MS65.28.5

Acta Cryst. (2005). A**61**, C85

Structural and Functional Insight into Celldefending Non-specific Nucleases

Hanna S. Yuan[a], Kuo-Chiang Hsia[a], Lyudmila G. Doudeva[a], Hsinchin Huang[a], Wei-Zen Yang[a], Woei-Chyn Chu[b], [a]*Institute of Molecular Biology, Academia Sinica, Taipei, Taiwan, ROC.* [b]*Institute of Biomedical Engineering, National Yang Ming University, Taipei, Taiwan, ROC.* E-mail: hanna@sinica.edu.tw

The bacterial toxin ColE7 bears an H-N-H motif that has been identified in hundreds of prokaryotic and eukaryotic endonucleases, involved in DNA homing, restriction, repair or chromosome degradation. The crystal structures of the nuclease domain of ColE7 in complex with an 8-bp [1], 12-bp and 18-bp duplex DNA have been determined respectively by X-ray diffraction methods. In each of the structure, the H-N-H motif is bound at the minor groove primarily to DNA phosphate groups, with little interaction to ribose groups and bases. This result provides a structural basis for sugar and sequence independent DNA recognition. Structural comparison shows that several families of endonucleases bind and bend DNA in a similar way to that of the H-N-H ColE7, indicating that endonucleases containing a similar His-metal finger fold of active site possess a universal mode for protein-DNA interactions [2].

[1] Hsia K.-C., Chak K.-F., Liang P.-H., Cheng Y.-S., Ku W.-Y., Yuan H. S., *Structure*, 2004, **12**, 205-214. [2] Hsia K.-C., Li C.-L., Yuan H. S., *Curr. Opin. Struct. Biol.*, 2005, **15**, 126–134.

Keywords: DNA-protein interactions, DNA recognition, endonucleases

---

MS66 TOPOLOGY OF CRYSTAL STRUCTURES: NETS, KNOTS AND SURFACES

Chairpersons: Davide M. Proserpio, Jean-Guillaume Eon

MS66.28.1

Acta Cryst. (2005). A**61**, C85

Self-dual Tilings and Interpenetrating Periodic Nets

Michael O'Keeffe, *Department of Chemistry and Biochemistry, Arizona State University.* E-mail: mokeeffe@asu.edu

Some self-dual 3-periodic tilings of ordinary space are described. Pairs of nets carried by these tilings (their 1-skeletons) can interpenetrate so that all the rings of one net are catenated with rings of the other and *vice versa*. For a special class of nets their natural tilings are self-dual and these are called *naturally self-dual* nets.

It is shown that a given net can have an infinite number of distinct self-dual tilings, but (probably) at most one natural self-dual tiling.

Four vertex-transitive naturally self-dual nets are identified and it is conjectured that this list is complete. They are among the minimal nets of Bonneau *et al.* [1]. It is shown that these, and closely-related, nets account for the great majority of observed [2] instances of interpenetration in crystal structures.

Some naturally self-dual tilings and their associated nets with more than one kind of vertex are also described and their importance in crystal chemistry indicated.

[1] Bonneau C., Delgado-Friedrichs O., O'Keeffe M., Yaghi O. M., *Acta Crystallogr.*, 2004, **A60**, 517. [2] Blatov V. A., Carlucci L., Ciani G., Proserpio D. M., *Cryst. Eng. Comm.*, 2004, **6**, 377.

Keywords: tilings, periodic nets, interpenetrating nets

MS66.28.2

Acta Cryst. (2005). A**61**, C85

Sphere Packings with Exceptional Properties

Elke Koch, *Institut for Mineralogy, Petrology and Crystallography, University of Marburg, D-35083 Marburg, Germany.* E-mail: elke.koch@staff.uni-marburg.de

Homogeneous sphere packings with different kinds of unusual and strange properties are discussed.

For most sphere-packing types there exists a minimal density, and the corresponding sphere packings show the highest inherent symmetry of that type. In the other cases the density decreases towards a boundary of the parameter range. So far, three exceptions are known: in one case, the minimum of density refers to parameter values very close to but not identical with those of highest inherent symmetry; two sphere-packing types exist the minimal densities of which occur not only at a single point but at a whole line of its parameter region.

Normally, the small rings of spheres within a sphere packing are not linked. Very few examples, however, have been found where such rings are catenated. In such a case, a purely graph-theoretical characterization of the type is not sufficient [1].

Some sphere packings may be intertwined in such a way that 2, 3, 4, 5 or 8 congruent or enantiomorphic copies interpenetrate each other without mutual contact. For such interpenetrating packings the contact numbers per sphere vary between 3 and 6. In a few cases, sphere packings of the same type may be fitted into each other in different ways. In addition, interpenetrations of two-periodic 6^3 and 48^2 nets of spheres have been derived. Here the nets are arranged in two or three sets of parallel nets [2, 3] with a mutual angle of 90° or 60°, respectively.

[1] Koch E., Sowa H., *Acta Cryst.*, 2004, A**60**, 239. [2] Fischer W., Koch E., *Acta Cryst.*, 1976, A**32**, 225. [3] Sowa H., Koch E., *Acta Cryst.*, 2004, **A60**, 158.

Keywords: sphere packings, interpenetration, catenation

MS66.28.3

Acta Cryst. (2005). A**61**, C85

Knotted Nets and Weavings – from 2D Hyperbolic to 3D Euclidean Patterns

Stephen T. Hyde[a], Stuart J. Ramsden[a,b], Vanessa Robins[a], [a]*Department of Applied Mathematics, Research School of Physical Sciences, Australian National University.* [b]*Vizlab, ANU Supercomputing Facility, Australian National University.* E-mail: Stephen.hyde@anu.edu.au

Crystalline patterns in 3D euclidean space can be constructed from tilings of 2D hyperbolic space, followed by projection onto three-periodic hyperbolic surfaces. We demonstrate the technique by projection onto the simpler three-periodic minimal surfaces. The edge arrays of finite tiles, that can be systematically enumerated using Delaney-Dress tiling theory, generate many - though not all - of the commonly encountered crystalline networks.

A variety of hyperbolic tilings can be formed using infinite tiles, whose edges are lines or trees. Projections of those examples generate more complex patterns. Packed trees result in multiple interpenetrating networks, which define “polycontinuous” space partitions. Packings of hyperbolic lines project to arrays of generalized helices, whose simplest examples are well-known rod packings. Generic examples are complex 3D weavings, whose knottedness can be captured by analyzing the homotopy of their quotient graphs (links) embedded in the relevant hyperbolic manifolds (the “minimal embeddings” of the links).

Keywords: patterns, minimal surfaces, knots and links

MS66.28.4

Acta Cryst. (2005). A**61**, C85-C86

The Nomenclature of Interpenetration

Stuart R. Batten, *School of Chemistry, Monash University 3800, Australia.* E-mail: stuart.batten@sci.monash.edu.au

The interpenetration of 1D, 2D and 3D networks (especially hydrogen bonded nets and coordination polymers) has become an important phenomenon in crystal engineering [1,2]. In such cases it is important that not only the topology of the interpenetrating networks is described, but also the topology of the interpenetration itself.

Therefore a simple descriptive nomenclature for describing the various modes of interpenetration is necessary. Interpenetration of 1D and 2D nets may be described as parallel or inclined interpenetration, depending on whether the mean directions of propagation (1D) (or mean planes (2D)) are co-linear (or parallel) or not, respectively. The overall topology of the entanglement may be of higher dimension than the individual networks, and thus descriptors of the form mD → nD, where mD is the dimensionality of the individual nets and nD is the dimensionality of the overall entanglement, can be used. It is also