Analysis Wizard offers three methods for initial structure determination: a) Direct method, b) Direct space method and c) Charge flipping method.


Keywords: Ab-initio crystal structure analysis, charge flipping method, rietveld method

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Recent Progress in joint charge and spin densities refinement
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Electron density, in all its representations, plays a key role in the understanding of the nature of interatomic interactions and chemical bonds. In case of molecular magnetic materials, as the experimental electron densities rely on high resolution X-ray diffraction experiments, it is necessary to go further and enrich the electronic model by the use of complementary techniques such as unpolarized and polarized neutron (PND) diffraction or Compton scattering. This implies to be able to include all these different experimental contributions into a unique electronic model, and to carry out a joint refinement. In this respect we are developing a new program to model the charge, spin and momentum densities (ANR CEDA project [*]).

We will report on the first charge and spin densities joint refinement applied to the molecular magnetic compound MnCuPb₈a, (Fig. 1 [1],[2]). The results are consistent with the previous separated studies of spin and charge densities. This method can bring new insights in the nature of interactions in the solid.

Fig.1. ORTEP view of the MnCuPb₈a complex chain structure at 100K


Keywords: charge, spin, densities

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Structure and magnetic order in CrOCl at low temperatures
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Keywords: phase transition, magnetic order, superstructure

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Probing the local sense of the Dzyaloshinskii-Moriya vector: neutrons vs x-rays
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