

$\bar{4}2c$

$\bar{4}2m$

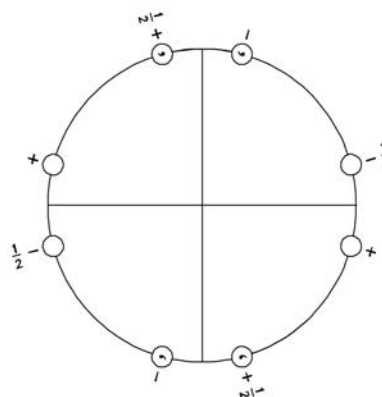
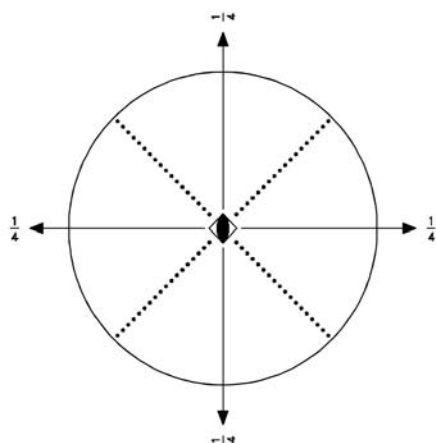
Tetragonal

No. 38

$\bar{4}2c$

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

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

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

Positions

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

I	$[2]\bar{4}11$ ($\bar{4}, 27$)	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)

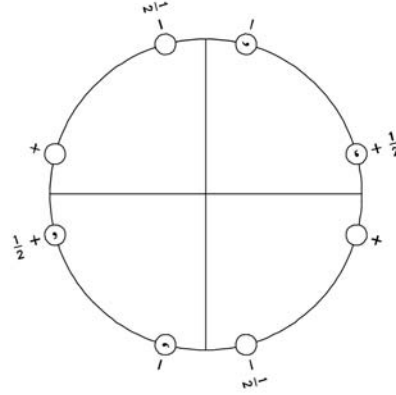
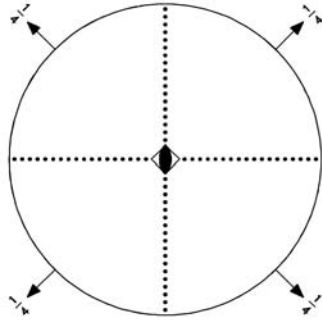
$\bar{4}c2$ $\bar{4}m2$

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>f</i> 1	(1) x, y, z (5) $x, \bar{y}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) $\bar{x}, y, z + \frac{1}{2}$	(3) y, \bar{x}, \bar{z} (7) $y, x, \bar{z} + \frac{1}{2}$	(4) \bar{y}, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	General: $l : l = 2n$ Special: no extra conditions
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] $\bar{2}c1$ ($\bar{2}c2$, 16) 1; 2; 5; 6
 [2] $\bar{2}12$ ($\bar{2}22$, 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)