

Refinement on electron diffraction data in MoPro: A quest for improved structure model

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The most conclusive and elucidating component of any small or macromolecular study is the proper structure determination. The two most commonly used tool for structure determination are being nuclear magnetic resonance spectroscopy (NMR) and X-ray diffraction. While both these techniques are extremely popular but have certain limitations. Recently a new technique 3D Electron Diffraction (3D ED) data collection for getting near to atomic resolution structures has taken a leap in last few years. In this method, once the intensities are extracted, the structures are obtained from the 3D ED data using similar tools as for X-ray diffraction structure determination like SHELX, olex2 etc. In general Independent atom model (IAM) are used for solving the structures, where a precomputed model of electrostatic potential is built using scattering factors from isolated, spherically averaged atoms or ions.¹ In reality the atoms in molecule are not isolated and spherical, moreover the usage of improper electron scattering factors in refinement may lead to physically unrealistic values. To overcome this, a aspherical TAAM refinement have been applied both for X-ray and ED refinement which largely improved the physical representation and refinement statistics of the structure.² We have chosen a model molecule β -glycine for this study for which 3D ED data is already available.³ Spherical and Aspherical TAAM refinement seemed to be possible in MoPro with the inclusion of electron scattering factors. Aspherical electron scattering TAAM model will be constructed using ELMAM2 and MATTS databank and refinement will be performed using MoPro. A comparison will be shown between reported data and spherical and aspherical TAAM refinement using MoPro and various statistics will be presented.

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[3] Broadhurst, E. T. *et al.* Polymorph evolution during crystal growth studied by 3D electron diffraction. *IUCrJ* **7**, 5–9 (2020).

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