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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 $C2/c$ (#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

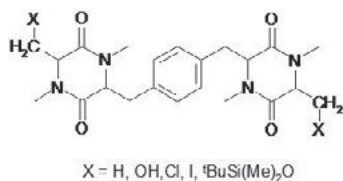
P09.02.14

Acta Cryst. (2008). A64, C478

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.



Keywords: molecular conformation, hydrogen bonding, halide interactions

P09.02.15

Acta Cryst. (2008). A64, C478

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

Acta Cryst. (2008). A64, C478-479

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