

$Pm\bar{3}$

$T_h^1$

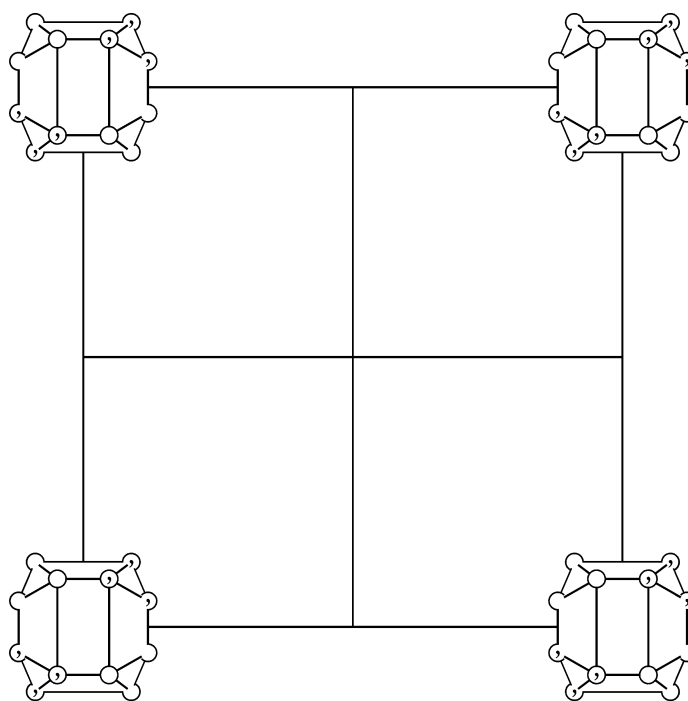
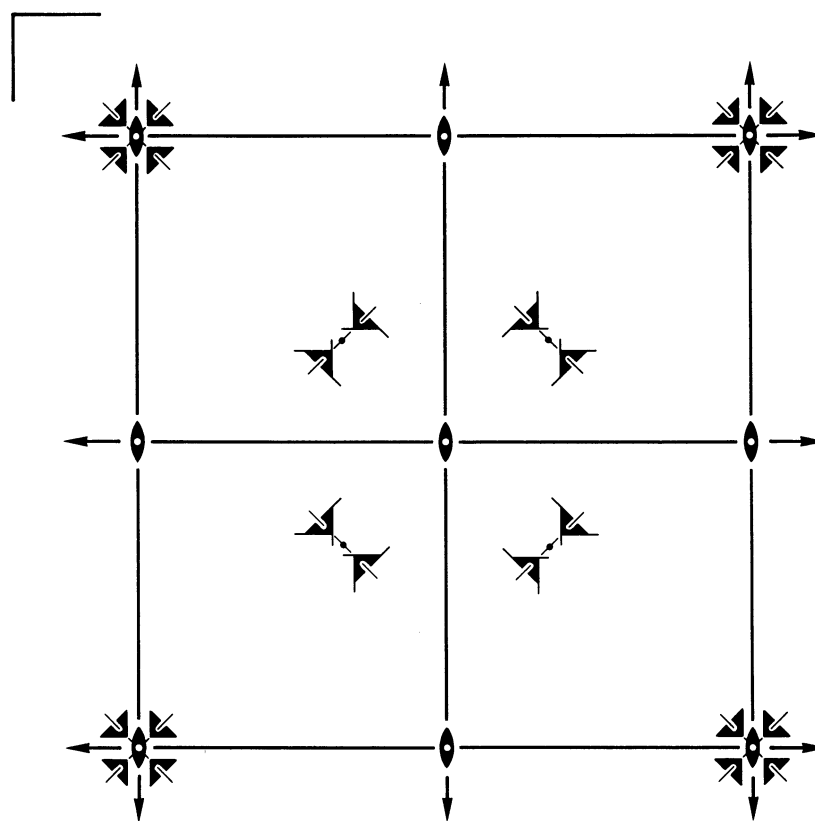
$m\bar{3}$

Cubic

No. 200

$P2/m\bar{3}$

Patterson symmetry  $Pm\bar{3}$



Origin at centre ( $m\bar{3}$ )

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; z \leq \min(x, y)$

Vertices  $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad 0, \frac{1}{2}, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

**Symmetry operations**

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3 <sup>+</sup> x,x,x	(6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x
(9) 3 <sup>-</sup> x,x,x	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) m x,y,0	(15) m x,0,z	(16) m 0,y,z
(17) $\bar{3}^+$ x,x,x; 0,0,0	(18) $\bar{3}^+$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0	(19) $\bar{3}^+$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0	(20) $\bar{3}^+$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0
(21) $\bar{3}^-$ x,x,x; 0,0,0	(22) $\bar{3}^-$ x, $\bar{x}$ , $\bar{x}$ ; 0,0,0	(23) $\bar{3}^-$ $\bar{x}$ , $\bar{x}$ ,x; 0,0,0	(24) $\bar{3}^-$ $\bar{x}$ ,x, $\bar{x}$ ; 0,0,0

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5); (13)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

 $h,k,l$  cyclically permutable

General:

24	<i>l</i>	1	(1) x,y,z	(2) $\bar{x}$ , $\bar{y}$ ,z	(3) $\bar{x}$ ,y, $\bar{z}$	(4) x, $\bar{y}$ , $\bar{z}$
			(5) z,x,y	(6) z, $\bar{x}$ , $\bar{y}$	(7) $\bar{z}$ , $\bar{x}$ ,y	(8) $\bar{z}$ ,x, $\bar{y}$
			(9) y,z,x	(10) $\bar{y}$ ,z, $\bar{x}$	(11) y, $\bar{z}$ , $\bar{x}$	(12) $\bar{y}$ , $\bar{z}$ ,x
			(13) $\bar{x}$ , $\bar{y}$ , $\bar{z}$	(14) x,y, $\bar{z}$	(15) x, $\bar{y}$ ,z	(16) $\bar{x}$ ,y,z
			(17) $\bar{z}$ , $\bar{x}$ , $\bar{y}$	(18) $\bar{z}$ ,x,y	(19) z,x, $\bar{y}$	(20) z, $\bar{x}$ ,y
			(21) $\bar{y}$ , $\bar{z}$ , $\bar{x}$	(22) y, $\bar{z}$ ,x	(23) $\bar{y}$ ,z,x	(24) y,z, $\bar{x}$

no conditions

Special: no extra conditions

12	<i>k</i>	<i>m</i> ..	$\frac{1}{2}$ ,y,z	$\frac{1}{2}$ , $\bar{y}$ ,z	$\frac{1}{2}$ ,y, $\bar{z}$	$\frac{1}{2}$ , $\bar{y}$ , $\bar{z}$	z, $\frac{1}{2}$ ,y	z, $\frac{1}{2}$ , $\bar{y}$
			$\bar{z}$ , $\frac{1}{2}$ ,y	$\bar{z}$ , $\frac{1}{2}$ , $\bar{y}$	y,z, $\frac{1}{2}$	$\bar{y}$ ,z, $\frac{1}{2}$	y, $\bar{z}$ , $\frac{1}{2}$	$\bar{y}$ , $\bar{z}$ , $\frac{1}{2}$
12	<i>j</i>	<i>m</i> ..	0,y,z	0, $\bar{y}$ ,z	0,y, $\bar{z}$	0, $\bar{y}$ , $\bar{z}$	z,0,y	z,0, $\bar{y}$
			$\bar{z}$ ,0,y	$\bar{z}$ ,0, $\bar{y}$	y,z,0	$\bar{y}$ ,z,0	y, $\bar{z}$ ,0	$\bar{y}$ , $\bar{z}$ ,0
8	<i>i</i>	.3.	x,x,x	$\bar{x}$ , $\bar{x}$ ,x	$\bar{x}$ ,x, $\bar{x}$	x, $\bar{x}$ , $\bar{x}$		
			$\bar{x}$ , $\bar{x}$ , $\bar{x}$	x,x, $\bar{x}$	x, $\bar{x}$ ,x	$\bar{x}$ ,x,x		
6	<i>h</i>	<i>m m 2</i> ..	x, $\frac{1}{2}$ , $\frac{1}{2}$	$\bar{x}$ , $\frac{1}{2}$ , $\frac{1}{2}$	$\frac{1}{2}$ ,x, $\frac{1}{2}$	$\frac{1}{2}$ , $\bar{x}$ , $\frac{1}{2}$	$\frac{1}{2}$ , $\frac{1}{2}$ ,x	$\frac{1}{2}$ , $\frac{1}{2}$ , $\bar{x}$
6	<i>g</i>	<i>m m 2</i> ..	x, $\frac{1}{2}$ ,0	$\bar{x}$ , $\frac{1}{2}$ ,0	0,x, $\frac{1}{2}$	0, $\bar{x}$ , $\frac{1}{2}$	$\frac{1}{2}$ ,0,x	$\frac{1}{2}$ ,0, $\bar{x}$
6	<i>f</i>	<i>m m 2</i> ..	x,0, $\frac{1}{2}$	$\bar{x}$ ,0, $\frac{1}{2}$	$\frac{1}{2}$ ,x,0	$\frac{1}{2}$ , $\bar{x}$ ,0	0, $\frac{1}{2}$ ,x	0, $\frac{1}{2}$ , $\bar{x}$
6	<i>e</i>	<i>m m 2</i> ..	x,0,0	$\bar{x}$ ,0,0	0,x,0	0, $\bar{x}$ ,0	0,0,x	0,0, $\bar{x}$
3	<i>d</i>	<i>m m m</i> ..	$\frac{1}{2}$ ,0,0	0, $\frac{1}{2}$ ,0	0,0, $\frac{1}{2}$			
3	<i>c</i>	<i>m m m</i> ..	0, $\frac{1}{2}$ , $\frac{1}{2}$	$\frac{1}{2}$ ,0, $\frac{1}{2}$	$\frac{1}{2}$ , $\frac{1}{2}$ ,0			
1	<i>b</i>	<i>m <math>\bar{3}</math></i> .	$\frac{1}{2}$ , $\frac{1}{2}$ , $\frac{1}{2}$					
1	<i>a</i>	<i>m <math>\bar{3}</math></i> .	0,0,0					

**Symmetry of special projections**Along [001]  $p2mm$  $\mathbf{a}' = \mathbf{a}$     $\mathbf{b}' = \mathbf{b}$ 

Origin at 0,0,z

Along [111]  $p6$  $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ 

Origin at x,x,x

 $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Along [110]  $p2mm$  $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$     $\mathbf{b}' = \mathbf{c}$ 

Origin at x,x,0