



[1] Schomaker V. Trueblood K.N., *Acta Cryst.*, **1968**, B24, 63. [2] Willis B.T.M., Pryor A.W. *Thermal Vibrations in Crystallography*, **1975**, Cambridge University Press, London. [3] TOPAS version 4.1, **2008**, Bruker AXS. [4] Brock C.P., Dunitz J. *Acta Cryst.*, **1982**, B38, 2218. [5] Capelli, S.C., Albinati A., Mason S.A., Willis B.T.M. *J. Phys. Chem. A*, **2006**, 110, 11695.

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Substitution Effects in Some Bismuth Based Rare Earth Manganites. Kiril Krezhov^a, Stefan Kovachev^a, Daniela Kovacheva^b, Erzhebet Svab^c, Françoise Bourée^d, Gilles André^d. ^a*Institute for Nuclear Research and Nuclear Energy*. ^b*Institute of General and Inorganic Chemistry, Sofia, Bulgaria*. ^c*Research Institute for Solid State Physics and Optics, Budapest, Hungary*. ^d*Laboratoire Leon Brillouin, CEA/Saclay, Gif-sur-Yvette, France*.

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In consistence with other authors we established that the characteristic signs attributed to the charge ordering (CO) and orbital ordering (OO) in the parent manganites $\text{Bi}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ and $\text{Bi}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ appear at $T_{\text{CO}} \approx 320$ K and $T_{\text{CO}} \approx 525$ K, respectively [1]. We investigated the magnetic ordering and CO/OO phenomena with respect to temperature and chemical doping in $\text{Bi}_{0.25}\text{R}_{0.25}\text{AA}_{0.5}\text{MnO}_3$ (R = La, Nd, Ho, Er, Tm) (A-site doping [1-3]) and $\text{Bi}_{0.5}\text{AA}_{0.5}\text{Fe}_x\text{Mn}_{1-x}\text{O}_3$ (B-site doping [4-6]), where AA stands for Ca or Sr. For both sets of Bi-based manganites prepared as polycrystalline powders by controlled solid-state reaction we correlated the structural findings from high-resolution X-ray and neutron powder diffraction with results for transport and magnetic properties. At 295 K $\text{Bi}_{0.25}\text{R}_{0.25}\text{Ca}_{0.5}\text{MnO}_3$ are in paramagnetic phase of small monoclinic distortion allowing for structural description in orthorhombic Pnma symmetry. A significant anisotropic distortion of the MnO_6 octahedra occurs in the characteristic manner associated with the particular orbital order of manganese ions at half doping level. The findings corroborate the conclusion that the effective Bi^{3+} ionic radius in Bi-Ca manganites is close in value to that of Nd^{3+} indicating that the lone pair character of $6s^2$ Bi^{3+} orbitals is rather constrained than dominant. Except for

$\text{Bi}_{0.25}\text{La}_{0.25}\text{Ca}_{0.5}\text{MnO}_3$ which undergoes a ferromagnetic transition at $T_{\text{C}} = 281$ K followed by a transition to an antiferromagnetic state at lower temperatures, the rest compounds become antiferromagnetic. At 10 K the ground magnetic state of most Ca-Bi compounds could be acceptably described by the insulating antiferromagnetic CE ordering. The RT cell parameters of $\text{Bi}_{0.5}\text{Ca}_{0.5}\text{Fe}_x\text{Mn}_{1-x}\text{O}_3$ ($0 \leq x \leq 0.6$) change monotonously with increasing x . The compounds are antiferromagnetic with T_{N} which decreases with increasing Fe-substitution. For $x \geq 0.1$ the antiferromagnetism is accompanied by a weak ferromagnetism. The CO-OO order in the neat form is suppressed at very low Fe-substitution ($x \leq 0.05$). Room temperature diffraction data of $\text{Bi}_{0.5}\text{Sr}_{0.5}\text{Fe}_x\text{Mn}_{1-x}\text{O}_3$ ($0 \leq x < 1.0$) show that the crystal structure is orthorhombic for $x \leq 0.3$ and cubic for $x > 0.4$. Unit cell volume increases with x . The charge/orbital order was observed for the compound without Fe. The magnetic state of the compounds with different Fe-content changes from paramagnetic to weak antiferromagnetic below T_{N} , in the range 116 K - 155 K. All Ca-Fe and Sr-Fe compounds are semiconductors between 100 K and 600 K and there was no magnetoresistivity effect in fields up to 7 kOe.

[1] Krezhov K., Kovacheva D., Svab E., Bourée F., Stamenov, P. *Physica B*, **2004**, 350/1-3S, E13. [2] Krezhov K., Kovacheva D., Svab E., Bourée F., *J. Phys: Condens. Matter*, **2005**, 17, S3139. [3] Tzankov D., Kovacheva D., Krezhov K., Puzniak R., Wiśniewski A., Sváb E., Mikhov M., *J. Phys: Condens. Matter*, **2005**, 17, 4319, [4] Krezhov K., *AIP Conf. Proc.*, **2007**, 899 (1), 263 [5] Krezhov K., *RAST07 IEEE Proceedings*, **2007**, 123. [6] Tzankov D., Kovacheva D., Krezhov K., Puzniak R., Wiśniewski A., Mikhov M., *J. Appl. Phys.* 103, **2008**, 053910.

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Molecular and Crystalline Structures of Three (S)-4-alkoxycarbonyl-2-azetidiones Containing Long Alkyl Side Chains From Synchrotron X-ray Powder Diffraction Data. Luis E. Seijas^a, Asiloé J. Mora^a, Gerzon E. Delgado^a, Francisco Lopéz-Carrasquero^b, Michela Brunelli^c, Andrew N. Fitch^d. ^a*Laboratorio de Cristalografía, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, 5101, Venezuela*. ^b*Laboratorio de Polímeros, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, 5101, Venezuela*. ^c*ILL Institut Laue-Langevin, BP 156, 38042 Grenoble cedex 9, France*. ^d*European Synchrotron Radiation Facility, BP 220, 38043 Grenoble cedex, France*.

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The (S)-4-alkoxycarbonyl-2-azetidiones are optically active β -lactam derivatives of aspartic acid, which are used as precursors of carbapenems-type antibiotics and poly- β -aspartates. The crystal structures of three (S)-4-alkoxycarbonyl-2-azetidione with alkyl chains with