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A century after the Braggs on precision and accuracy of single crystal X-ray results

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So far, more than 1.4 mln organic, inorganic and macromolecular structures have been solved and refined by single crystal X-ray analysis. It is incredible that the Independent Atom Model (IAM) of electron density, effectively introduced a century ago, is still the most common model used in structural analysis. Its success has dominated the whole field of X-ray diffraction for the past century and for years now plays, quite a negative role. When IAM was introduced, Max von Laue, the Braggs, were using home-made pieces of equipment which could have hardly supplied any qualitative information on diffraction spots. In consequence, the errors associated with the model of electron density were overshadowed by far larger diffraction hardware errors. However, within the past century, there has been an overwhelming progress in the design and production of X-ray hardware made for the needs of both small laboratories and large-scale facilities. This progress should also accelerate progress in the quality and complexity of models of electron density used to interpret experimental results. I will discuss the precision and accuracy of single crystal X-ray results obtained for multiple measurements of single crystals of oxalic acid as a function of the resolution of X-ray data and the quality of electron density model applied (IAM, multipole model (MM), Hirshfeld Atom Refinement (HAR) and Transferable Aspherical Atom Model of electron density (TAAM)). I will present a detailed comparison of structural, thermal and electronic parameters obtained for the same multiple diffraction data sets collected for single crystals of oxalic acid when different models of electron density are refined. Practical suggestions will be presented how to estimate and improve the quality of structural results. Among others with the newer models, one can obtain more precise and accurate information on positions of H-atoms or energy of intermolecular interactions in crystals.

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