

$\bar{4}2m$

$\bar{4}2m$

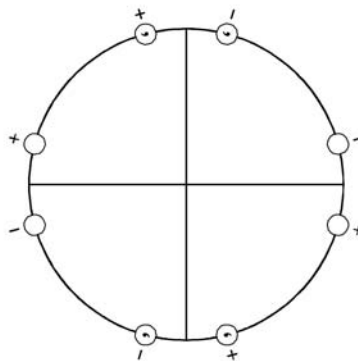
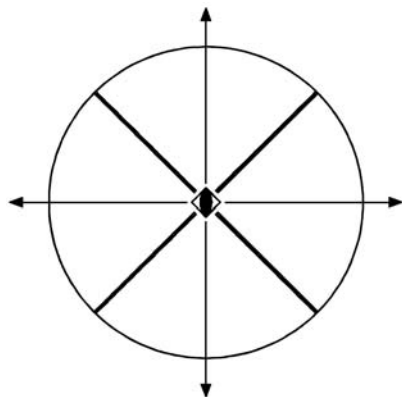
Tetragonal

No. 37

$\bar{4}2m$

Patterson symmetry $\bar{4}/mmm$

FIRST SETTING



Origin at $\bar{4}2m$

Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq 1; x \leq y$

Symmetry operations

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

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

Positions

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

Symmetry of special projections

Along [001] $4mm$	Along [100] $\bar{4}2mm$	Along [110] $\bar{4}11m$
Origin at $0, 0, z$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\bar{4}11$ ($\bar{4}, 27$)	1; 2; 3; 4
[2] $\bar{4}21m$ ($\bar{4}mm2, 15$)	1; 2; 7; 8
[2] $\bar{4}221$ ($\bar{4}222, 13$)	1; 2; 5; 6

IIa none

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

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\bar{4}2m$ ($\mathbf{c}' = 2\mathbf{c}$) (37)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $\bar{4}/mmm$ (39); [2] $\bar{4}_2/mmc$ (41)

II none

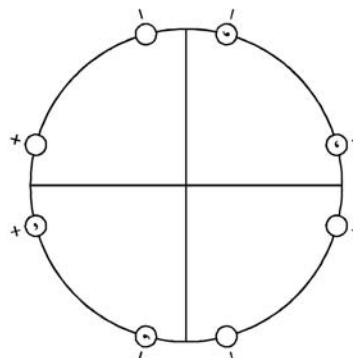
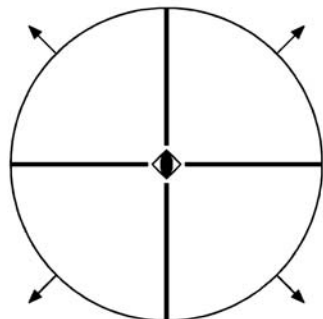
$\bar{4}m2$ $\bar{4}m2$

Tetragonal

No. 37

 $\bar{4}m2$ Patterson symmetry $\bar{4}m2$

SECOND SETTING

Origin at $\bar{4}m2$ Asymmetric unit $0 \leq x; 0 \leq y; 0 \leq z \leq 1; x \leq y$

Symmetry operations

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

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

Positions

	Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8	g 1	(1) x, y, z (5) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z	(3) y, \bar{x}, \bar{z} (7) y, x, \bar{z}	(4) \bar{y}, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$	General: no conditions Special: no extra conditions
4	f . m .	$x, 0, z$	$\bar{x}, 0, z$	$0, \bar{x}, \bar{z}$	$0, x, \bar{z}$	
4	e . . 2	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	
4	d . . 2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$x, \bar{x}, 0$	$\bar{x}, x, 0$	
2	c $2mm$.	$0, 0, z$	$0, 0, \bar{z}$			
1	b $\bar{4}m2$	$0, 0, \frac{1}{2}$				
1	a $\bar{4}m2$	$0, 0, 0$				

Symmetry of special projections

Along [001] $4mm$

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

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

Origin at $0, 0, z$

$\mathbf{a}' = \mathbf{c}$
Origin at $x, 0, 0$

$\mathbf{a}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

- I** [2] $\bar{4}11$ ($\bar{4}, 27$) 1; 2; 3; 4
 [2] $2m1$ ($2mm, 15$) 1; 2; 5; 6
 [2] 212 ($222, 13$) 1; 2; 7; 8

IIa none

IIb [2] $\bar{4}c2$ ($c' = 2c$) ($\bar{4}2c, 38$)

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [2] $\bar{4}m2$ ($c' = 2c$) ($\bar{4}2m, 37$)

Minimal non-isotypic non-enantiomorphic supergroups

I [2] $4/mmm$ (39); [2] $4_2/mmc$ (41)

II none