

$\bar{4}2/mmc$

$4/mmm$

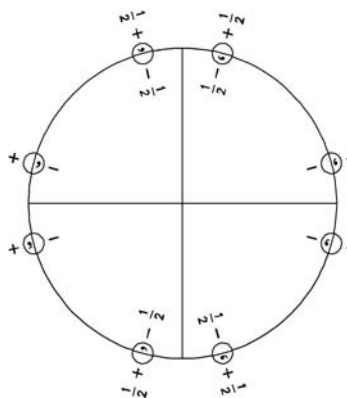
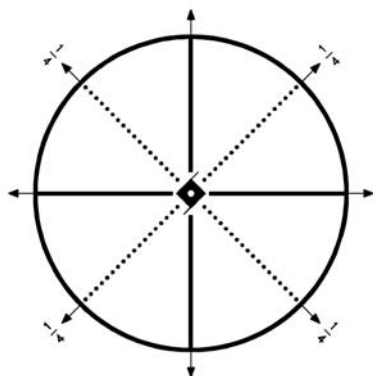
Tetragonal

No. 41

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

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

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

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] $4mm$

Origin at $0, 0, z$

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

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

Origin at $x, 0, 0$

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

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

Origin at $x, x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\bar{4}2c$ (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)

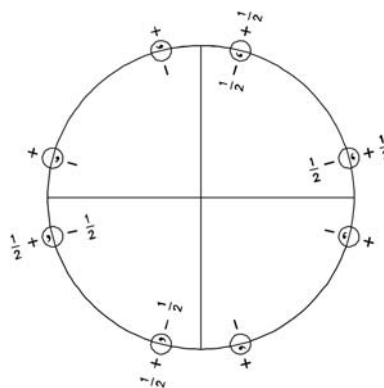
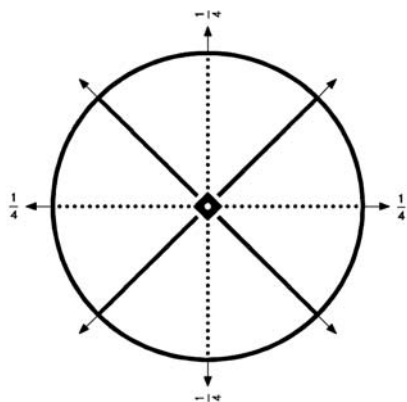
$\cancel{4}_2/mcm$ $4/mmm$

Tetragonal

No. 41

 $\cancel{4}_2/m2/c2/m$ Patterson symmetry $\cancel{4}/mmm$

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

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

I	$[2]\bar{4}c2 (\bar{4}2c, 38)$	1; 2; 7; 8; 11; 12; 13; 14
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	$[2]\bar{4}2/m2/c1 (\bar{4}ccm, 21)$	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 $[2]\bar{4}4/mmm (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (39)$