Oral presentation

Using aspherical Hirshfeld form factors in structure refinements against 3D ED data

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3D electron diffraction (3D ED) has emerged as an alternative to x-ray diffraction for structure elucidation of crystals in the sub-micrometer range [1]. With scattering cross-sections typically 10^4 times larger than x-rays, data can be routinely collected from nano-sized grains. Experiments performed in transmission electron microscopes or electron diffractometers allow to focus electron beams into diameters of tens of nanometers, allowing to collect single crystal data from microcrystalline samples. Further advantages include direct determination of absolute structure [2], easier localisation of light atoms including hydrogens [3] and an increased sensitivity to atomic charges [4]. Dynamical refinements taking multiple scattering of electrons into account allow to obtain precise structure models with R-factors comparable to x-ray diffraction [5].

We have recently focused on improving the modelling of 3D ED data by implementing refinement techniques from the quantum crystallography field. In our previous work, we showed that taking charge transfer among atoms into account through a spherical atom kappa formalism leads to improvements in structure accuracy [6]. We now focus on the implementation of aspherical form factors in 3D ED refinements obtained through the Hirshfeld atom refinement (HAR) formalism [7].

We present here the results on paracetamol. Our results show an improvement in wR(all) from 7.42% to 6.84%, with clearing of residues in difference Fourier maps [Fig. 1]. Comparison of bond lengths with reference values taken from neutron scattering also reveals a betteragreement, suggesting an overall improved accuracy of the refinement.

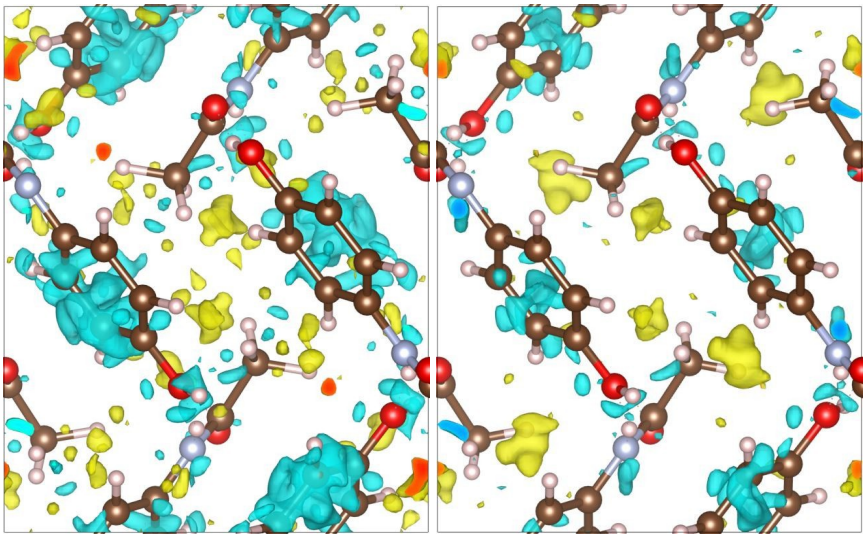

Figure 1. Comparison of Paracetamol difference Fourier maps before (left) and after (right) HAR at the same isosurface level 5.0 e^-/Å.

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