

***P*622**

***D*₆¹**

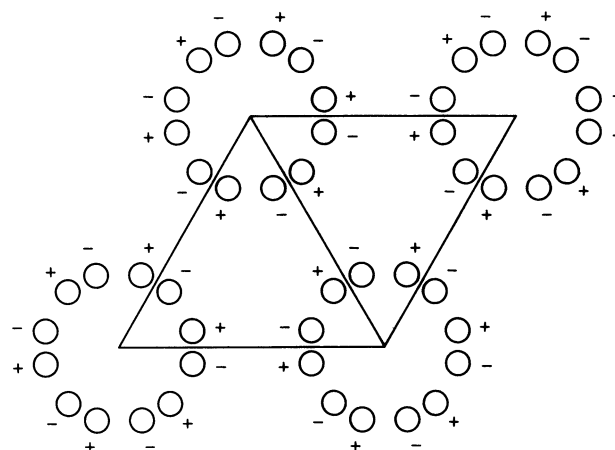
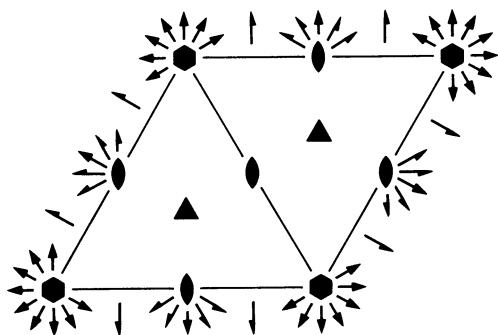
622

Hexagonal

No. 177

***P*622**

Patterson symmetry *P*6/*m**m**m*



Origin at 622

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

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

Symmetry operations

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

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>n</i>	1	(1) x, y, z	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$
			(4) \bar{x}, \bar{y}, z	(5) $y, \bar{x} + y, z$	(6) $x - y, x, z$
			(7) y, x, \bar{z}	(8) $x - y, \bar{y}, \bar{z}$	(9) $\bar{x}, \bar{x} + y, \bar{z}$
			(10) $\bar{y}, \bar{x}, \bar{z}$	(11) $\bar{x} + y, y, \bar{z}$	(12) $x, x - y, \bar{z}$

General:

no conditions

Special: no extra conditions

6	<i>m</i>	. . 2	$x, \bar{x}, \frac{1}{2}$	$x, 2x, \frac{1}{2}$	$2\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$\bar{x}, 2\bar{x}, \frac{1}{2}$	$2x, x, \frac{1}{2}$
6	<i>l</i>	. . 2	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$
6	<i>k</i>	. 2 .	$x, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$x, x, \frac{1}{2}$
6	<i>j</i>	. 2 .	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$x, x, 0$
6	<i>i</i>	2 . .	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$
4	<i>h</i>	3 . .	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z$	$\frac{2}{3}, \frac{1}{3}, \bar{z}$	$\frac{1}{3}, \frac{2}{3}, \bar{z}$		
3	<i>g</i>	2 2 2	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
3	<i>f</i>	2 2 2	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			
2	<i>e</i>	6 . .	$0, 0, z$	$0, 0, \bar{z}$				
2	<i>d</i>	3 . 2	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$				
2	<i>c</i>	3 . 2	$\frac{1}{3}, \frac{2}{3}, 0$	$\frac{2}{3}, \frac{1}{3}, 0$				
1	<i>b</i>	6 2 2	$0, 0, \frac{1}{2}$					
1	<i>a</i>	6 2 2	$0, 0, 0$					

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 $x, \frac{1}{2}x, 0$