

$\bar{4}/mcc$

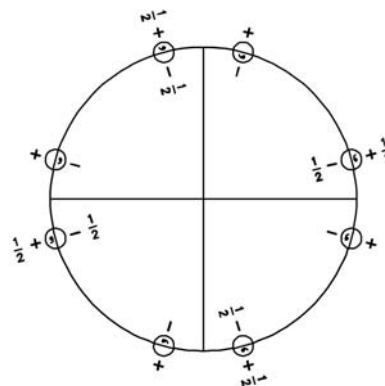
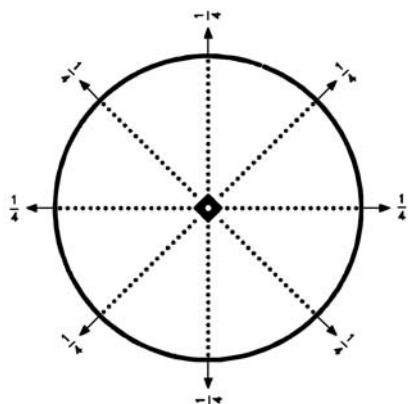
$4/mmm$

Tetragonal

No. 40

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

Patterson symmetry  $\bar{4}/mmm$



**Origin** at centre ( $4/m$ ) at  $4/mcc$

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

**Symmetry operations**

- |   |   |   |   |
|---|---|---|---|
| (1) 1<br>(1 0,0,0)  | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)                            | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0)                          | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0)                                |
| (5) 2 0,y, $\frac{1}{4}$<br>(2 <sub>y</sub>  0,0, $\frac{1}{2}$ ) | (6) 2 x,0, $\frac{1}{4}$<br>(2 <sub>x</sub>  0,0, $\frac{1}{2}$ ) | (7) 2 x,x, $\frac{1}{4}$<br>(2 <sub>xy</sub>  0,0, $\frac{1}{2}$ )                        | (8) 2 x, $\bar{x}$ , $\frac{1}{4}$<br>(2 <sub><math>\bar{xy}</math></sub>  0,0, $\frac{1}{2}$ ) |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0)                        | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0)                           | (11) $\bar{4}$ <sup>+</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>+</sup>  0,0,0) | (12) $\bar{4}$ <sup>-</sup> 0,0,z; 0,0,0<br>( $\bar{4}$ <sub>z</sub> <sup>-</sup>  0,0,0)       |
| (13) c x,0,z<br>(m <sub>y</sub>  0,0, $\frac{1}{2}$ )             | (14) c 0,y,z<br>(m <sub>x</sub>  0,0, $\frac{1}{2}$ )             | (15) c x, $\bar{x}$ ,z<br>(m <sub>xy</sub>  0,0, $\frac{1}{2}$ )                          | (16) c x,x,z<br>(m <sub><math>\bar{xy}</math></sub>  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
						General:
16	$g$ 1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z$	(3) $\bar{y}, x, z$	(4) $y, \bar{x}, z$	$l : l = 2n$
		(5) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	
		(9) $\bar{x}, \bar{y}, \bar{z}$	(10) $x, y, \bar{z}$	(11) $y, \bar{x}, \bar{z}$	(12) $\bar{y}, x, \bar{z}$	
		(13) $x, \bar{y}, z + \frac{1}{2}$	(14) $\bar{x}, y, z + \frac{1}{2}$	(15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(16) $y, x, z + \frac{1}{2}$	Special: no extra conditions
8	$f$ $m..$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, 0$	$y, \bar{x}, 0$	
		$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$	$y, x, \frac{1}{2}$	$\bar{y}, \bar{x}, \frac{1}{2}$	
8	$e$ $.2.$	$x, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$0, \bar{x}, \frac{1}{4}$	
		$\bar{x}, 0, \frac{3}{4}$	$x, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$0, x, \frac{3}{4}$	
8	$d$ $..2$	$x, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, x, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$	
		$\bar{x}, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	$x, \bar{x}, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$	
4	$c$ $4..$	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$	
2	$b$ $4/m..$	$0, 0, 0$	$0, 0, \frac{1}{2}$			
2	$a$ $422$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			

**Symmetry of special projections**

Along [001]  $4mm$

Along [100]  $\mu 2mm$

Along [110]  $\mu 2mm$

Origin at  $0, 0, z$

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

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Origin at  $x, 0, 0$

Origin at  $x, x, 0$

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

<b>I</b>	$[2]\mu\bar{4}2c$ (38)	1; 2; 5; 6; 11; 12; 15; 16
	$[2]\mu\bar{4}c2$ ( $\mu\bar{4}2c$ , 38)	1; 2; 7; 8; 11; 12; 13; 14
	$[2]\mu 4cc$ (36)	1; 2; 3; 4; 13; 14; 15; 16
	$[2]\mu 422$ (30)	1; 2; 3; 4; 5; 6; 7; 8
	$[2]\mu 4/m11$ ( $\mu 4/m$ , 28)	1; 2; 3; 4; 9; 10; 11; 12
	$[2]\mu 2/m2/c1$ ( $\mu ccm$ , 21)	1; 2; 5; 6; 9; 10; 13; 14
	$[2]\mu 2/m12/c$ ( $\mu ccm$ , 21)	1; 2; 7; 8; 9; 10; 15; 16

**IIa** none

**IIb** none

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

**IIc**  $[3]\mu 4/mcc$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (40)

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

**I** none

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