Topology I-Group Theory & Topology

MS21.01.01 EXPLORING NEW CRYSTALLOGRAPHIC SYMMETRIES IN PROTEIN MOLECULES. A. Janner, Institute for Theoretical Physics, Faculty of Science, Toernooiveld, NL-6581 ED Nijmegen, The Netherlands

Protein folding in the Cyclophilin A - Cyclosporin A complex (as described in the 2rma file of the Brookhaven Protein Data Base) reveals the existence of basic structural sites having symmetries like those in quasicrystals. Such sites also appear in protein molecules having a non-crystallographic rotational symmetry of order n after projecting the molecule along the rotational axis in a plane perpendicular to it. While this implies a regular polygonal arrangement, one also finds evidence of additional scaling relations arising from intersection points of associated star polygons in the plane. An analogous situation is observed in snow crystals (for the crystallographic value $n = 6$). In the cases considered so far of proteins of the chaperone type, this leads to a relation between the overall size of the molecule and that of the characteristic central hole. These basic structural sites have $\varphi(n)$ integral coordinates in the plane, where φ is the Euler function, mutually related by invertible integral matrices. This ensures the crystallographic nature of these symmetries, which appear to be of the multimetrical type (Janner, 1995, Acta Cryst. B51, 386401). In the case of the Cyclophilin A - Cyclosporin A complex the sites are defined in term of centroids of folding subunits of the ten monomers. The basic structural sites form, therefore, a kind of "Cheshire cat" molecule consisting of symmetryrelated points avoided by the polypeptide chains. The symmetry of the Cheshire cat Cyclophilin A - Cyclosporin A complex is larger than the Euclidean point group 52 of the molecule, as it includes pentagrammal scale-rotational symmetry elements, similar to those one finds in decagonal quasicrystals. This leads to multiple goldenratio distance relations. There are thus protein molecules with a multimetrical crystallographic order. This order is, however, still poorly understood.

MS21.01.02 ORBIFOLDS OF CUBIC CRYSTALLO-GRAPHIC GROUPS William D. Dunbar, Simon's Rock College, 84 Alford Road, Great Barrington, MA 01230

Associated with each crystallographic group G, there is the space X of equivalence classes of positions in Euclidean space, where two points in Euclidean space are considered equivalent if some symmetry of the group takes one to the other. This space X inherits a topological structure, and in fact a metric structure, from Euclidean space. X is an orbifold, i.e. a topological space in which every point has a neighborhood which is a quotient space of a finite group action on an open ball in Euclidean space (this generalizes the definition of a surface as a space in which every point has a neighborhood homeomorphic to a disk — the group in this case consists of the identity element alone). X will have singular points corresponding to (equivalence classes of) points in Euclidean space which are fixed by some symmetry of G.

When G is one of the 36 groups of cubic type, the orbifold X will be homeomorphic to a hypersphere in 12 cases and to projective space in 1 case, when G consists only of direct motions, X will be homeomorphic to a ball in 11 cases, to the suspension of the projective plane in 10 cases and to the cone on the projective plane in 2 cases, when G contains reflections and/or inversions. The singular sets of these orbifolds will be discussed, as well as the way they reveal subgroup relationships between the crystallographic groups, and some of the implications for the study of equivariant Morse functions.

MS21.01.03 DESCRIPTION OF TRIPLY-PERIODIC MINIMAL SURFACES. Andrew Fogden, Physical Chemistry 1, Center for Chemistry and Chemical Engineering, P.O. Box 124, S-221 00 Lund, Sweden

The special class of three-dimensionally periodic surfaces bearing uniform mean-curvature, and most notably the minimal (zero mean-curvature) surfaces, are reviewed with respect to their classification, mathematical description and their role in crystalline and liquid-crystalline structures, and illustrated with many examples and applications. The simplest and most familiar of these bicontinuous space partitions are the P, D and G minimal surfaces, possessing cubic symmetry and genus 3. The exact equation defining any minimal surface can be obtained via parametrisation in the complex plane, reducing the problem to the construction of its corresponding complex-analytic function. Using an elegant method of matching the distribution of functional singularities in the plane to the symmetry and topology in real space, a multitude of new minimal surfaces have been discovered, or verified, in recent years. This increased knowledge of minimal partitions has greatly helped in visualising and understanding the geometry underlying many complicated chemical and physical assemblies. These developments are illustrated by taking the 3 above-mentioned surfaces and considering the new families liberated by the different modes of distortion to lower symmetries. More elaborate topologies are also presented using the examples of the S´-S´´, H´-T and T-WP minimal surfaces. These specific cases are of relevance to the description of zeolitic framework structure-types and also to the structure of novel bicontinuous liquid-crystalline phases formed by surfactants in water. Fitting of the minimal surfaces to the strucural information is assessed. The exact equations of the simple minimal surfaces can be approximated to great accuracy as level surfaces (equipotentials) of three-dimensional Fourier series, in which only the lowest frequency contributions are retained. Inclusion of higher frequencies yields good representations of more complicated examples, for which the exact parametrisations become unwieldly. For surfaces with uniform, but non-zero, mean-curvature the generalised parametrisation is difficult to apply and a Fourier description becomes even more beneficial. This is illustrated by the uniformly-curved companions of the H´-T minimal surface, which undergo necking transformations to layered "mesh" geometries of connectivity 3 or 6.

MS21.01.04 TETRAHEDRAL NETS IN ZEOLITES, CLATHRATES, ETC: SUBUNITS & CONNECTIVITY Joseph V. Smith, Department of Geophysical Sciences, University of Chicago, Chicago, IL 60637, USA.

The tetrahedral atoms lie at the vertices of 4-connected 3D nets. The nets can be decomposed into subunits, including 2D nets, polyhedra, chains & columns. The Catalogs of the Consortium for Theoretical Frameworks contain ~1100 theoretical nets, ~200 of which occur in materials, & >1000 subunits which are being assembled by algorithms into new 3D nets. The 3D nets & subunits are ordered by topochemical features, allowing systematic recovery. Assembly of subunits into 3D nets allows speculations on crystallization mechanisms which are tested against observed co-crystallization of synthetic zeolites and stacking errors of natural & synthetic materials. A historical review of relevant aspects of mathematical topology is underway, including sphere packing & connectivity algorithms. Complex polyhedral units form a family of derivatives from symmetric prototypes. Systematic enumeration of 4-connected 3D nets, based on the conversion of some edges of a stack of 3-connected 2D nets, is completed for 2-, 3- &4-repeat chains, and for selected nets & chains particularly important for zeolite synthesis chemists. Classification of mixed (n,m)-connected nets has begun with initiat emphasis on octahedral-tetrahedral nets, & nets containing triangles.