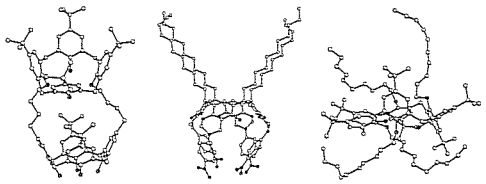
PS06.05.03 ALIPHATIC CHAINS IN CALIXARENE DERIVATIVES E. F. Paulus, Hoechst AG, D-65926 Frankfurt/Main; V. Böhmer, R. Arnecke, R. A. Jakobi, W. Wasikiewicz, Universität D-55099 Mainz, Germany.

The following 3 calixarenes with aliphatic chains were investigated by single crystal x-ray structure analysis:

In compound (I) two aliphatic chains $(CH_2)_4O$ are connecting the two calices of a couple calixarene of the head-to-tail type, in compound (II) four aliphatic chains $CH_3(CH_2)_{10}$ are substituents at the 4 bridging methylene groups and in compound (III) four of the six hydroxyl groups have the substituents $CH_3(CH_2)_9$. It can immediately be seen from the figures, that the aliphatic chains are mostly unfolded, backfolding is relatively seldom and occurs usually at the end of the chain. The following table gives the corresponding torsion angles, beginning at the hydroxyl ((I), (III)) or alkyl ((II)) end of the chain. Molecule (II) is on a special position and has therefore only two independent chains.

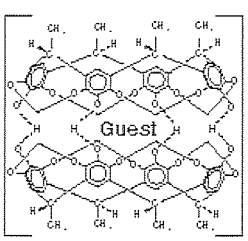
I	II		III			
-178.0(5)	169.7(4)	168.6(4)	-18(2)	-72(1)	73(1)	51(1)
-177.9(5)	-179.7(4)	-173.2(4)	-176(2)	-170(1)	170(1)	-178(1)
71.5(5)	179.7(4)	172.1(6)	100(3)	175(1)	-178(1)	175(1)
	176.0(5)	-179.3(6)	169(2)	-168(1)	179(1)	-180(1)
-72.0(6)	-177.1(5)	172.6(7)	-167(3)	-56(2)	70(1)	169(1)
177.0(5)	177.6(5)	173.7(8)	141(4)	-178(1)	151(2)	-71(2)
173.6(5)	-175.8(5)	170.5(9)	-18(8)	-163(2)	-177(2)	-92(3)
	178.8(6)	55.3(14)	-136(4)	178(1)	-46(4)	164(2)
	-179.8(6)	60.6(12)				

That these conformations of but low energy, but at the same time of low entropy, can occur, seems to be favoured by the high flexibility of the calixarenes. This can be seen by the fact, that the calixarene molecules are on special positions of not as high order of symmetry as is theoretically thinkable.



PS06.05.04 A NOVEL SUPRAMOLECULAR ASSEMBLY: SWITCHABLE ENCAPSULATION OF A GUEST MOLECULE BETWEEN TWO BOWL-SHAPED MOLECULES. Gunnar Olovsson, Robert G. Chapman, John C. Sherman and James Trotter, Department of Chemistry, 2036 Main Mall, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z1

The highly stable self-assembled complex **1**.pyrazine is formed via charged hydrogen bonds between the bowls, and van der Waals and electrostatic interactions between the bowls and the pyrazine guest molecule. The reaction is reversible (by adjusting the pH) and strongly guest-selective[1,2]. Larger assemblies are being developed with potential of nanotechnological applications, like for example drug delivery devices etc. ***Crystal structure: Tetragonal P4cc, a=b=22.661(3)Å, c=30.209(2)Å, V=15513(3)Å³.*** The pyrazine guest molecule sits on the 4-fold axis and is thus disordered. Each of the two crystallographically independent complexes of **1**.pyrazine is surrounded by 4 molecules of the counterion DBU ($[C_9H_{17}N_2]^+$). Nitrobenzene solvent and water are also present in the crystal.



1. Guest

(1) Chapman, R.G. and Sherman, J.C. (1995) J. Am. Chem. Soc. 117, 9081-9082.
(2) Grotzfeld, R.M., Branda, N. and Rebek, J. Jr. (1996) Science, 271, 487-489.

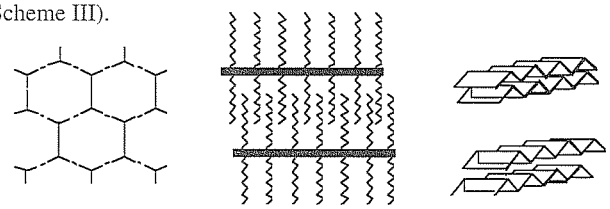
PS06.05.05 CRYSTAL ENGINEERING: HONEYCOMB NETWORKS, MOLECULAR LAMINATES AND SUPRAMOLECULAR BOXES: C. V. Krishnamohan Sharma, Michael J. Zaworotko, Department of Chemistry, Saint Mary's University, Halifax, Nova Scotia, B3H 3C3, Canada

Possibly general strategies for constructing a variety of supramolecular architectures will be discussed. A schematic representation of each of these strategies is depicted below.

Honeycomb Networks: The modular self assembly of trigonal molecules (either with triple functional hydrogen bond donor or acceptor sites) with complementary linear 'spacer' molecules results in hexagonal networks as shown in Scheme I.

Molecular Laminates: Alkyl group(s) that are supported by rigid two dimensional scaffolding may be used to generate a variety of molecular laminates by manipulating the nature of alkyl chain(s) (Scheme II).

Supramolecular Boxes: Alignment of corrugated sheets through directional forces precludes the expected close-packing between the layers, leading instead to formation of supramolecular boxes (Scheme III).



Scheme I **Scheme II** **Scheme III**

PS06.05.06 ON SUPRAMOLECULAR ARCHITECTURE WATER MOLECULES FORM IN HYDROPHOBIC HYDRATES. Janusz Lipkowski*, Konstantin Udachin #, Jerzy Narbutt & and Pawel Staszewski* * Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44, 01 224 Warszawa, Poland, # Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Lavrentyeva 3, 630090 Novosibirsk, Russia, & Institute of Nuclear Chemistry and Technology, Dorodna 16, 03 195 Warszawa, Poland

In the crystal structures of molecular hydrates different modes of hydration co-exist. These are: *hydrophilic hydration*, in which water is H-bonded to suitable moieties of the solvated molecule, *hydrophobic hydration* in which water molecules *enclathrate* lipophilic parts of molecules or guest moieties, and, ionic interactions if the guest species are solvated in ionized form (like, e.g. alkylammonium fluorides, from which fluoride anions are incorporated into water crystalline framework while the guest-alkylammonium is cationic). It is believed that x-ray studies on crystal structure of water, containing different solute species, may have some importance in understanding possible hydration patterns in solution phases.

In the paper some new x-ray structures of water structures in hydrates will be displayed. These include hydrophobic hydration pattern of Zr(acac) •10H 0 (as the example of hydrophobic hydration of metal chelates, which is of importance from the point of view of phase equilibria in liquid/liquid extractions), and a series of crown macrocycles and their complexes. In the latter case hydrophilic hydration occurs if the macrocycle is not complexing any guest species. Hydrophobic hydration is strongly dependent both upon geometry of the guest species and the hydrate stoichiometry. The most unexpected architectures found include different layered, channel and zeolite-like structures of water. Most of experimental work required low temperature (*Oxford Cryogenics*) since the compounds melt below 0° C.