

Assorted Space Groups

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1 *m* (Monoclinic)

Monoclinic

m

C_s^4

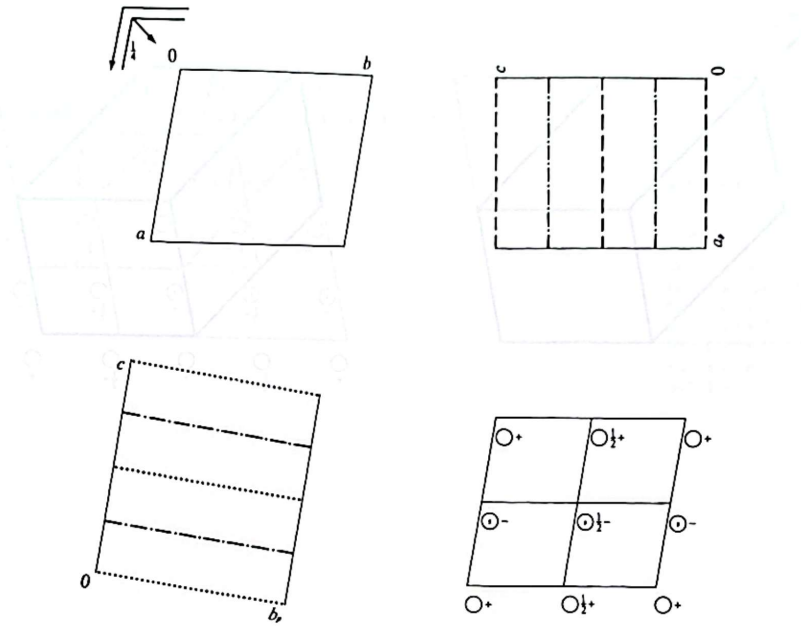
Cc

Patterson symmetry $A112/m$

$A11a$

No. 9

UNIQUE AXIS *c*, CELL CHOICE 1



Origin on glide plane *a*

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

For $(0, 0, 0)+$ set

(1) 1 (2) $a \ x, y, 0$

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

(1) $t(0, \frac{1}{2}, \frac{1}{2})$ (2) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, \frac{1}{2}$

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; (2)

Positions

Multiplicity		Coordinates
Wyckoff letter		$(0, 0, 0)+ \ (0, \frac{1}{2}, \frac{1}{2})+$
Site symmetry		

4 *a* 1 (1) x, y, z (2) $x + \frac{1}{2}, y, \bar{z}$

Reflection conditions

General:

$hkl: k + l = 2n$

$hk0: h, k = 2n$

$0kl: k + l = 2n$

$h0l: l = 2n$

$00l: l = 2n$

$h00: h = 2n$

$0k0: k = 2n$

Symmetry of special projections

Along $[001] \ p1$

$a' = \frac{1}{2}a \quad b' = \frac{1}{2}b$

Origin at $0, 0, z$

Along $[100] \ c11m$

$a' = b_p \quad b' = c$

Origin at $x, 0, 0$

Along $[010] \ p1g1$

$a' = \frac{1}{2}c \quad b' = a_p$

Origin at $0, y, 0$

227

2 $Pm\bar{3}m$

$Pm\bar{3}m$

No. 221

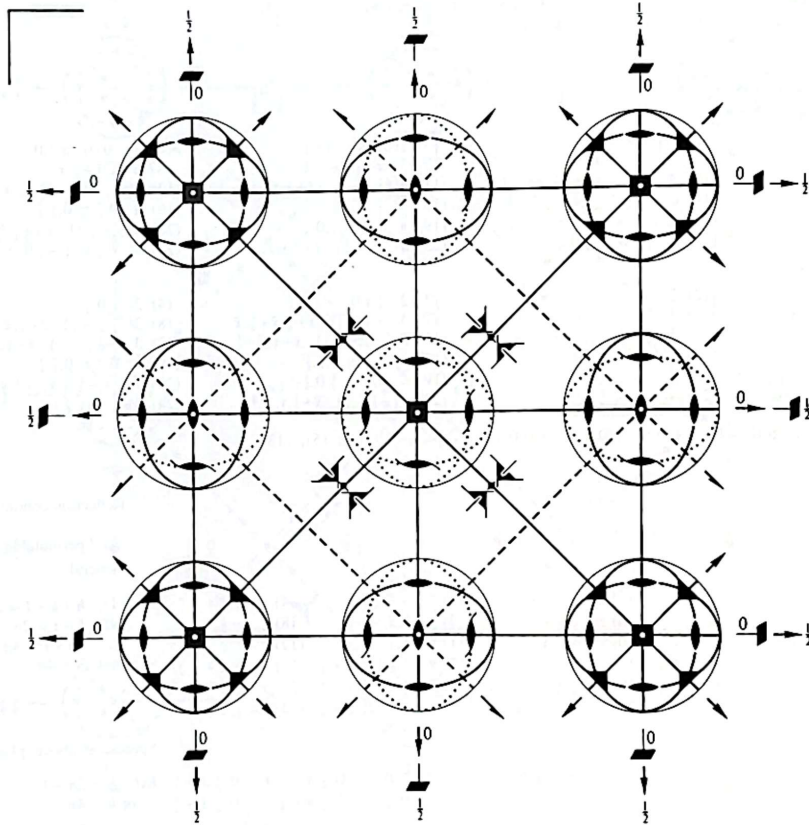
O_h^1

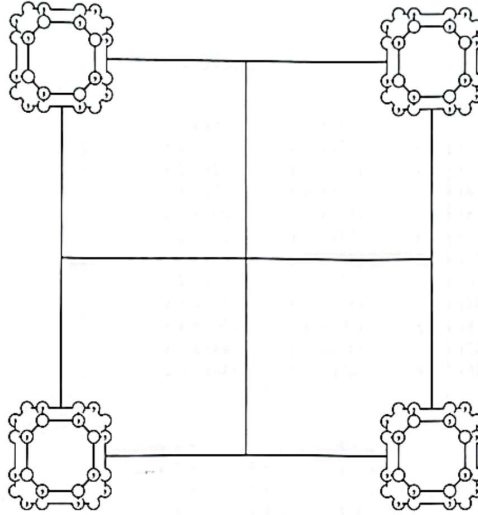
$P 4/m \bar{3} 2/m$

$m\bar{3}m$

Cubic

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

Symmetry operations

- | | | | |
|-------------------------------|---|---|---|
| (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) $m x,y,y$ | (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

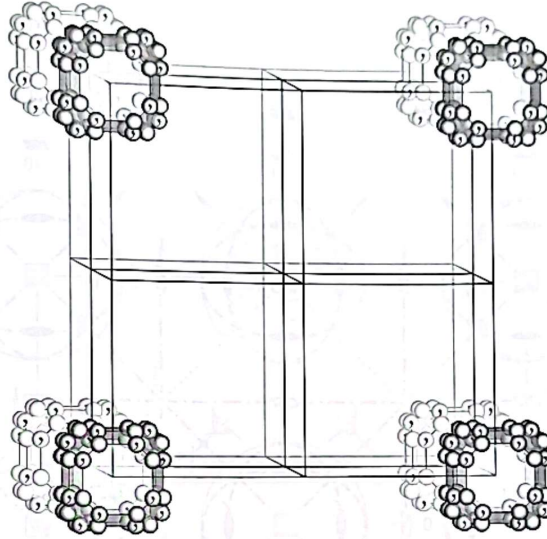
General:

no conditions

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

Special: no extra conditions

24	m	$\dots m$	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	$m \dots$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$	$\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, \bar{z}$	$z, \frac{1}{2}, y$	$z, \frac{1}{2}, \bar{y}$
			$\bar{z}, \frac{1}{2}, y$	$\bar{z}, \frac{1}{2}, \bar{y}$	$y, z, \frac{1}{2}$	$\bar{y}, z, \frac{1}{2}$	$y, \bar{z}, \frac{1}{2}$	$\bar{y}, \bar{z}, \frac{1}{2}$
			$y, \frac{1}{2}, \bar{z}$	$\bar{y}, \frac{1}{2}, \bar{z}$	$y, \frac{1}{2}, z$	$\bar{y}, \frac{1}{2}, z$	$\frac{1}{2}, z, \bar{y}$	$\frac{1}{2}, z, y$
			$\frac{1}{2}, \bar{z}, \bar{y}$	$\frac{1}{2}, \bar{z}, y$	$z, y, \frac{1}{2}$	$z, \bar{y}, \frac{1}{2}$	$\bar{z}, y, \frac{1}{2}$	$\bar{z}, \bar{y}, \frac{1}{2}$
24	k	$m \dots$	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$	$z, 0, y$	$z, 0, \bar{y}$
			$\bar{z}, 0, y$	$\bar{z}, 0, \bar{y}$	$y, z, 0$	$\bar{y}, z, 0$	$y, \bar{z}, 0$	$\bar{y}, \bar{z}, 0$
			$y, 0, \bar{z}$	$\bar{y}, 0, \bar{z}$	$y, 0, z$	$\bar{y}, 0, z$	$0, z, \bar{y}$	$0, z, y$
			$0, \bar{z}, \bar{y}$	$0, \bar{z}, y$	$z, y, 0$	$z, \bar{y}, 0$	$\bar{z}, y, 0$	$\bar{z}, \bar{y}, 0$
12	j	$m \cdot m2$	$\frac{1}{2}, y, y$	$\frac{1}{2}, \bar{y}, y$	$\frac{1}{2}, y, \bar{y}$	$\frac{1}{2}, \bar{y}, \bar{y}$	$y, \frac{1}{2}, y$	$y, \frac{1}{2}, \bar{y}$
			$\bar{y}, \frac{1}{2}, y$	$\bar{y}, \frac{1}{2}, \bar{y}$	$y, y, \frac{1}{2}$	$\bar{y}, y, \frac{1}{2}$	$y, \bar{y}, \frac{1}{2}$	$\bar{y}, \bar{y}, \frac{1}{2}$
12	i	$m \cdot m2$	$0, y, y$	$0, \bar{y}, y$	$0, y, \bar{y}$	$0, \bar{y}, \bar{y}$	$y, 0, y$	$y, 0, \bar{y}$
			$\bar{y}, 0, y$	$\bar{y}, 0, \bar{y}$	$y, y, 0$	$\bar{y}, y, 0$	$y, \bar{y}, 0$	$\bar{y}, \bar{y}, 0$
12	h	$m m 2 \dots$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$
			$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \bar{x}$	$0, \frac{1}{2}, x$
8	g	$\cdot 3 m$	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	$4 m \cdot m$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
6	e	$4 m \cdot m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
3	d	$4/m m \cdot m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$			
3	c	$4/m m \cdot m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			
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 $[001]$ $p4mm$
 $a' = a$ $b' = b$
 Origin at $0, 0, z$

Along $[111]$ $p6mm$
 $a' = \frac{1}{3}(2a - b - c)$ $b' = \frac{1}{3}(-a + 2b - c)$
 Origin at x, x, x

Along $[110]$ $p2mm$
 $a' = \frac{1}{2}(-a + b)$ $b' = c$
 Origin at $x, x, 0$

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); (25)

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:

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

96	l	1	(1) x, y, z	(2) $\bar{x}, \bar{y}, \bar{z}$	(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, \bar{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

Special: as above, plus

no extra conditions

48	k	$\dots m$	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	$\bar{z}, \bar{x}, \bar{x}$

no extra conditions

48	j	$m \dots$	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$	$z, 0, y$	$z, 0, \bar{y}$
			$\bar{z}, 0, y$	$\bar{z}, 0, \bar{y}$	$y, z, 0$	$\bar{y}, z, 0$	$y, \bar{z}, 0$	$\bar{y}, \bar{z}, 0$
			$y, 0, \bar{z}$	$\bar{y}, 0, \bar{z}$	$y, 0, z$	$\bar{y}, 0, z$	$0, z, \bar{y}$	$0, z, y$
			$0, \bar{z}, \bar{y}$	$0, \bar{z}, y$	$z, y, 0$	$z, \bar{y}, 0$	$\bar{z}, y, 0$	$\bar{z}, \bar{y}, 0$

no extra conditions

48	i	$\dots 2$	$\frac{1}{2}, y, \bar{y} + \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y} + \frac{1}{2}$	$\frac{1}{2}, y, y + \frac{1}{2}$	$\frac{1}{2}, \bar{y}, y + \frac{1}{2}$
			$\bar{y} + \frac{1}{2}, \frac{1}{2}, y$	$\bar{y} + \frac{1}{2}, \frac{1}{2}, \bar{y}$	$y + \frac{1}{2}, \frac{1}{2}, y$	$y + \frac{1}{2}, \frac{1}{2}, \bar{y}$
			$y, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$y, y + \frac{1}{2}, \frac{1}{2}$	$\bar{y}, y + \frac{1}{2}, \frac{1}{2}$
			$\frac{1}{2}, \bar{y}, y + \frac{1}{2}$	$\frac{1}{2}, y, y + \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y} + \frac{1}{2}$	$\frac{1}{2}, y, \bar{y} + \frac{1}{2}$
			$y + \frac{1}{2}, \frac{1}{2}, \bar{y}$	$y + \frac{1}{2}, \frac{1}{2}, y$	$\bar{y} + \frac{1}{2}, \frac{1}{2}, \bar{y}$	$\bar{y} + \frac{1}{2}, \frac{1}{2}, y$
			$\bar{y}, y + \frac{1}{2}, \frac{1}{2}$	$y, y + \frac{1}{2}, \frac{1}{2}$	$\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$y, \bar{y} + \frac{1}{2}, \frac{1}{2}$

no extra conditions

24	h	$m \dots m2$	$0, y, y$	$0, \bar{y}, y$	$0, y, \bar{y}$	$0, \bar{y}, \bar{y}$	$y, 0, y$	$y, 0, \bar{y}$
			$\bar{y}, 0, y$	$\bar{y}, 0, \bar{y}$	$y, y, 0$	$\bar{y}, y, 0$	$y, \bar{y}, 0$	$\bar{y}, \bar{y}, 0$

no extra conditions

24	g	$m m 2 \dots$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$0, \frac{1}{2}, x$	$0, \frac{1}{2}, \bar{x}$
			$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, x$	$\frac{1}{2}, 0, \bar{x}$

no extra conditions

16	f	$\dots 3m$	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

no extra conditions

12	e	$4m \dots m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
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no extra conditions

12	d	$\bar{4}m \dots 2$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$
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no extra conditions

8	c	$\dots \bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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$hkl: k, l = 2n$

6	b	$4/m m \dots m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
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no extra conditions

2	a	$m\bar{3}m$	$0, 0, 0$
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no extra conditions

CONTINUED

No. 225

$Fm\bar{3}m$

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

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq \min(x, \frac{1}{2}-x); z \leq y$
 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) 2 x,x,0 | (14) 2 x,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,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,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,y | (43) m 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 |

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|---|--|---|
| (1) $r(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0, \frac{1}{2}, \frac{1}{2}) 0, \frac{1}{2}, z$ | (3) $2(0, \frac{1}{2}, 0) 0, y, \frac{1}{2}$ | (4) 2 x, $\frac{1}{2}, \frac{1}{2}$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x - \frac{1}{2}, x - \frac{1}{2}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x - \frac{1}{2}, x + \frac{1}{2}, x$ | (10) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x + \frac{1}{2}, \frac{1}{2}$ | (14) $2(-\frac{1}{2}, \frac{1}{2}, 0) x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | (15) $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, \frac{1}{2}, z$ | (16) $4^-(0, 0, \frac{1}{2}) -\frac{1}{2}, \frac{1}{2}, z$ |
| (17) 4 ⁻ x, $\frac{1}{2}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) 0, y, y$ | (19) 2 0,y, $\frac{1}{2}, \bar{y}$ | (20) 4 ⁻ x, 0, $\frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \frac{1}{2}, y, \frac{1}{2}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x - \frac{1}{2}, \frac{1}{2}, x$ | (23) $4^-(0, \frac{1}{2}, 0) -\frac{1}{2}, y, \frac{1}{2}$ | (24) $2(-\frac{1}{2}, 0, \frac{1}{2}) \bar{x} + \frac{1}{2}, \frac{1}{2}, x$ |
| (25) $\bar{1}$ 0, $\frac{1}{2}, \frac{1}{2}$ | (26) b x,y, $\frac{1}{2}$ | (27) c x, $\frac{1}{2}, z$ | (28) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ |
| (29) $\bar{3}^+ x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{2}, 0, \frac{1}{2}$ | (31) $\bar{3}^+ x, \bar{x} + \frac{1}{2}, \bar{x}; 0, \frac{1}{2}, 0$ | (32) $\bar{3}^+ \bar{x} + 1, \bar{x} + \frac{1}{2}, x; \frac{1}{2}, 0, \frac{1}{2}$ |
| (33) $\bar{3}^- x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}; 0, 0, \frac{1}{2}$ | (35) $\bar{3}^- \bar{x} - 1, \bar{x} + \frac{1}{2}, x; -\frac{1}{2}, \frac{1}{2}, 0$ | (36) $\bar{3}^- \bar{x} + 1, x + \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, \frac{1}{2}$ |
| (37) $g(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x - \frac{1}{2}, x, z$ | (39) $\bar{4}^- -\frac{1}{2}, \frac{1}{2}, z; -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (40) $\bar{4}^- \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |
| (41) $\bar{4}^- x, 0, \frac{1}{2}; 0, 0, \frac{1}{2}$ | (42) m x,y, $\frac{1}{2}, \bar{y}$ | (43) $g(0, \frac{1}{2}, \frac{1}{2}) x, y, y$ | (44) $\bar{4}^- x, \frac{1}{2}, 0; 0, \frac{1}{2}, 0$ |
| (45) $\bar{4}^- -\frac{1}{2}, y, \frac{1}{2}; -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (46) $g(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (48) $g(\frac{1}{2}, 0, \frac{1}{2}) x - \frac{1}{2}, y, x$ |

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

- | | | | |
|---|---|---|--|
| (1) $r(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2(0, 0, \frac{1}{2}) \frac{1}{2}, 0, z$ | (3) 2 $\frac{1}{2}, y, \frac{1}{2}$ | (4) $2(\frac{1}{2}, 0, 0) x, 0, \frac{1}{2}$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, x - \frac{1}{2}, x$ | (6) $3^+(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x - \frac{1}{2}, x - \frac{1}{2}, x$ | (10) $3^- x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) $3^-(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x - \frac{1}{2}, \frac{1}{2}$ | (14) $2(\frac{1}{2}, -\frac{1}{2}, 0) x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | (15) $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, -\frac{1}{2}, z$ | (16) $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) x, \frac{1}{2}, \frac{1}{2}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \frac{1}{2}, y - \frac{1}{2}, y$ | (19) $2(0, -\frac{1}{2}, \frac{1}{2}) \frac{1}{2}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) x, -\frac{1}{2}, \frac{1}{2}$ |
| (21) $4^+ \frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x, 0, x$ | (23) $4^- 0, y, \frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, 0, x$ |
| (25) $\bar{1}$ $\frac{1}{2}, 0, \frac{1}{2}$ | (26) a x,y, $\frac{1}{2}$ | (27) $n(\frac{1}{2}, 0, \frac{1}{2}) x, 0, z$ | (28) c $\frac{1}{2}, y, z$ |
| (29) $\bar{3}^+ x - \frac{1}{2}, x - \frac{1}{2}, x; 0, 0, \frac{1}{2}$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}; 0, 0, \frac{1}{2}$ | (31) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \frac{1}{2}, \frac{1}{2}, 0$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \frac{1}{2}, -\frac{1}{2}, 0$ |
| (33) $\bar{3}^- x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{2}, \frac{1}{2}$ | (35) $\bar{3}^- \bar{x} + \frac{1}{2}, \bar{x} + 1, x; 0, \frac{1}{2}, \frac{1}{2}$ | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, x, \bar{x}; \frac{1}{2}, 0, 0$ |
| (37) $g(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, x, z$ | (39) $\bar{4}^- \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (40) $\bar{4}^- \frac{1}{2}, -\frac{1}{2}, z; \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$ |
| (41) $\bar{4}^- x, -\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$ | (42) $g(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) x, y + \frac{1}{2}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y - \frac{1}{2}, y$ | (44) $\bar{4}^- x, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |
| (45) $\bar{4}^- 0, y, \frac{1}{2}; 0, 0, \frac{1}{2}$ | (46) m $\bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, 0; \frac{1}{2}, 0, 0$ | (48) $g(\frac{1}{2}, 0, \frac{1}{2}) x, y, x$ |

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

- | | | | |
|--|---|--|---|
| (1) $r(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) 2 $\frac{1}{2}, \frac{1}{2}, z$ | (3) $2(0, \frac{1}{2}, 0) \frac{1}{2}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{2}, 0$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, x + \frac{1}{2}, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, x + \frac{1}{2}, x$ | (10) $3^- x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^-(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (14) 2 x, $\bar{x} + \frac{1}{2}, 0$ | (15) $4^- \frac{1}{2}, 0, z$ | (16) $4^- 0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) x, \frac{1}{2}, -\frac{1}{2}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \frac{1}{2}, y + \frac{1}{2}, y$ | (19) $2(0, -\frac{1}{2}, \frac{1}{2}) \frac{1}{2}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) x, \frac{1}{2}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \frac{1}{2}, y, -\frac{1}{2}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x + \frac{1}{2}, \frac{1}{2}, x$ | (23) $4^-(0, \frac{1}{2}, 0) \frac{1}{2}, y, \frac{1}{2}$ | (24) $2(\frac{1}{2}, 0, -\frac{1}{2}) \bar{x} + \frac{1}{2}, \frac{1}{2}, x$ |
| (25) $\bar{1}$ $\frac{1}{2}, \frac{1}{2}, 0$ | (26) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (27) a x, $\frac{1}{2}, z$ | (28) b $\frac{1}{2}, y, z$ |
| (29) $\bar{3}^+ x + \frac{1}{2}, x, x; \frac{1}{2}, 0, 0$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + 1, \bar{x}; 0, \frac{1}{2}, \frac{1}{2}$ | (31) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + 1, \bar{x}; 0, \frac{1}{2}, -\frac{1}{2}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x}, x; \frac{1}{2}, 0, 0$ |
| (33) $\bar{3}^- x, x + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (34) $\bar{3}^- x + 1, \bar{x} - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, \frac{1}{2}$ | (35) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; 0, \frac{1}{2}, 0$ | (36) $\bar{3}^- \bar{x} + 1, x - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, -\frac{1}{2}$ |
| (37) m $x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, 0) x, x, z$ | (39) $\bar{4}^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, 0$ | (40) $\bar{4}^- \frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$ |
| (41) $\bar{4}^- x, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (42) $g(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) x, y + \frac{1}{2}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x, y + \frac{1}{2}, y$ | (44) $\bar{4}^- x, \frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$ |
| (45) $\bar{4}^- \frac{1}{2}, y, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (46) $g(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$ | (48) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) x + \frac{1}{2}, y, x$ |

Generators selected (1); $r(1,0,0)$; $r(0,1,0)$; $r(0,0,1)$; $r(0,\frac{1}{2},\frac{1}{2})$; $r(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

Reflection conditions

h, k, l permutable

General:

192	l	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

$hkl: h+k, h+l, k+l=2n$
 $0kl: k, l=2n$
 $hhl: h+l=2n$
 $h00: h=2n$

Special: as above, plus

96	k	$\dots m$	x, x, z \bar{z}, \bar{x}, x x, x, \bar{z} $\bar{x}, \bar{z}, \bar{x}$	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x} $\bar{x}, \bar{x}, \bar{z}$ x, \bar{z}, x	\bar{x}, x, \bar{z} x, z, x x, \bar{x}, z z, x, \bar{x}	x, \bar{x}, \bar{z} \bar{x}, z, \bar{x} \bar{x}, x, z z, \bar{x}, x	z, x, x x, \bar{z}, \bar{x} x, z, \bar{x} \bar{z}, x, x	z, \bar{x}, \bar{x} \bar{x}, \bar{z}, x \bar{x}, z, x $\bar{z}, \bar{x}, \bar{x}$	no extra conditions
96	j	$m \dots$	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions
48	i	$m \cdot m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	no extra conditions
48	h	$m \cdot m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions
48	g	$2 \cdot mm$	$x, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{1}{4}$	$\bar{x}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \bar{x}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $x, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \bar{x}, \frac{1}{4}$ $\bar{x}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{1}{4}, \bar{x}$	$\frac{1}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{1}{4}, x$	$hkl: h=2n$
32	f	$\cdot 3m$	x, x, x x, x, \bar{x}	\bar{x}, \bar{x}, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x			no extra conditions
24	e	$4m \cdot m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions
24	d	$m \cdot mm$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{1}{4}, 0$	$hkl: h=2n$
8	c	$\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					$hkl: h=2n$
4	b	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						no extra conditions
4	a	$m\bar{3}m$	$0, 0, 0$						no extra conditions

5 $Fd\bar{3}m$

$Fd\bar{3}m$

O_h^7

$m\bar{3}m$

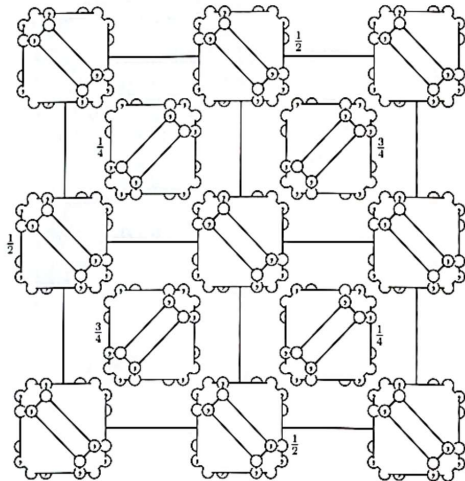
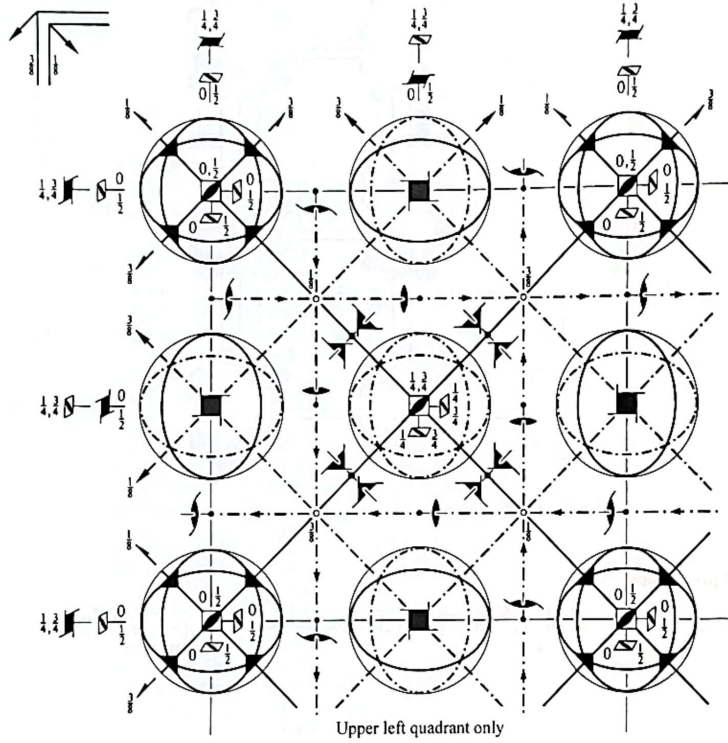
Cubic

No. 227

$F 4_1/d \bar{3} 2/m$

Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 1



672

Origin at $\bar{4}3m$, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre ($\bar{3}m$)

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

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

Symmetry operations

For $(0, 0, 0) + \text{set}$

- | | | | |
|---|---|--|---|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \quad 0, \frac{1}{2}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad \frac{1}{2}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{2}$ |
| (5) $3^+ x, x, x$ | (6) $3^+(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \quad \bar{x} + \frac{1}{6}, x + \frac{1}{6}, \bar{x}$ | (7) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{6}, \bar{x} - \frac{1}{6}, \bar{x}$ | (8) $3^+(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \quad \bar{x} + \frac{1}{6}, \bar{x} + \frac{1}{6}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- x, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x - \frac{1}{2}, \frac{1}{2}$ | (14) $2 \quad x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | (15) $4^-(0, 0, \frac{1}{2}) \quad \frac{1}{2}, \frac{1}{2}, z$ | (16) $4^-(0, 0, \frac{1}{2}) \quad 0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) \quad x, \frac{1}{2}, \frac{1}{2}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y + \frac{1}{2}, y$ | (19) $2 \quad \frac{1}{2}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \quad \frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x - \frac{1}{2}, \frac{1}{2}, x$ | (23) $4^-(0, \frac{1}{2}, 0) \quad \frac{1}{2}, y, \frac{1}{2}$ | (24) $2 \quad \bar{x} + \frac{1}{2}, \frac{1}{2}, x$ |
| (25) $\bar{1} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (26) $d(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, \frac{1}{2}$ | (27) $d(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{2}, z$ | (28) $d(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y, z$ |
| (29) $\bar{3}^+ x, x, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - 1, x + 1, \bar{x}; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (31) $\bar{3}^+ x, \bar{x} + 1, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + 1, \bar{x}, x; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x, x, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ | (35) $\bar{3}^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + 1, x + \frac{1}{2}, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ |
| (37) $g(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, \bar{x}, z$ | (38) $m \quad x, x, z$ | (39) $\bar{4}^- -\frac{1}{2}, \frac{1}{2}, z; -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (40) $\bar{4}^- \frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$ |
| (41) $\bar{4}^- x, -\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$ | (42) $g(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \quad x, y + \frac{1}{2}, \bar{y}$ | (43) $m \quad x, y, y$ | (44) $\bar{4}^+ x, \frac{1}{2}, 0; 0, \frac{1}{2}, 0$ |
| (45) $\bar{4}^+ 0, y, \frac{1}{2}; 0, 0, \frac{1}{2}$ | (46) $g(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$ | (48) $m \quad x, y, x$ |

For $(0, \frac{1}{2}, \frac{1}{2}) + \text{set}$

- | | | | |
|---|--|--|--|
| (1) $r(0, \frac{1}{2}, \frac{1}{2})$ | (2) $2 \quad 0, 0, z$ | (3) $2 \quad \frac{1}{2}, y, \frac{1}{2}$ | (4) $2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{2}, 0$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x - \frac{1}{2}, x - \frac{1}{2}, x$ | (6) $3^+ \bar{x} + \frac{1}{2}, x, \bar{x}$ | (7) $3^+ x, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x - \frac{1}{2}, x + \frac{1}{2}, x$ | (10) $3^- x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^-(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \quad \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x}, x, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, \frac{1}{2}$ | (14) $2(-\frac{1}{2}, \frac{1}{2}, 0) \quad x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | (15) $4^-(0, 0, \frac{1}{2}) \quad \frac{1}{2}, 0, z$ | (16) $4^-(0, 0, \frac{1}{2}) \quad \frac{1}{2}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) \quad x, \frac{1}{2}, -\frac{1}{2}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y - \frac{1}{2}, y$ | (19) $2 \quad \frac{1}{2}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) \quad x, 0, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \quad \frac{1}{2}, y, -\frac{1}{2}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{2}, x$ | (23) $4^-(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{2}$ | (24) $2(-\frac{1}{2}, 0, \frac{1}{2}) \quad \bar{x} + \frac{1}{2}, \frac{1}{2}, x$ |
| (25) $\bar{1} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (26) $d(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, \frac{1}{2}$ | (27) $d(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{2}, z$ | (28) $d(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y, z$ |
| (29) $\bar{3}^+ x, x, x + \frac{1}{2}, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (31) $\bar{3}^+ x, \bar{x} + \frac{1}{2}, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + 1, \bar{x} - \frac{1}{2}, x; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x - \frac{1}{2}, x - \frac{1}{2}, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ | (35) $\bar{3}^- \bar{x}, \bar{x} + 1, x; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + 1, x, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ |
| (37) $m \quad x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x - \frac{1}{2}, x, z$ | (39) $\bar{4}^- 0, 0, z; 0, 0, 0$ | (40) $\bar{4}^- \frac{1}{2}, -\frac{1}{2}, z; \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$ |
| (41) $\bar{4}^- x, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (42) $g(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \quad x, y + \frac{1}{2}, \bar{y}$ | (43) $g(0, \frac{1}{2}, \frac{1}{2}) \quad x, y, y$ | (44) $\bar{4}^- x, 0, 0; 0, 0, 0$ |
| (45) $\bar{4}^- \frac{1}{2}, y, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (46) $m \quad \bar{x}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, 0; \frac{1}{2}, 0, 0$ | (48) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x - \frac{1}{2}, y, x$ |

For $(\frac{1}{2}, 0, \frac{1}{2}) + \text{set}$

- | | | | |
|---|---|--|--|
| (1) $r(\frac{1}{2}, 0, \frac{1}{2})$ | (2) $2 \quad \frac{1}{2}, \frac{1}{2}, z$ | (3) $2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{2}$ | (4) $2 \quad x, 0, 0$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, x - \frac{1}{2}, x$ | (6) $3^+ \bar{x}, x, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x - \frac{1}{2}, x - \frac{1}{2}, x$ | (10) $3^- (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ | (11) $3^- \bar{x}, \bar{x}, x$ | (12) $3^- \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, \frac{1}{2}$ | (14) $2(\frac{1}{2}, -\frac{1}{2}, 0) \quad x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | (15) $4^-(0, 0, \frac{1}{2}) \quad \frac{1}{2}, 0, z$ | (16) $4^-(0, 0, \frac{1}{2}) \quad -\frac{1}{2}, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) \quad x, \frac{1}{2}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y, y$ | (19) $2(0, -\frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) \quad x, \frac{1}{2}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \quad \frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x + \frac{1}{2}, \frac{1}{2}, x$ | (23) $4^-(0, \frac{1}{2}, 0) \quad -\frac{1}{2}, y, \frac{1}{2}$ | (24) $2 \quad \bar{x} + \frac{1}{2}, \frac{1}{2}, x$ |
| (25) $\bar{1} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (26) $d(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, \frac{1}{2}$ | (27) $d(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{2}, z$ | (28) $d(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y, z$ |
| (29) $\bar{3}^+ x - \frac{1}{2}, x - \frac{1}{2}, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (31) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x + \frac{1}{2}, x, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + 1, \bar{x} - 1, \bar{x}; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ | (35) $\bar{3}^- \bar{x}, \bar{x} + \frac{1}{2}, x; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + \frac{1}{2}, x - \frac{1}{2}, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ |
| (37) $m \quad x, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, x, z$ | (39) $\bar{4}^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, 0$ | (40) $\bar{4}^- \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |
| (41) $\bar{4}^- x, 0, 0; 0, 0, 0$ | (42) $m \quad x, y + \frac{1}{2}, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, y - \frac{1}{2}, y$ | (44) $\bar{4}^- x, \frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$ |
| (45) $\bar{4}^- 0, y, 0; 0, 0, 0$ | (46) $g(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \quad \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{2}, y, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (48) $g(\frac{1}{2}, 0, \frac{1}{2}) \quad x, y, x$ |

For $(\frac{1}{2}, \frac{1}{2}, 0) + \text{set}$

- | | | | |
|--|--|--|--|
| (1) $r(\frac{1}{2}, \frac{1}{2}, 0)$ | (2) $2(0, 0, \frac{1}{2}) \quad \frac{1}{2}, 0, z$ | (3) $2 \quad 0, y, 0$ | (4) $2 \quad x, \frac{1}{2}, \frac{1}{2}$ |
| (5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, x + \frac{1}{2}, x$ | (6) $3^+ \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x} - \frac{1}{2}, \bar{x}$ | (8) $3^+ \bar{x}, \bar{x}, x$ |
| (9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, x + \frac{1}{2}, x$ | (10) $3^- x, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x + \frac{1}{2}, \frac{1}{2}$ | (14) $2 \quad x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | (15) $4^-(0, 0, \frac{1}{2}) \quad \frac{1}{2}, -\frac{1}{2}, z$ | (16) $4^-(0, 0, \frac{1}{2}) \quad 0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) \quad x, \frac{1}{2}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y, y$ | (19) $2(0, \frac{1}{2}, -\frac{1}{2}) \quad \frac{1}{2}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) \quad x, -\frac{1}{2}, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \quad \frac{1}{2}, y, \frac{1}{2}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{2}, x$ | (23) $4^-(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{2}$ | (24) $2(\frac{1}{2}, 0, -\frac{1}{2}) \quad \bar{x} + \frac{1}{2}, \frac{1}{2}, x$ |
| (25) $\bar{1} \quad \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (26) $d(\frac{1}{2}, \frac{1}{2}, 0) \quad x, y, \frac{1}{2}$ | (27) $d(\frac{1}{2}, 0, \frac{1}{2}) \quad x, \frac{1}{2}, z$ | (28) $d(0, \frac{1}{2}, \frac{1}{2}) \quad \frac{1}{2}, y, z$ |
| (29) $\bar{3}^+ x + \frac{1}{2}, x, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (30) $\bar{3}^+ \bar{x} - \frac{1}{2}, x + 1, \bar{x}; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (31) $\bar{3}^+ x + \frac{1}{2}, \bar{x} + 1, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x}, x; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ |
| (33) $\bar{3}^- x, x + \frac{1}{2}, x; \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; \frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{2}, \bar{x} + 1, x; -\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | (36) $\bar{3}^- \bar{x} + 1, x, \bar{x}; \frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$ |
| (37) $g(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, \bar{x}, z$ | (38) $g(\frac{1}{2}, \frac{1}{2}, 0) \quad x, x, z$ | (39) $\bar{4}^- \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (40) $\bar{4}^- 0, 0, z; 0, 0, 0$ |
| (41) $\bar{4}^- x, 0, \frac{1}{2}; 0, \frac{1}{2}, \frac{1}{2}$ | (42) $m \quad x, y, \bar{y}$ | (43) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x, y + \frac{1}{2}, y$ | (44) $\bar{4}^+ x, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |
| (45) $\bar{4}^+ -\frac{1}{2}, y, \frac{1}{2}; -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | (46) $m \quad \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- 0, y, 0; 0, 0, 0$ | (48) $g(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \quad x + \frac{1}{2}, y, x$ |

ORIGIN CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0, \frac{1}{2}, \frac{1}{2})$; $t(\frac{1}{2}, 0, \frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity	Coordinates
Wyckoff letter	
Site symmetry	$(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ $(\frac{1}{2}, 0, \frac{1}{2})+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

Reflection conditions

h, k, l permutable
General:

192	i	1	(1) x, y, z	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$
			(5) z, x, y	(6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$	(7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$	(8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$
			(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	(11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	(12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$
			(13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$
			(17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$
			(21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	(23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	(24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$
			(25) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(27) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(28) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$
			(29) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(30) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}$	(31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(32) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$
			(33) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(34) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	(35) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$	(36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$
			(37) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$	(38) y, x, z	(39) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$
			(41) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$	(42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y}$	(43) x, z, y	(44) $\bar{x}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$
			(45) $\bar{z} + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$	(46) $\bar{z}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x}$	(48) z, y, x

hkl : $h+k=2n$ and $h+l, k+l=2n$
 OkI : $k+l=4n$ and $k, l=2n$
 hhl : $h+l=2n$
 $h00$: $h=4n$

Special: as above, plus

96	h	$.2$	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}$	$\frac{1}{8}, y + \frac{1}{2}, y + \frac{1}{4}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$
			$\bar{y} + \frac{1}{2}, \frac{1}{8}, y$	$\bar{y} + \frac{1}{2}, \frac{7}{8}, \bar{y} + \frac{1}{4}$	$y + \frac{1}{2}, \frac{3}{8}, y + \frac{1}{4}$	$y + \frac{1}{2}, \frac{5}{8}, \bar{y}$
			$y, \bar{y} + \frac{1}{4}, \frac{1}{8}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}, \frac{7}{8}$	$y + \frac{1}{2}, y + \frac{1}{4}, \frac{3}{8}$	$\bar{y}, y + \frac{1}{4}, \frac{5}{8}$
			$\frac{1}{8}, \bar{y} + \frac{1}{2}, y$	$\frac{7}{8}, y + \frac{1}{2}, y + \frac{1}{4}$	$\frac{1}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}$	$\frac{5}{8}, y + \frac{1}{2}, \bar{y}$
			$y, \frac{1}{8}, \bar{y} + \frac{1}{4}$	$y + \frac{1}{2}, \frac{7}{8}, y + \frac{1}{4}$	$\bar{y} + \frac{1}{2}, \frac{3}{8}, \bar{y} + \frac{1}{4}$	$\bar{y}, \frac{5}{8}, y + \frac{1}{4}$
			$\bar{y} + \frac{1}{2}, y, \frac{1}{8}$	$y + \frac{1}{2}, y + \frac{1}{4}, \frac{7}{8}$	$\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{4}, \frac{3}{8}$	$y + \frac{1}{2}, \bar{y}, \frac{5}{8}$

no extra conditions

96	g	$.m$	x, x, z	$\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	$x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$
			z, x, x	$z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$	$\bar{z}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$
			x, z, x	$\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$
			$x + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$
			$x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$
			$z + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$z + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{z} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$

no extra conditions

48	f	$2.m\bar{m}$	$x, 0, 0$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$0, 0, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
			$\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$

hkl : $h=2n+1$
or $h+k+l=4n$

32	e	$.3m$	x, x, x	$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$
			$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$
			$x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$
			$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$

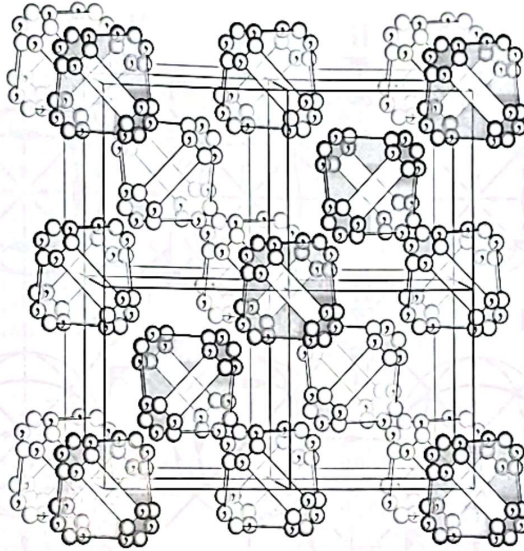
no extra conditions

16	d	$.\bar{3}m$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{3}{8}, \frac{7}{8}$
16	c	$.\bar{3}m$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$

hkl : $h=2n+1$
or $h, k, l=4n+2$
or $h, k, l=4n$

8	b	$\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$
8	a	$\bar{4}3m$	$0, 0, 0$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$

hkl : $h=2n+1$
or $h+k+l=4n$



Symmetry of special projections

Along $[001]$ $p4mm$

$$a' = \frac{1}{4}(a-b) \quad b' = \frac{1}{4}(a+b)$$

Origin at $0,0,z$

Along $[111]$ $p6mm$

$$a' = \frac{1}{6}(2a-b-c) \quad b' = \frac{1}{6}(-a+2b-c)$$

Origin at x,x,x

Along $[110]$ $c2mm$

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

Origin at $x,x,\frac{1}{4}$



6 $F\bar{4}3m$

$F\bar{4}3m$

No. 216

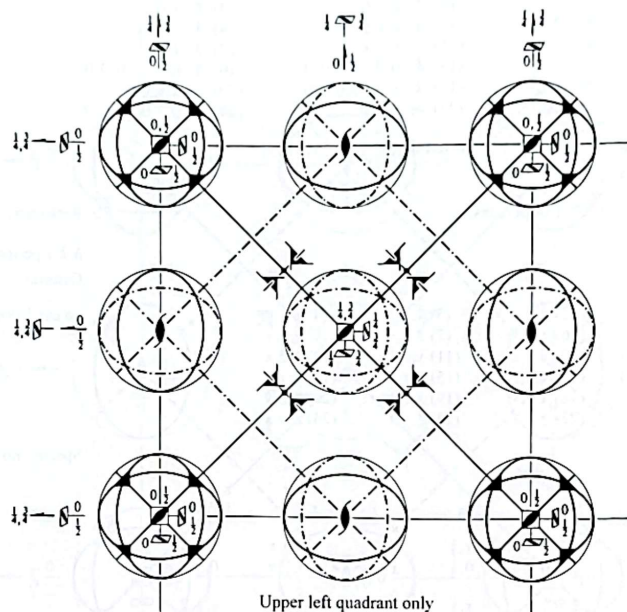
T_d^2

$F\bar{4}3m$

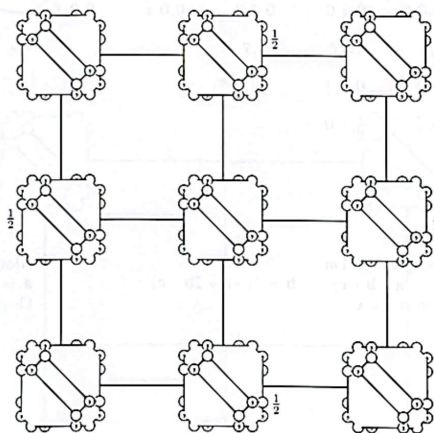
$\bar{4}3m$

Cubic

Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at $\bar{4}3m$

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

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) $3^+ \bar{x},\bar{x},\bar{x}$ | (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) $m x,x,z$ | (14) $m x,\bar{x},z$ | (15) $\bar{4}^+ 0,0,z; 0,0,0$ | (16) $\bar{4}^- 0,0,z; 0,0,0$ |
| (17) $m x,y,y$ | (18) $\bar{4}^+ x,0,0; 0,0,0$ | (19) $\bar{4}^- x,0,0; 0,0,0$ | (20) $m x,y,\bar{y}$ |
| (21) $m x,y,x$ | (22) $\bar{4}^- 0,y,0; 0,0,0$ | (23) $m \bar{x},y,x$ | (24) $\bar{4}^+ 0,y,0; 0,0,0$ |

Symmetry operations (continued)

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

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

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

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

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

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

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates
 $(0, 0, 0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ $(\frac{1}{2}, 0, \frac{1}{2})+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

Reflection conditions

h, k, l permutable
General:
 $hkl: h + k, h + l, k + l = 2n$
 $OkI: k, l = 2n$
 $hIh: h + l = 2n$
 $h00: h = 2n$

96	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) 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

Special: no extra conditions

48	h	$\dots m$	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	g	$2 . mm$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$
24	f	$2 . mm$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$
16	e	$. 3 m$	x, x, x	\bar{x}, \bar{x}, x	\bar{x}, x, \bar{x}	x, \bar{x}, \bar{x}		
4	d	$\bar{4} 3 m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
4	c	$\bar{4} 3 m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
4	b	$\bar{4} 3 m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
4	a	$\bar{4} 3 m$	$0, 0, 0$					

Symmetry of special projections

Along $[001]$ $p4mm$
 $a' = \frac{1}{2}a$ $b' = \frac{1}{2}b$
Origin at $0, 0, z$

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

Along $[110]$ $c1m1$
 $a' = \frac{1}{2}(-a + b)$ $b' = c$
Origin at $x, x, 0$

7 $P6_3mc$

Hexagonal

$6mm$

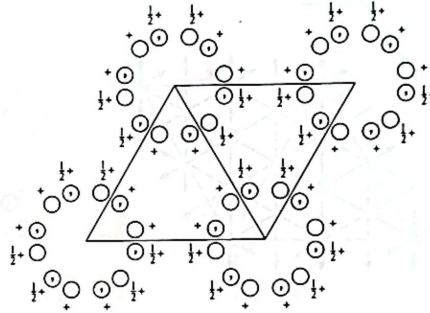
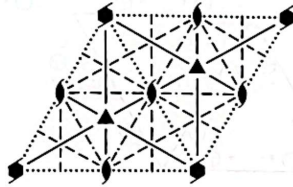
C_{6v}^4

$P6_3mc$

Patterson symmetry $P6/mmm$

$P6_3mc$

No. 186



Origin on $3m1$ on 6_3mc

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1; x \leq (1+y)/2; y \leq x/2$
 Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0$
 $0,0,1 \quad \frac{1}{2},0,1 \quad \frac{1}{2},\frac{1}{2},1$

Symmetry operations

- (1) 1
- (2) 3^+ $0,0,z$
- (3) 3^- $0,0,z$
- (4) $2(0,0,\frac{1}{2})$ $0,0,z$
- (5) 6^+ $(0,0,\frac{1}{2})$ $0,0,z$
- (6) 6^- $(0,0,\frac{1}{2})$ $0,0,z$
- (7) m x,\bar{x},z
- (8) m $x,2x,z$
- (9) m $2x,x,z$
- (10) c x,x,z
- (11) c $x,0,z$
- (12) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

12	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
			(7) \bar{y},\bar{x},z	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

General:

$hh\bar{2}hl: l = 2n$
 $000l: l = 2n$

Special: as above, plus

6	c	$.m.$	x,\bar{x},z	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$\bar{x},2\bar{x},z+\frac{1}{2}$	$2x,x,z+\frac{1}{2}$
2	b	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$				
2	a	$3m.$	$0,0,z$	$0,0,z+\frac{1}{2}$				

no extra conditions

$hkil: l = 2n$
 or $h-k = 3n+1$
 or $h-k = 3n+2$

$hkil: l = 2n$

Symmetry of special projections

Along $[001]$ $p6mm$
 $a' = a$ $b' = b$
 Origin at $0,0,z$

Along $[100]$ $p1g1$
 $a' = \frac{1}{2}(a+2b)$ $b' = c$
 Origin at $x,0,0$

Along $[210]$ $p1m1$
 $a' = \frac{1}{2}b$ $b' = \frac{1}{2}c$
 Origin at $x,\frac{1}{2}x,0$

8 $P4/n$

$P4/n$

C_{4h}^3

$4/m$

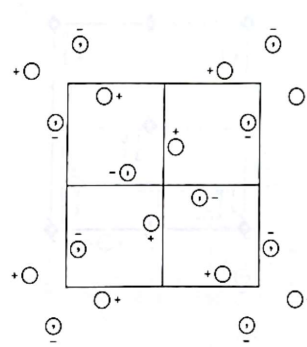
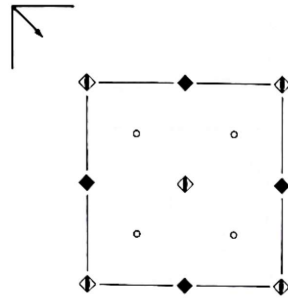
Tetragonal

No. 85

$P4/n$

Patterson symmetry $P4/m$

ORIGIN CHOICE 1



Origin at $\bar{4}$ on n , at $-\frac{1}{2}, \frac{1}{2}, 0$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- (1) $\bar{1}$ (2) 2 $0, 0, z$ (3) 4^+ $0, \frac{1}{2}, z$ (4) 4^- $\frac{1}{2}, 0, z$
 (5) $\bar{1}$ $\frac{1}{2}, \frac{1}{2}, 0$ (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ (7) 4^+ $0, 0, z; 0, 0, 0$ (8) 4^- $0, 0, z; 0, 0, 0$

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 g 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	General: $hkl: h + k = 2n$ $h00: h = 2n$
4 f 2..	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	Special: as above, plus $hkl: h + k = 2n$
4 e $\bar{1}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (7) y, \bar{x}, \bar{z}	$hkl: h, k = 2n$
4 d $\bar{1}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (8) \bar{y}, x, \bar{z}	$hkl: h, k = 2n$
2 c 4..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$	no extra conditions
2 b $\bar{4}..$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k = 2n$
2 a $\bar{4}..$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl: h + k = 2n$

Symmetry of special projections

Along $[001]$ $p4$
 $a' = \frac{1}{2}(a - b)$ $b' = \frac{1}{2}(a + b)$
Origin at $0, 0, z$

Along $[100]$ $p2mg$
 $a' = b$ $b' = c$
Origin at $x, \frac{1}{2}, 0$

Along $[110]$ $p2mm$
 $a' = \frac{1}{2}(-a + b)$ $b' = c$
Origin at $x, x, 0$

Tetragonal

4/m

C_{4h}^3

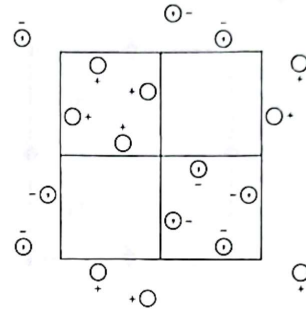
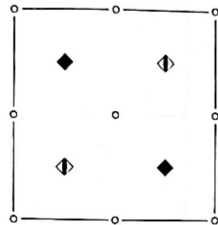
P4/n

Patterson symmetry P4/m

P4/n

No. 85

ORIGIN CHOICE 2



Origin at $\bar{1}$ on n , at $\frac{1}{2}, -\frac{1}{2}, 0$ from $\bar{4}$

Asymmetric unit $-\frac{1}{2} \leq x \leq \frac{1}{2}; -\frac{1}{2} \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$

Symmetry operations

- (1) 1 (2) $2 \frac{1}{2}, \frac{1}{2}, z$ (3) $4^+ \frac{1}{2}, \frac{1}{2}, z$ (4) $4^- \frac{1}{2}, \frac{1}{2}, z$
 (5) $\bar{1}$ 0,0,0 (6) $n(\frac{1}{2}, \frac{1}{2}, 0)$ x,y,0 (7) $\bar{4}^+ \frac{1}{2}, -\frac{1}{2}, z; \frac{1}{2}, -\frac{1}{2}, 0$ (8) $\bar{4}^- -\frac{1}{2}, \frac{1}{2}, z; -\frac{1}{2}, \frac{1}{2}, 0$

Generators selected (1); $r(1,0,0)$; $r(0,1,0)$; $r(0,0,1)$; (2); (3); (5)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
8 g 1	(1) x,y,z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (5) $\bar{x}, \bar{y}, \bar{z}$ (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (8) $\bar{y}, x + \frac{1}{2}, \bar{z}$	General: hkl: $h+k=2n$ h00: $h=2n$
4 f 2..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	Special: as above, plus hkl: $h+k=2n$
4 e $\bar{1}$	0,0, $\frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	hkl: $h,k=2n$
4 d $\bar{1}$	0,0,0 $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	hkl: $h,k=2n$
2 c 4..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
2 b $\bar{4}^+$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	hkl: $h+k=2n$
2 a $\bar{4}^-$	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	hkl: $h+k=2n$

Symmetry of special projections

Along [001] p4

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

Origin at $\frac{1}{2}, \frac{1}{2}, z$

Along [100] p2mg

$a' = b$ $b' = c$

Origin at x,0,0

Along [110] p2mm

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

Origin at x,x,0

9 *Pnma*

Pnma

No. 62

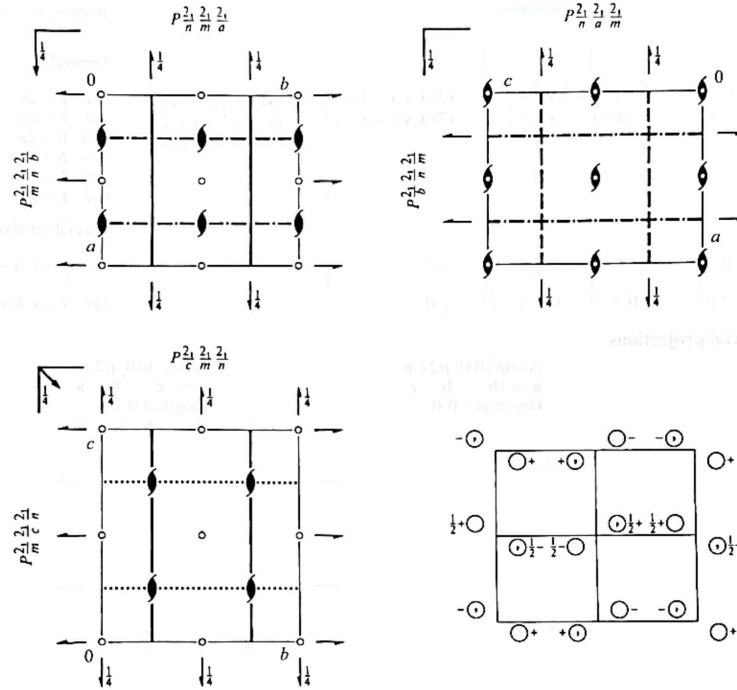
D_{2h}^{16}

$P 2_1/n 2_1/m 2_1/a$

mmm

Orthorhombic

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on 12, 1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

- | | | | |
|-----------------------|--|------------------------------------|--|
| (1) 1 | (2) $2(0, 0, \frac{1}{2}) \frac{1}{2}, 0, z$ | (3) $2(0, \frac{1}{2}, 0) 0, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) x, \frac{1}{2}, \frac{1}{2}$ |
| (5) $\bar{1} 0, 0, 0$ | (6) $a x, y, \frac{1}{2}$ | (7) $m x, \frac{1}{2}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2}) \frac{1}{2}, y, z$ |

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

8	<i>d</i>	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(7) $x, \bar{y} + \frac{1}{2}, z$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$

General:

- $Ok\bar{l}: k + l = 2n$
- $hk0: h = 2n$
- $h00: h = 2n$
- $0k0: k = 2n$
- $00l: l = 2n$

Special: as above, plus

4	<i>c</i>	$.m.$	$x, \frac{1}{2}, z$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \bar{z}$	$x + \frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$
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no extra conditions

4	<i>b</i>	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
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$hk\bar{l}: h + l, k = 2n$

4	<i>a</i>	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	----------	-----------	-----------	-------------------------------	---------------------	---

$hk\bar{l}: h + l, k = 2n$

Symmetry of special projections

Along $[001]$ $p2gm$
 $a' = \frac{1}{2}a$ $b' = b$
 Origin at $0, 0, z$

Along $[100]$ $c2mm$
 $a' = b$ $b' = c$
 Origin at $x, \frac{1}{2}, \frac{1}{2}$

Along $[010]$ $p2gg$
 $a' = c$ $b' = a$
 Origin at $0, y, 0$

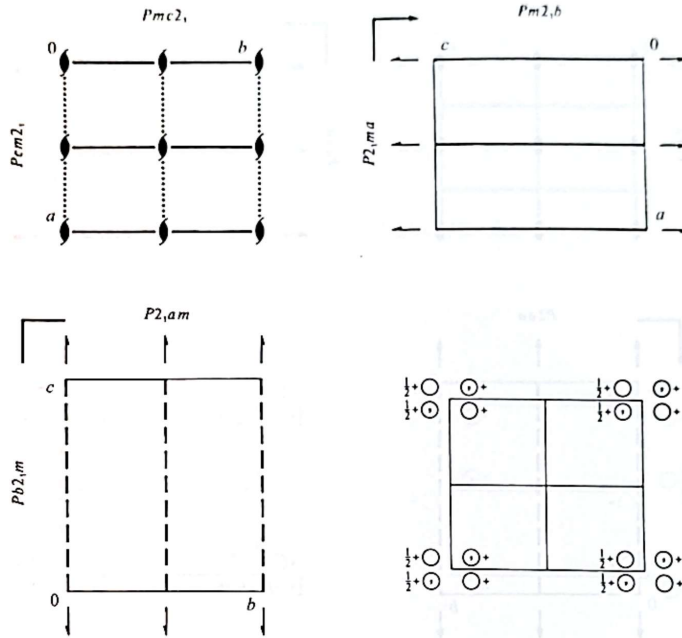
10 $Pmc2_1$

Orthorhombic
 Patterson symmetry $Pmmm$

$mm2$

C_{2v}^2
 $Pmc2_1$

$Pmc2_1$
 No. 26



Origin on $mc2_1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0, 0, \frac{1}{2})$ $0, 0, z$ (3) c $x, 0, z$ (4) m $0, y, z$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 c 1	(1) x, y, z (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (3) $x, \bar{y}, z + \frac{1}{2}$ (4) \bar{x}, y, z

Reflection conditions

General:

$h0l: l = 2n$
 $00l: l = 2n$

Special: no extra conditions

2 b $m..$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z + \frac{1}{2}$
2 a $m..$	$0, y, z$	$0, \bar{y}, z + \frac{1}{2}$

Symmetry of special projections

Along $[001]$ $p2mm$
 $a' = a$ $b' = b$
 Origin at $0, 0, z$

Along $[100]$ $p1g1$
 $a' = b$ $b' = c$
 Origin at $x, 0, 0$

Along $[010]$ $p11m$
 $a' = \frac{1}{2}c$ $b' = a$
 Origin at $0, y, 0$