Synthesis, Crystal and Magnetic Structure of the New Double Perovskite Ba₂MnMoO₆

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Z. Naturforsch **58b**, 571–576 (2003); received February 14, 2003

We describe the preparation and characterization of a new double perovskite of formula Ba_2MnMoO_6 . It has been obtained in polycrystalline form by thermal treatment, in a H_2/N_2 flow, of previously decomposed citrate precursors. This material has been studied by X-ray (XRD) and neutron powder diffraction (NPD): it crystallizes, at room temperature, in the cubic space group $Fm\bar{3}m$, and shows an almost perfect ordering between Mn^{2+} and Mo^{6+} cations at the B substructure. Below $T_N = 10.8$ K, it experiences a long range antiferromagnetic ordering that was followed from sequential NPD data. The low-temperature magnetic structure is defined by the propagation vector $\mathbf{k} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The ordered magnetic moment of Mn is found to be 4.04(8) μ_B at 2 K, suggesting a divalent oxidation state for Mn cations, in a high spin $t_{3g}^2 e_g^2$ (S = 5/2) electronic configuration.

Key words: Perovskite Structure, Neutron Diffraction, Magnetic Structure, Antiferromagnetic Ordering, Manganese