

calculate the aspherical atoms' parameters for atoms present in RNA and DNA molecules, and to enable the modelling of some other biological complexes of interest (e.g. minor groove binders). Reconstruction of the electron density enables us to perform interaction energy calculations for such systems.

Newly obtained pseudoatom models were first tested on a set of over 200 nucleic base pairs, and small charged molecular complexes. Electrostatic interaction energies were calculated for the densities reconstructed using UBDB (EPMM method) [2], and then compared against quantum calculations performed for the same systems (eg. adenine dimer, guanine-cytosine pair) at the two levels of theory *i.e.* first order electrostatic term HF/aug-cc-pVDZ and B3LYP/6-31G\*\*. Correlation between the electrostatic interaction energy values obtained using those methods is high, while the linear coefficient is close to one. UBDB+EPMM satisfactorily reconstructs the electrostatic interaction energy, and what is particularly important, it closely reproduces the energetical trends.

The total interaction energy was estimated for the sample structures (containing DNA and RNA bases and their modifications) using the UBDB databank, and other atom-atom potential methods. Quantum mechanical interaction energy calculations (force field) were also performed. We compared all the results to get a clear idea about the accuracy and limits of all those approaches and generally to validate all available methods in this field. Good estimation of total interaction energy is very important in the potential applications of our method in the drug design and molecular biology.

[1] Dominiak P. M., Volkov A., Li X., Messerschmidt M., Coppens P., *J. Chem. Theory Comput.* 2007, 3, 232. [2] Volkov A., Koritsanszky T., Coppens P., *Chem. Phys. Lett.* 2004, 391, 170.

**Keywords: electron density, intermolecular interactions, nucleic acids**

#### FA3-MS20-P04

**Hirshfeld surfaces from experimental charge density data.** Radosław Kamiński, Anna A. Hoser, Krzysztof Woźniak. *Department of Chemistry, University of Warsaw, Warszawa, Poland.*

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Crystal engineering methods have recently attracted much attention due to their potential applications in predicting and designing new functional materials. Hirshfeld surfaces[1] have become a very popular tool to understand the packing of molecules in the solid state as well as intermolecular interactions between them. However, typical surfaces are defined using spherical atomic densities, which is not always the best option; especially when dealing with very accurate experimental charge density data. Thus, the whole effort to gain electron density information from the solid state is not fully utilized when applying such surfaces in the analysis. Therefore, here we propose a new approach to obtain Hirshfeld surfaces utilizing the charge density data obtained from multipole refinement with the Hansen-Coppens formalism.[2] Our methodology is tested on simple molecular examples such as, for example,  $\alpha$ -oxalic acid dihydrate showing hidden potential of these inter-molecular surfaces.

[1] M. A. Spackman, D. Jayatilaka, *Cryst. Eng. Comm.*, 2009, 11, 19. [2] N. K. Hansen, P. Coppens, *Acta Cryst.*, 1978, A34, 909.

**Keywords: crystal engineering, charge density, Hirshfeld surfaces**

#### FA3-MS20-P05

**Magnetoelastic coupling in the triangular lattice antiferromagnet CuCrS<sub>2</sub> investigated by neutron and X-ray diffraction, neutron polarimetry and inelastic neutron scattering.** Julia C. E. Rasch<sup>a,b</sup>, Martin Boehm<sup>a</sup>, Clemens Ritter<sup>a</sup>, Hannu Mutka<sup>a</sup>, Jürg Schefer<sup>b</sup>, Lukas Keller<sup>b</sup>, Galina M. Abramova<sup>c</sup>, Antonio Cervellino<sup>d</sup> and Jörg F. Löffler<sup>c</sup>. <sup>a</sup>*Institut Laue-Langevin, 6 Rue Jules Horowitz, BP 156, FR-38042 Grenoble Cedex 9, France.* <sup>b</sup>*Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland.* <sup>c</sup>*L.V. Kirensky Institute of Physics, SB RAS, Krasnoyarsk RU-660036, Russia.* <sup>d</sup>*Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland.* <sup>e</sup>*Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland*  
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CuCrS<sub>2</sub> is a triangular lattice Heisenberg antiferromagnet with a rhombohedral crystal structure. We report on neutron and synchrotron powder diffraction results which reveal a monoclinic lattice distortion at the magnetic transition and verify a magnetoelastic coupling [1]. CuCrS<sub>2</sub> is therefore an interesting material to study the influence of magnetism on the relief of geometrical frustration. Polarimetry has been used to determine the magnetic structure to be a spin density wave and to exclude a helical arrangement. Because of the magnetoelastic coupling, the system is assumed to be able to select a magnetic ground state and to overcome frustration. Additionally a magnetic resonance mode has been found at  $\hbar\omega=12\text{meV}$  which evidences a dimerization of Cr ions in the triangular planes [2].

[1] Julia C. E. Rasch et al, *Phys. Rev.* 80 (2009) 104431, 1-6. [2] Julia C. E. Rasch et al, submitted to PRL.

**Keywords: magnetoelastic, polarimetry, frustration, VBS**

#### FA3-MS20-P06

**On the significance of low and zero intensity observations.** Julian Henn, Kathrin Meindl. *Institute of Inorganic Chemistry, University of Göttingen, Germany.*  
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Counting statistics determine the minimum error present in an X-ray measurement. Thus, weak and zero intensity observations are naturally insignificant. However, a weak intensity may appear as significant by accident due to large variations in the variance of an intensity measured with low redundancy  $N$ . We investigate the significance of weak and zero intensity observations for the optimistic limiting case of a Poisson distribution for the individual reflections [1]. In real measurements additional sources of error are present the contribution of which even reduces the significance of weak and zero intensity observations. The redundancies required for

approaching the true values are derived and numerical examples are given.

[1] Haight, F. A., "Handbook of the Poisson Distribution", John Wiley & Sons, Inc., New York, 1967.

**Keywords:** Poisson distribution, significance, low intensity observation

### FA3-MS20-P07

#### Remarks on an erroneous omission of an ellipse in the gap of the hyperbola in the dispersion curves.

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Based upon the Laue method, the biquadratic secular equation as the dispersion relation in X-ray diffraction is

$$|S_{ij}| = \begin{vmatrix} k^2 - \bar{k}_0^2 & K^2 C \chi_{-g} \\ K^2 C \chi_g & k^2 - \bar{k}_g^2 \end{vmatrix} \\ = k^4 - (\bar{k}_0^2 - \bar{k}_g^2) k^2 + \bar{k}_0^2 \cdot \bar{k}_g^2 - K^4 C^2 \chi_g^2 = 0, \quad (1)$$

where  $|\chi_{-g}| = |\chi_g|$ ,  $\bar{k}_g = \bar{k}_0 + \vec{g}$  ( $\vec{g}$  is the reciprocal lattice vector) and others are in general usage. The diagonal terms of  $S_{11}$  and  $S_{22}$  in eq. (1) represent the same two circles intersected at two points and the dispersion relations from eq. (1) near Brillouin zone boundary should be carefully examined. The roots of  $k^2$  in eq. (1) could be given by

$$k^2 = \frac{1}{2} \left\{ (\bar{k}_0^2 + \bar{k}_g^2) \pm \sqrt{(\bar{k}_0^2 - \bar{k}_g^2)^2 + 4 |K^4 C^2 \chi_g^2|} \right\}. \quad (2)$$

In case of  $|\bar{k}_0^2| \cong |\bar{k}_g^2|$ , eq. (2) could be expanded as

$$= \frac{1}{2} (\bar{k}_0^2 + \bar{k}_g^2) \pm |K^2 C \chi_g| \pm \frac{1}{8 |K^2 C \chi_g|} (\bar{k}_0^2 - \bar{k}_g^2)^2 \pm \dots \quad (3)$$

After mild calculation, the 2nd and 3rd terms in eq. (3) show hyperbola and ellipse in form like

$$y^2 = b^2 \pm (bx/a)^2 \quad (4)$$

as dispersion curves and the parameter  $2b$  in eq. (4) is simultaneously not only the transverse axis of hyperbola but also the diameter of ellipse. Therefore, the Bragg gap could not exist. By roughly approximating  $S_{11}$  and  $S_{22}$  at  $k^2 - \bar{k}_0^2 \cong 2\bar{k}_0 \cdot \Delta k \cong 2K \cdot \xi_0$  and  $k^2 - \bar{k}_g^2 \cong 2\bar{k}_g \cdot \Delta k \cong 2K \cdot \xi_g$ , since eq. (1) could be shared half and half by the central surfaces of the second order in eq. (4) and one half of a pair, i. e., ellipse has been eliminated by rough approximation, consequently another half of hyperbola of the popular dispersion curve could be given by

$$|S_{ij}| = \begin{vmatrix} 2\xi_0 & KC\chi_{-g} \\ KC\chi_g & 2\xi_g \end{vmatrix} = 4\xi_0\xi_g - K^2 C^2 \chi_g^2 = 0, \quad (5)$$

which could be defined by that products of the perpendiculars from an arbitrary point on hyperbola to its two asymptotes is a constant. The rough approximation that makes biquadratic eq. (1) a quadratic eq. (5) could not be accepted with no proofs and remarks. Further, all of drawings in eq. (5) in almost all

references have been shown by a simple coordinate mix-up. It is something very strange from mindlessness.

**Keywords:** dynamical theory of X-ray diffraction, Laue method, dispersion.

### FA3-MS20-P08

#### Experimental charge density studies, electrostatic and topological analysis of 1-(2'-Aminophenyl)-2-methyl-4-nitro-1H-imidazole crystals. Agneszka Paul<sup>a,b</sup>, Maciej Kubicki<sup>a</sup>, Claude Lecomte<sup>b</sup>, Christian Jelsch<sup>b</sup>. <sup>a</sup>Adam Mickiewicz University in Poznań, Poland. <sup>b</sup>Nancy University, CNRS, France.

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High resolution diffraction data of crystals of small organic molecules, such as 4-nitro-1H-imidazole derivatives, are achievable within a period of days, thanks to the development of the measurement devices.

Processing these data in the standard manner to solve and refine the structures and to obtain the information about the geometry and interactions is usually performed applying the Independent Atom Model (IAM). Within this approximation all atoms are treated as 'spherical balls' with the electron density concentrated around the nuclei. However, this assumption neglects transfer of the charge density into the bonding regions – especially for the covalent bonds – and the transfer associated with the intermolecular interactions.

To improve the electron density distribution model and to allow for the detailed analysis of the intra- and interactions in the molecules and in the supramolecular assemblies, such as the 1-(2'-Aminophenyl)-2-methyl-4-nitro-1H-imidazole, the Hansen-Coppens formalism [1] and Atoms-in-Molecule approach [2] for topological analysis are used. The multipole model has been implemented in the MoPro program suite [3] and allows electrostatic and topological calculations for both small molecules and biological macromolecules at subatomic resolution.

Within this poster the experimental charge density distribution of the title compound will be presented. The crystal structure of this 4-nitroimidazole derivative was published recently, using standard resolution data [4], however no detailed analysis of the influence of the substituents on the electron distribution was performed. The main observed interactions are the strong and weak hydrogen bonds (N-H...N, N-H...O and C-H...O, C-H...Cg (centroid of the aromatic ring), respectively). These regions, with a special attention paid to the nitro group (as hydrogen bond acceptor), will be analysed. This is a part of our project to investigate the weak interactions in the series of 4-nitro-1H-imidazole derivatives, to examine the influence of the different substituent groups on the charge density distribution within the aromatic ring.

[1] Coppens P., Koritsanszky T.S., Chem. Rev. (2001). 101, 1583-1627. [2] Bader R.F.W. (1990). Atoms in Molecules: A Quantum Theory. Oxford University Press. [3] Jelsch, C., Guillot B., Lagoutte, A. & Lecomte C.J. Applied Crystallography (2005). 38. 38-54. Advances in protein and small-molecules charge-density refinement methods using MoPro. [4] Kubicki M., Wagner P., Acta Cryst. (2007). C63, o454-o457.

**Keywords:** 4-nitro-1H-imidazole derivatives, multipole refinement, high resolution diffraction