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

Mohamed Souhassou¹, Youfack Bolivard, Nicolas Claiser, Maxime Deutsch, Claude Lacomte, Jean Michel Gillet², Pietro Cortona², Zeyin Yan², Iuri K labalin³, Béatrice Gillon³, Florence Porcher³, Arsen Gukasov¹, Yoshitaru Sakurai¹, Masayoshi Itou¹, Masahisa Ishii³

1. CRM² Université de Lorraine Nancy France
2. Laboratoire SPMS, CentraleSupelec, Université Paris-Saclay, France
3. Laboratoire Leon Brillouin, CEA/CNRS, France
4. JASRI/SPRING8, Japan
5. Gunma University, Japan

email: Mohamed.Souhassou@univ-lorraine.fr

High resolution X-ray (XRD) and polarized neutron diffractions (PND) are routinely utilized 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 pervoskite crystal. This compound is ferromagnetic 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, x ray diffraction, polarised neutron diffraction, magnetic compton scattering, joint refinement, magnetic materials

---

**MS24-O3** New antiferromagnets \([\text{CuX(pyz)}_2(\text{BF}_4)] \) with \( X = \text{Cl and Br} \)

Mariusz Kubus¹,², Arianna Lanza², Nicola Casati¹, Piero Macchi², Lukas Keller¹, Christoph Fiolka², Jürg Šchefer¹, Christian Ruegg¹, Karl Krämer²

1. Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
2. Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland
3. Laboratory for Synchrotron Radiation – Condensed Matter, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

email: mariusz.kubus@psi.ch

The structures of new compound \([\text{CuX(pyz)}_2(\text{BF}_4)] \) with \( X = \text{Cl} \) and \( \text{Br} \) and pyz = pyrazine were determined by single crystal X-ray diffraction. These tetragonal compounds crystallize in space group \( P4/nmb \). They are built from \([\text{CuX(pyz)}_2]^{2+} \) layers which are connected by \( X^- \) ions along the \( c \)-axis. Charge is compensated by \( \text{BF}_4^- \) ions in the voids of the 3D coordination compound. The antiferromagnetic interactions between the \( \text{Cu}^{2+} \) ions are mainly two-dimensional (2D) located within the \([\text{CuX(pyz)}_2]^{2+} \) 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 \( \mu = 0.76(8) \mu_\text{B}/\text{Cu}^{2+} \) at 1.5 K. The moments are antiferromagnetically coupled along the \( b \)- and \( c \)-axes. Long-range 3D magnetic order is observed below \( T_N = 3.9(1) \) K. A fit of a 2D Heisenberg model to the magnetic susceptibility data results in \( J_\parallel = 9.6 \) K.

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

---

s92

*Acta Cryst. (2016). A72, s92*