

Structure Determination of Organic Materials from Powder X-ray Diffraction Data: Opportunities for Multi-technique Synergy

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Structure determination of organic materials directly from powder X-ray diffraction (XRD) data [1,2] is nowadays carried out extensively by researchers in both academia and industry. Most work in this field exploits the direct-space strategy for structure solution [3,4] followed by Rietveld refinement. Although these techniques are now readily accessible and relatively straightforward to use, it is essential that the structural results obtained from such analysis are subjected to rigorous scrutiny before they can be assigned as incontrovertibly correct, and the lecture will present an overview of important issues that must be given careful attention in validating the correctness of crystal structures determined using these techniques. The lecture will discuss several aspects of validation that are important with regard to: (i) validation of the appropriate structural model for use in direct-space structure solution calculations, and (ii) validation of the final structure obtained from Rietveld refinement [5]. The lecture will emphasize that significant advantages can be gained by the synergistic utilization of information obtained from other experimental and computational techniques as an important component within the strategy for structure determination from powder XRD data [6-10], focusing on the important roles that solid-state NMR spectroscopy and periodic DFT calculations may play in extending the scope of structure determination of organic materials from powder XRD data.

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