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Structure Determination of Molecular Solids from Powder X-ray Diffraction Data

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Structure determination of organic molecular solids from powder X-ray diffraction (XRD) data [1] is nowadays carried out extensively by researchers in both academia and industry, and the development of new methodology in this field has made particularly significant impact in the pharmaceuticals industry within the last 20 years or so. However, although software for carrying out each stage of the procedure for structure determination from powder XRD data is now readily accessible and relatively straightforward to use, it is essential that the results from such structure determination calculations are subjected to careful scrutiny to confirm that the final structure obtained is actually correct. In this regard, it can be particularly advantageous to augment the analysis of the powder XRD data and to assist the scrutiny of the structural results by considering complementary structural information derived from other experimental and computational techniques. Techniques that can be particularly valuable in this regard include solid-state NMR spectroscopy, energy calculations (either on individual molecules or periodic crystal structures), vibrational spectroscopies, and techniques of thermal analysis (e.g. DSC and TGA). The lecture will give an overview of the current "state of the art" in the structure determination of organic materials from powder XRD data, giving emphasis [2,3] to the opportunities to enhance the structure determination process by making use of information derived from other experimental (especially solid-state NMR) and computational techniques. Recent results will be presented, with emphasis on raising issues of relevance to research on pharmaceutical materials.

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