

this time and its creative energies not by piles of reprints nor lists of citations, but by the visually attractive fruits of our labors.

From the earliest times, as crystallographers searched for ways to depict and explain their structural results, clusters and juxtapositions of atoms have taken on striking artistic forms. This mini-symposium and the accompanying exposition of contemporary art are dedicated to the presentation of the aesthetic aspects of structural studies.

From the ephemeral refresh rate of the computer terminal to the durability of a wooden or metal sculpture, these images and forms are a stimulation to the scientist first seeing them, who then manipulates parameters to create forms and images that rise above the ordinary to magnify aesthetic images of nature from the atomic and molecular scale. The artist in us aspires [1] to create images and sculptures of lasting value. The support of the US National Science Foundation and collaboration with the Smithsonian Institution are gratefully acknowledged.

[1] Meyer E., *IEEE Eighth International Conference on Information Visualisation*, London, 2004, 229-234.

Keywords: computer graphics, models, sculptures

MS31 SUPRAMOLECULAR CHEMISTRY

Chairpersons: Franco Ugozzoli, Claire Gervais

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Diffusion of Guests into Non-porous Crystals

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Crystals composed of purely organic compounds have largely been ignored as gas sorption substrates since such molecules usually pack with efficiencies in the narrow range of 60 to 67%. The host lattices of solvated inclusion compounds are often described as possessing zero-, one-, two- or three-dimensional solvent-accessible voids if the guest molecules are located in isolated cavities, channels, layers or networks of channels, respectively. It is therefore attractive to envision facile removal of the solvent molecules from these materials to yield highly porous host lattices analogous to those of zeolites. In reality, the process of desolvation almost always involves reassembly of the host molecules in the solid state to form one or more phases, where the pure compound is again efficiently packed. However, a few exceptions are known to exist. A low-density phase of sublimed *p*-*tert*-butylcalix[4]arene possesses lattice voids of *ca.* 235 Å³ [1]. Despite an apparent lack of porosity, these crystals readily and reversibly absorb volatile gases [2,3] at room temperature and ambient pressures. In this presentation, new developments in the understanding of such gas absorption will be discussed.

[1] Atwood J. L., Barbour L. J., Jerga A., Schottel B. L., *Science*, 2002, **298**, 1000. [2] Atwood J. L., Barbour L. J., Jerga A., *Angew. Chem. Int. Ed. Engl.*, 2004, **43**, 2948. [3] Atwood J. L., Barbour L. J., Thallapally P. K., Wirsig T. B., *Chem. Comm.*, 2005, 51.

Keywords: calixarene, gas absorption, single crystal

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Sandwiches and Cavities: The Supramolecular Chemistry of Hemimellitic Acid

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Prior to our investigations of its potential contribution to supramolecular chemistry, and despite its commercial availability as a crystalline dihydrate, hemimellitic acid (H₃HMA; benzene-1,2,3-tricarboxylic acid) appeared in only 8 crystal structures recorded in the Cambridge Structural Database (CSD; Version 5.26, November 2004).

The presence of carboxylic acid functionality in H₃HMA facilitates the formation of both organic-based hydrogen bonding arrays and metal-organic coordination frameworks, as has been previously demonstrated using trimesic and terephthalic acids.

H₃HMA forms solvent-inclusion clathrates with solvent molecules capable of hydrogen bonding, often with rectangular solvent-filled cavities running through the structure [1]. Co-crystallisation with molecules containing *N*-heterocycles has also led to hydrogen bonded structures, often with accompanying proton-transfer [2]. The most interesting findings undoubtedly result from a systematic study of the coordination of H₃HMA to monopositive (Group 1 metals) and dipositive (Group 2 and transition metals) cations [3]. Significant structural diversity has been observed within this series of complexes; trends within the series will be analysed.

[1] Dale S. H., Elsegood M. R. J., Coombs A. E. L., *CrystEngComm*, 2004, 328-335. [2] Dale S. H., Elsegood M. R. J., Kainth S., *manuscripts in preparation*. [3] Dale S. H., Elsegood M. R. J., Kainth S., *manuscripts in preparation*.

Keywords: supramolecular chemistry, hydrogen bonding, carboxylic acids

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Supramolecular Coordination Chemistry – the Challenge of the Outer Sphere

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Supramolecular coordination chemistry seeks to construct large complexes, either as discrete multinuclear complexes or as extended structures. Synthetic approaches may be classified into: (A) the use of large polynucleating ligands capable of binding several metal ions; (B) the use of bridging ligands such as 4,4'-bipyridine, cyanide or oxalate to link metals together; (C) linking complexes via interactions between groups located on the exterior of the complex, the outer sphere. This last approach is the subject of the lecture. It offers a number of advantages including easier synthesis than approach (A), and little or no perturbation of the properties of the metal centre. In favorable cases the binding of the metal can be used to activate the ligand to outer sphere association, and the interaction may be controlled by the external environment.

These ideas will be illustrated by a series of examples using hydrogen bonding and stacking interactions of heterocyclic ligands. Attention will be paid to how these interactions may be induced or suppressed.

Keywords: coordination compounds, supramolecular chemistry, crystal packing

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Structure Control by Hydrogen Bonding to Anions and Coordination to Cations

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A series of urea-containing pyridyl ligands have been prepared and used to bind ion pairs by hydrogen bonding to the anions and coordination to the cations. The new complexes are frequently coordination polymers or hydrogen bonded polymers, although discrete species that also persist in solution have also been observed (as in the figure). Common, reproducible and predictable hydrogen bonded motifs are observed across the series.

