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Keywords: electron diffraction tomography (EDT), dynamical refinement, synchrotron Rietveld refinement, octahedral molecular sieves (OMS), electrode materials

MS27-O4 Localization of hydrogen atoms in organic molecules using dynamical refinement of electron diffraction data

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Although, localization of hydrogen atoms in data from electron diffraction has been reported in special cases [1,2] reliable *ab initio* determination of hydrogen positions from single nano-crystals has not been achieved to the best of our knowledge. Our work focuses on pharmaceuticals and pharmaceutical co-crystals. The stability of these compounds under electron beam irradiation is low and data collection requires low-dose technique at low-temperature. Precession assisted electron diffraction tomography on single nano-crystals was used for data acquisition. Data were processes using programs PETS, Jana2006 and Dyngo. In favourable cases like in the case of paracetamol form I (S. G. $P2_1/n$), it was possible to localize a few of the hydrogen atoms in difference Fourier maps after kinematical refinement of the structure (R(obs) = 20 %). Dynamical approach provided an improved difference Fourier map, which revealed the complete set of hydrogen atoms (Figure 1). Dynamical refinement of the structure without the hydrogen atoms resulted in the R(obs) factor of 12 %. An addition of the hydrogen atoms into the model led to an addition improvement of the R(obs) slightly below 10 %, demonstrating the sensitivity of the result to the presence of the hydrogen atoms in the model.

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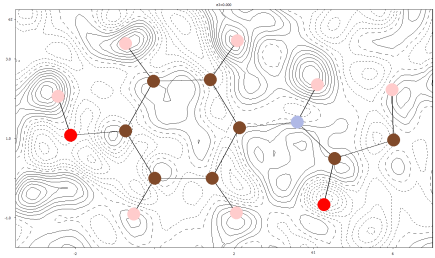

Figure 1. Difference Fourier map of the best plane through the paracetamol molecule overlayed by the structure obtained after refinement of the model with added hydrogen atoms.

Keywords: hydrogen atoms localization, single crystal electron diffraction, dynamical refinement