# On Precision and Accuracy of X-Ray Results as a Function of Resolution and Electron Density Model

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The Independent Atom Model (IAM) of electron density effectively introduced a century ago is still the most common model of electron density used in structural analysis. When this model was introduced, Max von Laue, the Braggs and their colleagues were using home-made pieces of equipment which could have hardly supplied qualitative information on diffraction spots. In consequence, the errors associated with the model of electron density used were overshadowed by far larger diffraction hardware errors. It is very surprising that although the quality of diffraction information collected in X-ray experiments in XXI century allows for far more thorough X-ray diffraction data quality, most crystallographers (with exception of the participants of this Conference) keep using 100 years old models of electron density effectively proving that even with the most modern scientific tools, one can step backward and do ca. 100 years old crystallography☺.

In our presentation, we will discuss precision and accuracy of X-ray results (structural parameters and ADPs and their errors) as a function of resolution of X-ray data and different models of electron density (IAM, experimental pseudatom- Hansen/Coppens, Hirshfeld Atom Refinement, and Transferable Aspherical Atom Model) applied in the refinements of multiple datasets obtained for hydrated oxalic acid. We will present a detailed comparison of structural, thermal and electronic parameters obtained for the same diffraction data sets when different models of electron density are refined against collected intensities of reflections. Some practical suggestions will be presented how to estimate and improve the quality of single crystal X-ray diffraction structural results. We have obtained our results using multiple (12) high resolution hkl datasets collected for oxalic acid trimmed to particular resolutions and applying different models of electron density.

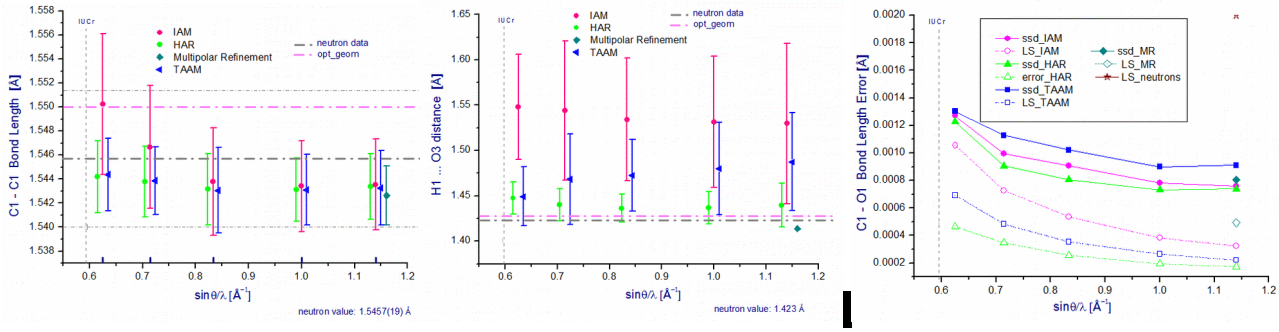


Fig. 1. Examples of relations obtained for different parameters of oxalic acid (the central C1C1 bond, the -C(1)OOH(1)…O(3)H2 hydrogen bonding, errors of C(1)O(1) bond); ssd stands for sample standard deviations (solid lines) whereas the dotted lines illustrate esds from LS refinement.

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