

Poster Presentation

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Local Structure of Iridate Pyrochlores from Hydrothermal Synthesis

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Iridate pyrochlores of general formula $M_2Ir_2O_7$ have potential applications in catalysis [1]. They also often exhibit unusual magnetic and electronic properties caused by spin-orbit coupling and geometric frustration [2]. A detailed understanding of structure is necessary to enable these properties to be understood and exploited. Because of the propensity of the pyrochlore structure to accommodate structural disorder, we have chosen to utilise the technique of total scattering to examine the structure of $M_2Ir_2O_7$ ($M = Bi, Nd$). The sensitivity of our measurements to all the constituent elements is maximised by the combination of both neutron and X-ray total scattering. We find no evidence for magnetic ordering in our samples of $Nd_2Ir_2O_7$, in contrast to literature reports [3]. By comparing the local structure of our samples with that of one reported to exhibit magnetic ordering, we explore the possibility of a structural origin for the differences in magnetic behaviour. We have found that synthesis method can directly influence the structure of these iridate pyrochlores. Local structural analysis provides evidences of A-site cation deficiency and partial oxidation of Ir(IV) to Ir(V) in samples produced by hydrothermal techniques. Irreversible changes to the lattice parameter upon heating these samples at 400 – 900 °C further support the inference that the cation content is somewhat variable. We report the results of reverse Monte Carlo (RMC) refinements using the program RMCProfile, which is capable of simultaneously fitting to X-ray and neutron data, and therefore provides structural models of the greatest possible accuracy. We also report the results of in situ X-ray total scattering measurements which provide local-scale insight into the interesting thermal behaviour and apparent flexible cation content of these materials.

[1] K. Sardar, S. C. Ball, J. D. B. Sharman, et al., *Chem. Mater.*, 2012, 24, 4192–4200., [2] M. C. Shapiro, S. C. Riggs, M. B. Stone, et al., *Phys. Rev. B*, 2012, 85, 214434., [3] S. M. Disseler, C. Dhital, T. C. Hogan, et al., *Phys. Rev. B*, 2012, 85, 174441.

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