

# Magnetic Ordering in the B-site Ordered Double Perovskite Ba<sub>2</sub>YO<sub>6</sub>

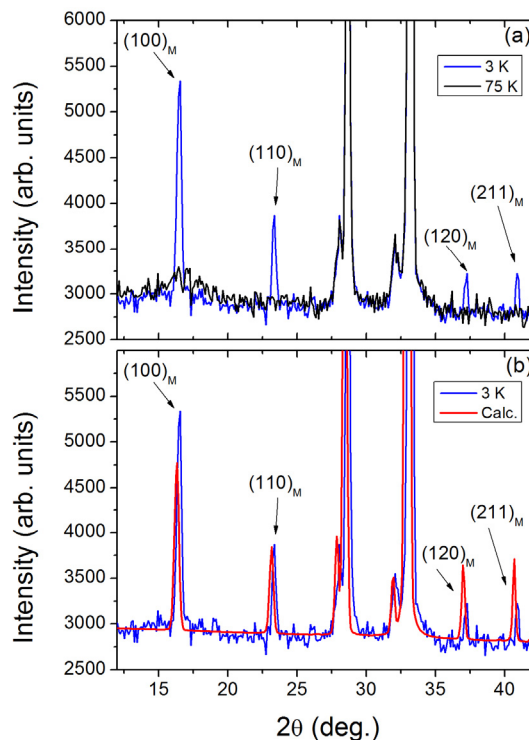
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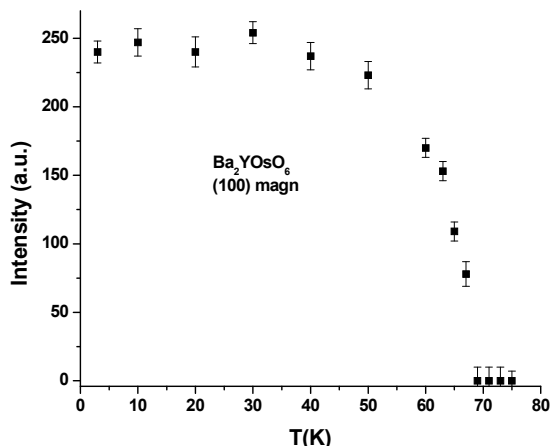
The ordered double perovskite (DP) structure was confirmed at 290 K and 3.5 K by refinement of neutron powder diffraction data as summarized in Table 1 below. The magnetic structure was determined to be antiferromagnetic Type I f.c.c. with  $T_c = 68$  K as indicated in figure 1. Figure 2 shows the temperature dependence of the magnetic (100) reflection showing  $T_c = 68$  K. A manuscript describing this work and related inelastic scattering is being written for submission to Physical Review B.

Table 1. Neutron diffraction refinement results of Ba<sub>2</sub>YO<sub>6</sub> at 290K. The refinement was done simultaneously with two wavelengths, 2.37Å and 1.33Å. The results provided for the 1.33Å are reported in () behind the 2.37Å results and the 3.5K refinement results are reported in [] below the 290K data.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> <sub>iso</sub> (Å <sup>2</sup> )
Ba	0.25	0.25	0.25	0.40(5) [0.01(5)]
Y	0.50	0.50	0.50	0.38(9) [0.12(8)]
Os	0	0	0	0.20 [0.15]
O	0.235(2) [0.235(2)]	0	0	0.235(2) [0.29(4)]
$a_0 = 8.3541(4)$ Å $[a_0 = 8.3435(4)$ Å] $R_{\text{Bragg}} = 1.93$ (3.26); $R_F = 1.41$ (1.97); $\chi^2 = 6.32$ (10.0) $[R_{\text{Bragg}} = 2.06$ (2.63); $R_F = 1.30$ (1.66); $\chi^2 = 7.04$ (14.1)]				



**Figure 1** Neutron diffraction patterns collected at 3.5 K and 75 K. The magnetic reflections are indexed with a propagation vector  $k = (1, 0, 0)$ . The broad peak at the (100) magnetic reflection position indicates short-range magnetic correlations at 75 K. (b) Structural and magnetic refinements (red line) of the diffraction pattern observed at 3K (blue line). The overfitting of the (120) and (211) magnetic reflections is ascribed to inaccuracies in the Os(5+) form factor.



**Figure 2** Temperature dependence of the magnetic (100) reflection