

$Ia\bar{3}$

$T_h^7$

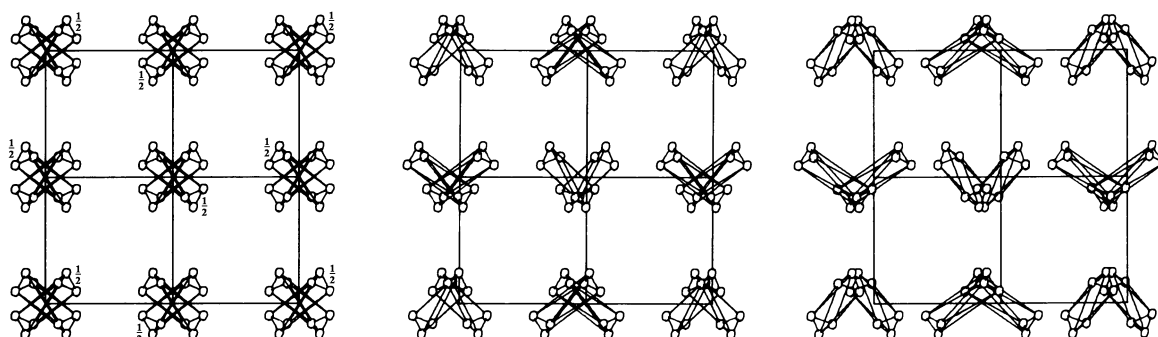
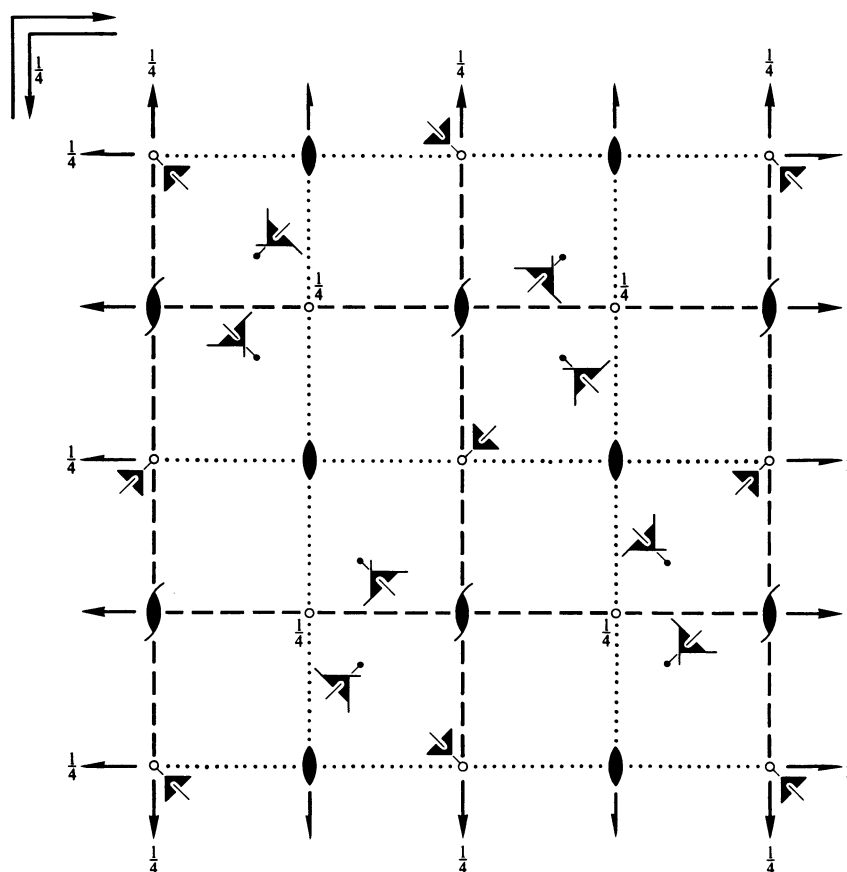
$m\bar{3}$

Cubic

No. 206

$I2_1/a\bar{3}$

Patterson symmetry  $Im\bar{3}$



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

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

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

**Symmetry operations**

For (0,0,0)+ set

- |                                   |   |   |  |
|-----------------------------------|---|---|--|
| (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) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{2}, 0, 0$                                      |

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

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

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ ; (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:	
48 <i>e</i> 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) $y + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$	$hkl : h + k + l = 2n$ $0kl : k, l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$	
24 <i>d</i> 2..	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, 0, \frac{3}{4}$ $x + \frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$	$\frac{3}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{4}, x + \frac{1}{2}, 0$	$0, \frac{1}{4}, x$ $0, \frac{3}{4}, \bar{x}$	$0, \frac{3}{4}, \bar{x} + \frac{1}{2}$ $0, \frac{1}{4}, x + \frac{1}{2}$ no extra conditions
16 <i>c</i> .3.	$x, x, x$ $\bar{x}, \bar{x}, \bar{x}$	$\bar{x} + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $x + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x$	no extra conditions	
8 <i>b</i> . $\bar{3}$ .	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : k, l = 2n$	
8 <i>a</i> . $\bar{3}$ .	0,0,0	$\frac{1}{2}, 0, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : k, l = 2n$	

Special: as above, plus

**Symmetry of special projections**

Along [001]  $p2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$     $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   
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]  $p2mg$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$     $\mathbf{b}' = \frac{1}{2}\mathbf{c}$   
Origin at  $x, x, 0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $I2_3$ (199)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Ia1$ ( $Ibca$ , 73)	(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)+
<b>IIa</b>	[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
<b>IIb</b>	none	

**Maximal isomorphic subgroups of lowest index**

**IIc** [27]  $Ia\bar{3}$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$ ) (206)

**Minimal non-isomorphic supergroups**

<b>I</b>	[2] $Ia\bar{3}d$ (230)
<b>II</b>	[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)