MEISALO, V. & INKINEN, O. (1967). *Acta Cryst.* **22**, 58–62.
MERISALO, M. & INKINEN, O. (1966). *Ann. Acad. Sci. Fenn. Ser. A6*, No. 207.
SANGER, P. L. (1969). *Acta Cryst.* A**25**, 694–702.
SCHOKNECHT, G. (1957). *Z. Naturforsch. Teil A*, **12**, 983–986.
SIROTA, N. N. (1962). *Dokl. Akad. Nauk USSR*, **142**, 1278–1281.
SIROTA, N. N. & SCHELEG, A. U. (1963). *Dokl. Akad. Nauk USSR*, **152**, 81–83.
STEWART, R. F. (1974). *Chem. Phys. Lett.* **26**, 121–125.
STEWART, R. F. (1977). *Chem. Phys. Lett.* **49**, 281–284.
STEWART, R. F. (1979). *Chem. Phys. Lett.* **65**, 335–342.
Tables of Physics Values (1976). Moscow: Atom Press.
TSIREL'SON, V. G., NOZIK, U. Z. & URUSOV, V. S. (1983). *Geochemistry (USSR)*, **3**. Submitted.
TSIREL'SON, V. G. & OZEROV, R. P. (1981). In *The Study of Matter by Diffraction Methods*, edited by L. A. FEIGIN, pp. 47–62. Kishinev: Shtiintsa.
VAN VLECK, J. H. & FRANK, A. (1929). *Proc. Natl Acad. Sci. USA*, **15**, 539–541.
VARNEK, A. A., TSIREL'SON, V. G. & OZEROV, R. P. (1981). *Dokl. Akad. Nauk USSR*, **257**, 382–385.
VIDAL-VALAT, G., VIDAL, J. P. & KURKI-SUONIO, K. (1978). *Acta Cryst.* A**34**, 594–602.
WEISS, K. J. (1966). *X-ray Determination of Electron Distribution*. Amsterdam: North-Holland.

Acta Cryst. (1983). A**39**, 415–421

Geometric Units in Tetragonal Crystal Structures

BY CHUNG CHIEH

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

(*Received* 20 *July* 1982; *accepted* 21 *December* 1982)

Abstract

Tetragonal space groups are classified from the geometric-unit view point by considering crystal structures as a result of combinations and permutations of some basic polyhedral units. There are nine patterns among two categories represented by four units packed on the $(1\bar{1}0)$ and (100) planes. Category (I) consists of five types with four units packed on the $(1\bar{1}0)$ plane. The centers of these units are 0,0,0; 0,0,$\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$ and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. In that order, the patterns can be represented by *ABCD*, *AA'BB'*, *ABA'B'*, *ABB'A'* and *AA'A''A''*. Each letter here represents an independent unit: primes are used to indicate one of the following orientation relationships: identity, fourfold rotation, mirror plane parallel to (110), and mirror plane parallel to (100). These units have the shape of tetragonal prisms and they stack in the same way as the crystallographic unit cells. Category (II) has four types packed on the (100) plane and the centers of these units are at 0,0,0; $0,\frac{1}{2},\frac{1}{4}$; 0,0,$\frac{1}{2}$ and $0,\frac{1}{2},\frac{3}{4}$. In that order, the patterns can be represented by *ACBD*, *ABA'B'*, *AA'BB'* and *AA'A''A''*. The ideal polyhedra for category (II) are truncated tetragonal prisms or flattened truncated octahedra depending on the axial ratio c/a. For simplicity, these polyhedra are transformed into tetragonal prisms so that all geometric units have the same shape. Units in category (II) stack in an interlocking fashion, like the work of a bricklayer. The overlap displacements for the interlocking are in the (001) direction. The symmetries of the geometric units in some space groups depend on the choice of origin, but a shift to equivalent origins changes neither the packing patterns nor the symmetries of the geometric units.

Introduction

Plato's hypothesis about the structure of matter is that all matter is the result of combinations and permutations of a few basic polyhedral units. From a geometric view point, these polyhedral units are made up of atoms, ions, or molecules. Furthermore, a polyhedral unit may contain a group of nested polyhedra whose vertices are marked by positions of symmetry-related atoms. This paper reports the exploration along this idea of combinations and permutations of some basic units for the tetragonal system.

The problem of space filling with polyhedra has fascinated many mathematicians and crystallographers alike for more than two thousand years (Senechal, 1981). For example, Dirichlet (1850) and Wigner & Seitz (1933) introduced methods for finding the polyhedra enclosing each of the lattice points. These polyhedra are called Dirichlet regions (or domains) or Wigner–Seitz cells.

For the cubic crystal system, it has been demonstrated that all geometric units have the shape of an Archimedean truncated octahedron (Chieh, 1979). The

0567-7394/83/030415-07$01.50

description of any cubic crystal structure can be made based on the arrangement of these units, and further detail is given as the arrangement of atoms within them. Subsequently, this idea is applied to the description of crystal structures whose geometric units have $\bar{4}3m$ symmetry (Chieh, 1980) and $m3m$ symmetry (Chieh, 1982).

After the publication of privileged origins (Burzlaff & Zimmerman, 1980), a revised classification of cubic space groups by the arrangement of geometric units was given by Chieh, Burzlaff & Zimmermann (1982).

Bradley & Jones (1933) used *cluster* to describe the γ-brass structures; this author recognized that this concept is actually derived from the geometric properties of space groups. Following our work with γ brasses (Booth, Brandon, Brizard, Chieh & Pearson, 1977), this concept was extended to all cubic crystals. Further description of crystal structures is done by grouping the atoms in the form of polyhedra, a geometric property of the point group, within the geometric unit. This same method was used by Chabot, Cenzual & Parthé (1981).

A few applications of the geometric unit concept follow. 1. The arrangement of many space-group symmetry elements in geometric units is easy to understand. The classification of space groups by this method provides an interesting linkage between crystallographic point groups and space groups. 2. Although the division of a unit cell into geometric units is independent of the origin, we can always select points of high symmetry to be centers of these units and thus allow the description of crystal structures within them by nested polyhedra as Chabot *et al.* (1981) termed it, or nested configurations of certain symmetry. 3. An arrangement of geometric units is usually common to several space groups and thus allows the study of correlation among crystal structures, furnishing a mean for the consideration of geometric and symmetric factors governing their stability. 4. The arrangement of geometric units can be described by a few simple easily understood and remembered invariant lattice complexes (Fischer, Burzlaff, Hellner & Donnay, 1973). 5. Geometric units are building blocks for crystals as are crystallographic unit cells. These blocks are polyhedra, which may or may not relate to a molecule. Often, we do see a relationship between geometric units and molecules as demonstrated in the two previous studies (Chieh, 1980, 1982). 6. For very complicated crystal structures, the task of describing or memorizing them is reduced to a problem, much simpler than other methods, of knowing the nesting of the polyhedra in the geometric units. 7. The classification of space groups by the geometric construction produces a new way for the study of systematics of crystal chemistry, and for the study of structural relationships.

Aside from the three pairs of enantiomorphic space groups $P4_1$, $P4_3$; $P4_122$, $P4_322$; and $P4_12_12$, $P4_32_12$, the representation patterns are unique to all other space groups in terms of the symmetry of the geometric units and orientation relationships, providing a one-to-one correspondence between space groups and the patterns.

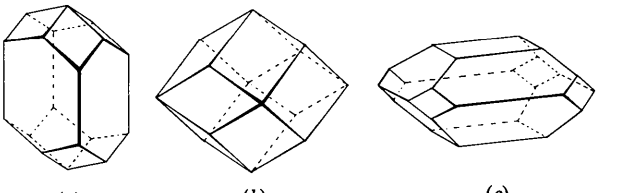
Dirichlet domains of tetragonal lattices

The two lattices, P and I, of the tetragonal system have the largest number (68) of space groups among the seven crystal classes. However, the geometric units and their arrangements in the tetragonal system can be derived in a manner similar to that of the cubic system, for which the Dirichlet domain of the I lattice was adopted as the basic geometric unit. Although Koch (1972) and Fischer, Koch & Hellner (1971) studied the Dirichlet domains, the discussion on the properties of the Dirichlet domains has not been widely available. These properties are key points for the discussion of geometric units; therefore Dirichlet domains for the tetragonal I lattice will be discussed before we deal with the classification of tetragonal space groups. The shape of the Dirichlet region for a P lattice is a tetragonal prism.

The Dirichlet domain or Wigner–Seitz cell for a body-centered tetragonal I cell has four shapes depending on the axial ratio, c/a. Three of them are shown in Fig. 1; the fourth is an Archimedean truncated octahedron, a special case when the tetragonal cell is metrically cubic. When c is greater than $\sqrt{2}a$, the polyhedron has the shape of a truncated tetragonal prism, Fig. 1(a). The top and bottom of the polyhedron consist of four congruent rhomboids. The angle subtended by the two opposite rhomboids at the apex is $2\tan^{-1}(c/\sqrt{2}a)$. The angles between adjacent rhomboids are $\cos^{-1}[1/(2r^2+1)]$, where $r = c/a$. The length of the edges for the prism is $(c^2 - 2a^2)/2c$, and the distance between the two apexes is obviously $c/2$.

For $c = \sqrt{2}a$, the Dirichlet domain is a rhombic dodecahedron (see Fig. 1b), the same as that for a cubic F lattice, and many of its properties are listed in *International Tables for X-ray Crystallography* (1972). When $c < \sqrt{2}a$, the Dirichlet domain is a flattened truncated octahedron, Fig. 1(c).

The packing of the Dirichlet domains on the $(1\bar{1}0)$ plane corresponding to the three shapes of Fig. 1 are



(a) (b) (c)

Fig. 1. Three of the four possible polyhedra for the Dirichlet domain of a tetragonal I lattice: (a) when $c > \sqrt{2}a$; (b) when $c = \sqrt{2}a$; and (c) when $c < \sqrt{2}a$.

shown in Fig. 2. Although Figs. 2(*a*) and (*c*) appear to be the same when one of them is viewed sideways, they represent different polyhedra. Fig. 2(*b*) represents packing on the (100) plane of an *F* cubic lattice. Regardless of the variation in the axial ratio, *c*/*a*, there is a great similarity in the arrangements of geometric units to those of the cubic system (Chieh, 1979).

Geometric units of the tetragonal system

The $(1\bar{1}0)$ plane is very useful in showing the packing of the geometric units for many tetragonal space groups. However, planar packing patterns on the $(1\bar{1}0)$ and (100) planes are employed, resulting in categories (I) and (II) respectively. For (I), the geometric units are derived from the Dirichlet domains of the lattice complex formed by the Wyckoff point set 4(*a*), 4(*b*), or 4(*c*) in the space group $I4/mcm$ (No. 140). This lattice complex, designated as *Cc* by Fischer *et al.* (1973), is primitive and has a cell volume of $\frac{1}{4}$ that of the original unit cell. The Dirichlet domains for these are tetragonal prisms with the four faces $(\pm 1,\pm 1,0)$. The packing of these on a $(1\bar{1}0)$ plane is shown in Fig. 3(*a*), which includes all patterns of category (I).

The geometric units can be derived from the Cheshire group (Hirshfeld, 1968) of the space groups in category (I). Aside from the hemimorphic space groups such as *P*4, *I*4*m etc.*, they all have Cheshire group of $(P4/mmm)_{vc}$, where the subscripts *vc* refer to a unit cell with $a' = (a - b)/2$, $b' = (a + b)/2$ and $c' = c/2$. The unit cell for the Cheshire group has the same volume as the geometric units.

Geometric units for category (II) can be derived from the Dirichlet domains of the lattice complex *Fc*, formed by the Wyckoff sets 8(*a*) or 8(*b*) of the space group $I4_1/acd$. This is an *I* lattice with $\frac{1}{8}$ of the volume of the original unit cell. Thus the Dirichlet domains are, in general, truncated tetragonal prisms or flattened truncated octahedra. The packing of these has been described in the previous section, but it should be pointed out that the $(1\bar{1}0)$ plane of the lattice complex *Fc* is the (100) plane of the original cell. In addition, the cell constants of the *I* lattice were given in the previous section: for the correct shape of the Dirichlet domain the appropriately transformed cell dimensions should be used.

It is desirable for all geometric units in the tetragonal system to have the same shape, and this is achieved by employing Escher's method of transformation. Many of his drawings can be visualized as the transformation of plane-covering polygons into lizards, knights, or whatever. Instead of the truncated tetragonal prism or flattened truncated octahedron, the tetragonal prism can be used as the basic geometric unit in filling space. When this is done, the resulting pattern looks like the work of a bricklayer; however, the relative arrangement of these units stays the same; the transformation of Fig. 2 is given in Fig. 3(*b*). Since we are not dealing with the crystal structures in terms of the lattice complex *Fc*, but the cell of the original tetragonal cell, Fig. 3 is labelled according to the latter.

At this point, we realize that a similar transformation can be done for the cubic system, *i.e.* use cubes rather than Archimedean truncated octahedra,

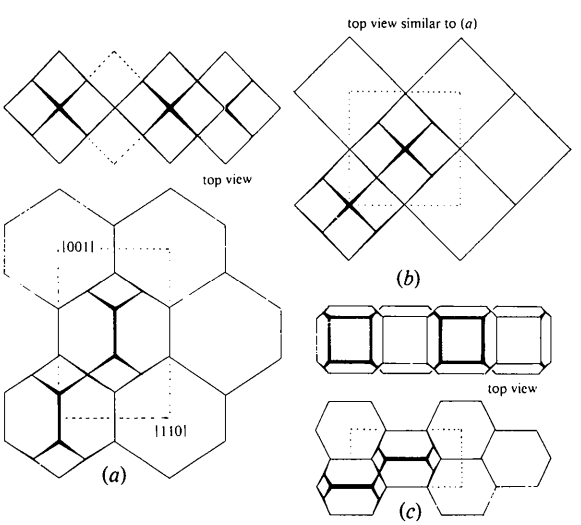


Fig. 2. Packing of the Dirichlet domain in the tetragonal system. (*a*) when $c > \sqrt{2}a$; (*b*) when $c = \sqrt{2}a$; and (*c*) when $c < \sqrt{2}a$.

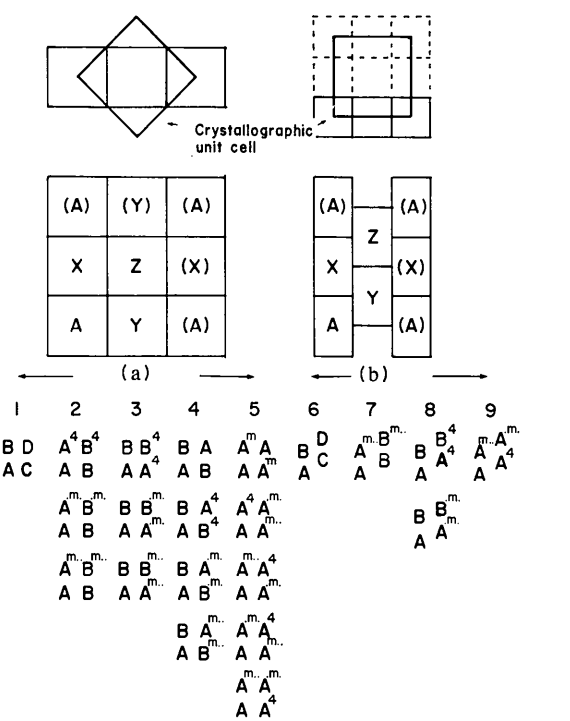


Fig. 3. Packing patterns of geometric units in the tetragonal system, categories (I) (*a*) and (II) (*b*).

although the latter conform with geometry and are aesthetically pleasing. Thus simple tetragonal prisms or cubes may be used instead of elaborate polyhedra. However, the latter have to be used if one wants to employ polyhedra with colored faces to conform with point-group symmetry and to study their arrangements for the derivation of space groups.

For the cubic system (Chieh, 1979), we constructed Dirichlet domains from two point sets which may have different site symmetries. The units will then have the site symmetries of these point sets. However, once the pattern is established, the polyhedra resulting from Dirichlet domains can be transformed into some simple and convenient forms. In the tetragonal system, all geometric units in a space group belong to the same point group. Both the cubic and tetragonal systems have two categories, but the unit cells are divided into two and 16 geometric units for the former, and into four and eight units for the latter.

Classification of tetragonal space groups by geometric units

The use of the Dirichlet domains of the I or of the P lattices or of any lattice complex is obviously convenient for the partition of a three-dimensional space. For simplicity, and for the purpose of keeping the same shape for all geometric units in the tetragonal system, and for reasons already given in the previous section, the tetragonal prism is adopted as the basic geometric unit.

In the classification of space groups from the geometric-unit point of view, the following rules are applied. 1. The number of classes should remain as few as possible. 2. All geometric units in the crystal structure of a space group should have the same point-group symmetry, which is one of the crystallographic point groups unless this is impossible. As a consequence, all equivalent origins are used as centers of geometric units. The aspect of equivalent origins can be derived from the Cheshire group of space groups (Hirshfeld, 1968), and it was further discussed by Koch & Fischer (1975). 3. The number of geometric units should be as few as possible, *i.e.* use Wyckoff sets with lowest multiplicity as their centers. 4. The centers of the geometric unit should coincide with points of high site symmetry as far as possible. However, there are a few space groups for which another origin could serve equally well. 5. Simple planes such as the (100) and $(1\bar{1}0)$ are considered for the packing patterns.

The classification of tetragonal space groups is given in Table 1. Categories (I) and (II) make use of the $(1\bar{1}0)$ and (100) planes, respectively. The (100) plane passes through the origin of the next cell along **a**, therefore, the x coordinate is 0 for all centers of geometric unit A. There are nine types (see Fig. 3 for a summary), one of which contains as many as 19 space groups.

The packing pattern on the $(1\bar{1}0)$ plane for category (I), see Fig. 3(*a*), consists of four geometric units; thus there are possibilities of having four, two or one independent units. The type with four independent units consists of six P-type space groups formed by the combination of unit-cell translations and the tetragonal point groups. The geometric unit D lies between two A units along the body diagonal, whereas the units B and C lie between two A's in the [001] and [110] directions respectively. Two hemimorphic space groups $P4$ and $P4mm$, and two pairs of enantiomorphs are also placed in type 1. For the hemimorphic and enantiomorphic pairs of space groups, it is easier to handle if we combine the A and B (similarly C and D) into a single unit. Units with hemimorphic point-group symmetries can be divided or combined along the polar axis without altering the symmetry. The Cheshire groups for these space groups degenerate to equivalences of planar groups.

Permutations of two each of two independent units in the four positions on a planar pattern, keeping one fixed at the origin, give rise to types 2, 3 and 4. In each of these types, there exist subclasses because of different symmetry relationships between geometric units. In some of the subclasses, there are hemimorphic space groups and enantiomorphic pairs. When the site symmetries are ambiguous, four-direction designations are used following the convention of Fischer *et al.* (1973).

The orientation relationships are indicated by superscripts 4, $m..$, and $.m.$ referring to fourfold rotation, mirror plane parallel to (100) and (010) respectively. When the mirror plane is parallel to either (100) or (010), a single m is used in the superscripts.

For type 5, all four units are the same, however, three of them may have different orientations with respect to the one at the origin. This type has the most number of subclasses, as seen from Table 1 and Fig. 3.

Again, there can be four, two or one independent units in category (II), the patterns of which also consist of four units on a (100) plane as shown in Fig. 3(*b*). This pattern,

$$\begin{matrix} & A & \\ B & & B \\ A & & \end{matrix},$$

is not permissible because of periodicity requirements, thus only four types instead of five are present in category (II). The centers of the four units from the bottom upward are 0,0,0; $0,\frac{1}{2},\frac{1}{4}$; $0,0,\frac{1}{2}$; and $0,\frac{1}{2},\frac{3}{4}$; respectively. It should be noticed, however, that these patterns do not stack right on top of each other but in a brick-wall fashion, *i.e.* the view from the [010] is the same as that from the [100].

Table 1. *Classification of tetragonal space groups by packing pattern of geometric units*

Type no.	Pattern		Space group number / Space group symbol / Wyckoff point set, site symmetry			
Packing pattern based on the (1$\bar{1}$0) plane						
			81	83	89	111
1	B D		$P\bar{4}$	$P4/m$	$P422$	$P\bar{4}2m$
	A C	A:	1(*a*) $\bar{4}$	1(*a*) 4/*m*	1(*a*) 422	1(*a*) $\bar{4}2m$
		B:	1(*b*) $\bar{4}$	1(*b*) 4/*m*	1(*b*) 422	1(*c*) $\bar{4}2m$
		C:	1(*c*) $\bar{4}$	1(*c*) 4/*m*	1(*c*) 422	1(*d*) $\bar{4}2m$
		D:	1(*d*) $\bar{4}$	1(*d*) 4/*m*	1(*d*) 422	1(*b*) $\bar{4}2m$
			115	123		
			$P\bar{4}2m$	$P4/mmm$		
		A:	1(*a*) $\bar{4}m2$	1(*a*) 4/*mmm*		
		B:	1(*d*) $\bar{4}m2$	1(*b*) 4/*mmm*		
		C:	1(*b*) $\bar{4}m2$	1(*c*) 4/*mmm*		
		D:	1(*c*) $\bar{4}m2$	1(*d*) 4/*mmm*		
			75	99		
			$P4$	$P4mm$		
		AB:	1(*a*)* 4	1(*a*)* 4*mm*		
		CD:	1(*b*)* 4	1(*b*)* 4*mm*		
			76	78	91	95
			$P4_1$	$P4_3$	$P4_122$	$P4_322$
		AB:	000† 4_1	000† 4_3	000† 4_12	000† 4_32
		CD:	$\frac{1}{2}\frac{1}{2}$0† 4_1	$\frac{1}{2}\frac{1}{2}$0† 4_3	$\frac{1}{2}\frac{1}{2}$0† 4_12	$\frac{1}{2}\frac{1}{2}$0† 4_32
			77	84	93	101
2	A^4 B^4		$P4_2$	$P4_2/m$	$P4_222$	$P4_2cm$
	A B	A:	2(*a*)* 2	2(*a*) 2/*m*	2(*a*) 222	2(*a*)* 2.*mm*
		B:	2(*b*)* 2	2(*b*) 2/*m*	2(*b*) 222	2(*b*)* 2.*mm*
			105	131	132	
			$P4_2mc$	$P4/mmc$	$P4_2/mcm$	
		A:	2(*a*)* 2*mm*.	2(*a*) *mmm*.	2(*a*) *m*.*mm*	
		B:	2(*b*)* 2*mm*.	2(*b*) *mmm*.	2(*c*) *m*.*mm*	
			103	112	124	
	$A^{m\cdot}B^{m\cdot}$		$P4cc$	$P\bar{4}2c$	$P4/mcc$	
	A B	A:	2(*a*)* 4	2(*e*) $\bar{4}$	2(*b*) 4/*m*	
		B:	2(*b*)* 4	2(*f*) $\bar{4}$	2(*d*) 4/*m*	
			116			
	$A^{m\cdot\cdot}B^{m\cdot\cdot}$		$P\bar{4}c2$			
	A B	A:	2(*c*) $\bar{4}$			
		B:	2(*d*) $\bar{4}$			
			85	90		
3	B B^4		$P4/n$	$P42_12$		
	A A^4	A:	2(*a*) $\bar{4}$	2(*a*) 2.22		
		B:	2(*b*) $\bar{4}$	2(*b*) 2.22		
			113	125	127	129
	B $B^{\cdot m\cdot}$		$P\bar{4}2_1m$	$P4/nbm$	$P4/mbm$	$P4/nmm$
	A $A^{\cdot m\cdot}$	A:	2(*a*) $\bar{4}$	2(*a*) 422	2(*a*) 4/*m*	2(*a*) $\bar{4}2m$
		B:	2(*b*) $\bar{4}$	2(*b*) 422	2(*b*) 4/*m*	2(*b*) $\bar{4}2m$
			100			
			$P4bm$			
		AB:	2(*a*)* 4			
			117			
	B $B^{m\cdot\cdot}$		$P\bar{4}b2$			
	A $A^{m\cdot\cdot}$	A:	2(*a*) $\bar{4}$			
		A:	2(*b*) $\bar{4}$			
			87	97	121	139
4	B A		$I4/m$	$I422$	$I\bar{4}2m$	$I4/mmm$
	A B	A:	2(*a*) 4/*m*	2(*a*) 422	2(*a*) $\bar{4}2m$	2(*a*) 4/*mmm*
		A:	2(*b*) 4/*m*	2(*b*) 422	2(*b*) $\bar{4}2m$	2(*a*) 4/*mmm*
			79	107		
			$I4$	$I4mm$		
		AB:	2(*a*)* 4	2(*a*)* 4*mm*		
			86	94	134	136
	B A^4		$P4_2/n$	$P4_22_12$	$P4_2/nnm$	$P4_2/mnm$
	A B^4	A:	2(*a*) $\bar{4}$	2(*a*) 222	2(*a*) $\bar{4}2m$	2(*a*) *mmm*
		B:	2(*b*) $\bar{4}$	2(*b*) 222	2(*b*) $\bar{4}2m$	2(*b*) *mmm*
			137			
			$P4_2/nmc$			
		A:	2(*a*) $\bar{4}m2$			
		B:	2(*b*) $\bar{4}m2$			
			102	92	96	
			$P4_2nm$	$P4_12_12$	$P4_32_12$	
		AB:	2(*a*)* *mm*	000† 4_1	000† 4_3	
			114	126	128	
	B $A^{\cdot m\cdot}$		$P\bar{4}2_1c$	$P4/nnc$	$P4/mnc$	
	A $B^{\cdot m\cdot}$	A:	2(*a*) $\bar{4}$	2(*a*) 422	2(*a*) 4/*m*	
		A:	2(*a*) $\bar{4}$	2(*a*) 422	2(*a*) 4/*m*	
			104			
			$P4nc$			
		AB:	2(*a*) 4			
			118			
	B $A^{m\cdot\cdot}$		$P\bar{4}n2$			
	A $B^{m\cdot\cdot}$	A:	2(*a*) $\bar{4}$			
		B:	2(*b*) $\bar{4}$			
			108	140		
5	A^m A		$I4cm$	$I4/mcm$		
	A A^m	A:	2(*a*) $\bar{4}$	4(*c*) 4/*m*		
			106	135		
	A^4 $A^{\cdot m\cdot}$		$P4_2bc$	$P4_2/mbc$		
	A $A^{\cdot m\cdot}$	A:	4(*a*)* 2	4(*a*) 2/*m*		
			138			
	$A^{m\cdot\cdot}A^4$		$P4_2/ncm$			
	A $A^{\cdot m\cdot}$	A:	4(*b*) $\bar{4}$			
			133			
	$A^{\cdot m\cdot}A^4$		$P4_2/mbc$			
	A $A^{m\cdot\cdot}$	A:	4(*d*) $\bar{4}$			
			130			
	$A^{m\cdot\cdot}A^{\cdot m\cdot}$		$P4/ncc$			
	A A^4	A:	4(*b*) $\bar{4}$			
Packing pattern based on the (100) plane						
			82	119		
6	D		$I\bar{4}$	$I\bar{4}m2$		
	B	A:	2(*a*) $\bar{4}$	2(*a*) $\bar{4}m2$		
	C	B:	2(*b*) $\bar{4}$	2(*b*) $\bar{4}m2$		
	A	C:	2(*c*) $\bar{4}$	2(*c*) $\bar{4}m2$		
		D:	2(*d*) $\bar{4}$	2(*d*) $\bar{4}m2$		
			120			
7	$B^{m\cdot\cdot}$		$I\bar{4}c2$			
	$A^{m\cdot\cdot}$	A:	4(*b*) $\bar{4}$			
	B	B:	4(*c*) $\bar{4}$			
	A					
			88	98	141	
8	B^4		$I4_1/a$	$I4_122$	$I4_1/amd$	
	B	A:	4(*a*) $\bar{4}$	4(*a*) 222	4(*a*) $\bar{4}m2$	
	A^4	B:	4(*b*) $\bar{4}$	4(*b*) 222	4(*b*) $\bar{4}m2$	
	A					
			80	109		
			$I4_1$	$I4_1md$		
		AB:	4(*a*)* 2	4(*a*)* *mm*		
			122			
	$B^{\cdot m\cdot}$		$I\bar{4}2d$			
	B	A:	4(*a*) $\bar{4}$			
	$A^{\cdot m\cdot}$	B:	4(*b*) $\bar{4}$			
	A					
			110	142		
9	$A^{\cdot m\cdot}$		$I4_1cd$	$I4_1/acd$		
	$A^{m\cdot\cdot}$	A:	8(*a*)* 2	8(*a*) $\bar{4}$		
	A^4					
	A					

* Singular points (0,0,0; $\frac{1}{2},\frac{1}{2},0$; 0,0,$\frac{1}{2}$; or $\frac{1}{2},\frac{1}{2},\frac{1}{2}$) for these Wyckoff point sets are used as centers of geometric units. The centers of the combined unit, AB, are singular points 0,0,$\frac{1}{4}$ for type 1, 3 and 4 and 0,0,$\frac{1}{8}$ for type 8.

† The origin is an arbitrary point on a 4_1 or 4_3 axis for these enantiomorphic pairs; see text for discussion.

The generations of A' from A on a (100) plane in type 8 for most space groups are accomplished by a 4_1 at $(0,\frac{1}{4},z)$. As a result, A is rotated by a fourfold axis to A', as is B to B'. There is no simple relationship for A and A' in $I\bar{4}2d$; these two are related to each other by diamond glide planes and, therefore, the relationship between A and A' is a mirror parallel to (110).

The number of subclasses for category (II) is smaller than that of category (I), possibly due to a small number of space groups in (II).

Discussion

The tetragonal space groups have been classified by the consideration of combinations and permutations of a few basic geometric units belonging to some point-group symmetries. Like the cubic system (Chieh, 1979), there is a maximum of four independent units for some space groups; unlike the cubic system, planar packing patterns of geometric units on $(1\bar{1}0)$ and (100) are required. It may be argued that the patterns in category (II) can be represented by sequences in the [011] direction, in which case, they become *ABCD*, *ABA'B'*, *AA'BB'* and *AA'A'A'*. Since there are planar patterns in the tetragonal system, there is no real advantage in using the linear sequence.

For the hemimorphic space groups, the centers of geometric units are not uniquely determined; in many cases, we choose to combine two units along the polar axis, so that only one singular point, namely $0,0,\frac{1}{4}$, of the Wyckoff set 0,0,*z* is required for the combined unit. Since we want to keep the number of types to a minimum, and the combination of units does not change their relative packing pattern in types 1, 3, 4, and 8, there is no need to create separate classes. Besides, two singular points of the same Wyckoff point set 2(*a*) can always be chosen as the centers of two geometric units. Thus A and B can still be separate units. Both choices result in the same pattern, although the sizes of the units would be different.

The classification follows the same principle used in the derivation of Cheshire groups (Hirshfeld, 1968), in the discussion of automorphism and normalizer (Koch & Fischer, 1975), and in the choice of origins (Burzalaff & Zimmermann, 1980). The fact that the geometric units have $\frac{1}{4}$ or $\frac{1}{8}$ of the volume of the tetragonal cell is related to the simple fact that the special *orbit* resulted in a super space group with $\frac{1}{4}$ or $\frac{1}{8}$ of the cell volume (Wondratschek, 1976; Matsumoto & Wondratschek, 1979).

To illustrate the application of geometric units, let us look at the crystal structure of $Nb_{78}Fe_{40}Si_{80}$, space group $P4_2/mcm$, $a = 23{\cdot}76$, $c = 4{\cdot}959$ Å (Steinmetz, Rogues, Courtois & Protas, 1979). This is a complicated structure with 198 atoms per unit cell. Because of the short *c* axis, it is convenient to project the unit on to a (001) plane as shown in Fig. 4. From Table 1, the space group is in type 2; thus one understands that the atoms in units A and B must have $z \leq \frac{1}{4}$, *i.e.* the asymmetric unit lies such that $0 \leq z \leq \frac{1}{4}$. When the published atomic coordinates are converted according to this scheme, the *z* coordinates are either 0 or $\sim\frac{1}{4}$. Atoms with $z = \sim\frac{1}{4}$ are shared between two A's or two B's, whereas atoms with $z = 0$ form a layer passing through the centers of units A and B. For the diagramatic display of the structure, one may use a graduated sheet with the unit cell and geometric units outlined; then the atoms are placed according to the coordinates. Since the point-group symmetry of the units is *m.mm*, *i.e.* vertical and horizontal mirror planes in Fig. 4, symmetry-related atoms can be generated easily with the help of just a ruler. The asymmetric unit is roughly indicated by the area where the atoms are labelled. Lists of atoms in the geometric units can be given in the order of their distances from the center of the unit, but in the present case in the order of their distances from the center of the square. The original atomic numbering is used. For correct

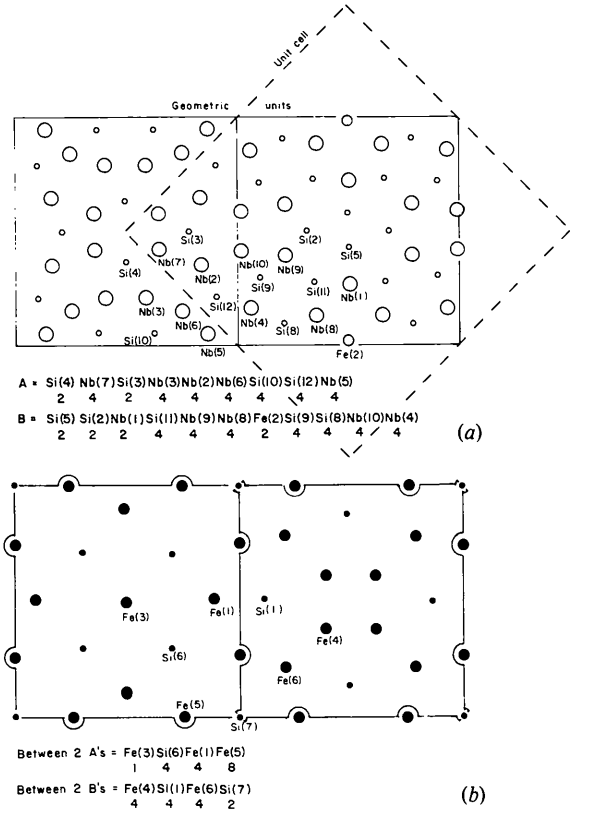


Fig. 4. Geometric units of $Nb_{78}Fe_{40}Si_{80}$, $a = 23{\cdot}76$, $c = 4{\cdot}959$ Å, $P4_2/mcm$, pattern $\begin{matrix} A^4B^4 \\ A\ B \end{matrix}$. (*a*) Layer through center of A and B, (*b*) layer shared between two A's and two B's. Lists of atoms, with original atomic numbering, for units A and B are given in order of their distances from the centers of the squares; their numbers per geometric unit are given under them.

stoichiometry, it should be noted that Fe(1) = $\frac{1}{2}$Fe + $\frac{1}{2}$Si, Fe(3) = $\frac{1}{2}$Fe + $\frac{1}{2}$Nb, and Fe(6) = $\frac{7}{8}$Fe + $\frac{1}{8}$Nb.

For the three enantiomorphic pairs of space groups $P4_1$ and $P4_3$, $P4_122$ and $P4_322$, and $P4_12_12$ and $P4_32_12$, it can be argued that there should be eight or four geometric units instead of using two per (unit) cell. However, under these circumstances, the geometric units will not have an identifiable axis in the [001] direction. All space-group symmetry operations have to be employed for the description of structures and there is no real advantage in applying the concept of the geometric unit.

In order that the geometric unit has a 4_1 axis, the origin was chosen at a 4_1 axis for space group $P4_12_12$, whereas *International Tables for X-ray Crystallography* (1969) chooses the origin at 2_12.

The symmetries of geometric units in some space groups depend on the choice of origin. For example, space group $P4_2/mbc$ has four Wyckoff sets with multiplicity four and their site symmetries are 222, $2/m$, $\bar{4}$, and $2/m$ (= $4_2/m$), respectively. Any one of these four can be used as the center of geometric unit A in type 5. If 4(*b*) is used instead of 4(*a*) as the center, the symmetry of the geometric unit is changed from $2/m$ to $\bar{4}$. Despite the shift of the origin, the packing pattern of the geometric units has not been affected.

Another property of the geometric representation is that the shift to equivalent origin changes neither the symmetry of the units nor the packing pattern. In space group $P\bar{4}$, for example, Wyckoff sites (*a*), (*b*), (*c*) and (*d*) are equivalent origins. The centers of the geometric units for the pattern can be any of the following combinations:

B D	(*b*)(*d*)	(*d*)(*b*)	(*a*)(*c*)	(*c*)(*a*)
A C	(*a*)(*c*)	(*c*)(*a*)	(*b*)(*d*)	(*d*)(*b*)

They correspond to the four equivalent origins.

This work was supported by the Natural Sciences and Engineering Research Council of Canada. The author thanks Drs H. Burzlaff, W. Fischer, E. Koch, W. B. Pearson, H. Wondratshek and H. Zimmermann for their interest in this work and for discussions to ensure that the classification was made in accordance with the theory of automorphism, group–subgroup relationship and equivalent origins.

References

Booth, M. H., Brandon, J. K., Brizard, R. Y., Chieh, C. & Pearson, W. B. (1977). *Acta Cryst.* B**33**, 30–36.

Bradley, A. J. & Jones, P. (1933). *J. Inst. Met.* **51**, 131–162.

Burzlaff, H. & Zimmermann, H. (1980). *Z. Kristallogr.* **153**, 151–179.

Chabot, B., Cenzual, K. & Parthé, E. (1981). *Acta Cryst.* A**37**, 6–11.

Chieh, C. (1979). *Acta Cryst.* A**35**, 946–952.

Chieh, C. (1980). *Acta Cryst.* A**36**, 819–826.

Chieh, C. (1982). *Acta Cryst.* A**38**, 346–349.

Chieh, C., Burzlaff, H. & Zimmermann, H. (1982). *Acta Cryst.* A**38**, 746–747.

Dirichlet, P. G. L. (1850). *Jahrb. Rein Angew. Math.* **40**, 209–227.

Fischer, W., Burzlaff, H., Hellner, E. & Donnay, J. D. H. (1973). *Space Groups and Lattice Complexes. Natl Bur. Stand. (US) Mongr.* No. 134.

Fischer, W., Koch, E. & Hellner, E. (1971). *Neues Jahrb. Mineral. Monatsh.* pp. 227–237.

Hirshfeld, E. F. (1968). *Acta Cryst.* A**24**, 301–311.

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

International Tables for X-ray Crystallography (1972). Vol. II. Birmingham: Kynoch Press.

Koch, E. (1972). *Wirkungsbereichspolyeder und Wirkungsbereichsteilungen zu kubischen Gittercomplexen mit weniger als drei Freiheitsgraden.* Inaugural-Dissertation Philipps-Universtät Marburg.

Koch, E. & Fischer, W. (1975). *Acta Cryst.* A**31**, 88–95.

Matsumoto, T. & Wondratschek, H. (1979). *Z. Kristallogr.* **150**, 181–198.

Senechal, M. (1981). *Math. Mag.* **54-5**, 227–243.

Steinmetz, J., Rogues, B., Courtois, A. & Protas, J. (1979). *Acta Cryst.* B**35**, 2509–2514.

Wigner, E. & Seitz, F. (1933). *Phys. Rev.* **43**, 804–810.

Wondratschek, H. (1976). *Z. Kristallogr.* **143**, 460–470.