Magnetic Scattering in $BaYFeO_4$

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$BaYFeO_4$ 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 **k** = (0 0 1/3) for 36 K < T < 48 K and **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.

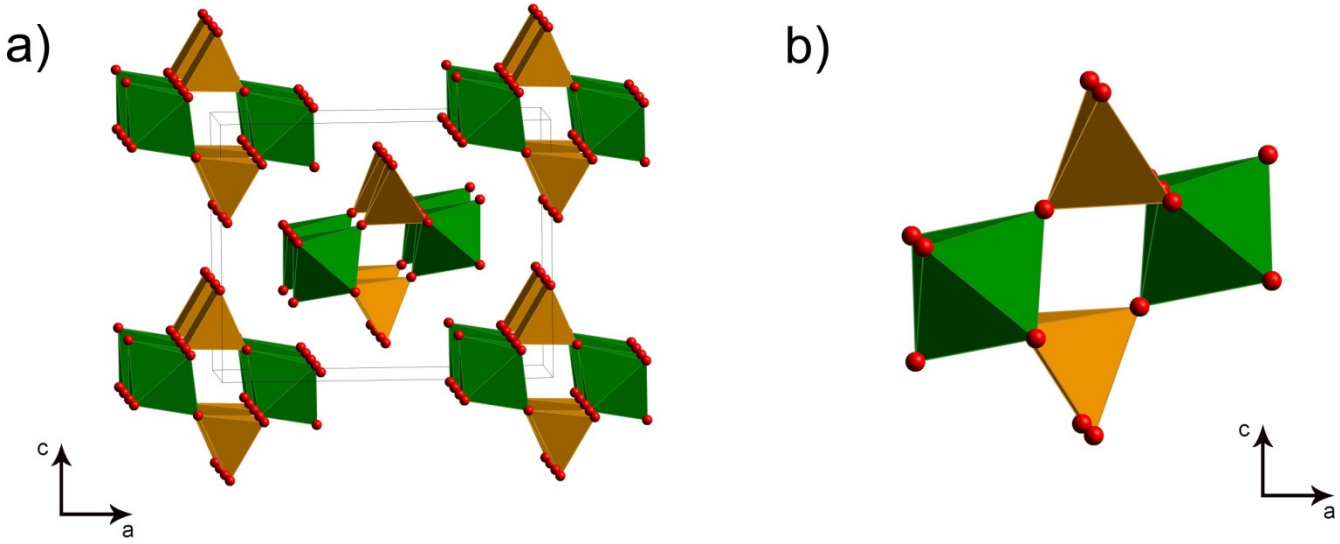

Figure 1 Crystal structure of $BaYFeO_4$. a) Columns of edge sharing rings $[Fe_4O_{18}]^{24-}$. b) $[Fe_4O_{18}]^{24-}$ ring formed by corner shared $[FeO_5]^{7-}$ and $[FeO_6]^{9-}$ polyhedra. $[FeO_5]^{7-}$ and $[FeO_6]^{9-}$ polyhedra are shown in gold and green, respectively, oxygen atoms are red spheres. Barium and yttrium atoms were omitted for clarity.

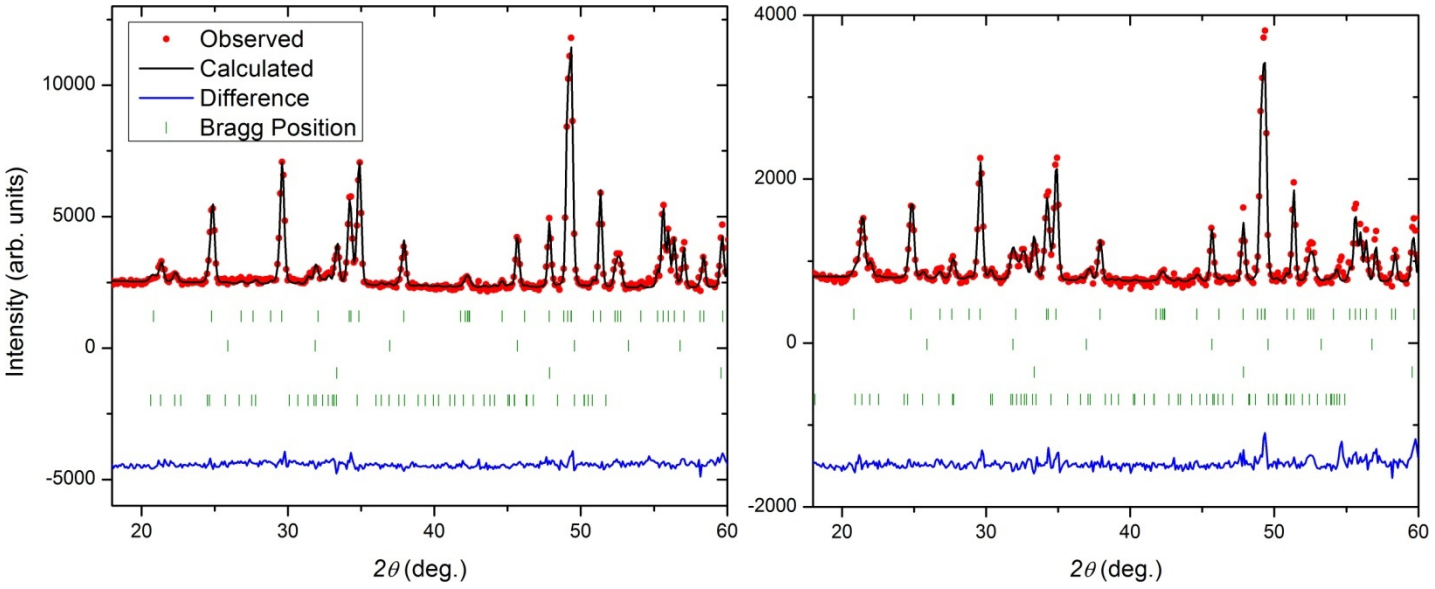

Figure 2 (left) Refinement of the neutron diffraction pattern at 6 K. (right) Refinement of the neutron diffraction pattern at 38 K.

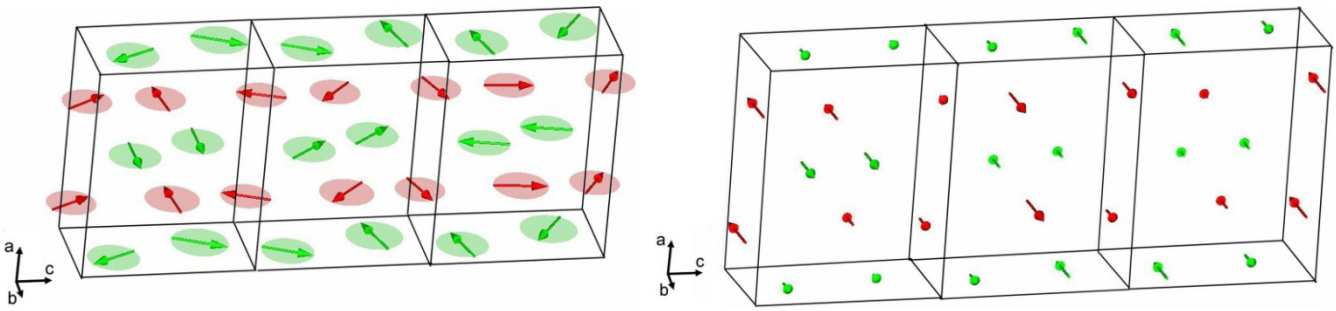

Figure 3 Refined magnetic structures. The octahedral Fe3+ sites are in green and the square pyramidal sites in red. (left) Refined magnetic structure at 6 K. (right) Refined magnetic structure at 38 K.