

$Pn\bar{3}$

T_h^2

$m\bar{3}$

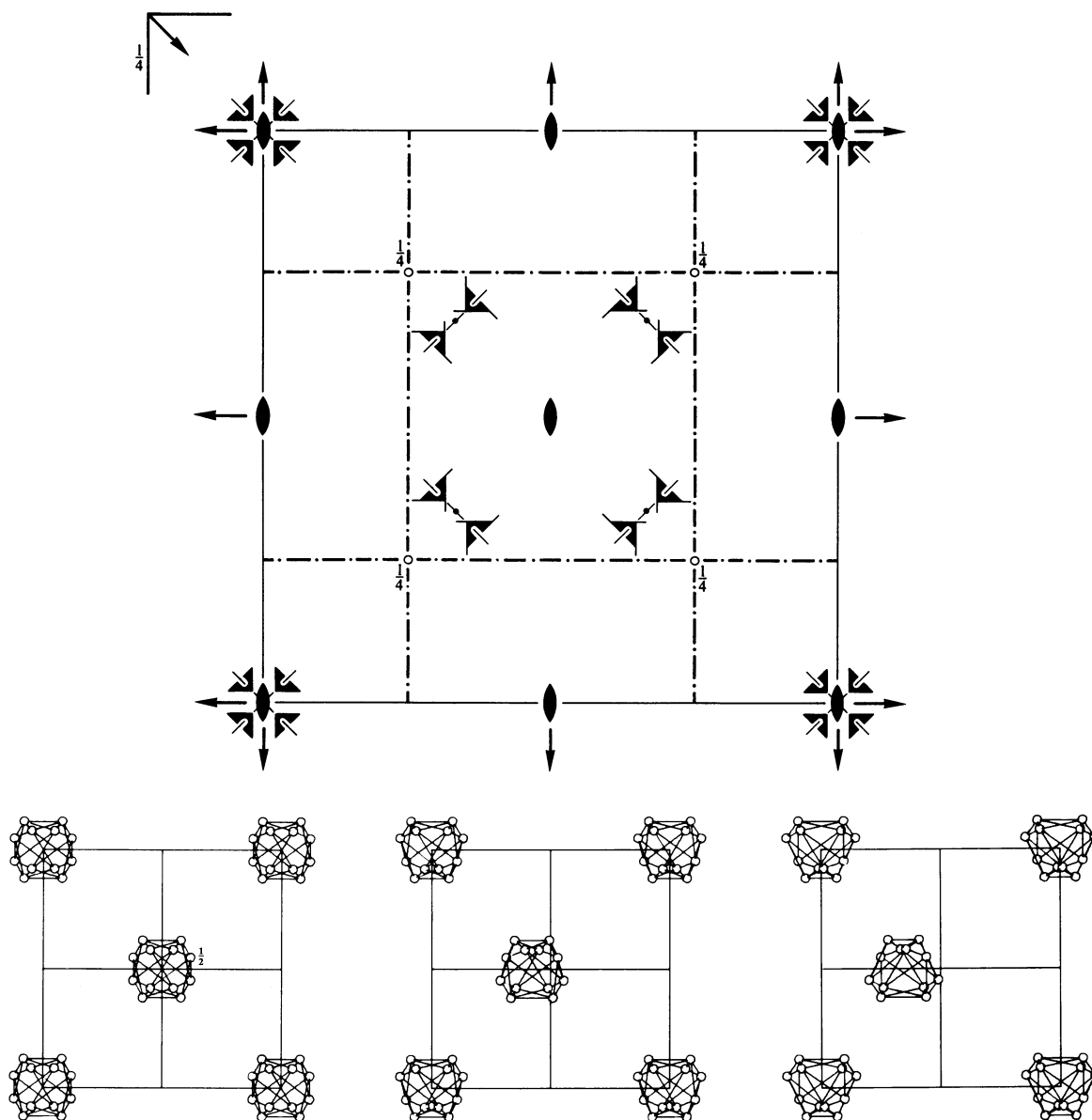
Cubic

No. 201

$P2/n\bar{3}$

Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 1



Origin at 23, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}$)

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

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

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) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (14) $n(\frac{1}{2}, \frac{1}{2}, 0)$ x,y, $\frac{1}{4}$ | (15) $n(\frac{1}{2}, 0, \frac{1}{2})$ x, $\frac{1}{4}$,z | (16) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}$,y,z |
| (17) $\bar{3}^+$ x,x,x; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (18) $\bar{3}^+$ $\bar{x}-1, x+1, \bar{x}$; $-\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ | (19) $\bar{3}^+$ x, $\bar{x}+1, \bar{x}$; $\frac{1}{4}, \frac{3}{4}, -\frac{1}{4}$ | (20) $\bar{3}^+$ $\bar{x}+1, \bar{x}, x$; $\frac{3}{4}, -\frac{1}{4}, \frac{1}{4}$ |
| (21) $\bar{3}^-$ x,x,x; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (22) $\bar{3}^-$ x+1, $\bar{x}-1, \bar{x}$; $\frac{1}{4}, -\frac{1}{4}, \frac{3}{4}$ | (23) $\bar{3}^-$ $\bar{x}, \bar{x}+1, x$; $-\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ | (24) $\bar{3}^-$ $\bar{x}+1, x, \bar{x}$; $\frac{3}{4}, \frac{1}{4}, -\frac{1}{4}$ |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		h, k, l cyclically permutable General:
24 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) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (16) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (17) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (18) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}$ (19) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (20) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (21) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (22) $y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (23) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (24) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0kl : k + l = 2n$ $h00 : h = 2n$
		Special: as above, plus
12 g 2..	$x, \frac{1}{2}, 0$ $\bar{x}, \frac{1}{2}, 0$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $\frac{1}{2}, 0, x$ $\frac{1}{2}, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $0, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
12 f 2..	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $0, 0, x$ $0, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$
8 e .3.	x, x, x \bar{x}, \bar{x}, x \bar{x}, x, \bar{x} x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions
6 d 222..	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $0, 0, \frac{1}{2}$	$hkl : h + k + l = 2n$
4 c . $\bar{3}$.	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4 b . $\bar{3}$.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
2 a 23.	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projectionsAlong $[001] c2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along $[111] p6$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x Along $[110] p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, \frac{1}{4}$ **Maximal non-isomorphic subgroups****I** [2] $P23$ (195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12[3] $Pn1$ ($Pn\bar{3}$, 48) 1; 2; 3; 4; 13; 14; 15; 16[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 5; 9; 13; 17; 21[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 6; 12; 13; 18; 24[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 7; 10; 13; 19; 22[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 8; 11; 13; 20; 23**IIa** none**IIb** [2] $Fd\bar{3}$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (203)**Maximal isomorphic subgroups of lowest index****IIc** [27] $Pn\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (201)**Minimal non-isomorphic supergroups****I** [2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)**II** [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)