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Charge, Spin and Momentum Densities simultaneous refinement. From the method to the code. Jean-Michel Gillet[a], Yurii Ciumacov[a], Pietro Cortona[a], Pierre Becker[a], Mohamed Souhassou[b], Nicolas Claiser[b], Maxime Deutsch[b], Sebastien Pillet[b], Claude Lecomte[b], Beatrice Gillon[c], Dominique Luneau[d], Ana Borta[d], Olga Iasco[d]. [a]*Laboratoire de Cristallographie, Résonance Magnétique et Modélisations, Institut Jean Barriol, Université des Sciences et Techniques, BP 70239, boulevard des Aiguillettes, Vandoeuvre-lès-Nancy, France.*[c]. [b]*Laboratoire Structures et Propriétés des Matériaux Solides, UMR CNRS 8580, Ecole Centrale Paris, Grande Voie des Vignes, 92290 Châtenay-Malabry, France.* [c]*Laboratoire Leon Brillouin, CEA-Saclay, 91191 Gif sur Yvette, France.* [d]*Laboratoire Multimatériaux et Interfaces, Université Claude Bernard, 43 boulevard du 11 novembre 1918, 69622 Villeurbanne Cedex, France.*
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We present the latest progress of the Convergence of spin, charge and momentum Electron Density Analysis project.
In the last decade, few methods have been proposed to build a quantum model with the goal to refine some of its important features using a set of different experiments. Among these experiments, high resolution x-rays and polarized neutrons diffraction, convergent beam electron diffraction, magnetic and non magnetic X-rays Compton scattering are the most popular.
The joint refinement of charge and spin electron densities in position and momentum spaces from a set of different experiments, as those previously mentioned, requires the use of a common quantity known as the "one particle reduced density matrix" (1-RDM). Its role will be briefly presented.
We will then explain the model(s), the method and the strategies that were adopted in constructing a general joint refinement computer code.
Results from preliminary tests will be described as well as possible future joint studies.

Keywords: electron density, spin density, charge density, momentum density, density matrix, refinement.

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Spin density distributions in molecular magnetic materials. Javier Campo. *Materials Science Institute of Aragón, (CISC-University of Zaragoza), C/ Pedro Cerbuna 12, 50009 Zaragoza, Spain.*
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A good understanding of the magnetic interaction mechanisms, which are strongly influenced by the spin density distribution on the molecules, has a great importance in the design of new molecular magnets with high ordering temperatures. Moreover, we will show how spin density investigations can seed light to fundamental problems in molecular magnetism, such as the anisotropy in molecular clusters.
The aim of this contribution is to understand the particular magnetic behavior, through the analysis of the experimental and computational determination of the spin density distribution and the magnetic coupling constants of different magnetic molecular materials; the family $A_2FeX_5{\cdot}H_2O$ (A=alkali, X=Cl, Br), the thiazyl-based magnets p-X-$C_6F_4CNSSN{\cdot}$ (X=Br, NO_2, CN) and the Mn-based molecular cluster $Mn_3L_4(ClO_4)_2(H_2O)_2$, (HL=2-methoxy-6-(pyridine-2-hydrazonomethyl)phenol).
Although the family $A_2FeX_5{\cdot}H_2O$ had been extensively studied we were interested in these 3D low anisotropy antiferromagnetic series because still remained an interesting open question: why are their transition temperatures relatively high considering that in these compounds there are no μ-bridging groups between the iron ions, such as Fe-O-Fe or Fe-X-Fe linkages, but all the super-exchange pathways are of the type Fe-X···X-Fe or Fe-O···X-Fe? Our results shown a high spin density delocalization (20 %) to the halogen atoms being the more important at the X_4-halogen belonging to the H bond [1].
On the other hand the sulphur based free-radical family represents an alternative to the classical nitrogen-oxygen one for the design of purely organic magnets. In fact, the dithiadiazolyl radical family includes the organic material with the highest known transition temperature into a phase showing spontaneous magnetization and the organic magnet with the second highest transition temperature into a ferromagnetic phase. The subject addressed in our studies was to explore and understand the magnetic interaction mechanisms, via the spin density determination and *ab initio* modelizations, in this free-radical family and to investigate its suitability for achieving ferromagnetic interactions [2].
The Mn3 cluster has been described as an almost lineal trimer of Mn(II) in a high spin configuration with two isotropic magnetic interactions. One striking fact is the experimental EPR g factor of 2.14 for such an isotropic system. Due to its isotropic and not degenerate nature, the system is an ideal benchmark to investigate the interplay of the magnetic interactions in systems with several magnetic centers and more than one electron per magnetic center. An in deep study of the system through the combination of several experimental and theoretical methods has allowed us to demonstrate the isotropic nature of the system and the ferromagnetic character of the intra-molecular magnetic interactions.

[1] J. Campo, J. Luzón, F. Palacio, G. J. McIntyre, A. Millán, A. R. Wildes, *Phys Rev B.* 78, 054415 (2008). [2] J. Luzón, J. Campo, F. Palacio, G. J. McIntyre, J M. Rawson, R. J. Less, C. M. Pask, A. Alberola, R. D. Farley, D. M. Murphy, and A. E. Goeta *Phys Rev B.* 81(2010)

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On the *ab-initio* calculation of all-atom ADPs for molecules in crystal structures. Birger Dittrich[a].
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Thermal motion and electron density are convoluted, and one can not distinguish between them from X-ray diffraction data alone [1]. The ability to calculate atomic displacement parameters (ADPs) for molecules in crystal structures would allow application of charge-density methodology to datasets of 'normal resolution' (fulfilling the Acta C limit), since a