Charge, Spin & Momentum Density I
Multipole & Maximum Entropy Refinement

MS09.01.01 A COMPARISON OF SERIAL AND IMAGING PLATE DATA COLLECTION: THE LOW TEMPERATURE CHARGE DENSITY OF *Dl*-HISTIDINE. Michael Carducci, Robert Bolotovsky and Philip Coppens (Chemistry Department, State University of New York at Buffalo, Buffalo, NY 14260-3000 USA).

In response to the long (and often difficult) data collection requirements of accurate low temperature intensities for charge density analysis, many laboratories are turning from serial scintillation counters to area detectors. For comparison of these two techniques we present data sets of *dl*-histidine collected at 110K on a CAD4 with sealed tube source and scintillation counter (1) and on a modified Huber 4-circle goniometer with rotating anode source and Fuji imaging plates. The imaging plate system allows collection, in days, of data sets which required a month or more to be collected serially, but possessing different strengths and limitations compared to "standard" serial data.

Imaging plate data was processed using HIPPO (2) and modified versions of the Blessing software (3) also used to process the serial data. Each data set was subject to several identical refinements using the XD multipolar refinement package. In each case, the same positional and thermal parameters were obtained within 2 sigma and reasonable molecular geometries and rigid bond tests were obtained. In kappa and multipolar refinements, the charges and multipolar populations were found to be dependent on the refinement model and the treatment of discordant data during processing. We compare the differences between data sets with the observed charge densities of *dl*-histidine.

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MS09.01.02 TRANSFERABILITY OF ELECTRON DENSITY: APPLICATION TO MACROMOLECULAR SYSTEMS. V. Pichon-Pesme, H. Lachekar, C. Lecomte, LCM3B, URA CNRS n° 809, Université Henri Poincaré, Nancy 1, BP 239, 54506 Vandoeuvre-lès-Nancy Cédex, France

Because electron density is a local property, e- density studies of the peptide molecules show that the nonspherical part of the deformation density (i.e. the P_{lm} parameters of Hansen-Coppens model) and the P_v valence population parameters remain essentially the same for a given atom in the same environment. We have determined for each chemical type of a given atom a small set of pseudoatom multipole parameters and we have used them to describe aspherical form factors.

The refinement of the structure of a peptide for which only low resolution data are available was improved by the use of these aspherical factors[1]. The statistical indices decreased by about 30 %, the molecule pass the rigid bond test very well. On leu-enkephalin, we will show a comparison between the multipole refinement[2] and a structure refinement with aspherical form factors and net atomic charges derived from our previous studies on other peptides. The agreement factors, the experimental deformation density map, the result of rigid bond test are comparable in both cases. These results lead us to consider this method for bigger molecules like small protein. Then, we are creating a data bank containing all the multipole parameters for each type of atom for the 20 amino acid residues. The preliminary results applied to high resolution data of a scorpio toxin will be shown.

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MS09.01.03 IMAGING OF DIFFRACTION DATA BY MEM. Makoto Sakata, Dept. of Applied Physics, Nagoya University, Nagoya 464-01 JAPAN.

The recent works of charge and nuclear densities in crystalline materials using the Maximum Entropy Method (MEM) is reviewed. Recently MEM has been introduced and developed as a new method for accurate structure analysis[1,2]. The MEM is promising in material science since the high resolution density distribution can be obtained directly from the limited number of diffraction data. The concept of Imaging of Diffraction Data is introduced to describe the role of MEM analysis in these works. Assuming that the phase problem is solved by direct method or some other way, it is possible to reconstruct real space image, such as the electron density distribution in the case of X-ray diffraction[2], the nuclear density distribution in the case of neutron diffraction[3], or the spin density distribution in the case of polarized neutron diffraction[4], directly from the experimental diffraction data. This process can be done without using any crystal structure model. This fact may provide a new approach in crystallography, in which all the sophisticated analyses, such as multipole or topological analysis[5] of charge density and anharmonicities in nuclear density[6] can be done based on the real space images of diffraction data instead of the reciprocal quantities of structure factors.

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MS09.01.04 RETRIEVAL OF SPIN DENSITIES FROM POLARIZED NEUTRON DIFFRACTION DATA USING MAXIMUM ENTROPY. R. J. Papoular, Laboratoire Leon Brillouin, CEN-Saclay, 91191 Gif-sur-Yvette Cedex, France

In this work, Maximum-Entropy (MaxEnt) is viewed as a powerful and flexible regularizing tool used to solve an ill-posed linear inverse problem: the retrieval of model-free 3-dimensional magnetization densities $m(\mathbf{r})$ from scarce and noisy data sets of measured flipping ratios. Beside the ability of MaxEnt to reduce truncation effects of the standard Fourier synthesis drastically (Papoular et al, 1990, Europhys. Lett, 429-434), it also brings forth three radical improvements:

• **The retrieval of a 2D projection is now a 3D reconstruction problem, which makes use of all the experimental data** This results from the nonlinearity of the MaxEnt algorithm. In extreme cases, quite decent projections can be obtained even without a single Bragg reflection from the horizontal scattering plane (Papoular et al, 1995, Acta Cryst, A51, 295-300).

• **Previous chemical knowledge can be introduced as a 3D nonuniform prior spin density in real space.** This is particularly valuable when the neutron data are too scarce and/or noisy. The features not present in the data are then taken from the best available model for the spin density prior to the experiment (Zheludev et al, 1995, Acta Cryst., A51, 450-455).

• **The retrieval of spin densities pertaining to acentric structures can now be achieved,** once the flipping ratios pertaining to acentric Bragg peaks have been suitably linearized (Papoular et al, 1994, Phys. Rev. Lett., 72, 1486-1489).

Resulting MaxEnt density maps can and should be used to improve on already existing models, e.g. via a refined multipole expansion.

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