

**FA3-MS02-O1****Resolution Dependent Scaling, Minor Disorder, Parameter Correlations: Possible Pitfalls for Experimental Charge Densities.** Birger Dittrich.

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In charge density research the electron-density distribution (EDD)  $\rho(r)$  of a system of interest can be obtained from high-resolution single-crystal diffraction data using rigid pseudo-atoms [1]. As part of such a procedure, multipole parameters of a chosen multipole model are least-squares refined. To make sure that these parameters—and hence our derived EDD—bear physical meaning, we first need to verify our data quality.

We will show that resolution-dependent ‘systematic errors’, indicated by subsets of a data set with different scale factors, can remain for current CCD data of three different suppliers (Bruker, MAR, Oxford Diffraction) even after carefully correcting for LP, absorption and, if necessary, extinction. A comparison to scintillation-counter data is made. Validation of resolution-dependent scaling can be achieved by refinement with fixed database parameters calculated from *ab-initio* computations [2],[3] or by Hirshfeld-atom refinement [4].

Apart from data quality, validating the experimental least-squares-refined EDD is equally important for obtaining a physically meaningful result. It entails the identification of real physical effects arising in the crystal that can bias our multipole parameters, namely easily overlooked minor disorder and/or large amplitude vibrations. Like before, we can identify such effects and therefore validate our experimental results by theoretical predictions [5].

Finally we would like to exemplify the importance of non-unique results that can arise when parameter correlations exceed 70%. All three points mentioned will be substantiated by recent case studies.

[1] Stewart, R.F., *Acta Cryst. A.*, **1976**, 32, 565; Hansen, N. and Coppens, P., *Acta Cryst. A.*, **1978**, 34, 981. [2] Dittrich, B., Hübschle, C.B., Luger, P., and Spackman, M.A., *Acta Cryst. D.*, **2006**, 62, 1325. [3] Dominiak, P. M., Volkov, A., Li, X., Messerschmidt, M., and Coppens, P., *J. Chem. Theory Comput.*, **2007**, 3, 232. [4] Jayatilaka, D., Dittrich, B., *Acta Cryst. A.*, **2008**, 64, 383. [5] Dittrich, B., Warren, J. E., Fabbiani, F. P. A., Morgenroth, W., and Corry, B., *Phys. Chem. Chem. Phys.*, **2009**, 11, 2601.

**Keywords:** charge density; validation; multipole refinements

**FA3-MS02-O2**

**Getting the Most from Image Plate Data.** Vladimir V. Zhurov<sup>a</sup>, Elizabeth A. Zhurova<sup>a</sup>, Alan Pinkerton<sup>a</sup>.  
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The steps we take for obtaining the best possible information from high quality X-ray diffraction data using image plate

detectors will be presented. These steps will include sample preparation for He-temperature experiments, a description of the low temperature attachment, running the experiment at He temperature, data collection strategy and details of data processing.

Features of the VIIPP integration software [1,2] and its recent developments will be reported.

A possibility of obtaining subtle electron density features together with anharmonic thermal parameters will be discussed based on several data sets for the compound RDX at different temperatures. Anisotropic thermal parameters for hydrogen atoms obtained from He-temperature data for RDX, HMX and meltdrum’s acid will also be reported.

[1] Zhurov, V. V.; Zhurova, E. A.; Chen, Y.-S.; Pinkerton, A. A. *J. Appl. Crystallogr.* **2005**, 38, 827. [2] Zhurova, E. A.; Zhurov, V. V.; Tanaka, K. *Acta Crystallogr.* **1999**, B55, 917.

**Keywords:** charge density; accurate data processing; data collection on non-routine samples

**FA3-MS02-O3**

**A Copper(II)-Copper(II) Bond in a Dimeric Molecule of a Mineral.** Federica Bertolotti<sup>a</sup>, Alessandra Forni<sup>a</sup>, Giuliana Gervasio<sup>a</sup>, Domenica Marabello<sup>a</sup>.  
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Copper(II) acetate monohydrated, mineral hoganite, shows a dimeric structure with four acetate residuals bridging a metal-metal moiety. The ferromagnetism of the compound has been attributed to spin pairing obtained either through a direct Cu(II)-Cu(II) bond or through the carboxylate ligands. A low temperature (100K) X-ray data collection and a subsequent multipolar analysis has supplied maps of electron densities. The topological study of the maps revealed the presence of a direct metal-metal bond, which has been confirmed by theoretical DFT calculations on the isolated molecule. Experimental and theoretical topological parameters will be reported.

