

Tetragonal-Packed Crystal Structures

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Abstract

The tetragonal packing arrangement is a new type of sphere packing [Baur (1981). *Mater. Res. Bull.* **16**, 339–345], in which the coordination number is eleven. It may be regarded formally as a special distortion of hexagonal close packing in which the sixfold axis is lost but a new fourfold axis is created. It may be described as a corrugated layer structure in which two equivalent sets of layers, at 90° to each other, occur. Various interstitial sites, including distorted and undistorted, tetrahedral and octahedral sites are present in a tetragonal-packed array. Structures which have an approximately tetragonal-packed anion array include rutile, Li_4GeO_4 , $\beta\text{-BeO}$ and its derivatives. The hollandite structure may be regarded as a tetragonal-packed structure on a unit-cell scale. Distorted structures whose oxide array is intermediate between hexagonal-close-packed and tetragonal-packed occur in, for example, Li_4SiO_4 , Li_3PO_4 , $\text{Li}_2\text{ZnSiO}_4$ and $\text{Li}_3\text{Zn}_{0.5}\text{GeO}_4$. The tetragonal-packed anion arrangement, and its various distorted forms, appears to be an important component of many solid electrolytes, especially Li^+ -ion conductors.

Introduction

Baur (1981) has recently shown that a new type of periodic sphere packing exists in which 71.87% of space is occupied. The sphere coordination number is eleven and he has named this arrangement tetragonal close packing (t.c.p.). He has identified this packing arrangement in several oxide structures, including rutile, β -beryllia and Li_4GeO_4 . We have also been aware (West, 1980) of the existence and properties of this packing arrangement for some time and present a summary of our conclusions here. Although many of these are the same as those of Baur, our approach is rather different and we have extended more widely our considerations to solid electrolytes.

Tetragonal packing – symmetry considerations

The new packing arrangement has a sphere density of 71.87%, which is somewhat less than the value of 74.05% in cubic and hexagonal close packing. For this reason, we prefer the name ‘tetragonal packing’ (t.p.), instead of the ‘tetragonal close packing’ proposed by Baur.

The t.p. arrangement may be readily visualized by regarding it as a special distortion of hexagonal close packing (h.c.p.); the close-packed layers in h.c.p., which are perpendicular to a sixfold symmetry axis, are corrugated in the t.p. arrangement and, therefore, lose their sixfold symmetry (Table 1). However, whereas h.c.p. contains c.p. layers in only one orientation, the t.p. arrangement contains identical, corrugated layers in two orientations at 90° to each other. This is shown in Fig. 1; in the t.p. arrangement (a), corrugated layers run horizontally and vertically but in h.c.p. (b), planar c.p. layers run horizontally only. Strongly corrugated layers (dashed) run vertically in (b) and these become partially straightened in the t.p. arrangement (a).

The t.p. arrangement contains fourfold symmetry with a 4_2 screw axis perpendicular to the plane of the paper, (a). Hence, although structural distortions normally lead to a loss of symmetry, this is accompanied in the present case by the creation of new symmetry, *i.e.* the fourfold axis. We believe, therefore,

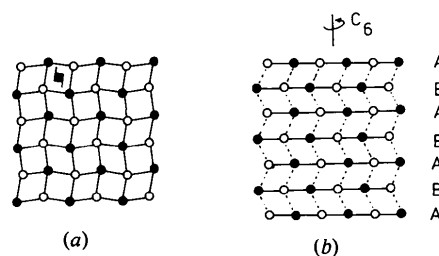


Fig. 1. Arrangement of spheres in (a) tetragonal packing, in projection down the fourfold axis, and (b) hexagonal close packing, with the sixfold axis vertically in the plane of the paper. Solid and open circles represent spheres at different heights.

Table 1. *Symmetry of hexagonal close packing and tetragonal packing*

	h.c.p.	t.p.
Principal symmetry axis	Sixfold	Fourfold
Number of equivalent packing orientations	1	2
Coordination number	12	11
Sphere density	74.05%	71.87%

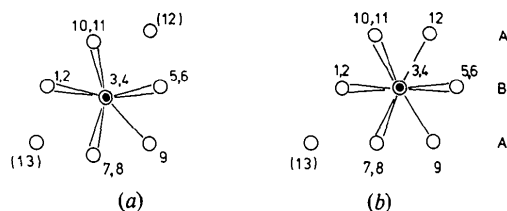


Fig. 2. Coordination numbers of (a) eleven in tetragonal packing, with two next-nearest neighbours, and (b) twelve in hexagonal close packing.

as does Baur, that the new t.p. arrangement, with its own symmetry characteristic (Table 1), should be regarded as a separate and independent packing arrangement.

The unit cell of a t.p. arrangement of spheres is tetragonal. The spheres are placed in positions $4(f)$ of space group $P4_2/mnm$; i.e. $x, x, 0$; $\bar{x}, \bar{x}, 0$; $\frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2}$; $\frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{2}$; $x = 0.2929$. The c/a ratio is, ideally, equal to 0.5858.

The sphere coordination number is eleven in t.p. in contrast to the value of twelve in h.c.p. and cubic close packed (c.c.p.) structures. This is shown in Fig. 2. The twelve equidistant neighbours around the shaded sphere in h.c.p. are shown in (b), but in t.p. (a) sphere number 12 is outside the first coordination sphere of the shaded atom. Sphere 13 is equivalent to sphere 12 in (a) and is moved closer to the shaded sphere, compared with its position in h.c.p. (b). Hence, the coordination number is eleven nearest neighbours with two next-nearest neighbours.

Cation sites in structures containing t.p. anions

(a) Undistorted tetrahedral and octahedral sites

Close-packed structures (h.c.p. and c.c.p.) contain two tetrahedral and one octahedral site per packing atom or anion. In t.p. structures, however, the nature of these interstitial sites is altered considerably: half of the sites remain the same shape but the other half become grossly distorted. Thus, one half of the octahedral sites are undistorted and are occupied by, for example, Ti in rutile (in fact, the coordination of Ti is slightly distorted since the oxide arrangement is not ideally t.p.). Similarly, one half of the tetrahedral sites are undistorted and are occupied by Be in β -BeO.

Table 2. *Coordinates of positions in a tetragonal, t.p. unit cell (space group $P4_2/mnm$)*

Position	Wyckoff notation	Coordinates
t.p. atom (P)	$4(f)$	$x, x, 0$; $x = 0.2929$
Octahedral site (E)	$2(a)$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
Tetrahedral site (B)	$4(g)$	$x, \bar{x}, 0$; $x = 0.3535$
Distorted octahedral site (A)	$4(c)$	$\frac{1}{2}, 0, 0$
Distorted tetrahedral site (D)	$4(d)$	$\frac{1}{2}, 0, \frac{1}{2}$
Distorted tetrahedral site (C)	$8(i)$	$x, y, 0$; $x = 0.5976, y = 0.0690$

The coordinates of these undistorted cation positions in the tetragonal unit cell are given in Table 2. The structure of rutile is shown in Fig. 3 in a familiar projection down the tetragonal c axis. A parallelogram with a bar across the short diagonal represents an octahedron, edge-on, such that parallel to c run columns of edge-sharing TiO_6 octahedra. The other half of the octahedral sites, which are grossly distorted in rutile, appear as squares, at X, X' , in projection. These distorted sites have the four equatorial bonds much longer than the two axial bonds; they are discussed in more detail later.

The structure of β -BeO may also be represented by Fig. 3. In this case, a parallelogram with a bar across the short diagonal represents a pair of edge-sharing, BeO_4 tetrahedra. The similarity in the oxide arrangements in rutile and β -BeO was noted by Smith, Cline & Austerman (1965). Their atomic coordinates, $x = 0.310$ for O and $x = 0.336$ for Be, are close to the ideal

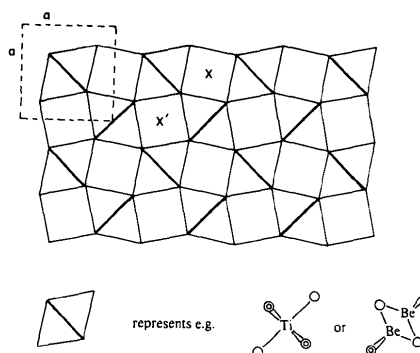


Fig. 3. Projection of the rutile structure down the tetragonal c axis. The same diagram also represents the β -BeO structure.

Table 3. Distances and angles in a tetragonal, t.p. unit cell

Distances are relative to a value of unity for the shortest distance between neighbouring t.p. atoms.

Position 1	Label (Fig. 4)	Position 2	Label (Fig. 4)	Distance	Number of equivalent distances	Description
0.2929, 0.2929, 0	<i>P</i>	0.2071, 0.7929, 0.5	<i>P'</i>	1.0000	11	t.p. atom-t.p. atom, nearest distance
0.2929, 0.2929, 0	<i>P</i>	0.7071, -0.2929, 0	<i>P''''</i>	1.2247	2	t.p. atom-t.p. atom, next-nearest distance
0.2929, 0.2929, 0	<i>P</i>	0.5000, 0.5000, 0.5000	<i>E</i>	0.7071	6	Octahedral site-t.p. atom
0.2929, 0.2929, 0	<i>P</i>	0.3535, 0.6465, 0	<i>B</i>	0.6123	4	Tetrahedral site-t.p. atom
0.2929, 0.2929, 0	<i>P</i>	0.5000, 0, 0	<i>A</i>	0.6123	2	Distorted octahedral site-t.p. atom
0.7929, 0.2071, 0.5000	<i>P''</i>	0.5000, 0, 0	<i>A</i>	0.7906	4	
0.2929, 0.2929, 0	<i>P</i>	0.5976, 0.0690, 0	<i>C</i>	0.6455	4	Distorted tetrahedral site-t.p. atom
0.2929, 0.2929, 0	<i>P</i>	0.5000, 0, 0.2500	<i>D</i>	0.6614	4	Distorted tetrahedral site-t.p. atom
0.3535, 0.6465, 0	<i>B</i>	0.3535, 0.6465, 1.0000	<i>B'''</i>	1.0000	2	Tetrahedral site-tetrahedral site, with common corner
0.3535, 0.6465, 0	<i>B</i>	0.1465, 0.1465, 0.5000	<i>B''</i>	1.0504	8	
0.3535, 0.6465, 0	<i>B</i>	0.6465, 0.3535, 0	<i>B'</i>	0.7071	1	Tetrahedral site-tetrahedral site, with common edge

Table 3 (cont.)

Central atom	Coordinated atom 1	Coordinated atom 2	Angle	Number of equivalent angles
Octahedral (<i>E</i>)	<i>P</i>	<i>P'</i>	90°	12
Distorted octahedral atom (<i>A</i>)	<i>P</i>	<i>P''</i>	90°	8
	<i>P''</i>	<i>P''''</i>	78° 28'	2
	<i>P''</i>	<i>P''''</i>	101° 32'	2
Tetrahedral atom (<i>B</i>)	<i>P</i>	<i>P'</i>	109° 29'	6
Distorted tetrahedral site (<i>D</i>)	<i>P''</i>	<i>P''''</i>	135° 34'	2
	<i>P</i>	<i>P''</i>	98° 14'	4
Distorted tetrahedral site (<i>C</i>)	<i>P</i>	<i>P''</i>	101° 32'	5
	<i>P</i>	<i>P''''</i>	143° 06'	1
Packing atom (<i>P</i>)	<i>E</i>	<i>E'</i>	90°	1
	<i>E</i>	<i>E''</i>	135°	2
Packing atom (<i>P</i>)	<i>B</i>	<i>B'</i>	70° 34'	1
	<i>B</i>	<i>B''</i>	118° 06'	4
	<i>B''</i>	<i>B''''</i>	109° 29'	1

values (Table 2), especially considering that the structure of β -BeO was solved from powder X-ray diffraction data recorded at very high temperature, ~2373 K.

A selection of bond distances and angles in an ideal t.p. structure is given in Table 3. In order to facilitate comparison between the different sites, all distances are given relative to a value of unity for the shortest distance between the packing atoms; hence each packing atom has 11 like nearest neighbours at a distance of 1.0000 and two next-nearest neighbours at a distance of 1.2247. On this basis, the tetragonal cell dimensions are $a = b = 1.7071$, $c = 1.0000$. From Table 3, the octahedral (*E*) and tetrahedral (*B*) sites both have undistorted coordination but the coordination of the packing atoms is less regular. For instance, in a rutile structure which is distorted to be ideally t.p., the anion (*P*) is coordinated to three cations in a planar arrangement but the angles are 90, 135 and 135° (instead of $3 \times 120^\circ$). Hence, it is not possible for both anion and cation simultaneously to have undis-

torted coordination. A similar effect occurs with the β -BeO structure; if the Be coordination is undistorted tetrahedral and the anion array is ideally t.p., then the (OBe_4) tetrahedron is grossly distorted, with one angle as small as 70° 34'.

It seems likely, therefore, that ideal, undistorted t.p. structures will occur rarely, if at all. Instead, structural distortions occur in order that (i) the anion coordination is somewhat more regular and (ii) cation-cation repulsions are minimized.

(b) Distorted sites

Octahedral. Half of the tetrahedral and octahedral sites in an h.c.p. structure suffer considerable distortion in a t.p. structure. These distorted sites are all located in the columns of square cross section in projection, centred at X, X' in Fig. 3. An unusual consequence of the structural distortion in the t.p. structure is that the number of distorted tetrahedral and octahedral sites in these columns in the t.p. array is double the number of equivalent, undistorted sites in an h.c.p. array. Two of the distorted octahedral sites are shown at A, A' in Fig. 4; they have coordinates $\frac{1}{2}, 0, 0$ and $\frac{1}{2}, 0, \frac{1}{2}$ and belong to the set of 4(c) sites (Table 2). In an h.c.p. array, position *A* would correspond to an octahedral site and position A' to a two-coordinate site situated midway along an octahedron edge. In Fig. 4, however, the four *P* atoms at $z = \pm \frac{1}{2}$ are displaced so as to be further from *A* and the two *P* atoms at $z = 0$ are moved closer to *A*, compared with their positions in an undistorted octahedral coordination (e.g. as at site *E*). On the other hand, the two *P* atoms at $z = \frac{1}{2}$ are displaced so as to be further from A' and the four *P* atoms at $z = 0, 1$ are closer to A' than in an h.c.p. structure. Consequently, sites A, A' are similar, grossly distorted octahedral sites in which four bonds are considerably longer than the other two (Table 3). In addition, the coordination is further distorted such that four of the twelve angles are not equal to 90° (Table 3).

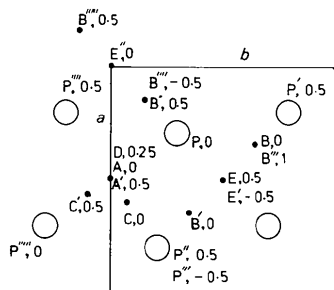


Fig. 4. Distorted and undistorted sites for cations in a tetragonal-packed anion structure.

This means that the four equatorial bonds of the distorted octahedron are rectangular-planar instead of square-planar. The two sites A, A' have four P atoms in common: P, P'', P''', P'''' (Fig. 4). On comparing the sizes of the undistorted (E) and distorted (A) octahedral sites (Fig. 4 and Table 3), it can be seen that while four of the $A-P$ bonds are $\sim 12\%$ longer than the $E-P$ bonds, two of the $A-P$ bonds are $\sim 13\%$ shorter.

Tetrahedral. Two types of distorted tetrahedral sites may be identified. Sites D lie midway between the distorted octahedral sites A, A' and have coordinates such as $\frac{1}{2}, 0, \frac{1}{4}$ in a $4(d)$ set (Fig. 4 and Table 2). These sites are considerably larger than the undistorted, B sites with $D-P$ bonds about 8% longer than $B-P$ bonds, but the angles are rather different from the ideal tetrahedral values.

Sites C are equivalent to the sites B in an h.c.p. structure but are distorted in the t.p. structure. In addition, there are twice as many of these C sites (C, C') – eight per unit cell – as there are B sites. The $C-P$ bonds are $\sim 5\%$ longer than the $B-P$ bonds but the tetrahedra are distorted with one very large angle, $143^\circ 6'$.

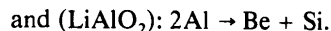
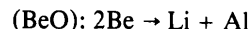
From a consideration of the shapes of the distorted octahedral and tetrahedral sites, it seems more likely that the tetrahedral sites would be occupied and an unusual feature of the t.p. structures is the large number of available tetrahedral sites. Normal close-packed structures (h.c.p. and c.c.p.) contain two undistorted tetrahedral sites per packing atom or anion. However, the t.p. structure contains twice as many (one undistorted and three distorted) tetrahedral sites per packing atom. While the distorted sites are unlikely to be occupied by highly charged cations such as Si, Ge or Ti, they may be occupied by smaller alkali ions, especially Li^+ . The distorted nature of these sites and especially the size and shape of the faces or bottle-necks between adjacent sites may account for high Li^+ -ion conductivity in a considerable number of oxides with t.p. and related structures.

More complex, t.p.-related structures

Structures containing ideally t.p. anions appear to occur rather infrequently, probably because, as stated earlier, it is not possible to satisfy the requirement that both anions and cations have a regular, symmetrical coordination within a t.p. anion framework. Thus, Baur (1981) gives a list of structures which contain essentially t.p. anions and the c/a ratio in these is usually considerably different from the ideal value of 0.5858. We consider some of these and other distorted t.p. structures in more detail.

$\gamma\text{-LiAlO}_2$ and $\gamma\text{-Li}_2\text{BeSiO}_4$

These two structures are derived from the $\beta\text{-BeO}$ structure by a direct cation-substitution mechanism (Baur, 1981; Howie & West, 1974; West, 1975):



Thus, whereas $\beta\text{-BeO}$ contains pairs of edge-sharing BeO_4 tetrahedra, LiO_4 and AlO_4 tetrahedra form edge-sharing pairs in $\gamma\text{-LiAlO}_2$, and in $\gamma\text{-Li}_2\text{BeSiO}_4$, LiO_4 , BeO_4 and LiO_4 , SiO_4 tetrahedra form edge-sharing pairs. Because of the considerable difference in size of LiO_4 and the other tetrahedra, a considerable structural distortion occurs but, apart from this, the structures may be regarded as t.p. $\gamma\text{-NaAlO}_2$ and $\gamma\text{-NaFeO}_2$ also appear to have the $\gamma\text{-LiAlO}_2$ structure (West, 1975).

Li_4GeO_4 (Völlenkle & Wittmann, 1969)

This is a more distant relative of the $\beta\text{-BeO}$ structure. Although it has a large orthorhombic unit cell, the structure may be referred to the tetragonal pseudocell (Fig. 4), in order to show the relation to $\beta\text{-BeO}$. Sites B, B' contain Li^+ ions which, therefore, form columns of edge-sharing tetrahedra parallel to the tetragonal c axis. Sites B'' and B''' which are occupied by Be in $\beta\text{-BeO}$, are alternately empty and contain Ge atoms. The remaining Li^+ ions occupy, in ordered fashion, one quarter of the C sites, which are empty in $\beta\text{-BeO}$. The oxide ions are approximately t.p.

Structures which are intermediate between t.p. and h.c.p.

t.p. structures may be regarded as distorted h.c.p. structures and *vice versa*, as shown in Fig. 1. In some complex structures, however, the anion layers are only partially distorted so as to be intermediate between h.c.p. and t.p., as shown in the following examples.

Li_4SiO_4 (Völlenkle, Wittmann & Nowotny, 1968; Tranqui, Shannon, Chen, Ijima & Baur, 1979)

The arrangement of some of the oxide ions is shown in Fig. 5; corrugated layers of oxide ions run vertically in a t.p. type of array. Horizontally, however, the layers have both corrugated and planar segments that form ribbons parallel to the monoclinic c axis. A planar ribbon is shown by the line $R-R'$, in projection, whereas atoms $S-S'$ form part of a corrugated ribbon. In the b direction planar ribbons alternate with corrugated ribbons (not shown) and *vice versa*. The structure, therefore has features of both h.c.p. and t.p. structures.

$\gamma\text{-Li}_3\text{PO}_4$, $\gamma\text{-Li}_2\text{ZnSiO}_4$, $\text{Li}_3\text{Zn}_{0.5}\text{GeO}_4$, etc. (West, 1975; Plattner & Völlenkle, 1979; Zemmann, 1960; Hong, 1978)

The family of γ -tetrahedral oxides, in which all atoms have coordination number 4, has been discussed above with the structures of $\beta\text{-BeO}$, $\gamma\text{-LiAlO}_2$ and $\gamma\text{-Li}_2\text{BeSiO}_4$. It also includes compounds such as Li_3XO_4 : $X = \text{P, As, V}$, and Li_2MYO_4 : $\text{MY} = \text{MgSi, MgGe, ZnGe, ZnSi, CoSi}$, as well as solid solutions based on these systems which contain interstitial Li^+ ions, e.g. $\text{Li}_{2+2x}\text{Zn}_{1-x}\text{GeO}_4$ (LISICON).

The oxide arrangement in these structures is also intermediate between that of h.c.p. and t.p. but in a

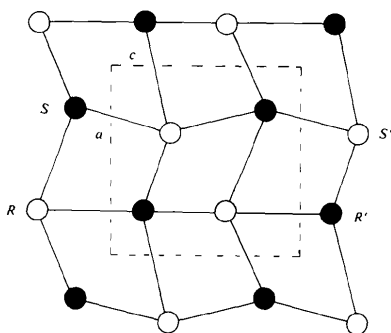


Fig. 5. Arrangement of oxide ions in Li_4SiO_4 . Solid and open circles represent atoms at two different b heights. The unit cell contains atoms at essentially four different b heights and only half of the structure is shown.

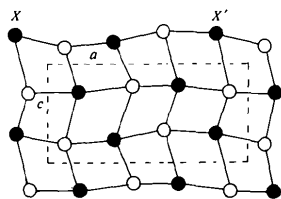


Fig. 6. Oxide arrangement in γ -tetrahedral structures such as $\gamma\text{-Li}_3\text{PO}_4$ and $\text{Li}_{3,0}\text{Zn}_{0,5}\text{GeO}_4$. Only half of the structure in the b direction is shown.

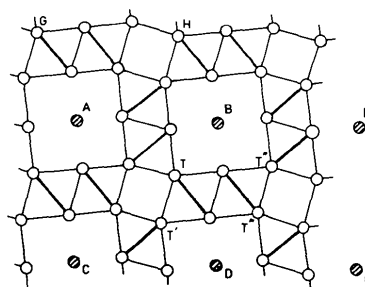


Fig. 7. Arrangement of oxide ions in the hollandite structure. Open circles are oxide ions. Shaded circles are large cations such as K^+ , Ba^{2+} or Pb^{2+} .

different way to Li_4SiO_4 . The oxide arrangement in $\text{Li}_3\text{Zn}_{0,5}\text{GeO}_4$ is shown in Fig. 6. Corrugated layers run vertically as in a t.p. arrangement. Corrugated layers also run horizontally but the repeat unit is now twice that in a t.p. arrangement and contains four atoms in projection, e.g. from X to X' . Hence, the horizontal layers are considerably more planar than in a t.p. arrangement and may be regarded as intermediate between t.p. and h.c.p.

The hollandite structure (Byström & Byström, 1950, 1951)

This structure also has characteristics of both h.c.p. and t.p. structures, not by virtue of a partial distortion, as in the above cases, but as a kind of intergrowth on an atomic scale. The structure is shown in Fig. 7. Corrugated layers run vertically and horizontally but, considered over the structure as a whole, the corrugation is different from that in t.p. structures. The volume element (in projection) enclosed by $ABCD$ is t.p., as are adjacent volume elements such as $BDEF$. However, a change in sign of the corrugation does not occur to either side of B and D . Hence, the sequence from, for example, G to H contains a three-atom repeat unit of the type \dots zig-zig-zag \dots as opposed to the two-atom repeat \dots zig-zag \dots in t.p. structures. The structure may therefore be regarded as built of columns which have a t.p. structure but the interface between adjacent columns is more like h.c.p., with planar segments of oxide layers across the interface; e.g., the area enclosed by T, T', T'', T''' appears to be h.c.p.

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An Electron Diffraction Study of the Structures of Sulphur Hexafluoride below 94 K

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Abstract

Single-crystal electron diffraction patterns were obtained from SF₆ crystals condensed in an environmental cell in a 200 kV transmission electron microscope. Between 50 ± 5 K and 94 K the lattice was found to be hexagonal, with $a = 8.01$ (12) and $c = 4.83$ (7) Å. Consideration of the packing of SF₆ molecules shows that this phase is isostructural with UCl₆, having space group $P\bar{3}m1$ with $Z = 3$. At lower temperatures ($T < 50 \pm 5$ K) this structure was found to distort slightly to a C face-centred monoclinic (or conceivably even lower symmetry) lattice with $a = 8.01$ (12), $b = 13.9$ (2), $c = 4.83$ (7) Å and $\beta = 92.5$ (5)° with $Z = 6$. These observations are correlated with previous NMR and Raman-scattering results.

Introduction

Sulphur hexafluoride belongs to a group of transition-metal and Group VIa hexafluorides which all have broadly similar structural properties (Taylor, 1976). With the exception of the actinide hexafluorides they condense initially into an orientationally disordered body-centred cubic structure, which is characterized by rapid molecular reorientation and low barriers to molecular self-diffusion. At lower temperatures a phase transition occurs to a lower-symmetry structure. The crystallography of the low-temperature phase of several transition-metal hexafluorides has been determined

(Levy, Taylor & Wilson, 1975). They have been found to be isostructural with UF₆ (Levy, Taylor & Wilson, 1976), being orthorhombic, with space group $Pnma$ and $Z = 4$. It appears, however, that no low-temperature crystallographic work has been carried out on SF₆ or any of the other Group VIa hexafluorides.

SF₆ condenses at 222.4 K and undergoes a phase transition to the low-temperature phase at 94 K. Neutron diffraction (Taylor & Waugh, 1976; Dolling, Powell & Sears, 1979) and NMR (Blinic & Lahajnar, 1967) studies of the high-temperature phase confirm the b.c.c. structure and the orientational disorder of the molecules. Some orientational order is present since the S–F bonds tend to be aligned along $\langle 100 \rangle$ directions.

NMR of the low-temperature phase (Garg, 1977) suggests that molecules occupy two inequivalent lattice sites, with a fraction of $\sim \frac{1}{4}$ of the molecules still undergoing quite rapid reorientation while the rest are orientationally more ordered. The results of a study of the Raman spectrum (Gilbert & Drifford, 1972) appear to confirm the presence of two inequivalent lattice sites.

In the present work, selected-area electron diffraction was used to study the low-temperature phase of SF₆. The advantage of this method over X-ray or neutron diffraction lies in the fact that the diffraction pattern is collected from an area of crystal only $\sim 1 \mu\text{m}^2$ in size. Hence single-crystal patterns could be obtained even though it was not possible to prepare crystals larger than a few μm in diameter. Because of the dynamical nature of electron diffraction, it was not possible to determine the structure factors. However, having found the unit-cell dimensions, it was possible to determine the approximate atomic positions from consideration of the packing of SF₆ molecules.

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