}^{4+}$  ions and the other which contains 8-fold coordinated  $\text{A}^{3+}$  ions. By varying the size of the  $\text{A}^{3+}$  ion, the strength of the Ir 5d electronic correlations can be systematically tuned, resulting in a gradual changeover from insulating ( $\text{A} = \text{Y}$ ) to metallic ( $\text{A} = \text{Pr}$ ) properties [1]. It has been proposed that certain pyrochlore iridates, such as  $\text{Y}_2\text{Ir}_2\text{O}_7$  and  $\text{Eu}_2\text{Ir}_2\text{O}_7$ , could provide the first experimental realization of a topological semimetal (TSM) [2,3]. A TSM is an exotic topologically ordered phase, similar to a topological insulator (TI). However, unlike a TI, a TSM can display topologically protected conducting states in both surface and bulk, and its topological properties are not destroyed by the presence of magnetic order.

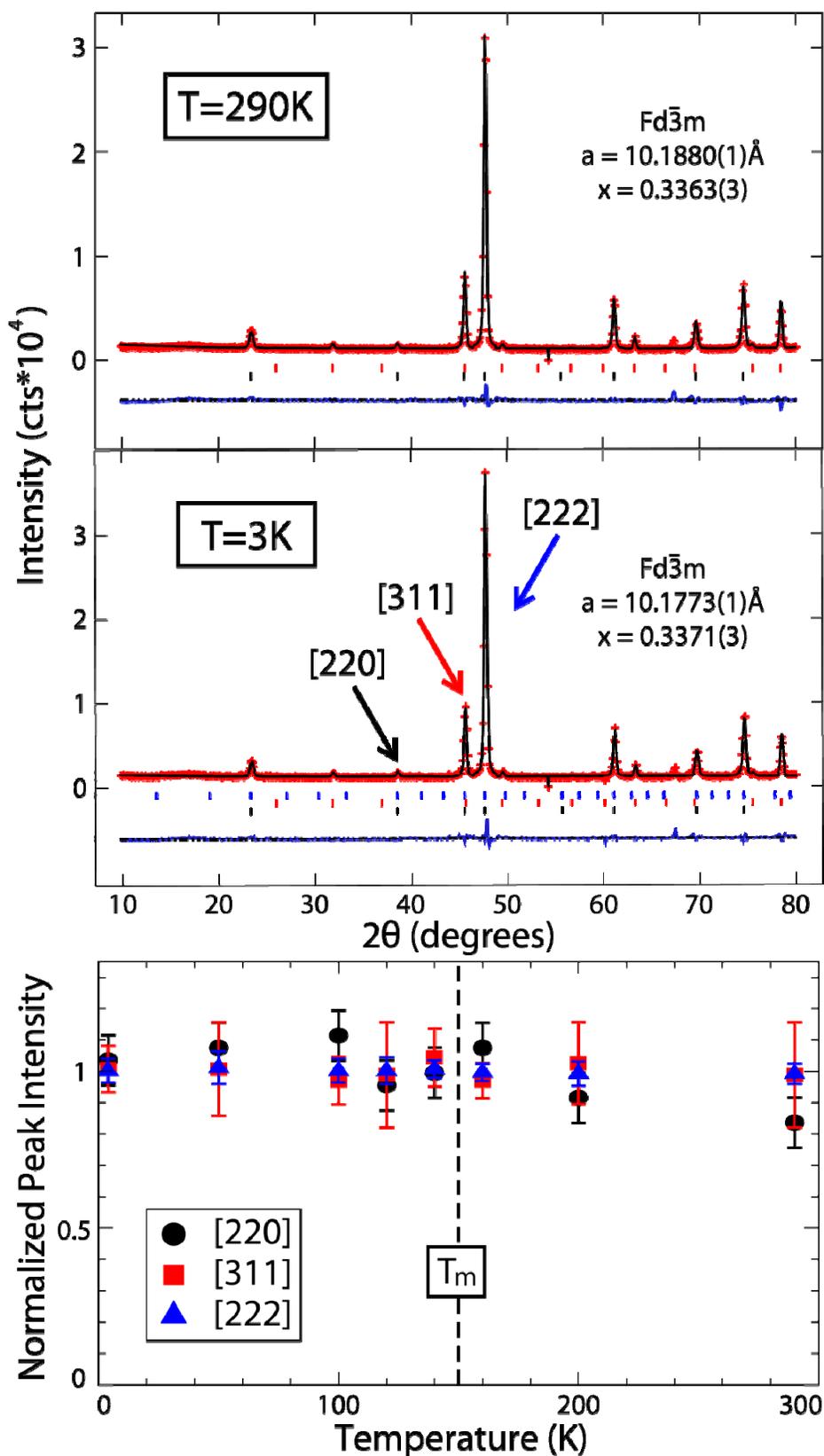
In spite of significant interest, the magnetic ground state of the  $\text{A}_2\text{Ir}_2\text{O}_7$  compounds has remained surprisingly elusive.  $\text{Y}_2\text{Ir}_2\text{O}_7$  is believed to undergo a magnetic phase transition at  $T_m = 150$  K [4], marked by a small anomaly in the magnetic susceptibility and significant hysteresis between field-cooled and zero-field-cooled magnetization. Although  $\mu\text{SR}$  results suggest the presence of commensurate magnetic order below  $T_m$  [5], there has been no conclusive evidence of long-range magnetic order from elastic neutron scattering. Theoretical calculations for  $\text{Y}_2\text{Ir}_2\text{O}_7$  [2,3] predict a  $\text{Q} = 0$  magnetic ground state with an “all-in, all-out” spin configuration (i.e. with the four spins on each  $\text{Ir}^{4+}$  tetrahedra pointing either inwards or outwards along the local  $\langle 111 \rangle$  axes).

In an attempt to determine the nature of this magnetic ground state, neutron powder diffraction measurements were performed on a 3.5 g sample of  $\text{Y}_2\text{Ir}_2\text{O}_7$  using the C2 diffractometer. Measurements were collected at two different neutron wavelengths ( $\lambda = 2.37$  Å and  $\lambda = 1.33$  Å), for temperatures ranging from  $T = 290$  K (well within the paramagnetic phase) to  $T = 3$  K (well within the suggested magnetically ordered phase).

Figure 1 shows two representative Rietveld refinements, carried out at  $\lambda = 2.37$  Å for  $T = 290$  K and  $T = 3$  K. The same  $\text{Fd-}3\text{m}$  space group can be used to model  $\text{Y}_2\text{Ir}_2\text{O}_7$  at temperatures above and below  $T_m$ , indicating that (1) no structural phase transitions are observed between 290 K and 3 K, and (2) no superlattice magnetic Bragg peaks develop below  $T_m$  (i.e. there is no evidence of  $\text{Q} \neq 0$  magnetic order down to  $T = 3$  K). In addition, the temperature dependence of the [220], [311], and [222] Bragg peaks, shown in the bottom panel of Figure 1, indicates that no  $\text{Q} = 0$  magnetic scattering develops below  $T_m$  either. Magnetic structure refinements, performed with an “all-in, all-out” trial spin configuration, allow us to place a conservative upper bound of  $0.5 \mu_B/\text{Ir}$  on the size of the ordered moment in  $\text{Y}_2\text{Ir}_2\text{O}_7$ . These results are consistent with two independent neutron powder diffraction studies which have recently been reported in the literature [5,6].

## References

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**Figure 1** Rietveld refinements performed within the paramagnetic ( $T = 290\text{ K}$ , top) and magnetically ordered ( $T = 3\text{ K}$ , middle) phases of  $\text{Y}_2\text{Ir}_2\text{O}_7$ . The vertical dashed lines denote the positions of  $\text{Y}_2\text{Ir}_2\text{O}_7$  nuclear peaks (black),  $\text{Y}_2\text{O}_3$  impurity peaks (red), and  $\text{Y}_2\text{Ir}_2\text{O}_7$  magnetic peaks (blue) assuming an “all-in, all-out” spin configuration. The temperature dependence of the [220], [311], and [222] Bragg peaks (bottom) reveals no observable magnetic scattering intensity below  $T_m$ .