MS20 Electric, opto-electronic and magnetic properties from elastic and inelastic scattering plus properties of materials from quantum crystallography

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Experimental charge density and phase transition studies of a new hybrid perovskite: the complementarity between powder diffraction, single-crystal diffraction and magnetic measurements

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Abstract

Crystal structure of bis(1,2diaminepropane) di-μ-chloro-bis[diaquadichloromanganate(II)] dichloride, is built as layers of centrosymmetric dinuclear units made of two (MnIICl4(H2O)2)- octahedra (figure 1) sharing one edge along the a direction and distributed in the basal ac plane. These doubly negative charged layers are separated along the b axis positively charged di-amine propane layers. Non-coordinated chloride anions make the electroneutrality and stabilize the structure through hydrogen bonds with coordinated water molecules, and the ammonium groups of organic layers. We modelled the experimental charge density based on high-resolution single crystal diffraction experiment in order to calculate the electrostatic properties of this material, explaining how the electrostatic interactions contribute largely to the stability of the structure.

Differential scanning calorimetry (DSC) reveal a two-step transition (main peaks at T= 366 K and T= 375 K) ascribed to the release of the coordinated water molecules. Meanwhile, SQUID magnetometry show very different magnetic behaviour after the transitions. Below 346 K the temperature dependence of the product of the magnetic susceptibly with temperature (cT) is almost constant down to 10K (Figure 1). After heating up to 390 K the cT temperature dependence is no more constant but decrease rapidly with temperature. To understand such a change and using combined powder and single crystal diffraction experiments we investigate the determination of the high temperature resulting structure. This reveals that the dinuclear Mn(II) units rearrange in trinuclear Mn(II) units. This structural description is according perfectly with simulation of the magnetic behaviour.

Figure 1. a) 3D view of the structures at 100K before (along the a axis) and after (along the b axis) high temperature heating. b) Temperature dependence of magnetic behaviour.