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Beyond IAM refinement for 3D ED data: aspherical scattering factors

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In recent years we observe spectacular development of the methods for 3D electron diffraction (3D ED). Currently, there are available structures from refinements in the dynamical approach [1] with R-factors below 10% and resolution around dmin = 0.5Å. For such data, residual electrostatic potential on bonding paths or lone electron pairs regions can be observed. It gives us an opportunity to use more sophisticated, aspherical models and get closer to obtaining the correct electrostatic potential from the experiment.

We proposed Transferable Aspherical Atom Model (TAAM) refinements against 3D ED data in kinematic approximation [2]. Next, we coupled TAAM with dynamical refinement in Jana2020 [3]. Here, we present refinements of 1-methyluracil crystal structure against dmin = 0.56 Å data with TAAM in the dynamical approach. We use several TAAM versions. TAAM fits to the experimental data better than standard IAM, what is evidenced by a visible clearing of the residual density map (Fig. 1), lowering of the maximum and minimum values and lowering of R-factor. However, after detailed analysis we see the insufficiency of TAAM.

By comparing experimental refinements and theoretical simulations we discuss possibilities of the refinement of the valence populations of multipole model directly against experimental 3D ED data. We show how big impact on electron scattering factors have even small changes in multipole model parameters and how huge impact on the Fourier electrostatic potential maps have incorrect scattering factors. These results help us to understand what we really see on the residual electrostatic potential maps.

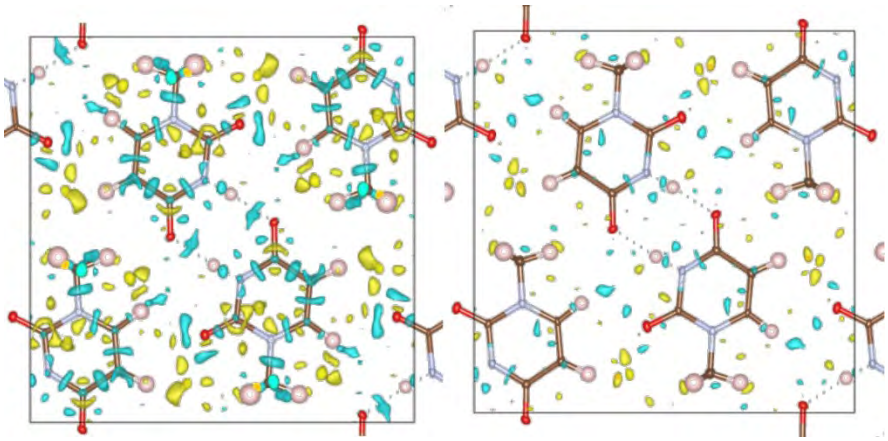

Figure 1. Residual density maps for dynamical IAM refinement (left) and dynamical TAAM refinement (right). Contour level 0.04 eÅ^{-1}, yellow: positive, cyan: negative.

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