**MS24-O2 Spin, charge and momentum densities of YTiO3 perovskite**

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High resolution X-ray (XRD) and polarized neutron diffractions (PND) are routinely used to model charge and spin densities of localized electrons, while inelastic Compton scattering (ICS) is a valuable mean for determining delocalized electrons. Our objective is to construct a unique electron density model common to these three experimental data sets. We have demonstrated that a joint refinement of a multipolar model based on polarized neutron and X-ray diffraction data is possible and brings more insight in the electron distribution [1]. The inclusion of ICS data implies to go beyond the atom centered model to take into account bicentric terms. As the multipolar model is thus no more adapted, a new model based on atomic orbitals under development will be discussed and applied to a YTiO3 perovskite crystal. This compound is ferrimagnetic at low temperature (below 29K), suggesting that a single d electron (0.84mB/mol) mainly localized on the Ti atom gives rise to the magnetic interactions.


**Keywords**: charge spin densities, xray diffraction, polarised neutron diffraction, magnetic conption scattering, joint refinement, magnetic materials

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**MS24-O3 New antiferromagnets [CuX(pyz)]_2[BF_4] with X = Cl and Br.**

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The structures of new compound [CuX(pyz)]_2[BF_4] with X = Cl and Br and pyz = pyrazine were determined by single crystal X-ray diffraction. These tetragonal compounds crystallize in space group P4/nmm. They are built from [Cu(pyz)]_2[BF_4] layers which are connected by X ions along the c-axis. Charge is compensated by BF_4 ions in the voids of the 3D coordination compound. The antiferromagnetic interactions between the Cu^{2+} ions are mainly two-dimensional (2D) located within the [Cu(pyz)]_2[BF_4] layers. This results in a broad maximum of the magnetic susceptibility around 9 K. Towards lower temperature a kink is observed at 4 K which indicates long-range 3D magnetic order. The magnetic unit cell is doubled along the c-axis (k = 0,0,1/2) and the ordered magnetic moment amounts to \( \mu = 0.76(8) \mu_B/Cu^{2+} \) at 1.5 K. The moments are antiferromagnetically coupled along the b- and c-axes. Long-range 3D magnetic order is observed below \( T_N = 3.0(1) \) K. A fit of a 2D Heisenberg model to the magnetic susceptibility data results in \( J_{||} = 9.6 \) K.

**Keywords**: 2D antiferromagnet, copper, pyrazine, DMC, XRD, ESR