Acta Cryst. (1987). B43, 1-14

Application of Coincidence Site Lattices for Crystal Structure Description. Part I: $\Sigma = 3$

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(*Received 28 May 1985; accepted 29 April 1986*)

Abstract

The coincidence site lattice (CSL) theory, usually used to find models for grain boundaries, is shown to give a quantitative and accurate description of crystal structures. The CSL model with $\Sigma = 3$ gives building blocks which are defined and symbolized in terms of 2, 3, 4 or 5 integral numbers, *i.e.* (K, L), (K, L, P), (K, L, P, Q) or (K, L, P, Q, S). The assembly rule of building blocks in a c.c.p.-related crystal is analyzed in terms of 17 space groups. The relationship between a group and its subgroup is discussed. Two formulae which can calculate the coordinates of the atoms of a building block and a crystal structure are given. The following structure types have been analyzed: SiF_4, α-Mn, γ-brass, Fe_3W_3C, $Al_{10}V$, pyrochlore, zunyite, $Mg_{44}Rh_7$, Na_6Tl, Cu_4Cd_3, $Ge_{38}P_8I_8$ and Li_7VN_4.

1. Introduction

The empirical use of building blocks of atoms has been very fruitful in the description of complex crystal structures. The building blocks were almost always found to be units of simpler structures. Complex structures were described by letting the simpler blocks repeat by the classical operations of translation, reflection and rotation (Andersson, 1981; Andersson & Hyde, 1982).

By strictly describing and defining building blocks according to the symmetry of a crystal and repeating it with twin, rotation or reflection operations, we have arrived at a general and quantitative method for calculating atomic positions of even the most complex cubic inorganic structures. The mathematical concept used here is the same as that used in the study of grain boundaries and their coincidence site lattices (CSL), *viz.* matrix algebra.

It can be shown that for a rotation matrix of a cubic lattice

$$R = \frac{1}{N}\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

then $V_c = NV_1$ for p.c., b.c.c. and f.c.c. (Grimmer, Bollmann & Warrington, 1974) where V_1 is the volume for a standard cubic unit and V_c the volume for a structure unit derived from the CSL. They also showed that $N = \Sigma$ for these three cubic cases, with $\Sigma = 3, 5, 7, \ldots$ ($\Sigma = 1$ is simple translation), where Σ is the CSL parameter. A simplified method to find such a parameter has been derived by one of us (Yang, 1980, 1982). The smaller is Σ, the larger is the coincidence coefficient and the lower is the grain-boundary energy in most cases.

The CSL model for description of the structure is very closely related to unit-cell twinning (Andersson & Hyde, 1974) and we shall discuss it in § 4.

2. Building blocks

Twins with {111} composition lattice plane have the smallest $\Sigma = 3$. Such twinning is very common in metals, alloys, inorganic compounds and minerals. A cubic crystal includes at least three twofold axes in the ⟨100⟩ directions and four threefold axes in the ⟨111⟩ directions. If twinning occurs in one of the ⟨111⟩ directions, it will appear in the other three directions, therefore both a matrix and its twins have a T_d symmetry; we then call the matrix a T_d polyhedron. Consequently the T_d polyhedron and its twins are called building blocks.

2.1. *Symbol to describe a building block*

We can choose a rhombohedral unit cell with $a = Kd$ [d is the edge of a tetrahedron and equal to $(3/2)^{1/2}d_{111}$] and $\alpha = 60°$ from an f.c.c. lattice, as shown in Fig. 1 with $a = 2d$. A T_d polyhedron can be obtained by cutting the rhombohedron with two planes perpendicular to its long diagonal; the spacing between these planes is Kd_{111}. However, there are $(2K+1)$ ways to cut it and $(2K+1)$ different T_d polyhedra can be obtained. As shown in Fig. 1, for example, we can cut the rhombohedral unit cell at layers 0 and 2, at layers 1 and 3, 2 and 4, 3 and 5, 4 and 6, and denote the resulting polyhedra by symbols (2, 0), (2, 1), (2, 2), (2, 3), (2, 4). Generally, we use (K, L) to indicate a T_d polyhedron, where K means that the polyhedron has height Kd_{111} in the ⟨111⟩ direction, and L means that the polyhedron is obtained by cutting the rhombohedral unit cell at the Lth and the $(L+K)$th layers. Then we see that (K, L_1)

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0108-7681/87/010001-18$01.50

is equal to (K, L_2) but they have opposite orientations for $L_1 = K - i$, $L_2 = K + i$, $i = 0, 1, 2, \ldots, K$. For example, $(2, 1)$ as well as $(2, 3)$ are truncated tetrahedra; however, a hexagon of $(2, 1)$ is in the $[111]$ direction, and that of $(2, 3)$ is in $-[111]$. Now, one can easily see that $(1, 0)$ is a tetrahedron, $(1, 1)$ an octahedron, $(2, 0)$ the tetrahedron with edge $= 2d$, $(2, 2)$ the octahedron with edge $= 2d$ *etc.*

There exist twins with composition plane $\{111\}$ in a complicated c.c.p.-related crystal. One can use (K, L, P) to represent a (K, L) polyhedron with four twins of P atomic layers parallel to the $\{111\}$ lattice planes. We use (K, L, P, Q) or (K, L, P, Q, S) to denote a (K, L) polyhedron with second-order or third-order twins, where Q and S denote the numbers of the layers of the twins. Models of the building blocks $(1, 0), (1, 1), (2, 0), (2, 1), (2, 2), (2, 0, 1), (3, 0)$, $(1, 0, 1, 1, 1)$, $(1, 0, 1)$, $(1, 2, 1)$, $(1, 1, 1)$, $(1, 1, 1, 1)$, $(1, 1, 1, \bar{1}, 1)$, $(3, 0, 1)$, $(2, 1, 2)$, $(4, 1, 1)$, $(4, 5, 1)$, $(4, 3, 1)$ are shown in Figs. 2(*a*)–(*g*).

2.2. *Calculating the atomic positions of a building block*

2.2.1. *The formula for a (KL) polyhedron.* Let axes $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ of a cubic unit cell be transformed into $\mathbf{d}_1$, $\mathbf{d}_2$, $\mathbf{d}_3$ of a rhombohedral unit cell. Then

$$\mathbf{d}_1 = (3/2n)(\mathbf{a}_2 + \mathbf{a}_3) \qquad (2.2.1a)$$

$$\mathbf{d}_2 = (3/2n)(\mathbf{a}_3 + \mathbf{a}_1) \qquad (2.2.1b)$$

$$\mathbf{d}_3 = (3/2n)(\mathbf{a}_1 + \mathbf{a}_2) \qquad (2.2.1c)$$

where n is the number of atomic layers parallel to (111) from $[000]$ to $[111]$.

Consequently, we obtain

$$a = n(2^{1/2})d/3 \qquad \text{where } d = |\mathbf{d}_i|. \qquad (2.2.2)$$

This formula is a fundamental one in c.c.p.-related structures, and it was empirically derived earlier (Andersson, 1980).

In matrix notation, (2.2.1*a*) to (2.2.1*c*) can be combined as

$$\begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \end{pmatrix} = \frac{3}{2n} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}.$$

Let $m_1\mathbf{d}_1 + m_2\mathbf{d}_2 + m_3\mathbf{d}_3 = x\mathbf{a}_1 + y\mathbf{a}_2 + z\mathbf{a}_3$ where m_1, m_2, m_3 are integers; then

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{3}{2n} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix}.$$

This formula can be used to calculate all the coordinates of a (K, L) polyhedron by choosing suitable integers m_1, m_2, m_3. But, in this case, the centre of the (K, L) polyhedron does not coincide with the origin of the cubic unit cell. It would be better to put the center of the (K, L) polyhedron at the origin of the cubic unit cell. Translate the (K, L) polyhedron a distance $(K + L)(3/4)d(2/3)^{1/2}$ along the $-[111]$ direction, then we get

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{3}{4n} \begin{pmatrix} 0 & 2 & 2 & \bar{1} \\ 2 & 0 & 2 & \bar{1} \\ 2 & 2 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{pmatrix} \qquad (2.2.3a)$$

where

$$m_4 = K + L$$

$$0 \leq m_i \leq K \qquad i = 1, 2, 3$$

$$L \leq m_1 + m_2 + m_3 \leq m_4.$$

A Friauf polyhedron is different from a truncated tetrahedron. For a Friauf polyhedron, there is no atom at the center of hexagons, but there are atoms inside it and out from the hexagons. Therefore, m_i $(i = 1, 2, 3)$ have to satisfy more conditions to exclude the atoms at the center of the hexagons of a Friauf polyhedron, namely

$$m_1 + m_2 + m_3 = \begin{cases} \text{odd: } m_i \text{ not all odd} \\ \text{even: } m_i \text{ all even.} \end{cases}$$

Thus 111, 311, 511, 331, ... are forbidden number groups by the first condition and 013, 123, ... violate the second condition, while 002, 024, ... are permitted number groups.

However, in order to include the atomic coordinates at the center of a Friauf polyhedron and outside the hexagons of a Friauf polyhedron, we have to choose $m_i (i = 1, 2, 3) =$ odd first, and then calculate x, y, z from (2.2.3*a*); then

$$(x_1' \, y_1' \, z_1') = (x \, y \, z) + \left(\frac{3}{4n} \, \frac{3}{4n} \, \frac{3}{4n}\right) \qquad (2.2.3b)$$

$$(x_2' \, y_2' \, z_2') = (x \, y \, z) - \left(\frac{3}{4n} \, \frac{3}{4n} \, \frac{3}{4n}\right) \qquad (2.2.3c)$$

are coordinates of the center of a Friauf polyhedron and outside the hexagons of a Friauf polyhedron.

All these conditions are obtained by an inductive method.

2.2.2. *The formula for a twin part of a building block.* Let a cubic crystal be reflected by the (111) lattice

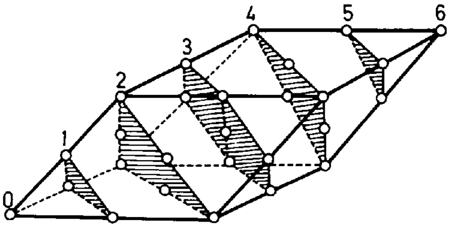


Fig. 1. Construction of T_d polyhedra.

plane through the origin; then

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 1 & \bar{2} & \bar{2} \\ \bar{2} & 1 & \bar{2} \\ \bar{2} & \bar{2} & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad (2.2.4)$$

where xyz are the coordinates of the matrix, and XYZ are those of the twin (Grimmer, Bollmann & Warrington, 1974).

If the mirror plane (111) is translated $(K+L)\times(1/4)(2/3)^{1/2}d$ along the [111] direction, then

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \frac{1}{4n}\begin{pmatrix} \bar{8} & \bar{2} & \bar{2} & 5 \\ \bar{2} & \bar{8} & \bar{2} & 5 \\ \bar{2} & \bar{2} & \bar{8} & 5 \end{pmatrix}\begin{pmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{pmatrix} \qquad (2.2.5)$$

where

$$m_4 = K + L$$

$$0 \le m_i (i = 1, 2, 3) \le K$$

$$m_4 - P \le m_1 + m_2 + m_3 \le m_4 - 1.$$

If $P = 1$ then $m_1 + m_2 + m_3 = m_4 - 1$. Usually, $P = 1$.

For a Friauf polyhedron, $m_i(i = 1, 2, 3)$ in (2.2.5) have to satisfy more conditions which are exactly the same as for (2.2.3a).

The formula for a crystal is as follows:

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \frac{3U_i}{4n}\begin{pmatrix} 0 & 2 & 2 & \bar{1} \\ 2 & 0 & 2 & \bar{1} \\ 2 & 2 & 0 & \bar{1} \end{pmatrix}\begin{pmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{pmatrix} + \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} \qquad (2.2.6)$$

for a (K, L) polyhedron, and

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \frac{U_i}{4n}\begin{pmatrix} \bar{8} & \bar{2} & \bar{2} & 5 \\ \bar{2} & \bar{8} & \bar{2} & 5 \\ \bar{2} & \bar{2} & \bar{8} & 5 \end{pmatrix}\begin{pmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{pmatrix} + \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} \qquad (2.2.7)$$

for the twin part of the building block, where $x_0y_0z_0$ are coordinates of the center of a building block in a crystal and U_i is a symmetry matrix $(i = 1, 2, 3, 4)$, with

$$U_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad U_2 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix},$$

$$U_3 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}, \qquad U_4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

U_i and $x_0y_0z_0$ depend on the space group, and are given in Table 1. $(x_0y_0z_0)$ is the complex with 23 or $43m$ symmetry.

We can conclude from Table 1 that:

1. All of the space groups in Table 1 include 23 or $\bar{4}3m$ symmetry.

2. The space groups $P23$, $I23$, $Pn3$, $P4_232$, $P\bar{4}3n$, $P\bar{4}3m$, $I\bar{4}3m$ and $Pn3m$ contain two building blocks, which are located around (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The space groups $P23$, $I23$ and $I\bar{4}3m$ have the same $x_0y_0z_0$ and U_i, but their building blocks differ. Two building blocks of $P23$ are independent and different from each other; however, those of $I23$ are the same. The $x_0y_0z_0$ and U_i of $I23$ and $I\bar{4}3m$ look exactly the same, but $I23$ is one of the subgroups of $I\bar{4}3m$. The building blocks of $I\bar{4}3m$ have higher symmetry than that of $I23$. A similar relationship exists between space groups $Pn3$ and $Pn3m$.

3. $Fm3$, $F432$ and $Fm3m$ consist of eight building blocks. $Fm3$ is a subgroup of $Fm3m$ although they have the same U_i and $x_0y_0z_0$.

4. The space groups $Fd3$, $F4_132$, $F\bar{4}3c$ and $Fd3m$ consist of 16 building blocks in two different types. $Fd3$ and $Fd3m$ have the same U_i and $x_0y_0z_0$, but $Fd3$ is a subgroup of $Fd3m$.

5. The space groups $F23$ and $F\bar{4}3m$ consist of 16 building blocks in four different types; $F23$ is a subgroup of $F\bar{4}3m$.

6. A group and its subgroup can consist of the same building blocks. In that case, the supergroup probably consists of homogeneous atoms and the subgroup of heterogeneous atoms, or a small atomic displacement occurs in the subgroup. All the group-subgroup relationships have been given in Fig. 3.

7. The space groups in Table 1 are divided into two types. Group type II can accommodate all of the building blocks; however, group type I can accommodate only building blocks which have special positions such as $x00$, $xx0$, xxx, xxz, and cannot accommodate the coordinates xyz. If group type I includes general positions xyz, they must have other positions xzy at the same time, which is not given in Table 2.

2.3. *The coordinates of a building block*

All of the coordinates of a building block are given in Table 2. Since n in (2.2.3a,b,c) and (2.2.5) depends on the crystal structures, we give only $4nx$, $4ny$, $4nz$ and $4nX$, $4nY$, $4nZ$ $(t_1t_2t_3)$, which are independent of the crystal structure. The coordinates in Table 2 have to be divided by $4n$ when the coordinates of the atoms in a crystal are calculated. Table 2 only gives the coordinates of building blocks which appear very often in a crystal. For simplicity, we assume that a building block has the following symmetry elements:

$$\begin{array}{llllll} xyz & yzx & zxy & xzy & zyx & yxz \\ x\bar{y}\bar{z} & y\bar{z}\bar{x} & z\bar{x}\bar{y} & x\bar{z}\bar{y} & z\bar{y}\bar{x} & y\bar{x}\bar{z} \\ \bar{x}y\bar{z} & \bar{y}z\bar{x} & \bar{z}x\bar{y} & \bar{x}z\bar{y} & \bar{z}y\bar{x} & \bar{y}x\bar{z} \\ \bar{x}\bar{y}z & \bar{y}\bar{z}x & \bar{z}\bar{x}y & \bar{x}\bar{z}y & \bar{z}\bar{y}x & \bar{y}\bar{x}z. \end{array}$$

Only independent coordinates are given in Table 2.

Table 1. U_i *and* $x_0y_0z_0$ *for* 17 *space groups*

Space group	Space group type	Number of complex sets	Complex 1 matrix	Complex 2 matrix	Complex 3 matrix	Complex 4 matrix	Remarks
$P23$	I	2	000 U_1	½½½ U_1			
$F23$	I	4	000 0½½ ½0½ ½½0 U_1	¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ U_1	½½½ ½00 0½0 00½ U_1	¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1	
$I23$	I	1	000 ½½½ U_1				
$Pn3$	I	1	000 ½½½ U_1 U_2				
$Fm3$	I	1	¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ ¾¾¾ ¼¼¾ ¼¾¼ ¾¼¼ U_1 U_2				Origin at 23
$Fd3$	I	2	000 0½½ ½0½ ½½0 ¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ U_1 U_2	½½½ ½00 0½0 00½ ¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1 U_2			Origin at 23
$P4_232$	I	1	000 ½½½ U_1 U_3				
$F432$	I	1	¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ ¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1 U_3				
$F4_132$	I	2	000 0½½ ½0½ ½½0 ¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ U_1 U_3	½½½ ½00 0½0 00½ ¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1 U_3			
$P\bar{4}3n$	I	1	000 ½½½ U_1 U_4				
$F\bar{4}3c$	I	2	000 0½½ ½0½ ½½0 ½½½ ½00 0½0 00½ U_1 U_4	¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ ¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1 U_4			
$P\bar{4}3m$	II	2	000 U_1	½½½ U_1			
$F\bar{4}3m$	II	4	000 0½½ ½0½ ½½0 U_1	¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ U_1	½½½ ½00 0½0 00½ U_1	¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1	
$I\bar{4}3m$	II	1	000 ½½½ U_1 U_1				
$Pn3m$	II	1	000 ½½½ U_1 U_2				
$Fm3m$	II	1	¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ ¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1 U_2				
$Fd3m$	II	2	000 0½½ ½0½ ½½0 ¼¼¼ ¼¾¾ ¾¼¾ ¾¾¼ U_1 U_2	½½½ ½00 0½0 00½ ¾¾¾ ¾¼¼ ¼¾¼ ¼¼¾ U_1 U_2			Origin at $\bar{4}3m$

The group type I does not have such high symmetry. Its symmetry elements are only the left half of the group type II. There is no difference between the two types of space groups for the positions such as $x00$, $xx0$, xxx, xxz. It can be seen that most of the building blocks in Table 2 satisfy this except the building blocks $(2,2,1)$, $(4,3,1)$, $(4,5,1)$, $(4,7,1)$ and $(2,0,1,\bar{1},1)$. Coordinates such as xyz of a building block have to be divided into xyz and xzy in group type I as mentioned in § 2.2.2.

The coordinates of the building blocks $(1,1,1,1)$, $(1,0,1,1)$ $(1,0,1,1,1)$ having higher-order twins cannot be calculated by (2.2.3*a*) and (2.2.5) and we have to use other formulae which are much more complicated than (2.2.3*a*) and (2.2.5). This is not described in this paper.

The coordinates of the second-order twin of the building block $(1,0,1,1)$ would be $(1/3\ 1/3\ 31/3)$, according to the rigorous second-order twinning formula if the factor $1/4n$ is omitted. The coordinates $(\bar{1}/3\ \bar{1}/3\ 31/3)$ can be obtained from $(1/3\ 1/3\ 31/3)$ in terms of symmetry operations. These two positions of $(\bar{1}/3\ \bar{1}/3\ 31/3)$ and $(1/3\ 1/3\ 31/3)$ are very close together. The distance between them is 0·9428 which is much shorter than the edge (8·485) of a tetrahedron, namely 11% of a tetrahedron edge. The average of the coordinates of these two positions is $(0\ 0\ 31/3)$ which is very close to the coordinates $(0\ 0\ 31{\cdot}045/3)$ of the vertex of the capped triangle (Nyman & Andersson, 1979) on the edge of the central tetrahedron of a *stella quadrangula*.

In common with the building block $(1,0,1,1)$, the coordinates $(80/9\ 80/9\ \overline{13}/9)$ of a building block $(1,0,1,1,1)$, which are very close to the coordinates $(80{\cdot}091/9\ 80{\cdot}091/9\ 13{\cdot}045/9)$ of the vertex of the capped triangle on the edge of the outer tetrahedron of a *stella quadrangula*, are the average of the coordinates $(77/9\ 83/9\ \overline{13}/9)$ and $(83/9\ 77/9\ \overline{13}/9)$ which are calculated by the formula of the third-order twin. Similarly, the coordinates $(9/3\ 9/3\ \overline{40}/3)$ are the average of $(8/3\ 10/3\ \overline{40}/3)$ and $(10/3\ 8/3\ \overline{40}/3)$. Stereoview pictures of the building blocks $(1,0,1,1,1)$ are given in Figs. 4(*a*) and (*b*). It can be seen that some pairs of atoms of the second- or third-order twins are so close together that they have to be replaced by one atom at the middle of these two atoms. Now, we can easily realize that, in fact, a building block $(1,0,1)$ is a *stella quadrangula*; $(1,0,1,1)$ the triangular capping of a *stella quadrangula*; $(1,0,1,1,1)$ a double triangular capping, and $(1,1,1,1)$ an octahedral capping pyrochlore unit (Andersson, 1978). All of the twins of building blocks in Table 2 share atoms in the (111), $(1\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, $(\bar{1}\bar{1}1)$ lattice planes with a central T_d polyhedron. Of

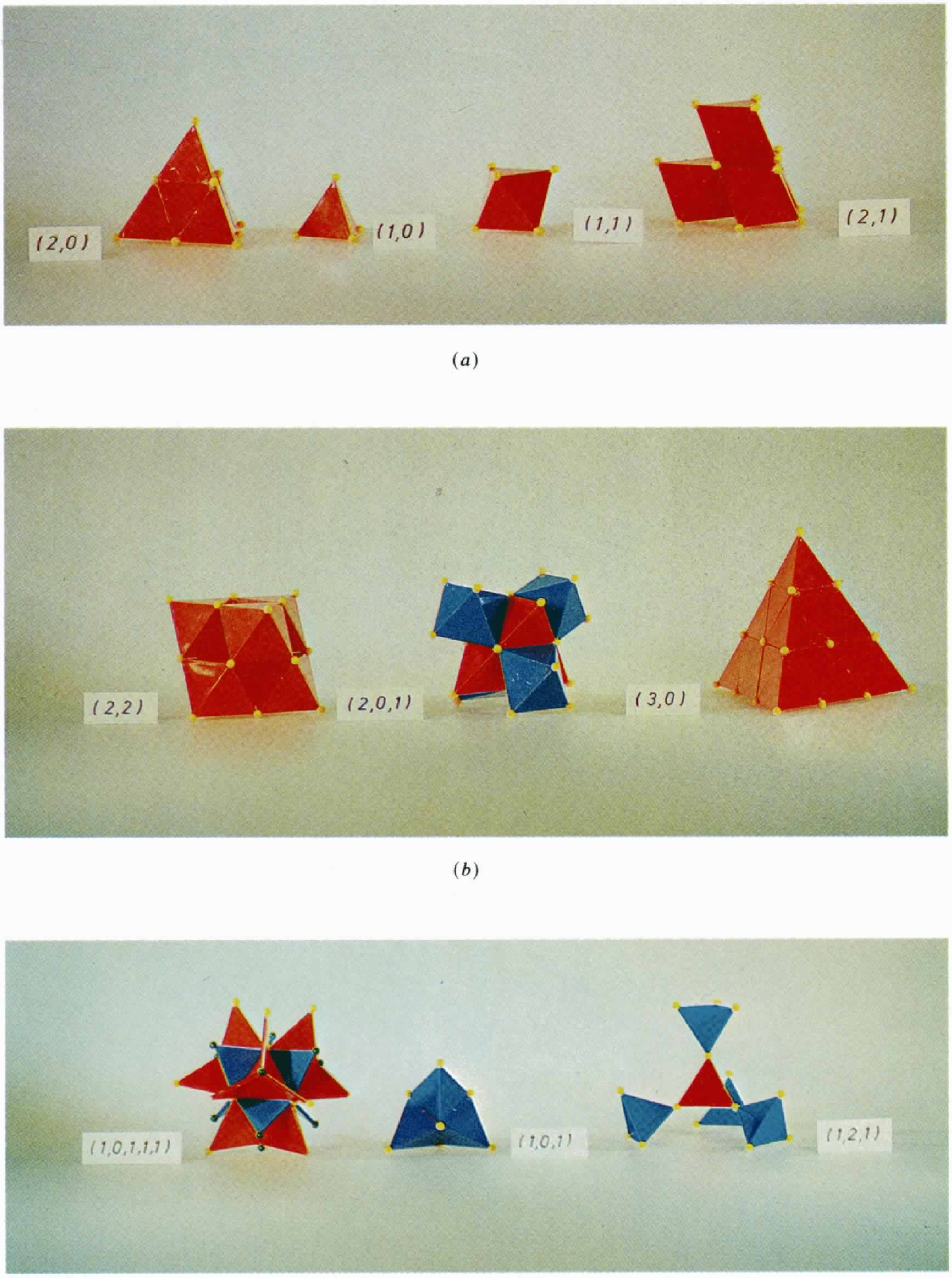
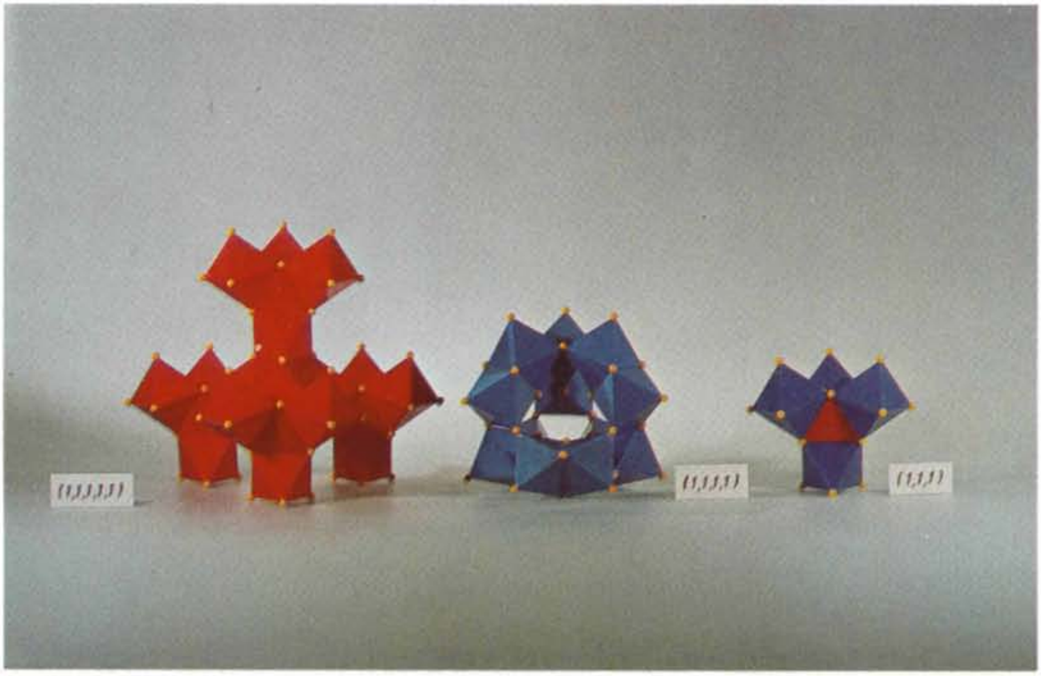
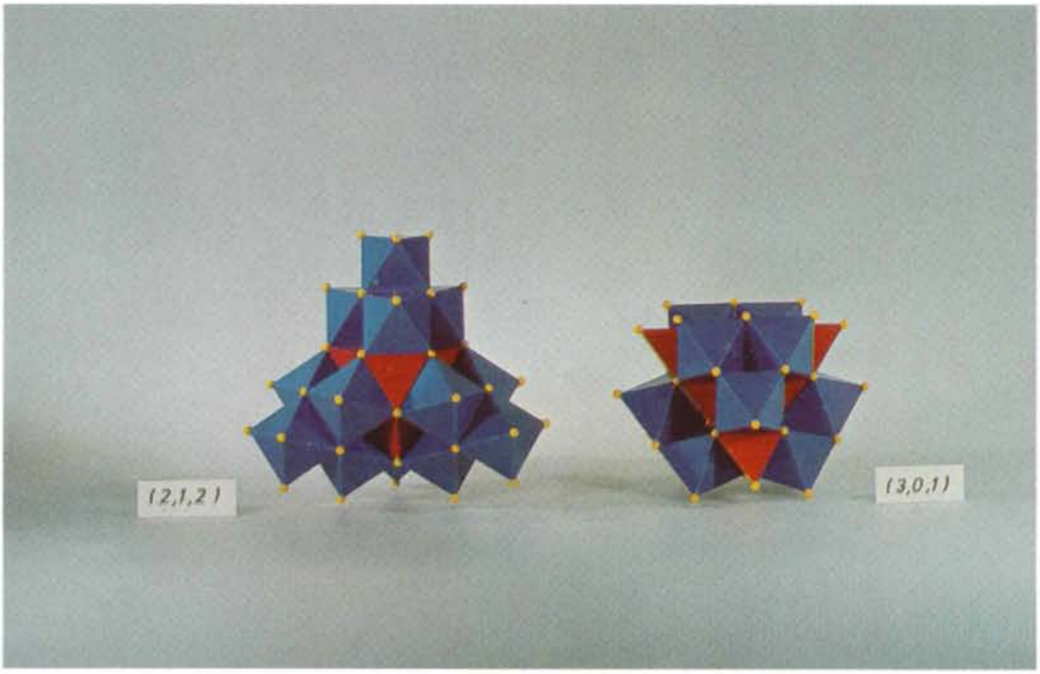


Fig. 2. (*a*)–(*g*) Models of building blocks used to describe c.c.p.-related structures.

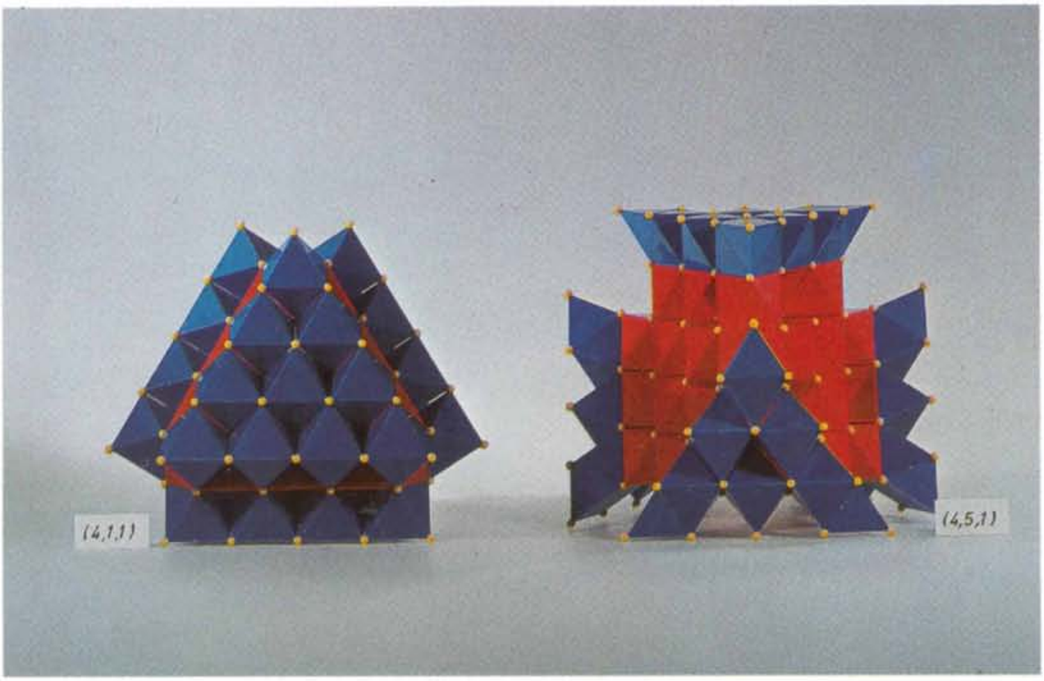


(*d*)



(*e*)

Fig. 2 (*cont.*) (*d*) (*e*)



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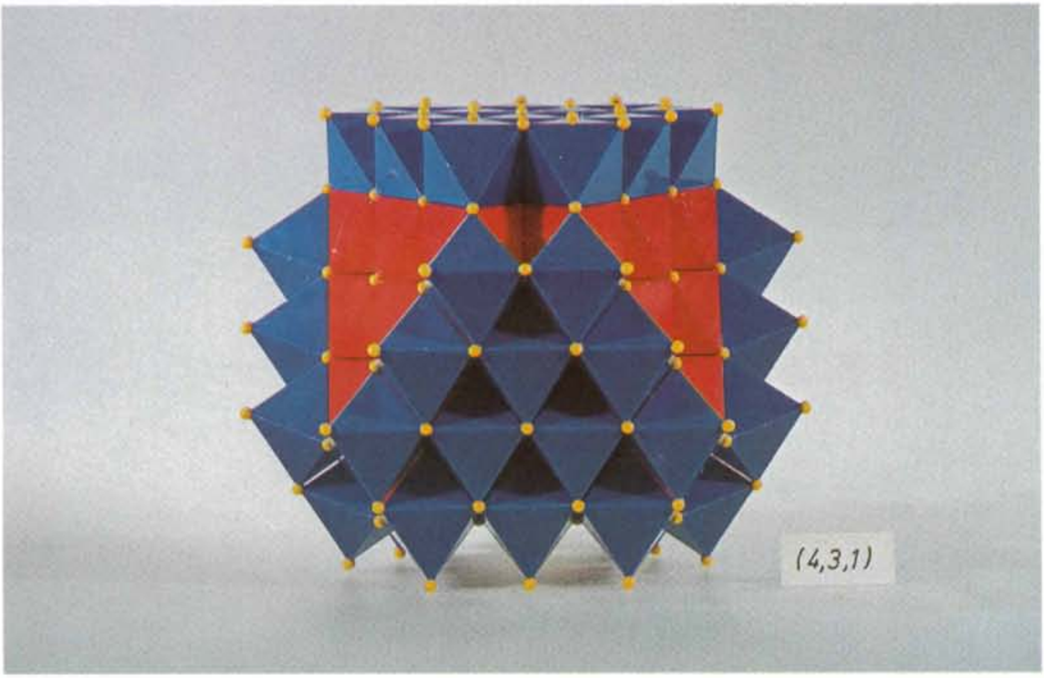


(*g*)

Fig. 2 (*cont.*) (*f*) (*g*)

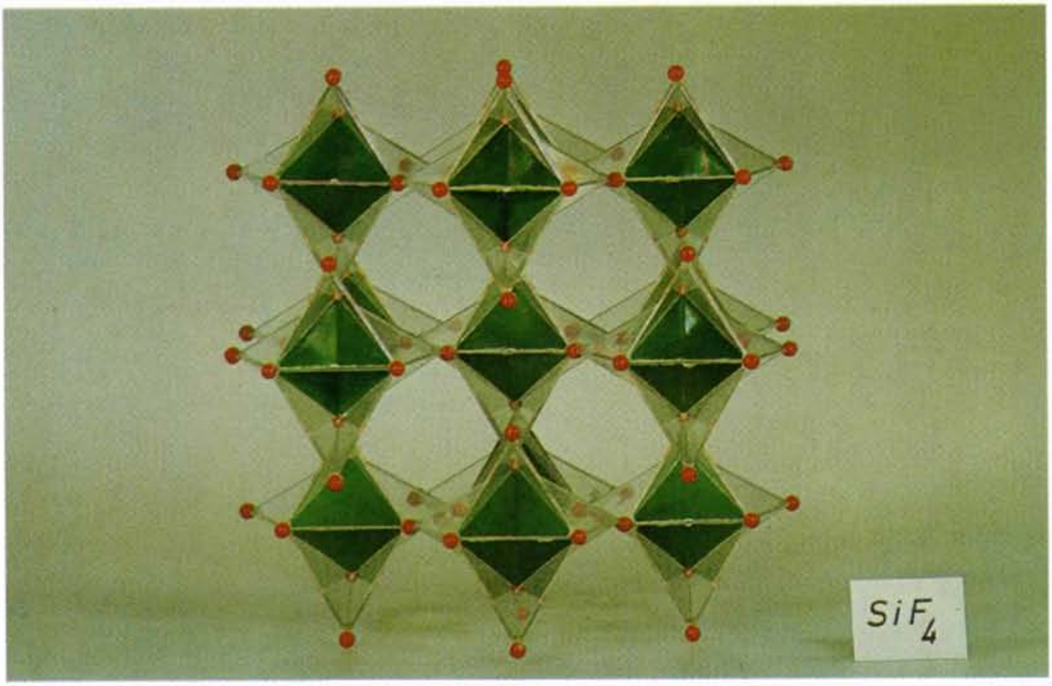


Fig. 5. The structure of SiF_4.

Table 2. *The coordinates of building blocks*

Building block	$m_1m_2m_3$ and coordinates ($t_1t_2t_3$) ($t_1=4nx$ or $4nX$, $t_2=4ny$ or $4nY$, $t_3=4nz$ or $4nZ$)										
(0,0)	$m_1m_2m_3$	0 0 0									
	$t_1t_2t_3$	0 0 0									
(1,0)	$m_1m_2m_3$	0 0 0									
	$t_1t_2t_3$	$\bar{3}\ \bar{3}\ \bar{3}$									
(1,0,1)	$m_1m_2m_3$	0 0 0	0 0 0*								
	$t_1t_2t_3$	$\bar{3}\ \bar{3}\ \bar{3}$	5 5 5								
(1,1)	$m_1m_2m_3$	1 1 0									
	$t_1t_2t_3$	0 0 6									
(1,1,1)	$m_1m_2m_3$	1 1 0	0 0 1*								
	$t_1t_2t_3$	0 0 6	8 8 2								
(1,2)	$m_1m_2m_3$	1 1 1									
	$t_1t_2t_3$	3 3 3									
(1,2,1)	$m_1m_2m_3$	1 1 1	1 1 0*								
	$t_1t_2t_3$	3 3 3	5 5 11								
(2,0)	$m_1m_2m_3$	0 0 0	1 1 0								
	$t_1t_2t_3$	$\bar{6}\ \bar{6}\ \bar{6}$	0 0 6								
(2,0,1)	$m_1m_2m_3$	0 0 0	1 1 0	0 0 1*							
	$t_1t_2t_3$	$\bar{6}\ \bar{6}\ \bar{6}$	0 0 6	8 8 2							
(2,1)	$m_1m_2m_3$	1 1 1	0 0 2								
	$t_1t_2t_3$	3 3 3	$3\ 3\ \bar{9}$								
(2,1,1)	$m_1m_2m_3$	1 1 1	0 0 2	1 1 0*	0 0 2*						
	$t_1t_2t_3$	3 3 3	$3\ 3\ \bar{9}$	5 5 11	$11\ 11\ \bar{1}$						
(2,1,2)	$m_1m_2m_3$	1 1 1	0 0 2	1 1 0*	0 0 2*	1 0 0*					
	$t_1t_2t_3$	3 3 3	$3\ 3\ \bar{9}$	5 5 11	$11\ 11\ \bar{1}$	7 13 13					
(2,2)	$m_1m_2m_3$	1 1 1	2 1 1	2 2 0							
	$t_1t_2t_3$	0 0 0	0 6 6	0 0 12							
(2,2,1)	$m_1m_2m_3$	1 1 1	3 1 1	2 2 0	1 1 1*	2 1 0*					
	$t_1t_2t_3$	0 0 0	0 6 6	0 0 12	8 8 8	2 8 14					
(2,3)	$m_1m_2m_3$	1 1 1	2 2 1								
	$t_1t_2t_3$	$\bar{3}\ \bar{3}\ \bar{3}$	3 3 9								
(2,3,1)	$m_1m_2m_3$	1 1 1	2 2 1	2 2 0*	1 1 2*						
	$t_1t_2t_3$	$\bar{3}\ \bar{3}\ \bar{3}$	3 3 9	5 5 17	11 11 5						
(2,4)	$m_1m_2m_3$	2 2 2	2 2 1								
	$t_1t_2t_3$	6 6 6	0 0 6								
(2,4,1)	$m_1m_2m_3$	2 2 2	2 2 1	2 2 1*							
	$t_1t_2t_3$	6 6 6	0 0 6	8 8 14							
(3,0)	$m_1m_2m_3$	0 0 0	0 0 2	1 1 1							
	$t_1t_2t_3$	$\bar{9}\ \bar{9}\ \bar{9}$	$3\ 3\ \bar{9}$	3 3 3							
(3,0,1)	$m_1m_2m_3$	0 0 0	0 0 2	1 1 1	1 1 0*	0 0 2*					
	$t_1t_2t_3$	$\bar{9}\ \bar{9}\ \bar{9}$	$3\ 3\ \bar{9}$	3 3 3	5 5 11	$11\ 11\ \bar{1}$					

Building block	$m_1m_2m_3$ and coordinates ($t_1t_2t_3$) ($t_1=4nx$ or $4nX$, $t_2=4ny$ or $4nY$, $t_3=4nz$ or $4nZ$)											
(4,1)F	$m_1m_2m_3$	0 0 4	0 0 3	2 2 1	$1\ 1\ 1^+$	$1\ 1\ 1^-$						
	$t_1t_2t_3$	$9\ 9\ \overline{15}$	$3\ 3\ \overline{15}$	3 3 9	0 0 0	$\bar{6}\ \bar{6}\ \bar{6}$						
(4,1,1)F	$m_1m_2m_3$	0 0 4	0 0 3	2 2 1	$1\ 1\ 1^+$	$1\ 1\ 1^-$	1 1 1*	1 1 3*	2 2 0*	0 0 4*		
	$t_1t_2t_3$	$9\ 9\ \overline{15}$	$3\ 3\ \overline{15}$	3 3 9	0 0 0	$\bar{6}\ \bar{6}\ \bar{6}$	10 10 10	12 12 0	5 5 17	$17\ 17\ \bar{7}$		
(4,3)F	$m_1m_2m_3$	0 0 4	1 0 4	2 2 3	2 2 2	1 1 1	3 3 1					
	$t_1t_2t_3$	$3\ 3\ \overline{21}$	$3\ 9\ \overline{15}$	9 9 3	3 3 3	$\bar{6}\ \bar{6}\ \bar{6}$	0 0 12					
(4,3,1)F	$m_1m_2m_3$	0 0 4	1 0 4	2 2 3	2 2 2	1 1 1	3 3 1	0 2 4*	2 2 2*	3 3 1*	$1\ 1\ 1^+$	
	$t_1t_2t_3$	$3\ 3\ \overline{21}$	$3\ 9\ \overline{15}$	9 9 3	3 3 3	$\bar{6}\ \bar{6}\ \bar{6}$	0 0 12	$23\ 11\ \bar{1}$	11 11 11	6 6 18	$\overline{12}\ \overline{12}\ \overline{12}$	$18\ 18\ \bar{6}$
(4,5)F	$m_1m_2m_3$	1 3 3	3 3 3	2 2 2	2 2 4	4 4 1	4 3 2					
	$t_1t_2t_3$	12 0 0	6 6 6	$\bar{3}\ \bar{3}\ \bar{3}$	$9\ 9\ \bar{3}$	3 3 21	3 9 15					
(4,5,1)F	$m_1m_2m_3$	1 3 3	3 3 3	2 2 2	2 2 4	4 4 1	4 3 2	4 4 0*	2 2 4*	3 3 3*	$3\ 3\ 1^+$	
	$t_1t_2t_3$	12 0 0	6 6 6	$\bar{3}\ \bar{3}\ \bar{3}$	$9\ 9\ \bar{3}$	3 3 21	3 9 15	5 5 29	17 17 5	12 12 12	10 10 22	
(4,7)F	$m_1m_2m_3$	1 1 1	3 3 3	2 2 4	4 4 2	4 4 3						
	$t_1t_2t_3$	0 0 0	6 6 6	$3\ 3\ \bar{9}$	3 3 15	9 9 15						
(4,7,1)F	$m_1m_2m_3$	1 1 1	3 3 3	2 2 4	4 4 2	4 4 3	4 4 2*					
	$t_1t_2t_3$	0 0 0	6 6 6	$3\ 3\ \bar{9}$	3 3 15	9 9 15	11 11 23					
(5,0)F	$m_1m_2m_3$	0 0 0	0 0 4	0 0 3	2 2 1	$1\ 1\ 1^+$	$1\ 1\ 1^-$					
	$t_1t_2t_3$	$\overline{15}\ \overline{15}\ \overline{15}$	$9\ 9\ \overline{15}$	$3\ 3\ \overline{15}$	3 3 9	0 0 0	$\bar{6}\ \bar{6}\ \bar{6}$					
(5,0,1)F	$m_1m_2m_3$	0 0 0	0 0 4	0 0 3	2 2 1	$1\ 1\ 1^+$	$1\ 1\ 1^-$	1 1 1*	1 1 3*	2 2 0*	0 0 4*	
	$t_1t_2t_3$	$\overline{15}\ \overline{15}\ \overline{15}$	$9\ 9\ \overline{15}$	$3\ 3\ \overline{15}$	3 3 9	0 0 0	$\bar{6}\ \bar{6}\ \bar{6}$	10 10 10	12 12 0	5 5 17	$17\ 17\ \bar{7}$	
(1,0,1,1)	$m_1m_2m_3$	0 0 0	0 0 0*	0 0 0**								
	$t_1t_2t_3$	$\bar{3}\ \bar{3}\ \bar{3}$	5 5 5	0 0 31/3								
(1,1,1,1)	$m_1m_2m_3$	1 1 0	0 0 1*	0 0 1**	0 1 0**							
	$t_1t_2t_3$	0 0 6	8 8 2	$\frac{16}{3}\ \frac{16}{3}\ \frac{46}{3}$	$\frac{9}{3}\ \frac{9}{3}\ \frac{\overline{40}}{3}$							
(2,0,1,1)	$m_1m_2m_3$	0 0 0	1 1 0	0 0 1*	0 0 1**	0 1 0**						
	$t_1t_2t_3$	$\bar{6}\ \bar{6}\ \bar{6}$	0 0 6	8 8 2	$\frac{16}{3}\ \frac{16}{3}\ \frac{46}{3}$	$\frac{9}{3}\ \frac{9}{3}\ \frac{\overline{40}}{3}$						
(2,0,1,$\bar{1}$,1)	$m_1m_2m_3$	0 0 0	1 1 0	0 0 1*								
	$t_1t_2t_3$	$\bar{6}\ \bar{6}\ \bar{6}$	0 0 6	8 8 2	2 2 14	0 10 16	8 8 14	16 16 6	14 14 14			
(1,0,1,1,1)	$m_1m_2m_3$	0 0 0	0 0 0*	0 0 0**	0 0 0	***						
	$t_1t_2t_3$	$\bar{3}\ \bar{3}\ \bar{3}$	5 5 5	$0\ 0\ \frac{31}{3}$	$\frac{80}{9}\ \frac{80}{9}\ \frac{13}{9}$							
(2,5)F	$m_1m_2m_3$	$1\ 1\ 1^+$	$1\ 1\ 1^-$	0 0 2								
	$t_1t_2t_3$	0 0 0	6 6 6	$3\ 3\ \bar{9}$								
(2,3)F	$m_1m_2m_3$	$1\ 1\ 1^+$	$1\ 1\ 1^-$	2 2 1								
	$t_1t_2t_3$	0 0 0	$\bar{6}\ \bar{6}\ \bar{6}$	3 3 9								
(2,1,2)F	$m_1m_2m_3$	$1\ 1\ 1^+$	$1\ 1\ 1^-$	0 0 2	0 0 2*	0 0 1*						
	$t_1t_2t_3$	0 0 0	$\bar{6}\ \bar{6}\ \bar{6}$	$3\ 3\ \bar{9}$	$11\ 11\ \bar{1}$	13 13 7						
(3,3,1)	$m_1m_2m_3$	1 2 2	0 3 3	1 2 3	2 2 2	1 1 1						
	$t_1t_2t_3$	6 0 0	18 0 0	12 6 0	6 6 6	$\bar{6}\ \bar{6}\ \bar{6}$						

course, the twins of a building block can share atoms in the $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$ lattice planes with a T_d polyhedron as well. We use (K, L, P, Q, S) to denote the former, $-(K, L, P, Q, S)$ the latter. The coordinates of the building block $-(K, L, P, Q, S)$ are just the negative of the (K, L, P, Q, S) coordinates so that we do not show them in Table 2. The building block $(K, L, P, \bar{Q}, S)$ means that the twinning plane of the twin P is the (111) lattice plane and that of the twin Q is $-(111)$, so that the orientation of the twin Q is the same as that of the central T_d polyhedron.

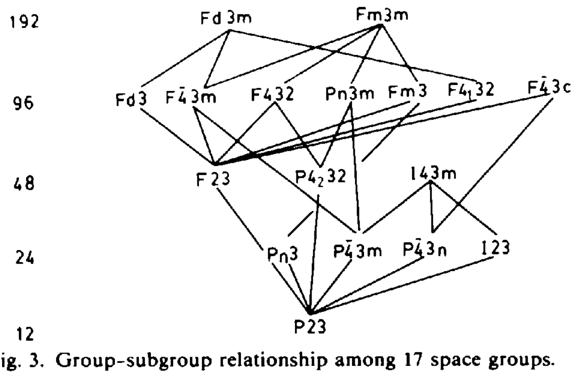


Fig. 3. Group-subgroup relationship among 17 space groups.

Those with the letter F consist of Friauf polyhedra. The symbol * means first-order twin; ** second; *** third. 111^+ and 111^- means that $t_1t_2t_3$ $(4nx'_1, 4ny'_1, 4nz'_1$ or $4nx'_2, 4ny'_2, 4nz'_2)$ are calculated by (2.2.3b) and (2.2.3c) respectively.

3. The description of a c.c.p.-related structure in terms of a building block

3.1. SiF_4

SiF_4 is cubic, space group $I\bar{4}3m$, $a = 5{\cdot}41$ Å. It was shown in Table 1 that a crystal of $I\bar{4}3m$ includes two building blocks of the same type; one is around (000), the other around $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$.

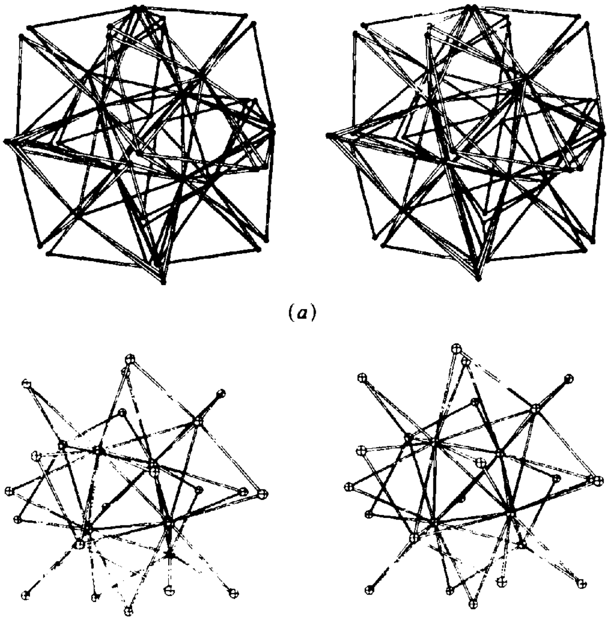
Table 3. SiF_4, *cubic*, $a = 5{\cdot}41$ Å, *space group* $I\bar{4}3m$

Atomic	Experimental coordinates			Calculated coordinates			Calculated				Building block				
position	x	y	z	x	y	z	t_1	t_2	t_3	$m_1\ m_2\ m_3$	symbol	n	U	$x_0\ y_0\ z_0$	Δd (Å)
2 Si in (a)	0	0	0												
8 F in (a)	0·17	0·17	0·17	0·1875	0·1875	0·1875	−5	−5	−5	0 0 0*	−(1, 0, 1)	4	U_1	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$	0·164
							3	3	3	0 0 0	−(1, 0, 1)	4	U_1	0 0 0	

Table 4. α-Mn, *cubic*, $a = 8{\cdot}89$ Å, *space group* $I\bar{4}3m$

Atomic	Experimental coordinates			Calculated coordinates			Calculated				Building block				
position	x	y	z	x	y	z	t_1	t_2	t_3	$m_1\ m_2\ m_3$	symbol	n	U	$x_0\ y_0\ z_0$	Δd (Å)
2 Mn(1) in 2(a)	0	0	0	0	0	0	0	0	0	1 1 1	−(2, 1, 2)F	8	U_1	0 0 0	0·000
8 Mn(2) in 8(c)	0·31787	0·31787	0·31787	0·31250	0·31250	0·31250	$\bar{6}$	$\bar{6}$	$\bar{6}$	1 1 1	−(2, 1, 2)F	8	U_1	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$	0·083
24 Mn(3) in 24$(g)_1$	0·35706	0·35706	0·03457	0·34375	0·34375	0·03125	11	11	1	0 0 2*	−(2, 1, 2)F	8	U_1	0 0 0	0·170
24 Mn(4) in 24$(g)_2$	0·08958	0·08958	0·28194	0·09375	0·09375	0·28125	$\overline{13}$	$\overline{13}$	$\bar{7}$	0 0 1*	−(2, 1, 2)F	8	U_1	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$	0·053
							3	3	9	0 0 2	−(2, 1, 2)F	8	U_1	0 0 0	

SiF_4 consists of two −(1, 0, 1) building blocks as shown in Table 3. The Si atom is located at the center of the central tetrahedron of the −(1, 0, 1) building block forming a strong Si-F bond, bringing the F atoms closer together so that the edge of a central tetrahedron is shorter than that of the outer ones. The edge of a central tetrahedron is 2·601 Å, and that of the outer ones is 2·969 Å. The building block around (000) shares an atom with that around $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, *i.e.* the atom at the vertex of an outer tetrahedron of −(1, 0, 1) at (000) belongs to the central tetrahedron of −(1, 0, 1) at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The deviation of the calculated atomic positions from the experimentally determined positions is 0·164 Å. The average F-F distance is 2·869 Å. The average percentage of the atomic deviation (APAD), $\Delta d/d$, is 5·7. The structure is shown in Fig. 5.


(*a*)

(*b*)

Fig. 4. (*a*) Stereoview of building block (1, 0, 1, 1, 1). (*b*) Stereoview of building block in γ-brass.

3.2. α-Mn

α-Mn (Oberteuffer & Ibers, 1970) is cubic, $a = 8{\cdot}89$ Å, space group $I\bar{4}3m$. It can be seen from Table 4 that the building blocks located at (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ are −(2, 1, 2). They each share three atoms, whose coordinates are (0·08958 0·08958 0·28194), (0·08959 0·28194 0·08958) and (0·28194 0·08958 0·08958). The deviation of the positions 8(c), 24$(g)_1$, 24$(g)_2$ from the experimental positions are 0·083, 0·170 and 0·053 Å respectively. The average interatomic distance of Mn is 2·3573 Å. The APAD of α-Mn is 4·4. This description of α-Mn in terms of a −(2, 1, 2) building block is quite accurate and is the same as used by Samson (1964).

3.3. γ-*Brass*

γ-Brass (Brandon, Brizard, Chieh, McMillan & Pearson, 1974) is cubic, $a = 8{\cdot}878$ Å, space group $I\bar{4}3m$. Bradley & Jones (1933) have described γ-brass in terms of clusters, each containing 26 atoms. Nyman & Andersson (1979) have described it as doubly triangle-capped *stella quadrangula*. From Table 5, one can find that γ-brass consists of two building blocks −(1, 0, 1, 1, 1) located around (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. In fact, three different descriptions lead to the same result. However, it seems that the method in terms of the building block −(1, 0, 1, 1, 1) has more relationships with other structures and building blocks and it is physically more meaningful. The APAD of γ-brass is 4·2. A model of the structure is shown in Nyman & Andersson's (1979) paper, using the same building block unit (1, 0, 1, 1, 1).

3.4. Fe_3W_3C

Fe_3W_3C (Bojarski & Leciejewicz, 1967) is cubic, $a = 11{\cdot}087$ Å, space group $Fd3m$. The crystal of this

Table 5. *γ-Brass* (Cu_5Zn_8), *cubic*, $a = 8{\cdot}878$ Å, *space group* $I\bar{4}3m$

Atomic	Experimental coordinates			Calculated coordinates			Calculated				Building block				
position	x	y	z	x	y	z	t_1	t_2	t_3	$m_1\ m_2\ m_3$	symbol	n	U	$x_0\ y_0\ z_0$	Δd (Å)
IT 8(*c*) (*xxx*)	0·1089	0·1089	0·1089	0·1071	0·1071	0·1071	3	3	3	0 0 0	−(1, 0, 1, 1, 1)	7	U_1	0 0 0	0·0277
OT 8(*c*) (*xxx*)	−0·1720	−0·1720	−0·1720	−0·1786	−0·1786	−0·1786	$\bar{5}$	$\bar{5}$	$\bar{5}$	0 0 0*	−(1, 0, 1, 1, 1)	7	U_1	0 0 0	0·1015
OH 12(*e*) (*x*00)	0·3558	0	0	0·3690	0	0	31/3	0	0	0 0 0**	−(1, 0, 1, 1, 1)	7	U_1	0 0 0	0·1172
CO 24(*g*) (*xxz*)	0·3128	0·3128	0·0366	0·3175	0·3175	0·0516	80/9	80/9	13/9	0 0 0***	−(1, 0, 1, 1, 1)	7	U_1	0 0 0	0·1457

Table 6. Fe_3W_3C, *cubic*, $a = 11{\cdot}087$ Å, *space group* $Fd3m$

Atomic	Experimental coordinates			Calculated coordinates			Calculated				Building block				
position	x	y	z	x	y	z	t_1	t_2	t_3	$m_1\ m_2\ m_3$	symbol	n	U	$x_0\ y_0\ z_0$	Δd (Å)
16 Fe(1) in (*d*)	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$	$\bar{5}$	$\bar{5}$	$\bar{5}$	0 0 0*	−(1, 0, 1)	10	U_2	$\frac{3}{4}\ \frac{3}{4}\ \frac{3}{4}$	0.000
							5	5	5		(1, 0, 1)	10	U_1	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$	
32 Fe(2) in (*e*)	−0·1703	−0·1703	−0·1703	−0·1750	−0·1750	−0·1750	3	3	3	0 0 0	−(1, 0, 1)	10	U_2	$\bar{\frac{1}{4}}\ \bar{\frac{1}{4}}\ \bar{\frac{1}{4}}$	0·0899
48 W in (*f*)	0·1978	0	0	0·1875	0	0	$\bar{2}$	$\bar{8}$	$\bar{8}$	0 0 1	−(1, 1, 1)	8	U_2	$\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$	0·1142
							6	0	0	0 1 1	(1, 1, 1)	8	U_1	0 0 0 0	
16 C in (*c*)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$									

Table 7. $Al_{10}V$, *cubic*, $a = 14{\cdot}516$ Å, *space group* $Fd3m$

Atomic	Experimental coordinates			Calculated coordinates			Calculated				Building block				
position	x	y	z	x	y	z	t_1	t_2	t_3	$m_1\ m_2\ m_3$	symbol	n	U	$x_0\ y_0\ z_0$	Δd (Å)
96 Al (*g*)	0·0654	0·0654	0·3009	0·0682	0·0682	0·2955	3	3	−9	0 0 2	(2, 1)F	11	U_1	0 0 $\frac{1}{2}$	0·0972
							−8	−8	−2	0 0 1*	(1, 1, 1)	11	U_2	$\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$	
48 Al (*f*)	0·1407	0	0	0·1364	0	0	6	0	0	1 1 0	−(1, 1, 1)	11	U_1	0 0 0	0·0624
16 Al (*d*)	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$												
16 V (*c*)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$												
8 Al*(*b*)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	1 1 1	(2, 1)F	11	U_1	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$	0·0000

* Occupancy of these sites 0–10%.

space group consists of 16 building blocks of two different types. One of them is around (000), $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ and their face-centered related positions. The two building blocks at (000), $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ have an inverse center at $(\frac{1}{8}\frac{1}{8}\frac{1}{8})$. Therefore, they can be symbolized as (K, L, P, Q, S) and $-(K, L, P, Q, S)$ respectively. Those at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ and $(\frac{3}{4}\frac{3}{4}\frac{3}{4})$ have an inverse center at $(\frac{5}{8}\frac{5}{8}\frac{5}{8})$. The building blocks at (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ can be independent and different.

It has been shown (Table 6) that Fe_3W_3C consists of two different types of building blocks (1, 1, 1) and (1, 0, 1). The building blocks (1, 1, 1) and −(1, 1, 1) located at (000) and $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ respectively share three atoms. Their coordinates are (0·1978 0 0), (0 0·1978 0) and (0 0 0·1978). The building blocks (1, 0, 1) and −(1, 0, 1) located at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ and $(\frac{3}{4}\frac{3}{4}\frac{3}{4})$ share only one atom, whose coordinates are $(\frac{5}{8}\frac{5}{8}\frac{5}{8})$. Fe_3W_3C has two different values of *n*, namely 8 and 10, for the building blocks (1, 1, 1) and (1, 0, 1) respectively. The average interatomic distance of (1, 1, 1) is 2·9219 Å, and that of (1, 0, 1) is 2·3419 Å. The reason that *n* for the (1, 1, 1) building blocks is different from that for (1, 0, 1) is that they consist of different atoms of different sizes. The (1, 1, 1) consists of W atoms, (1, 0, 1) of Fe atoms. Carbon is located at the center of the outer octahedron of the building block (1, 1, 1). The APAD's of the building blocks (1, 1, 1) and (1, 0, 1) are 3·9 and 2·6 respectively. Co_3W_3C and Co_2W_4C are isomorphous structures of Fe_3W_3C. The structure built with these two building blocks is shown in an earlier paper (Nyman, Andersson, Hyde & O'Keeffe, 1978).

3.5. $Al_{10}V$

$Al_{10}V$ (Brown, 1957) is cubic, $a = 14{\cdot}516$ Å, space group *Fd*3*m*. The construction and distribution of the building blocks of $Al_{10}V$ (Table 7) is the same as that of Fe_3W_3C. The building blocks (2, 1)*F* and −(2, 1)*F* are located at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, $(\frac{3}{4}\frac{3}{4}\frac{3}{4})$ respectively in the unit cell of $Al_{10}V$. They have an inverse center in $(\frac{5}{8}\frac{5}{8}\frac{5}{8})$ which is also the center of a hexagonal prism formed by two hexagons of (2, 1)*F* and −(2, 1)*F*. An Mg atom is situated at the center of the hexagonal prism. The building blocks −(1, 1, 1) and (1, 1, 1) are located at (000) and $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ respectively. The (1, 1, 1) at $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ shares three atoms at (0·0654 0·0654 0·3009), (0·0654 0·3009 0·0654) and (0·3009 0·0654 0·0654) with (2, 1)*F* at $(00\frac{1}{2})$. One V atom at $(\frac{1}{8}\frac{1}{8}\frac{1}{8})$ locates the centre of the icosahedron formed by the building blocks −(1, 1, 1) and (1, 1, 1). The APAD of the building block (2, 1)*F* and −(2, 1)*F* is 3·2 and that of (1, 1, 1) and −(1, 1, 1) is 3·5. $Al_{18}Cr_2Mg_3$ is an isomorphous structure of $Al_{10}V$. The structure has been described earlier by Nyman, Andersson, Hyde & O'Keeffe (1978).

Table 8. *Pyrochlore* $[(NaCa)_2Nb_2O_6F]_8$, *cubic*, $a = 10{\cdot}40$ Å, *space group* $Fd3m$

Atomic position	Experimental coordinates			Calculated coordinates			Calculated						Building block symbol	n	U				Δd (Å)
	x	y	z	x	y	z	t_1	t_2	t_3	m_1	m_2	m_3				x_0	y_0	z_0	
16 Nb in 16(d)	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$																
8 F in 8(d)	0	0	0																
16 Ca in 16(c)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	3	3	3	0	0	0	−(1, 0)	6	U_1	0	0	0	0·0
							$\bar{3}$	$\bar{3}$	$\bar{3}$	0	0	0	(1, 0)	6	U_2	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	
48 O in 48(f)	x	0 ($x = 0{\cdot}316, 0{\cdot}313, 0{\cdot}322, 0{\cdot}330$)	0	0·3125	0	0	2	8	8	0	0	1	(1, 1, 1)	8	U_2	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	
							$\bar{6}$	0	0	0	1	1	−(1, 1, 1)	8	U_1	$-\frac{1}{2}$	0	0	

Table 9. *Zunyite* $[Al_{13}Si_5O_{20}(OH, F)_{18}Cl]$, *cubic*, $a = 13{\cdot}820$ Å, *space group* $F\bar{4}3m$

Atomic position	Experimental coordinates			Calculated coordinates			Calculated						Building block symbol	n	U				Δd (Å)
	x	y	z	x	y	z	t_1	t_2	t_3	m_1	m_2	m_3				x_0	y_0	z_0	
4 Cl in (b)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	0	0	(0, 0)	11	U_1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	
4 SiI in (c)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$																
16 SiII in (e)	0·1143	0·1143	0·1143	0·1136	0·1136	0·1136													0·0168
4 AlI in (d)	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$													
48 AlII in (h)	0·0853	0·0853	−0·2333																
16 OI in (e)	−0·1750	−0·1750	−0·1750	−0·1818	−0·1818	−0·1818	$\bar{8}$	$\bar{8}$	$\bar{8}$	1	1	1*	−(2, 2, 1)	11	U_1	0	0	0	0·1628
							3	3	3	0	0	0	(2, 1, 1)	11	U_1	$\bar{\frac{1}{4}}$	$\bar{\frac{1}{4}}$	$\bar{\frac{1}{4}}$	
16 OII in (e)	0·1818	0·1818	0·1818	0·1818	0·1818	0·1818	$\bar{3}$	$\bar{3}$	$\bar{3}$	0	0	0	−(1, 2, 1)	11	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·0000
24 OIII (OH, F) in (f)	0·2780	0	0	0·2727	0	0	1	$\overline{11}$	11	0	0	2*	(2, 1, 1)	11	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	0·0735
							12	0	0	0	2	2	−(2, 2, 1)	11	U_1	0	0	0	
							14	8	2	2	1	0*	−(2, 2, 1)	11	U_1	$\frac{1}{2}$	0	$\frac{1}{2}$	
48 OIV (OH, F) in (h)	0·1793	0·1793	0·5466	0·1818	0·1818	0·5455	−3	−3	−9	0	0	1	(2, 1, 1)	11	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	0·0514
							−5	−5	11				(2, 1, 1)	11	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	
48 OV (OH, F) in (h)	0·1385	0·1385	0·0003	0·1364	0·1364	0	6	6	0	3	1	1	−(2, 2, 1)	11	U_1	0	0	0	0·0413
							−5	−5	−11	1	1	3	−(1, 2, 1)	11	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	

3.6. $[(Na,Ca)_2Nb_2O_6F]_8$ (*pyrochlore*)

This compound (Perrault, 1968) is cubic, space group $Fd3m$ as Fe_3W_3C and $Al_{10}V$, $a = 10{\cdot}4$ Å. From Table 8, building blocks −(1, 0) and (1, 0) which are occupied by Ca atoms and centered by F atoms are located at (000) and ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$). The oxygen constitutes building blocks (1, 1, 1) and −(1, 1, 1) which are located at ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$) and ($\frac{3}{4}\frac{3}{4}\frac{3}{4}$) respectively. The Nb atom is situated at the center of the outer octahedron of (1, 1, 1) and −(1, 1, 1). The n of building block (1, 0) is 6, and that of (1, 1, 1) is 8, because they are constructed by different atoms, namely calcium and oxygen respectively. Building block (1, 0) is an ideal polyhedron, and the APAD's of (1, 1, 1) and −(1, 1, 1) are 0·2, 0·02, 0·9, 1·3, 6·5 for five different pyrochlores.

3.7. *Zunyite*

Zunyite $[Al_{13}Si_5O_{20}(OH,F)_{18}Cl]$ (Kamb, 1960) is cubic, $a = 13{\cdot}820$ Å, space group $F\bar{4}3m$. the crystal of $F\bar{4}3m$ consists of 16 building blocks of four different types located at (000), ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$), ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$), ($\frac{3}{4}\frac{3}{4}\frac{3}{4}$) as well as their 12 corresponding face-centered related positions. From Table 9, building blocks −(2, 2, 1), −(1, 2, 1), (0, 0) and (2, 1, 1) in zunyite are located at (000), ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$), ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$) and ($\frac{3}{4}\frac{3}{4}\frac{3}{4}$) respectively. The (2, 2, 1) is the building block originally used by Pauling to describe this structure, while (2, 1, 1) is the well known Keggin unit. The oxygen positions constitute quite regular building blocks (2, 1, 1), −(2, 2, 1) and −(1, 2, 1) whose APAD's are 2·4, 2·2 and 1·2 respectively. 4 SiI in (c) are located at the center of a central tetrahedron of a building block −(1, 2, 1). 16 SiII in (e) are located at the center of a tetrahedron of the twin part of a building block −(2, 2, 1). Chlorine is surrounded by 18 oxygens and the average interatomic distance between O and Cl is 3·452 Å which is much longer than the distances of both Si–O and O–O. 4 AlI in (d) are in the centers of tetrahedra in the truncated tetrahedra of (2, 1, 1). 48 AlII in (h) are in the octahedra of the twin part of (2, 1, 1). 48 AlII form a truncated tetrahedron (2, 1) with $n = 8{\cdot}25$.

We conclude that oxygen constitutes the framework of building blocks −(2, 2, 1), −(1, 2, 1) and (2, 1, 1). Building blocks −(2, 2, 1), −(1, 2, 1) and (2, 1, 1) share atoms with each other. −(2, 2, 1) and (2, 1, 1) share all the atoms with each other, and −(2, 1, 1) share most of the atoms. The APAD's of the −(2, 2, 1), −(1, 2, 1) and −(2, 1, 1) blocks are 2·2, 1·2 and 2·2 respectively.

3.8. $Mg_{44}Rh_7$ *and* Na_6Tl

$Mg_{44}Rh_7$ (Westin & Edshammar, 1971) is cubic, $a = 20{\cdot}110$ Å, and has the space group $F\bar{4}3m$ as for zunyite. The assembly rule of building blocks in $Mg_{44}Rh_7$ is similar to zunyite. Building blocks (1, 0, 1, 1, 1), −(1, 1, 1, 1, 1), (3, 0, 1) and (1, 0, 1, 1, 1) in $Mg_{44}Rh_7$ are located at (000), ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$), ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$) and ($\frac{3}{4}\frac{3}{4}\frac{3}{4}$) and their 12 corresponding face-centered related positions, as shown in Table 10. They share atoms with

Table 10. $Mg_{44}Rh_7$, *cubic*, $a = 20\cdot110$ Å, *space group* $F\bar{4}3m$

Atomic position	Experimental coordinates			Calculated coordinates			Calculated						Building block symbol	n	U				Δd (Å)
	x	y	z	x	y	z	t_1	t_2	t_3	m_1	m_2	m_3				x_0	y_0	z_0	
24 Rh(1) in 24(g)	$\frac{1}{4}$	$\frac{1}{4}$	0·5867	$\frac{1}{4}$	$\frac{1}{4}$	0·5655	0	0	$-\frac{31}{3}$	0	0	0^{**}	(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	0·4271
16 Rh(2) in 16(e)	0·0833	0·0833	0·0833	0·0893	0·0893	0·0893	5	5	5	0	0	0^{*}	(1, 0, 1, 1, 1)	14	U_1	0	0	0	0·2094
16 Rh(3) in 16(e)	0·3488	0·3488	0·3488	0·3393	0·3393	0·3393	$\bar{9}$	$\bar{9}$	$\bar{9}$	0	0	0^{*}	(3, 0, 1)	14	U_1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0·3246
48 Mg(1) in 48(h)	0·0525	0·0525	0·3380	0·0536	0·0536	0·3393	3	3	$\bar{9}$	0	0	2	(3, 0, 1)	14	U_1	0	0	$\frac{1}{2}$	0·0366
48 Mg(2) in 48(h)	0·1072	0·1072	0·2141	0·1071	0·1071	0·2143	$\bar{8}$	$\bar{8}$	$\bar{2}$	0	0	1	−(1, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·0049
48 Mg(3) in 48(h)	0·1949	0·1949	0·4806	0·1963	0·1963	0·4821	11	11	$\bar{1}$	0	0	2^{*}	(3, 0, 1)	14	U_1	0	0	$\frac{1}{2}$	0·0500
				0·1964	0·1964	0·4881	$-\frac{9}{3}$	$-\frac{9}{3}$	$\frac{40}{3}$	0	0	1^{**}	−(1, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·1510
48 Mg(4) in 48(h)	0·0961	0·0961	0·7206	0·0913	0·0913	0·7242	$-\frac{80}{9}$	$-\frac{80}{9}$	$-\frac{13}{9}$	0	0	0^{***}	(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	0·2653
				0·0893	0·0893	0·6964	5	5	11	1	1	0^{*}	(3, 0, 1)	14	U_1	0	0	$\frac{1}{2}$	
48 Mg(5) in 48(h)	0·1565	0·1565	0·9795	0·1587	0·1587	0·9742	$\frac{80}{9}$	$\frac{80}{9}$	$-\frac{13}{9}$	0	0	0^{***}	(1, 0, 1, 1, 1)	14	U_1	0	0	1	0·0868
				0·1548	0·1548	0·9761	$-\frac{16}{3}$	$-\frac{16}{3}$	$-\frac{46}{3}$	0	0	0^{**}	−(1, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	
24 Mg(6) in 24(g)	$\frac{1}{4}$	$\frac{1}{4}$	0·3553	$\frac{1}{4}$	$\frac{1}{4}$	0·3571	0	0	6	1	1	0	−(1, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·0363
24 Mg(7) in 24(f)	0	0	0·1824	0	0	0·1845	0	0	$\frac{31}{3}$	0	0	0^{**}	(1, 0, 1, 1, 1)	14	U_1	0	0	0	0·0484
16 Mg(8) in 16(e)	0·6956	0·6956	0·6956	0·6965	0·6965	0·6965	$\bar{3}$	$\bar{3}$	$\bar{3}$	0	0	0	(1, 0, 1, 1, 1)	14	U_1	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0·0314
16 Mg(9) in 16(e)	0·8338	0·8338	0·8338	0·8393	0·8393	0·8393	5	5	5	0	0	0^{*}	(1, 0, 1, 1, 1)	14	U_1	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0·1919
16 Mg(10) in 16(e)	0·5618	0·5618	0·5618	0·5535	0·5535	0·5535	3	3	3	1	1	1	(3, 0, 1)	14	U_1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.2896
16 Mg(11) in 16(e)	0·9476	0·9476	0·9476	0·9465	0·9465	0·9465	$\bar{3}$	$\bar{3}$	$\bar{3}$	0	0	0	(1, 0, 1, 1, 1)	14	U_1	1	1	1	0·0384

Table 11. Na_6Tl, *cubic*, $a = 24\cdot115$ Å, *space group* $F\bar{4}3m$

Atomic position		Experimental coordinates			Calculated coordinates			Calculated						Building block symbol	n	U				Δd (Å)
		x	y	z	x	y	z	t_1	t_2	t_3	m_1	m_2	m_3				x_0	y_0	z_0	
Na 48(h)$_1$	xxz	0·14228	0·14228	0·03346	0·14286	0·14286	0·03571	8	8	2	0	0	1^{*}	(2, 0, 1, 1)	14	U_1	0	0	0	0·0578
Na 48(h)$_2$	xxz	0·08984	0·08984	0·26791	0·09524	0·09524	0·27381	$\frac{16}{3}$	$\frac{16}{3}$	$\frac{46}{3}$	0	0	1^{**}	(2, 0, 1, 1)	14	U_1	0	0	0	0·2033
					0·09127	0·09127	0·27579	$-\frac{80}{9}$	$-\frac{80}{9}$	$-\frac{13}{9}$	0	0	0^{***}	−(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	
Na 48(h)$_3$	xxz	0·05604	0·05604	0·76942	0·05357	0·05357	0·76190	$\frac{9}{3}$	$\frac{9}{3}$	$-\frac{40}{3}$	0	1	0^{**}	(2, 0, 1, 1)	14	U_1	0	0	0	0·1379
					0·05357	0·05357	0·76785	$\overline{11}$	$\overline{11}$	1	0	0	2^{*}	−(2, 1, 1)F	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	
Na 48(h)$_4$	xxz	0·15395	0·15395	0·52856	0·15873	0·15873	0·52579	$\frac{80}{9}$	$\frac{80}{9}$	$\frac{13}{9}$	0	0	0^{***}	(1, 0, 1, 1, 1)	14	U_1	0	0	$\frac{1}{2}$	0·1764
Na 48(h)$_5$	xxz	0·19809	0·19809	0·90985	0·19643	0·19643	0·91071	$\bar{3}$	$\bar{3}$	9	1	1	2^{*}	−(2, 1)F	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	0·2153
Na 24(f)	$x00$	0·10858	0	0	0·10714	0	0	6	0	0	0	1	1	(2, 0, 1, 1)	14	U_1	0	0	0	0·0348
Tl 24(f)	$x00$	0·33516	0	0	0·31548	0	0	$-\frac{31}{3}$	0	0	0	0	0^{**}	(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{2}$	0	0	0·4753
Na 24(g)	$x\frac{1}{4}\frac{1}{4}$	0·06815	$\frac{1}{4}$	$\frac{1}{4}$	0·06548	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{31}{3}$	0	0	0	0	0^{**}	−(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·0645
Na 16(e)$_1$	xxx	0·30267	0·30267	0·30267	0·30357	0·30357	0·30357	3	3	3	0	0	0	−(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·0217
Na 16(e)$_2$	xxx	0·41542	0·41542	0·41542	0·41071	0·41071	0·41071	$\bar{5}$	$\bar{5}$	$\bar{5}$	0	0	0^{*}	(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0·1970
Na 16(e)$_3$	xxx	0·55549	0·55549	0·55549	0·55357	0·55357	0·55357	3	3	3	0	0	0	(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0·0720
Tl 16(e)$_1$	xxx	0·67234	0·67234	0·67234	0·64286	0·64286	0·64286	$\bar{6}$	$\bar{6}$	$\bar{6}$	1	1	1	−(2, 1, 1)F	14	U_1	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	1·23
Tl 16(e)$_2$	xxx	0·16755	0·16755	0·16755	0·16083	0·16083	0·16083	$\bar{5}$	$\bar{5}$	$\bar{5}$	0	0	0^{*}	−(1, 0, 1, 1, 1)	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0·2811
Tl 16(e)$_3$	xxx	0·90136	0·90136	0·90136	0·89285	0·89285	0·89285	$\bar{6}$	$\bar{6}$	$\bar{6}$	0	0	0	(2, 0, 1, 1)	14	U_1	1	1	1	0·3589
Void 4d	$\frac{1}{4}\frac{1}{4}\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	0	0	0	0	0	0	−(2, 1, 1)F	14	U_1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	0·0000

each other. For instance, (1, 0, 1, 1, 1) around (000) and −(1, 1, 1, 1) around ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$) share three atoms, (0·1565 0·1565 −0·0205), (0·1565 −0·0205 0·1565) and (−0·0205 0·1565 0·1565). Building block −(1, 1, 1, 1) around ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$) is connected to building block (3, 0, 1) around (00$\frac{1}{2}$) and they share three atoms (0·1949 0·1969 0·4806), (0·1949 −0·4806 −0·1919) and (−0·4806 0·1949 −0·1949). The building block (3, 0, 1) around (00$\frac{1}{2}$) is in contact with (1, 0, 1, 1, 1) around ($\frac{1}{4}\frac{1}{4}\frac{3}{4}$) and shares three atoms (0·0961 0·0961 0·7206), (0·0961 1·7206 0·0961) and (1·7206 0·0961 0·0961). The APAD's of building blocks (1, 0, 1, 1, 1), −(1, 1, 1, 1), (3, 0, 1) and (1, 0, 1, 1, 1) are 2·9, 5·0, 2·5 and 8·6 respectively. The APAD of the building block (1, 0, 1, 1, 1) around ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$) and that of (1, 0, 1, 1, 1) around ($\frac{3}{4}\frac{3}{4}\frac{3}{4}$) are quite different, because they are independent of each other, and have no related symmetry.

Na_6Tl (Samson & Hansen, 1972) is not isomorphic with $Mg_{44}Rh_7$, but very similar. Na_6Tl has building blocks (2, 0, 1, 1) and (2, 1, 1) instead of −(1, 1, 1, 1) and (3, 0, 1) in $Mg_{44}Rh_7$. Building block (2, 0, 1, 1) in Na_6Tl has one more atom (666) [*i.e.* Tl(16) in (e)$_3$] than the building block (1, 1, 1, 1) in $Mg_{44}Rh_7$, and (3, 0, 1) in $Mg_{44}Rh_7$ has one more atom (999) [*i.e.* 16Rh(3) in 16(e)] and one less atom (666) [*i.e.* Tl(16)-(e)$_1$] than Na_6Tl. As a result, Na_6Tl has 15 independent positions, *i.e.* one more independent position than $Mg_{44}Rh_7$, and three different positions from $Mg_{44}Rh_7$, as shown in Tables 10 and 11. A model of $Mg_{44}Rh_7$ is shown in Fig. 2 of an earlier paper (Andersson, 1978).

3.9. Cu_4Cd_3

Cu_4Cd_3 (Samson, 1967) is cubic, $a = 25\cdot871$ Å, space group $F\bar{4}3m$. It contains 1124 atoms in the unit cell and it is one of the most complicated inorganic compounds. The assembly rule for the building blocks of Cu_4Cd_3 is similar to zunyite, $Mg_{44}Rh_7$ and Na_6Tl, but its unit cell is much bigger. The description of Cu_4Cd_3 is very simple in terms of building blocks in

Table 12. Cu_4Cd_3, *cubic*, $a = 25{\cdot}871$ Å, *space group* $F\bar{4}3m$

Atomic position		Experimental coordinates x	y	z	Calculated coordinates x	y	z	Calculated t_1 9	t_2 15	t_3 $\bar{3}$	m_1	m_2	m_3	x_0	y_0	z_0	U	Building block symbol	n	Δd (Å)
1 Cu	$96(i)_1$	0·1018	0·1714	0·4662	0·1022	0·1705	0·4659	0	10	16	2	1	4	0	0	$\frac{1}{2}$	U_1	$-(4,5,1)$	22	0·0266
2 Cu	$96(i)_2$	0·0036	0·1362	0·2256	0·0000	0·1389	0·2222	$\bar{3}$	$\bar{3}$	$\overline{15}$				0	0	0	U_1	$-(2,0,1,\bar{1},1)$	18	0·1459
3 Cu	$48(h)_1$	0·2142	0·2142	0·0813	0·2159 0·7222	0·2159 0·2222	0·0795 0·0833	16 $\bar{9}$	16 $\bar{9}$	6 $\overline{15}$	0	0	2	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	U_1 U_1	$(4,1,1)$ $-(2,0,1,\bar{1},1)$	22 18	0·0732
4 Cu	$48(h)_2$	0·1476	0·1476	0·0784	0·1477	0·1477	0·0795	$\overline{17}$	$\overline{17}$	$\bar{7}$	0	0	1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	U_1	$(4,1,1)$	22	0·0286
5 Cu	$48(h)_3$	0·0560	0·0560	0·1683	0·0568	0·0568	0·1704	5 $\overline{12}$	5 $\overline{12}$	$\overline{29}$ 0	4	4	0	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	$\frac{1}{4}$ $\frac{1}{2}$	U_1	$(4,1,1)$ $-(4,5,1)$	22	0·0617
6 Cu	$48(h)_4$	0·1138	0·1138	0·2499	0·1136	0·1136	0·2500	10 3	10 3	$\overline{22}$ $\overline{21}$	1	1	3	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	$\frac{1}{4}$ $\frac{1}{2}$	U_1	$(4,1,1)$ $-(4,5,1)$	22	0·0078
7 Cu	$48(h)_5$	0·0339	0·0339	0·2604	0·0341	0·0341	0·2613	$\bar{3}$	$\bar{3}$	9	0	0	4	0	0	$\frac{1}{2}$	U_1	$-(4,5,1)$	22	0·0244
8 Cu	$48(h)_6$	0·2157	0·2157	0·3517	0·2157	0·2157	0·3522	$\bar{5}$	$\bar{5}$	17	2	2	0	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	U_1	$(4,1,1)$	22	0·0149
9 Cu	$48(h)_7$	0·1931	0·1931	0·4424	0·1932	0·1932	0·4432	17 9	17 9	$\bar{5}$ 3	2	2	4	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	$\frac{1}{4}$ $\frac{1}{2}$	U_1	$(4,1,1)$ $(4,5,1)$	22	0·0210
10 Cu	$48(h)_9$	0·1026	0·1026	0·5335	0·1023	0·1023	0·5335	$-\frac{16}{3}$	$-\frac{16}{3}$	$-\frac{46}{3}$	2	2	3	0	0	$\frac{1}{2}$	U_1	$-(4,5,1)$	22	0·0110
11 Cu	$48(h)_{10}$	0·1793	0·1793	0·5474	0·1798	0·1798	0·5482	8	8	$\overline{14}$				$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	U_1	$-(2,0,1,1)$	19	0·0276
12 $\frac{2}{3}$Cd + $\frac{1}{3}$Cu	$48(h)_{11}$	0·1060	0·1060	0·8117	0·1111	0·1111	0·8055	6	6	18				0	0	1	U_1	$-(2,0,1,\bar{1},1)$	18	0·2460
13 Cd	$48(h)_{12}$	0·0663	0·0663	0·7043	0·0681	0·0681	0·7045	$\bar{8}$	$\bar{8}$	$\bar{2}$				0	0	$\frac{1}{2}$	U_1	$(4,3,1)$	22	0·0661
14 $\frac{1}{2}$Cu + $\frac{1}{2}$Cd	$48(h)_{13}$	0·1498	0·1498	0·7244	0·1447	0·1447	0·7237	2	2	$\overline{14}$				$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	U_1	$-(2,0,1,1)$	19	0·1874
15 $\frac{2}{3}$Cu + $\frac{1}{3}$Cd	$48(h)_{14}$	0·0354	0·0354	0·8091	0·0278	0·0278	0·8055	$-\frac{9}{3}$	$-\frac{9}{3}$	$\frac{40}{3}$				0	0	1	U_1	$-(2,0,1,\bar{1},1)$	18	0·2932
16 $\frac{1}{2}$Cu + $\frac{1}{2}$Cd	$48(h)_{15}$	0·2130	0·2130	0·9138	0·2105	0·2105	0·9254	8	8	$\bar{2}$				$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	U_1	$-(2,0,1,1)$	19	0·3137
17 Cd	$48(h)_{16}$	0·1119	0·1119	0·9796	0·1111	0·1111	0·9722	6	0	0	0	0	1	0	0	0	U_1	$(2,0,1,\bar{1},1)$	18	0·1936
18 Cd	$24(f)_1$	0·0876	0	0	0·0833	0	0	$\overline{12}$	0	0	1	1	0	0	0	0	U_1	$-(2,0,1,\bar{1},1)$	18	0·1926
19 Cd	$24(f)_2$	0·3635	0	0	0·3636	0	0				1	1	3	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	U_1	$-(4,5,1)$	22	0·0045
20 Cu	$24(g)_1$	0·5006	$\frac{1}{4}$	$\frac{1}{4}$				$\bar{6}$	0	0										
21 Cu	$24(g)_2$	0·6793	$\frac{1}{4}$	$\frac{1}{4}$	0·6710	$\frac{1}{4}$	$\frac{1}{4}$	6	6	6	0	0	1	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	U_1	$-(2,0,1,1)$	19	0·2121
22 Cu	$16(e)_1$	0·0744	0·0744	0·0744	0·0833	0·0833	0·0833	$\bar{6}$	$\bar{6}$	$\bar{6}$				0	0	0	U_1	$(2,0,1,\bar{1},1)$	18	0·3988
23 Cd	$16(e)_2$	0·1815	0·1815	0·1815	0·1818 0·1944	0·1818 0·1944	0·1818 0·1944	14 $\overline{12}$	14 $\overline{12}$	14 $\overline{12}$	1	1	1	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	$\frac{1}{4}$ 0	U_1	$(4,1,1)$ $-(2,0,1,\bar{1},1)$	22 18	0·0134 0·5780
24 Cd	$16(e)_3$	0·3632	0·3632	0·3632	0·3636	0·3636	0·3636	10 $\bar{6}$	10 $\bar{6}$	10 $\bar{6}$	3	3	3	$\frac{1}{2}$ $\frac{1}{4}$	$\frac{1}{2}$ $\frac{1}{4}$	$\frac{1}{2}$ $\frac{1}{4}$	U_1	$-(4,5,1)$ $(4,1,1)$	22	0·0179
25 Cd	$16(e)_4$	0·4315	0·4315	0·4315	0·4318	0·4318	0·4318	3	3	3	1	1	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	U_1	$-(4,5,1)$	22	0·0134
26 Cu	$16(e)_5$	0·5346	0·5346	0·5346	0·5340	0·5340	0·5340	11	11	11	2	2	2	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	U_1	$-(4,5,1)$	22	0·0269
27 Cu	$16(e)_7$	0·6262	0·6262	0·6262	0·6250	0·6250	0·6250	6	6	6				$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	U_1	$(4,3,1)$	22	0·0518
28Cu	$16(e)_8$	0·8203	0·8203	0·8203	0·8289	0·8289	0·8289	0	0	0				$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	U_1	$-(2,0,1,1)$	19	0·3719
29 Cu	$4(c)$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				1	1	1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	U_1	$(4,1,1)$	22	

Table 2. Building blocks $-(2,0,1,\bar{1},1)$, $(4,1,1)$, $-(4,5,1)$ and $-(2,0,1,1)$ distribute around (000), $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ and $(\frac{3}{4}\frac{3}{4}\frac{3}{4})$ and their 12 corresponding face-centered related positions respectively. The APAD's for them are 7·2, 1·2, 1·9, 6·9 respectively. An obvious feature of this compound is that it has three different n values for different building blocks. They are 22 for $(4,1,1)$ and $-(4,5,1)$, 19 for $-(2,0,1,1)$ and 18 for $-(2,0,1,1)$. The reason why different building blocks have different n is that the octahedron and tetrahedron for different building blocks have a different composition of Cu and Cd. The Cu atomic percentages of octahedra and tetrahedra in the building blocks $-(4,5,1)$ and $(4,1,1)$ are 100; however, those of $(-2,0,1,1)$ and $-(2,0,1,\bar{1},1)$ are 73·9 and 60·4 respectively. The average Cu-Cu distance is 2·4945 Å, and that of Cu-Cd is 2·9750 Å. The ratio of atomic distances of Cu-Cd and Cu-Cu is 22 : 18·76. Therefore, the higher the Cu atomic percentage of a building block, the larger is n. This is also the reason why the APAD's of the building blocks $-(2,0,1,\bar{1},1)$ and $-(2,0,1,1)$ are much bigger than those of the building blocks $-(4,5,1)$ and $(4,1,1)$. The interatomic distances in the octahedra and tetrahedra of the building blocks $-(4,5,1)$ and $(4,1,1)$ are entirely Cu-Cu distances.

The deviations of atoms of these two building blocks are, of course, very small. However, some of the interatomic distances of building blocks $-(2,0,1,\bar{1},1)$ and $(2,0,1,1)$ are those of Cu-Cd, some are Cu-Cu. Of course, their deviations are much bigger than those of $-(4,5,1)$ and $(4,1,1)$. Like other compounds, the building blocks in Cu_4Cd_3 share atoms with each other. As shown in Table 12, $-(4,5,1)$ shares atoms $48(h)_3$, $48(h)_4$, $48(h)_7$ and $16(e)_3$ *with* $(4,1,1)$, and $(4,1,1)$ shares atoms $48(h)_1$ and $16(e)_2$ with $-(2,0,1,\bar{1},1)$. $(2,0,1,1)$ does not share atoms with any building block, but atoms $48(h)_{10}$ *of* $(2,0,1,1)$ *and* $48(h)_1$ *of* $(2,0,1,\bar{1},1)$ constitute icosahedra with $16(e)_8$ of $-(2,0,1,1)$ located at the center of the icosahedra. A model of Cu_4Cd_3 was shown in Figs. 2 to 5 of Andersson's (1980) paper.

3.10. $Ge_{38}P_8I_8$

$Ge_{38}P_8I_8$ (Menke & von Schnering, 1973) is cubic, $a = 10{\cdot}507$ Å, space group $P\bar{4}3n$. This space group consists of two building blocks around (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ of the same type. $Ge_{38}P_8I_8$ consists of four frameworks which are $-(1,0,1)$, $(1,0,1)$, dodecahedron and truncated octahedron as shown in Table 13. The centers of these frameworks coincide with

Table 13. $Ge_{38}P_8I_8$, *cubic*, $a = 10{\cdot}507$ Å, *space group* $P\bar{4}3n$

Atomic position	Experimental coordinates *x*	*y*	*z*	Calculated coordinates *x*	*y*	*z*	Calculated t_1	t_2	t_3	Building block symbol	*n*	*U*	x_0	y_0	z_0	Δd (Å)
24 Ge(1) in (*i*)	−0·0009	0·1186	0·3072	0	0·1158	0·3032				Dodecahedron	4					0·0499
							−5	−5	−5	(1, 0, 1)		U_4	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	
8 Ge(2) in (*e*)	0·1842	0·1842	0·1842	0·1875	0·1875	0·1875	3	3	3	−(1, 0, 1)	4	U_1	0	0	0	0·0600
							5	5	11	(1, 2, 1)		U_4	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	
6 Ge(3) in (*c*)	0	$\frac{1}{4}$	$\frac{1}{2}$							Truncated octahedron	4					0·0000
							5	5	−11	−(1, 2, 1)		U_4	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	
8 P in (*e*)	0·8152	0·8152	0·8152	0·8125	0·8125	0·8125	5	5	5	−(1, 0, 1)	4	U_4	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0·0491
							−3	−3	−3	(1, 0, 1)		U_1	1	1	1	
6 I(1) in (*d*)	0	$\frac{1}{2}$	$\frac{1}{4}$	0	$\frac{1}{2}$	$\frac{1}{4}$				Truncated octahedron	4					0·0000
2 I(2) in (*a*)	0	0	0	0	0	0				Truncated octahedron	4					0·0000

each other, so they interpenetrate each other. The −(1, 0, 1) framework is occupied by Ge, (1, 0, 1) by P. The two frameworks are located at (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. As a result, the atoms of one framework are located at the centre of the outer tetrahedron of the other, but the central tetrahedron of these two frameworks is occupied by an I atom. These two frameworks are exactly the same as that of the F atoms in SiF_4. In addition, frameworks (1, 0, 1) and −(1, 0, 1) can be replaced by −(1, 2, 1) and (1, 2, 1) respectively since they share all the atoms with each other. The third framework is a dodecahedron which consists of 24 Ge(1) in (*i*) and building blocks (1, 0, 1) and −(1, 0, 1). The integer *n* for building blocks (1, 0, 1) and −(1, 0, 1) is 4. The eight atoms of the central tetrahedron of (1, 0, 1) and −(1, 0, 1) belong to a dodecahedron. The positions of these eight atoms which determine the rest of the dodecahedron were calculated and are given in Table 13. The dodecahedron of $Ge_{38}P_8I_8$ consists of 20 atoms, *i.e.* 16 Ge and 4 P, and is centered by atom I.

The average interatomic distance between an I atom and atoms on the dodecahedron is 3·41 Å, and that between atoms on the dodecahedron itself is 2·40 Å. The coordinates of the nearest two atoms of the two dodecahedra at (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ respectively are (0·1842 0·1842 0·1842) and (0·3152 0·3152 0·3152). The distance between these two atoms is 2·38 Å and very close to 2·40 Å. The fourth framework is a truncated octahedron. Its centres are also in (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The truncated octahedron consists of four hexagons with edge = $(2^{1/2}/2)a$ whose centers are at $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$, $(\frac{\bar{1}}{4}\frac{\bar{1}}{4}\frac{1}{4})$, $(\frac{1}{4}\frac{\bar{1}}{4}\frac{\bar{1}}{4})$ and $(\frac{\bar{1}}{4}\frac{1}{4}\frac{\bar{1}}{4})$ respectively. The distance between the atom in the hexagon and 24 Ge(1) in (*i*) is 2·45 Å which also is very close to 2·40 Å. The APAD's of (1, 0, 1), (1, 2, 1), dodecahedron and truncated octahedron are 1·8, 1·4, 2·2 and 0·0 respectively. It is concluded that this structure is very close to an ideal model. $P\bar{4}3n$ is a subgroup of $I\bar{4}3m$. $Ge_{38}P_8I_8$ will change into $I\bar{4}3m$ from $P\bar{4}3n$, if the coordinates of 24 Ge(1) in (*i*), (−0·0009 0·1186 0·3072), are replaced by (0·0000 0·1186 0·3072), and 6 I(1) in (*d*) is replaced by 6 Ge. Therefore, the chemical formula will change into $Ge_{44}P_8I_2$. But these two structures can be described by the same building blocks. Of course, $P\bar{4}3n$ is also a subgroup of $Pm3n$. The $Ge_{38}P_8I_8$ will become $Pm3n$ if the coordinates of 8 P in (*e*) of $Ge_{38}P_8I_8$ change into (0·8158 0·8158 0·8158) from (0·8152 0·8152 0·8152) and 8 P atoms are replaced by Ge. The chemical formula of $Ge_{38}P_8I_8$ will become $Ge_{46}I_8$ correspondingly. In fact, the assumed structure is an isomorphous structure of $Ge_{46}K_8$, $Sn_{46}K_8$, $Si_{46}Na_8$, and $Ge_{38}P_8Br_8$ and $Ge_{38}As_8I_8$ are isomorphous with $Ge_{38}P_8I_8$.

3.11. Li_7VN_4

Li_7VN_4 (Juza, Geiren & Haug, 1959) is cubic, $a = 9{\cdot}60$ Å, space group $P\bar{4}3n$. It contains four frameworks which are the building blocks (2, 2), (2, 1), −(2, 0) and truncated octahedra as shown in Table 14. The dominant unit is the building block (2, 2). There exist three layers of atoms parallel to the (111) lattice plane between (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ because $n = 6$. Accordingly, the distance between two surfaces of two building blocks (2, 2) around (000) and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ is one atomic layer or the height of an octahedron. These two surfaces constitute four trigonal prisms; one is a central trigonal prism and three are outer ones. Building block (2, 2) has six octahedra, eight tetrahedra and 32 trigonal prisms around it. The six atoms at the vertices of the central octahedron of building block (2, 0) are located at the center of the octahedron of building block (2, 2). The four atoms at the vertices of the outer tetrahedron of building block −(2, 0) are situated at the center of the central trigonal prisms. The four N atoms at the vertices of the central tetrahedron of building block (2, 1) are located in four of the eight tetrahedra of building block (2, 2), but not at the center. The three N atoms at the vertices of the triangle of building block (2, 1) are located in the outer trigonal prisms. The hexagon which constitutes a truncated octahedron is parallel to the bottom of a trigonal prism and is half the height of the trigonal prisms, as shown in Fig. 6, which is projected along [111]. Li_7VN_4 will become $I\bar{4}3m$ and its chemical formula will become 'Li_2N', if 6 V(2) in 6(*c*) are replaced by 6 Li (antifluorite). Building blocks (2, 2), −(2, 0) and truncated

Table 14. Li_7VN_4, *cubic*, $a = 9{\cdot}60$ Å, *space group* $P\bar{4}3n$

Atomic position	Experimental coordinates x	y	z	Calculated coordinates x	y	z	Calculated t_1	t_2	t_3	m_1	m_2	m_3	Building block symbol	n	U	x_0	y_0	z_0	Δd (Å)
2 V(1) in 2(*a*)	0	0	0	0	0	0	0	0	0	1	1	1	(2, 2)	6	U_1	0	0	0	0·0000
6 V(2) in 6(*c*)	$\frac{1}{4}$	$\frac{1}{2}$	0	$\frac{1}{4}$	$\frac{1}{2}$	0							Truncated octahedron						0·0000
8 N(3) in 8(*e*)	0·120	0·120	0·120	0·125	0·125	0·125	3	3	3	1	1	1	(2, 1)	6	U_1	0	0	0	0·0831
24 N(4) in 24(*i*)	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	$\bar{3}$	$\bar{3}$	$\bar{9}$	0	0	2	(2, 1)	6	U_4	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0·0000
6 Li(1) in 6(*b*)	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	12	0	0	2	2	0	(2, 2)	6	U_4	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0·0000
6 Li(2) in 6(*d*)	$\frac{1}{4}$	0	$\frac{1}{2}$	$\frac{1}{4}$	0	$\frac{1}{2}$							Truncated octahedron						0·0000
8 Li(3) in 8(*e*)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	6	6	6	0	0	0	−(2, 0)	6	U_1	0	0	0	0·0000
12 Li(4) in 12(*f*)	$\frac{1}{4}$	0	0	$\frac{1}{4}$	0	0	6	0	0	1	1	0	−(2, 0)	6	U_4	0	0	0	0·0000
24 Li(5) in 24(*i*)	$\frac{1}{4}$	$\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{4}$	0	6	6	0	3	1	1	(2, 2)	6	U_1	0	0	0	0·0000

octahedra are ideal polyhedra. The APAD of (2, 1) is 0·7. Accordingly, Li_7VN_4 consists of almost ideal building blocks.

4. Discussion

Up to now, we have described 12 c.c.p. crystals which belong to four space groups, $I\bar{4}3m$, $Fd3m$, $F\bar{4}3m$ and $P\bar{4}3n$. The integers n of all the building blocks are 4, 6, 7, 8, 10, 11, 14, 18, 19, 22. We can conclude that all these structures or their dominant parts can be described by the building blocks in Table 2. The rest of the atoms of these structures are located at the centers of the tetrahedra or octahedra of these building blocks or at the center of a trigonal prism, hexagonal prism, icosahedron, dodecahedron or a big cavity formed by these building blocks. (111)-twinning in c.c.p.-related structures changes the orientation of a tetrahedron and an octahedron. Second-order and third-order twinning changes their orientation progressively. The building blocks (2, 0, 1) and (1, 1, 1), (2, 1, 1) and (2, 0, 1, 1), (2, 0, 1) and (1, 1, 1, 1), $(2, 0, 1, \bar{1}, 1)$ and $(2, 0, 1, \bar{1}, 1)$ *etc.* can all form icosahedra and naturally there is an atom located at the center and this atom is a component part of these building blocks. But in most cases it is a heterogeneous atom. Consequently, (111)-twinning of a T_d polyhedron creates a method of forming a trigonal prism, hexagonal prism, icosahedron *etc.* Such polyhedra, tetrahedra and octahedra can together accommodate quite a range of heterogeneous atom sizes and compound compositions. The same space groups have the same assembly rule of building blocks which is independent of the size of a unit cell. The structural difference between the smallest and the biggest unit cell in the same space group lies only in the size of building blocks. The structural description of a complicated c.c.p.-related crystal can be simplified greatly if we use building blocks. There exists a very close relationship between a group and its subgroup, and c.c.p.-related structures belonging to the space groups given in Table 1 can be described with these methods.

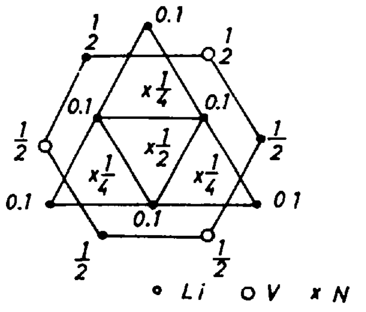


Fig. 6. Part of the structure of Li_7VN_4.

The CSL model with $\Sigma = 3$ is quite an accurate model for a description of c.c.p.-related structures. APAD's of building blocks range from 0 to 8·6 for 12 crystals and the average APAD of all the building blocks in this paper is 3·2, as shown in Table 15.

As mentioned in the introduction, there exists a very close relationship between the CSL model for structure description and unit-cell twinning. For example, $\Sigma = 11$, which is twinning of (113) (Andersson & Hyde, 1974; Hyde, Andersson, Bakker, Plug & O'Keeffe, 1978), can describe hundreds of compounds. As a matter of fact, $\Sigma = 3$ can describe not only h.c.p. and c.c.p. structures but also pentagonal Frank-Kasper phases *etc.* $\Sigma = 5$ is suitable for describing some phases of tetragonal, orthorhombic, monoclinic systems. The CSL model for structure description is a rather general one. For instance, there almost always exists a CSL among domains which are related by a crystallographic operation such as reflection, rotation, threefold and fourfold axes and intergrowth *etc.* We shall demonstrate this in a series of papers.

5. Concluding remarks

The CSL model with $\Sigma = 3$ used to describe c.c.p. structures has the following advantages:

1. *General.* The structure of a c.c.p.-related crystal can always be described with twin operations in a unit cell. All the c.c.p.-related structures which we have studied can be described with the CSL of $\Sigma = 3$ and using the building blocks given in Table 2.

2. *Quantitative structure description.* In order to describe some of these structures quantitatively, two formulae were derived earlier, (2, 2, 2) and

$$(x, y, z) = m/4n \qquad (5.1)$$

Table 15. *Summary of results for c.c.p. structures*

Compound	Crystal system	Space group	Lattice constant (Å)	Building block 1 symbol	center	n	APAD	Building block 2 symbol	center	n	APAD
SiF_4	Cubic	$I\bar{4}3m$	5·41	−(1, 0, 1)	0 0 0	4	5·7	−(1, 0, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	4	5·7
γ-Brass Cu_5Zn_8	Cubic	$I\bar{4}3m$	8·878	−(1, 0, 1, 1, 1)	0 0 0	7	4·2	−(1, 0, 1, 1, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	7	4·2
α-Mn	Cubic	$I\bar{4}3m$	8·89	−(2, 1, 2)	0 0 0	8	4·4	−(2, 1, 2)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	8	4·4
$[(Na.Ca)_2Nb_2O_6F]$	Cubic	$Fd3m$	10·40	−(1, 0)	0 0 0	6	0	(1, 1, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	8	0·2 ~ 6·5
Fe_3W_3C	Cubic	$Fd3m$	11·087	(1, 1, 1)	0 0 0	8	3·9	(1, 2, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	10	2·6
Zunyite	Cubic	$F\bar{4}3m$	13·820	−(2, 2, 1)	0 0 0	11	2·2	(0, 0)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	11	0·0
$Al_{10}V$	Cubic	$Fd3m$	14·516	−(1, 1, 1)	0 0 0	11	3·5	(2, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	11	3·5
$Mg_{44}Rh_7$	Cubic	$F\bar{4}3m$	20·110	(1, 0, 1, 1, 1)	0 0 0	14	8·4	(3, 0, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	14	5·0
Na_6Tl	Cubic	$F\bar{4}3m$	24·115	(2, 0, 1, 1)	0 0 0	14	3·3	−(1, 0, 1, 1, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	14	4·2
Cu_4Cd_3	Cubic	$F\bar{4}3m$	25·871	$-(2, 0, 1, \bar{1}, 1)$	0 0 0	18	7·2	−(4, 5, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	22	1·2
$Ge_{38}P_8I_8$	Cubic	$P\bar{4}3n$	10·507	−(1, 0, 1) (1, 0, 1)	0 0 0	4	1·8 1·4	−(1, 0, 1) (1, 0, 1)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	4	1·8 1·4
Li_7VN_4	Cubic	$P\bar{4}3n$	9·60	(2, 2)	0 0 0	6	0·0	(2, 2)	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	6	0·0
					Building block 3				Building block 4		
$[(Na.Ca)_2Nb_2O_6F]$	Cubic	$Fd3m$	10·40	(1, 0)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	6	0	−(1, 1, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	8	0·2 ~ 6·5
Fe_3W_3C	Cubic	$Fd3m$	11·087	−(1, 1, 1)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	8	3·9	−(1, 2, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	10	2·6
Zunyite	Cubic	$F\bar{4}3m$	13·820	−(1, 2, 1)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	11	1·2	(2, 1, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	11	2·4
$Al_{10}V$	Cubic	$Fd3m$	14·516	(1, 1, 1)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	11	3·5	−(2, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	11	3·5
$Mg_{44}Rh_7$	Cubic	$F\bar{4}3m$	20·110	−(1, 1, 1, 1)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	14	2·5	(1, 0, 1, 1, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	14	2·9
Na_6Tl	Cubic	$F\bar{4}3m$	24·115	−(1, 0, 1, 1, 1)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	14	6·4	−(2, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	14	8·6
Cu_4Cd_3	Cubic	$F\bar{4}3m$	25·871	(4, 1, 1)	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	22	1·4	−(2, 0, 1, 1)	$\frac{3}{4}\frac{3}{4}\frac{3}{4}$	19	6·9

by one of us (Andersson, 1980). However, (5.1) has to be modified, because (*a*) the limit of integer m was not given, and (*b*) xyz are not independent since they are the three coordinates of one and the same atom. (5.1) was thus an oversimplification and (2.2.6) and (2.2.7) have solved these problems. These formulae give the true description of the coordinates of atoms in a crystal. Finally we can derive the accuracy of a description of a crystal structure.

3. *Symbolism for a building block.* Earlier building blocks were given special names like pyrochlore unit, Keggin unit, *stella quadrangula*, truncated tetrahedron, Friauf polyhedron *etc.* The relationship among these building blocks was not obvious. We can now denote them in terms of two, three, four or five integers, *i.e.* (K, L), (K, L, P), (K, L, P, Q) or (K, L, P, Q, S) which can be used in the formulae (2.2.6) and (2.2.7). There is a common relation of $\Sigma = 3$ among them.

4. *The convenience of building a model of a c.c.p. structure.* The shortest interatomic distances and their average value can be calculated from the coordinates of a structure. Then n can be calculated by (2.2.2). The assembly rule for building blocks in a c.c.p. structure is determined by its space group. The building blocks of a structure can easily be found in terms of n and space group. The relationship among these building blocks can be found easily by means of shared atoms. For example, $Al_{10}V$ is of space group $Fd3m$ and consists of two kinds of building blocks, (2, 1) and (1, 1, 1), which share three atoms on the triangle surface of (2, 1) and on the triangle surface of the outer octahedron of (1, 1, 1). Putting these two surfaces together, the model of $Al_{10}V$ can be built. This is easily programmed, and the structure description can be made with computer graphics.

5. *The possibility of solving an unknown complex and c.c.p.-related structure.* Given n and the space group of a structure, various building blocks can be derived. The distance between two building blocks must be $n/2$ or $n/4$, and building blocks must share atoms. This algebraic method seems to us to be much simpler and more straightforward than the stochastic, geometrical method used by Samson (1964). This we hope to demonstrate in a forthcoming paper.

We are grateful for valuable discussions with S. T. Hyde, Physics Department, Monash, Melbourne. QBY thanks the Royal Swedish Academy of Engineering for financial support. This research is supported by the Swedish Research Council, which is gratefully acknowledged.

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An Alternative Description of the Structure of $NaCd_2$

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(*Received* 13 *January* 1986; *accepted* 29 *April* 1986)

Abstract

A new description of the ordered part of the crystal structure of $NaCd_2$ is proposed. A framework of cadmium Friauf polyhedra, related to but different from that of Cu_4Cd_3, interpenetrates a partially disordered sodium-cadmium structure. Using matrix algebra developed for the coincidence site lattice theory, atomic coordinates can be calculated which are very close to those experimentally determined.

Introduction

The crystal structure of $NaCd_2$ (β-Mg_2Al_3 is isostructural) is cubic, $Fd3m$, with $a = 30{\cdot}56$ Å, and approximately 1192 atoms in the unit cell, as determined by Samson (Samson, 1962, 1965). According to Samson's description, the unit cube contains 672 icosahedra, 252 Friauf polyhedra, and 244 miscellaneous, more or less irregular polyhedra.

Derivation and description

From Samson's data for β-Mg_2Al_3 the structure was plotted with cubic axes. Two different building blocks consisting of Friauf polyhedra were derived, and these could be joined together in the space group $Fd3m$. The derived structure contained the cadmium atoms numbered 1, 2, 3, 4, 5 and 6 (from the structure of $NaCd_2$) and is shown in Fig. 2. These building blocks are red, yellow and green, the red and yellow building blocks being identical units, but in opposite orientations.

In a parallel article (Yang & Andersson, 1987), we give an exact and general description of the cubic structures that contain building blocks, using matrix algebra and symmetry considerations. It was also pointed out that this method could be used for a direct determination of complex structures. It was decided to carry out a test on $NaCd_2$, as Samson's structure determination of this compound had resulted in a relatively high R factor, *viz.* 0·17. Crystals of $NaCd_2$ were prepared in silica tubes. Complete data were collected using a Nicolet diffractometer with Mo $K\alpha$ radiation, from a suitable crystal sealed in a glass capillary.

From the general formula

$$a = n(2^{1/2})d/3$$

as derived by Yang & Andersson (1987), d is the shortest interatomic distance and was determined from the three-dimensional Patterson synthesis to be 0·09744 Å; $n = 21{\cdot}77 \approx 22$. The space group of $NaCd_2$ is $Fd3m$, which is composed of 16 building blocks of two types.

The nearest two building blocks are those located at (000) and $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ respectively. We assume that the building block around (000) is ($KLPQS$); then that around $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ must be $-(KLPQS)$. The interface between these two building blocks is the (111) lattice plane through $(\frac{1}{8}\frac{1}{8}\frac{1}{8})$. Let ($xyz$) be the coordinates of the atoms in the interface. Then

$$(x\mathbf{a}+y\mathbf{b}+\mathbf{c})(\mathbf{a}+\mathbf{b}+\mathbf{c}) = x+y+z = 3/8$$

and

$$t_1+t_2+t_3 = 4n(x+y+z) = 33.$$

The only building block in Table 2 of our parallel paper (Yang & Andersson, 1987) which has $t_1+t_2+t_3 = 33$, *i.e.* coordinates $(23\;11\;\bar{1})$ or (11 11 11), is (4, 3, 1). The interface of two building blocks, as shown in Fig. 1, consists of these two independent coordinates according to symmetry operations.

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0108-7681/87/010014-04$01.50