

$Pm\bar{3}m$

O_h^1

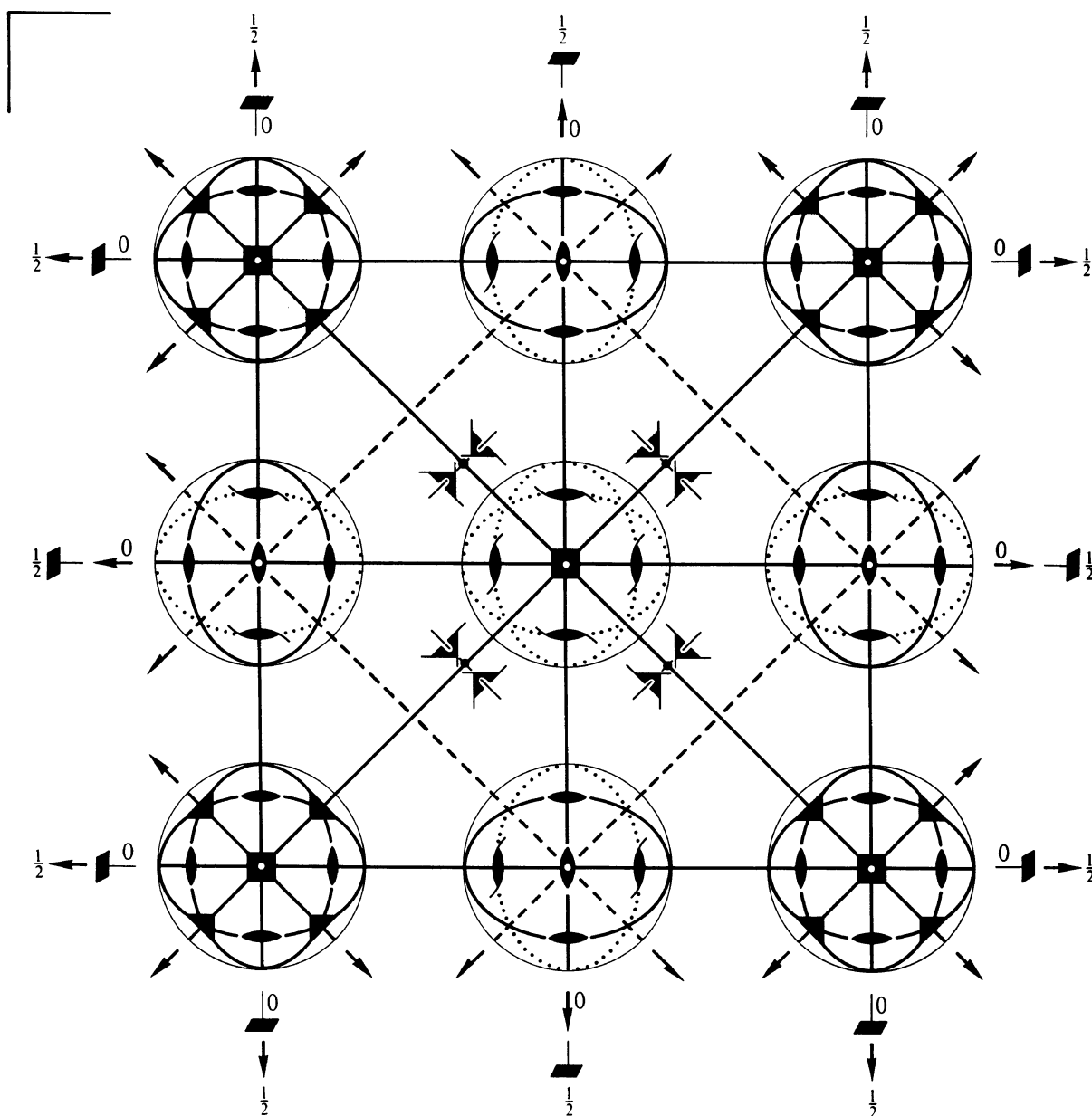
$m\bar{3}m$

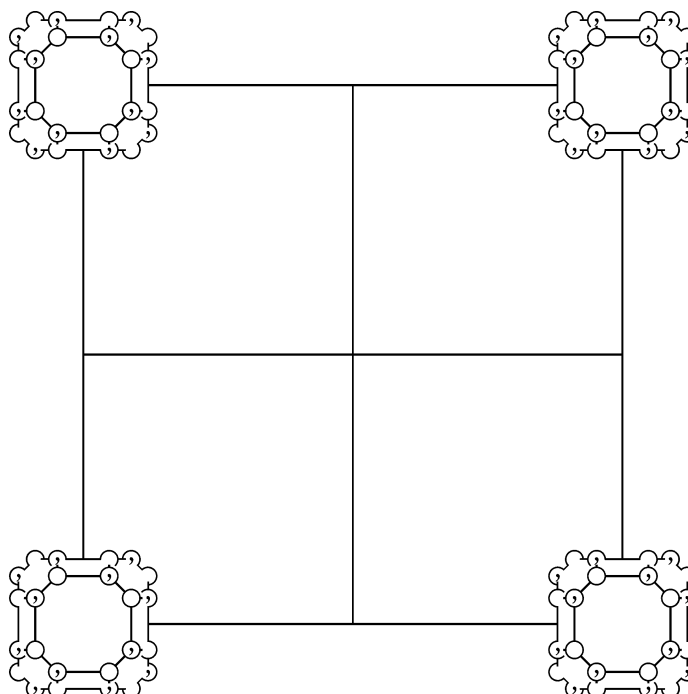
Cubic

No. 221

$P 4/m \bar{3} 2/m$

Patterson symmetry $Pm\bar{3}m$





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

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

Symmetry operations

- | | | | |
|------------------------------------|--|--|--|
| (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) 2 $x,x,0$ | (14) 2 $x,\bar{x},0$ | (15) 4^- $0,0,z$ | (16) 4^+ $0,0,z$ |
| (17) 4^- $x,0,0$ | (18) 2 $0,y,y$ | (19) 2 $0,y,\bar{y}$ | (20) 4^+ $x,0,0$ |
| (21) 4^+ $0,y,0$ | (22) 2 $x,0,x$ | (23) 4^- $0,y,0$ | (24) 2 $\bar{x},0,x$ |
| (25) $\bar{1}$ $0,0,0$ | (26) m $x,y,0$ | (27) m $x,0,z$ | (28) m $0,y,z$ |
| (29) $\bar{3}^+$ x,x,x ; $0,0,0$ | (30) $\bar{3}^+$ \bar{x},x,\bar{x} ; $0,0,0$ | (31) $\bar{3}^+$ x,\bar{x},\bar{x} ; $0,0,0$ | (32) $\bar{3}^+$ \bar{x},\bar{x},x ; $0,0,0$ |
| (33) $\bar{3}^-$ x,x,x ; $0,0,0$ | (34) $\bar{3}^-$ x,\bar{x},\bar{x} ; $0,0,0$ | (35) $\bar{3}^-$ \bar{x},\bar{x},x ; $0,0,0$ | (36) $\bar{3}^-$ \bar{x},x,\bar{x} ; $0,0,0$ |
| (37) m x,\bar{x},z | (38) m x,x,z | (39) $\bar{4}^-$ $0,0,z$; $0,0,0$ | (40) $\bar{4}^+$ $0,0,z$; $0,0,0$ |
| (41) $\bar{4}^-$ $x,0,0$; $0,0,0$ | (42) m x,y,\bar{y} | (43) $\bar{4}^-$ x,y,y | (44) $\bar{4}^+$ $x,0,0$; $0,0,0$ |
| (45) $\bar{4}^+$ $0,y,0$; $0,0,0$ | (46) m \bar{x},y,x | (47) $\bar{4}^-$ $0,y,0$; $0,0,0$ | (48) m x,y,x |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

h, k, l permutable

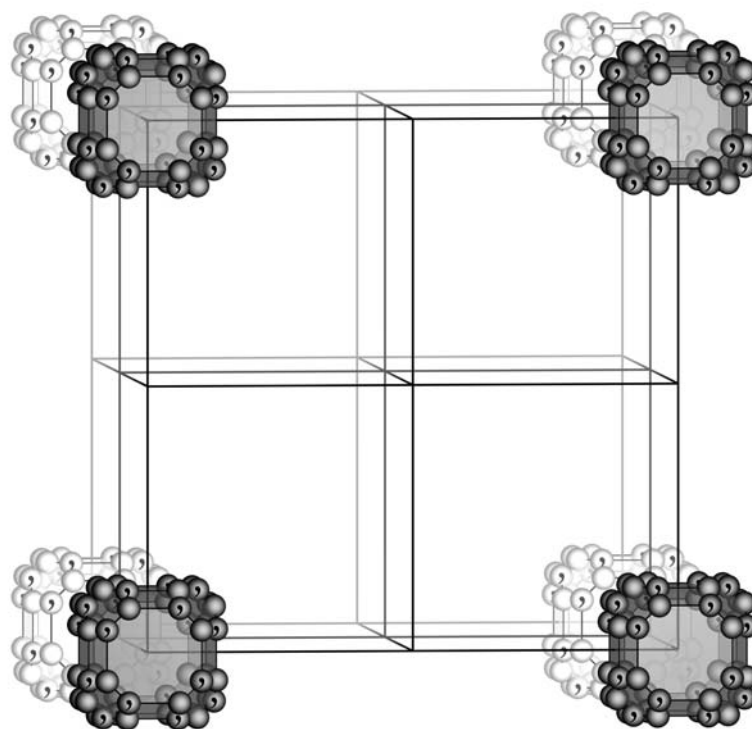
General:

48	n	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, \bar{z}	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) y, \bar{x}, z	(16) \bar{y}, x, z
			(17) x, z, \bar{y}	(18) \bar{x}, z, y	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) x, \bar{z}, y
			(21) z, y, \bar{x}	(22) z, \bar{y}, x	(23) \bar{z}, y, x	(24) $\bar{z}, \bar{y}, \bar{x}$
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) x, y, \bar{z}	(27) x, \bar{y}, z	(28) \bar{x}, y, z
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) \bar{z}, x, y	(31) z, x, \bar{y}	(32) z, \bar{x}, y
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) y, \bar{z}, x	(35) \bar{y}, z, x	(36) y, z, \bar{x}
			(37) \bar{y}, \bar{x}, z	(38) y, x, z	(39) \bar{y}, x, \bar{z}	(40) y, \bar{x}, \bar{z}
			(41) \bar{x}, \bar{z}, y	(42) x, \bar{z}, \bar{y}	(43) x, z, y	(44) \bar{x}, z, \bar{y}
			(45) \bar{z}, \bar{y}, x	(46) \bar{z}, y, \bar{x}	(47) z, \bar{y}, \bar{x}	(48) z, y, x

no conditions

Special: no extra conditions

24	m	$. . m$	x, x, z	\bar{x}, \bar{x}, z	\bar{x}, x, \bar{z}	x, \bar{x}, \bar{z}	z, x, x	z, \bar{x}, \bar{x}
			\bar{z}, \bar{x}, x	\bar{z}, x, \bar{x}	x, z, x	\bar{x}, z, \bar{x}	x, \bar{z}, \bar{x}	\bar{x}, \bar{z}, x
			x, x, \bar{z}	$\bar{x}, \bar{x}, \bar{z}$	x, \bar{x}, z	\bar{x}, x, z	x, z, \bar{x}	\bar{x}, z, x
			$\bar{x}, \bar{z}, \bar{x}$	x, \bar{z}, x	z, x, \bar{x}	z, \bar{x}, x	\bar{z}, x, x	$\bar{z}, \bar{x}, \bar{x}$
24	l	$m . .$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$	$\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, \bar{z}$	$z, \frac{1}{2}, y$	$z, \frac{1}{2}, \bar{y}$
			$\bar{z}, \frac{1}{2}, y$	$\bar{z}, \frac{1}{2}, \bar{y}$	$y, z, \frac{1}{2}$	$\bar{y}, z, \frac{1}{2}$	$y, \bar{z}, \frac{1}{2}$	$\bar{y}, \bar{z}, \frac{1}{2}$
			$y, \frac{1}{2}, \bar{z}$	$\bar{y}, \frac{1}{2}, \bar{z}$	$y, \frac{1}{2}, z$	$\bar{y}, \frac{1}{2}, z$	$\frac{1}{2}, z, \bar{y}$	$\frac{1}{2}, z, y$
			$\frac{1}{2}, \bar{z}, \bar{y}$	$\frac{1}{2}, \bar{z}, y$	$z, y, \frac{1}{2}$	$z, \bar{y}, \frac{1}{2}$	$\bar{z}, y, \frac{1}{2}$	$\bar{z}, \bar{y}, \frac{1}{2}$
24	k	$m . .$	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$	$z, 0, y$	$z, 0, \bar{y}$
			$\bar{z}, 0, y$	$\bar{z}, 0, \bar{y}$	$y, z, 0$	$\bar{y}, z, 0$	$y, \bar{z}, 0$	$\bar{y}, \bar{z}, 0$
			$y, 0, \bar{z}$	$\bar{y}, 0, \bar{z}$	$y, 0, z$	$\bar{y}, 0, z$	$0, z, \bar{y}$	$0, z, y$
			$0, \bar{z}, \bar{y}$	$0, \bar{z}, y$	$z, y, 0$	$z, \bar{y}, 0$	$\bar{z}, y, 0$	$\bar{z}, \bar{y}, 0$
12	j	$m . m2$	$\frac{1}{2}, y, y$	$\frac{1}{2}, \bar{y}, y$	$\frac{1}{2}, y, \bar{y}$	$\frac{1}{2}, \bar{y}, \bar{y}$	$y, \frac{1}{2}, y$	$y, \frac{1}{2}, \bar{y}$
			$\bar{y}, \frac{1}{2}, y$	$\bar{y}, \frac{1}{2}, \bar{y}$	$y, y, \frac{1}{2}$	$\bar{y}, y, \frac{1}{2}$	$y, \bar{y}, \frac{1}{2}$	$\bar{y}, \bar{y}, \frac{1}{2}$
12	i	$m . m2$	$0, y, y$	$0, \bar{y}, y$	$0, y, \bar{y}$	$0, \bar{y}, \bar{y}$	$y, 0, y$	$y, 0, \bar{y}$
			$\bar{y}, 0, y$	$\bar{y}, 0, \bar{y}$	$y, y, 0$	$\bar{y}, y, 0$	$y, \bar{y}, 0$	$\bar{y}, \bar{y}, 0$
12	h	$m m 2 . .$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$
			$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \bar{x}$	$0, \frac{1}{2}, x$
8	g	$. 3 m$	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
			x, x, \bar{x}	$\bar{x}, \bar{x}, \bar{x}$	x, \bar{x}, x	\bar{x}, x, x		
6	f	$4 m . m$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
6	e	$4 m . m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
3	d	$4/m m . m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$			
3	c	$4/m m . m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
1	b	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
1	a	$m\bar{3}m$	$0, 0, 0$					



Symmetry of special projections

Along $[001]$ $p4mm$

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at $0, 0, z$

Along $[111]$ $p6mm$

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

Origin at x, x, x

Along $[110]$ $p2mm$

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

Origin at $x, x, 0$