

alignment programs.

An extension of ESPript named ENDscript has been made available at the same electronic address [2]. It enables the creation from a single Protein Data Bank identifier, of a multiple sequence alignment figure adorned with secondary structures of each sequence of known structure. ENDscript uses programs such as BLAST, CLUSTAL and PHYLODENDRON to work on protein sequences and such as DSSP and CNS to work on protein coordinates. Similar structures are superimposed in turn with the program PROFIT. Final 3D figures are drawn with MOLSCRIPT, BOBSCRIPT and DINO, so as to show sequence conservation as well as structure conservation.

[1] Gouet P., Courcelle E., Stuart D. I., Metz F., *Bioinformatics*, 1999, **15**, 305. [2] Gouet P., Courcelle E., *Bioinformatics*, 2002, **18**, 767.

**Keywords:** bioinformatics, sequence homology, protein structure comparison

### MS30 ART AND CRYSTALLOGRAPHY

**Chairpersons:** Edgar Meyer, Cristina Acidini

#### MS30.26.1

*Acta Cryst.* (2005). A61, C43

#### Plastic Visions in Art and Science

Martin Kemp, *Department of the History of Art, University of Oxford.*

E-mail: martin.kemp@trinity.ox.ac.uk

Techniques of instrumental seeing, such as sonar, electron microscopy and X-ray diffraction, pose particular problems in spatial visualisation and representation. However, the basic skills of mental modelling and graphic representation have existed in various guises in art, architecture, technology and science since the Renaissance (at least). The kinds of skills demanded in crystallography will be set in a broader context of visualization through the selective examination of key episodes from the era of Leonardo to the present day. Some of the examples will be drawn from my regular column in *Nature*, which has in part appeared in book form [1].



Buckminster Fuller, Dome for Expo '67, Montreal

[1] Kemp M.K., *Visualisations. The Nature Book of Art and Science*, 2000.

**Keywords:** X-ray diffraction techniques, molecular modelling, computer modelling solids

#### MS30.26.2

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#### M.C. Escher and the Crystallographers

Doris Schattschneider, *Dept. of Math. and Comp. Sci., Moravian College PPHAC, 1200 Main St., Bethlehem, PA 18018-6650 USA.* E-mail: schattdo@moravian.edu

Forty-five years ago, a relatively unknown Dutch graphic artist,

M.C. Escher, gave a standing-room-only lecture to the Fifth International Congress of the IUCr in Cambridge, England. There was an accompanying exhibit of his work that amazed the crystallographers. His pioneering work in exploring colour symmetry was a rare instance of an artist investigating a field before "official crystallography even thought about [it]." [1] Escher's quest to understand periodic tilings (which he called 'regular divisions of the plane') was stimulated in 1935 by two articles in *Zeitschrift für Kristallographie*; roughly 20 years later crystallographers (notably, Caroline MacGillavry and J.D.H. and Gabrielle Donnay) sought him out to learn from his work. In 1960, Escher's book *The Graphic Work of M.C. Escher* contained a crystallographer's explanation of symmetry and symmetry groups. In 1965, the IUCr published [1] for which MacGillavry had collaborated with Escher.

We discuss how Escher's quest to understand the subject of coloured periodic tilings differed from that of the crystallographers', and how even today, some of his original investigations are worthy of further scientific inquiry.

[1] MacGillavry C.H., *Symmetry Aspects of M.C. Escher's Periodic Drawings*, IUCr, Utrecht, 1965. [2] Schattschneider D., *M.C. Escher: Visions of Symmetry*, Freeman W.H., New York, 1990, Harry Abrams, New York, 2004.

**Keywords:** M.C. Escher, colour symmetry, crystallographic teaching

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#### Ancient Crystalline Materials for the Arts of Beauty

Georges Tsoucaris, Philippe Walter, *Centre de recherche et de restauration des musées de France-CNRS UMR 171, Paris, France.*

E-mail: Georges.Tsoucaris@culture.fr

#### Dedicated to the memory of HUBERT CURIEN

Recent progress in the analysis and structural characterisation of materials has had an increasing impact on studies of archaeological specimens. We shall mainly focus on cosmetic chemicals, also used as pigments and medicines. Many crystalline compounds found in Egyptian tombs have been identified. The structural information has ultimately revealed that the Egyptians had developed a *wet chemical synthesis of lead-containing compounds not occurring in nature*. Archaeological data (2000-1200 BC) and Greco-Roman texts (50 AD) have been crucial in tracing back this technology about 1500 years earlier than it has been previously assumed [1].

Greek texts from the 4<sup>th</sup> century BC describe a remarkable method of synthesis and comment on the widespread use of ceruse (lead white) still continuing until the present day. A marked difference in the historical use of cosmetics by the Egyptian and Greco-Roman societies will be emphasised.

The archaeological materials may suffer alterations over the centuries. Time may be then viewed as a "fourth dimension" for the purpose of approaching the significance of "molecular messengers" in "Molecular and Structural Archaeology". Thus we have observed by X-ray diffraction a keratin  $\alpha$ -helix, still perfectly preserved, in human hair 2500 years old. In contrast the structure of skin elements has been altered by the mummification process.

[1] Walter P., Martinetto P., Tsoucaris G., Breniaux R., Lefebvre M.A., Richard G., Talabot J., Dooryhée E., *Nature*, 1999, **397**, 483-484.

**Keywords:** structural analysis, archaeological materials, lead

#### MS30.26.4

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#### Art in Crystallography in Art

Edgar Meyer, *Dept. of Biochemistry & Biophysics, Texas A&M University and Molecular Sculpture Laboratory, University of New Mexico, Taos.* E-mail: E-Meyer@tam.u.edu

What is our legacy to future generations? Over the last 50 years, crystallography has changed science, society, and the world. When one considers the enormous impact our structural studies have had on the material, chemical, and life sciences, we find ourselves challenged to present to a discerning public the fruits of our research in a form that is appealing to the eye and of lasting value. Posterity will know

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

#### MS31.26.1

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#### Diffusion of Guests into Non-porous Crystals

Jerry L. Atwood<sup>a</sup>, Leonard J. Barbour<sup>b</sup>, Praveen K. Thallapally<sup>a</sup>,  
<sup>a</sup>*Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211.* <sup>b</sup>*University of Stellenbosch, Department of Chemistry, 7602 Matieland, South Africa.* E-mail: atwoodj@missouri.edu

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 Å<sup>3</sup> [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

#### MS31.26.2

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#### Sandwiches and Cavities: The Supramolecular Chemistry of Hemimellitic Acid

Sophie H. Dale<sup>a</sup>, Augusta E. L. Coombs<sup>a</sup>, William Clegg<sup>a</sup>, Mark R. J. Elsegood<sup>b</sup>, Sarita Kainth<sup>b</sup>,  
<sup>a</sup>*School of Natural Sciences, University of Newcastle-upon-Tyne, Newcastle-upon-Tyne, UK.* <sup>b</sup>*Chemistry Department, Loughborough University, Loughborough, UK.* E-mail: S.H.Dale@newcastle.ac.uk

Prior to our investigations of its potential contribution to supramolecular chemistry, and despite its commercial availability as a crystalline dihydrate, hemimellitic acid (H<sub>3</sub>HMA; 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 H<sub>3</sub>HMA 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.

H<sub>3</sub>HMA 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 H<sub>3</sub>HMA 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

#### MS31.26.3

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#### Supramolecular Coordination Chemistry – the Challenge of the Outer Sphere

Alan F. Williams, *Department of Inorganic Chemistry, University of Geneva, Switzerland.* E-mail: Alan.Williams@chiam.unige.ch

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

#### MS31.26.4

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#### Structure Control by Hydrogen Bonding to Anions and Coordination to Cations

Jonathan W. Steed, David R. Turner, *Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, UK.* E-mail: jon.steed@durham.ac.uk

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.

