

$P6_3/mcm$

$D_{6h}^3$

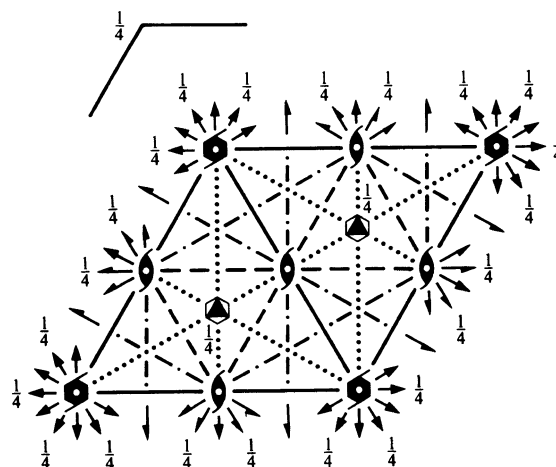
$6/mmm$

Hexagonal

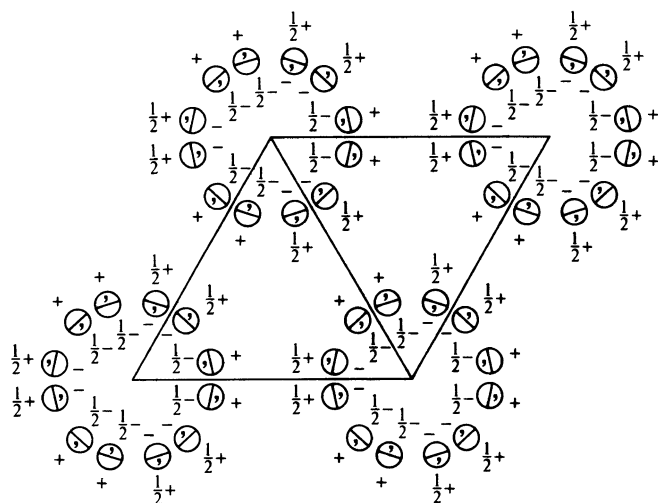
No. 193

$P 6_3/m 2/c 2/m$

Patterson symmetry  $P6/mmm$



For  $\bar{1}$  and  $\bar{6}$  see  $P6_3/m$  (No. 176)



Origin at centre ( $\bar{3}1m$ ) at  $\bar{3}c2/m$

Asymmetric unit  $0 \leq x \leq \frac{2}{3}$ ;  $0 \leq y \leq \frac{1}{3}$ ;  $0 \leq z \leq \frac{1}{4}$ ;  $x \leq (1+y)/2$ ;  $y \leq \min(1-x, x)$

Vertices  $0, 0, 0$   $\frac{1}{2}, 0, 0$   $\frac{2}{3}, \frac{1}{3}, 0$   $\frac{1}{2}, \frac{1}{2}, 0$   
 $0, 0, \frac{1}{4}$   $\frac{1}{2}, 0, \frac{1}{4}$   $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$   $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$

**Symmetry operations**

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

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (4); (7); (13)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

								General:	
24	$l$	1	(1) $x, y, z$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (10) $\bar{y}, \bar{x}, \bar{z}$ (13) $\bar{x}, \bar{y}, \bar{z}$ (16) $x, y, \bar{z} + \frac{1}{2}$ (19) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (22) $y, x, z$	(2) $\bar{y}, x - y, z$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (8) $x - y, \bar{y}, \bar{z} + \frac{1}{2}$ (11) $\bar{x} + y, y, \bar{z}$ (14) $y, \bar{x} + y, \bar{z}$ (17) $\bar{y}, x - y, \bar{z} + \frac{1}{2}$ (20) $\bar{x} + y, y, z + \frac{1}{2}$ (23) $x - y, \bar{y}, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x - y, x, z + \frac{1}{2}$ (9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{2}$ (12) $x, x - y, \bar{z}$ (15) $x - y, x, \bar{z}$ (18) $\bar{x} + y, \bar{x}, \bar{z} + \frac{1}{2}$ (21) $x, x - y, z + \frac{1}{2}$ (24) $\bar{x}, \bar{x} + y, z$			$h\bar{h}0l: l = 2n$ $000l: l = 2n$	
								Special: as above, plus	
12	$k$	$..m$	$x, 0, z$ $0, \bar{x}, z + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$	$0, x, z$ $x, x, z + \frac{1}{2}$ $0, \bar{x}, \bar{z}$	$\bar{x}, \bar{x}, z$ $0, x, \bar{z} + \frac{1}{2}$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z + \frac{1}{2}$ $x, 0, \bar{z} + \frac{1}{2}$ $x, x, \bar{z}$	no extra conditions		
12	$j$	$m..$	$x, y, \frac{1}{4}$ $y, x, \frac{1}{4}$	$\bar{y}, x - y, \frac{1}{4}$ $x - y, \bar{y}, \frac{1}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{x} + y, \frac{1}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{y}, \bar{x}, \frac{3}{4}$	$y, \bar{x} + y, \frac{3}{4}$ $\bar{x} + y, y, \frac{3}{4}$	$x - y, x, \frac{3}{4}$ $x, x - y, \frac{3}{4}$	no extra conditions
12	$i$	$..2$	$x, 2x, 0$ $\bar{x}, 2\bar{x}, 0$	$2\bar{x}, \bar{x}, 0$ $2x, x, 0$	$x, \bar{x}, 0$ $\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, \frac{1}{2}$ $x, 2x, \frac{1}{2}$	$2x, x, \frac{1}{2}$ $2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$ $x, \bar{x}, \frac{1}{2}$	$hkil: l = 2n$
8	$h$	$3..$	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \bar{z} + \frac{1}{2}$ $\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$ $\frac{2}{3}, \frac{1}{3}, z$			$hkil: l = 2n$
6	$g$	$m2m$	$x, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	no extra conditions
6	$f$	$..2/m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil: l = 2n$
4	$e$	$3.m$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$			$hkil: l = 2n$
4	$d$	$3.2$	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, 0$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$			$hkil: l = 2n$
4	$c$	$\bar{6}..$	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$	$\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$			$hkil: l = 2n$
2	$b$	$\bar{3}.m$	$0, 0, 0$	$0, 0, \frac{1}{2}$					$hkil: l = 2n$
2	$a$	$\bar{6}2m$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$					$hkil: l = 2n$

**Symmetry of special projections**Along  $[001]$   $p6mm$  $\mathbf{a}' = \mathbf{a}$     $\mathbf{b}' = \mathbf{b}$ Origin at  $0, 0, z$ Along  $[100]$   $p2mm$  $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$     $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at  $x, 0, 0$ Along  $[210]$   $p2gm$  $\mathbf{a}' = \frac{1}{2}\mathbf{b}$     $\mathbf{b}' = \mathbf{c}$ Origin at  $x, \frac{1}{2}x, 0$