

$P\bar{3}1c$

D_{3d}^2

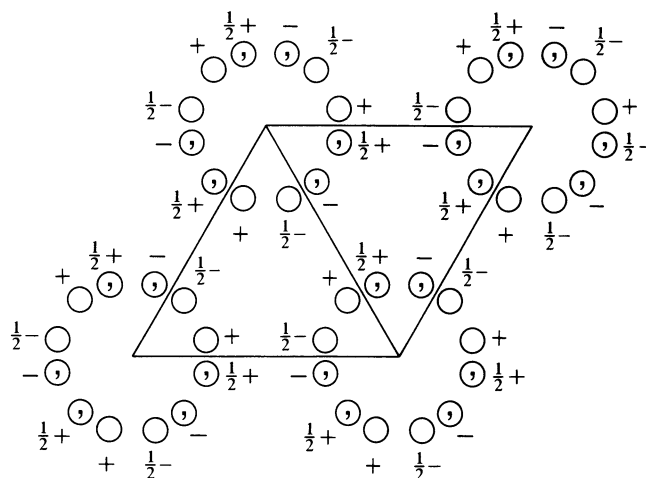
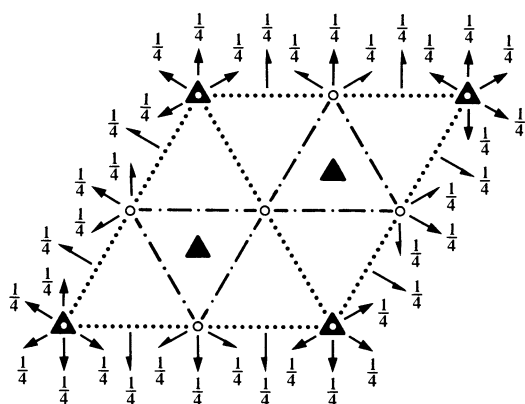
$\bar{3}1m$

Trigonal

No. 163

$P\bar{3}12/c$

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



Origin at centre ($\bar{3}$) at $\bar{3}1c$

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

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

Symmetry operations

- | | | |
|-----------------------------------|---------------------------------------|---------------------------------------|
| (1) 1 | (2) 3^+ $0, 0, z$ | (3) 3^- $0, 0, z$ |
| (4) 2 $x, \bar{x}, \frac{1}{4}$ | (5) 2 $x, 2x, \frac{1}{4}$ | (6) 2 $2x, x, \frac{1}{4}$ |
| (7) $\bar{1}$ $0, 0, 0$ | (8) $\bar{3}^+$ $0, 0, z$; $0, 0, 0$ | (9) $\bar{3}^-$ $0, 0, z$; $0, 0, 0$ |
| (10) c x, x, z | (11) c $x, 0, z$ | (12) c $0, y, z$ |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
12 <i>i</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (5) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$ (6) $x, x - y, \bar{z} + \frac{1}{2}$ (7) $\bar{x}, \bar{y}, \bar{z}$ (8) $y, \bar{x} + y, \bar{z}$ (9) $x - y, x, \bar{z}$ (10) $y, x, z + \frac{1}{2}$ (11) $x - y, \bar{y}, z + \frac{1}{2}$ (12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$	General: $hh\bar{2}hl$: $l = 2n$ $000l$: $l = 2n$
6 <i>h</i> ..2	$x, \bar{x}, \frac{1}{4}$ $x, 2x, \frac{1}{4}$ $2\bar{x}, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$ $\bar{x}, 2\bar{x}, \frac{3}{4}$ $2x, x, \frac{3}{4}$	Special: as above, plus no extra conditions
6 <i>g</i> $\bar{1}$	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkil$: $l = 2n$
4 <i>f</i> 3..	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{1}{3}, \frac{2}{3}, \bar{z} + \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, \bar{z}$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
4 <i>e</i> 3..	$0, 0, z$ $0, 0, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, z + \frac{1}{2}$	$hkil$: $l = 2n$
2 <i>d</i> 3.2	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$ $\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>c</i> 3.2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$ $\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$hkil$: $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>b</i> $\bar{3}$..	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkil$: $l = 2n$
2 <i>a</i> 3.2	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkil$: $l = 2n$

Symmetry of special projections

Along $[001]$ $p6mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along $[100]$ $p2gm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along $[210]$ $p2$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

Maximal non-isomorphic subgroups

I	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P312$ (149)	1; 2; 3; 4; 5; 6
	[2] $P\bar{3}11$ ($P\bar{3}$, 147)	1; 2; 3; 7; 8; 9
	{ [3] $P112/c$ ($C2/c$, 15)	1; 4; 7; 10
	{ [3] $P112/c$ ($C2/c$, 15)	1; 5; 7; 11
	{ [3] $P112/c$ ($C2/c$, 15)	1; 6; 7; 12

IIa none

IIIb [3] $H\bar{3}1c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{3}c1$, 165); [3] $R\bar{3}c$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + 2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (167);
[3] $R\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (167)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{3}1c$ ($\mathbf{c}' = 3\mathbf{c}$) (163); [4] $P\bar{3}1c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (163)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

II [3] $H\bar{3}1c$ ($P\bar{3}c1$, 165); [2] $P\bar{3}1m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (162)