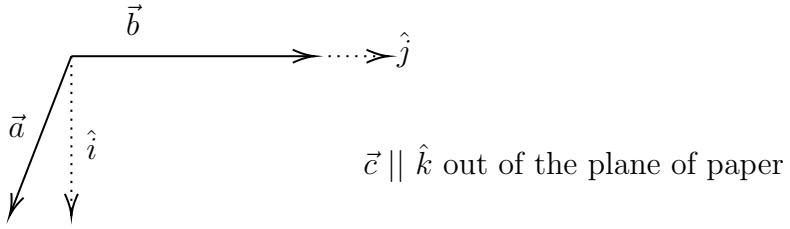
Assignment 3

Diffraction, Scattering, Structure Factors
Please no AI-generated solutions. Would be your loss!

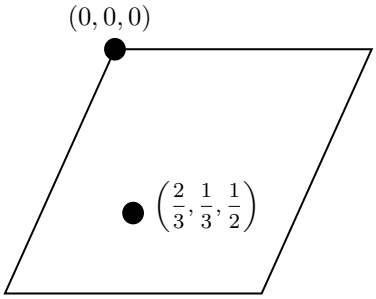
Question 1



(a) Find the unit translation vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$ of the (P) hexagonal lattice in terms of the unit vectors $\hat{i}$, $\hat{j}$, and $\hat{k}$ as shown above.

(b) Find the reciprocal lattice in terms of $\hat{i}$, $\hat{j}$, and $\hat{k}$.

(c) Elements like Co and Mg crystallize in the (P) hexagonal lattice in the manner shown. Their fractional coordinates are:



The basis has two atoms. This arrangement of atoms is often called hexagonal-close-packed (or hcp for short). Find the lattice structure factor S_{hkl} for the (P) hexagonal lattice.

(d) Find the basis structure factor $S_{hk\ell}$. Hence, determine the overall structure factor.

(e) How many possible values of the intensity of diffracted X-ray peaks exist, and what are their relative magnitudes (ignoring the dependence of f on θ)?

Question 2

Fe has a BCC structure. Note that only reflections for which $h + k + \ell =$ even are allowed (as seen in class). For Fe, $a = 0.2866\,\text{nm}$.

(a) Make a table of d-values for planes $\{hk\ell\}$ from which X-ray reflections can be produced. Put the entries in order of decreasing d-values and list the first five entries.

(b) Find the corresponding scattering angles.

Question 3

A BCC structure with a basis at $(0, 0, 0)$ has a lattice parameter $a = 0.5\,\text{nm}$.

(a) X-rays of wavelength $0.25\,\text{nm}$ are shone onto a single crystal. Using the Ewald construction, identify the reflecting planes, reflecting directions, and angles in 3D.

(b) In a Laue experiment, a range of X-ray wavelengths between $0.25\,\text{nm}$ and $0.3\,\text{nm}$ are incident on the same crystal. Using the Ewald construction, now identify all the reflecting planes and directions in the $[uv0]$ plane.

Question 4

The dichalcogenide MoS_2 crystallizes in the space group No. 11 ($P2_1/m$). Show that for 00ℓ reflections from a general position $4f$, one must satisfy the condition $\ell = 2n$. For this, you would need to find the structure factor for the atoms at the $4f$ positions.

Question 5

A single crystal has scattered X-ray beams with the following $\sin^2\theta$ values:

$$
\begin{gathered}
0.0700 \\
0.0763 \\
0.1400 \\
0.1463 \\
0.2163 \\
0.2762 \\
0.2800 \\
0.2863 \\
0.3500 \\
0.3563
\end{gathered}
$$

For a cubic crystal, the d-spacing is given by:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}.$$

For a tetragonal crystal:

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}.$$

(a) Show that the crystal does not belong to the cubic system.

(b) Let's determine whether it belongs to the tetragonal class. Show that for tetragonal crystals we can write:

$$\sin^2\theta = AN + BM,$$

where N and M are integers. What are the allowed values for N and M?

(c) Tabulate your data and determine A and B, and hence determine the lattice parameters a and c. Conclude that the crystal is tetragonal.

Question 6

In class, we showed that the atomic scattering function is:

$$f_a \propto \int_{r=0}^{R} dr\ r^2\ \rho(r) \int_0^{\pi} d\phi \sin\phi\ e^{-i\frac{4\pi}{\lambda}\sin\theta\cos\phi}.$$

(a) Solve the angular part with a suitable substitution.

(b) Given $\rho(r) \propto e^{-r/b}$, where b is a constant, find f_a (correct upto a scaling factor).

(c) Plot f_a versus $\sin\theta$.

Question 7

$BaTiO_3$ is $Pm\bar{3}m$. The basis is:

$$\begin{aligned} &\text{Ba} && [0,0,0], \\ &\text{Ti} && \left[\frac{1}{2},\frac{1}{2},\frac{1}{2}\right], \\ &\text{O} && \left[\frac{1}{2},\frac{1}{2},0\right], \left[\frac{1}{2},0,\frac{1}{2}\right], \left[0,\frac{1}{2},\frac{1}{2}\right]. \end{aligned}$$

(a) Sketch this unit cell.

(b) Find $S_{(001)}$ where the atomic form factors are f_{Ba}, f_{Ti}, f_{O}, i.e. find $S_{(hk\ell)}$ for $h = 0, k = 0, \ell = 1$. You are required to find the structure factors for both the lattice and the basis. Then multiply the two together.

Question 8

Copper ($Fm\bar{3}m$) is illuminated with X-rays ($\lambda = 154$pm).

(a) Show that for the scattering angle θ,

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+\ell^2) = \frac{\lambda^2}{4a^2}N = A \times N.$$

where $N = h^2 + k^2 + \ell^2$ must be an integer.

(b) A real experiment yields the scattering directions tabulated in the given table. Complete the table below and in the process verify that the crystal system is cubic. Find the unit cell size.

$\sin^2\theta$	N	$h\ k\ \ell$
0.1365		
0.1820		
0.3640		
0.5005		
0.5460		
0.7280		
0.8645		
0.9100		

Question 9

Diamond belongs to the $Fd\bar{3}m$ space group with C atoms in the $8a$ positions.

(a) Show that these atomic positions are compatible with a basis set of C atoms at $0, 0, 0$ and $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$.

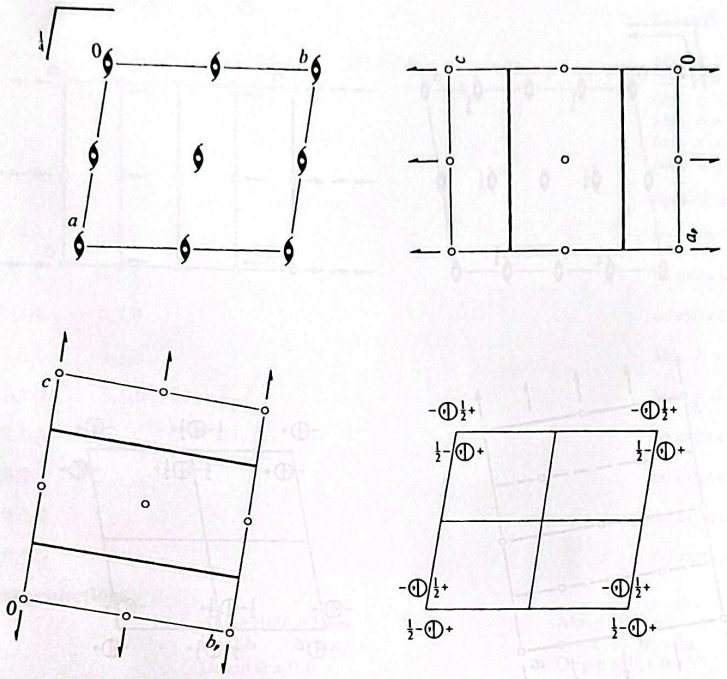
(b) Find the $S_{hk\ell}^{\text{basis}}$, and hence the systematic absences.

(c) How many distinct values for the intensities for the scattered X-rays exist?

Monoclinic $2/m$ C_{2h}^2 $P2_1/m$

Patterson symmetry $P112/m$ $P112_1/m$ No. 11

UNIQUE AXIS c



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

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

Symmetry operations

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

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	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
2	e	m	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

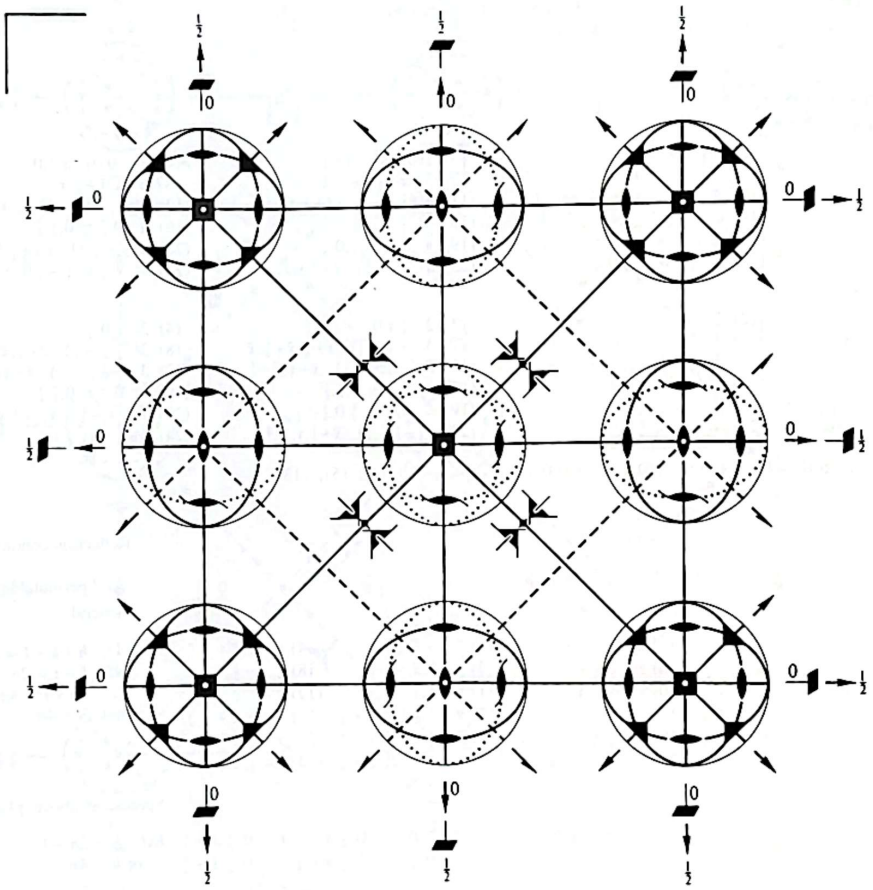
Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

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

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



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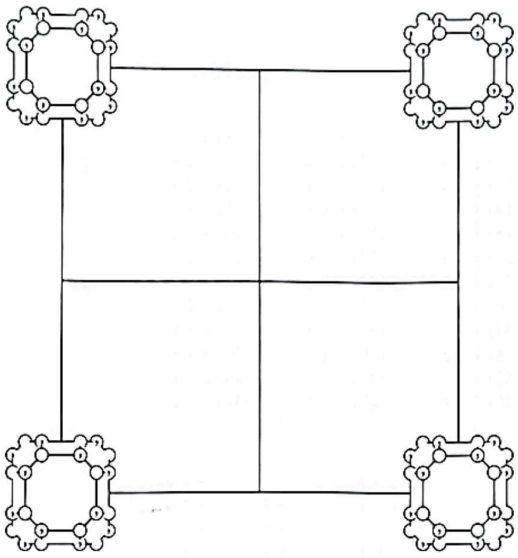
CONTINUED No. 221 $Pm\bar{3}m$



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+ x̄,x,x̄
(7) 3+ x,x̄,x̄
(8) 3+ x̄,x̄,x
(9) 3- x,x,x
(10) 3- x,x̄,x̄
(11) 3- x̄,x̄,x
(12) 3- x̄,x,x̄
(13) 2 x,x,0
(14) 2 x,x̄,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,ȳ
(20) 4+ x,0,0
(21) 4+ 0,y,0
(22) 2 x,0,x
(23) 4- 0,y,0
(24) 2 x̄,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) $\bar{3}$+ x̄,x,x̄; 0,0,0
(31) $\bar{3}$+ x,x̄,x̄; 0,0,0
(32) $\bar{3}$+ x̄,x̄,x; 0,0,0
(33) $\bar{3}$- x,x,x; 0,0,0
(34) $\bar{3}$- x,x̄,x̄; 0,0,0
(35) $\bar{3}$- x̄,x̄,x; 0,0,0
(36) $\bar{3}$- x̄,x,x̄; 0,0,0
(37) m x,x̄,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,ȳ
(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 x̄,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) $\bar{x},y,z$	
			(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	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$	Special: no extra conditions
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$	
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$	
24	l	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$	
			$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$	
			$y,\frac{1}{2},\bar{z}$	$\bar{y},\frac{1}{2},\bar{z}$	$y,\frac{1}{2},z$	$\bar{y},\frac{1}{2},z$	$\frac{1}{2},z,\bar{y}$	$\frac{1}{2},z,y$	
			$\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{z},y$	$z,y,\frac{1}{2}$	$z,\bar{y},\frac{1}{2}$	$\bar{z},y,\frac{1}{2}$	$\bar{z},\bar{y},\frac{1}{2}$	
24	k	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$	
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$	
12	j	$m.m2$	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$	
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$	
12	i	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
12	h	$mm2..$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$	$0,\frac{1}{2},x$	
8	g	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
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	$m\bar{3}m$	$0,0,0$						

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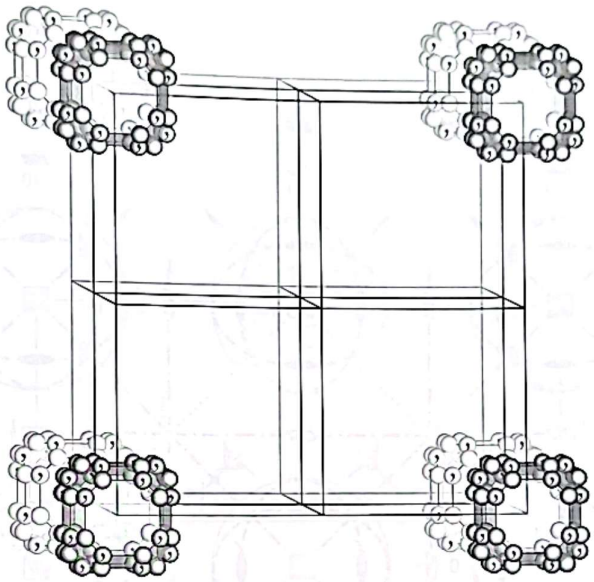
No. 221 $Pm\bar{3}m$



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 $x,x,0$

CONTINUED No. 225 $Fm\bar{3}m$

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

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

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

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) 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

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

$Fm\bar{3}m$ No. 225 CONTINUED

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)

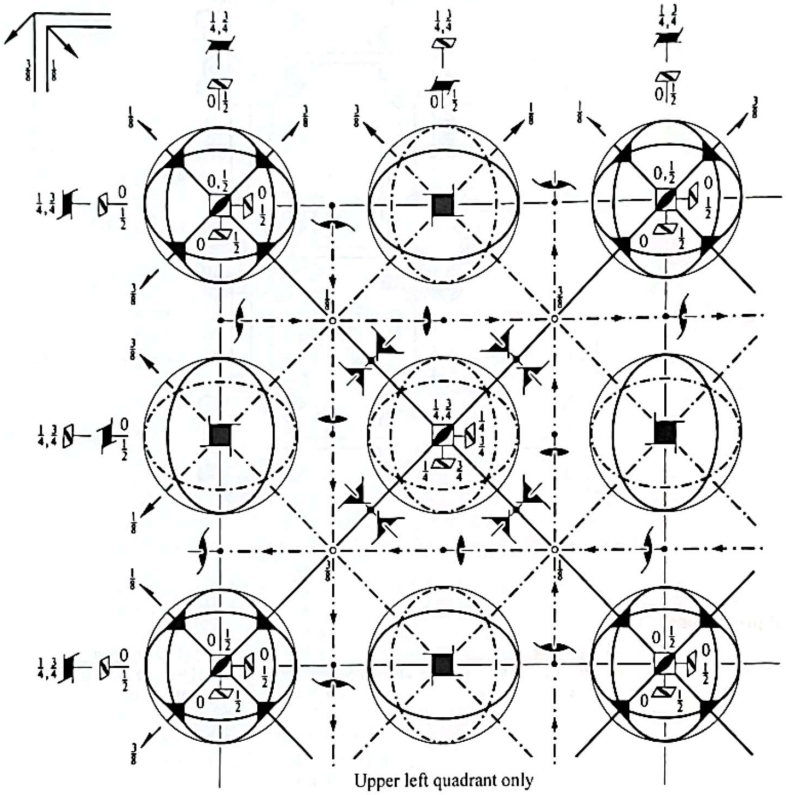
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	(0,½,½)+	(½,0,½)+	(½,½,0)+			Reflection conditions
									h,k,l permutable General:
192	*l*	1	(1) *x,y,z* (5) *z,x,y* (9) *y,z,x* (13) *y,x,z̄* (17) *x,z,ȳ* (21) *z,y,x̄* (25) *x̄,ȳ,z̄* (29) *z̄,x̄,ȳ* (33) *ȳ,z̄,x̄* (37) *ȳ,x̄,z* (41) *x̄,z̄,y* (45) *z̄,ȳ,x*	(2) *x̄,ȳ,z* (6) *z,x̄,ȳ* (10) *ȳ,z,x̄* (14) *ȳ,x̄,z̄* (18) *x̄,z,y* (22) *z,ȳ,x* (26) *x,y,z̄* (30) *z̄,x,y* (34) *y,z̄,x* (38) *y,x,z* (42) *x,z̄,ȳ* (46) *z̄,y,x̄*	(3) *x̄,y,z̄* (7) *z̄,x̄,y* (11) *y,z̄,x̄* (15) *y,x̄,z* (19) *x̄,z̄,ȳ* (23) *z̄,y,x* (27) *x,ȳ,z* (31) *z,x,ȳ* (35) *ȳ,z,x* (39) *ȳ,x,z̄* (43) *x,z,y* (47) *z,ȳ,x̄*	(4) *x,ȳ,z̄* (8) *z̄,x,ȳ* (12) *ȳ,z̄,x* (16) *ȳ,x,z* (20) *x,z̄,y* (24) *z̄,ȳ,x̄* (28) *x̄,y,z* (32) *z,x̄,y* (36) *y,z,x̄* (40) *y,x̄,z̄* (44) *x̄,z,ȳ* (48) *z,y,x*			*hkl*: $h+k,h+l,k+l=2n$ *0kl*: $k,l=2n$ *hhl*: $h+l=2n$ *h*00: $h=2n$
									Special: as above, plus
96	*k*	. . *m*	*x,x,z* *z̄,x̄,x* *x,x,z̄* *x̄,z̄,x̄*	*x̄,x̄,z* *z̄,x,x̄* *x̄,x̄,z̄* *x,z̄,x*	*x̄,x,z̄* *x,z,x* *x,x̄,z* *z,x,x̄*	*x,x̄,z̄* *x̄,z,x̄* *x̄,x,z* *z,x̄,x*	*z,x,x* *x,z̄,x̄* *x,z,x̄* *z̄,x,x*	*z,x̄,x̄* *x̄,z̄,x* *x̄,z,x* *z̄,x̄,x̄*	no extra conditions
96	*j*	*m* . .	0,*y,z* *z̄*,0,*y* *y*,0,*z̄* 0,*z̄,ȳ*	0,*ȳ,z* *z̄*,0,*ȳ* *ȳ*,0,*z̄* 0,*z̄,y*	0,*y,z̄* *y,z*,0 *y*,0,*z* *z,y*,0	0,*ȳ,z̄* *ȳ,z*,0 *ȳ*,0,*z* *z,ȳ*,0	*z*,0,*y* *y,z̄*,0 0,*z,ȳ* *z̄,y*,0	*z*,0,*ȳ* *ȳ,z̄*,0 0,*z,y* *z̄,ȳ*,0	no extra conditions
48	*i*	*m* . *m*2	½,*y,y* *ȳ*,½,*y*	½,*ȳ,y* *ȳ*,½,*ȳ*	½,*y,ȳ* *y,y*,½	½,*ȳ,ȳ* *ȳ,y*,½	*y*,½,*y* *y,ȳ*,½	*y*,½,*ȳ* *ȳ,ȳ*,½	no extra conditions
48	*h*	*m* . *m*2	0,*y,y* *ȳ*,0,*y*	0,*ȳ,y* *ȳ*,0,*ȳ*	0,*y,ȳ* *y,y*,0	0,*ȳ,ȳ* *ȳ,y*,0	*y*,0,*y* *y,ȳ*,0	*y*,0,*ȳ* *ȳ,ȳ*,0	no extra conditions
48	*g*	2 . *mm*	*x*,¼,¼ ¼,*x*,¾	*x̄*,¾,¼ ¾,*x̄*,¾	¼,*x*,¼ *x*,¼,¾	¼,*x̄*,¾ *x̄*,¼,¼	¼,¼,*x* ¼,¼,*x̄*	¾,¼,*x̄* ¼,¾,*x*	*hkl*: $h=2n$
32	*f*	. 3 *m*	*x,x,x* *x,x,x̄*	*x̄,x̄,x* *x̄,x̄,x̄*	*x̄,x,x̄* *x,x̄,x*	*x,x̄,x̄* *x̄,x,x*			no extra conditions
24	*e*	4 *m* . *m*	*x*,0,0	*x̄*,0,0	0,*x*,0	0,*x̄*,0	0,0,*x*	0,0,*x̄*	no extra conditions
24	*d*	*m* . *mm*	0,¼,¼	0,¾,¼	¼,0,¼	¼,0,¾	¼,¼,0	¾,¼,0	*hkl*: $h=2n$
8	*c*	$\bar{4}$ 3 *m*	¼,¼,¼	¼,¼,¾					*hkl*: $h=2n$
4	*b*	$m\bar{3}m$	½,½,½						no extra conditions
4	*a*	$m\bar{3}m$	0,0,0						no extra conditions

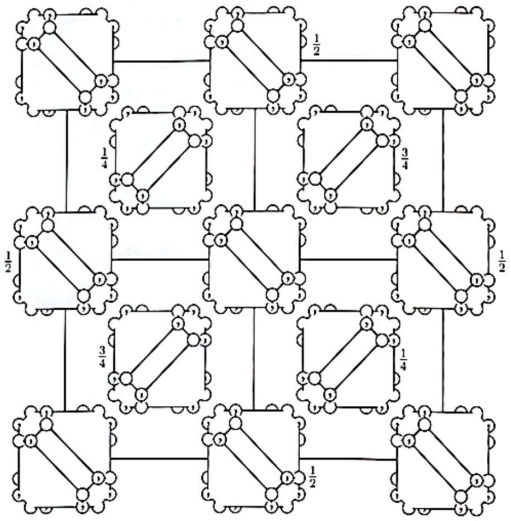
$F\,d\,\bar{3}\,m$ O_h^7 $m\bar{3}m$ Cubic

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 $0\le x\le\frac{1}{3};\quad 0\le y\le\frac{1}{8};\quad -\frac{1}{8}\le z\le\frac{1}{8};\quad y\le\min(\frac{1}{2}-x,x);\quad -y\le z\le y$

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) $2(\frac{1}{4},0,\frac{1}{2})\ x-\frac{1}{4},\frac{1}{8},x$
(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) $\bar{3}^-\ x+\frac{3}{4},\bar{x}-1,\bar{x};\ \frac{5}{8},-\frac{1}{8},\frac{7}{8}$
(35) $\bar{3}^-\ \bar{x}+\frac{1}{2},\bar{x}+\frac{3}{4},x;\ -\frac{1}{8},\frac{7}{8},\frac{5}{8}$
(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) $g(\frac{1}{4},\frac{1}{4},-\frac{1}{4})\ x,y+\frac{1}{4},\bar{y}$
(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) $3^-(\frac{1}{3},\frac{1}{4},-\frac{1}{3})\ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-\ \bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ x,x,\frac{1}{8}$
(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) $2(\frac{1}{4},0,\frac{1}{4})\ x,\frac{1}{8},x$
(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) $d(\frac{1}{4},0,\frac{3}{4})\ x,\frac{1}{8},z$
(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) $4^-(0,\frac{3}{4},0)\ -\frac{1}{4},y,\frac{1}{2}$
(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) $\bar{3}^+\ \bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x;\ \frac{7}{8},-\frac{1}{8},\frac{5}{8}$
(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) $2\ x,\bar{x}+\frac{1}{2},\frac{1}{8}$
(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) $2(\frac{1}{4},0,\frac{3}{4})\ x,\frac{1}{8},x$
(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) $\bar{3}^+\ \bar{x}+1,\bar{x},x;\ \frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^-\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{3}{8},\frac{1}{8}$
(34) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{3}{8},\frac{3}{8}$
(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

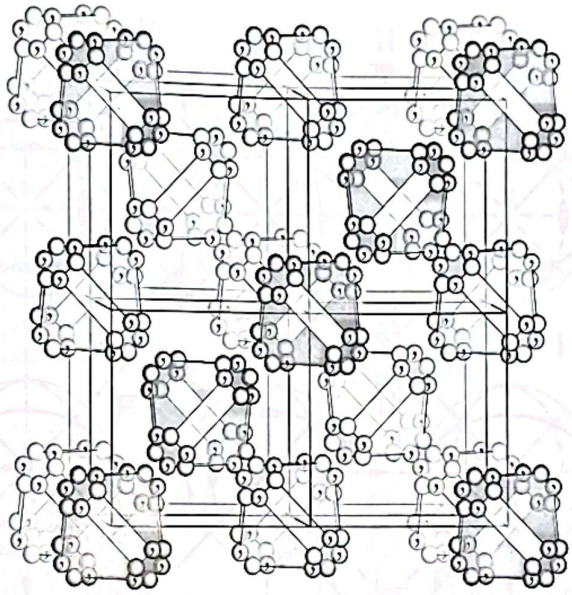
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

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 $h+l,k+l=2n$
	(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) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	$0kl$: $k+l=4n$ and $k,l=2n$
	(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) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	hhl: $h+l=2n$
	(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) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	$h00$: $h=4n$
	(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) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{3}{4}$	(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	$x,0,0$	$\bar{x},\frac{1}{4},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	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 $\bar{4}$ 3 m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$			hkl: $h=2n+1$ or $h+k+l=4n$
8 a $\bar{4}$ 3 m	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			

CONTINUED

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

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