MOLECULAR COCRYSTALS AND SALTS: 'FULL' STRUCTURAL CHARACTERISATION FROM POWDER DIFFRACTION DATA

M. Tremayne, L. Thompson, A. Cowell, G. Cutts and D. Bell
School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK.
Email: m.tremayne@bham.ac.uk

Molecular cocrystals are becoming increasingly important within the pharmaceutical industry as they represent a new source of solid-state materials which have the potential to provide optimal physical properties while retaining the chemical properties of the individual components. Although initial identification of a new adduct form is often performed using powder diffraction, subsequent structural rationalisation of these materials is usually carried out using single crystal techniques. The ability to determine the crystal structures of these materials from powder diffraction data is vital when crystals of suitable quality cannot be obtained from traditional solvent-mediated cocrystal synthesis, but becomes even more invaluable when a stoichiometry or form is available only from synthesis by solvent-drop or dry grinding.

The development of direct space structure solution techniques has been a driving factor in the increasing number and complexity of crystal structures that can be determined by powder X-ray diffraction data. This presentation will focus on some of our recent work on the development and application of the differential evolution structure solution technique (DE) which employs evolutionary principles to guide a highly efficient global optimisation process.

Examples will be chosen to demonstrate application to multicomponent molecular systems (molecular cocrystals and salts based primarily on isonicotinamide, nicotinamide and dicarboxylic acid synthons) prepared from both solution and solid-based synthesis. The accuracy and reliability of the structural details obtained from both laboratory and synchrotron data will be discussed including interpretation of protonation and isomerisation within the adducts presented. The ability for structure solution from multi-phase powder diffraction data will also be discussed.