

$I4_1cd$

C_{4v}^{12}

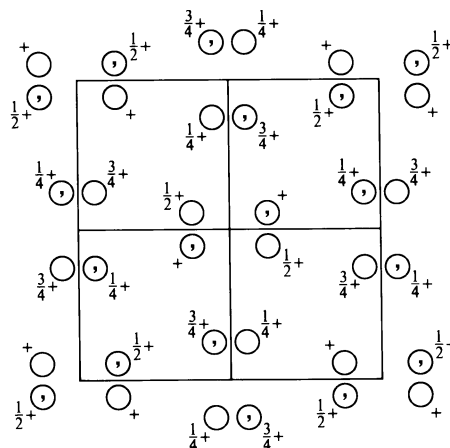
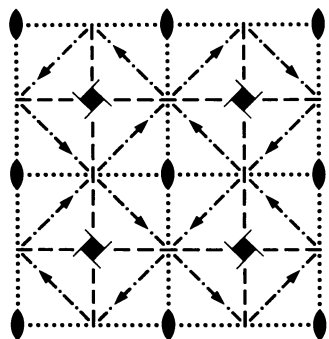
$4mm$

Tetragonal

No. 110

$I4_1cd$

Patterson symmetry $I4/mmm$



Origin on $2c1$

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

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

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

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

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

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
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$				General:
16 <i>b</i> 1	(1) x, y, z (5) $x, \bar{y}, z + \frac{1}{2}$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (7) $\bar{y}, \bar{x} + \frac{1}{2}, z + \frac{3}{4}$	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (8) $y + \frac{1}{2}, x, z + \frac{1}{4}$	$hkl : h + k + l = 2n$ $hk0 : h + k = 2n$ $0kl : k, l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$
8 <i>a</i> 2..	$0, 0, z$	$0, \frac{1}{2}, z + \frac{1}{4}$	$0, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{3}{4}$	Special: as above, plus $hkl : 2h + l = 4n$

Symmetry of special projections

Along [001] $p4gm$

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

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

Along [100] $p1m1$

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

Origin at $x, 0, 0$

Along [110] $c1m1$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

- I** [2] $I4_111(I4_1, 80)$ (1; 2; 3; 4)+
 [2] $I2c1(Iba2, 45)$ (1; 2; 5; 6)+
 [2] $I21d(Fdd2, 43)$ (1; 2; 7; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1cd(\mathbf{c}' = 3\mathbf{c})$ (110); [9] $I4_1cd(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})$ (110)

Minimal non-isomorphic supergroups

I [2] $I4_1/acd$ (142)

II [2] $C4_2md(\mathbf{c}' = \frac{1}{2}\mathbf{c})$ ($P4_2nm$, 102)