

$I\bar{4}3m$

$T_d^3$

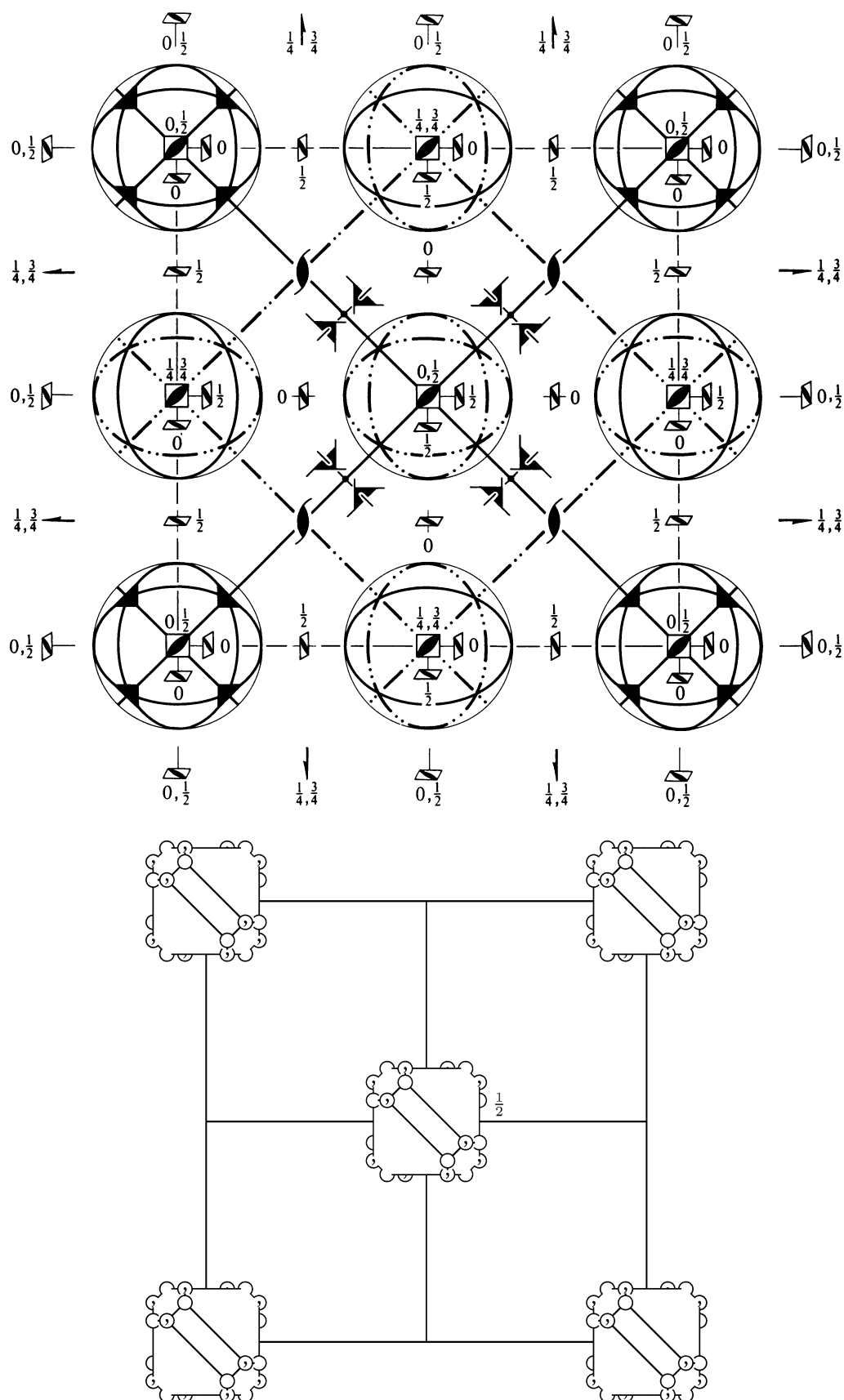
$\bar{4}3m$

Cubic

No. 217

$I\bar{4}3m$

Patterson symmetry  $Im\bar{3}m$



Origin at  $\bar{4}3m$

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

**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

 $h, k, l$  permutable

General:

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) y,x,z	(14) $\bar{y}, \bar{x}, z$	(15) y, $\bar{x}, \bar{z}$	(16) $\bar{y}, x, \bar{z}$
			(17) x,z,y	(18) $\bar{x}, z, \bar{y}$	(19) $\bar{x}, \bar{z}, y$	(20) x, $\bar{z}, \bar{y}$
			(21) z,y,x	(22) z, $\bar{y}, \bar{x}$	(23) $\bar{z}, y, \bar{x}$	(24) $\bar{z}, \bar{y}, x$

 $hkl: h+k+l=2n$  $OkL: k+l=2n$  $hhl: l=2n$  $h00: h=2n$ 

Special: no extra conditions

24	$g$	$. . m$	x,x,z $\bar{z}, \bar{x}, x$	$\bar{x}, \bar{x}, z$ $\bar{z}, x, \bar{x}$	$\bar{x}, x, \bar{z}$ x,z,x	x, $\bar{x}, \bar{z}$ $\bar{x}, z, \bar{x}$	z,x,x x, $\bar{z}, \bar{x}$	z, $\bar{x}, \bar{x}$ $\bar{x}, \bar{z}, x$
24	$f$	2..	$x, \frac{1}{2}, 0$ $\frac{1}{2}, x, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x}, 0$	0,x, $\frac{1}{2}$ x,0, $\frac{1}{2}$	0, $\bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, x$ 0, $\frac{1}{2}, x$	$\frac{1}{2}, 0, \bar{x}$ 0, $\frac{1}{2}, \bar{x}$
12	$e$	2.mmm	x,0,0	$\bar{x}, 0, 0$	0,x,0	0, $\bar{x}, 0$	0,0,x	0,0, $\bar{x}$
12	$d$	4..	$\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, \frac{1}{2}, 0$	0, $\frac{1}{4}, \frac{1}{2}$	0, $\frac{3}{4}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$
8	$c$	.3m	x,x,x	$\bar{x}, \bar{x}, x$	$\bar{x}, x, \bar{x}$	x, $\bar{x}, \bar{x}$		
6	$b$	42.m	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	$a$	43m	0,0,0					

**Symmetry of special projections**Along [001]  $p4mm$  $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$      $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ 

Origin at 0,0,z

Along [111]  $p31m$  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$      $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ 

Origin at x,x,x

Along [110]  $p1m1$  $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$      $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ 

Origin at x,x,0