MS28-O4 On precision and accuracy of X-ray results – How to get better quality results from different X-ray diffraction experiments

Krzysztof Wozniak[1], Fabiola Sanjuan-Szklarz[1], Magdalena Woinska[1], Slawomir Domagała[1], Paulina Dominiak[1]

1. Biological and Chemical Research Centre, Chemistry Department, Warsaw University, Zwirki i Wigury 101, 02-089 Warszawa, Poland

email: kwozniak@chem.uw.edu.pl

Although everything seems to be already well known in the field of routine structural single crystal X-ray analysis and ca. 1.1 mln structures have been solved and refined so far, even commonly used approaches and models should be critically re-evaluated. It is incredible that 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. One would even say that its success has dominated the whole field. 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. However, within the past century there is an overwhelming progress in design and production of X-ray hardware which is made for needs of both small laboratories and large scale facilities. This progress in sophisticated X-ray hardware should also accelerate progress in the quality and complexity of models of electron density used to interpret experimental results. However, it is very surprising that although the quality of diffraction information collected in X-ray experiments in XXI century allows these days for far more thorough structural data quality, almost all crystallographers 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 my presentation, I will discuss precision and accuracy of results as a function of resolution of X-ray data when IAM, experimental charge density studies, Hirshfeld Atom Refinement, and Transferable Aspherical Atom Model are applied. I will present a detailed comparison of structural, thermal and electronic parameters obtained for the same diffraction data sets when different models of electron density (IAM, TAAM, HAR, MM) 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. The Authors acknowledge financial support within the Polish NCN MAESTRO grant, decision number DEC-2012/04/A/ST5/00609.

Figure 1. Symbolic consequences of application of the Independent Atom Model.

Keywords: Accuracy, precision, IAM, charge density, HAR, TAAM