MS44-01 | Crystal Structure of New and Highly Complex Organic Molecules Solved by 3D Electron Diffraction

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3D electron diffraction allows data collection on nanocrystalline domains, which can be used as kinematical intensities in ab-initio structure solution methods. The development of single electron detectors for diffraction and of fast recording protocols based on continuous rotation of the sample have dramatically reduced the electron dose necessary for collecting a data set with a large coverage. With total doses of less than 1 el/Å^2 very beam sensitive samples like organic and macromolecular crystals can now be studied by electron diffraction in nanocrystalline form. Examples of structure solution on known pharmaceutical compounds based on simulated annealing will be presented, as the structure solution attempted in case of low quality 3DED data. Combining STEM imaging with weak beams and the sensitivity of direct electron detectors we will show how it is possible to record high quality 3DED data on organic crystals without the need to work under cryo condition. Standard precession assisted step-wise 3DED data collection allowed the structure solution of metaxalone and of the unknown crystal structure of orthocetamol.