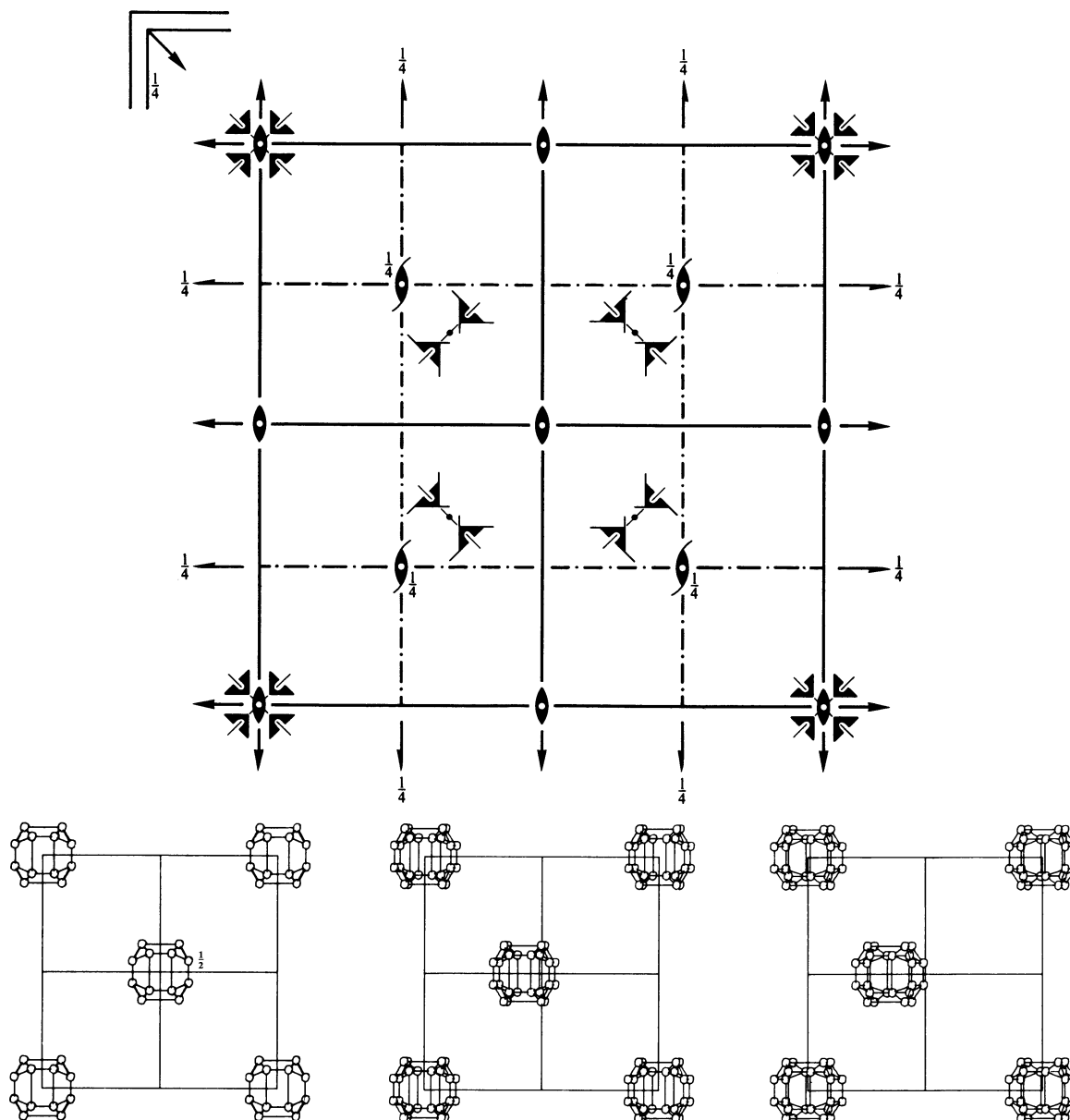


$I\bar{m}\bar{3}$
 T_h^5
 $m\bar{3}$

Cubic

No. 204

 $I2/m\bar{3}$

 Patterson symmetry $I\bar{m}\bar{3}$

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

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq x; z \leq y$
Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

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) $\bar{1}$ $0,0,0$ | (14) m $x,y,0$ | (15) m $x,0,z$ | (16) m $0,y,z$ |
| (17) $\bar{3}^+$ $x,x,x; 0,0,0$ | (18) $\bar{3}^+$ $\bar{x},x,\bar{x}; 0,0,0$ | (19) $\bar{3}^+$ $x,\bar{x},\bar{x}; 0,0,0$ | (20) $\bar{3}^+$ $\bar{x},\bar{x},x; 0,0,0$ |
| (21) $\bar{3}^-$ $x,x,x; 0,0,0$ | (22) $\bar{3}^-$ $x,\bar{x},\bar{x}; 0,0,0$ | (23) $\bar{3}^-$ $\bar{x},\bar{x},x; 0,0,0$ | (24) $\bar{3}^-$ $\bar{x},x,\bar{x}; 0,0,0$ |

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

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

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)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}) +$	h,k,l cyclically permutable General: $hkl : h+k+l = 2n$ $0kl : k+l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$
48 h 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) \bar{x},\bar{y},\bar{z} (14) x,y,\bar{z} (15) x,\bar{y},z (16) \bar{x},y,z (17) \bar{z},\bar{x},\bar{y} (18) \bar{z},x,y (19) z,x,\bar{y} (20) z,\bar{x},y (21) \bar{y},\bar{z},\bar{x} (22) y,\bar{z},x (23) \bar{y},z,x (24) y,z,\bar{x}	Special: as above, plus
24 g $m..$	$0,y,z$ $0,\bar{y},z$ $0,y,\bar{z}$ $0,\bar{y},\bar{z}$ $z,0,y$ $z,0,\bar{y}$ $\bar{z},0,y$ $\bar{z},0,\bar{y}$ $y,z,0$ $\bar{y},z,0$ $y,\bar{z},0$ $\bar{y},\bar{z},0$	no extra conditions
16 f $.3.$	x,x,x \bar{x},\bar{x},x \bar{x},x,\bar{x} x,\bar{x},\bar{x} \bar{x},\bar{x},\bar{x} x,x,\bar{x} x,\bar{x},x \bar{x},x,x	no extra conditions
12 e $mm2..$	$x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$ $\frac{1}{2},x,0$ $\frac{1}{2},\bar{x},0$ $0,\frac{1}{2},x$ $0,\frac{1}{2},\bar{x}$	no extra conditions
12 d $mm2..$	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$	no extra conditions
8 c $.\bar{3}.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$hkl : k,l = 2n$
6 b $mmm..$	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	no extra conditions
2 a $m\bar{3}.$	$0,0,0$	no extra conditions

Symmetry of special projections

Along [001] $c2mm$	Along [111] $p6$	Along [110] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I23$ (197)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Im1$ ($Immm$, 71)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
IIa	[2] $Pn\bar{3}$ (201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Im\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (204)

Minimal non-isomorphic supergroups

I	[2] $Im\bar{3}m$ (229)
II	[4] $Pm\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (200)