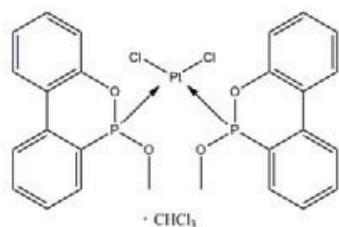


FA4-MS04-P08

Molecular Association in the Dichloridobis(2-methoxydibenzo[c,e]-[1,2]oxaphosphorine-κ-P) platinum(II): Trichloromethane 1:1 Solvate. Tamas Holczbauer^a, Csaba Németh^b, Éva Pfeifer^b, János Mink^b, Andrea Kerényi^c, György Keglevich^c, Mátyás Czugler^a. ^{a,b}*Hung. Acad. Sci., Chemical Research Center, Structural Chemistry.* ^a*X-ray Diffraction, and* ^b*Department of Molecular Spectroscopy,* ^c*University of Technology and Economics, Department of Organic Chemistry and Technology, Budapest, Hungary.*
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The X-ray structure determination of the oxaphosphorine-platinum-dichloride complex showed that it crystallized with one chloroform solvent molecule. The solvent molecules are stuck in channels made up by the complex molecules. These open solvent tubes are parallel to the crystallographic a axis and penetrate the macroscopic crystals throughout. Each chloroform molecule connects to its complex molecule via a pronounced C-H ... O bond. The chloroform molecules are clearly disordered. To decide the dynamic or static nature of disorder X-ray diffraction data were collected at low and at room temperatures, too. IR and Raman spectroscopy were also used to determine the binding angles and the intermolecular C-H ... O bonds' characteristics. The understanding of the role of the chloroform molecule in the solid phase is important for the structure and stability of the crystal. As a first step we reported the LT crystal structure of the title associate [1]. RT structure and spectroscopic results will be compared and analyzed in light of a possible disorder model.



Scheme of the asymmetric unit of the crystal

[1] Holczbauer, T., Keglevich, Gy, Kerényi, A., Czugler, M., *Acta Crystallogr.*, **2009**, E65; m347-m348.

Keywords: inclusion complex; molecular channel; disorder

FA4-MS04-P09

Structural Investigations of Cd Complexes of Bisphosphonate Ester Derivatives. Jonna Jokiniemi^a, Jouko J. Vepsäläinen^b, Harri Nätkinniemi^a, Sirpa Peräniemi^b, Markku Ahlgrén^a. ^a*Department of Chemistry, University of Joensuu, P.O.Box 111, 80101, Joensuu, Finland.* ^b*Laboratory of Chemistry, Department of Biosciences, University of Kuopio, P.O. Box 1627, 70211, Kuopio, Finland.*
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Bisphosphonic acids have attracted close attention because of their utility in supramolecular chemistry and crystal engineering [1,2]. Usually, the metal bisphosphonates form polymeric materials and microporous solids, with properties that offer a diversity of practical applications in catalysis, ion-exchange and sorption [2-4]. Hydrogen bonds are predominant in these architectures, producing one-, two- and three-dimensional networks. In our continuing research for bisphosphonate ester derivatives, we have prepared three new Cd complexes of (dichloromethylene) bisphosphonic acid P,P-diphenyl, monophenyl and monoethyl ester derivatives. The structures of these compounds were characterized by single crystal X-ray diffraction. All three compounds show a different layered structure. The Cd complex of monophenyl ester derivative consists of 1-D chains with four independent octahedral Cd atoms joined by two bisphosphonate ligands. The chains are connected into layers by phosphonate O atoms, and the adjacent layers are held together by weak π - π stacking interactions. The Cd complex of diphenyl ester derivatives shows a new type of layered structure for metal bisphosphonates, where the bisphosphonate ligand coordinates tridentately to three Cd²⁺ ions. Each CdO₆ octahedron is connected to three CPO₃ tetrahedra and each tetrahedron to three octahedra leading to a 2-D framework consisting of 12-membered cyclic cores. In Cd compound of monoethyl ester derivative, the asymmetric unit contains two independent Cd²⁺ cations connected by bisphosphonate ligands, to form a Cd-bisphosphonate layer. The layers are further interconnected into a 3-D supramolecular network by extensive hydrogen bonds.

[1] A. Clearfield, C.V. Krishnamohan Sharma, B. Zhang, *Chem. Mater.*, **2001**, 13, 3099. [2] R. Fu, S. Hu, X. Wu, *Cryst. Growth Des.*, **2007**, 7, 1134. [3] A. Clearfield, *Progress in Inorganic Chemistry: Metal Phosphonate Chemistry*, ed. K. D. Karlin, Wiley, New York, **1998**, vol 47, pp. 371-510 and references therein. [4] Maeda, K. *Microporous Mesoporous Mater.*, **2004**, 73, 47 and reference therein.

Keywords: bisphosphonates; coordination complexes; single crystal X-ray analysis

FA4-MS04-P10

Supramolecular Chemistry of Reinecke Salt Derivatives. Mátyás Czugler^a, Veronika Kudar^a. ^a*X-ray Diffraction, Structural Chemistry, Chemical Research Center, Budapest, Hungary.*
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One of the oldest complex anion salts, used for long in the analytical chemistry of mainly foodstuffs and of inorganic chemistry is the Reinecke salt, conceived in the 1860s. Apart from early attempts no systematic structural studies were reported for this long-known substance, however. Crystallization of such compounds poses formidable problems as the title salt generally forms rather awkward precipitates. Nevertheless, series of complexes of derivatives of the parent compound were prepared in our laboratory and about half a dozen structure determinations by single crystal X-ray diffraction followed these experiments.

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].

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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.

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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