

$P6_122$

D_6^2

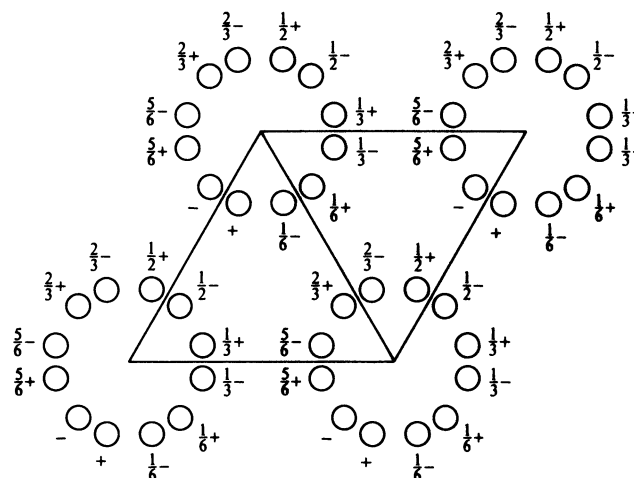
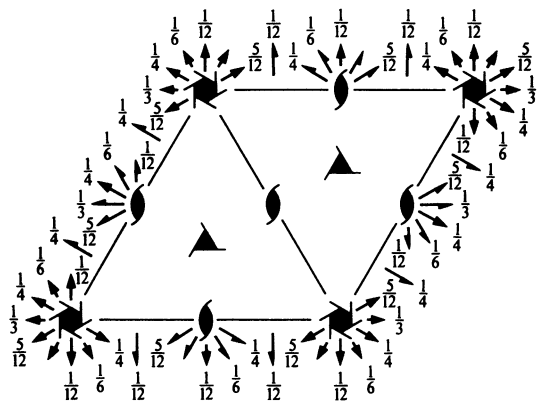
622

Hexagonal

No. 178

$P6_122$

Patterson symmetry $P6/mmm$



Origin on $2[100]$ at $6_1(2, 1, 1)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{12}$
 Vertices $0, 0, 0 \quad 1, 0, 0 \quad 1, 1, 0 \quad 0, 1, 0$
 $0, 0, \frac{1}{12} \quad 1, 0, \frac{1}{12} \quad 1, 1, \frac{1}{12} \quad 0, 1, \frac{1}{12}$

Symmetry operations

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

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>c</i> 1	(1) x, y, z (2) $\bar{y}, x - y, z + \frac{1}{3}$ (3) $\bar{x} + y, \bar{x}, z + \frac{2}{3}$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{5}{6}$ (6) $x - y, x, z + \frac{1}{6}$ (7) $y, x, \bar{z} + \frac{1}{3}$ (8) $x - y, \bar{y}, \bar{z}$ (9) $\bar{x}, \bar{x} + y, \bar{z} + \frac{2}{3}$ (10) $\bar{y}, \bar{x}, \bar{z} + \frac{5}{6}$ (11) $\bar{x} + y, y, \bar{z} + \frac{1}{2}$ (12) $x, x - y, \bar{z} + \frac{1}{6}$	General: $000l: l = 6n$
6 <i>b</i> .. 2	$x, 2x, \frac{1}{4} \quad 2\bar{x}, \bar{x}, \frac{7}{12} \quad x, \bar{x}, \frac{11}{12} \quad \bar{x}, 2\bar{x}, \frac{3}{4} \quad 2x, x, \frac{1}{12} \quad \bar{x}, x, \frac{5}{12}$	Special: as above, plus $hh\bar{2}hl: l = 2n$ or $l = 3n + 1$ or $l = 3n + 2$
6 <i>a</i> . 2 .	$x, 0, 0 \quad 0, x, \frac{1}{3} \quad \bar{x}, \bar{x}, \frac{2}{3} \quad \bar{x}, 0, \frac{1}{2} \quad 0, \bar{x}, \frac{5}{6} \quad x, x, \frac{1}{6}$	$h\bar{h}0l: l = 2n$ or $l = 3n + 1$ or $l = 3n + 2$

Symmetry of special projections

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

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

Along $[210]$ $p2gm$ $\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{2}x, \frac{1}{12}$