

Some of these crystals also represent problem cases as the ensuing crystals are generally small and extremely prone for different kinds of twinning. Still, a first classification of such systems seems to be feasible. Results of these investigations will be reported concurrently.

Keywords: supramolecular assembly; disorder; crystallization

FA4-MS04-P11

High Performance Organic Field Effect Transistors, Textured by Self-assembly. Jens W. Andreasen^a, Claudia M. Duffy^b, Hoi N. Tsao^c, Dag W. Breiby^d, Wojciech Pisula^e, Masahiko Ando^e, Takashi Minakata^f, Don Cho^e, Ali Rouhanipour^e, Martin M. Nielsen^g, Henning Sirringhaus^b, Klaus Müllen^e. ^aSolar Energy Programme, Risø National Laboratory for Sustainable Energy, Technical University of Denmark. ^bOptoelectronics Group, Cavendish Laboratory, University of Cambridge. ^cMax Planck Institute for Polymer Research. ^dDepartment of Physics, Norwegian University of Science and Technology. ^eHitachi Cambridge Laboratory. ^fAsahi-KASEI Corporation. ^gCentre for Molecular Movies, Niels Bohr Institute, University of Copenhagen. E-mail: jewa@risoe.dtu.dk

It is often stated that the penetration of so-called pervasive computing in society depends on the availability of cheap, even disposable, electronics for RFID tags, sensors, flexible displays and matching backplane circuits. Organic field effect transistors (OFETs) are expected to be the building block for these devices, but have been hampered by their low mobility. The performance of organic field effect transistors is seriously compromised by trapping and scattering sites that may comprise structural defects and grain boundaries. Thus, it is crucial to control the formation of such sites, minimizing their occurrence frequency in the completed device, preferably as an integral part of facile processing, i.e. by self-assembly. Research has to a large degree focused on device models based on spin-coated thin films, but in practice, real devices will be manufactured by printing techniques. It is therefore important to determine the process of self-organization of organic molecules using either industrial, or simulated industrial deposition methods. Examples are inkjet or coating methods using molecules in solution. It is well established that texture can be induced by crystallisation from solvent in confined geometries with substantial impact on the charge transport properties of organic semiconductors [1]. We present two cases that may be regarded as laboratory equivalents of the "slot die" and the "immersion/dip coating" techniques of the coating industry, and demonstrate the self-organization effect of these techniques. The first example uses the zone-casting technique [2] which is closely related to the roll-to-roll slot-die coating method. With this method, we demonstrate thin-film deposition of large area (several mm²) crystalline monodomains of the small-molecule organic semiconductor, pentacene [3]. The second example employs the dip-coating

method with a high-mobility conjugated copolymer, cyclopentadithiophenebenzothiadiazole, which shows a doubling of the charge mobility in the processed device because of crystalline texture [4]. The thin film crystalline texture was in both cases determined by comparing grazing incidence X-ray diffraction data with simulations [5].

[1] Cavallini M.; Stolar P.; Moulin J.F.; Surin M.; Leclere P.; Lazzaroni R.; Breiby D.W.; Andreasen J.W.; Nielsen M.M.; Sonar P.; Grimsdale A.C.; Mullen K.; Biscarini F., *Nano Lett.*, **2005**, *5*, 2422. [2] Tracz, A.; Pakula, T.; Jeszka, J. K. *Mater. Sci. (Pol.)* **2004**, *22*, 415 [3] Duffy C.M.; Andreasen J.W.; Breiby D.W.; Nielsen M.M.; Ando M.; Minakata T.; Sirringhaus H. *Chem. Mater.*, **2008**, *20*, 7252. [4] Tsao H.N.; Cho D.; Andreasen J.W.; Rouhanipour A.; Breiby D.W.; Pisula W.; Mullen K., *Adv. Mater.*, **2009**, *21*, 209. [5] Breiby D.W.; Bunk O.; Andreasen J.W.; Lemke H.T.; Nielsen M.M., *J. Appl. Cryst.* **2008**, *41*, 262.

Keywords: organic electronics; conjugated organic compounds; grazing incidence X-ray diffraction

FA4-MS04-P12

Variation in the Supramolecular Assembly of the Molecular Container *p*-Sulfonatocalix[4]arene, a Well-Known Supramolecular Building Block. Clive L. Oliver^a, Leonard J. Barbour^b. ^aDepartment of Chemistry, University of Cape Town, South Africa. ^bDepartment of Chemistry, University of Stellenbosch, South Africa. E-mail: Clive.Oliver@uct.ac.za

The well-known supramolecular building block *p*-sulfonatocalix[4]arene (mostly occurring in its anionic form) crystallizes in a variety of different packing arrangements, depending on the co-crystallized components. It has especially attracted attention when it crystallizes in large, spherical arrangements of twelve calixarene anions residing on the vertices of an icosahedron or cuboctahedron, respectively, the former mimicking the geometry of the many viruses [1,2]. Here we report a variety of novel arrangements of the *p*-sulfonatocalix[4]arene anion some of which include large, multi-component assemblies not conforming to the geometries of the previously reported Platonic and Archimedean solids.

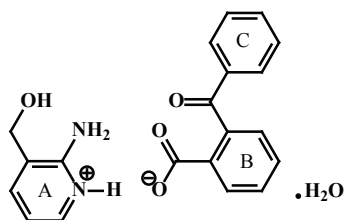
[1] Orr, G.W., Barbour, L.J., Atwood, J.L., *Science*, **1999**, *285*, 1049. [2] Atwood, J.L., Barbour, L.J., Dalgarno, S.J., Hardie, M.J., Raston, C.L., Webb, H.R., *J. Am. Chem. Soc.*, **2004**, *126*, 13170.

Keywords: supramolecular; assembly; variation

FA4-MS04-P13

Structure of 2-amino-3-hydroxymethylpyridinium 2-Benzoylbenzoate Monohydrate. Hakkı Yasin Odabaşoğlu^a, Mustafa Odabaşoğlu^b, Orhan Büyükgüngör^c. ^aPamukkale University, Textile Engineering, Denizli-Turkey. ^bPamukkale University, Chemistry Program, Denizli-Turkey. ^cOndokuz Mayıs University, Department of Physics, Samsun-Turkey. E-mail: yasinodabasoglu@gmail.com

The title crystal is obtained with the reaction of (2-aminopyridin-3-yl)methanol (2-aminopyridine used in manufacture of pharmaceuticals, hair dyes and other dyes) and 2-benzoylbenzoic acid. The cotton fabrics which treated benzophenone derivatives have powerful antibacterial properties against *S. aureus* and *E. coli*, and benzoylbenzoic acid derivatives treated cotton fabric demonstrated pesticide degradation ability, under UV irradiation [1]. Furthermore, the copper (II) complexes of 2-aminopyridinium carboxylates have important properties in the applications of pharmaceuticals, fungicides, oxygen transfer, oxidative addition, homogenous hydrogenation, gas occlusion compounds, and solvent extractions processes [2,3]. Hydrogen bonding plays a key role in molecular recognition [4] and crystal engineering research [5]. The design of highly specific solid-state structures is of considerable significance in organic chemistry due to their important applications in the development of new optical, magnetic and electronic systems [6]. With this in mind, the synthesis and structure determination of the title compound (I), were undertaken.



The crystal structure of the title compound exhibit four N-H...O, three O-H...O and two π ... π interactions. The dihedral angle between the A/B, A/C and B/C aromatic rings are $4.42(14)^\circ$, $78.59(14)^\circ$ and $82.04(14)^\circ$ respectively.

[1] Hong, K.H., Sun, *G. Carbohydrate Polymers* 71, **2008**, 598–605. [2] R.N. Yang, D.M. Wang, Y.M. Hou, B.Y. Xue, D.M. Jin, L.R. Chen, B.S. Luo, *Acta Chem. Scand.* 49, **1995**, 771–773. [3] N. Lah, G. Giester, J. Lah, P. Segegin, I. Leban, *New J. Chem.* 25, **2001**, 753–759. [4] S.P. Goswami, K. Ghosh, *Tetrahedron Lett.* 38, **1997**, 4503–4506. [5] S.P. Goswami, A.K. Mahapatra, G.D. Nigam, K. Chinnakli, H.-K. Fun, *Acta Crystallogr. C* 54, **1998**, 1301–1302. [6] J.M. Lehn, *Angew. Chem. Int. Ed. Engl.* 29, **1990**, 1304.

Keywords: 2-aminopyridine; 2-benzoylbenzoic acid; hydrogen bonding; X-ray crystal structure

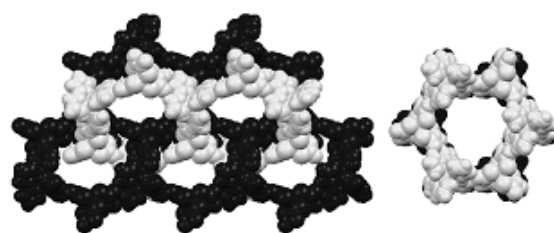
FA4-MS04-P14

Chiral Supramolecular Chemistry Crystal Structure Synthesis-Constructing Channel Structures Based on D_3 Metal Complexes. S. N. Abdul Halim^a, C. J. Adams^a, A. G. Orpen^a. ^a*School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK.*

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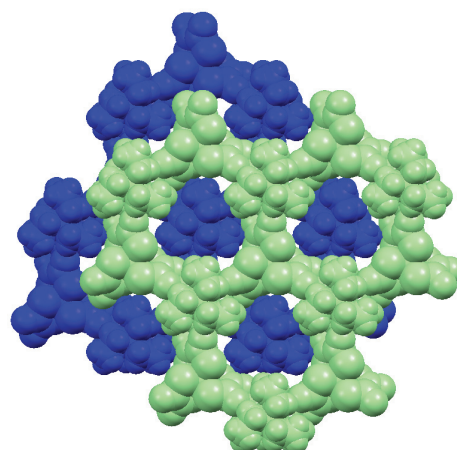
A series of cationic metallotectons containing 2,2'-biimidazole, ethylenediamine and sepulchrate ligands have been crystallized with anionic metallotectons with dithiooxalate and oxalate ligands. The D_3 metal complexes

undergo molecular recognition to obtain a range of chicken-wire networks through persistent hydrogen-bonding patterns adopted by certain functional groups, which act as templates and rely on the robustness of such motifs to create new solid-state structures. The structures typically contain rings of alternating Δ -anions and Λ -cations and *vice versa*. The use of chiral Δ -complexes as tectons remains largely unexploited and can open new perspectives in controlling and directing the individual chelate rings and their relative stabilities. Here we show how the tecton stereochemistry, their supramolecular behaviour lead to formation of structures containing solvent-filled channel and / or occluded regions.



Structure Type A
Iba2

Structure Type E
R3



Keywords: chiral supramolecular chemistry; crystal engineering; octahedral metal complexes