MS25-P08 | REFINEMENT OF ORGANIC CRYSTAL STRUCTURE WITH MULTIPOLAR ELECTRON SCATTERING FACTORS

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Electron diffraction (ED) is based on scattering of electron beam on electrostatic potential. This recently fast advancing method allows to obtain crystal structures of nanocrystals at atomic resolutions, for both small and macro- molecules [1,2]. However, for this purpose, it is necessary to use proper scattering factors [3]. Different models, already known for x-ray diffraction, can be implemented for ED.

In this study, we present comparison of refinements of IAM and TAAM (Transferable Aspherical Atom Model) with parameters of multipolar model with Hansen-Coppens formalism taken from UBDB [4]. For both models are used electron scattering factors implemented in DiSCaMB library [5] and interfaced with Olex2[6]. The TAAM accounts for the fact that atoms in molecules bear partial charge and are not spherical. Refinements are performed against experimental electron structure factors [1] and theoretical electron structure factors computed in Crystal14 [7]. Results show the possibilities and limitations of the TAAM method. We discuss e.g. improvement of fitting statistics (R1), anisotropic displacement parameters and hydrogen atoms positions obtained from refinements of TAAM instead of IAM.

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