Oral Contributions

[MS13] Charge and spin density measurements of materials

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[MS13-01] Experimental Spin-Resolved Electron Densities: Results of a Joint Refinement of XRD and PND Data

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Since the first works of Stewart on modelling charge density [1], huge improvements of X-ray sources, detectors and software has significantly increased the resolution and the qualities of diffraction data allowing an accurate determination of the charge density of a growing number of molecules. However, despite the technological improvement, no dramatic change of the experimental model was reached since the multipolar model of Hansen & Coppens in 1978 [2]. At the same time polarised neutron diffraction (PND) experiments were developed [3] to get access to the spin density at the molecular scale and the multipolar Hansen & Coppens model was adapted to model this quantity.
These two quantities (charge and spin densities) are described by a similar multipolar atom centred model with a common parameterization, therefore a combined treatment of X-ray diffraction (XRD) and PND data, is not only possible but also useful as stated by Becker & Coppens in 1985 [4]. Recently an extended Hansen & Coppens model and the corresponding refinement program were developed [5, 6] in order to allow the joint refinement of data sets coming from three different experiments (X-ray, unpolarised and polarised neutron diffraction). By combining different data sets, the new model gives access to electron density with spin up ($\rho\uparrow$) and electron density with spin down ($\rho\downarrow$) separately. These two quantities ($\rho\uparrow$ and $\rho\downarrow$) can be observed experimentally for the first time, and this observation allows a further comparison with theoretical models. In a first part the presentation will focus on the common model and the refinement procedure. The second part will describe its application to the case of an end-to-end azido double-bridged copper(II) complex (Cu2L2(N3)2 where L=1,1,1-triuoro-7-(dimethylamino)-4-methyl-5-aza-3-hepten-2-onato) [7]. The experimental results will be presented and compared to the theoretical densities.

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