

$P31c$

$C_{3v}^4$

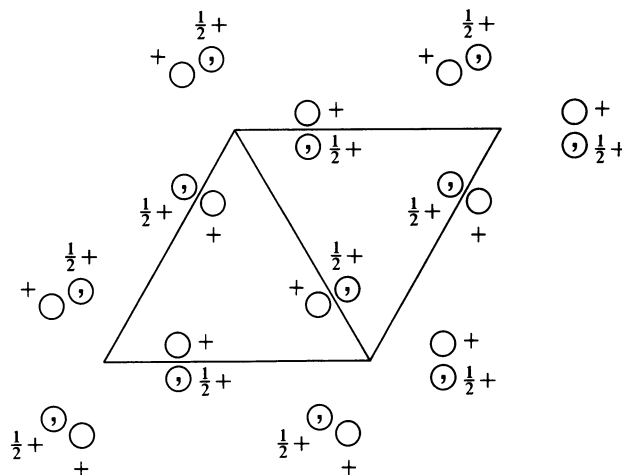
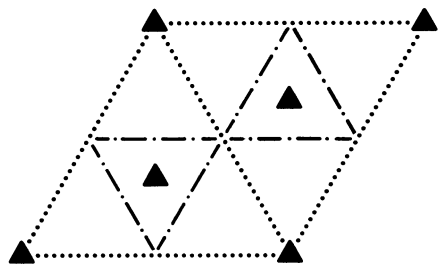
$31m$

Trigonal

No. 159

$P31c$

Patterson symmetry  $P\bar{3}1m$



Origin on  $31c$

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

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

Symmetry operations

- (1) 1 (2)  $3^+$   $0, 0, z$  (3)  $3^-$   $0, 0, z$   
 (4)  $c$   $x, x, z$  (5)  $c$   $x, 0, z$  (6)  $c$   $0, y, z$

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
6 <i>c</i> 1	(1) $x, y, z$ (4) $y, x, z + \frac{1}{2}$	(2) $\bar{y}, x - y, z$ (5) $x - y, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x} + y, \bar{x}, z$ (6) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$ : $l = 2n$ $000l$ : $l = 2n$  Special: as above, plus $hkil$ : $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$  $hkil$ : $l = 2n$
2 <i>b</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$		
2 <i>a</i> 3..	$0, 0, z$	$0, 0, z + \frac{1}{2}$		

**Symmetry of special projections**

Along [001]  $p31m$   
 $\mathbf{a}' = \mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
Origin at  $0, 0, z$

Along [100]  $p1g1$   
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$      $\mathbf{b}' = \mathbf{c}$   
Origin at  $x, 0, 0$

Along [210]  $p1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \frac{1}{2}\mathbf{c}$   
Origin at  $x, \frac{1}{2}x, 0$

**Maximal non-isomorphic subgroups**

**I** [2]  $P311$  ( $P3, 143$ ) 1; 2; 3  
 $\left\{ \begin{array}{l} [3] P11c (Cc, 9) \quad 1; 4 \\ [3] P11c (Cc, 9) \quad 1; 5 \\ [3] P11c (Cc, 9) \quad 1; 6 \end{array} \right.$

**IIa** none

**IIb** [3]  $H31c$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) ( $P3c1, 158$ ); [3]  $R3c$  ( $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$ ) (161);  
[3]  $R3c$  ( $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$ ) (161)

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $P31c$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (159); [4]  $P31c$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) (159)

**Minimal non-isomorphic supergroups**

**I** [2]  $P\bar{3}1c$  (163); [2]  $P6cc$  (184); [2]  $P6_3mc$  (186); [2]  $P\bar{6}2c$  (190)

**II** [3]  $H31c$  ( $P3c1, 158$ ); [2]  $P31m$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (157)