Magnetic Scattering in BaYFeO₄

Corey Thompson and J.E. Greedan¹

¹ Department of Chemistry and Brockhouse Institute for Materials Research, McMaster University

BaYFeO₄ is a newly discovered Fe-based oxide with a rather complex crystal structure in spite of the apparently simple chemical formula, Fig. 1. Magnetic susceptibility data show two very weak maxima at 48 K and 36 K. Neutron diffraction data were collected over the range 6 K – 50 K and 290 K in order to determine the magnetic structures. Magnetic reflections were indeed seen and indexed with propagation vectors \( \mathbf{k} = (0 0 1/3) \) for \( 36 K < T < 48 K \) and \( \mathbf{k} = (0 0 0.358) \) for \( 6 K < T < 36 K \). Fits to the neutron diffraction data for both T ranges are shown in Fig. 2 and the refined magnetic structures in Fig. 3. A manuscript based on this work has been submitted recently to Inorganic Chemistry.

Figure 1 Crystal structure of BaYFeO₄. a) Columns of edge sharing rings \([\text{Fe}_4\text{O}_{18}]^{24+}\). b) \([\text{Fe}_4\text{O}_{18}]^{24+}\) ring formed by corner shared \([\text{FeO}_5]^7\) and \([\text{FeO}_6]^9\) polyhedra. \([\text{FeO}_5]^7\) and \([\text{FeO}_6]^9\) polyhedra are shown in gold and green, respectively, oxygen atoms are red spheres. Barium and yttrium atoms were omitted for clarity.

Figure 2 (left) Refinement of the neutron diffraction pattern at 6 K. (right) Refinement of the neutron diffraction pattern at 38 K.
Figure 3 Refined magnetic structures. The octahedral Fe$^{3+}$ sites are in green and the square pyramidal sites in red. (left) Refined magnetic structure at 6 K. (right) Refined magnetic structure at 38 K.