

group. The O atoms maintain a close packed arrangement. The *M1* sites and the other hydrogen bonds link the layers. Astonishingly, this structural motive is found in compounds with quite different chemical formulas. They are worth mentioning because of some unique structural features. In medenbachite, $\text{Bi}_2\text{FeCu}(\text{AsO}_4)_2(\text{O},\text{OH})_2(\text{OH})_2$, the Bi and (O,OH) atoms are intercalated between the brucite-like layers. In $\text{KCu}_3(\text{OH})_2[(\text{AsO}_4)\text{H}(\text{AsO}_4)]$ some of the vacant positions are occupied by $\text{Cu}^{[2+4]}$ cations, an extremely rare environment for Cu^{2+} atoms. Again, a symmetry restricted hydrogen bond occurs, but it links between the brucite-like layers. In $\text{Cu}_2\text{O}(\text{SO}_4)$ (dolerophanite) all hydrogen and *M1* atoms are missing; in addition to the *M2* and XO_4 tetrahedra, two trigonal bipyramidally coordinated Cu^{2+} atoms share a common O-O edge in the centre of a vacant cation position.

Keywords: tsumcorite; H_3O_2 group; $\text{Cu}^{[2+4],5}\text{O}_6$ coordination figures

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Charge and Orbital Ordering in Layered Perovskites. Markus Braden^a, O.J. Schumann^a, M. Cwik^a, M. Kosmala^a, M.T. Fernandez-Diaz^b, M. Meven^c, A. Cousson^d. ^a*II. Physikalisches Institut, Köln, Germany.* ^b*Institut Laue Langevin, Grenoble, France;* ^c*FRM-II, Garching, Germany.* ^d*Laboratoire Léon Brillouin, Saclay, France.*

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Charge and orbital order is observed in many transition-metal oxides in a wide range of doping. The most famous examples are the stripe phases in the cuprates and the charge and orbital ordered states in manganates that exhibit colossal magneto resistivity. At least in the latter materials, the key role of the charge and orbital ordering for the understanding of the main physical mechanism has been well established. In spite of the large interest in these phenomena, there have been very little precise crystallographical studies determining the small structural distortions related with the electronic ordering. We have performed several single-crystal diffraction experiments mostly using neutrons in order to analyze the charge and orbital order in layered perovskites, $\text{La}_{2-x}\text{A}_x\text{MeO}_4$ (A=Sr, Ca and Me=Mn, Ni and Co), focusing on the half-doping concentration range. By analyzing the weak superstructure reflections we may clearly establish the character of the charge order in single-layered cobaltates, manganates and nickelates as well as that of the orbital order in manganates and in cobaltates. The precise analysis of the charge and orbital order in $\text{La}_{2-x}\text{A}_x\text{MeO}_4$ allows one to quantitatively understand the magnetic ordering schemes appearing in all these phases and, in the case of the manganates, yield an insight why these materials can so easily switch between ferromagnetic metallic and antiferromagnetic insulating states.

Keywords: charge and orbital order; neutron diffraction; electronic structure and magnetism

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Novel Li Vacancy Ordered Structure of Stage-2 $\text{Li}_{0.38}\text{BC}$ Phase. Bora Kalkan^a, Engin Ozdas^a.

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The existence of several borocarbides with crystal structures highly related to MgB_2 , in which one of these, the layered LiBC has been predicted based on the electronic structure calculations that this compound should become superconducting on doping with holes. However, the superconducting features for Li off-stoichiometric borocarbide compounds have not been observed in any experimental studies, because of the difficulties in the sample preparation. In this work, the effects of synthesis conditions on the structure of Li_xBC samples with the different Li content and the phase stability were investigated. The structural studies showed that the intercalation process has a staging behavior as Li intercalated graphite and a novel Li vacancy ordered structure for off-stoichiometric stage-2 $\text{Li}_{0.38}\text{BC}$ phase. The temperature dependence of the conductivity shows semiconducting behavior over the whole temperature range and the hopping type conduction improved by the hole doping.

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Keywords: layered materials; solid-state reactions; novel structures