

$Pa\bar{3}$

T_h^6

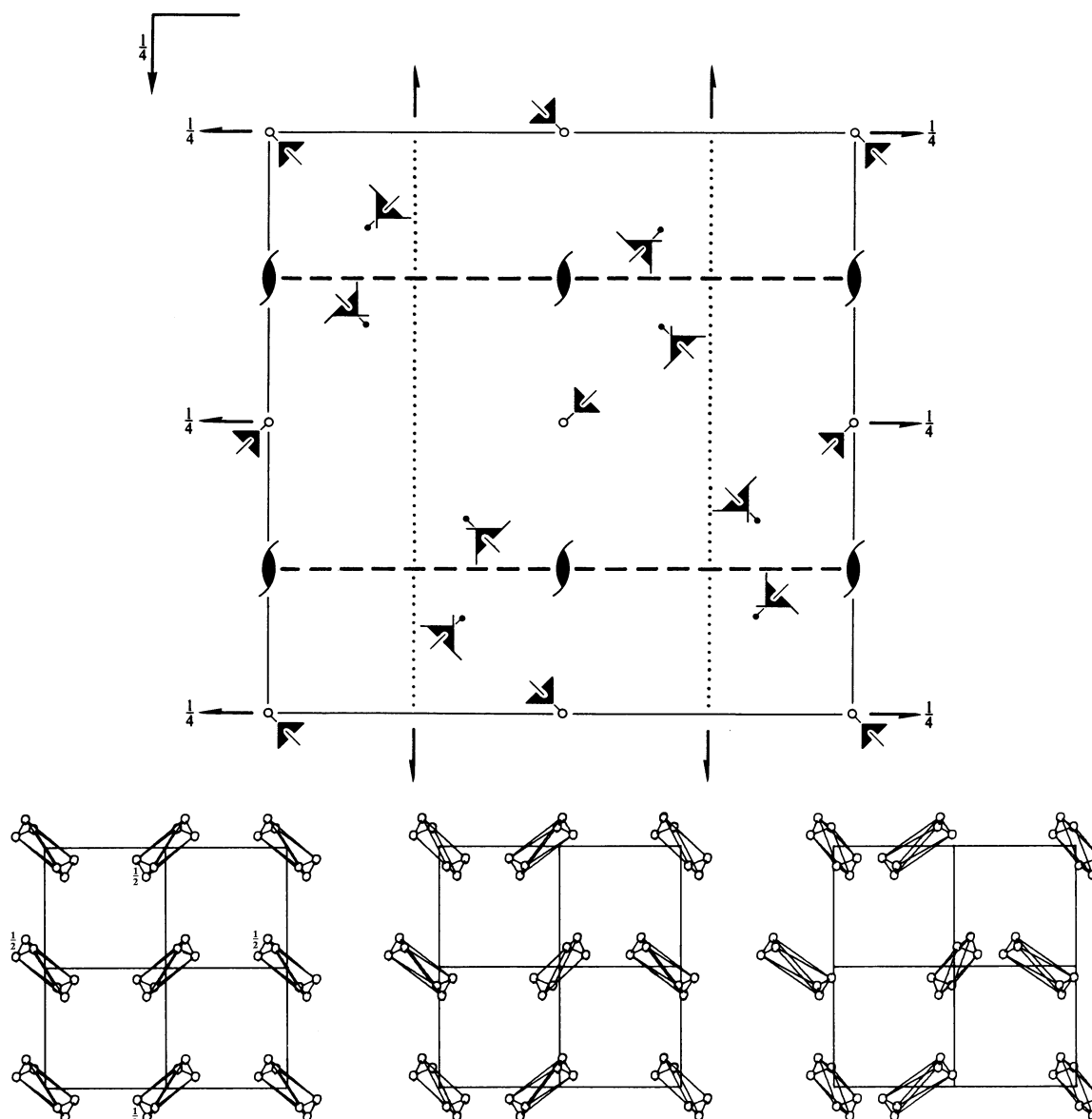
$m\bar{3}$

Cubic

No. 205

$P2_1/a\bar{3}$

Patterson symmetry $Pm\bar{3}$



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

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

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

Symmetry operations

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

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 d 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $\bar{x}, \bar{y}, \bar{z}$ (17) $\bar{z}, \bar{x}, \bar{y}$ (21) $\bar{y}, \bar{z}, \bar{x}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y}$ (10) $\bar{y}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (14) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (18) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ (22) $y, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x}$ (15) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (19) $z + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (23) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (16) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (20) $z, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (24) $y + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$	$0kl : k = 2n$ $h00 : h = 2n$
8 c .3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x$	Special: as above, plus no extra conditions
4 b . $\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 a . $\bar{3}$.	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$

Symmetry of special projections

Along $[001]$ $p2gm$

$$\mathbf{a}' = \frac{1}{2}\mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at $0, 0, z$

Along $[111]$ $p6$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$$

Origin at x, x, x

$$\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Along $[110]$ $p2gg$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$$

Origin at $x, x, 0$

$$\mathbf{b}' = \mathbf{c}$$

Maximal non-isomorphic subgroups

I	[2] $P2_13$ (198)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pa1$ ($Pbca$, 61)	1; 2; 3; 4; 13; 14; 15; 16
	$\left\{ \begin{array}{l} [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \\ [4] P1\bar{3} (R\bar{3}, 148) \end{array} \right.$	1; 5; 9; 13; 17; 21
		1; 6; 12; 13; 18; 24
		1; 7; 10; 13; 19; 22
		1; 8; 11; 13; 20; 23

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[27] Pa\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (205)

Minimal non-isomorphic supergroups

I none

II [2] $Ia\bar{3}$ (206); [4] $Fm\bar{3}$ (202)