

$\bar{4}2/mmc$

$4/mmm$

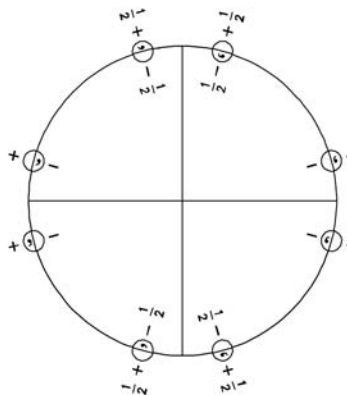
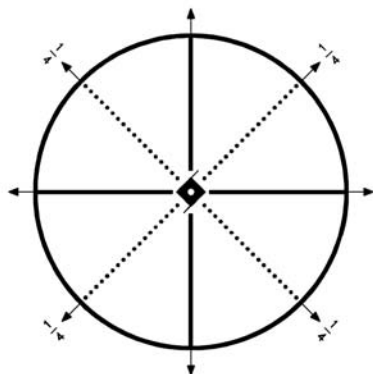
Tetragonal

No. 41

$\bar{4}2/m2/m2/c$

Patterson symmetry  $\bar{4}/mmm$

FIRST SETTING



**Origin** at centre ( $mmm$ ) at  $4_2/m2/mc$

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

**Symmetry operations**

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

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

**Positions**

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

**Symmetry of special projections**

Along [001]  $4mm$

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

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

Origin at  $0, 0, z$

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

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

Origin at  $x, 0, 0$

Origin at  $x, x, 0$

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

<b>I</b>	$[2]\bar{4}2c$ (38)	1; 2; 5; 6; 11; 12; 15; 16
	$[2]\bar{4}m2$ ( $\bar{4}2m, 37$ )	1; 2; 7; 8; 11; 12; 13; 14
	$[2]\bar{4}_2mc$ ( $\bar{4}_2cm, 35$ )	1; 2; 3; 4; 13; 14; 15; 16
	$[2]\bar{4}_222$ (32)	1; 2; 3; 4; 5; 6; 7; 8
	$[2]\bar{4}_2/m11$ ( $\bar{4}_2/m, 29$ )	1; 2; 3; 4; 9; 10; 11; 12
	$[2]\bar{4}2/m12/c$ ( $\bar{4}ccm, 21$ )	1; 2; 7; 8; 9; 10; 15; 16
	$[2]\bar{4}2/m2/m1$ ( $\bar{4}mmm, 20$ )	1; 2; 5; 6; 9; 10; 13; 14

**IIa** none

**IIb** none

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

**IIc**  $[3]\bar{4}_2/mmc$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (41)

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

**I** none

**II**  $[2]\bar{4}/mmm$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (39)

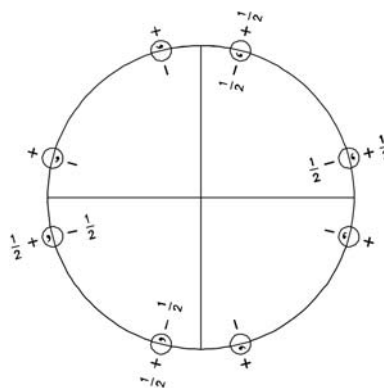
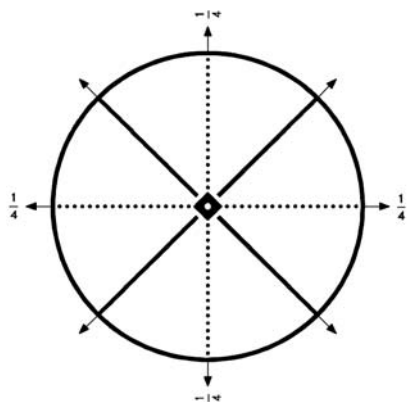
$\bar{4}2/mcm$  $4/mmm$ 

Tetragonal

No. 41

 $\bar{4}2/m2/c2/m$ Patterson symmetry  $\bar{4}4/mmm$ 

## SECOND SETTING

**Origin** at centre ( $mmm$ ) at  $4_2/mc2/m$ **Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq \frac{1}{2}; x \leq y$ **Symmetry operations**

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

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

**Positions**

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

**Symmetry of special projections**

Along [001]  $4mm$

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

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

Origin at  $0, 0, z$

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

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

Origin at  $x, x, 0$

Origin at  $x, x, 0$

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

<b>I</b>	$[2]\bar{4}c2(\bar{4}2c, 38)$	1; 2; 7; 8; 11; 12; 13; 14
	$[2]\bar{4}2m(37)$	1; 2; 5; 6; 11; 12; 15; 16
	$[2]\bar{4}_2cm(35)$	1; 2; 3; 4; 13; 14; 15; 16
	$[2]\bar{4}_222(32)$	1; 2; 3; 4; 5; 6; 7; 8
	$[2]\bar{4}_2/m11(\bar{4}_2/m, 29)$	1; 2; 3; 4; 9; 10; 11; 12
	$[2]\bar{4}2/m2/c1(\bar{4}ccm, 21)$	1; 2; 5; 6; 9; 10; 13; 14
	$[2]\bar{4}2/m12/m(\bar{4}mmm, 20)$	1; 2; 7; 8; 9; 10; 15; 16

**IIa** none

**IIb** none

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

**IIc**  $[3]\bar{4}_2/mcm(\mathbf{c}' = 3\mathbf{c})(\bar{4}_2/mmc, 41)$

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

**I** none

**II**  $[2]\bar{4}4/mmm(\mathbf{c}' = \frac{1}{2}\mathbf{c})(39)$