

Hexagonal

6

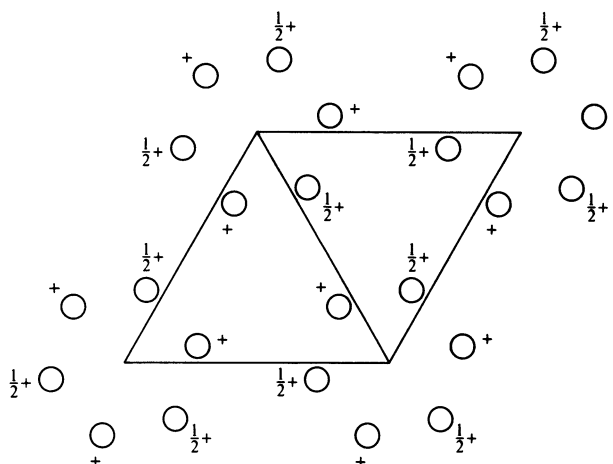
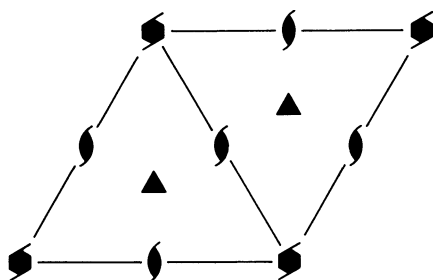
$C_6^6$

$P6_3$

Patterson symmetry  $P6/m$

$P6_3$

No. 173



Origin on 3 on 6<sub>3</sub>

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)  $2(0, 0, \frac{1}{2}) 0, 0, z$
- (5)  $6^-(0, 0, \frac{1}{2}) 0, 0, z$
- (6)  $6^+(0, 0, \frac{1}{2}) 0, 0, z$

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 c 1	(1) $x, y, z$ (2) $\bar{y}, x - y, z$ (3) $\bar{x} + y, \bar{x}, z$ (4) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (5) $y, \bar{x} + y, z + \frac{1}{2}$ (6) $x - y, x, z + \frac{1}{2}$	General: $000l: l = 2n$  Special: as above, plus $hkil: l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 b 3..	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$	$hkil: l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 a 3..	$0, 0, z$ $0, 0, z + \frac{1}{2}$	$hkil: l = 2n$

Symmetry of special projections

Along [001] $p6$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ 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] $p1g1$ $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, \frac{1}{2}x, 0$
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