and co-crystal former.
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Keywords: pharmaceutical co-crystal, polymorph, phase transformations

P09.01.10

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New crystal forms of gabapentin

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Gabapentin (GBP) is an API used against epilepsy, neuropathic pain and in the treatment of limb tremor[1]. Several polymorphs of GBP have been reported and characterized, but only SCX of Form II was known until very recently. Our group managed to obtain two new SCX structures of different polymorphs[2,3]. These new forms are not as stable as Form II, proved by several experiments. Form IV can even be considered a disappearing polymorph [3] because it readily transforms into another form. New crystal forms of GBP were obtained on acidifying the solution. We obtained GBP chloride hemihydrate, an ethyl ester of GBP and a co-crystal of GBP-lactam and benzoic acid [Fig.1] in different crystallization conditions. All these structures were determined by SCXRD, presenting different physicochemical properties and supramolecular arrangements [5]. Intramolecular interactions are only observed in Form IV and GBP Cl hemi-hydrate.

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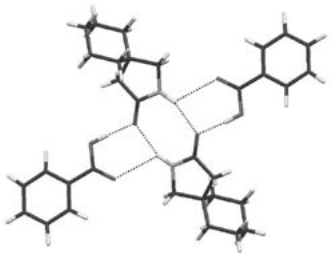
[5]V. Andre et al CrystEngComm, in submission.



Keywords: crystal engineering, cocrystal, polymorphism

P09.02.11

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Molecular cocrystals of peganole with peganine

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Earlier we studied solid solutions of biologically active derivatives of tricyclic quinazolines, the peganole (**1**) with the 6-bromopeganole (**2**) in different stoichiometry [1] using by single crystal X-ray diffraction methods. In all solid solutions, centrosymmetrical hydrogen-bonding interactions are found between the molecules of **1** and **2**, which forms dimers, by O-H...N hydrogen bonding associations. Recently have been prepared of cocrystal of peganole (**1**) and peganine (**3**) in the ratio of 1:1 which similar dimers connected with hydrogen bonds O-H...N. Individual **1** crystallizes as racemate. As against it **3** crystallizes in enantiomorfic forms, that confirm X-ray analysis of single crystals of **3** received by us and the literature [2]. In the unit cell of cocrystals both enantiomorphic forms of each substance (**1** and **3**) are located. Thus, individually peganine crystallizes in enantiomorph form, but in cocrystal take part both enantiomorfic forms. Probably, racemat peganole promote to cocrystallization of racemate peganine.

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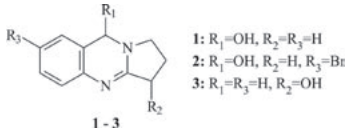

Keywords: cocrystals, solid solutions, hydrogen bonds

P09.02.12

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Subtle relationships between the structures of some aspirin derivatives

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Prompted by the identification of a second polymorph of the simple analgesic molecule aspirin, we have made a structural systematics study of some simple derivatives of aspirin. The main aim of this was to see how robust are the packing features in the two phases of the parent molecule, which have 2D similarity, in view of the small changes in the molecular shape and the possibility that the substituent groups may themselves have some involvement in defining intermolecular interactions. Compounds selected were those in which one aromatic ring proton was replaced by a small substituent group. Two relevant structures were already known - 3-methyl aspirin and 6-methyl aspirin. Further examples, namely 4-Me, 5-Me, 5-F, 5-Cl, 5-Br, 5-I, and 5-NO_2 aspirin were synthesised from substituted salicylic acid derivatives. Structure determinations of the new compounds, and detailed comparisons of all structures using the XPac method (Gelbrich and Hursthouse (2005) CrystEngComm 7: 324-336.) revealed that the family contained two isostructural sets − the 5-Cl-, 5-Br- and 5-I- derivatives, and the 5-F-, 5-O_2N- and 5-Me derivatives. A number of lower dimensional similarities were also identified. The poster will describe the relationships found between the structures.

Keywords: aspirin derivatives, systematics of crystal structures, structural motifs

P09.02.13

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The influence of hydrogen bonding on generation and stabilization of self-assembled layer structure

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The crystal structure of 6-[4-(trans-4-pentylcyclohexyl)phenoxy] hexane-1,2-diol (hereafter, CP2OH) has been determined by X-ray diffraction techniques. The CP2OH molecule crystallizes in the monoclinic crystal system with space group *C*2/*c* (#15). The asymmetric unit consists of one crystallographically independent molecule of CP2OH, and the unit cell contains eight molecules of CP2OH. The CP2OH molecules crystallize in sheets of layered arrangement along [010] direction. The unit distance of 30 Å exists between neighbouring layers along the [010] direction. In each sheet of the layered structure of CP2OH, the molecules are aligned in an inclined manner in which the terminal hydroxyl groups lie in a head-to-head fashion generated by hydrogen bonding interactions. The driving force behind the generation and stabilization of each sheet of the layered structure is attributed to the hydrogen bonded network between the terminal hydroxyl groups in the self assembled driven interactions amongst the CP2OH molecules. The intermolecular interactions are generally driven by hydrogen bonding and are also orientation dependent.

Keywords: hydrogen bonding, self-assembly, layered structure

P09.02.14

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Intermolecular interaction-directed conformations of bridged bis(1,4-piperazine-2,5-diones)

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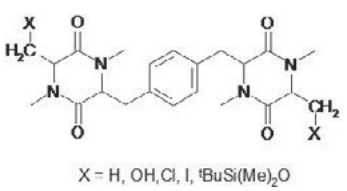
Recent synthetic work to chart a new and efficient route to xylylene-bridged bis(1,4-piperazine-2,5-diones) crossed over into organic crystal engineering, yielding some unexpected and intriguing results. In this class of compounds, molecular flexibility via rotation at the benzyl bridges permits the adoption of several conformers. S and C shapes are possible, depending on the relative position of the piperazinedione rings and the side chain substituent X. An S shape is clearly the least sterically hindered and is observed with both bulky (tert-butyldimethylsilyloxy) and small (hydrogen) substituents. Variation of side chain substituent from hydrogen to hydroxyl and halogen groups, however, showed that several compounds readily crystallize in a potentially energetically unfavourable C shaped conformation. The molecular conformation appears to be directed by hydrogen bonding and halide...halide interactions in the crystal packing, with the stabilization provided by these interactions overcoming steric hindrance. This poster will highlight some of these sterically strained compounds and discuss associated synthetic and crystallographic problems.



X = H, OH,Cl, I, ^{t}BuSi(Me)$_2$O

Keywords: molecular conformation, hydrogen bonding, halide interactions

P09.02.15

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Polymorphism from a solution perspective: Rationalisation at the molecular level

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Polymorphism is the formation of different crystal structures by the same chemical compound. It is an important phenomenon associated with crystallization because the crystal polymorphs have different physical properties, especially solubility differences which impact on chemical reactivity and bio-availability. The existence of polymorphic solid forms has far-reaching implications on patent ownership in the pharmaceutical industry. The critical stage in determining the outcome of a crystallization process for a polymorphic system is the nucleation state. This is believed to be a non-crystalline state of a few tens of molecules, formed via self-assembly from solution, present just prior to crystallisation. It is the structure of this state, and how it is influenced, which is key to understanding and controlling polymorph formation. To address this we have developed a protocol that strives to relate experimental and theoretical data, via artificial neural network analysis. This allows both experimental polymorph prediction and the identification of the molecular-level parameters (or combinations of) that influence the polymorph selection process. Our first target system was that of the well-studied polymorphic pharmaceutical carbamazepine. Polymorph screening experiments revealed a strong solvent and temperature dependence on the polymorph obtained from each experiment. Our work has focused on identifying the molecular-level parameters that are influential in the selection process, and consequently developing an ability to determine the polymorphic outcome of a crystallisation experiment.

Keywords: polymorphism, neural networks, molecular modelling

P09.02.16

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Characteristic network structure constructed from various block-like molecules

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Construction of molecular networks has recently drawn much attention in respect to the useful applications such as catalytic activity, gas adsorption and molecular channels for clathration. It is known that 3-D bulky molecule can construct a highly ordered aggregation in crystalline state. Precise control of topology, size and direction of functional group are required to such block molecules. We synthesized various block molecules based on stereochemistry of tertiary aromatic amide which prefers cis (folded) conformation and studied the crystal structures of them and their metal complexes. The simple cyclic aromatic triamide 1 constructed a 2-D coordination network with lanthanide metal cations in the crystalline state. Spherical aromatic amide 2 aggregated into a channel-shaped network via weak intermolecular interactions. Furthermore, complex