The evolution of SDPD for molecular organics: from routine PXRD to DFT-D

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The development of methods for crystal structure determination from powder diffraction data (SDPD) has seen consistent evolution, from early attempts to apply programs designed to deal with single-crystal data through to programs tailored specifically to overcome the challenges associated with the limited information content of powder data. Whether based around reciprocal space or real space approaches, SDPD is widely accepted as a powerful alternative to single-crystal-based structure determination, and it's important that structures obtained by SDPD are finalised to a high standard prior to deposition or publication.

Energy minimisation using dispersion-corrected density functional theory (DTF-D) has been shown to be a powerful approach to validating crystal structures [1,2] and is one that, with the ever-increasing availability of multi-core CPUs, is now easily accessible to routine practitioners of PXRD. Here, after a brief overview of how SDPD techniques have evolved over the years, and how PXRD fits into the current array of methods available for crystal structure determination, I will outline a systematic approach to determining high-quality molecular crystal structures using PXRD [3], that includes not only the diffraction data, but also factors in DFT-D as a key component of the solution and refinement processes.

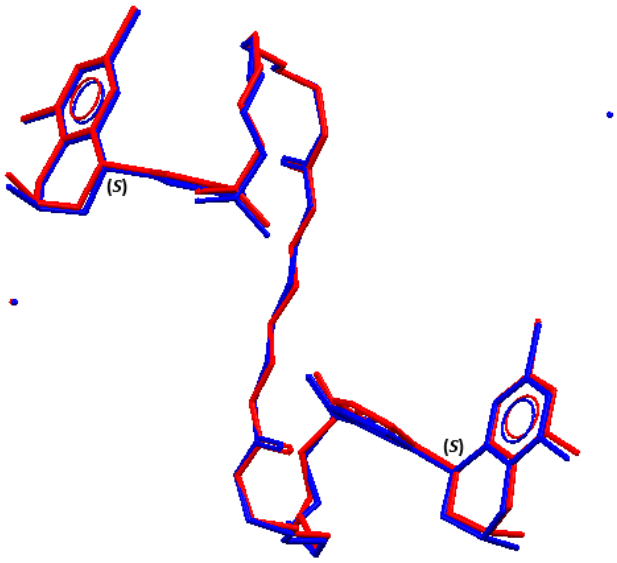


Figure 1. *The asymmetric unit of tenapanor dihydrochloride solved from 2.4Å PXRD data using DASH [4]. The refined structure is shown in red and the fixed-cell DFT-D optimised structure in in blue, RMSD 0.204Å.* N_{atoms}*=144,* N_{DOF}*=45.*

[1] J. van de Streek and M.A. Neumann, Acta Cryst. B (2010). 66(5) 544-558
[2] J. van de Streek and M.A. Neumann, Acta Cryst. B (2014). 70(6) 1020-1032
[3] E. Kabova et al. Acta Cryst. C (2025). 81(10) 559-569
[4] W.I.F. David et al. J. Appl. Cryst. (2006) 39 910-915