

Poster Presentations

[MS25-P17] Exploiting the Synergy of Powder X-ray Diffraction and Solid-State NMR Spectroscopy in a Powerful Strategy for Structure Determination of Organic Materials

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In the emerging field organic molecular solids the NMR crystallography has become an excellent technique for understanding the packing of organic materials and for characterisation of intermolecular contacts and interactions. We report a strategy for structure determination of organic materials where complete solid-state NMR spectral data is utilized within the context of structure determination from powder XRD data. Following the powder XRD data, first-principles techniques within the GIPAW approach [1] are exploited to calculate the solid-state NMR data for the structure, followed by careful scrutiny of the agreement with experimental solid-state NMR data [2]. The successful application of the strategy [3] is demonstrated by structure determination of the 1:1 cocrystal of indomethacin and nicotinamide. The ¹H and ¹³C chemical shifts calculated for the crystal structure determined from the powder XRD data are in excellent agreement with those measured experimentally. The key feature of this combined strategy is that the quality of the structure determined is assessed both against experimental powder XRD data and against experimental solid-state NMR data, thus providing a very robust validation of the veracity of the structure. Furthermore, via correction (DFT-D-TS) [4] we investigate the competition

between dispersion forces and hydrogen bonding forces in molecular packing.

References:

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