

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

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Plastic Visions in Art and Science

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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

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M.C. Escher and the Crystallographers

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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

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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 4th 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 α -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

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Art in Crystallography in Art

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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