

$P4_2/nmc$

D_{4h}^{15}

$4/mmm$

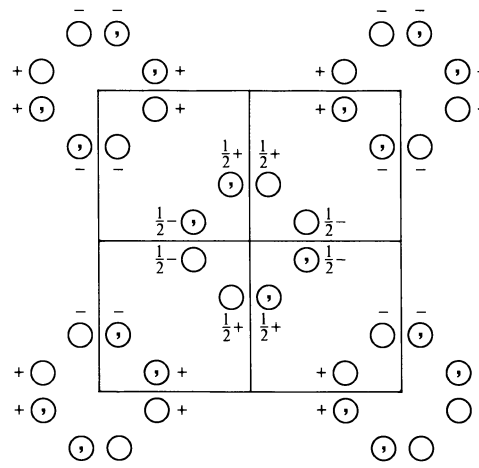
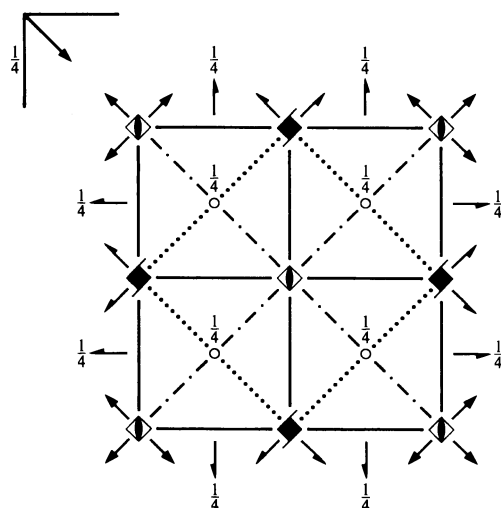
Tetragonal

No. 137

$P 4_2/n 2_1/m 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}m2/n$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>h</i> 1	(1) x,y,z (2) \bar{x},\bar{y},z (3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) y,x,\bar{z} (8) \bar{y},\bar{x},\bar{z} (9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (11) y,\bar{x},\bar{z} (12) \bar{y},x,\bar{z} (13) x,\bar{y},z (14) \bar{x},y,z (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	General: $hk0: h+k=2n$ $hhl: l=2n$ $00l: l=2n$ $h00: h=2n$ Special: as above, plus no extra conditions
8 <i>g</i> $.m.$	$0,y,z$ $\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\bar{y},z$ $\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $y,0,\bar{z}$ $y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\bar{y},0,\bar{z}$	
8 <i>f</i> $..2$	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},\bar{x},0$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x,\bar{x},0$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x,0$	$hkl: h+k+l=2n$
8 <i>e</i> $\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$hkl: h,k,l=2n$
4 <i>d</i> $2mm.$	$0,\frac{1}{2},z$ $0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}$	$hkl: l=2n$
4 <i>c</i> $2mm.$	$0,0,z$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$	$hkl: h+k+l=2n$
2 <i>b</i> $\bar{4}m2$	$0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	$hkl: h+k+l=2n$
2 <i>a</i> $\bar{4}m2$	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkl: h+k+l=2n$

Symmetry of special projections

Along $[001]$ $p4mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$ $\mathbf{c}' = \mathbf{c}$
 Along $[100]$ $p2mg$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Along $[110]$ $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $0,0,z$
 Origin at $x,\frac{1}{4},\frac{1}{4}$
 Origin at $x,x,0$

Tetragonal

$4/mmm$

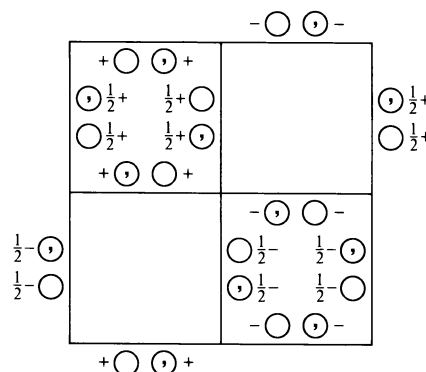
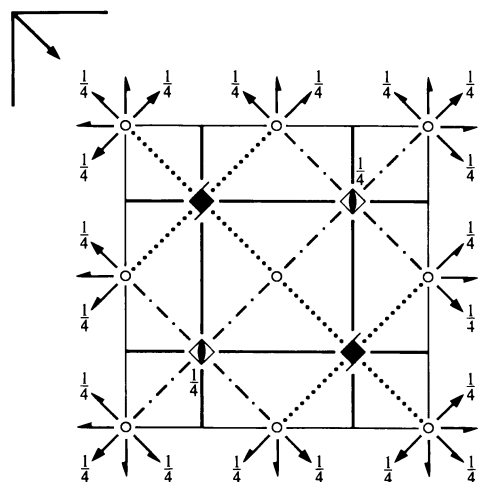
D_{4h}^{15}

$P4_2/nmc$

Patterson symmetry $P4/mmm$

$P 4_2/n 2_1/m 2/c$ No. 137

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $n2_1(c,n)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}m2$

Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|------------------------------------|---|---|---|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0,0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2(0, \frac{1}{2}, 0) 0, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, \frac{1}{4}$ | (8) $2 x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) $m x, \frac{1}{4}, z$ | (14) $m \frac{1}{4}, y, z$ | (15) $c x + \frac{1}{2}, \bar{x}, z$ | (16) $c x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>h</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (6) $x + \frac{1}{2}, \bar{y}, \bar{z}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y} + \frac{1}{2}, z$ (14) $\bar{x} + \frac{1}{2}, y, z$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	General: $hk0: h + k = 2n$ $hhl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$
8 <i>g</i> $.m.$	$\frac{1}{4}, y, z$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, z$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}$ $y, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, y + \frac{1}{2}, \bar{z}$ $\frac{3}{4}, \bar{y}, \bar{z}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\bar{y}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	no extra conditions
8 <i>f</i> $..2$	$x, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{1}{4}$	$hkl: h + k + l = 2n$
8 <i>e</i> $\bar{1}$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$hkl: h, k, l = 2n$
4 <i>d</i> $2mm.$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$hkl: l = 2n$
4 <i>c</i> $2mm.$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$hkl: h + k + l = 2n$
2 <i>b</i> $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: h + k + l = 2n$
2 <i>a</i> $\bar{4}m2$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl: h + k + l = 2n$

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 $\frac{1}{4}, \frac{1}{4}, z$

Along $[100] p2mg$

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

Origin at $x, 0, 0$

Along $[110] p2mm$

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

Origin at $x, x, 0$