

$\bar{4}2c$

$\bar{4}2m$

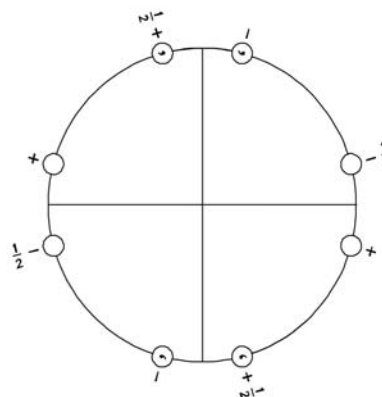
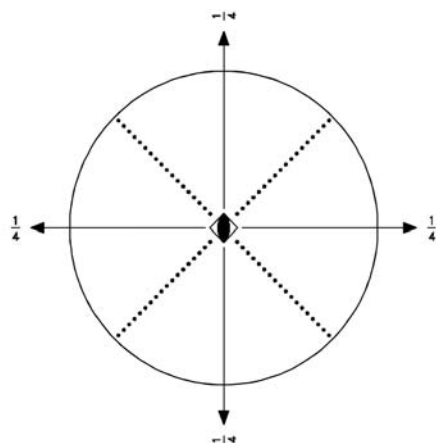
Tetragonal

No. 38

$\bar{4}2c$

Patterson symmetry  $\bar{4}/mmm$

FIRST SETTING



Origin at  $\bar{4}1c$

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

Symmetry operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                                       | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                         | (3) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0) | (4) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0) |
| (5) 2 $0,y,\frac{1}{4}$<br>( $2_y$  0,0, $\frac{1}{2}$ ) | (6) 2 $x,0,\frac{1}{4}$<br>( $2_x$  0,0, $\frac{1}{2}$ ) | (7) $c$ $x,\bar{x},z$<br>( $m_{xy}$  0,0, $\frac{1}{2}$ ) | (8) $c$ $x,x,z$<br>( $m_{xy}$  0,0, $\frac{1}{2}$ )       |

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

**Positions**

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry |                  | Coordinates  |  |  |  | Reflection conditions |
|---|------------------|--|--|--|--|-----------------------|
| <b>General:</b>                                   |                  |  |  |  |  |                       |
| $l : l = 2n$                                      |                  |  |  |  |  |                       |
| <b>Special: no extra conditions</b>               |                  |  |  |  |  |                       |
| 8   | $f$ 1            | (1) $x, y, z$<br>(5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ | (2) $\bar{x}, \bar{y}, z$<br>(6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ | (3) $y, \bar{x}, \bar{z}$<br>(7) $\bar{y}, \bar{x}, z + \frac{1}{2}$ | (4) $\bar{y}, x, \bar{z}$<br>(8) $y, x, z + \frac{1}{2}$ |                       |
| 4   | $e$ 2..          | 0, 0, $z$  | 0, 0, $\bar{z}$  | 0, 0, $\bar{z} + \frac{1}{2}$  | 0, 0, $z + \frac{1}{2}$                                  |                       |
| 4   | $d$ .2.          | 0, $y, \frac{1}{4}$                                      | 0, $\bar{y}, \frac{1}{4}$  | $y, 0, \frac{3}{4}$  | $\bar{y}, 0, \frac{3}{4}$                                |                       |
| 4   | $c$ .2.          | $x, 0, \frac{1}{4}$                                      | $\bar{x}, 0, \frac{1}{4}$  | 0, $\bar{x}, \frac{3}{4}$  | 0, $x, \frac{3}{4}$                                      |                       |
| 2   | $b$ $\bar{4}$ .. | 0, 0, 0  | 0, 0, $\frac{1}{2}$  |  |  |                       |
| 2   | $a$ 222.         | 0, 0, $\frac{1}{4}$                                      | 0, 0, $\frac{3}{4}$  |  |  |                       |

**Symmetry of special projections**

Along [001]  $4mm$

Origin at 0, 0,  $z$

Along [100]  $\bar{4}2mm$

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

Origin at  $x, 0, \frac{1}{4}$

Along [110]  $\bar{4}11m$

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

Origin at  $x, x, 0$

**Maximal non-isotypic non-enantiomorphic subgroups**

|          |                                      |            |
|----------|--------------------------------------|------------|
| <b>I</b> | $[2]\bar{4}11$ ( $\bar{4}, 27$ )     | 1; 2; 3; 4 |
|          | $[2]\bar{4}21c$ ( $\bar{4}cc2, 16$ ) | 1; 2; 7; 8 |
|          | $[2]\bar{4}221$ ( $\bar{4}222, 13$ ) | 1; 2; 5; 6 |

**IIa** none

**IIb** none

**Maximal isotypic subgroups and enantiomorphic subgroups of lowest index**

**IIc**  $[3]\bar{4}2c$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (38)

**Minimal non-isotypic non-enantiomorphic supergroups**

**I**  $[2]\bar{4}/mcc$  (40);  $[2]\bar{4}_2/mmc$  (41)

**II**  $[2]\bar{4}2m$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (37)

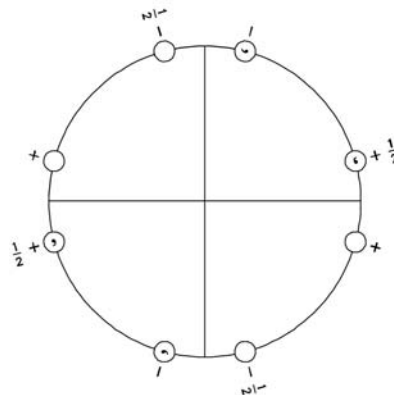
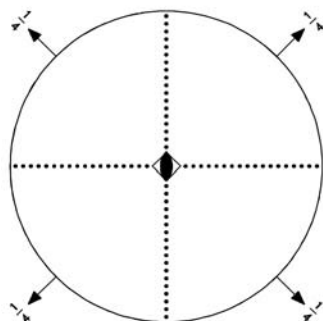
$\bar{4}c2$  $\bar{4}m2$ 

Tetragonal

No. 38

 $\bar{4}c2$ Patterson symmetry  $\bar{4}/mmm$ 

## SECOND SETTING

Origin at  $\bar{4}c1$ Asymmetric unit  $0 \leq x; 0 \leq z \leq \frac{1}{4}$ 

## Symmetry operations

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                               | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)                 | (3) $\bar{4}^+$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^+$  0,0,0)   | (4) $\bar{4}^-$ $0,0,z; 0,0,0$<br>( $\bar{4}_z^-$  0,0,0)               |
| (5) $c$ $x,0,z$<br>( $m_y$  0,0, $\frac{1}{2}$ ) | (6) $c$ $0,y,z$<br>( $m_x$  0,0, $\frac{1}{2}$ ) | (7) 2 $x,x,\frac{1}{4}$<br>( $2_{xy}$  0,0, $\frac{1}{2}$ ) | (8) 2 $x,\bar{x},\frac{1}{4}$<br>( $2_{\bar{xy}}$  0,0, $\frac{1}{2}$ ) |

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

**Positions**

| Multiplicity,<br>Wyckoff letter,<br>Site symmetry |                       | Coordinates  |  |  |  | Reflection conditions |
|---|-----------------------|--|--|--|--|-----------------------|
| <b>General:</b>                                   |                       |  |  |  |  |                       |
| $l : l = 2n$                                      |                       |  |  |  |  |                       |
| <b>Special: no extra conditions</b>               |                       |  |  |  |  |                       |
| 8   | <i>f</i> 1            | (1) $x, y, z$<br>(5) $x, \bar{y}, z + \frac{1}{2}$ | (2) $\bar{x}, \bar{y}, z$<br>(6) $\bar{x}, y, z + \frac{1}{2}$ | (3) $y, \bar{x}, \bar{z}$<br>(7) $y, x, \bar{z} + \frac{1}{2}$ | (4) $\bar{y}, x, \bar{z}$<br>(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ |                       |
| 4   | <i>e</i> 2..          | 0, 0, $z$  | 0, 0, $\bar{z}$  | 0, 0, $z + \frac{1}{2}$  | 0, 0, $\bar{z} + \frac{1}{2}$  |                       |
| 4   | <i>d</i> ..2          | $x, x, \frac{3}{4}$                                | $\bar{x}, \bar{x}, \frac{3}{4}$                                | $x, \bar{x}, \frac{1}{4}$                                      | $\bar{x}, x, \frac{1}{4}$  |                       |
| 4   | <i>c</i> ..2          | $x, x, \frac{1}{4}$                                | $\bar{x}, \bar{x}, \frac{1}{4}$                                | $x, \bar{x}, \frac{3}{4}$                                      | $\bar{x}, x, \frac{3}{4}$  |                       |
| 2   | <i>b</i> $\bar{4}$ .. | 0, 0, 0  | 0, 0, $\frac{1}{2}$  |  |  |                       |
| 2   | <i>a</i> 2.22         | 0, 0, $\frac{1}{4}$                                | 0, 0, $\frac{3}{4}$  |  |  |                       |

**Symmetry of special projections**

Along [001]  $4mm$

Origin at 0, 0,  $z$

Along [100]  $\bar{4}11m$

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

Origin at  $x, 0, 0$

Along [110]  $\bar{4}2mm$

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

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

**Maximal non-isotypic non-enantiomorphic subgroups**

**I** [2] $\bar{4}11$  ( $\bar{4}$ , 27) 1; 2; 3; 4  
 [2] $\bar{4}2c1$  ( $\bar{4}cc2$ , 16) 1; 2; 5; 6  
 [2] $\bar{4}212$  ( $\bar{4}222$ , 13) 1; 2; 7; 8

**IIa** none

**IIb** none

**Maximal isotypic subgroups and enantiomorphic subgroups of lowest index**

**IIc** [3] $\bar{4}c2$  ( $\mathbf{c}' = 3\mathbf{c}$ ) ( $\bar{4}2c$ , 38)

**Minimal non-isotypic non-enantiomorphic supergroups**

**I** [2] $\bar{4}/mcc$  (40); [2] $\bar{4}_2/mmc$  (41)

**II** [2] $\bar{4}2m$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (37)