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Keywords: hydrogen bonding, supramolecular synthons, coordination networks

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Cocrystallization of amino acids

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Cocrystals are multi-component systems where intermolecular interactions are used to form supramolecular networks containing more than one molecular entity. Cocrystals offer potential benefits in manufacturing of Active Pharmaceutical Ingredients in solid state with improved pharmaceutical properties like solubility, stability, manufacturability and bioavailability.

A series of hydrophobic amino acids L- Leucine, L- Isoleucine and L- Valine were selected to develop cocrystals by employing different crystallization strategies under various conditions of temperature and pressure. Crystals suitable for single crystal X-Ray diffraction were grown and the structures of these novel forms were resolved. Raman spectroscopy was also used to aid in the identification of these new forms. The final structures were compared to the pure forms of the amino acids so that structural similarities could be drawn.

Keywords: amino acids, cocrystallization, X-ray diffraction

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The XPac dissimilarity index as a quantitative descriptor of isostructurality

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We investigate the crystal structures formed by closely related organic molecules. In this way, it should be possible to examine the effects of incremental changes in molecular shape, van der Waals interactions and other, more directed intermolecular forces on the crystal packing. A 9×8 matrix of 4,4'-benzenesulfonamido-2-pyridines was obtained by the systematic variation of the substituents R^1 at the benzene and R^2 at the pyridine ring. R^1 and R^2 can be CN, CF_3 , I, Br, Cl, F, Me or H (and R^1 additionally OMe). 103 crystal structures were determined in total, at least one for each of the 72 compounds investigated. The computer program XPac [1] was used to establish the packing relationships between individual crystal structures.

One particular 1D stack of N-H...N bonded dimers was identified as the common building block of 37 crystals. These in turn belong to eight distinct 3D packing types. The most frequent of these fundamental structure types comprises all compounds with $R^1 = CF_3$, I, Br, Cl, F,

Me, H and $R^2 = CF_3$ or I. Thus, this fundamental 3D crystal packing arrangement is maintained even if $R^1 = H$ is exchanged against $R^1 = I$, which leads to an approximate doubling of the effective distance at R^1 and increases the molecular volume by 11 %.

A detailed picture of the incremental changes in geometry that occur within this series of 14 isostructures was obtained from matrix maps. These are collections of XPac dissimilarity indices x which have been calculated for individual crystal structure pairs. An inspection of XPac δ -plots provides additional information. It was found that the structural change in this series is predominantly translational and occurs in the direction of the crystallographic c -axes, which lies approximately parallel to the C- R^1 bond. Within the common 1D stack of N-H...N bonded dimers, the relative orientation of the molecules varies with the volume of R^1 .

The analogous geometrical analysis of another series from the same compound class showed that in this case a common basic 3D packing arrangement is maintained only approximately and with substantial geometrical alterations. Therefore, the relationship between these crystals is homeostructural rather than isostructural.

This systematic investigation of 4,4'-benzenesulfonamido-2-pyridines provides a set of universal reference values for the study of packing similarity in molecular crystals.

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Structure of nanosized crystals by total x-ray diffraction

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Nanosized crystals show diffraction patterns with a few, if any, Bragg-like peaks and a pronounced diffuse component that are difficult to be analyzed in the traditional way. The problem has a solution based on an approach involving high-energy x-ray diffraction coupled to atomic pair distribution functions analysis [1]. In the talk, the foundations of the approach will be introduced and its great potential in characterizing the atomic scale structure, size and shape of nanosized crystals illustrated with examples from several recent studies [2-6].

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Contrasting p and T -induced amorphization using ZrW_2O_8 and ZIF-4 as case studies

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