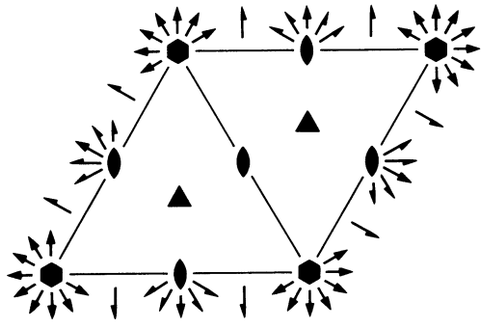
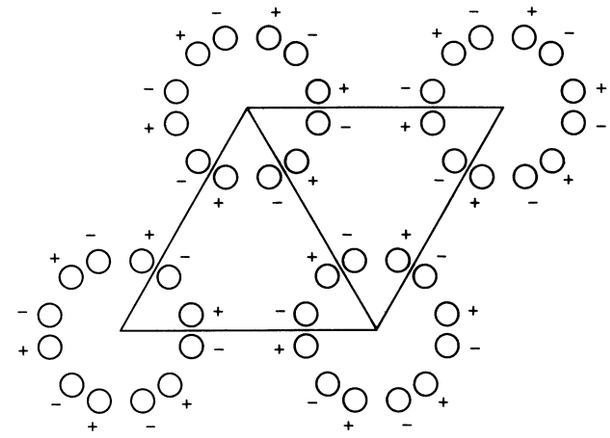
International Tables for Crystallography (2006). Vol. A, Space group 177, pp. 566–567.

$P622$ D_6^1 622 Hexagonal

No. 177 $P622$ Patterson symmetry $P6/mmm$





Origin at 622

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

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 $2x,x,0$

Maximal isomorphic subgroups of lowest index

IIc [2] $P622$ ($\mathbf{c}' = 2\mathbf{c}$) (177); [3] $H622$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P622$, 177)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6/mcc$ (192)

II none

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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	n	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(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) $x,x-y,\bar{z}$				
									Special: no extra conditions
6	m	. . 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	l	. . 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	k	. 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	j	. 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	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	h	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	g	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	f	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	6 . .	$0,0,z$	$0,0,\bar{z}$					
2	d	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	3 . 2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	6 2 2	$0,0,\frac{1}{2}$						
1	a	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 $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P611$ ($P6$, 168) 1; 2; 3; 4; 5; 6
[2] $P321$ (150) 1; 2; 3; 7; 8; 9
[2] $P312$ (149) 1; 2; 3; 10; 11; 12
{ [3] $P222$ ($C222$, 21) 1; 4; 7; 10
{ [3] $P222$ ($C222$, 21) 1; 4; 8; 11
{ [3] $P222$ ($C222$, 21) 1; 4; 9; 12

IIa none

IIb [2] $P6_322$ ($\mathbf{c}'=2\mathbf{c}$) (182); [3] $P6_422$ ($\mathbf{c}'=3\mathbf{c}$) (181); [3] $P6_222$ ($\mathbf{c}'=3\mathbf{c}$) (180)

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