

1, 5 and 7. It is clear that the use of a higher NMIN gives better results for the average phase deviation as well as a lower number of phases with an error of over 250 mcycles. An E map calculated from the phases obtained with NMIN equal to 7 revealed 162 atoms among the 240 strongest unique peaks; this number is not much larger than in the case of NMIN = 1, but the peaks were much higher, although the number of contributing reflections was smaller.

The alternative procedure was also tested using $\Delta_3 = 0$ in (6), which is equivalent to the use of the usual formula (5). From the results given in the lower half of Table 3 it can be concluded that: (a) the final phase sets are almost centrosymmetric and (b) the use of a higher number for NMIN only slightly slows down the appearance of the other enantiomorph. For the sake of comparison an E map was calculated from the phases obtained with $\Delta_3 = 0$ and NMIN = 7. Only 93 out of the 243 strongest unique peaks could be identified as atoms.

The total computing time for the tangent extension procedure mentioned above ranged from 78 to 105 c.p.u.s (on a Cyber 73 computer). The procedure based on the graphical determination of new phases took 147 s c.p.u. time for the 400 atom structure despite the fact that only ± 1300 unique triplets were used in the final refinement cycles. Our conclusion is that the procedure based on graphical phase determination is rather expensive and difficult to optimize for accepting new phases. Since the procedure using (5) leads to a maximum number of more or less correct phases in a minimum of time, it is to be preferred. If this procedure

is combined with a refinement procedure based on (6) the results are sufficiently enantiomorph specific to lead to a correct solution, starting from a medium-sized phase set.

The main conclusion of this paper is that with a relatively simple improvement in the estimates used, the centering tendency of the tangent formula is efficiently blocked. However, since it is expected that better estimates will improve the quality of the final map, this will be an important part of our future efforts.

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The Archimedean Truncated Octahedron, and Packing of Geometric Units in Cubic Crystal Structures

BY CHUNG CHIEH

Guelph–Waterloo Center for Graduate Work in Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

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Abstract

Any cubic crystal structure can be divided into small units in the form of congruent semi-regular (Archimedean) truncated octahedra. The centers of these polyhedra can be chosen at invariant equivalent positions for most cubic space groups. The part of a

crystal structure enclosed by an Archimedean polyhedron is called a geometric unit (or unit for short); however, the boundary of the unit may be relaxed to include a whole molecule or ion in case the geometric division is not convenient. Based on the properties and arrangements of such geometric units, there is an interesting relationship among the 36 cubic space

groups. All units in a crystal structure of any one of 16 space groups are equivalent. There are 14 space groups to accommodate crystal structures with two types of independent units. Only crystal structures of space groups $F23$ and $F\bar{4}3m$ consist of four types of independent units. The remaining four space groups are in the class with three types of geometric units. The arrangement of geometric units is represented by a sequence of one period along the body diagonals of a unit cell. The sequence of geometric units is a simple version of the packing map on a (110) plane. This packing map reveals structural features.

Introduction

There is a continuous interest among scientists in the search for ways to represent crystal structures such that a correlation among them can easily be recognized (Pearson, 1967; Loeb, 1970; Wells, 1977). In the cubic system, it is the multitude and variety of the crystals and the complexity of their interrelations that confound a systematologist. In an effort to tabulate structural data in a systematic way, the writer is confronted with the problem of choosing a suitable unit that can be represented by a formula. It is now realized that a unit can be chosen such that it is the part of a structure enclosed by a semi-regular truncated octahedron (*vide infra*) whose center is located at an invariant position. In 29 out of 36 cubic space groups, these invariant equivalent positions have the highest symmetry. The origin and body center always serve as centers for these polyhedra. This choice offers many advantages for representing and describing cubic crystal structures.

This paper reports the validity of this choice. It is divided into three sections. To begin with, the geometry and properties of the semi-regular truncated octahedron will be discussed. The cubic space groups will then be classified according to the symmetry and properties of the geometric units; examples are given to show how the geometric unit concept is applied to represent crystal structures. The paper is concluded by a discussion.

The Archimedean truncated octahedron

In a mathematical sense, a polyhedron is a solid bounded by plane polygons. An octahedron and a cube are two of the five possible regular polyhedra whose faces are congruent regular polygons and whose polyhedral angles are congruent (Wells, 1977). The common volume enclosed by both a cube and an octahedron in normal crystallographic orientations (*i.e.* their symmetry elements coinciding) is a truncated

octahedron. When a cube truncates the octahedron at points which divide the octahedral edges into three equal parts, the resulting solid is a semi-regular truncated octahedron, Fig. 1(a). It is also called an *Archimedean truncated octahedron*. This is not a regular polyhedron because not all faces are congruent. There are six square faces and eight hexagonal faces. Since all edges have the same length, it is usually referred to as a *semi-regular polyhedron*.

Table 1 shows specific dimensions of a truncated octahedron which is Archimedean. Some of these properties are important in crystal chemistry. For example, knowing that hexagonal faces are closer to the center (0.8660) than square faces (1.0), an inscribed sphere that just touches the hexagonal faces will not make contact with the square faces.

All symmetry elements of the octahedron (or the cube) are retained in the Archimedean truncated octahedron; therefore its point group is $m\bar{3}m$. The threefold axes are normal to the hexagonal faces as are the fourfold axes to the square faces. The twofold axes pass through the mid-points of opposite edges running between pairs of hexagonal faces. Three projections from 4-, 2- and 3-axes are shown in Fig. 1(b), in which the projection from a twofold axis is the most important one. It is a view from a [110] direction and it will be used frequently in the next section. The profile of this view is a truncated rhombus.

Packing of congruent Archimedean truncated octahedra fills the entire space leaving no gap. This packing gives a structure with a body-centered cubic cell. The arrangement of polyhedra in the geometric structure is the same as that of atoms in a b.c.c. structure. Two views of this packing are shown in Fig. 1, one along a [001], (c), and one along a [110] direction, (d). These are not exact projections of a

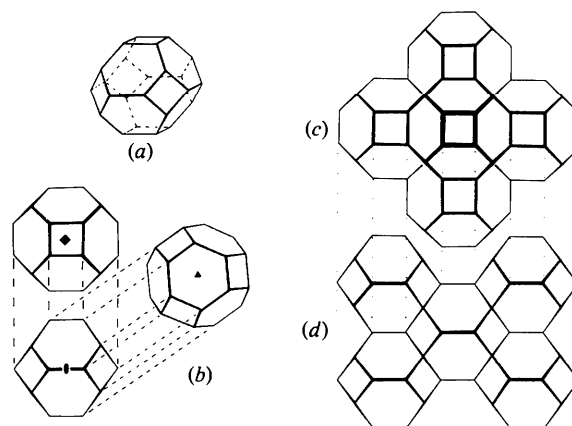


Fig. 1. (a) The Archimedean truncated octahedron, (b) views from four, two and threefold axes; the space filling packing viewed from (c) [001] and (d) [110] directions.

Table 1. Measures of an Archimedean truncated octahedron

Items	Measures	
	Normalized to unit distance between polyhedron center and square face center	Normalized to unit length for edges
Coordinates of vertices	$0, \pm\frac{1}{2}, 1; 0, \pm 1, \pm\frac{1}{2}$ $\pm\frac{1}{2}, \pm 1, 0; \pm 1, \pm\frac{1}{2}, 0$ $\pm 1, 0, \pm\frac{1}{2}; \pm\frac{1}{2}, 0, \pm 1$	$0, \pm 1/\sqrt{2}, \pm\sqrt{2}; 0, \pm\sqrt{2}, \pm 1/\sqrt{2}$ $\pm 1/\sqrt{2}, \pm\sqrt{2}, 0; \pm\sqrt{2}, \pm 1/\sqrt{2}, 0$ $\pm\sqrt{2}, 0, \pm 1/\sqrt{2}; \pm 1/\sqrt{2}, 0, \pm\sqrt{2}$
Edge	$1/\sqrt{2} = 0.7071$	1
Polyhedron center to vertices	$\sqrt{5}/2 = 1.1180$	$\sqrt{10}/2 = 1.5811$
Polyhedron center to mid edge	$3\sqrt{2}/4 = 1.0607$	$3/2 = 1.5$
Polyhedron center to centers of square faces	1	$\sqrt{2} = 1.4142$
Polyhedron center to centers of hexagonal faces	$\sqrt{3}/2 = 0.8660$	$\sqrt{6}/2 = 1.2247$
Vertex to centers of square faces	$1/2 = 0.5$	$1/\sqrt{2} = 0.7071$
Vertex to centers of hexagonal faces	$1/\sqrt{2} = 0.7071$	1
Area of a square face	$1/2$	1
Area of a hexagonal face	$3\sqrt{3}/4 = 1.2990$	$3\sqrt{3}/2 = 2.5981$
Total surface of polyhedron	$3 + 6\sqrt{3} = 13.3923$	$6 + 12\sqrt{3} = 26.7846$
Volume of polyhedron	4	$8\sqrt{2} = 11.3137$

particular aggregation because some polyhedra present in one are omitted in the other for clarity. The central Archimedean truncated octahedra in both (c) and (d) are at the body centers of the unit cells, if the centers of the other four polyhedra are defined as the origins. The stacking in a (110) plane, (d), has the advantage that all the Archimedean truncated octahedra are on the same level. The two Archimedean polyhedra per unit cell can equally be represented in a diagram.

Classification of cubic space groups by geometric units

Since the packing of Archimedean truncated octahedra fills the entire space, this polyhedron may be considered as a basic unit in a crystal structure. The part of a structure enclosed by this polyhedron is an idealized geometric unit. The natural boundaries between molecules or ions in some crystals may not be the same as those of the Archimedean truncated octahedra defined in the geometric sense; in this case we use the molecule or ion as a geometric unit. This relaxed definition simply means that some polyhedra in a structure have 'bumps' which fit into the 'craters' of the others in the same structure. Nevertheless, the packing pattern is still the same as that of the Archimedean truncated octahedra. With the structure added as a property, the point-group symmetry of a geometric unit is not necessarily the same as that of an Archimedean truncated octahedron.

Any cubic crystal structure can be described as packing of geometric units along $\langle 111 \rangle$ directions. (i)

All geometric units in some structures are identical; however, they may pack in one of the following ways: $A, A\bar{A}$, and AA' along the $\langle 111 \rangle$ directions, column 2 of Table 2, where \bar{A}, A' and \bar{A}' indicate units related to A by $\bar{1}, 4-$ and $\bar{4}$ -axes respectively. (ii) In crystal structures of $Fd\bar{3}c$, the packing sequence is $AA'\bar{A}'\bar{A}$. (iii) For crystal structures of space groups $Ia\bar{3}d, I\bar{4}3d$ and $I4_132$, there are two kinds of packing sequences running antiparallel to each other in $\langle 111 \rangle$ directions. (iv) Two types of geometrical units, A and B , may be present and they combine to give various packing sequences. (v) There are cases that need three or, at most, four types of geometric units to describe cubic crystal structures.

In this approach, a structure is divided into congruent Archimedean truncated octahedra which, whenever possible, are chosen in such a way that their centers correspond to invariant equivalent positions with the highest point symmetry in a space group, e.g. $2(a) \bar{4}3m$ 0,0,0, of $I\bar{4}3m$. The point group of the geometric unit is the site symmetry of its center. For example, the geometric unit in the $I\bar{4}3m$ crystal structure of hexamethylenetetramine (Dickinson & Raymond, 1923) consists of a molecule, $C_6H_{12}N_4$, which belongs to a point group $\bar{4}3m$. The unit is shown in Fig. 2. The profile of the Archimedean truncated octahedron outlines the actual area when viewed from a twofold axis. A crystal structure of any one of the five symorphic I -type space groups have identical geometric units and their arrangement on a (110) plane can be represented by Fig. 1(d).

Geometric units centered on equivalent points must

be identical. Their orientations are not always the same. For example, the two geometric units at 0,0,0 and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ for Cu₂O, a *Pn3m* structure, are related to each other by an inversion center, Fig. 3(a); therefore, we can represent the arrangement of geometric units by $A\bar{A}$.

The helvite, Mn₄(BeSiO₄)₃S, structure belongs to *P43n* (Holloway, Giordano & Peacor, 1972). In this structure, the sulfur is located at the center of the geometric unit, Fig. 3(b). There are four Mn atoms bound to the sulfur tetrahedrally. We see three in Fig. 3(b) because the fourth one is directly underneath the

one that is in front of the page. In addition to the sulfur, each Mn atom is bonded to three oxygen atoms which each bond unsymmetrically to a Si and a Be atom. The Si and Be atoms are located at the vertices of an Archimedean truncated octahedron and they are shared among the geometric units. The dotted and dashed lines indicate the geometric units and the boundary of a (110) plane in the cell respectively. The orientations of the two geometric units are related by a 90° rotation about (001). This relationship in a sequence is indicated by AA' in Table 2. The helvite

Table 2. Classification of cubic space groups according to the properties and arrangement of geometric units

m: multiplicity; *w*: Wyckoff notation; *ss*: site symmetry.

Number of geometric unit types	Geometric unit(s) in a period	Equivalent position(s) as center(s) of unit(s)												Space group	
		<i>m</i>	<i>w</i>	<i>ss</i>	<i>m</i>	<i>w</i>	<i>ss</i>	<i>m</i>	<i>w</i>	<i>ss</i>	<i>m</i>	<i>w</i>	<i>ss</i>		
1	<i>A</i>	2	<i>a</i>	23											<i>I23</i>
		2	<i>a</i>	<i>m3</i>											<i>Im3</i>
		2	<i>a</i>	43											<i>I432</i>
		2	<i>a</i>	$\bar{4}3m$											<i>I43m</i>
		2	<i>a</i>	<i>m3m</i>											<i>Im3m</i>
	$\bar{A}\bar{A}$	2	<i>a</i>	23											<i>I2,3</i>
		2	<i>a</i>	43											<i>Pn3</i>
		2	<i>a</i>	$\bar{4}3m$											<i>Pn3n</i>
	AA'	2	<i>a</i>	23											<i>Pn3m</i>
		2	<i>a</i>	<i>m3</i>											<i>P43n</i>
		2	<i>a</i>	23											<i>Pm3n</i>
	$AA'/\bar{A}'\bar{A}$	16	<i>a</i>	23											<i>P4,32</i>
		16	<i>a</i>	$\bar{3}$											<i>Fd3c</i>
		16	<i>c</i> †	3											<i>Ia3d</i>
		16	<i>e</i> †	3											<i>I43d</i>
	2	<i>AB</i>	1	<i>a</i>	23	1	<i>b</i>	23							
1			<i>a</i>	<i>m3</i>	1	<i>b</i>	<i>m3</i>								<i>P23</i>
1			<i>a</i>	43	1	<i>b</i>	43								<i>Pm3</i>
1			<i>a</i>	$\bar{4}3m$	1	<i>b</i>	$\bar{4}3m$								<i>P432</i>
1			<i>a</i>	<i>m3m</i>	1	<i>b</i>	<i>m3m</i>								<i>P43m</i>
$\bar{A}\bar{A}\bar{B}\bar{B}$		8	<i>a</i>	23	8	<i>b</i>	23								<i>Pm3m</i>
		8	<i>a</i>	$\bar{4}3m$	8	<i>b</i>	$\bar{4}3m$								<i>P2,3</i>
		8	<i>a</i>	23	8	<i>b</i>	23								<i>P4,32</i>
		8	<i>a</i>	43	8	<i>b</i>	43								<i>P4,32</i>
		8	<i>a</i>	$\bar{4}3m$	8	<i>b</i>	$\bar{4}3m$								<i>P4,32</i>
		8	<i>a</i>	$\bar{3}$	8	<i>b</i>	$\bar{3}$								<i>Fd3</i>
		8	<i>a</i>	23	8	<i>b</i>	23								<i>Fd3m</i>
$AA'BB'$		8	<i>a</i>	23	8	<i>b</i>	23								<i>F4,32</i>
		8	<i>a</i>	43	8	<i>b</i>	<i>m3</i>								<i>F4,32</i>
		8	<i>a</i>	23	8	<i>b</i>	23								<i>F43c</i>
		8	<i>a</i>	43	8	<i>b</i>	<i>m3</i>								<i>Fm3c</i>
	8	<i>a</i>	$\bar{3}$	8	<i>b</i>	$\bar{3}$								<i>Fm3c</i>	
3	$ACB\bar{C}$	4	<i>a</i>	<i>m3</i>	4	<i>b</i>	<i>m3</i>	8	<i>c</i>	23					<i>Ia3</i>
		4	<i>a</i>	<i>m3m</i>	4	<i>b</i>	<i>m3m</i>	8	<i>c</i>	$\bar{4}3m$					<i>Fm3</i>
	$ACBC'$	4	<i>a</i>	43	4	<i>b</i>	43	8	<i>c</i>	23					<i>Fm3m</i>
		4	<i>a</i>	$\bar{3}$	4	<i>b</i>	$\bar{3}$	8†	<i>c</i>	3					<i>F432</i>
		4	<i>a</i>	$\bar{3}$	4	<i>b</i>	$\bar{3}$	8†	<i>c</i>	3					<i>Pa3</i>
4	$ACBD$	4	<i>a</i>	23	4	<i>c</i>	23	4	<i>b</i>	23	4	<i>d</i>	23		<i>F23</i>
		4	<i>a</i>	$\bar{4}3m$	4	<i>c</i>	$\bar{4}3m$	4	<i>b</i>	$\bar{4}3m$	4	<i>d</i>	$\bar{4}3m$		<i>F43m</i>

* See Fig. 5 for arrangements of geometric units on a (110) plane. Geometric units \bar{A} , A' and \bar{A}' have orientations related to A by symmetries $\bar{1}$, 4, and 4 followed by $\bar{1}$. Other orientation relations are indicated by $\bar{\sim}$.

† Geometric units centered on singular points of 16(c), 8(c), or 16(e).

structure is the same as that of sodalite and it is usually referred to as such.

An F cell consists of 16 geometric units. There are four kinds that are independent of lattice translation and four of each kind per cell. On a (110) plane lie two of each kind and along the body diagonal is one of each kind within the boundary of a unit cell. This is indicated in Fig. 4. Those that are equivalent by lattice translation are labeled with the same letter. The sequence in a period consists of four geometric units,

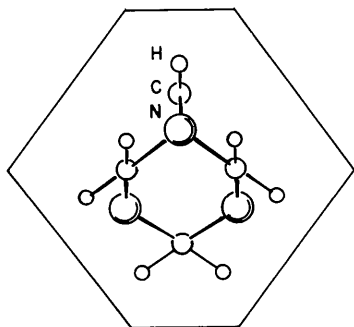


Fig. 2. A geometric unit in the $I43m$ crystal structure of hexamethylenetetramine, $\text{NH}_4(\text{CH}_2)_6$.

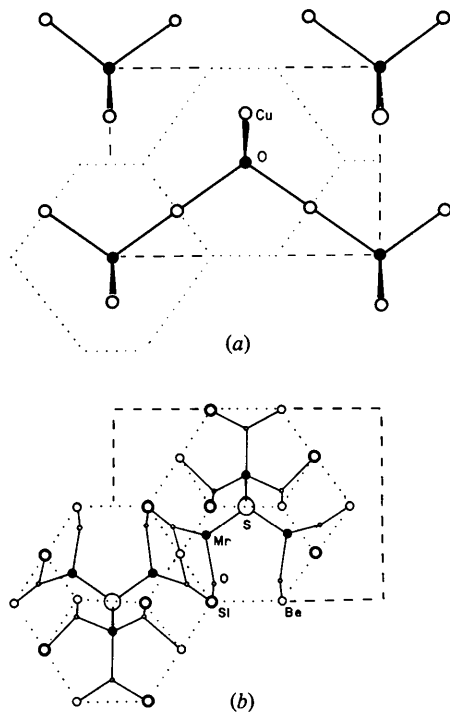


Fig. 3. The arrangements of geometric units: (a) in Cu_2O , an example of AA repeating sequence; (b) in helvite $[\text{Mn}_4(\text{BeSiO}_4)_3\text{S}]$, an example of AA' repeating sequence.

that is one of each kind. For crystal structures of space group $Fd3c$ all four units are identical, however, with four orientations, Fig. 5(a). This unit belongs to point group 23, Table 2.

For crystal structure of space groups $Ia3d$, $Pa3$ and $Ia3$, the unit cell can be divided into geometric units in the same way as that of an F cell. Geometric units at $\frac{1}{2}, \frac{1}{2}, 0$; $0, \frac{1}{2}, \frac{1}{2}$ and $\frac{1}{2}, 0, \frac{1}{2}$ are no longer equivalent to the one at the origin in these space groups. These are compared in Fig. 5. The geometric units pack in two kinds of repeating sequence in an I lattice. One passes through the origin whereas the other passes through the center of a face in the unit cell. For example, this type of arrangement is indicated by $AA'/\bar{A}\bar{A}'$ in Table 2. There are also two types of packing sequences of geometric unit in P lattices. Each sequence consists of four units, Table 2 and Fig. 5(c).

The crystal structures of pyrite, FeS_2 , belongs to $Pa3$. It is usually described as a pseudo NaCl structure with groups of Fe and S_2 in place of Na and Cl (Pearson, 1972). This description is attributed to the

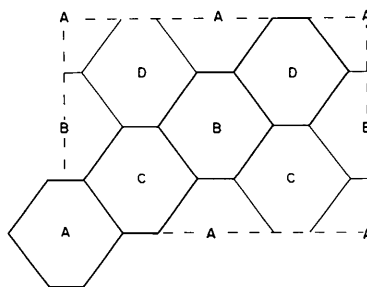


Fig. 4. Dividing of an F cell into 16 congruent Archimedean truncated octahedra showing only those with centers on a (110) plane.

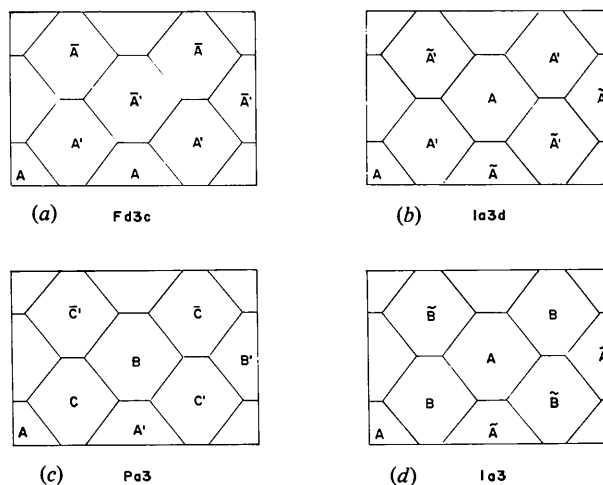


Fig. 5. Comparison of orientation orders of geometric unit for space groups $Fd3c$ (a), $Ia3d$ (b), $Pa3$ (c), and $Ia3$ (d).

similar arrangements of geometric units in an F cell and in a structure of $Pa3$, compare Fig. 5(a) and (c). The orientation of geometric units in the structure with space group $Pa3$ is an important feature that can be recognized in Fig. 5(c). However, the centers for units indicated by C 's are only singular points ($x = \frac{1}{4}$) of equivalent positions $8(c) x, x, x; \frac{1}{2} + x, \frac{1}{2} - x, \bar{x}; etc.$ The pyrite structure is common to many compounds. This is illustrated in Fig. 6(a), in which the Fe atom is labeled as A and A' . Being a single atom, A and A' have no orientation difference. Units B and B' , S_2 , have distinct orientations. The directionality of the unit B resulted in four orientations for the spaces centered on C, C', \bar{C} and \bar{C}' . The labels of geometric units in Fig. 6(a) are the same as those in Fig. 5(c). If S_2 is replaced by a single sphere, Fig. 6(a) represents a NaCl structure.

The molecular compound dodecachloropentasilane silicon tetrachloride, $Si(SiCl_3)_4 \cdot SiCl_4$ crystallizes in $F43c$ with $Z = 8$ (Fleming, 1972). Each molecule can be considered as a unit and they stack along the body diagonals of the cell with sequence $ABA'B'$, Table 2, where A and B represent $Si(SiCl_3)_4$ and $SiCl_4$ in any order. The molecule $SiCl_4$ which belongs to $\bar{4}3m$ point group is located at a site with 23 point symmetry but the other molecule $Si(SiCl_3)_4$ has only a 23 point symmetry which is consistent with the site. The arrangement of these two types of molecules on a (110) plane is shown in Fig. 6(b).

The five F -type symorphic space groups belong to two classes, Table 2, one with three geometric unit types and one with four. For the class that has three

geometric unit types, we use the f.c.c. close-packed spheres as an example to demonstrate the use of this concept. This structure belongs to $Fm3m$. Fig. 6(c) shows a view of the packing when the model is cut from a (110) plane. The two circles in the central part of the diagram represent two spheres lying on the two face centers behind the page. The Archimedean truncated octahedron profiles show the boundary of idealized geometric units. The three units are a sphere, S , two tetrahedral holes, T and \bar{T} , and an octahedral hole, O . The repeating sequence, $STOT$, not only gives the proper ratio for spheres to holes of an f.c.c. packing, but also indicates the orientation and symmetry, $\bar{4}3m$, of tetrahedral holes. If we use T to indicate tetrahedral holes and use the symbols of the element that constitute the geometric unit, the NaCl structure has a repeating sequence of $NaTC\bar{I}\bar{T}$. This indicates that the octahedral holes of the f.c.c. closed packing are occupied. Note that the repeating sequence can start with any geometric unit; it is origin independent.

Crystal structures of space groups $F23$ and $F\bar{4}3m$ have four independent geometric units. The zinc blende structure belongs to $F\bar{4}3m$ and is shown in Fig. 6(d). The unit centered at $B(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is the empty space enclosed by a cage structure of four S and six Zn atoms, whereas the cage around D consists of four Zn and six S atoms. The sequence is $ZnS-(S_4Zn_6)-(Zn_4S_6)$.

Discussion

It has been demonstrated that cubic crystal structures can conveniently be represented by geometric units that have the shape of an Archimedean truncated octahedron. The centers of these units usually coincide with invariant positions possessing the highest point symmetry in most space groups. The arrangement of these units can be represented by a sequence which specifies their relative positions and orientations along the body diagonals of the cubic unit cell.

Packing maps of geometric units on (110) planes are useful and perhaps second only to three-dimensional models in showing crystal structure. Thus the concept of geometric units provides a base for summarizing crystal structural data in a simple way. Crystal structures can be classified and tabulated in terms of geometric units.

In a few cases, the sequences for several space groups are the same. This sequence is origin independent; in cases with more than one unit we can start with any of them. These properties allow us to manipulate the representation in order to find correlations among crystal structures. Table 2 also presents an interesting relationship among the cubic space groups.

In the discussion of molecular or ionic crystal structures, it is necessary to retain the natural aggre-

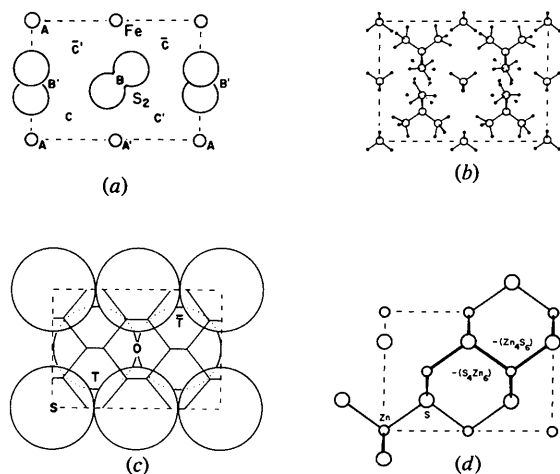


Fig. 6. Structures with unit cell divided into geometric units of an F cell: (a) pyrite, FeS_2 , a $Pa3$ structure; (b) dodecachloropentasilane silicon tetrachloride, $Si(SiCl_3)_4 \cdot SiCl_4$, a crystal structure with a repeating sequence of $ABA'B'$ in space group $F43c$; (c) geometric units in a f.c.c. structure, space group $Fm3m$; (d) four geometric unit types in the zinc blende structure, space group $F\bar{4}3m$.

gates as an isolated identity. Therefore, the arbitrary geometric boundary should not be adhered to as a golden rule when applying this concept, but the fact that parts of a molecule may extend from one unit into surrounding units is not seen as a hindrance, so long as appropriate symmetries with regard to the center of the unit are obeyed. However, for metallic compounds where no natural boundary exists, the Archimedean truncated octahedron can be used as a guideline for dividing a structure into its geometric units.

A common structural feature for normal γ brasses is that they all consist of 26-atom clusters (Bradley & Jones, 1933). The cubic γ -brass clusters all have $\bar{4}3m$ point symmetry and they can be regarded as geometric units. Crystal structures of both $I\bar{4}3m$ and $Pn\bar{3}m$ consist of a single geometric unit type that has a $\bar{4}3m$ point group. Although there are many $I\bar{4}3m$ γ brasses, Cu_2O is the only well characterized structure with a space group $Pn\bar{3}m$. This is probably due to the fact that the 26 atom clusters cannot have the A, \bar{A} arrangement. Both $P\bar{4}3m$ and $Fd\bar{3}m$ are in the class with two types of geometric unit that has point symmetry $\bar{4}3m$. For the same reason that no γ -brass structure belongs to space group $Pn\bar{3}m$, γ brasses with two types of cluster always belong to $P\bar{4}3m$. The space group $F\bar{4}3m$ can accommodate four geometric unit types that all belong to the $\bar{4}3m$ point group. Indeed, alloys $\text{Sn}_{11}\text{Cu}_{41}$, $\text{Sn}_3\text{Cu}_9\text{Ni}$, $\text{Sn}_2\text{Al}_2\text{Cu}_{12}$, $\text{Pt}_5\text{Hg}_{21}$ and $\text{Pt}_3\text{Zn}_{11}$ are γ brasses with this space group.

Another common structure type with space group $I\bar{4}3m$ is α -Mn. The geometric unit of this structure is a 29-atom cluster. Unlike γ brasses, no structure with two or four types of 29-atom cluster was ever found. Recently, Fornasini, Chabot & Parthé (1978) reported the crystal structure of $\text{Sm}_{11}\text{Cd}_{45}$ which belongs to $I\bar{4}3m$. Interestingly enough, among the four geometric unit types, two are similar to the clusters found in γ -brass except that there is an extra atom at the center. The other two are exactly like the 29-atom cluster found in α -Mn.

Representation of crystal structures by lattice complexes treats all equivalent positions in a space group

as isolated points (Fisher, Burzlaff, Hellner & Donnay, 1973). The present method associates atoms in a crystal structure with the invariant points in most space groups. This association gives rise to the geometric units which fill space, forming crystals. The centers of geometric units form a few simple lattice complexes that can easily be understood, thus avoiding the use of complicated nomenclatures in the lattice-complex scheme. The combination of geometric units and lattice-complex concepts will simplify the description and systemization of cubic crystal structures.

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