Assignment 2

Space Groups, Reciprocal Lattice Space, Miller Indices
Please no AI-generated solutions. Would be your loss!
Relevant space groups are attached towards the end.

Question 1

Let's understand some nomenclature here. Consider the orthorhombic space group $Pmc2_1$. The notation tells us that the lattice type is primitive, and there is:

(a) a mirror plane perpendicular to the x (or a) axis,

(b) a glide plane perpendicular to the y (or the b) axis. This means mirror planes passing through the (010) and (020) and each followed by translation $\vec{c}/2$.

(c) A $\mathbf{2}_1$ screw axis along the z (or the c) axis.

Use a clinographic projection to find out the 4 equivalent positions in the unit cell, showing your working as you go along.

Question 2

Diamond belongs to the $Fd\bar{3}m$ with atoms in the $8a$ positions. The relevant pages for this space group, taken from the International Table of crystallography are shown towards the end of this Assignment.

(a) What is the underlying crystal system?

(b) What is the underlying Bravais lattice?

(c) Draw a clinographic projection showing all 8 atoms inside the unit cell. This projection can be drawn by looking down the z (or the c) axis. Identify the 8 atoms by suitable labels and mark the fractional elevation of atoms (if $z > 0$).

(d) A four fold screw axis exists at $(\frac{1}{2}, \frac{1}{4}, 0)$. Mark its position and demonstrate the action of $\mathbf{4}_1, \mathbf{4}_2, \mathbf{4}_3$ screw operations on any atom of your choice. Clarify your working.

(e) A diamond glide plane also exists at the height $z = \frac{1}{8}$ following by the translation of $\frac{\vec{a}}{4} + \frac{\vec{b}}{4}$. Show by its action on any atom of your choice that this is indeed a symmetry operation.

(f) The m in the $Fd\bar{3}m$ space group symbol denotes a mirror plane along the face diagonal. Verify that it indeed exists in this structure.

(g) The diamond structure has a centre of inversion at $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$. Verify this statement.

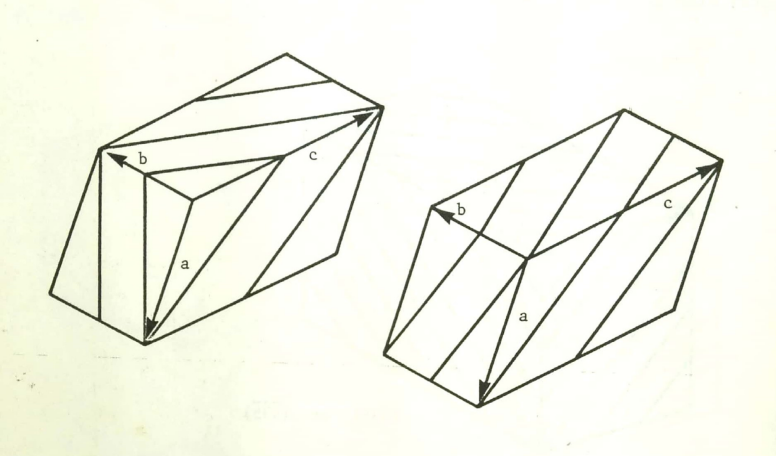
(h) In the diamond structure, there are two kinds of $8a$ positions. Show that for each kind, there is a distinct set of vectors joining the atom with its nearest neighbour.

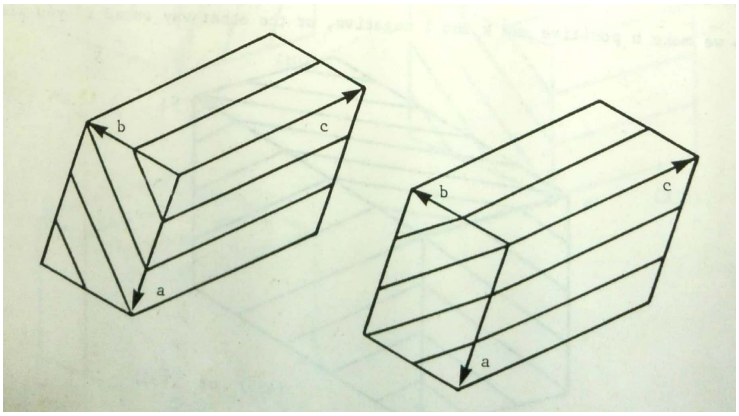
(i) A closely related structure is Zincblende (ZnS) which belongs to the space group $F\bar{4}3m$. By looking up the entry of this space group, draw a clinographic projection by placing Zn at the $4a$ site and S at the $4c$ sites. Where are all the atoms located inside the unit cell?

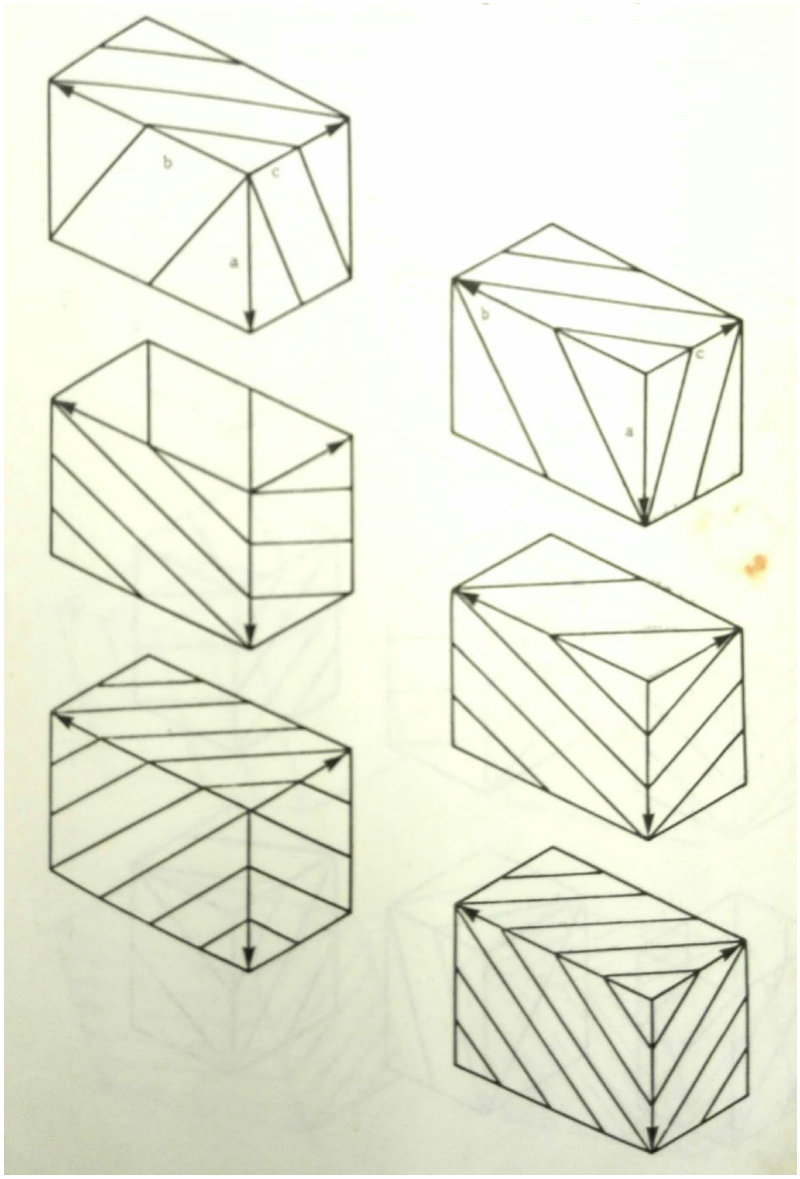
(j) Does this zincblende structure have a center of symmetry?

Question 3

Give the Miller indices to all the planes shown in the following **10** diagrams. Note the origin is specified on the top right owner.

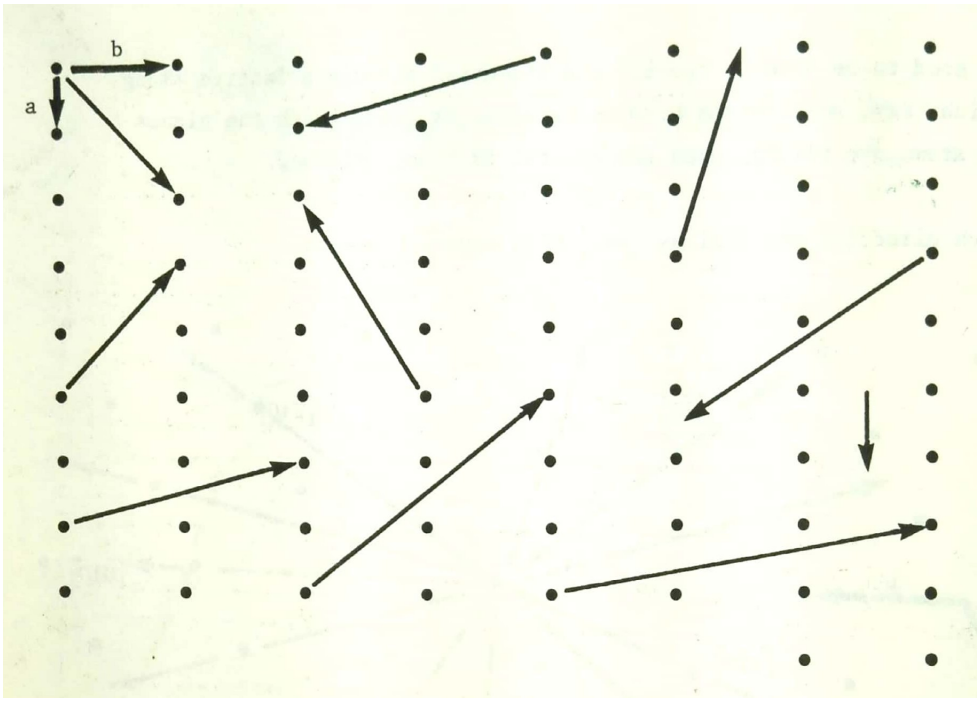


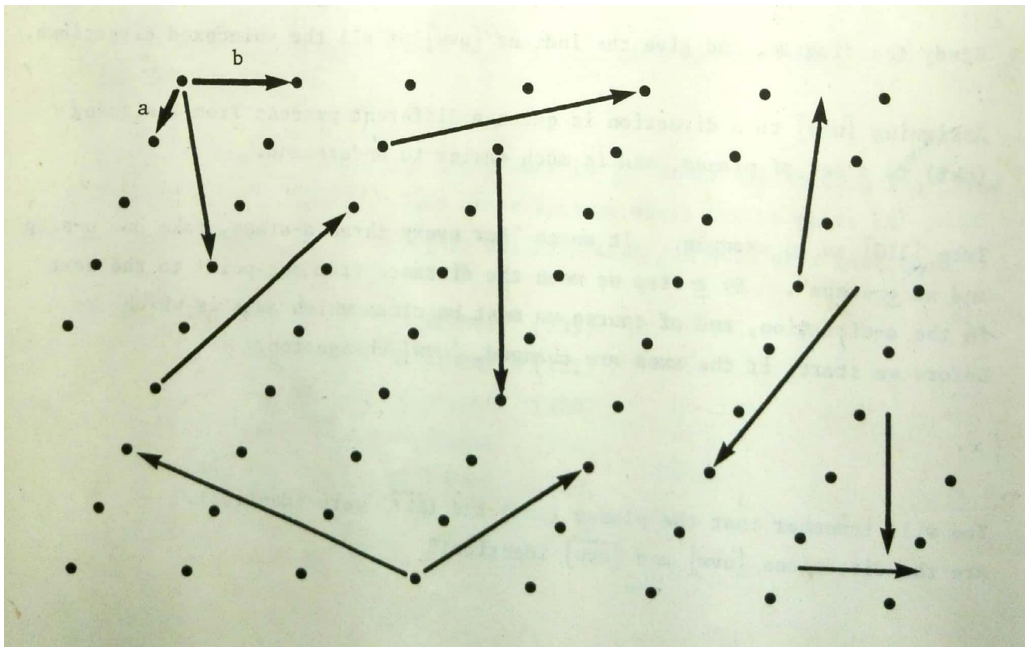

b
c
a
b
c
a


b
c
a
b
c
a

Question 4

Give the Miller indices $[uvw]$ of all directions shown below for the orthorhombic and monoclinic lattices, respectively. Be sure of the axis before starting. For simplicity here, all directions shown are in the plane of the paper, so $w = 0$ in all cases.





Question 5

Show that the reciprocal lattice of a face-centered cubic direct lattice is a body-centered lattice. Start by picking any lattice point and forming the primitive unit cell by identifying $\vec{a}$, $\vec{b}$ and $\vec{c}$ that connect the lattice point to the three neighbouring points. Then, form $\vec{a}^*$, $\vec{b}^*$ and $\vec{c}^*$.

Question 6

(a) Show clearly, with all steps, that the Fourier transformation of a direct lattice is indeed the reciprocal lattice.

(b) Prove the shift theorem used in Fourier theory, i.e., if in 1D,

$$\mathcal{F}(f(x)) = \hat{F}(k)$$
$$\mathcal{F}(f(x-a)) = \hat{F}(k)e^{-ika}$$

Question 7

For the $Im\bar{3}m$ space group, answer the following questions.

(a) What symmetry operation takes $x,\ y,\ z$ to $z,\ y,\ x$?

(b) What symmetry operation takes $x,\ y,\ z$ to $z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}$?

Show your working, preferably with a sketch and geometrical considerations. Recall that glide planes are written in the form

$$a, \quad b, \quad c, \quad n(\cdots), \quad d(\cdots),$$

where the entries inside parentheses indicate the direction of the translation component that follows the mirror reflection.

Question 8

Consider the space group $P4/n$ ($C_{4\mathrm{h}}^3$).

(a) From the point group $C_{4\mathrm{h}}$ construct its projection seen along the c-axis, showing the general locations.

(b) Show that there exists a centre of inversion $\bar{1}$ at $\frac{1}{4}, \frac{1}{4}, 0$.

(c) Is there a glide plane included in the "symmetry operations", and what is its action on a general location $x,\ y,\ z$?

Question 9

What coordinates are generated from a point $x,\ y,\ z$ if we apply:

(a) a c-glide at $x,\ \frac{1}{4},\ z$ followed by a 2, screw rotation about an axis through $[0, y, \frac{1}{4}]$?

(b) an n-glide at $x,\ 0,\ z$ followed by a 4_2 screw about $[\frac{1}{4}, 0, z]$?

(c) What happens in (a) if the two operations are applied in reverse?

Question 10

Lead zirconate-titanate $PbZrO_3$ (PZT) is a perovskite which belongs to the $Pm\bar{3}m$ space group. Its motif is:

$$\begin{aligned} \text{Pb}: &\quad 000 \\ \text{Zr}: &\quad \frac{1}{2}\frac{1}{2}\frac{1}{2}, \\ \text{3 O}: &\quad \frac{1}{2}00, \qquad 0\frac{1}{2}0, \qquad 00\frac{1}{2}, \end{aligned}$$

(a) Draw its structure (preferably in $3D$) and identify the Wycoff positions.

(b) Explain how a Zr atom is surrounded by O atoms.

Question 11

Gadolinium orthoferrite, $GdFeO_3$, is orthorhombic with lattice parameters $a = 5.349$ Å, $b = 5.611$ Å, $c = 7.669$ Å and space group $Pbmn$ (or $Pnma$). The coordinates of the atoms in the unit cell are:

$$\begin{aligned} \text{Gd}^{3+}: &\quad \pm(x, \tfrac{1}{2}+y, \tfrac{1}{4});\ \pm\left(\tfrac{1}{2}-x,\ y,\ \tfrac{1}{4}\right) \text{ with } x = 0.984,\ y = 0.063. \\ \text{Fe}^{3+}: &\quad (0,0,0);\ (0,0,\tfrac{1}{2});\ (\tfrac{1}{2},\tfrac{1}{2},0);\ (\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}). \\ \text{O}^{2-}: &\quad \pm(x, \tfrac{1}{2}+y, \tfrac{1}{4});\ \pm\left(\tfrac{1}{2}-x,\ y,\ \tfrac{1}{4}\right) \text{ with } x = 0.101,\ y = 0.467. \\ \text{O}^{2-}: &\quad \pm(x, \tfrac{1}{2}+y, z);\ \pm(x, \tfrac{1}{2}+y, \tfrac{1}{2}-z);\ \pm\left(\tfrac{1}{2}+x,\ \bar{y},\ \bar{z}\right);\ \pm\left(\tfrac{1}{2}+x,\ \bar{y},\ \tfrac{1}{2}+z\right) \\ &\qquad \text{with } x = 0.696,\ y = 0.302,\ z = 0.051. \end{aligned}$$

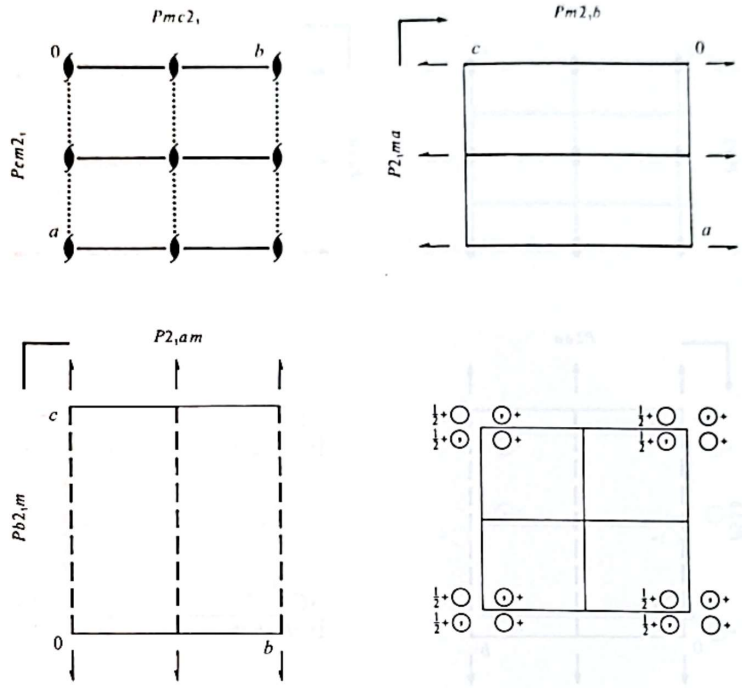
Draw an accurate plan on the (001) plane of one unit cell of the structure, using a scale of 20 mm to 1 Å. Mark on the plan all the symmetry elements present. The ferric cations are in six-fold coordination to oxygen anions, each Fe^{3+} having as its nearest neighbours six O^{2-} situated at the apices of a nearly regular octahedron. Identify the six nearest

neighbours of the Fe^{3+} ion at $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

How many independent Fe–O distances are there?

Orthorhombic $mm2$ C_{2v}^2 $Pmc2_1$

Patterson symmetry $Pmmm$ $Pmc2_1$ No. 26



Origin on $mc2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) c $x,0,z$ (4) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
4 c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	$h0l$: $l=2n$ $00l$: $l=2n$
					Special: no extra conditions
2 b m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$			
2 a m . .	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

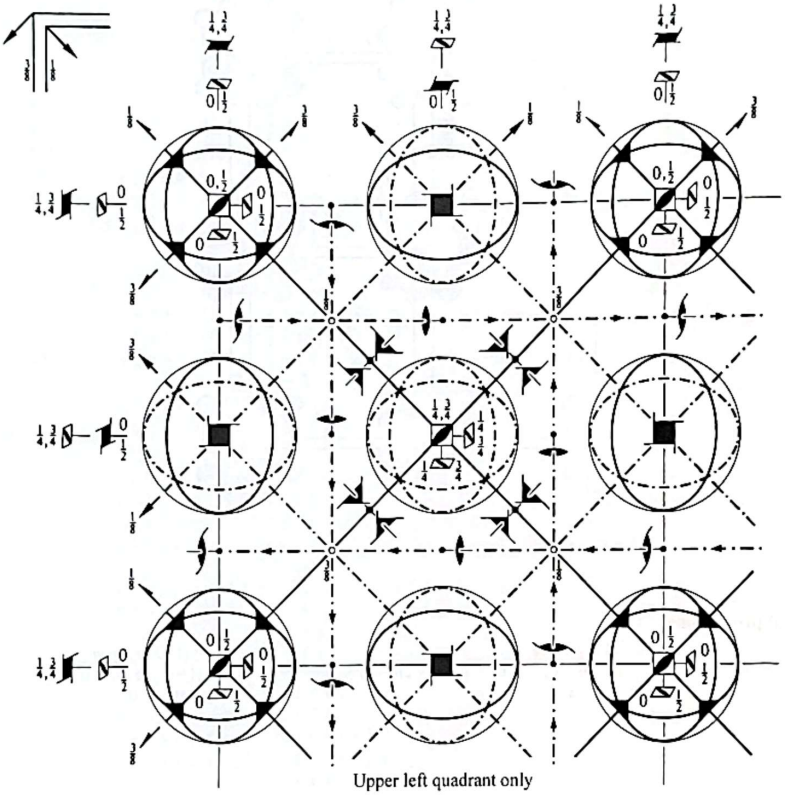
Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

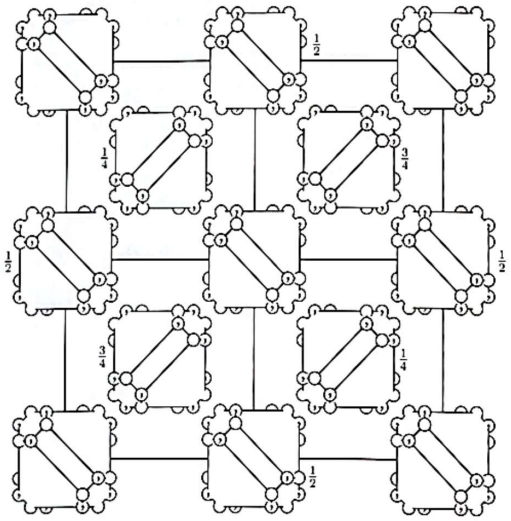
$F\,d\,\bar{3}\,m$ O_h^7 $m\bar{3}m$ Cubic

No. 227 $F\ 4_1/d\ \bar{3}\ 2/m$ Patterson symmetry $F\,m\bar{3}\,m$

ORIGIN CHOICE 1



Upper left quadrant only



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No. 227 $F\,d\,\bar{3}\,m$

Origin at $\bar{4}\,3m$, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre $(\bar{3}m)$

Asymmetric unit $0\le x\le\frac{1}{2};\quad 0\le y\le\frac{1}{8};\quad -\frac{1}{8}\le z\le\frac{1}{8};\quad y\le\min(\frac{1}{2}-x,x);\quad -y\le z\le y$

Vertices $0,0,0\quad \frac{1}{2},0,0\quad \frac{3}{8},\frac{1}{8},\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}\quad \frac{3}{8},\frac{1}{8},-\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},-\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) $2(0,0,\frac{1}{4})\ 0,\frac{1}{4},z$
(3) $2(0,\frac{1}{4},0)\ \frac{1}{4},y,0$
(4) $2(\frac{1}{4},0,0)\ x,0,\frac{1}{4}$
(5) $3^+\ x,x,x$
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-\ x,x,x$
(10) $3^-\ x,\bar{x}+\frac{1}{2},\bar{x}$
(11) $3^-\ \bar{x}+\frac{1}{2},\bar{x},x$
(12) $3^-\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ x,x-\frac{1}{4},\frac{3}{8}$
(14) $2\ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{1}{4})\ \frac{1}{2},\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})\ 0,\frac{1}{4},z$
(17) $4^-(\frac{3}{4},0,0)\ x,\frac{1}{2},\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})\ \frac{3}{8},y+\frac{1}{4},y$
(19) $2\ \frac{1}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)\ x,0,\frac{1}{4}$
(21) $4^+(0,\frac{1}{4},0)\ \frac{3}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})\ x-\frac{1}{4},\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)\ \frac{1}{4},y,\frac{1}{2}$
(24) $2\ \bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(26) $d(\frac{1}{4},\frac{3}{4},0)\ x,y,\frac{1}{8}$
(27) $d(\frac{1}{4},0,\frac{1}{4})\ x,\frac{3}{8},z$
(28) $d(0,\frac{1}{4},\frac{3}{4})\ \frac{1}{8},y,z$
(29) $\bar{3}^+\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(30) $\bar{3}^+\ \bar{x}-1,x+1,\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{7}{8}$
(31) $\bar{3}^+\ x,\bar{x}+1,\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{1}{8}$
(32) $\bar{3}^+\ \bar{x}+1,\bar{x},x;\ \frac{7}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^-\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(34) $\bar{3}^-\ x+\frac{3}{2},\bar{x}-1,\bar{x};\ \frac{5}{8},-\frac{1}{8},\frac{7}{8}$
(35) $\bar{3}^-\ \bar{x}+\frac{1}{2},\bar{x}+\frac{3}{2},x;\ -\frac{1}{8},\frac{7}{8},\frac{5}{8}$
(36) $\bar{3}^-\ \bar{x}+1,x+\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{5}{8},-\frac{1}{8}$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})\ x+\frac{1}{4},\bar{x},z$
(38) $m\ x,x,z$
(39) $\bar{4}^-\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+\ \frac{1}{2},0,z;\ \frac{1}{2},0,0$
(41) $\bar{4}^-\ x,-\frac{1}{4},\frac{1}{4};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})\ x,y+\frac{1}{4},\bar{y}$
(43) $m\ x,y,y$
(44) $\bar{4}^+\ x,\frac{1}{2},0;\ 0,\frac{1}{2},0$
(45) $\bar{4}^+\ 0,y,\frac{1}{2};\ 0,0,\frac{1}{2}$
(46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})\ \bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-\ \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(48) $m\ x,y,x$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) $2\ 0,0,z$
(3) $2\ \frac{1}{4},y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x-\frac{1}{3},x-\frac{1}{6},x$
(6) $3^+\ \bar{x}+\frac{1}{2},x,\bar{x}$
(7) $3^+\ x,\bar{x},\bar{x}$
(8) $3^+\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x-\frac{1}{6},x+\frac{1}{6},x$
(10) $3^-\ x+\frac{1}{2},\bar{x},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-\ \bar{x},x,\bar{x}$
(13) $2(\frac{1}{4},\frac{3}{4},0)\ x,x,\frac{1}{8}$
(14) $2(-\frac{1}{4},\frac{1}{4},0)\ x,\bar{x}+\frac{1}{2},\frac{3}{8}$
(15) $4^-(0,0,\frac{1}{4})\ \frac{1}{4},0,z$
(16) $4^+(0,0,\frac{1}{2})\ \frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)\ x,\frac{1}{2},-\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})\ \frac{3}{8},y-\frac{1}{4},y$
(19) $2\ \frac{1}{8},y+\frac{3}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)\ x,0,\frac{1}{4}$
(21) $4^+(0,\frac{3}{4},0)\ \frac{1}{2},y,-\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})\ x,\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)\ 0,y,\frac{3}{4}$
(24) $2(-\frac{1}{4},0,\frac{1}{4})\ \bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}\ \frac{1}{8},\frac{3}{8},\frac{3}{8}$
(26) $d(\frac{1}{4},\frac{1}{4},0)\ x,y,\frac{1}{8}$
(27) $d(\frac{1}{4},0,\frac{1}{4})\ x,\frac{1}{8},z$
(28) $d(0,\frac{3}{4},\frac{1}{4})\ \frac{3}{8},y,z$
(29) $\bar{3}^+\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$
(30) $\bar{3}^+\ \bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{8},\frac{5}{8},\frac{7}{8}$
(31) $\bar{3}^+\ x,\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{8},\frac{3}{8},-\frac{1}{8}$
(32) $\bar{3}^+\ \bar{x}+1,\bar{x}-\frac{1}{2},x;\ \frac{7}{8},-\frac{5}{8},\frac{1}{8}$
(33) $\bar{3}^-\ x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$
(34) $\bar{3}^-\ x+1,\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{5}{8},\frac{7}{8}$
(35) $\bar{3}^-\ \bar{x},\bar{x}+1,x;\ -\frac{1}{8},\frac{7}{8},\frac{1}{8}$
(36) $\bar{3}^-\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{3}{8},\frac{1}{8},-\frac{1}{8}$
(37) $m\ x+\frac{1}{2},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\ x-\frac{1}{4},x,z$
(39) $\bar{4}^-\ 0,0,z;\ 0,0,0$
(40) $\bar{4}^+\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-\ x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})\ x,y+\frac{1}{4},\bar{y}$
(43) $g(0,\frac{1}{2},\frac{1}{2})\ x,y,y$
(44) $\bar{4}^+\ x,0,0;\ 0,0,0$
(45) $\bar{4}^+\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) $m\ \bar{x},y,x$
(47) $\bar{4}^-\ \frac{1}{4},y,0;\ \frac{1}{2},0,0$
(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\ x-\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) $2\ \frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)\ 0,y,\frac{1}{4}$
(4) $2\ x,0,0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},x-\frac{1}{6},x$
(6) $3^+\ \bar{x},x,\bar{x}$
(7) $3^+\ x+\frac{1}{2},\bar{x},\bar{x}$
(8) $3^+\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x-\frac{1}{6},x-\frac{1}{3},x$
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-\ \bar{x},\bar{x},x$
(12) $3^-\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\ x,x,\frac{1}{8}$
(14) $2(\frac{1}{4},-\frac{1}{4},0)\ x,\bar{x}+\frac{1}{2},\frac{3}{8}$
(15) $4^-(0,0,\frac{1}{4})\ \frac{1}{4},0,z$
(16) $4^+(0,0,\frac{1}{2})\ -\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)\ x,\frac{1}{4},0$
(18) $2(0,\frac{3}{4},\frac{3}{4})\ \frac{1}{8},y,y$
(19) $2(0,-\frac{1}{4},\frac{1}{4})\ \frac{3}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)\ x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)\ \frac{1}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})\ x+\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{1}{4},0)\ -\frac{1}{4},y,\frac{1}{2}$
(24) $2\ \bar{x}+\frac{3}{4},\frac{1}{8},x$
(25) $\bar{1}\ \frac{3}{8},\frac{1}{8},\frac{3}{8}$
(26) $d(\frac{3}{4},\frac{3}{4},0)\ x,y,\frac{1}{8}$
(27) $d(\frac{1}{4},0,\frac{3}{4})\ x,\frac{3}{8},z$
(28) $d(0,\frac{1}{4},\frac{1}{4})\ \frac{1}{8},y,z$
(29) $\bar{3}^+\ x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$
(30) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{3}{8}$
(31) $\bar{3}^+\ x-\frac{1}{2},\bar{x}+\frac{3}{2},\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{5}{8}$
(32) $\bar{3}^+\ \bar{x}+\frac{3}{2},x+\frac{1}{2},x;\ \frac{7}{8},-\frac{1}{8},\frac{5}{8}$
(33) $\bar{3}^-\ x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$
(34) $\bar{3}^-\ x+1,\bar{x}-1,\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{7}{8}$
(35) $\bar{3}^-\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{8},\frac{3}{8},\frac{1}{8}$
(36) $\bar{3}^-\ \bar{x}+\frac{3}{2},x-\frac{1}{2},\bar{x};\ \frac{7}{8},-\frac{5}{8}$
(37) $m\ x,\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\ x+\frac{1}{4},x,z$
(39) $\bar{4}^-\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},0$
(40) $\bar{4}^+\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-\ x,0,0;\ 0,0,0$
(42) $m\ x,y+\frac{1}{2},\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\ x,y-\frac{1}{4},y$
(44) $\bar{4}^+\ x,\frac{1}{4},-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+\ 0,y,0;\ 0,0,0$
(46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})\ \bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(48) $g(\frac{1}{2},0,\frac{1}{2})\ x,y,x$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) $2(0,0,\frac{1}{2})\ \frac{1}{4},0,z$
(3) $2\ 0,y,0$
(4) $2\ x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},x+\frac{1}{3},x$
(6) $3^+\ \bar{x},x+\frac{1}{2},\bar{x}$
(7) $3^+\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{3},x+\frac{1}{6},x$
(10) $3^-\ x,\bar{x},\bar{x}$
(11) $3^-\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ x,x+\frac{1}{4},\frac{3}{8}$
(14) $2\ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{3}{4})\ \frac{1}{2},-\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})\ 0,\frac{1}{4},z$
(17) $4^-(\frac{1}{4},0,0)\ x,\frac{3}{4},0$
(18) $2(0,\frac{1}{4},\frac{1}{4})\ \frac{1}{8},y,y$
(19) $2(0,\frac{1}{4},-\frac{1}{4})\ \frac{3}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)\ x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)\ \frac{1}{2},y,\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})\ x,\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)\ 0,y,\frac{1}{4}$
(24) $2(\frac{1}{4},0,-\frac{1}{4})\ \bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}\ \frac{3}{8},\frac{3}{8},\frac{1}{8}$
(26) $d(\frac{3}{4},\frac{1}{4},0)\ x,y,\frac{3}{8}$
(27) $d(\frac{1}{4},0,\frac{1}{4})\ x,\frac{1}{8},z$
(28) $d(0,\frac{3}{4},\frac{3}{4})\ \frac{1}{8},y,z$
(29) $\bar{3}^+\ x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$
(30) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+1,\bar{x};\ -\frac{5}{8},\frac{1}{8},\frac{7}{8}$
(31) $\bar{3}^+\ x+\frac{1}{2},\bar{x}+1,x;\ \frac{1}{8},\frac{7}{8},-\frac{1}{8}$
(32) $\bar{3}^+\ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^-\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{3}{8},\frac{1}{8}$
(34) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{3}{8}$
(35) $\bar{3}^-\ \bar{x}-\frac{1}{2},\bar{x}+1,x;\ -\frac{3}{8},\frac{7}{8},\frac{1}{8}$
(36) $\bar{3}^-\ \bar{x}+1,x,\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{1}{8}$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})\ x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{2},\frac{1}{2},0)\ x,x,z$
(39) $\bar{4}^-\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+\ 0,0,z;\ 0,0,0$
(41) $\bar{4}^-\ x,0,\frac{1}{2};\ 0,0,\frac{1}{2}$
(42) $m\ x,y,\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\ x,y+\frac{1}{4},y$
(44) $\bar{4}^+\ x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+\ -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) $m\ \bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-\ 0,y,0;\ 0,0,0$
(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\ x+\frac{1}{4},y,x$

$Fd\bar{3}m$ No. 227

CONTINUED

ORIGIN CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	h,k,l permutable General:
192 i 1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$ and $h+l,k+l=2n$ $0kl$: $k+l=4n$ and $k,l=2n$ hhl: $h+l=2n$ $h00$: $h=4n$
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$	
	(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	
	(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	
	(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	
	(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
	(25) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{3}{4}$	(27) $x+\frac{3}{4},\bar{y}+\frac{3}{4},z+\frac{1}{4}$	(28) $\bar{x}+\frac{3}{4},y+\frac{1}{4},z+\frac{3}{4}$	
	(29) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(30) $\bar{z}+\frac{3}{4},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{4}$	(32) $z+\frac{3}{4},\bar{x}+\frac{3}{4},y+\frac{1}{4}$	
	(33) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(34) $y+\frac{3}{4},\bar{z}+\frac{3}{4},x+\frac{1}{4}$	(35) $\bar{y}+\frac{3}{4},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{3}{4}$	
	(37) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
	(41) $\bar{x}+\frac{1}{2},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}$	(43) x,z,y	(44) $\bar{x},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	
	(45) $\bar{z}+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}$	(48) z,y,x	
					Special: as above, plus
96 h ..2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{7}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{5}{8},\bar{y},y+\frac{1}{4}$	no extra conditions
	$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{7}{8},\bar{y}+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{8},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{5}{8},\bar{y}$	
	$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{3}{8}$	$\bar{y},y+\frac{1}{4},\frac{5}{8}$	
	$\frac{1}{8},\bar{y}+\frac{1}{4},y$	$\frac{3}{8},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{7}{8},\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2}$	$\frac{5}{8},y+\frac{1}{4},\bar{y}$	
	$y,\frac{1}{8},\bar{y}+\frac{1}{4}$	$y+\frac{1}{2},\frac{3}{8},y+\frac{3}{4}$	$\bar{y}+\frac{1}{2},\frac{7}{8},\bar{y}+\frac{3}{4}$	$\bar{y},\frac{5}{8},y+\frac{1}{4}$	
	$\bar{y}+\frac{1}{4},y,\frac{1}{8}$	$y+\frac{3}{4},y+\frac{1}{2},\frac{3}{8}$	$\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2},\frac{7}{8}$	$y+\frac{1}{4},\bar{y},\frac{5}{8}$	
96 g ..m	x,x,z	$\bar{x},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	no extra conditions
	z,x,x	$z+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$	$\bar{z},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	
	x,z,x	$\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	
	$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	
	$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{3}{4},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{z}+\frac{3}{4},x+\frac{3}{4}$	
	$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$z+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{z}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
48 f 2 . mm	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	hkl: $h=2n+1$ or $h+k+l=4n$
	$\frac{3}{4},x+\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},x+\frac{3}{4}$	
32 e .3 m	x,x,x	$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$					no extra conditions
	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$					
	$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$					
	$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$					
16 d .$\bar{3}$ m	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{7}{8}$			hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16 c .$\bar{3}$ m	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$			
8 b $\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$					hkl: $h=2n+1$ or $h+k+l=4n$
8 a $\bar{4}3m$	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$					

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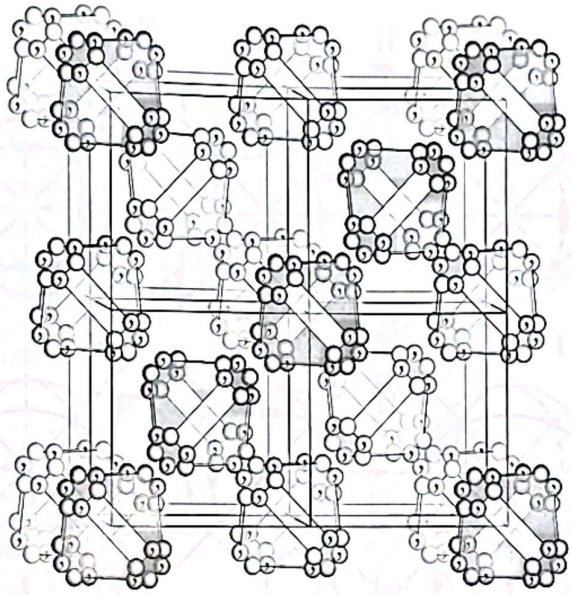
No. 227 $Fd\bar{3}m$



Symmetry of special projections

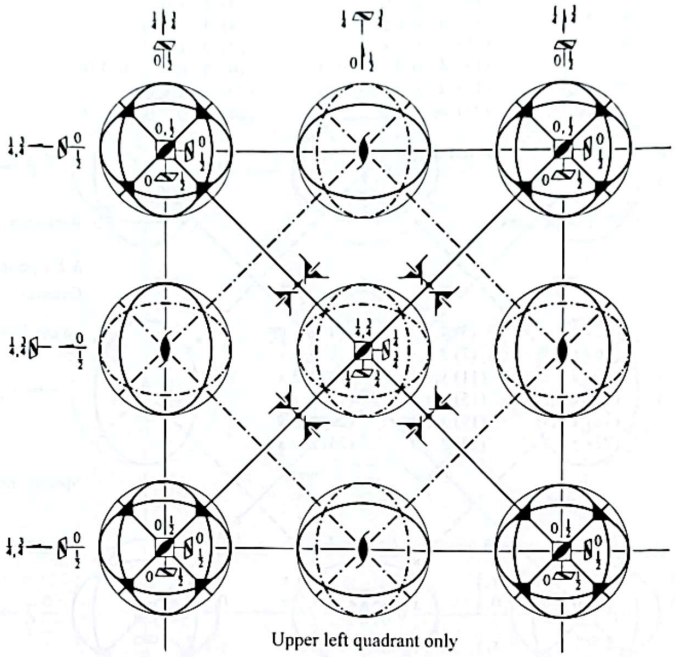
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

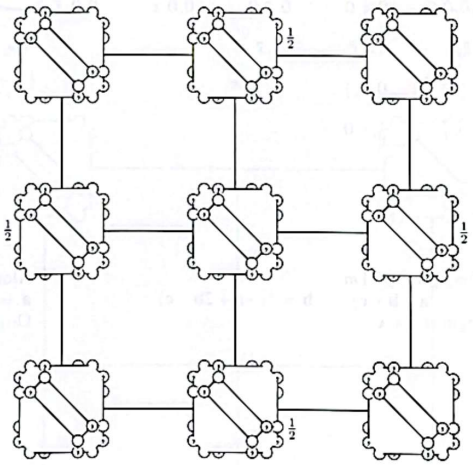
Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{8}$

$F\bar{4}3m$ T_d^2 $\bar{4}3m$ Cubic

No. 216 $F\bar{4}3m$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at $\bar{4}3m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) m x,x,z	(14) m $x,\bar{x},z$	(15) $\bar{4}^+$ 0,0,z; 0,0,0	(16) $\bar{4}^-$ 0,0,z; 0,0,0
(17) m x,y,y	(18) $\bar{4}^+$ x,0,0; 0,0,0	(19) $\bar{4}^-$ x,0,0; 0,0,0	(20) m $x,y,\bar{y}$
(21) m x,y,x	(22) $\bar{4}^-$ 0,y,0; 0,0,0	(23) m $\bar{x},y,x$	(24) $\bar{4}^+$ 0,y,0; 0,0,0

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CONTINUED No. 216 $F\bar{4}3m$

Symmetry operations *(continued)*

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$ (6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$ (7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ (8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$ (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ (12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{2},\frac{1}{2})$ $x-\frac{1}{4},x,z$ (14) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$ (15) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z;$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (16) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z;$ $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(17) $g(0,\frac{1}{2},\frac{1}{2})$ x,y,y (18) $\bar{4}^+$ $x,\frac{1}{2},0;$ $0,\frac{1}{2},0$ (19) $\bar{4}^-$ $x,0,\frac{1}{2};$ $0,0,\frac{1}{2}$ (20) m $x,y+\frac{1}{2},\bar{y}$
(21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{2})$ $x-\frac{1}{4},y,x$ (22) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4};$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (23) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ (24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4};$ $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) 2 $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$ (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ (7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ (8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$ (10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$ (11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$ (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},x,z$ (14) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$ (15) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z;$ $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ (16) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z;$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$ (18) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4};$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (19) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4};$ $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ (20) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{2},0,\frac{1}{2})$ x,y,x (22) $\bar{4}^-$ $\frac{1}{2},y,0;$ $\frac{1}{2},0,0$ (23) m $\bar{x}+\frac{1}{2},y,x$ (24) $\bar{4}^+$ $0,y,\frac{1}{2};$ $0,0,\frac{1}{2}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$ (6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$ (7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$ (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$ (10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$ (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z (14) m $x+\frac{1}{2},\bar{x},z$ (15) $\bar{4}^+$ $\frac{1}{2},0,z;$ $\frac{1}{2},0,0$ (16) $\bar{4}^-$ $0,\frac{1}{2},z;$ $0,\frac{1}{2},0$
(17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$ (18) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4};$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ (19) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4};$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (20) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x+\frac{1}{4},y,x$ (22) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4};$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ (23) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ (24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4};$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$		Reflection conditions
								h,k,l permutable
								General:
96	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$		hkl: $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$		$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$		hhl: $h+l=2n$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$		$h00$: $h=2n$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$		
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$		
								Special: no extra conditions
48	h	$..m$	x,x,z $\bar{z},\bar{x},x$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$	$\bar{x},x,\bar{z}$ x,z,x	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$	z,x,x $x,\bar{z},\bar{x}$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$
24	g	$2..mm$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$
24	f	$2..mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
16	e	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
4	d	$\bar{4}3m$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$					
4	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$					
4	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	a	$\bar{4}3m$	$0,0,0$					

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$Im\bar{3}m$ No. 229 CONTINUED

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

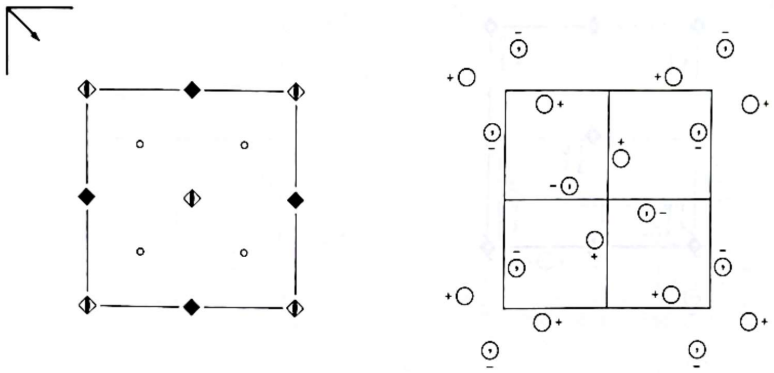
Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates (0,0,0)+	Coordinates $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+	Reflection conditions
			h,k,l permutable General:
96 l 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $y,x,\bar{z}$ (14) $\bar{y},\bar{x},\bar{z}$ (15) $y,\bar{x},z$ (16) $\bar{y},x,z$ (17) $x,z,\bar{y}$ (18) $\bar{x},z,y$ (19) $\bar{x},\bar{z},\bar{y}$ (20) $x,\bar{z},y$ (21) $z,y,\bar{x}$ (22) $z,\bar{y},x$ (23) $\bar{z},y,x$ (24) $\bar{z},\bar{y},\bar{x}$ (25) $\bar{x},\bar{y},\bar{z}$ (26) $x,y,\bar{z}$ (27) $x,\bar{y},z$ (28) $\bar{x},y,z$ (29) $\bar{z},\bar{x},\bar{y}$ (30) $\bar{z},x,y$ (31) $z,x,\bar{y}$ (32) $z,\bar{x},y$ (33) $\bar{y},\bar{z},\bar{x}$ (34) $y,\bar{z},x$ (35) $\bar{y},z,x$ (36) $y,z,\bar{x}$ (37) $\bar{y},\bar{x},z$ (38) y,x,z (39) $\bar{y},x,\bar{z}$ (40) $y,\bar{x},\bar{z}$ (41) $\bar{x},\bar{z},y$ (42) $x,\bar{z},\bar{y}$ (43) x,z,y (44) $\bar{x},z,\bar{y}$ (45) $\bar{z},\bar{y},x$ (46) $\bar{z},y,\bar{x}$ (47) $z,\bar{y},\bar{x}$ (48) z,y,x		hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $h00$: $h=2n$
			Special: as above, plus
48 k ..m	x,x,z $\bar{x},\bar{x},z$ $\bar{x},x,\bar{z}$ $x,\bar{x},\bar{z}$ z,x,x $z,\bar{x},\bar{x}$ $\bar{z},\bar{x},x$ $\bar{z},x,\bar{x}$ x,z,x $\bar{x},z,\bar{x}$ $x,\bar{z},\bar{x}$ $\bar{x},\bar{z},x$ $x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{x},z$ $\bar{x},x,z$ $x,z,\bar{x}$ $\bar{x},z,x$ $\bar{x},\bar{z},\bar{x}$ $x,\bar{z},x$ $z,x,\bar{x}$ $z,\bar{x},x$ $\bar{z},x,x$ $\bar{z},\bar{x},\bar{x}$		no extra conditions
48 j m..	$0,y,z$ $0,\bar{y},z$ $0,y,\bar{z}$ $0,\bar{y},\bar{z}$ $z,0,y$ $z,0,\bar{y}$ $\bar{z},0,y$ $\bar{z},0,\bar{y}$ $y,z,0$ $\bar{y},z,0$ $y,\bar{z},0$ $\bar{y},\bar{z},0$ $y,0,\bar{z}$ $\bar{y},0,\bar{z}$ $y,0,z$ $\bar{y},0,z$ $0,z,\bar{y}$ $0,z,y$ $0,\bar{z},\bar{y}$ $0,\bar{z},y$ $z,y,0$ $z,\bar{y},0$ $\bar{z},y,0$ $\bar{z},\bar{y},0$		no extra conditions
48 i ..2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\frac{3}{4},y,y+\frac{1}{2}$ $\frac{1}{4},\bar{y},y+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $y+\frac{1}{2},\frac{3}{4},y$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y,y+\frac{1}{2},\frac{3}{4}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},\bar{y},y+\frac{1}{2}$ $\frac{1}{4},y,y+\frac{1}{2}$ $\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\frac{3}{4},y,\bar{y}+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},\bar{y}$ $y+\frac{1}{2},\frac{1}{4},y$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $\bar{y}+\frac{1}{2},\frac{3}{4},y$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$ $y,y+\frac{1}{2},\frac{1}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$ $y,\bar{y}+\frac{1}{2},\frac{3}{4}$		no extra conditions
24 h m . $m2$	$0,y,y$ $0,\bar{y},y$ $0,y,\bar{y}$ $0,\bar{y},\bar{y}$ $y,0,y$ $y,0,\bar{y}$ $\bar{y},0,y$ $\bar{y},0,\bar{y}$ $y,y,0$ $\bar{y},y,0$ $y,\bar{y},0$ $\bar{y},\bar{y},0$		no extra conditions
24 g $mm2$..	$x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$ $\frac{1}{2},x,0$ $\frac{1}{2},\bar{x},0$ $0,\frac{1}{2},x$ $0,\frac{1}{2},\bar{x}$ $0,x,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $x,\frac{1}{2},0$ $\bar{x},\frac{1}{2},0$ $\frac{1}{2},0,\bar{x}$ $\frac{1}{2},0,x$		no extra conditions
16 f . $3m$	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x,x,\bar{x}$ $\bar{x},\bar{x},\bar{x}$ $x,\bar{x},x$ $\bar{x},x,x$		no extra conditions
12 e $4m$. m	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$		no extra conditions
12 d $\bar{4}m$ .2	$\frac{1}{4},0,\frac{1}{2}$ $\frac{3}{4},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{4},0$ $\frac{1}{2},\frac{3}{4},0$ $0,\frac{1}{2},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$		no extra conditions
8 c . $\bar{3}m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$		hkl: $k,l=2n$
6 b $4/mm$. m	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$		no extra conditions
2 a $m\bar{3}m$	$0,0,0$		no extra conditions

$P4/n$ C_{4h}^3 $4/m$ Tetragonal

No. 85 $P4/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1



Origin at $\bar{4}$ on n, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,\frac{1}{2},z$ (4) 4^- $\frac{1}{2},0,z$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$ (7) $\bar{4}^+$ $0,0,z$; $0,0,0$ (8) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	g 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
		(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$	$h00$: $h=2n$
						Special: as above, plus
4	f 2..	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl: $h+k=2n$
4	e $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	d $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h,k=2n$
2	c 4..	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	b $\bar{4}$..	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a $\bar{4}$..	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

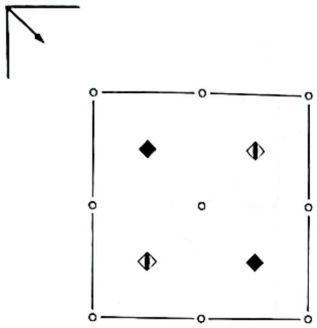
Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

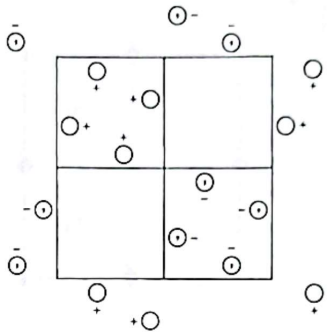
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Tetragonal $4/m$ C_{4h}^3 $P4/n$

Patterson symmetry $P4/m$ $P4/n$ No. 85

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{2}$

Symmetry operations

(1) 1 (2) $2\ \frac{1}{4},\frac{1}{4},z$ (3) $4^+\ \frac{1}{4},\frac{1}{4},z$ (4) $4^-\ \frac{1}{4},\frac{1}{4},z$
(5) $\bar{1}\ 0,0,0$ (6) $n(\frac{1}{2},\frac{1}{2},0)\ x,y,0$ (7) $\bar{4}^+\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},0$ (8) $\bar{4}^-\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},\bar{x},\bar{z}$	(8) $\bar{y},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
							Special: as above, plus
4	f	2..	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl: $h+k=2n$
4	e	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k=2n$
4	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h,k=2n$
2	c	4..	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	b	$\bar{4}$..	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}$..	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl: $h+k=2n$

Symmetry of special projections

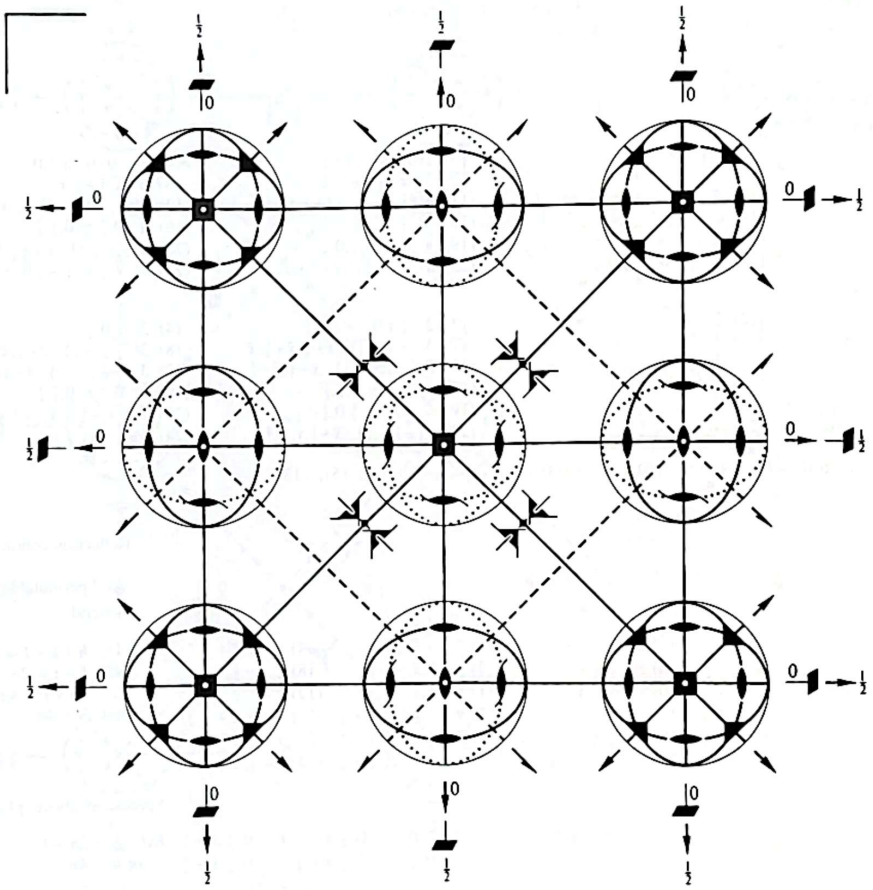
Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

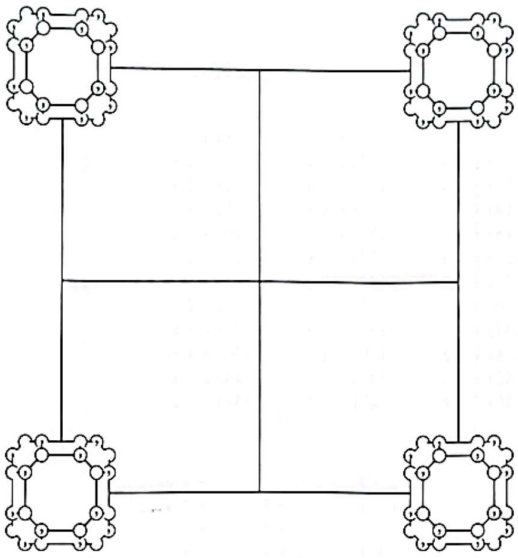
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$Pm\bar{3}m$ O_h^1 $m\bar{3}m$ Cubic

No. 221 $P\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$



CONTINUED No. 221 $Pm\bar{3}m$



Origin at centre $(m\bar{3}m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
(2) 2 0,0,z
(3) 2 0,y,0
(4) 2 x,0,0
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 x,x,0
(14) 2 $x,\bar{x},0$
(15) 4^- 0,0,z
(16) 4^+ 0,0,z
(17) 4^- x,0,0
(18) 2 0,y,y
(19) 2 $0,y,\bar{y}$
(20) 4^+ x,0,0
(21) 4^+ 0,y,0
(22) 2 x,0,x
(23) 4^- 0,y,0
(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ 0,0,0
(26) m x,y,0
(27) m x,0,z
(28) m 0,y,z
(29) $\bar{3}^+$ x,x,x; 0,0,0
(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; 0,0,0
(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; 0,0,0
(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; 0,0,0
(33) $\bar{3}^-$ x,x,x; 0,0,0
(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; 0,0,0
(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; 0,0,0
(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; 0,0,0
(37) m $x,\bar{x},z$
(38) m x,x,z
(39) $\bar{4}^-$ 0,0,z; 0,0,0
(40) $\bar{4}^+$ 0,0,z; 0,0,0
(41) $\bar{4}^-$ x,0,0; 0,0,0
(42) m $x,y,\bar{y}$
(43) m x,y,y
(44) $\bar{4}^+$ x,0,0; 0,0,0
(45) $\bar{4}^+$ 0,y,0; 0,0,0
(46) m $\bar{x},y,x$
(47) $\bar{4}^-$ 0,y,0; 0,0,0
(48) m x,y,x

$Pm\bar{3}m$ No. 221

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
48	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	h,k,l permutable General:
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$	
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	no conditions
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$	
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x	
24	m	$..m$	x,x,z $\bar{z},\bar{x},x$ $x,x,\bar{z}$ $\bar{x},\bar{z},\bar{x}$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{z},x$	$\bar{x},x,\bar{z}$ x,z,x $x,\bar{x},z$ $z,x,\bar{x}$	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$ $\bar{x},x,z$ $z,\bar{x},x$	z,x,x $x,\bar{z},\bar{x}$ $x,z,\bar{x}$ $\bar{z},x,x$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$ $\bar{x},z,x$ $\bar{z},\bar{x},\bar{x}$
24	l	$m..$	$\frac{1}{2},y,z$ $\bar{z},\frac{1}{2},y$ $y,\frac{1}{2},\bar{z}$ $\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{y},z$ $\bar{z},\frac{1}{2},\bar{y}$ $\bar{y},\frac{1}{2},\bar{z}$ $\frac{1}{2},\bar{z},y$	$\frac{1}{2},y,\bar{z}$ $y,z,\frac{1}{2}$ $y,\frac{1}{2},z$ $z,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{z}$ $\bar{y},z,\frac{1}{2}$ $\bar{y},\frac{1}{2},z$ $z,\bar{y},\frac{1}{2}$	$z,\frac{1}{2},y$ $y,\bar{z},\frac{1}{2}$ $\frac{1}{2},z,\bar{y}$ $\bar{z},y,\frac{1}{2}$	$z,\frac{1}{2},\bar{y}$ $\bar{y},\bar{z},\frac{1}{2}$ $\frac{1}{2},z,y$ $\bar{z},\bar{y},\frac{1}{2}$
24	k	$m..$	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$
12	j	$m.m2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
12	i	$m.m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
12	h	$mm2..$	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$
8	g	$.3m$	x,x,x $x,x,\bar{z}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$ $x,\bar{x},x$	$x,\bar{x},\bar{z}$ $\bar{x},x,x$		
6	f	$4m.m$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	$4/mm.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\bar{3}m$	$0,0,0$					

Special: no extra conditions

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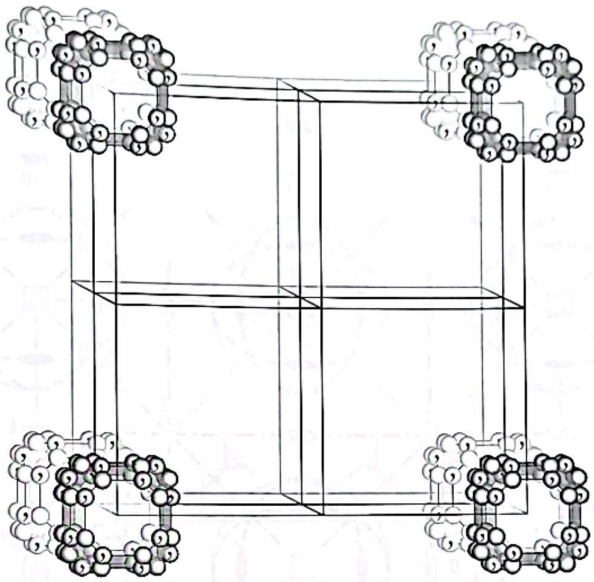
No. 221 $Pm\bar{3}m$



Symmetry of special projections

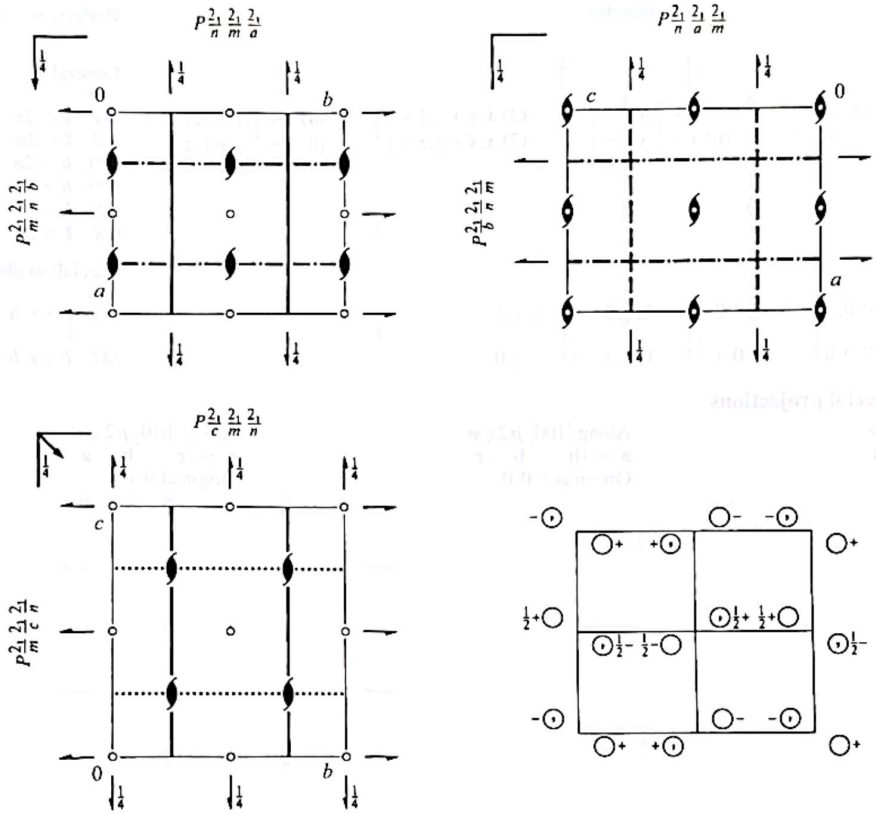
Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$Pnma$ D_{2h}^{16} mmm Orthorhombic

No. 62 $P\ 2_1/n\ 2_1/m\ 2_1/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

(1) 1
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) $2(0,\frac{1}{2},0)$ $0,y,0$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$
(6) a $x,y,\frac{1}{4}$
(7) m $x,\frac{1}{4},z$
(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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No. 62 *Pnma*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 *d* 1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
					Special: as above, plus
4 *c* . *m* .	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4 *b* $\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+l,k=2n$
4 *a* $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l,k=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p2gg$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$