

$I4_1/a$

C_{4h}^6

$4/m$

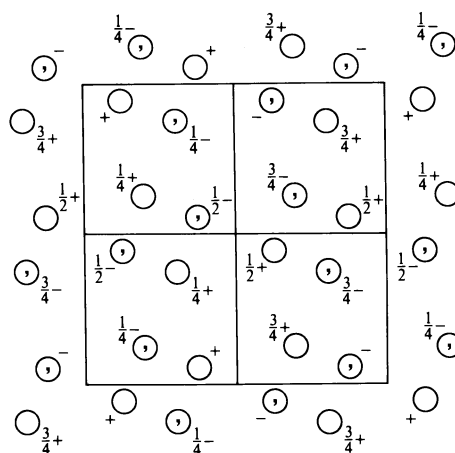
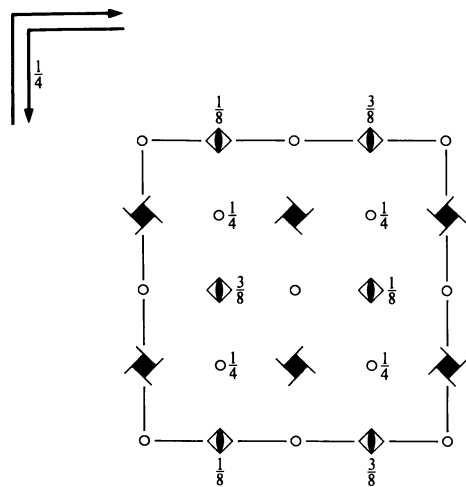
Tetragonal

No. 88

$I4_1/a$

Patterson symmetry $I4/m$

ORIGIN CHOICE 2



Origin at $\bar{1}$ on glide plane b , at $0, \frac{1}{4}, \frac{1}{8}$ from $\bar{4}$

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

Symmetry operations

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

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

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

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

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)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$				
16 <i>f</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{y} + \frac{3}{4}, x + \frac{1}{4}, z + \frac{1}{4}$ (7) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(4) $y + \frac{3}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$ (8) $\bar{y} + \frac{1}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{4}$	<p>General:</p> <p>$hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$</p> <p>Special: as above, plus</p> <p>$hkl : l = 2n + 1$ or $2h + l = 4n$</p> <p>$hkl : l = 2n + 1$ or $h, k = 2n, h + k + l = 4n$</p> <p>$hkl : l = 2n + 1$ or $2h + l = 4n$</p>
8 <i>e</i> 2..	$0, \frac{1}{4}, z$	$\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}$	$0, \frac{3}{4}, \bar{z}$	$\frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{3}{4}$	
8 <i>d</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	} $hkl : l = 2n + 1$ or $h, k = 2n, h + k + l = 4n$
8 <i>c</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	
4 <i>b</i> $\bar{4}..$	$0, \frac{1}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{7}{8}$	}		$hkl : l = 2n + 1$ or $2h + l = 4n$
4 <i>a</i> $\bar{4}..$	$0, \frac{1}{4}, \frac{1}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{3}{8}$			

Symmetry of special projections

Along $[001]$ $p4$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at $\frac{1}{4}, 0, z$

Along $[100]$ $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, \frac{1}{4}$

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

Maximal non-isomorphic subgroups

- I** $[2]I\bar{4}(82)$ (1; 2; 7; 8)+
- $[2]I4_1(80)$ (1; 2; 3; 4)+
- $[2]I2/a(C2/c, 15)$ (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[3]I4_1/a(\mathbf{c}' = 3\mathbf{c})(88)$; $[5]I4_1/a(\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b})(88)$

Minimal non-isomorphic supergroups

I $[2]I4_1/amd(141)$; $[2]I4_1/acd(142)$

II $[2]C4_2/a(\mathbf{c}' = \frac{1}{2}\mathbf{c})(P4_2/n, 86)$