

$P6_222$

$D_6^4$

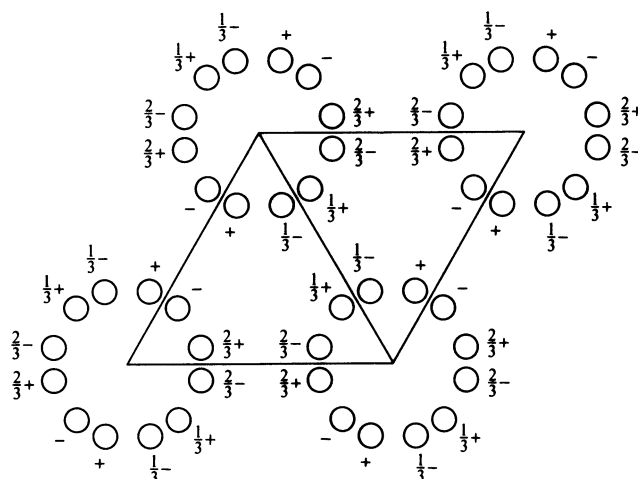
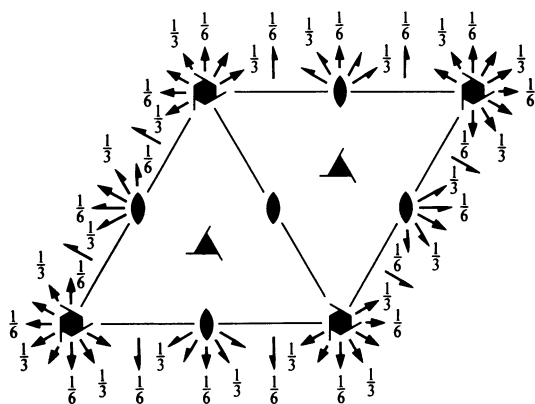
622

Hexagonal

No. 180

$P6_222$

Patterson symmetry  $P6/mmm$



**Origin** at 222 at  $6_2(2, 1, 1)(1, 2, 1)$

**Asymmetric unit**  $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{6}; y \leq x$

Vertices  $0, 0, 0 \quad 1, 0, 0 \quad 1, 1, 0$

$0, 0, \frac{1}{6} \quad 1, 0, \frac{1}{6} \quad 1, 1, \frac{1}{6}$

**Symmetry operations**

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

**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
								General:
12	<i>k</i> 1	(1) $x, y, z$ (4) $\bar{x}, \bar{y}, z$ (7) $y, x, \bar{z} + \frac{2}{3}$ (10) $\bar{y}, \bar{x}, \bar{z} + \frac{2}{3}$	(2) $\bar{y}, x - y, z + \frac{2}{3}$ (5) $y, \bar{x} + y, z + \frac{2}{3}$ (8) $x - y, \bar{y}, \bar{z}$ (11) $\bar{x} + y, y, \bar{z}$	(3) $\bar{x} + y, \bar{x}, z + \frac{1}{3}$ (6) $x - y, x, z + \frac{1}{3}$ (9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{1}{3}$ (12) $x, x - y, \bar{z} + \frac{1}{3}$				000 $l$ : $l = 3n$
								Special: as above, plus
6	<i>j</i> ..2	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{6}$	$x, \bar{x}, \frac{5}{6}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{6}$	$\bar{x}, x, \frac{5}{6}$	no extra conditions
6	<i>i</i> ..2	$x, 2x, 0$	$2\bar{x}, \bar{x}, \frac{2}{3}$	$x, \bar{x}, \frac{1}{3}$	$\bar{x}, 2\bar{x}, 0$	$2x, x, \frac{2}{3}$	$\bar{x}, x, \frac{1}{3}$	no extra conditions
6	<i>h</i> .2.	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{6}$	$\bar{x}, \bar{x}, \frac{5}{6}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{6}$	$x, x, \frac{5}{6}$	no extra conditions
6	<i>g</i> .2.	$x, 0, 0$	$0, x, \frac{2}{3}$	$\bar{x}, \bar{x}, \frac{1}{3}$	$\bar{x}, 0, 0$	$0, \bar{x}, \frac{2}{3}$	$x, x, \frac{1}{3}$	no extra conditions
6	<i>f</i> 2..	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z + \frac{2}{3}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{3}$	$0, \frac{1}{2}, \bar{z} + \frac{2}{3}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{3}$	$hkil$ : $h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$
6	<i>e</i> 2..	$0, 0, z$	$0, 0, z + \frac{2}{3}$	$0, 0, z + \frac{1}{3}$	$0, 0, \bar{z} + \frac{2}{3}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{3}$	$hkil$ : $l = 3n$
3	<i>d</i> 222	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{6}$	$\frac{1}{2}, \frac{1}{2}, \frac{5}{6}$				$hkil$ : $h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$
3	<i>c</i> 222	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{2}{3}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{3}$				$hkil$ : $h = 2n + 1$ or $k = 2n + 1$ or $l = 3n$
3	<i>b</i> 222	$0, 0, \frac{1}{2}$	$0, 0, \frac{1}{6}$	$0, 0, \frac{5}{6}$				$hkil$ : $l = 3n$
3	<i>a</i> 222	$0, 0, 0$	$0, 0, \frac{2}{3}$	$0, 0, \frac{1}{3}$				$hkil$ : $l = 3n$

**Symmetry of special projections**

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

Along [100]  $p2mm$   
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along [210]  $p2mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, \frac{1}{2}x, \frac{1}{6}$