Notes

s9'.m1.o5 **Investigation of molecular magnetism by high resolution X-ray diffraction : application to several organic and organometallic compounds.** S. Pillet[a], M. Souhassou[a], C. Lecomte[a], Y. Pontillon[b], C. Mathonière[c], P. Rabu[d] & C. Massobrio[d]. [a] *LCM3B, UHP Nancy I, BP 239, 54506 Vandoeuvre ;* [b] *ILL, 6 rue Jules Horowitz, 38042 Grenoble ;* [c] *ICMCB, 87 avenue du Docteur Albert Schweitzer, 33 608 Pessac ;* [d] *IPCMS, Strasbourg*

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One of the most used methods to investigate interatomic or intermolecular magnetic coupling is polarised neutron diffraction (PND). PND, thanks to the neutron magnetic moment, gives direct access to the global spin density distribution of the sample. Charge density and its topological analysis can also bring very precise information on the way these interactions take place. The spin density distribution is directly related to the unpaired electron carriers, while electron density distribution shows the whole interatomic or intermolecular interactions. Thus by careful join inspection of spin and electron densities, one can bring more insights of the magnetic interactions.

Electron density analysis is a powerful approach often used to investigate interatomic or intermolecular bonds, and therefore could help understanding magnetic interactions which arise from charge transfer, hydrogen bond or super-exchange mechanisms. Furthermore, in the case of organometallic compounds, an estimation of the 3d electron distribution (due to the crystal field and bond effects) around each metal atom is directly available from the multipole expansion of the modelled electron density. This electron distribution in the 3d orbitals is of major importance to study and explain the metal-ligand bonds.

Comparison of results obtained from both polarised neutron and X-ray diffraction techniques is performed on molecular compounds exhibiting different kind of magnetic effects. The magnetic interactions in a 3D ferromagnetic purely organic free radical (Nit(SMe)Ph)[1,2], an ordered ferrimagnetic bimetallic chain compound[3] $MnCu(Pba)(H_2O)_3.2H_2O$, and an antiferromagnetic ladder compound[4] $Cu_2(OH)_3NO_3$ are discussed.

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