PS21.01.09 PREDICTION OF MODELS FOR TETRAHEDRAL FRAMEWORKS BASED ON THE ENUMERATION OF GRAPHS. H.-J. Klein, Inst. f. Informatik u. Prakt. Mathematik, Universität Kiel, 24098 Kiel, Germany

For tetrahedral frameworks with corner sharing tetrahedra a graph-based method ist presented which allows to generate models of frameworks in a systematic way. Under reasonable assumptions concerning bond lengths the method is complete insofar as it generates all hypothetical models with a given number of non-equivalent tetrahedra.

Tetrahedral frameworks can be described by graphs with nodes representing tetrahedra and lines representing links between these tetrahedra. Because of space group symmetries, it is possible to transform the infinite graphs for ideal structures into finite directed graphs wit nodes corresponding to central atoms of tetrahedra in a fixed asymmetric unit and with lines having symmetry operations as labels. This kind of non-redundant description is well suited for generating for each space group all graphs representing frameworks with a given maximal number of translationally non-equivalent tetrahedra. Enumeration can be done in a goal-directed way by incorporating restriction conditions concerning topological properties of structures. Thus, complete enumeration of graphs becomes feasible for interesting classes of structures, e.g. zeolites or structures where all tetrahedra are topologically equivalent.

To check whether graphs can be realized geometrically as tetrahedral frameworks, nodes are placed into the centre of gravity of their immediate neighbours in the graph. Using the knowledge of bond lengths and Wyckoff positions, the cell parameters and the arrangement of atoms are refined for realizable graphs by applying simulated annealing techniques and gradiant methods.

Our approach is applicable more generally to classes of crystal structures with only one type of polyhedron and one type of link between polyhedra. Completeness and adaptability are the main features in which it differs from other approaches for the prediction of structures.

PS21.01.10 THE FUNDAMENTAL REGIONS OF THE POINT SYMMETRY GROUPS AS THE BASIS OF THE CLASSIFICATION OF THE STRUCTURAL STATES OF SUBSTANCE. N. V. Fyodorova, V. M. Talanov, State Technical University, Novocherkassk, 346400, Russia

We suggest the classification of types of the structural states of substance on the basis of the analysis of the point symmetry groups fundamental regions. The following types of the structural states are examine: isosymmetric, enantiomorphous, anti-isostructural, the states of the local increase of symmetry (extraordinary, exceptional), irrational (quasicrystalline) states.

The own isosymmetric states are possible in the 18 point groups (4-3m, 432, m3-, 23, 6/mmm, 6-2m, 6mm, 622, 4/mmm, 4-2m, 4mm, 422, 3-m, 3m, 32, mmm, mm2, 222), in which the fundamental regions are limited by the structural elements of the same types. In the six of them (432, 23, 622, 422, 32, 222), exactly in the turning groups having more then one symmetry axis, there are geometrically and crystallographically enantiomorphous varieties of structural states. The turning groups 2, 3, 4 and 6 occupy the special place, because in this groups the geometrically enantiomorphous states are possible not in the all classes of objects. The own anti-isostructural states are possible in 11 groups (4-3m, 432, 23, 6-2m, 622, 4-2m, 422, 3-m, 3m, 32, 222).

The directions of the local increase of symmetry are subdivided on the two types: extraordinary and exceptional. the first type take place in the 26 point groups (exept m3-m, 6/m, 4/m, 2/m, 1-, 1), in the 6 from which (6/mmm, 6mm, 622, 4/mmm, 4mm, 422) there are irrational extraordinary directions; the second type are observed in the 11 point groups (m3-,23, 4/mmm, 4-2m, 422, 4/m, 4-, 3-m, 32, 3-, 2/m), moreover in all these groups there are irrational exceptional directions.

PS21.01.11 TRANSITIONS BETWEEN DIFFERENT CRYSTALLINE COORDINATE SYSTEMS. V. A. Liopo, Phys. & Engin. Dept., Grodno State University, Grodno, BELARUS. 230023

Position of atoms in crystal may be described in 3-D space either in crystallophysic (CP) or in crystallographic (CG) systems. If P and G are matrix-generators of matrical representations of point groups in CP and CG systems respectively the relations between them are

$$G = M^{-1} \cdot P \cdot M, \qquad P = M \cdot G \cdot M^{-1}$$

M, M^{-1} are metrical tensors of direct and resiprocal lattice respectively [1]. Let symmetry of crystal is described in N-D space, and N x N matrix (N) is matrix-generator of N-D point group. Relation between N and 3-D matrix- generator (T) are

$$N \cdot P = P \cdot T, \qquad \prod \cdot N = T \cdot \prod.$$

Matrix P is N x 3 ones and matrix $\prod$ is 3 x N matrix. There are two types of transition between N-d and 3-d spaces. They are

$$\prod N^2 \cdot P = T \cdot \prod \cdot P \cdot T, \qquad N \cdot P \cdot \prod \cdot N = P \cdot T^2 \prod$$

For N - T pair the matrices of transition are P and $\prod$ and these matrices are ambiguons.

1. Liopo, V. A. Kristallographia (Russian). V. 30. N 6. P. 1181-1182. (1985).

PS21.01.12 THE DENSITY OF ELLIPSES PACKINGS WITH SIX CONTACTING NEIGHBOURS. Takeo Matsumoto and Masaharu T anemura, Dept. Earth Sciences, Faculty of Science, Kanazawa University, Japan and Institute of Statistical Mathematics, Tokyo, Japan

In contrast with the closeset packing of circles, with plane group,p6mm,periodic close packings of identical ellipses do not always have the maximum density $\rho=\pi\sqrt{12} = 0.9069.....$

Nowacki(1948) and Grünbaum & Shephard (1987) have shown altogether seven different close packings of ellipses, with six contacting neighbours, namely, c2mm, p2, p2gg, p31m, p3 and two p2gg's pasckings in plane groups.

Matsumoto(1968) and Matsumoto & Nowacki(1966) have shown that the first two of the above densest packings of ellipses, c2mm (2 a 2mm) and p2(1 a 2) always attain the above maximum density. That of the third, p2gg (2 a 2) cannot exceed this maximum density. The former two packings,c2mm and p2, are derived from the densest packing of circles,p6mm (1 a 6mm), by affine transformation,while the p2gg packing of ellipses can never attain the maximum density of ρ.

Tanemura & Matsumoto(1992) have recently indicated that the density of p31m(3 c m) packing of ellipses, the fourth one of the above list,never exceeds the maximum density, and shows a maximum only for the case of axial ratio = 1,where the packing is equivalent to the p6mm packing of circles.

Matsumoto & Tanemura(1995) have also shown that the density of p3(3 d 1) packing of ellipses, the fifth one of the above list, never exceeds the maximum density through numerical computations and series expansions. This maximum density is attained only by the closest packing of circles, p6mm.

We are now calculating the density of two p2gg's (both 4 c 1) packings, the last ones of the above list, by numerical calculations and by expanding forms in terms of $\varepsilon = k-1$ (k = axial ratio) and θ (tilting angle of ellipse). For these two cases, each density cannot exceed the maximum density.