Acta Cryst. (2002). A58 (Supplement), C59 STRUCTURE, MAGNETISM AND SUPERCONDUCTIVITY OF RUTHENOCUPRATES

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The ruthenocuprates have tetragonal perovskite-related structures containing distinct CuO₂ and RuO₂ layers. Superconductivity arises from doping of the CuO₂ planes, and the Ru spins show an independent magnetic ordering transition. The intrinsic order is near-antiferromagnetic, but a field-induced spin flop or metamagnetic transition to a ferromagnetic state is easily observed. Structural studies of RuSr₂GdCu₂O₈, show that local symmetry-breaking rotations and tilts of the RuO6 octahedra lead to domains seen by HREM [1,2]. The structure and conducting/magnetic properties result from overlap between Cu dx2-y2 and Ru t2g bands which is confirmed by doping Ru by Sn and Nb resulting in hole and electron doping, respectively [3,4,5]. A new ruthenocuprate Pb₂Sr₂RuCu₂O₈ with Pb₂Cl layers replacing Gd in the latter structure. The material is non-superconducting, but a variable temperature and field neutron diffraction study shows the magnetic properties to be very similar to those of RuSr₂GdCu₂O₈.

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THE SUPERCONDUCTING BISMUTH-BASED MIXED OXIDES <u>E.V. Antipov</u>¹ A.N. Baranov¹ N.R. Khasanova¹ J.S. Pshirkov¹ S.N. Putilin¹ C. Bougerol² O.I. Lebedev³ G. Van Tendeloo³

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The present work is focused on the synthesis and the characterization of mixedvalence bismuthates with 3- or 2-dimensional perovskite-like structures and on the elucidation of structural criteria affecting superconductivity in these compounds.

Single-phase samples of the Sr_{1-x}K_xBiO₃ and Ba_{1-x}K_xBiO₃ solid solutions have been prepared for the broad range of K-concentration: $x = 0.25 \cdot 0.65$ (for Sr) and $x = 0.35 \cdot 1.0$ (for Ba). For the Sr-based bismuthates, the symmetry of the structure changes from monoclinic to orthorhombic (x = 0.25) and finally to tetragonal ($x = 0.35 \cdot 0.65$) upon increasing the K-concentration, while it remains cubic for the Ba-based one. Increasing the K-content results in decreasing the Bi-O distances for both structures and in reducing the network distortions for Sr_{1-x}K_xBiO₃. Suppression of superconductivity due to overdopping occurs in Ba-based perovskite at x exceeding 0.70, while strong structure distortions cause a similar effect in Sr_{1-x}K_xBiO₃ at $x = 0.3 \cdot 0.4$. The influence of the formal Bi valence on the superconducting properties of Ba_{1-x}K_xBiO₃ was revealed from XANES and XRPD studies.

The layered type $(Sr,A)_3Bi_2O_7$ and $(Ba,A)_3Bi_2O_7$ phases belonging to the Ruddlesden-Popper homologous series were obtained for A = K or Rb. A strong buckling of the (BiO_2) layers in their structures occurs due to the partial ordering of alkaline- and alkaline-earth cations between two independent positions. The formation of the one-layer $(Ba,K)_2BiO_4$ bismuthate has been revealed by Electron Microscopy and XRPD studies. Both types of compounds are considered as possible candidates for new superconducting materials among bismuthates.

Keywords: SUPERCONDUCTIVITY BI MIXED OXIDES PEROVSKITE

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EVIDENCE AGAINST LATTICE EXPANSION AS THE SOLE EXPLANATION FOR TC INCREASE IN CHLOROFORM- AND BROMOFORM- INTERCALATED C₆₀

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CHCl₃ and CHBr₃ intercalated C₆₀ has attracted particular interest after superconductivity up to T_c = 117 K was discovered. We have determined the structure using synchrotron x-ray powder-diffraction. The expansion due to intercalation mainly takes place in one dimension, leaving planes of C₆₀ molecules on an approximately hexagonal, slightly expanded lattice. We have performed tight-binding band structure calculations for the surface layer. In spite of the slight expansion of the layers, the density of states at the Fermi energy is smaller for C₆₀·2CHCl₃ and C₆₀·2CHBr₃ than for C₆₀. This suggests that the expansion alone cannot explain the increase of T_c.

Keywords: INTERCALATED C60, POWDER DIFFRACTION, SUPERCONDUCTIVITY

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X-RAY DIFFRACTION STUDY OF THE SUPERCONDUCTOR MoRuP PREPARED AT HIGH PRESSURE W. Wong-Ng¹ J. A. Kaduk² I. Shirotani³

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In recent years, ternary transition phosphides with chemical formula of MM'P, where M and M' represent 3d, 4d and 5d transition metals, received increased attention because of the interesting superconductivity properties. There are two structure types for MM'P, both of which exhibit layer characteristic. The first structure type is hexagonal (Fe₂P-type) and the second type is referred to as the anti-PbCl₂ type (or Co₂Si), which is orthorhombic. In the hexagonal structure, each layer is occupied by either M and P, or M' and P; and there is a two-dimensional intraplanar M-network. Another feature of the structure is the triangular clusters of M'3. In the orthorhombic MRuP structure, all layers are filled with M, M' and P. The two-dimensional intraplanar M network is broken up and only M chains with a relatively large separation between each atom remain. The phase transformation to the orthorhombic phase is accompanied by a drop in the superconducting transition temperature.

This paper summarizes the x-ray diffraction characterization of the new superconductor, MoRuP, by using powder Rietveld refinement technique. A comparison of the structures of MoRuP with the Zr- and the Nb analogs will also be made.

Keywords: MoRuP SUPERCONDUCTOR CRYSTAL STRUCTURE