[MS17-02] Electron Crystallography of Molecular Crystals.

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Structure analysis of nanocrystalline organic materials, especially those existing as a phase mixture, is still a challenging task. X-ray powder diffraction (XRPD) and nuclear magnetic resonance (NMR) are powerful methods delivering bulk information. With the development of Automated electron Diffraction Tomography (ADT) [1, 2] a new tool has become available to collect single crystal electron diffraction data from individual nanocrystals. Successful application of the new technique for "ab initio" structure analysis was demonstrated for a variety of material systems: organic compounds [3], inorganic-organic hybrids [4], metal-organic frameworks [5] and a number of inorganic materials (minerals [6], zeolites [7]). Electron radiation damage leads to the decay of crystallinity in organic samples and, as a result, to modification / elimination of Bragg reflections [8]. The first stages of decay mainly affect high resolution reflections, thus making the data inappropriate for direct methods structure analysis. Nevertheless, the reduced resolution data can still be efficiently used for unit cell parameter determination, thus allowing polymorphs to be distinguished [9] and for the indexing of complex powder diffraction profiles. 3D reciprocal space reconstructed from electron diffraction data provides the possibility to identify and structurally describe disorder effects. Addressing each crystal individually, electron diffraction can efficiently describe polyphasic systems thus supporting XRPD and NMR analysis.

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