Enhancing Structure Determination from Powder X-Ray Diffraction Data Through Multi-Technique Synergy

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Structure determination of organic materials directly from powder X-ray diffraction (XRD) data [1,2] is now carried out extensively by researchers in academia and industry. Most research in this field uses the direct-space strategy for structure solution followed by Rietveld refinement. Although the structure determination process is generally carried out solely using powder XRD data, significant advantages may be gained by augmenting the process of structure determination from powder XRD data by utilizing information from other experimental and computational techniques. This type of multi-technique strategy may be particularly advantageous in tackling complex and challenging structure determination problems, both by providing independent information that directly facilitates the structure solution process and by allowing rigorous validation of the final structure obtained in the Rietveld refinement. The lecture will focus on the use of solid-state NMR data, three-dimensional electron diffraction (3D-ED) data and periodic DFT-D calculations to enhance the process of structure determination of organic materials from powder XRD data [3-11], and the lecture will highlight several examples from recent research.

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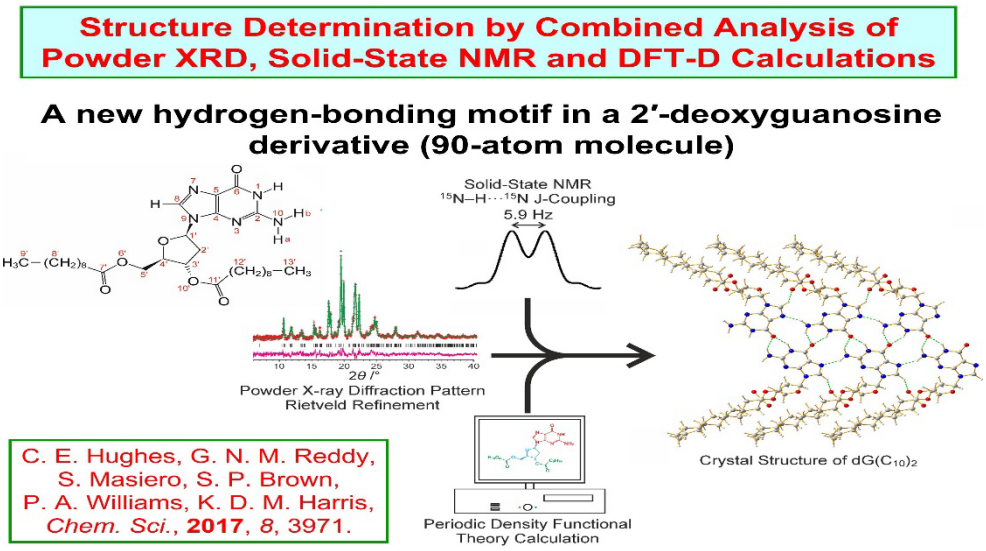

Figure 1