

Descriptors for Complex Inorganic Structures*

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It will be found that everything depends on the composition of the forces with which the particles of matter act upon one another; and from these forces, as a matter of fact, all phenomena of Nature take their origin. Roger Joseph Bos-covich (1711—1787) *Theoria Philosophiae Naturalis*, Venice, 1763. (sec. I.5).

Considering the great variety of natural structures built of atoms we may ask how we are to describe them. We may ask, further, whether there are any natural descriptions. Pauling's Rules laid the foundations for understanding the ionic structures in terms of coordination polyhedra. Here we elaborate on certain geometrical aspects of this by considering (a) quantitative dissection into coordination polyhedra; (b) specific atomic volumes; (c) minimal surfaces as large-scale features of silicate structures, and (d) complexity.

HIERARCHY

In most types of materials, especially biological, but also inorganic materials, all the component atoms are not on the same level, contributing directly and equally to the structure, as they might be, for example, in a large crystal of sodium chloride. Usually, atoms are recognisably organised into clusters and these clusters into bigger groupings and so on hierarchically. In organic structures the molecules are obvious, and exist even in solution or in the vapour. An individual atom does not usually 'belong' directly to the macroscopic assembly as a whole, but only as a member of a component group, one of an array of such subunits. We seek to discern and describe this hierarchic structure for inorganic materials as an essential way of reducing the number of parameters necessary for the intellectual perception of the structure.

Many arguments, most clearly those put forward by Simon in *The Architecture of Complexity*,¹ demonstrate that hierarchy is intrinsic to the process of building structures because of the much greater probability of formation which such structures have. The question is one of identifying substructures and of locating the boundaries between them, that is, of partitioning space. We use, albeit unconsciously, what might be called the Democritean Exclusion Principle — »No two atoms can have the same x, y, z, t coordinates« — which might be derived from the Pauli Exclusion Principle and the cost of overlapping wave functions by the Correspondence Principle. This is really just the principle of closest packing as a way of minimising the energy of the

* Dedicated to Professor D. Grdenić on occasion of his 65th birthday.

system. Given the components of an isolated system it would be expected that the system would settle to the state of least energy or, more accurately, to a state in which the probabilities of a spectrum of energy states E_i were in proportion to $\exp(-E_i/KT)$. It is also evident, however, that for example various protein molecules are not to be regarded as phases in the system C/H/O/N/S. Here there is a natural description which has guided the system through special paths in phase space to their very improbable synthesis.

DESCRIPTORS

Materials which are crystalline are invariably described in terms of crystallographic axes together with the space group (which describes the redundancy of the parameters). These derive, physically, from the symmetrical packing of the ions and are, in a sense secondary. The primary description is in terms of the coordination polyhedra and although formulated 50 years ago by Linus Pauling, this view has stood the test of time, being physically well-grounded. We may ask whether it is possible to build up a precise description of an ionic structure working outwards from ionic coordination. This would correspond to the precise descriptions of organic molecules by bond distances, bond angles and torsion angles.

We will take example of nickel sulphate, since it was used by Evans.² Beevers and Schwartz³ gave a network for nickel sulphate which represented the distribution of lines of force from positive to negative ions. This enshrined Pauling's Rules. Assignment of fluxes depended on the symmetry of the coordination polyhedra which, for example with Ca ions, was often low.

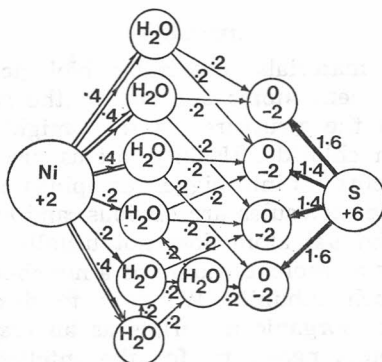


Figure 1. Distribution of electric flux in $\text{Ni}_2\text{SO}_4 \cdot 7\text{H}_2\text{O}$ (after Beevers and Schwartz³).

From the exact definition of coordination proposed by Frank and Kasper⁴ which involved the division of the structure into Voronoi polyhedra it is possible to construct a more quantitative network for the flux distribution in an ionic structure. Frank and Kasper characterised an ion as coordinated to another if it contributed to the definition of a vertex of the Voronoi polyhedron about the latter. Various descriptions have been given as to how to dissect systems of points into Voronoi polyhedra.

There are three main ways of calculating the Voronoi dissection: (a) that used by Fischer, Mackay,⁵ Finney⁶ and others where a tetrahedron of four atoms defines a potential Voronoi vertex as the centre of the sphere

TABLE I
 Exact Calculation of the Solid Angles (as Fractions of a Sphere) Subtended by one Atom at Those Coordinated to it in the Voronoi Dissection of $\text{Ni}_2\text{SO}_4 \cdot 7\text{H}_2\text{O}$

	Ni	S	O ₁	O ₂	O ₃	O ₄	(H ₂ O) ₁	(H ₂ O) ₂	(H ₂ O) ₃	(H ₂ O) ₄	(H ₂ O) ₅	(H ₂ O) ₆	(H ₂ O) ₇
Ni	—	—	—	—	—	—	.1604	.1735	.1781	.1814	.1472	.1594	—
S	—	—	.2433	.2332	.2726	.2475	—	—	.0005	.0021	—	.0008	—
O ₁	—	.2433	.0156	.0559	.0358	.0678	.0154	.0261	.0051	.1797	—	.0075	.0398
O ₂	—	.2332	.0559	—	.0483	.0522	.0041	.1655	.1669	.1271	.0316	.0346	.0626
O ₃	—	.2726	.0358	.0483	—	.0431	.1577	.0426	.1525	.0817	.0514	.0079	.0289
O ₄	—	.2475	.0678	.0522	.0431	—	.1437	.1419	.0308	.0056	.1513	.0707	.0039
(H ₂ O) ₁	.1604	—	.0154	.0041	.1577	.1437	—	.0687	.0720	.0181	.0512	.0710	.0036
(H ₂ O) ₂	.1735	—	.0261	.0238	.0426	.1419	.0238	—	.0038	.0470	.0605	.0784	.0036
(H ₂ O) ₃	.1781	.0005	.0051	.1669	.1525	.0308	.0038	.0070	—	.0218	.0006	.0306	.0817
(H ₂ O) ₄	.1814	.0021	.1797	.1271	.0016	.0056	.0181	.0470	.0664	—	.0724	.0545	.0001
(H ₂ O) ₅	.1472	—	.0726	.0316	.0514	.1513	.0512	.0006	.0065	.0724	.0003	.1514	.0191
(H ₂ O) ₆	.1594	.0008	.0075	.0346	.0079	.0176	.0784	.0125	.0306	.0545	.1514	.0001	.0488
(H ₂ O) ₇	—	—	.0398	.0626	.0039	.0000	.1446	.1446	.0817	.1232	.1232	.1459	—
			.1475		.0036		.0556		.0817	.0488			

circumscribed about the tetrahedron. In fact any definable point in the tetrahedron will give a unique dissection which is a variant of the Voronoi dissection. The algorithm requires careful book-keeping.

(b) The set-theory algorithm of Brostow, Dussault and Fox⁷ which partitions all atoms into sets according as they lie on one side or another of particular planes. Following from this method, it might be pointed out that, if only the signs of the volumes of all tetrahedra (with atoms at the four vertices) were known, then the complete structure would be defined to a considerable accuracy. Of course there would be a very large number of such tetrahedra, rising as the fourth power of the number of points. This consideration offers a method for calculating the quantity of information (in bits) contained in an arrangement of points.

(c) If it is required only to find the volumes of the Voronoi polyhedra (defined as the region about an atom within which all points are nearer to the atom in question than to any other) then this can be done by a Monte-Carlo method which is far simpler than making a complete dissection and can be used for the radical plane and other variants.⁸

The comparison of absolute and statistical calculations of the volumes of the Voronoi polyhedra for nickel sulphate heptahydrate.

The third column gives the volumes of the Voronoi polyhedra for the radical plane dissection (Radii: Ni, 0.68; S, 0.30; O and water 1.32 Å).

Ion.	/Absolute./	Stat calcn./	Radical plane (Stat.)
Ni	8.5	8.20	3.07
S	6.19	6.49	0.049
O1	21.73	21.81	22.10
O2	18.38	18.10	19.42
O3	19.70	19.66	20.98
O4	18.00	18.88	18.68
water 1	21.19	20.78	24.39
water 2	20.73	21.03	22.58
water 3	20.71	20.10	20.39
water 4	21.20	20.10	22.09
water 5	20.09	19.03	22.00
water 6	21.23	21.95	21.02
water 7	26.26	27.81	27.12

The statistical estimate, which has an r.m.s. error with respect to the full calculation, of 0.76 Å³ was made by taking 5000 random points and simply calculating which atom was nearest. 5000 points were also used for the radical plane calculation. The programme is very simple and can readily be carried out on a micro-computer.

Fischer, Koch and Hellner⁹ have shown that the radical plane variant is valuable, since this enables each type of ion to be given its characteristic radius.

The conservation of flux (Pauling's rule) corresponds to Kirchoff's node equations, but it is difficult to find adequate equivalents for the loop equations. Circuits are not uniquely defined in three dimensions. Brown¹⁰ has shown how, adding equalising conditions, the network equations can be solved for the bond strengths.

SPECIFIC VOLUME

The simplest property which atoms have is that of volume. Is it possible to predict the density of compounds from their composition? If Vegard's Law applies there is no difficulty, but departures from it will indicate conformational features. Following the suggestions of Sugden's development of the »parachor«,¹¹ a measurement of the volumes of organic molecules under conditions of normalised surface tension, a similar study has been made of inorganic materials. In principle, the cell volumes of all known crystal structures could be used to provide, by some least squares procedure, the specific volumes of each kind of ion in the solid state. Sugden found it necessary to introduce constitutional factors, (double bond, benzene rings, etc.) as well as compositional and a similar procedure has been followed in this example. We show that information on constitution can also be obtained from volume (or density) measurements of inorganic compounds.

From the unit cell data and the composition of compounds of CaO, Al₂O₃, SiO₂ and H₂O (designated in cement terminology, respectively, C, A, S, H), »X-ray densities« can be calculated, so that the volume of the structure can be attributed to its oxide composition. The volume changes clearly depend on the shapes of the oxygen coordination polyhedra.

This has been done for 83 such compounds, the volumes being fitted by least squares with an overall r. m. s. disagreement of 10.3% between observed and calculated densities, the density being calculated purely on the basis of the composition. The specific volumes obtained were:

Associated with each cation.		or with each oxygen ion:	
0.5 A	23.2 Å ³	or 0.333 A	15.47 Å ³
C	28.9	C	28.9
S	38.0	0.5 S	19.0
0.5 H	11.5	H	23.0

It is evident that the Si atom, with tetrahedral coordination, implying an open structure, makes a disproportionately large contribution to the volume.

If interactions are included and the volume is calculated as:

$$v = \sum_i n_i v_i + (\sum_{i,j} n_i n_j v_{ij}) / \sum_i n_i$$

where n_i is the fractional number of the atoms of type i .
the specific volumes become:

0.5 A	22.8	or per oxygen	0.33 A	15.20
C	28.8		C	28.8
S	40.6		0.5 S	20.3
0.5 H	14.3		H	28.6

and the interaction terms are:

$$v(\text{Al}, \text{Ca}) = 39.6; v(\text{Al}, \text{Si}) = -19.6; v(\text{Al}, \text{H}) = -26.6$$

$$v(\text{Ca}, \text{Si}) = -24; v(\text{Ca}, \text{H}) = -21$$

$$v(\text{Si}, \text{H}) = 2.7.$$

The r. m. s. deviation is reduced to 7.7%. This indicates that, if Al_2O_3 and CaO are both present, the volume is abnormally increased, i. e. packing is less dense, probably showing that the Al is in tetrahedral positions. The largest deviations are:

CAS2	— 12% less dense than expected
Grossularite	+ 16% more dense
CAS2H5	— 13%
C4A	— 11%
Mullite	— 11%
Portlandite	— 12%
C6S2H3	— 14%
K-phase	— 13%
Lawsonite	+ 14%
Ice	— 13%

Without the interaction terms the density of calcium aluminates is much underestimated. This probably shows that in Ca aluminates the Al tends to be tetrahedral rather than octahedral. A factor for the tetrahedral/octahedral ratio of the Al coordination could have been included specifically in the least squares fitting of the specific volumes. The volumes may be compared with those resulting from the radical plane dissections mentioned above.

PERIODIC SURFACES OF MINIMUM AREA

Structures which exhibit prominent internal membranes or symmetrical surfaces occur most obviously in foams or soap bubbles, where the surface tension clearly determines the configuration. Similar circumstances are to be recognized in assemblies of cells, and in metal grains at temperatures sufficiently high for annealing and grain growth to take place, driven by the minimisation of the area of the grain interfaces.

In, for example, the packing of equal air bubbles, used by W. L. Bragg and J. F. Nye as a model of the recrystallisation of metals, the packing can be periodic. Similar crystalline structures, periodic in three dimensions, and often of cubic symmetry, can be seen in certain phases of lyotropic crystals¹² or in mesophases. Even the Fermi surface in reciprocal space may show this kind of figure. A range of silicate structures, especially of molecular sieve materials,^{13,14} although rigid at room temperatures, would appear to have been formed by the action of the surface tension of the silicate membranes.¹⁵ In a wide range of clathrate materials the structuring forces are those of surface tension complicated by the presence of guest molecules around which the surface must form (as in the synthesis, for example, of silicalite). It should be possible to discuss the formation of silicates (and of silicalite) in the same way as is discussed the folding of protein chains so as to segregate hydrophobic and hydrophilic regions.

Although we speak of surface or membranes, the forces operating are, of course, only interatomic forces and »surface tension or interfacial energy« is just a simplified description of the collective effect of interatomic forces at a scale of resolution at which individual atoms are not separately discernable.

Several of the geometrical structures to be discussed occur on a variety of scales and are geometrical invariants and worth description in their own right.

The mathematical condition which defines the particular structures under a variety of conditions, is simply that of the minimisation of the interfacial area and thus of the energy. Such principles of hydrophobicity and hydrophilicity are widely used in discussions of protein folding. If the pressure is the same on both sides of the membrane, as in the cases following, this requires that the mean curvature should everywhere be zero. If the equation for the surface is expressed as $z = f(x, y)$, then the condition for zero mean curvature, the Laplace-Young equation is $H = 0$ where:

$$H = \frac{(1 + f_y f_y) f_{xx} - 2 f_x f_y f_{xy} + (1 + f_x f_x) f_{yy}}{2(1 + f_x f_x + f_y f_y)^{3/2}}$$

here f_x represents the first partial differential of z with respect to x , etc.

The corresponding expression for the area of the element $dx \cdot dy$ is $dA = [1 + f_x f_x + f_y f_y]^{1/2} dx \cdot dy$. The particular boundary conditions for which a solution has been found by Schwarz¹⁶ are for a quadrilateral lying in two planes in space, but neither Schwarz nor Nitsche¹⁷ gave computations of coordinates or areas but expressed the results as a complex integral. In the present work computations of $z = f(x, y)$ were made from first principles, repeatedly massaging the film into the position in which the mean curvature was everywhere zero.* The two principle periodic structures were also first described in detail by Schwarz.¹⁶ They are of particular interest as geometrical absolutes, comparable to the semi-regular polyhedra, since they each divide space into two identical regions. That is, the space on one side of the boundary surface is exactly congruent with space on the other side. Wells¹⁸ gives a drawing (Figure 2) of the corresponding figure with polyhedral faces.

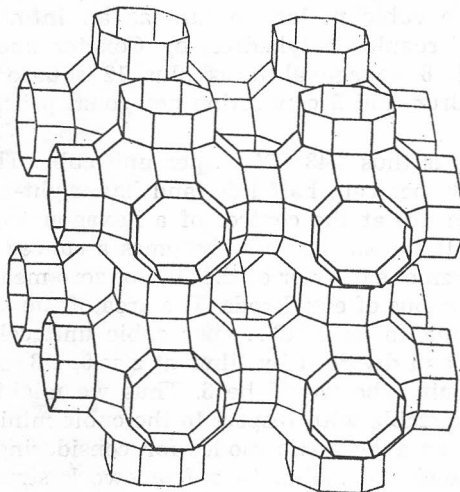


Figure 2. The bonds in a primitive cubic structure with octahedral coordination can be inflated, to a surface with polygonal faces to give an infinite semi-regular polyhedron (which is, in fact, body-centred cubic, since the surface divides space into two congruent regions and 0, 0, 0, is identical with 1/2, 1/2, 1/2). The figure is after Wells.¹⁸ When the polygonal faces are smoothed to zero mean curvature, the minimal surface found by Schwarz¹⁶ results.

* The programme is available from the author.

The topology of the two structures is best described by using the concept of inflation. The first structure, referred to as the simple cubic partition, is derived from the simple cubic packing of spheres, one sphere per lattice point, by the inflation of the bonds between the spheres (six bonds in the cube edge directions) until they form cylindrical tunnels, six radiating from each sphere. The surface may be either panelled with regular polygons, or may be a smooth minimal surface, but in either case the unfilled space between the tunnels is exactly congruent to the tunnel system, which thus occupies one half of the volume of each cell. The congruence could be achieved by a displacement of $(1/2, 1/2, 1/2)$.

The second structure, the diamond cubic pattern, bears a similar relationship to the diamond cubic structure. Here the bonds are inflated so that each sphere is connected by four tunnels radiating tetrahedrally. As in diamond, there are 8 such spheres per unit cell and the two non-connected spaces are interlaced as in the »double-diamond« structures of Cu_2O and of high pressure ice, and are related by a translation of $(1/2, 0, 0)$. Schwarz' tetrahedral surface has been observed by Longley and McIntosh¹⁹ for a lipid-water phase and the octahedral by Donnay and Pawson and Nissen for a natural sea-urchin spine (a calcite deposit).²⁰

In, for example, the structure of Faujasite (a zeolite), we may discern a recursive or fractal²¹ or hierarchic operation. We may conceptually take the structure of cristobalite (like that of diamond) which is made of linked SiO_4 tetrahedra and replace each of these tetrahedra with a larger tetrahedron, itself made of linked SiO_4 tetrahedra to obtain the structure of Faujasite. Thus the whole topology of connected SiO_4 tetrahedra may be seen again on a larger scale in the various polytypes of faujasite found by Thomas.²²

When the simple cubic pattern occurs as an infinite polyhedron (first recognised as a semi-regular polyhedron by Coxeter and Petrie²³) it has, in each cubic unit cell, 8 hexagonal faces plus 12 square faces making up a truncated cuboctahedron and 3 connecting octagonal prisms each of 8 squares (Figure 2).

The surface area is thus $2.435674 \dots$ per unit cube. The asymmetric unit, of which there are 96 per cell, half left- and half right-handed, is a triangle, the vertices of which are at the centres of a hexagon and two adjacent non-equivalent squares. If the surface now becomes a curved minimal surface the asymmetric unit is then one quarter of the film of zero mean curvature bounded by the edges of a rhombus of equal rods. The area of the surface had now been computed and is found to be $2.346 \dots$ per cubic unit cell of unit volume. If we take a unit cube and divide it by films at $z = 0, 1/3$ and $2/3$, then the area of the surface per unit cube would be 3. Thus we might expect that such a structure would be unstable with respect to the cubic minimal surface division. We have taken this as a heuristic model for considering the transformation of a layer silicate, such as kaolin, to a framework structure such as ultramarine. The transformation could be described in terms of catastrophe theory such as may be used in describing the transition of a cylindrical soap film between two rings from one surface to two as the separation is smoothly increased or the pressure is changed.

As an infinite polyhedron, the diamond cubic partition with 8 cuboctahedra per unit cell, each sharing 4 of their hexagonal faces with their neighbours, has 8×4 hexagons and 6×8 squares. This structure can be regarded as

composed of close-packed cuboctahedra (the tetrakaidehedra of Thomson²⁴ half of which belong to one semi-space and half to the other.

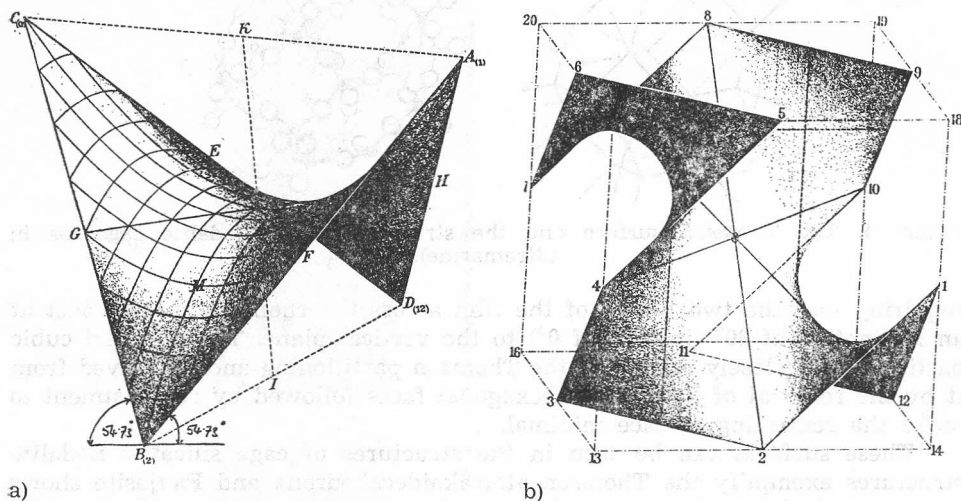


Figure 3. Figure (a) shows the quadrilateral panel, 24 of which fit together, in the way shown by figure (b), to give eventually a unit cell of an infinite, periodic, minimal surface, also found by Schwarz.¹⁶ The minimal surface corresponds to the diamond structure with tubular surfaces replacing the tetrahedral bonds, as in the structure of faujasite.

If the side of the unit cube is a , then the length of each edge is $a(2^{1/2})/3$. The surface of the unit cube is thus 2.049038. If the interface is made a minimal surface, the unit of pattern becomes a saddle slung over four edges of a tetrahedron of edge-length $a/(8^{1/2})$. The vertices of the tetrahedron lie at the centres of hexagonal faces. There are 96 tetrahedra per unit cube. Again, the problem reduces to one of the calculation of the area of a minimal surface over a quadrilateral frame, the result of which is 1.8227 per unit cube.

The Thomson Cube

W. Thomson (Lord Kelvin)²⁴ examined the question of the division of space with minimum partitional area and showed that for a periodic structure the best figure was the cuboctahedron (which he called the 'tetrakaidehedron' from its 14 faces). This is the Voronoi polyhedron for the bodycentred-cubic close packing.

The structure consists of closed cells and the area of surface, with 6 square faces and 8 hexagonal faces per cubic unit cell is 3.348076. However, the edges do not meet at 120° so that some curving of the cell edges and faces can take place to reduce the interfacial area to that of a minimal surface. Kelvin showed how this could be done by expanding the displacement of the hexagonal faces (the square faces remaining flat) a series of spherical harmonics. Lifshitz²⁵ gave an estimate of 0.103% for the reduction in area for curving the surfaces.

The program used for calculating the minimal film over a quadrilateral can be used for the Thomson partitioning. The programme was adapted by

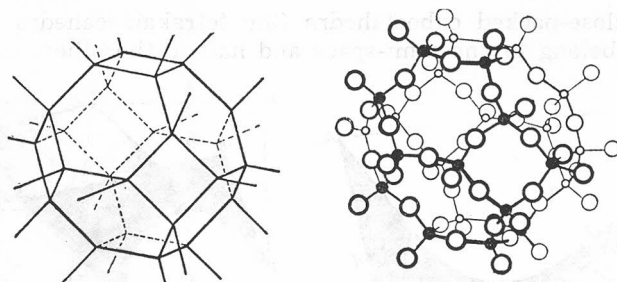


Figure 4. The Thomson surface and the structure of the sodalite cage (as in ultramarine).

requiring that the two halves of the film across the rhombus should meet at an inclination of 30° (instead of 0°) to the vertical plane. The diamond cubic partitioning is closely related to the Thomson partitioning and is derived from it by the removal of half of the hexagonal faces followed by readjustment to make the remaining surface minimal.

These surfaces can be seen in the structures of cage silicates. Sodalite structures exemplify the Thomson »tetrakaidecahedron« and Faujasite shows the tetrahedral inflation. A number of other minimal surfaces, for example, Neovius' surfaces with 12 and 8 coordination can be recognised in the infinite polyhedra described by Wells.¹⁸

TABLE II

The Minimal Surface are Built from Panels of Film Which are Quadrilateral Frames, Carrying »Soap-Films«.²⁶ These Frames are Rhombs, Folded out of the Plane so as to Have a Dihedral Angle. The Area of the Soap-Film, the Minimal Surface, Varies with the Dihedral Angle as Follows:

Dihedral half-angle of frame	Area	Saddle point
35.26°	2.3470	$z(0,0) = 0.1977$
30°	2.4325	0.1658
45°	2.125	0.2697
54.73°	1.8227	0.35355
0°	2.598076	0.0

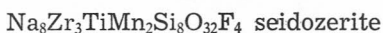
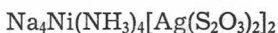
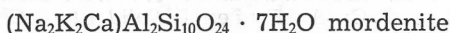
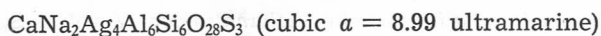
The area of the quadrilateral film with unit edges and one unit diagonal, folded symmetrically upwards about this diagonal, to make two equal half angles with the horizontal plane, $z = 0$, is tabulated, as is the height of the saddle-point of the film:

Cubic partitioning	3.
Thompson cube	2.598076
Wells (infin. polyhedron)	2.435675
Cycloid of revolution	2.346175
Spheres in primitive cubic lattice	3.141593
Surface of rhombic dodecahedron	2.121320
Diamond cubic	2.049038
Surface of 3 right circular cylinders intersecting at right angles	2.617074

THE COMPLEXITY OF CRYSTALS

Finally, we may ask whether there is a limit to the complexity of crystal structures, in the sense of asking if there is an upper limit to the number of parameters necessary to specify a crystal structure. This may also be investigated empirically using published tables such as »Crystal Data« (and could be done better when the Inorganic Data File is accessible interactively by machine).

We might ask first what might be the maximum number of chemical elements which may occur in an inorganic crystal structure, where each atom is in as definite position, solid solution being excluded. In »Crystal Data« (2nd. edn., 1963) we find 20 or more phases with 6 different elements and a few with 7 elements but probably none with 8. Some examples are:



We note that many on our list of compounds are cubic, and thus have high symmetry (the order of the symmetry group is high — the maximum being 192 for the group Fm3m) and that many have distinct subunits, such as complex (but symmetrical) phosphotungstate type ions or silicate frameworks. From these tentative observations we propose the hypothesis: »The greater the number of compositional parameters, the smaller the number of structural parameters«. A complex silicate framework, such a one of the infinite polyhedra described, driven by surface tension to its equilibrium conformation, has almost no parameters, given the topological connections.

It is assumed here that we are dealing here with crystals produced from melts or solutions or from the »primitive soup« and not from the crystallisation of molecules which may have been synthesised by biochemical pathways under the control of »informational molecules«.

We conclude that, with the appearance of data bases of inorganic structures, the study of inorganic crystal chemistry is entering a new phase. We are grateful to Professor Sten Andersson and his school for personal communications on this subject.

REFERENCES

1. H. A. Simon, *Proc. Amer. Phil. Soc.* **106** (1962) 467.
2. R. C. Evans, *Crystal Chemistry*, Cambridge University Press, 1939.
3. C. A. Beevers and C. M. Schwartz, *Zeit. Krist.*, **91** (1935) 157.
4. F. C. Frank and J. S. Kasper, *Acta Cryst.* **11** (1958) 184.
5. A. L. Mackay, *Jour. Microscopy* **95** (1972) 217.

6. J. L. Finney, *Proc. Roy. Soc.*, **A319** (1970) 479.
7. W. Brostow, J.-P. Dussault and B. L. Fox, *Jour. Comp. Physics*, **29** (1978) 81.
8. A. L. Mackay, unpublished work.
9. W. Fischer, E. Koch and E. Hellner, *Neues Jahrbuch der Mineralogie Monatsheft*, No. 5 (1971) 227.
10. I. D. Brown, *Acta Cryst.*, **B33** (1977) 1305.
11. S. Sugden, *Jour. Chem. Soc.*, **125** (1924) 1177.
12. K. Fontell, *Mol. Cryst. Liq. Cryst.* **63** (1981) 59.
13. L. Faelth and S. Andersson, *Zeit. Krist.*, **160** (1982) 313.
14. S. Andersson and B. G. Hyde, *Zeit. Krist.* **158** (1982) 119.
15. A. L. Mackay, *IUC Regional Conference*, Copenhagen, 1979, Paper no. 73-P1-5a in Abstracts.
16. H. A. Schwarz, *Gesammelte mathematische Abhandlungen* (2 vols.), Springer, 1890.
17. J. C. C. Nitsche, *Vorlesungen ueber Minimalflaechen*, Springer Berlin, 1975.
18. A. F. Wells, *Three-dimensional nets and polyhedra*, Wiley, New York, 1977.
19. W. Longley and T. J. MacIntosh, *Nature* **303** (1983) 612.
20. G. Donnay and D. L. Pawson, *Science*, **166** (1969) 1147; and H.-U. Nissen, *Science*, **166** (1969) 1150.
21. B. Mandelbrot, *Fractals*, Freeman, San Francisco, 1977.
22. J. M. Thomas, S. Ramdas, G. R. Millward, J. Klinowski, M. Audier, J. Gonzalez-Calbet and C. A. Fyfe, *J. Solid State Chem.*, **45** (1982) 368.
23. H. S. M. Coxeter, *Twelve Geometric Essays*, S. Illinois Press, (1968); and *Proc. Lond. Math. Soc.*, Ser. 2, **43** (1937) 33.
24. W. Thomson, *Phil. Mag*, **4** (1877) 503.
25. J. Lifschitz, *Science*, **97** (1943) 26.
26. C. Isenberg, *The Science of Soap Films and Soap Bubbles*, Tieto, Clevedon, 1978.

SAŽETAK

Deskriptori za kompleksne anorganske strukture

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Uzimajući u obzir veliku raznolikost struktura pitamo se kako da ih opišemo. Možemo se i dalje zapitati, postoji li uopće nekakav prirodni način njihova opisanja. Paulingova pravila dovela su do osnove za razumijevanje ionskih struktura u smislu koordinacijskih poliedara. Ovaj članak obrađuje neke geometrijske aspekte pri čemu uzima u obzir: (a) kvantitativno razdvajanje u koordinacijske poliedre; (b) specifični atomski volumen; (c) minimalne površine kao slike silikatnih struktura u velikom, i (d) kompleksnost.