

s7.m1.o5 Hole and Electron Doping in $\text{Bi}_{1-x}\text{Ca}_x\text{MnO}_3$ ($0 \leq x \leq 1$) Investigated by Neutron and Synchrotron X-Ray Diffraction. J.L. García-Muñoz¹, M.A.G. Aranda², A. LLobet^{1,3}, C. Frontera¹, J.A. Alonso⁴, C. Ritter⁵, ¹*Institut de Ciència de Materials de Barcelona, C.S.I.C. Spain.* ²*Departamento de Química Inorgánica, Cristalografía y Mineralogía, U. de Málaga. Spain.* ³*Laboratoire Louis Néel, CNRS, Grenoble, France.* ⁴*Instituto de Ciencia de Materiales de Madrid, C.S.I.C. Spain.* ⁵*Institute Laue Langevin, Grenoble, France.*

Notes

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The $\text{Bi}_{1-x}\text{Ca}_x\text{MnO}_3$ family of manganites ($0 \leq x \leq 1$) has been investigated, between 1.5 and 350 K, by means of high resolution neutron (NPD) and synchrotron x-ray (SXR) powder diffraction measurements. A detailed description is given of the different charge and magnetic structures found increasing the concentration of e_g electrons from $x=0$ to $x=1$. Based on joint refinements of neutron and synchrotron diffraction data, the different structural transitions are described and analysed. In particular, the compositions $x=1/4, 1/3, 1/2, 2/3, 3/4, 0.85$ and $7/8$ have been thoroughly investigated. Seven different magnetic phases have been identified associated to particular orbital/charge orderings and structures. Charge ordering is not detected for $x > 0.75$. A metal-insulator transition is only observed in the highly doped region (around $x=0.85$) where there is significant CMR effects.

Examples of macroscopic phase segregation coinciding with electronic localisation phenomena are discussed in terms of the stability of different orbital orderings and the observation of tiny compositional fluctuations. The results are relevant to the phase separation problem.