s2.m1.p11 **Experimental Charge Density Studies of Polydentate Diazine Ligands.** C. Wilson[a], S. Dahaoui[a,*], D. S. Yufit[b], J.A.K. Howard[b] and L.K. Thompson[c]. *[a]School of Chemistry, University of Nottingham, Nottingham, NG7 2RD; [b]Departments of Chemistry, University of Durham, Durham DH1 3LE, UK & [c]Memorial University of Newfoundland, St. John's, Newfoundland A1B 3X7, Canada. [*](actual address: LCM3B, Université Nancy I, BP 239, 54506 Vaondouevre-lès-Nancy France).*
Keywords: charge density, transition metal, low temperature.

Polynuclear transition metal complexes with interesting magnetic properties have been successfully created through the use of PAHAP ($C_{12}N_6H_{12}$), a nitrogen rich tetradentate ligand and its modifications[1]. The suitably separated bridging sites of these ligands allow metal centres to be brought into close proximity and the ligands provide a pathway for intramolecular spin-exchange interactions. Structural differences have been shown to have a pronounced effect on the magnetic behaviour of these complexes, for example the rotation of the Cu magnetic planes about the N-N bond in Cu dimers of these ligands.

We are currently extending our structural studies to experimental charge density studies of these ligands and their simple copper complexes through low temperature X-ray and neutron diffraction data. We aim to gain insight into the subtle factors affecting the coordination modes of these ligands and to investigate the electronic differences corresponding to those observed in the structures of the complexes. This will allow us to make comparisons between the free and complexed ligands and to the proposed models of the magnetic interactions. Results of these studies will be presented.

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s2.m1.p12 **LAPW Study of the Existence of Non Nuclear Maxima in the Electron Density.** G.K.H. Madsen[1], P. Blaha[1], K. Schwarz[1], J. O. Sofo[2], C. Gatti[3] *[1]Technische Universität Wien, A-1060 Vienna, Austria [2]Centro Atomico Bariloche, AR-8400 Bariloche, Argentina [3]CSRSRC-CNR, I-20133 Milano, Italy.*
Keywords: charge spin densities.

Maxima in the electron density are generally found at the positions of the nuclei. There are however a few well documented cases, where maxima have been found at positions other than the nuclear. Based on theoretical LCAO calculations and experimentally derived electron densities the excistence of these Non-Nuclear Maxima (NNM) in the solid state has been reported in several studies[1]. However, the effect is small and has been claimed to depend on the basis set used to obtain the wavefunction or the method used to derive the electron density from the experimental structure factors.

We will present Full potential Linearized Augmented Plane Wave (FLAPW) calculations[2] to examine fine details of the electron density. In the FLAPW method the basis set is controlled by only one parameter, namely the planewave cut-off. Therefore the calculations can be systematically improved to reach basis set convergence. Our studies confirm the excistence of NNM in several simple metals and in the periodic arrays of F-centers that can be formed inside sodalite host-lattices.

The FLAPW method divides space into atomic spheres and an interstitial region. This will be discussed with respect to the use of topological methods for the analyses the electron density[3]. Furthermore the mechanisms which lead to the formation of NNM will be discussed.

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