



Figure 1. ORTEP drawing of the $[\text{Fe}(\text{C}(\text{SiMe}_3)_3)]^-$ anion at 100 K. Atoms are depicted as 50 % probability ellipsoids. Orange, petrol blue and grey refer to iron, silicon and carbon, respectively. Hydrogen atoms have been omitted for clarity.

Keywords: Electron density, single molecule magnet, synchrotron radiation, topological analysis

MS24-O2 Spin, charge and momentum densities of YTiO_3 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 YTiO_3 perovskite 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.

Reference 1. "First spin-resolved electron distributions in crystals from combined polarized neutron and X-ray diffraction experiments". Maxime Deutsch, Béatrice Gillon, Nicolas Claiser, Jean-Michel Gillet, Claude Lecomte, and Mohamed Souhassou, *IUCrJ*. 2014 May 1; 1(Pt 3): 194–199.

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