

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

T_h^5

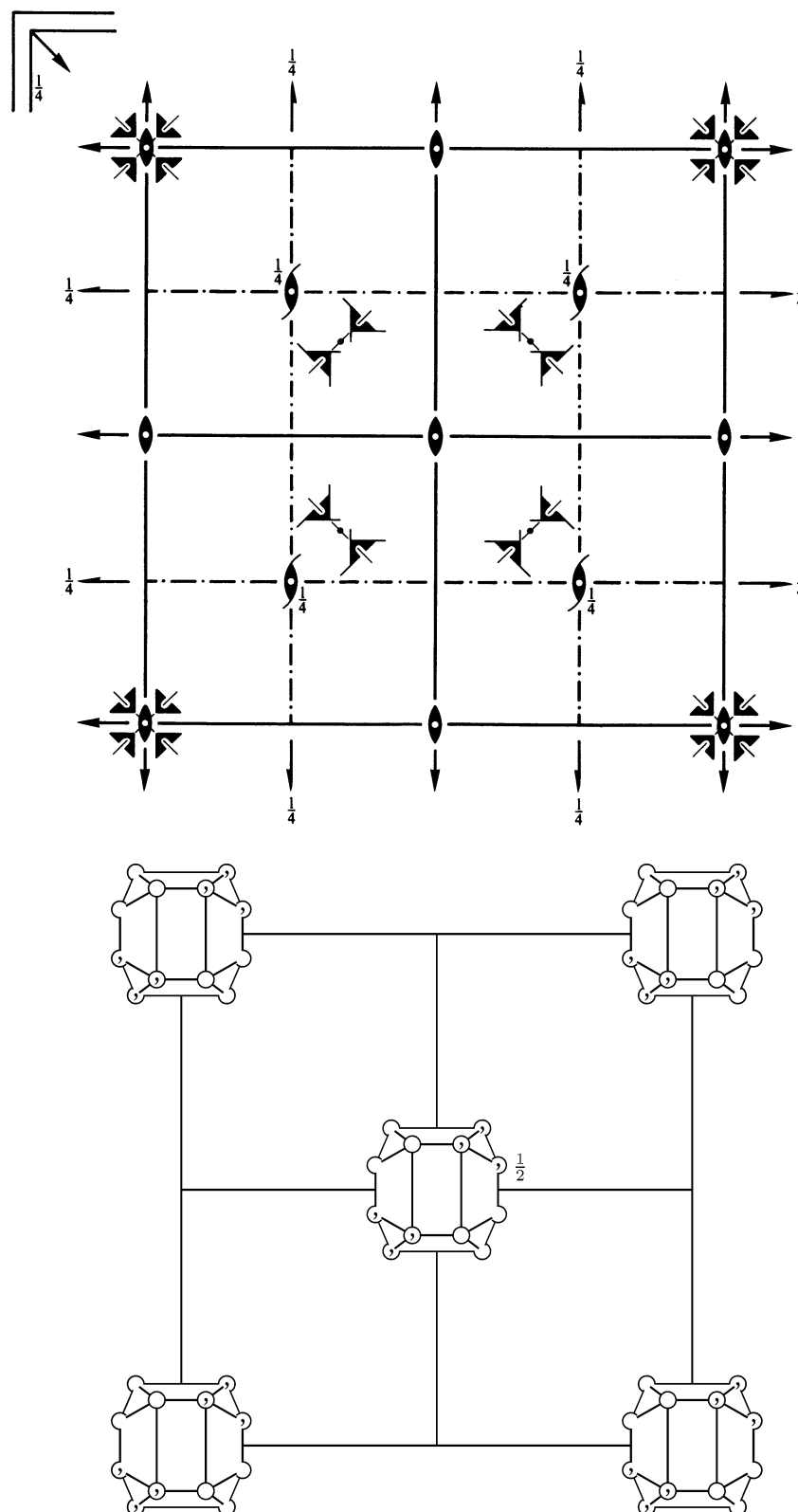
$m\bar{3}$

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) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}, \frac{1}{4}, z$	(3) 2(0, $\frac{1}{2}, 0$) $\frac{1}{4}, y, \frac{1}{4}$	(4) 2($\frac{1}{2}, 0, 0$) $x, \frac{1}{4}, \frac{1}{4}$
(5) 3 ⁺ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x	(6) 3 ⁺ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x}$	(7) 3 ⁺ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$	(8) 3 ⁺ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$
(9) 3 ⁻ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x,x,x	(10) 3 ⁻ ($-\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x}$	(11) 3 ⁻ ($\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}$) $\bar{x} + \frac{2}{3}, \bar{x} + \frac{1}{3}, x$	(12) 3 ⁻ ($\frac{1}{6}, -\frac{1}{6}, \frac{1}{6}$) $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$
(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); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (13)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates (0,0,0)+ ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+	Reflection conditions <i>h, k, l</i> cyclically permutable General: Special: as above, plus
48 <i>h</i> 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}	$hkl: h+k+l=2n$ $Ok: k+l=2n$ $hhl: l=2n$ $h00: h=2n$
24 <i>g</i> <i>m</i> . .	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 <i>f</i> . 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 <i>e</i> <i>m m</i> 2 . .	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 <i>d</i> <i>m m</i> 2 . .	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 <i>c</i> . $\bar{3}$.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: k, l=2n$
6 <i>b</i> <i>m m m</i> . .	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 <i>a</i> <i>m</i> $\bar{3}$.	0,0,0	no extra conditions

Symmetry of special projectionsAlong [001] *c*2*mm* $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0,0,z

Along [111] *p*6 $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$

Origin at x,x,x

 $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Along [110] *p*2*mm* $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,x,0