

$\bar{4}2cm$

$4mm$

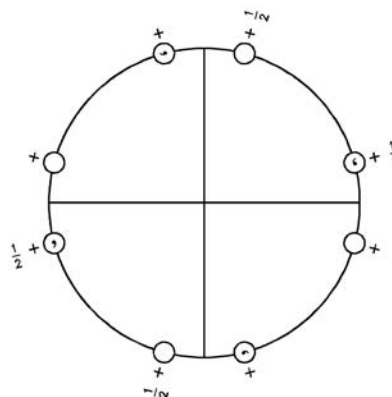
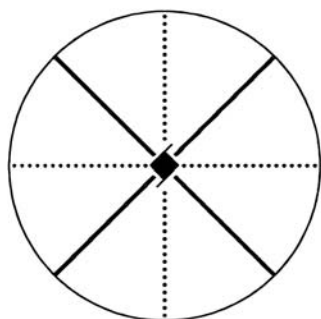
Tetragonal

No. 35

$\bar{4}2cm$

Patterson symmetry $\bar{4}/mmm$

FIRST SETTING



Origin on $2mm$ on 4_2cm

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

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) $c x,0,z$ | (6) $c 0,y,z$ | (7) $m x,\bar{x},z$ | (8) $m x,x,z$ |

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

Positions

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

Symmetry of special projections

Along [001] $4mm$	Along [100] $\mu 11m$	Along [110] $\mu 11m$
Origin at $0, 0, z$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\mu 4_2 11 (\mu 4_2, 25)$	1; 2; 3; 4
	$[2]\mu 2c1 (\mu cc2, 16)$	1; 2; 5; 6
	$[2]\mu 21m (\mu mm2, 15)$	1; 2; 7; 8

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\mu 4_2 cm (\mathbf{c}' = 3\mathbf{c}) (35)$

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\mu 4_2 / m m c (41)$

II $[2]\mu 4 m m (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (34)$

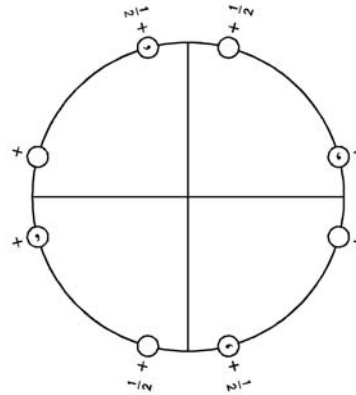
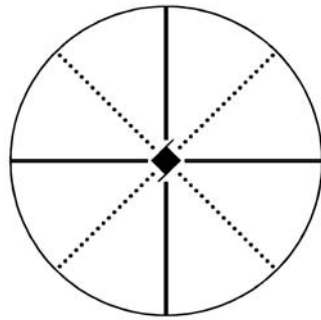
$\bar{4}2m$ $4mm$

Tetragonal

No. 35

 $\bar{4}2m$ Patterson symmetry $\bar{4}2m$

SECOND SETTING

**Origin** on $2mm$ on 4_2mc **Asymmetric unit** $0 \leq x; 0 \leq y; 0 \leq z \leq 1; x \leq y$ **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) $m x,0,z$ | (6) $m 0,y,z$ | (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:
8 <i>c</i> 1	(1) x, y, z (5) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) \bar{x}, y, z	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $y, x, z + \frac{1}{2}$	$l : l = 2n$
4 <i>b</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z + \frac{1}{2}$	$0, \bar{x}, z + \frac{1}{2}$	Special: no extra conditions
2 <i>a</i> 2 <i>mm</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$			

Symmetry of special projections

Along [001] $4mm$	Along [100] $\mu 11m$	Along [110] $\mu 11m$
Origin at $0, 0, z$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ Origin at $x, x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\mu 4_2 11 (\mu 4_2, 25)$	1; 2; 3; 4
	$[2]\mu 21c (\mu cc2, 16)$	1; 2; 7; 8
	$[2]\mu 2m1 (\mu mm2, 15)$	1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\mu 4_2 mc (\mathbf{c}' = 3\mathbf{c}) (\mu 4_2 cm, 35)$

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\mu 4_2 / m m c (41)$

II $[2]\mu 4 m m (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (34)$