

**FA4-MS03-O1****Complexation of Camphor by  $\alpha$ -Cyclodextrin.**

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Complexes of  $\alpha$ -cyclodextrin with camphor were prepared by diffusion method: solution of cyclodextrin in water or water/alcohol was exposed to slowly diffusing vapors of camphor. Two principal crystalline phases were obtained in this way. First, needle shaped crystals form having the 1 : 2 guest/host molecular ratio. In the second step flattened needles of a different structure form. In both phases substantial amounts of solvent molecules are present and are able to reversible sorption/desorption, at which swelling/contraction of the unit cell takes place. It was measured by powder diffraction on a series of samples. Lattice parameters: (I)  $a=13.7894$ ,  $b=24.4785$ ,  $c=30.9833$ ,  $P2_12_12_1$ ; (II)  $a=16.170$ ,  $b=72.140$ ,  $c=16.460$ ,  $\beta=119.300$ ,  $P2_1$ . The II structure is very sensitive to the changes of composition of the mother solution. When exposed (crystals under mother liquor) to open air, the crystals crack even when covered with the liquid due to slow change of its composition (alcohol evaporating faster than water). Similar effect occurs when adding water to the mother solution. This will be illustrated by microscope movie and x-ray powder diffractograms showing the lattice contraction effects. Camphor molecules included within the double-cyclodextrin cavity are strongly held and desorb completely above 250 °C only.

**Keywords:** cyclodextrin; camphor; supramolecular inclusion compound

**FA4-MS03-O2**

**Structure-Property Relationships of Two Host-Guest Systems.** Len Barbour. Department of Chemistry, University of Stellenbosch, Stellenbosch, South Africa.

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Unraveling the link between structure and function is one of the core pursuits in the field of materials science. Single-crystal X-ray diffraction studies provide a valuable means of elucidating intermolecular interactions and this information can be utilized to great effect with regard to explaining interesting and useful properties of materials. A number of inclusion compounds have been studied using two different host systems: Dianin's compound and a series of related diyne-diol compounds. These systems exhibit interesting properties, which include polar ordering of guests, anomalous thermal expansion, recrystallisation on guest-loss (as opposed to host rearrangement), self-inclusion [1] and porosity. The structure-property relationships of a number of crystalline systems will be discussed.

[1] Lloyd, G. O.; Alen, J.; Bredenkamp, M. W.; de Vries, E. J. C.; Esterhuysen, C.; Barbour, L. J. *Angew. Chem. Int. Ed.* **2006**, *45*, 5354.

**Keywords:** diynes; Dianin's compound; host-guest interactions

**FA4-MS03-O3**

**Molecular Shape and Polarity Relationships for Cocrystal Screening.** László Fábán<sup>a,b</sup>, Tomislav Friščić<sup>a,c</sup>, Shyam Karkj<sup>a,c</sup>, William Jones<sup>c,a</sup>.

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We have recently found [1] that cocrystals in the Cambridge Structural Database (CSD) [2] are usually formed by molecules of similar shapes and polarities. The relative influence of supramolecular synthons and shape similarity was investigated by screening experiments. The experiments involved pairs of molecules with (a) similar (strong) synthons and similar shapes, (b) similar synthons and different shapes and (c) different (strong or weak) synthons and similar shapes. Cocrystals were obtained only in the first case, that is, if both strong synthons and similar molecular shapes favoured their formation.

Statistical data on shape and polarity descriptors calculated for cocrystals in the CSD were used to derive cut-off values for likely cocrystal formation. If both the shape and polarity descriptors of two molecules differ by less than these cut-off values then the molecules are considered 'likely' to form a cocrystal, otherwise they are 'unlikely' to cocrystallise. Screening experiments on more than 200 compound pairs were analysed using this scheme. The results show that by performing only the 'likely' experiments the efficiency of screening can be increased by 50% while losing only 15% of the cocrystals.

[1] Fábán L. *Cryst. Growth. Des.*, **2009**, *9*, DOI: 10.1021/cg800861m. [2] Allen, F.H. *Acta Cryst.*, **2002**, B58, 380.

**Keywords:** cocrystals; screening experiments; molecular descriptors

**FA4-MS03-O4**

**Diffuse Scattering from Layered Organic Materials.** Lynne H. Thomas<sup>a</sup>, Gavin A. Craig<sup>a</sup>, Derek S. Middlemiss<sup>b</sup>, Chick C. Wilson<sup>a</sup>.

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Organic materials with a layered crystal structure characteristically tend to have strong intermolecular interactions within the planes but much weaker interactions between the planes. Such systems often are subject to faults in the crystal packing that may occur during crystal growth or by the application of external forces such as

pressure or temperature. The planes of molecules may slip relative to one another creating stacking faults or molecules may individually displace from their planes in such a way as to enhance or relieve any interactions that may take place between the planes. Such movements, if correlated over short distances, can give rise to structured diffuse scattering. This diffuse scattering may manifest itself as features connected to Bragg peaks such as long tails, or as those located in between and well separated from the Bragg peaks. Each of the materials to be presented here shows characteristic diffuse scattering, the location of which can give us insight, in a qualitative manner, into the possible causes of the disorder. Quantitative computational modelling can provide information into the short-range order in these materials and the length scales over which it occurs. In order to measure the complete diffuse scattering pattern it is necessary to record large areas of reciprocal space. We have made use of our in-house Rigaku RAPID diffractometer possessing a large area image plate. The exploitation of the large dynamic range and low background associated with an image plate allows rapid measurement of large regions of reciprocal space whilst enhancing the weaker scattering, all on a laboratory diffractometer. It is also possible to expose the image plate for long times and thus record scattering that is much weaker and more diffuse in nature than the Bragg scattering. We will report measurements that we have made on two materials, phloroglucinol dihydrate, and the co-crystal of 3-fluorobenzoic acid with 4-acetylpyridine. Preliminary quantum mechanical calculations into these materials, that will aid quantitative modelling of the disordered structures, will also be presented.

**Keywords:** diffuse X-ray scattering; disordered molecular crystals; molecular cocrystals