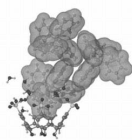


**P.06.06.19***Acta Cryst.* (2005). A61, C287**Exploiting Phenyl Embraces and  $\pi$ -stacking in the Assembly of Supramolecular Arrays of Tetraphenylphosphonium and *p*-sulfonatocalix[n]arene (n=4,6,8)**Alexandre N. Sobolev, Mohamed Makha, Colin L. Raston, Allan H. White, *Chemistry, M313, School of Biomedical and Chemical Sciences, University of Western Australia, Crawley, WA 6009, Australia*. E-mail: ans@chem.uwa.edu.au

The interactions between  $\text{Ph}_4\text{P}^+$  cations and *p*-sulfonatocalix[n]arene anions offer the possibility of building up new materials based on interactions between the anions and cations beyond their electrostatic attraction, such as the possibility of a phenyl ring of the cation residing in the cavity of the calixarene. In developing this concept, we have embarked on a systematic study of the ability of the  $\text{Ph}_4\text{P}^+$ -*p*-sulfonatocalix[n]arene system to generate extensive self-assembled arrays. We report herein the formation of materials built up from  $\text{Ph}_4\text{P}^+$  cations and different sizes calix[n]arenes with n = 4 (see Figure), n = 6 and n = 8.

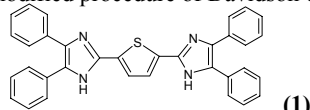


[1] Makha M., Raston C. L., Sobolev A. N., White A. H., *Chem. Commun.*, 2004, 9, 1066. [2] Makha M., Raston C. L., Sobolev A. N., White A. H., *Chem. Commun.*, 2005, *in press*.

**Keywords:** calixarene complexes, crystal engineering, self-assembly molecular chemistry

**P.06.07.1***Acta Cryst.* (2005). A61, C287**Chromotropism of Imidazole, 2,2'-(2,5-thiophenediyl)bis[4,5-diphenyl]**Natalya Fridman, Menahem Kaftory, Shammai Speiser, *Department of Chemistry Technion - Israel Institute of Technology, Haifa 32000, Israel*. E-mail: fridmann@tx.technion.ac.il

We have prepared new doublelophineimidazole derivative, Imidazole, 2,2'-(2,5-thiophene-diyl)bis[4,5-diphenyl] (**1**), according to slightly modified procedure of Davidson et al. [1].



(**1**) shows solvatochromism, halochromism and photochromism in solution and tribochromism, photochromism and thermochromism in the solid state. We have measured the absorption and the fluorescence spectra of (**1**) in aprotic solvent MeCN at different pH. We have measured the absorption and the fluorescence spectra of (**1**) with different periods of irradiation time in neutral MeCN solution and in basic MeCN solution. It was shown that the fluorescence intensity decreases with increasing irradiation time for both solutions.

When (**1**) was triturated in mortar, the light green colour turned to dark green irreversibly. It was found that (**1**) crystallized as inclusion compound in two different colours: yellow and green, depending on the guest molecules. Crystallization of (**1**) from MeCN:Acetone (10:1) yields long solvate yellow needles with the ratio of host-guest (1:2 MeCN:2 H<sub>2</sub>O). Crystallization of (**1**) from dry MeCN yields large solvate green prisms with the ratio of host-guest (1:2). When the yellow crystals were allowed to stand at room temperature, the yellow needles lost two molecules of water and gradually turned into green needles. The spectroscopic behavior of (**1**) in solutions of different pH, before and after irradiation, the packing pattern of two different inclusion compounds of (**1**) are presented.

[1] Davidson D., Weiss M., Jelling M., *J. Org. Chem.*, 1937, 2, 319.

**Keywords:** colour, conjugate compounds, X-ray structure

**P.06.07.2***Acta Cryst.* (2005). A61, C287**Selective Enclathration of Picolines**Kirsten C. Corin<sup>a</sup>, Susan A. Bourne<sup>a</sup>, Luigi R. Nassimbeni<sup>a</sup>, Fumio

Toda<sup>b</sup>, <sup>a</sup>*Department of Chemistry, University of Cape Town, Cape Town, South Africa*. <sup>b</sup>*Department of Chemistry, Faculty of Science, Okayama University of Science, Okayama, Japan*. E-mail: kirsten@science.uct.ac.za

The host 1,1,2,2-tetraphenyl-1,2-ethane diol has been employed to separate the isomers 2-picoline (2-pic), 3-picoline (3-pic), and 4-picoline (4-pic) by selective enclathration. The crystal structures are all stabilized by (host)-O-H...N(guest) hydrogen bonds.

For any pair of guests, competition experiments were carried out by setting up vials containing the host and mixtures of the guests such that the mole fraction of a given guest varied systematically from 0 to 1. This was also done for all three guests simultaneously. The crystals obtained were analyzed by gas chromatography to give the relative amounts of each guest incorporated within the crystal. The experiments show that enclathration preferentially takes place in the order 4-pic > 3-pic > 2-pic.

The effect of adding a "neutral" (non-competitive) solvent was investigated. The effect of benzene and methanol as "neutral" solvents shows that the former is incorporated as a guest in the 4-pic structure, and enhances the enclathration of 4-pic over 3-pic. Methanol displays no such effect.

[1] Dohi K., Tanaka K., Toda F., *J. Chem. Soc. Jpn., Chem. Ind. Chem.*, 1986, 7, 927.

**Keywords:** inclusion compounds, selectivity, separation

**P.06.07.3***Acta Cryst.* (2005). A61, C287**Anisotropy in the Photodimerization of 9-Acetylanthracene in Inclusion Compound**Irena Zouev, M. Kaftory, *Department of Chemistry Technion - Israel Institute of Technology, Haifa 2000, Israel*. E-mail: charisha@technion.ac.il

Besides their intrinsic and basic scientific significance, organic solid-state photoreactions are attractive for a variety of reasons. They are useful as a means for synthesizing novel products that may be very difficult, if not impossible, to prepare by other means. The advantage of these reactions is that they are friendly to the environment.

Solid-state photochemical reactions are highly dependent on the geometry of the reacting compound and its product. An important advantage in the understanding of the reaction mechanism, the course of the reaction, and the reaction control factors lies in the ability to follow the geometrical changes during the reaction.

In inclusion compounds, the guest molecules occupy space formed by the host molecules. If the host molecules provide topochemical conditions required for bimolecular reactions and the guest molecules are photochemically active, regio- and stereo-selective reactions are anticipated.

Photochemical [4 + 4] dimerization reaction of 9-acetylanthracene inclusion compound was studied using the chromophore absorption spectra tail irradiation method[1]. X-ray diffraction data was collected after irradiation for different periods of time. The interesting finding is that only one of the two crystallographic independent pairs of 9-acetylanthracene undergo solid state photodimerization to ca. 40% conversion to the head-to-tail dimer without destruction of the single crystallinity nature.

[1] Enkelman V., Wegner G., *J. Am. Chem. Soc.*, 1993, 115, 10390.

**Keywords:** inclusion compounds, photochemistry, topochemistry

**P.06.07.4***Acta Cryst.* (2005). A61, C287-C288**Temperature Dependent Selectivity of Inclusion**Lidiya Yu. Izotova<sup>a</sup>, D.M. Ashurov<sup>a</sup>, B.T. Ibragimov<sup>a</sup>, E. Weber<sup>b</sup>, S.A. Talipov<sup>a</sup>, <sup>a</sup>*Institute of Bioorganic Chemistry, Tashkent, Uzbekistan*. <sup>b</sup>*Institute of Organic Chemistry of Technical University Bergakademie, Freiberg, Germany*. E-mail: ckrystal@uzsci.net

Trans-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic acid (DEDA) is a versatile host, capable to form inclusion complexes with both polar and non polar solvents[1]. At the room temperature