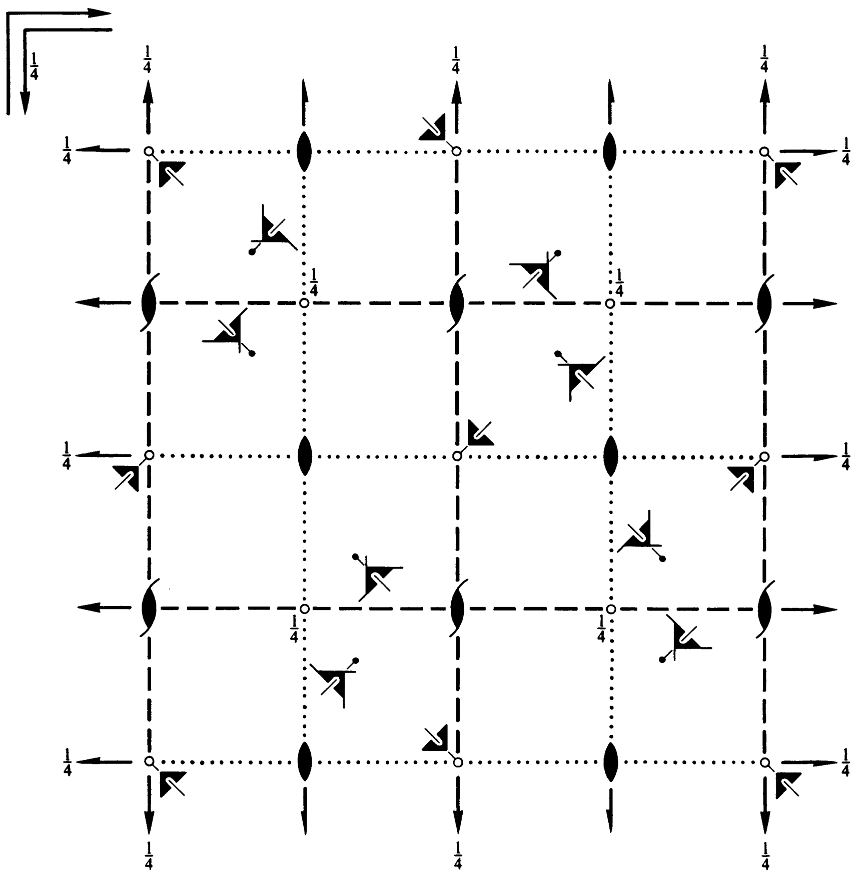
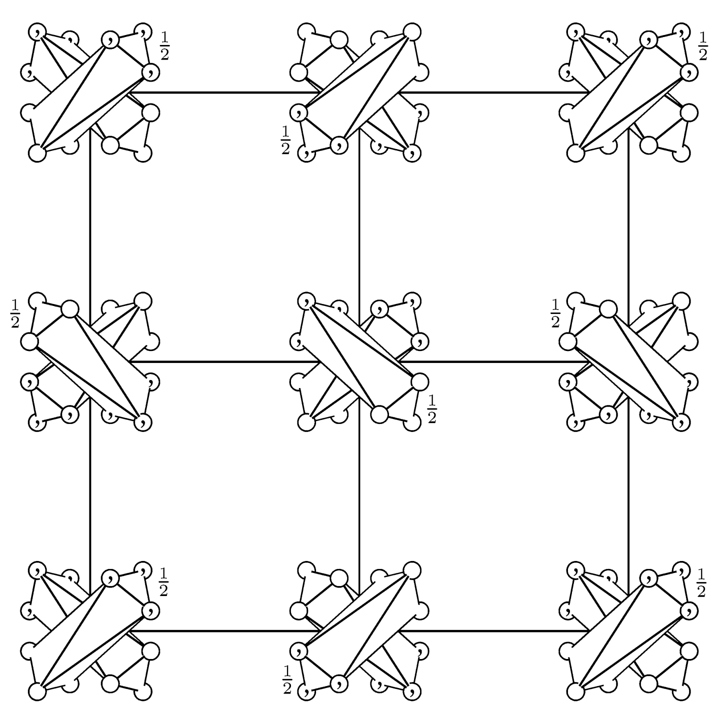
$Ia\bar{3}$ T_h^7 $m\bar{3}$ Cubic

No. 206 $I2_1/a\bar{3}$ Patterson symmetry $Im\bar{3}$





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

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

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

Symmetry operations

For (0,0,0)+ set

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

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

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$						Reflection conditions
									h,k,l cyclically permutable General:
48	e	1	(1) x,y,z	(2) $\bar{x}+\tfrac{1}{2},\bar{y},z+\tfrac{1}{2}$	(3) $\bar{x},y+\tfrac{1}{2},\bar{z}+\tfrac{1}{2}$	(4) $x+\tfrac{1}{2},\bar{y}+\tfrac{1}{2},\bar{z}$			hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z+\tfrac{1}{2},\bar{x}+\tfrac{1}{2},\bar{y}$	(7) $\bar{z}+\tfrac{1}{2},\bar{x},y+\tfrac{1}{2}$	(8) $\bar{z},x+\tfrac{1}{2},\bar{y}+\tfrac{1}{2}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z+\tfrac{1}{2},\bar{x}+\tfrac{1}{2}$	(11) $y+\tfrac{1}{2},\bar{z}+\tfrac{1}{2},\bar{x}$	(12) $\bar{y}+\tfrac{1}{2},\bar{z},x+\tfrac{1}{2}$			hhl: $l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\tfrac{1}{2},y,\bar{z}+\tfrac{1}{2}$	(15) $x,\bar{y}+\tfrac{1}{2},z+\tfrac{1}{2}$	(16) $\bar{x}+\tfrac{1}{2},y+\tfrac{1}{2},z$			$h00$: $h=2n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\tfrac{1}{2},x+\tfrac{1}{2},y$	(19) $z+\tfrac{1}{2},x,\bar{y}+\tfrac{1}{2}$	(20) $z,\bar{x}+\tfrac{1}{2},y+\tfrac{1}{2}$			
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\tfrac{1}{2},x+\tfrac{1}{2}$	(23) $\bar{y}+\tfrac{1}{2},z+\tfrac{1}{2},x$	(24) $y+\tfrac{1}{2},z,\bar{x}+\tfrac{1}{2}$			
									Special: as above, plus
24	d	$2\,.\,.$	$x,0,\tfrac{1}{4}$	$\bar{x}+\tfrac{1}{2},0,\tfrac{3}{4}$	$\tfrac{1}{4},x,0$	$\tfrac{3}{4},\bar{x}+\tfrac{1}{2},0$	$0,\tfrac{1}{4},x$	$0,\tfrac{3}{4},\bar{x}+\tfrac{1}{2}$	no extra conditions
			$\bar{x},0,\tfrac{3}{4}$	$x+\tfrac{1}{2},0,\tfrac{1}{4}$	$\tfrac{3}{4},\bar{x},0$	$\tfrac{1}{4},x+\tfrac{1}{2},0$	$0,\tfrac{3}{4},\bar{x}$	$0,\tfrac{1}{4},x+\tfrac{1}{2}$	
16	c	$.\,3\,.$	x,x,x	$\bar{x}+\tfrac{1}{2},\bar{x},x+\tfrac{1}{2}$	$\bar{x},x+\tfrac{1}{2},\bar{x}+\tfrac{1}{2}$	$x+\tfrac{1}{2},\bar{x}+\tfrac{1}{2},\bar{x}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\tfrac{1}{2},x,\bar{x}+\tfrac{1}{2}$	$x,\bar{x}+\tfrac{1}{2},x+\tfrac{1}{2}$	$\bar{x}+\tfrac{1}{2},x+\tfrac{1}{2},x$			
8	b	$.\,\bar{3}\,.$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	$\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}$	$\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}$	$\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}$			hkl: $k,l=2n$
8	a	$.\,\bar{3}\,.$	$0,0,0$	$\tfrac{1}{2},0,\tfrac{1}{2}$	$0,\tfrac{1}{2},\tfrac{1}{2}$	$\tfrac{1}{2},\tfrac{1}{2},0$			hkl: $k,l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\tfrac{1}{2}\mathbf{a}$ $\mathbf{b}'=\tfrac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\tfrac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\tfrac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mg$
$\mathbf{a}'=\tfrac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\tfrac{1}{2}\mathbf{c}$
Origin at $x,x,0$