

stoichiometry of the inclusion compounds can be controlled by the composition of the liquid guest mixture. The selectivity of a host molecule towards a given guest in a binary mixture of guests G1 and G2 can be determined by competition experiments, in which the inclusion compounds are crystallised in a mixture of guests of known composition and the ensuing crystals analysed by a suitable analytical technique. The resulting analysis of the enclathrated guests yields the selectivity profile which may be of three main types: (i) Zero selectivity, where the mole fraction of the captured guest = that in the starting solution; (ii) A given guest is strongly favoured over the complete range; (iii) The selectivity is strongly concentration dependent [2]. The question which arises is what is the structure of the harvested crystals? Thus if a host compound H forms inclusion compounds H.G1 and H.G2, what is the structure of the crystals derived from the 50:50 mixture of G1 and G2? Is it a mixture of the original compounds, a new compound, or a combination of both? We have studied this problem using bulky Hosts containing Hydroxyl moieties which capture a variety of guests and have obtained unusual results. Thus, with the host H1 = 1,4-bis(9-hydroxyfluoren-9-yl)benzene dissolved in an equimolar mixture of morpholine (MORPH) and 4-picoline (4PIC) the ensuing crystals contain both H1.2(MORPH) and H1.2(4PIC) in the unit cell, with the host adopting both cis- and trans-configurations. The related host H2 = 2,2'-bis(hydroxydiphenylmethyl)1,1'-binaphthyl, yields three distinct polymorphs of the apohost and nine different inclusion compounds when crystallised from pyridine, morpholine, benzene and their various mixtures. The structures of these inclusion compounds, their thermal stabilities and their kinetics of decomposition will be discussed.

[1] Ibragimov B.T., *CrystEngComm*, 2007, 9, 111.

[2] Nassimbeni L.R., in *Separations and Reactions in Organic Supramolecular Chemistry*, eds F Toda and R Bishop, Wiley, Chichester, 2004, Chapter 5.

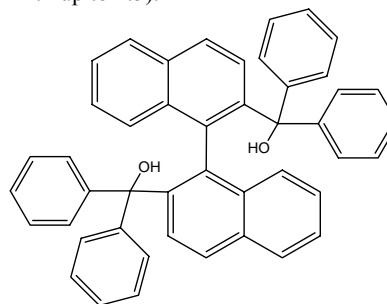
#### MS18 P05

**A bis(hydroxydiphenylmethyl) substituted 1,1'-binaphthyl diol host compound: polymorphism and clathrates with multiple guest species** [Hong Su](#) and Luigi R Nassimbeni, *Department of Chemistry, University of Cape Town, Rondebosch 7701, Cape Town, South Africa*. Email: [hong.su@uct.ac.za](mailto:hong.su@uct.ac.za)

**Keywords:** polymorphism, clathrates, single-crystal X-ray analysis

The host compounds based on the scissor-type design proved to be effective clathrate formers[1]. The diol host compound under our study is 2,2'-bis-(diphenylhydroxymethyl)binaphthylene (**H**) (see scheme). Three polymorphous crystalline forms, A, B and C, were discovered during our study, one of which was previously published[2]. All these three forms has been found to co-exist in solution of equal mole ratio of acetone/2-butanol solvent mixture at ambient conditions. Lattice energies were calculated from their respective atomic coordinates using atom-atom pair potentials with Gavezzotti's program OPIX. The results are  $-215.4 \text{ kJ mol}^{-1}$ ,  $-232.1 \text{ kJ mol}^{-1}$  and  $-210.5 \text{ kJ mol}^{-1}$  for forms A, B and C respectively. This places the stability of these three polymorphous forms in the order B>A>C. This was proved by several slurry experiments using different

solvents, from which form B were constantly obtained. We have carried out competition experiments with three solvents, i.e. pyridine, morpholine and benzene, in different combinations of mixtures at different crystallisation temperatures. A series of clathrates with multiple guest species were obtained: **H**·Morpholine·2Pyridine, **H**·3Morpholine·2Pyridine, **H**·Morpholine·1.5Benzene, **H**·2Morpholine·0.5Benzene, **H**·2Pyridine·Benzene and **H**·Morpholine·Pyridine·Benzene. Analysis of the crystal structures reveals that the molecular structure of **H** is similar in all these compounds. The most characteristic feature of **H** molecule is the presence of an intramolecular hydrogen bond between the two hydroxyls and an intermolecular hydrogen bond to a respective guest. Pyridine is more likely to form hydrogen bond to **H**. Benzene is always hold in the lattice by weak van der Waals interactions. Our study shows a flexible polymorphic host structure with the ability to form clathrates with remarkable high guest ratios (host:guest ratio from 1:1 up to 1:5).



[1] Part 11: Johnson L., Nassimbeni L. R., Weber E., Skobridis K., *J. Chem. Soc., Perkin Trans. 2*, 1992, 2131.

[2] Weber E., Skobridis K., Wierig A., Barbour L. J., Caira M. R., Nassimbeni L. R., *Chem. Ber.* 1993, 126, 1141.

#### MS18 P06

**Inclusion complexes of  $\beta$ -cyclodextrin with the Drugs Triclosan and Tolbutamide.** [A. Paulidou](#), I. M. Mavridis, *Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", P. O. Box 60228, Aghia Paraskevi 15310, Athens, Greece*  
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**Keywords:** beta-cyclodextrin; triclosan; tolbutamide

Cyclodextrins (CDs) are well known cyclic oligosaccharides, water soluble, used for micro encapsulation of organic molecules inside their relatively apolar cavity, thus they are used extensively to solubilize and/or stabilize apolar/unstable molecules, especially drugs. Triclosan [5-chloro-2-(2,4-dichlorophenoxy)phenol] is a wide spectrum antibacterial agent, infused in an increasing number of consumer products. Inclusion of triclosan in  $\beta$ -cyclodextrin ( $\beta$ CD) cavity finds application in the release of the drug in a controlled way. The  $\beta$ CD/triclosan complex has been crystallized from a water/ethanol mixture and data were collected by synchrotron radiation at 100K (triclinic P1,  $a=15.189 \text{ \AA}$ ,  $b=15.23 \text{ \AA}$ ,  $c=16.293 \text{ \AA}$ ,  $\alpha=91.066^\circ$ ,  $\beta=91.049^\circ$ ,  $\gamma=100.709^\circ$ ). The structure has been refined up to  $R_I=0.0658$ .