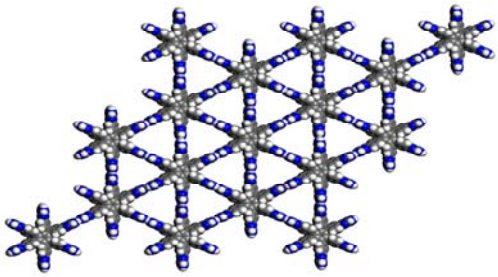
MS19 O1

Guidelines for Engineering Molecular Crystals James D. Wuest, *Département de Chimie, Université de Montréal, Montréal, Québec H3C 3J7, Canada.* E-mail: james.d.wuest@umontreal.ca

Keywords: supramolecular chemistry, crystal engineering, materials science

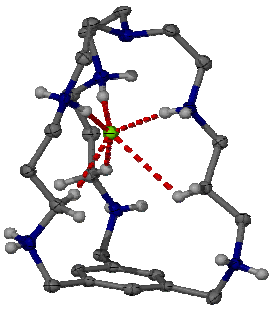
No reliable method exists for predicting the structure of molecular crystals in detail, and the relationship between the structure and properties of crystals remains poorly understood. Our limited knowledge of these subjects is an obstacle to progress in many areas of science and technology, and attempts to engineer crystals for specific applications have remained largely empirical activities. A promising strategy in crystal engineering uses molecules with arrays of well-oriented sticky sites that direct association according to reliable motifs, linked to cores that orient the sticky sites and introduce other desirable molecular properties. In favorable cases, the oriented sticky sites play a dominant role in association and place each molecule in a predetermined position relative to its neighbors, leading to the programmed construction of particular networks. The concepts that underlie this strategy are simple and qualitative, but they are powerful enough to lead consistently to the discovery of molecular crystals with properties not previously observed. The approach can also be used to direct 2D crystallization and to thereby nanopattern surfaces. Guidelines for engineering 2D and 3D molecular crystals will be illustrated by referring to recent published and unpublished work of the Wuest group.



MS19 O2

Anion Binding as a Trigger in Sensing and in Supramolecular Gels Jonathan W. Steed Chemistry Department, Durham University, Durham DH1 3LE, UK. E-mail: Jon.steed@durham.ac.uk

We have designed a number of anion-binding containers exhibiting dynamic conformational behaviour. These systems range from macrobicyclic cryptands (**1**) exhibiting conformational twisting to tripodal (**2**) and tetrapodal hosts (**3**) exhibiting significant flexibility of the pendant arms. The containers' dynamic properties are modulated by anion binding. Anion binding may also be used to modulate self-assembly and hence rheological properties in supramolecular gel phase systems. This lecture explores the scope and uses of this kind of fundamental process in preparing new supramolecular sensors and materials.



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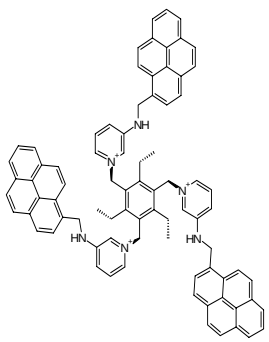

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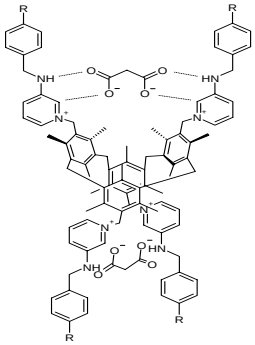

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Gels: Stanley, C. E.; Clarke, N.; Anderson, K. M.; Lenthall, J. P.; Steed, J. W., *Chem. Commun.* 2006, 3199-3201.
Confomational Effects: Turner, D. R.; Paterson, M. J.; Steed, J. W., *J. Org. Chem.* 2006, *71*, 1598-1608.

MS19 O3

Structural characterization of α-cyclodextrin/lipid complexes. Delphine Gallois-Montbrun[a], Sylviane Lesieur[a], Sax Mason[b], François Bonhomme[a], Bernard Fraisse[c], Nouredine Ghermani[a,c], Thierry Prangé[d], , Geneviève Le Bas[a], [a]*UMR CNRS 8612, Université Paris Sud, Châtenay-Malabry, France.* [b]*ILL, Grenoble, France.* [c]*UMR CNRS 8580, ECP, Châtenay-Malabry, France.* [d]*UMR CNRS 8015, Université Paris V, France.*
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Keywords: cyclodextrins, supramolecular assemblies, X-ray neutron single-crystal diffraction

A systematic study of complexes formed from α-cyclodextrin and monoalkyl amphiphiles was performed as a model of intermolecular interactions between lipids and carbohydrates which are so important in biological structures and processes. We observed that depending on the crystallization conditions (temperature, hydration level) and the characteristics of the lipid (chain-length, nature of its polar head group) these complexes crystallize in different crystalline forms. Three different forms were identified : a triclinic P1 (pseudo-hexagonal) lattice (this packing mode was already observed for polyiodide complexes[1]), a hexagonal lattice with R3 symmetry and a monoclinic C2 lattice[2,3]. The last two structures had not been described before for α-cyclodextrin inclusion complexes. In all cases, the complexes crystallize in channel-type structures, where head to head dimers of α-cyclodextrin molecules are stacked like coins in a roll and the alkyl chain of the guest compound is embedded in the tubular cavity of the cyclodextrins.