

$P 6_3/m m c$  $D_{6h}^4$  $6/m m m$ 

Hexagonal

No. 194

 $P 6_3/m 2/m 2/c$ Patterson symmetry  $P 6/m m m$ Origin at centre ( $\bar{3} m 1$ ) at  $\bar{3} 2/m c$ 

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry,  
Coordinates

## Patterson peaks (U, V, W (Multiplicity))

24	l 1	x,y,z; -y,x-y,z; etc. $0, 0, 0$ (24) $x-y, -x+y, 2z$ (2) $2x-y, 0, 1/2+2z$ (2) $0, 0, 1/2+2z$ (12) $0, -x+2y, 0$ (4)	$x+y, -x+2y, 0$ (4) $y, 2y, 2z$ (2) $0, -x+2y, 1/2+2z$ (2) $x+y, -x+2y, 1/2+2z$ (2) $x-y, -x+y, 1/2$ (4)	$2x, 2y, 1/2$ (2) $2x, x, 2z$ (2) $2x, 2y, 2z$ (1) $x+y, x+y, 0$ (4) $y, 2y, 1/2$ (4)	$x-y, x, 1/2$ (4) $x+y, x+y, 1/2+2z$ (2) $x-y, x, 2z$ (2) $2x-y, 0, 0$ (4) $2x, x, 1/2$ (4)
12	k . m .	x,2x,z; -2x,-x,z; etc. $0, 0, 0$ (12) $-x, x, 2z$ (2)	$3x, 3x, 0$ (4) $2x, x, 2z$ (1)	$2x, x, 1/2$ (2) $3x, 3x, 1/2+2z$ (2)	$-x, x, 1/2$ (4) $0, 0, 1/2+2z$ (6)
12	j m . .	x,y,1/4; -y,x-y,1/4; etc. $0, 0, 0$ (12) $x-y, -x+y, 1/2$ (2) $2x-y, 0, 0$ (2)	$x+y, -x+2y, 0$ (2) $y, 2y, 1/2$ (2) $0, -x+2y, 0$ (2)	$2x, 2y, 1/2$ (1) $2x, x, 1/2$ (2)	$x-y, x, 1/2$ (2) $x+y, x+y, 0$ (2)
12	i . 2 .	x,0,0; 0,x,0; etc. $0, 0, 0$ (12) $2x, 0, 0$ (2)	$x, -x, 0$ (4) $x, x, 0$ (4)	$2x, 0, 1/2$ (2) $0, 0, 1/2$ (12)	$x, x, 1/2$ (4) $x, -x, 1/2$ (4)
6	h m m 2	x,2x,1/4; -2x,-x,1/4; etc. $0, 0, 0$ (6)	$3x, 3x, 0$ (2)	$2x, x, 1/2$ (1)	$-x, x, 1/2$ (2)
6	g . 2/m .	1/2,0,0; 0,1/2,0; etc. $0, 0, 0$ (6)	$1/2, 1/2, 0$ (4)	$0, 0, 1/2$ (6)	$1/2, 1/2, 1/2$ (4)
4	f 3 m .	1/3,2/3,z; 2/3,1/3,1/2+z; etc. $0, 0, 0$ (4)	$2/3, 1/3, 1/2$ (2)	$2/3, 1/3, 2z$ (1)	$0, 0, 1/2+2z$ (2)
4	e 3 m .	0,0,z; 0,0,1/2+z; etc. $0, 0, 0$ (4)	$0, 0, 1/2$ (4)	$0, 0, 2z$ (2)	$0, 0, 1/2+2z$ (2)
2	d $\bar{6} m 2$	1/3,2/3,3/4; 2/3,1/3,1/4 $0, 0, 0$ (2)	$2/3, 1/3, 1/2$ (1)		
2	c $\bar{6} m 2$	1/3,2/3,1/4; 2/3,1/3,3/4 $0, 0, 0$ (2)	$2/3, 1/3, 1/2$ (1)		
2	b $\bar{6} m 2$	0,0,1/4; 0,0,3/4 $0, 0, 0$ (2)	$0, 0, 1/2$ (2)		
2	a $\bar{3} m .$	0,0,0; 0,0,1/2 $0, 0, 0$ (2)	$0, 0, 1/2$ (2)		

## Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

1, l	$x1-x2, y1-y2, z1-z2$ (2) $x1+y2, y1-x2+y2, z1-z2$ (2) $x1+x2-y2, y1+x2, z1-z2$ (2) $x1+x2, y1+y2, 1/2+z1-z2$ (2) $x1-y2, y1+x2-y2, 1/2+z1-z2$ (2) $x1-x2+y2, y1-x2, 1/2+z1-z2$ (2) $x1-y2, y1-x2, z1+z2$ (2) $x1-x2+y2, y1+y2, z1+z2$ (2) $x1+x2, y1+x2-y2, z1+z2$ (2) $x1+y2, y1+x2, 1/2+z1+z2$ (2) $x1+x2-y2, y1-y2, 1/2+z1+z2$ (2) $x1-x2, y1-x2+y2, 1/2+z1+z2$ (2) $x1+x2, y1+y2, z1+z2$ (2) $x1-y2, y1+x2-y2, z1+z2$ (2) $x1-x2+y2, y1-x2, z1+z2$ (2) $x1-x2, y1-y2, 1/2+z1+z2$ (2) $x1+y2, y1-x2+y2, 1/2+z1+z2$ (2) $x1+x2-y2, y1+x2, 1/2+z1+z2$ (2) $x1+y2, y1+x2, z1-z2$ (2) $x1+x2-y2, y1-y2, z1-z2$ (2) $x1-x2, y1-x2+y2, z1-z2$ (2) $x1-y2, y1-x2, 1/2+z1-z2$ (2) $x1-x2+y2, y1+y2, 1/2+z1-z2$ (2) $x1+x2, y1+x2-y2, 1/2+z1-z2$ (2)	$x1+x2, y1+x2-y2, 1/4+z1$ (1) $x1+y2, y1+x2, 3/4+z1$ (1) $x1+x2-y2, y1-y2, 3/4+z1$ (1) $x1-x2, y1-x2+y2, 3/4+z1$ (1) $-x1+x2, -y1+y2, 3/4-z1$ (1) $-x1-y2, -y1+x2-y2, 3/4-z1$ (1) $-x1-x2+y2, -y1-x2, 3/4-z1$ (1) $-x1-x2, -y1-y2, 1/4-z1$ (1) $-x1+y2, -y1-x2+y2, 1/4-z1$ (1) $-x1+x2-y2, -y1+x2, 1/4-z1$ (1) $-x1+y2, -y1+x2, 1/4-z1$ (1) $-x1+x2-y2, -y1-y2, 1/4-z1$ (1) $-x1-x2, -y1-x2+y2, 1/4-z1$ (1) $-x1-y2, -y1-x2, 3/4-z1$ (1) $-x1-x2+y2, -y1+y2, 3/4-z1$ (1) $-x1+x2, -y1+x2-y2, 3/4-z1$ (1)
1, k	$x1-x2, y1-2x2, z1-z2$ (2) $x1+2x2, y1+x2, z1-z2$ (2) $x1-x2, y1+x2, z1-z2$ (2) $x1+x2, y1+2x2, 1/2+z1-z2$ (2) $x1-2x2, y1-x2, 1/2+z1-z2$ (2) $x1+x2, y1-x2, 1/2+z1-z2$ (2) $x1-2x2, y1-x2, z1+z2$ (2) $x1+x2, y1+2x2, z1+z2$ (2) $x1+x2, y1-x2, z1+z2$ (2) $x1+2x2, y1+x2, 1/2+z1+z2$ (2) $x1-x2, y1-2x2, 1/2+z1+z2$ (2) $x1-x2, y1+x2, 1/2+z1+z2$ (2)	$x1-x2, y1, z1$ (2) $x1, y1-x2, z1$ (2) $x1+x2, y1+x2, z1$ (2) $x1+x2, y1, 1/2+z1$ (2) $x1, y1+x2, 1/2+z1$ (2) $x1-x2, y1-x2, 1/2+z1$ (2) $x1+x2, y1, z1$ (2) $x1, y1+x2, z1$ (2) $x1-x2, y1-x2, z1$ (2) $x1-x2, y1, 1/2+z1$ (2) $x1, y1-x2, 1/2+z1$ (2) $x1+x2, y1+x2, 1/2+z1$ (2)
1, j	$x1-x2, y1-y2, 3/4+z1$ (1) $x1+y2, y1-x2+y2, 3/4+z1$ (1) $x1+x2-y2, y1+x2, 3/4+z1$ (1) $x1+x2, y1+y2, 1/4+z1$ (1) $x1-y2, y1+x2-y2, 1/4+z1$ (1) $x1-x2+y2, y1-x2, 1/4+z1$ (1) $x1-y2, y1-x2, 1/4+z1$ (1) $x1-x2+y2, y1+y2, 1/4+z1$ (1)	$1/2+x1, y1, z1$ (2) $x1, 1/2+y1, z1$ (2) $1/2+x1, 1/2+y1, z1$ (2) $1/2+x1, y1, 1/2+z1$ (2)
	1, i	$x1-x2, y1, z1$ (2) $x1, y1-x2, z1$ (2) $x1+x2, y1+x2, z1$ (2) $x1+x2, y1, 1/2+z1$ (2) $x1, y1+x2, 1/2+z1$ (2) $x1-x2, y1-x2, 1/2+z1$ (2) $x1+x2, y1, z1$ (2) $x1, y1+x2, z1$ (2) $x1-x2, y1-x2, z1$ (2) $x1-x2, y1, 1/2+z1$ (2) $x1, y1-x2, 1/2+z1$ (2) $x1+x2, y1+x2, 1/2+z1$ (2) $x1-x2, y1-2x2, 3/4+z1$ (1) $x1+2x2, y1+x2, 3/4+z1$ (1) $x1-x2, y1+x2, 3/4+z1$ (1) $x1+x2, y1+2x2, 1/4+z1$ (1) $x1-2x2, y1-x2, 1/4+z1$ (1) $x1+x2, y1-x2, 1/4+z1$ (1) $-x1+x2, -y1+2x2, 3/4-z1$ (1) $-x1-2x2, -y1-x2, 3/4-z1$ (1) $-x1+x2, -y1-x2, 3/4-z1$ (1) $-x1-x2, -y1-2x2, 1/4-z1$ (1) $-x1+2x2, -y1+x2, 1/4-z1$ (1) $-x1-x2, -y1+x2, 1/4-z1$ (1)
	1, h	$1/2+x1, y1, z1$ (2) $x1, 1/2+y1, z1$ (2) $1/2+x1, 1/2+y1, z1$ (2) $1/2+x1, y1, 1/2+z1$ (2)
	1, g	

	$x1, 1/2+y1, 1/2+z1$ (2)		$x1-x2, 2x1-x2, 1/2+z1$ (2)
	$1/2+x1, 1/2+y1, 1/2+z1$ (2)		$x1-x2, 2x1-2x2, 3/4+z1$ (1)
l, f	$2/3+x1, 1/3+y1, z1-z2$ (1)		$x1+2x2, 2x1+x2, 3/4+z1$ (1)
	$1/3+x1, 2/3+y1, 1/2+z1-z2$ (1)		$x1+x2, 2x1+2x2, 1/4+z1$ (1)
	$1/3+x1, 2/3+y1, z1+z2$ (1)		$x1-2x2, 2x1-x2, 1/4+z1$ (1)
	$2/3+x1, 1/3+y1, 1/2+z1+z2$ (1)		$-x1+x2, -2x1+2x2, 3/4-z1$ (1)
	$2/3-x1, 1/3-y1, -z1+z2$ (1)		$-x1-2x2, -2x1-x2, 3/4-z1$ (1)
	$1/3-x1, 2/3-y1, 1/2-z1+z2$ (1)		$-x1-x2, -2x1-2x2, 1/4-z1$ (1)
	$1/3-x1, 2/3-y1, -z1-z2$ (1)		$-x1+2x2, -2x1+x2, 1/4-z1$ (1)
	$2/3-x1, 1/3-y1, 1/2-z1-z2$ (1)	k, g	$1/2+x1, 2x1, z1$ (2)
l, e	$x1, y1, z1-z2$ (2)		$x1, 1/2+2x1, z1$ (2)
	$x1, y1, 1/2+z1-z2$ (2)		$1/2+x1, 2x1, 1/2+z1$ (2)
	$x1, y1, z1+z2$ (2)		$x1, 1/2+2x1, 1/2+z1$ (2)
	$x1, y1, 1/2+z1+z2$ (2)	k, f	$2/3+x1, 1/3+2x1, z1-z2$ (1)
l, d	$2/3+x1, 1/3+y1, 1/4+z1$ (2)		$1/3+x1, 2/3+2x1, 1/2+z1-z2$ (1)
	$1/3+x1, 2/3+y1, 3/4+z1$ (2)		$1/3+x1, 2/3+2x1, z1+z2$ (1)
l, c	$2/3+x1, 1/3+y1, 3/4+z1$ (2)		$2/3+x1, 1/3+2x1, 1/2+z1+z2$ (1)
	$1/3+x1, 2/3+y1, 1/4+z1$ (2)		$2/3-x1, 1/3-2x1, -z1+z2$ (1)
l, b	$x1, y1, 3/4+z1$ (2)		$1/3-x1, 2/3-2x1, 1/2-z1+z2$ (1)
	$x1, y1, 1/4+z1$ (2)		$1/3-x1, 2/3-2x1, -z1-z2$ (1)
l, a	$x1, y1, z1$ (2)		$2/3-x1, 1/3-2x1, 1/2-z1-z2$ (1)
	$x1, y1, 1/2+z1$ (2)	k, e	$x1, 2x1, z1-z2$ (2)
k, k	$x1-x2, 2x1-2x2, z1-z2$ (2)		$x1, 2x1, 1/2+z1-z2$ (2)
	$x1+2x2, 2x1+x2, z1-z2$ (2)		$x1, 2x1, z1+z2$ (2)
	$x1+x2, 2x1+2x2, 1/2+z1-z2$ (2)		$x1, 2x1, 1/2+z1+z2$ (2)
	$x1-2x2, 2x1-x2, 1/2+z1-z2$ (2)	k, d	$2/3+x1, 1/3+2x1, 1/4+z1$ (2)
	$x1-2x2, 2x1-x2, z1+z2$ (2)		$1/3+x1, 2/3+2x1, 3/4+z1$ (2)
	$x1+x2, 2x1+2x2, z1+z2$ (2)	k, c	$2/3+x1, 1/3+2x1, 3/4+z1$ (2)
	$x1+2x2, 2x1+x2, 1/2+z1+z2$ (2)		$1/3+x1, 2/3+2x1, 1/4+z1$ (2)
	$x1-x2, 2x1-2x2, 1/2+z1+z2$ (2)	k, b	$x1, 2x1, 3/4+z1$ (2)
k, j	$x1-x2, 2x1-y2, 3/4+z1$ (1)		$x1, 2x1, 1/4+z1$ (2)
	$x1+y2, 2x1-x2+y2, 3/4+z1$ (1)	k, a	$x1, 2x1, z1$ (2)
	$x1+x2-y2, 2x1+x2, 3/4+z1$ (1)		$x1, 2x1, 1/2+z1$ (2)
	$x1+x2, 2x1+y2, 1/4+z1$ (1)	j, j	$x1-x2, y1-y2, 0$ (2)
	$x1-y2, 2x1+x2-y2, 1/4+z1$ (1)		$x1+y2, y1-x2+y2, 0$ (2)
	$x1-x2+y2, 2x1-x2, 1/4+z1$ (1)		$x1+x2-y2, y1+x2, 0$ (2)
	$-x1+x2, -2x1+y2, 3/4-z1$ (1)		$x1+x2, y1+y2, 1/2$ (2)
	$-x1-y2, -2x1+x2-y2, 3/4-z1$ (1)		$x1-y2, y1+x2-y2, 1/2$ (2)
	$-x1-x2+y2, -2x1-x2, 3/4-z1$ (1)		$x1-x2+y2, y1-x2, 1/2$ (2)
	$-x1-x2, -2x1-y2, 1/4-z1$ (1)		$x1-y2, y1-x2, 1/2$ (2)
	$-x1+y2, -2x1-x2+y2, 1/4-z1$ (1)		$x1-x2+y2, y1+y2, 1/2$ (2)
	$-x1+x2-y2, -2x1+x2, 1/4-z1$ (1)		$x1+x2, y1+x2-y2, 1/2$ (2)
k, i	$x1-x2, 2x1, z1$ (2)		$x1+y2, y1+x2, 0$ (2)
	$x1, 2x1-x2, z1$ (2)		$x1+x2-y2, y1-y2, 0$ (2)
	$x1+x2, 2x1+x2, z1$ (2)		$x1-x2, y1-x2+y2, 0$ (2)
	$x1+x2, 2x1, 1/2+z1$ (2)	j, i	$x1-x2, y1, 1/4$ (2)
	$x1, 2x1+x2, 1/2+z1$ (2)		$x1, y1-x2, 1/4$ (2)

	$x1+x2, y1+x2, 1/4$ (2)	i, d	$2/3+x1, 1/3, 1/4$ (2)
	$x1+x2, y1, 3/4$ (2)	i, c	$2/3+x1, 1/3, 3/4$ (2)
	$x1, y1+x2, 3/4$ (2)	i, b	$x1, 0, 3/4$ (4)
	$x1-x2, y1-x2, 3/4$ (2)	i, a	$x1, 0, 0$ (4)
j, h	$x1-x2, y1-2x2, 0$ (2)		$x1, 0, 1/2$ (4)
	$x1+2x2, y1+x2, 0$ (2)	h, h	$x1-x2, 2x1-2x2, 0$ (2)
	$x1-x2, y1+x2, 0$ (2)		$x1+2x2, 2x1+x2, 0$ (2)
	$x1+x2, y1+2x2, 1/2$ (2)		$x1+x2, 2x1+2x2, 1/2$ (2)
	$x1-2x2, y1-x2, 1/2$ (2)		$x1-2x2, 2x1-x2, 1/2$ (2)
	$x1+x2, y1-x2, 1/2$ (2)	h, g	$1/2+x1, 2x1, 1/4$ (2)
j, g	$1/2+x1, y1, 1/4$ (2)		$x1, 1/2+2x1, 1/4$ (2)
	$x1, 1/2+y1, 1/4$ (2)	h, f	$2/3+x1, 1/3+2x1, 1/4-z2$ (2)
	$1/2+x1, 1/2+y1, 1/4$ (2)		$1/3+x1, 2/3+2x1, 3/4-z2$ (2)
j, f	$2/3+x1, 1/3+y1, 1/4-z2$ (2)	h, e	$x1, 2x1, 1/4-z2$ (2)
	$1/3+x1, 2/3+y1, 3/4-z2$ (2)		$x1, 2x1, 3/4-z2$ (2)
j, e	$x1, y1, 1/4-z2$ (2)	h, d	$2/3+x1, 1/3+2x1, 1/2$ (1)
	$x1, y1, 3/4-z2$ (2)		$1/3+x1, 2/3+2x1, 0$ (1)
j, d	$2/3+x1, 1/3+y1, 1/2$ (1)		$2/3-x1, 1/3-2x1, 1/2$ (1)
	$1/3+x1, 2/3+y1, 0$ (1)		$1/3-x1, 2/3-2x1, 0$ (1)
	$2/3-x1, 1/3-y1, 1/2$ (1)	h, c	$2/3+x1, 1/3+2x1, 0$ (1)
	$1/3-x1, 2/3-y1, 0$ (1)		$1/3+x1, 2/3+2x1, 1/2$ (1)
j, c	$2/3+x1, 1/3+y1, 0$ (1)		$2/3-x1, 1/3-2x1, 0$ (1)
	$1/3+x1, 2/3+y1, 1/2$ (1)		$1/3-x1, 2/3-2x1, 1/2$ (1)
	$2/3-x1, 1/3-y1, 0$ (1)	h, b	$x1, 2x1, 0$ (2)
	$1/3-x1, 2/3-y1, 1/2$ (1)		$x1, 2x1, 1/2$ (2)
j, b	$x1, y1, 0$ (2)	h, a	$x1, 2x1, 1/4$ (2)
	$x1, y1, 1/2$ (2)	g, f	$1/6, 1/3, -z2$ (2)
j, a	$x1, y1, 1/4$ (2)		$5/6, 2/3, 1/2-z2$ (2)
i, i	$x1-x2, 0, 0$ (4)	g, e	$1/2, 0, -z2$ (4)
	$x1, -x2, 0$ (4)		$1/2, 0, 1/2-z2$ (4)
	$x1+x2, 0, 1/2$ (4)	g, d	$1/6, 1/3, 1/4$ (2)
	$x1, x2, 1/2$ (4)	g, c	$1/6, 1/3, 3/4$ (2)
	$x1+x2, 0, 0$ (4)	g, b	$1/2, 0, 3/4$ (4)
	$x1, x2, 0$ (4)	g, a	$1/2, 0, 0$ (4)
	$x1-x2, 0, 1/2$ (4)		$1/2, 0, 1/2$ (4)
	$x1, -x2, 1/2$ (4)	f, f	$0, 0, z1-z2$ (4)
i, h	$x1-x2, -2x2, 3/4$ (2)		$2/3, 1/3, 1/2+z1-z2$ (2)
	$x1+2x2, x2, 3/4$ (2)		$2/3, 1/3, z1+z2$ (2)
	$x1-x2, x2, 3/4$ (2)		$0, 0, 1/2+z1+z2$ (4)
i, g	$1/2+x1, 0, 0$ (4)	f, e	$1/3, 2/3, z1-z2$ (2)
	$x1, 1/2, 0$ (4)		$1/3, 2/3, 1/2+z1-z2$ (2)
	$1/2+x1, 0, 1/2$ (4)		$1/3, 2/3, z1+z2$ (2)
	$x1, 1/2, 1/2$ (4)		$1/3, 2/3, 1/2+z1+z2$ (2)
i, f	$2/3+x1, 1/3, -z2$ (2)	f, d	$0, 0, 1/4+z1$ (2)
	$1/3+x1, 2/3, 1/2-z2$ (2)		$2/3, 1/3, 3/4+z1$ (1)
i, e	$x1, 0, -z2$ (4)		$0, 0, 1/4-z1$ (2)
	$x1, 0, 1/2-z2$ (4)		$2/3, 1/3, 3/4-z1$ (1)

- f, c  $0, 0, 3/4+z1$  (2)  
 $2/3, 1/3, 1/4+z1$  (1)  
 $0, 0, 3/4-z1$  (2)  
 $2/3, 1/3, 1/4-z1$  (1)
- f, b  $1/3, 2/3, 3/4+z1$  (2)  
 $1/3, 2/3, 1/4+z1$  (2)
- f, a  $1/3, 2/3, z1$  (2)  
 $1/3, 2/3, 1/2+z1$  (2)
- e, e  $0, 0, z1-z2$  (4)  
 $0, 0, 1/2+z1-z2$  (4)  
 $0, 0, z1+z2$  (4)  
 $0, 0, 1/2+z1+z2$  (4)
- e, d  $2/3, 1/3, 1/4+z1$  (2)  
 $1/3, 2/3, 3/4+z1$  (2)
- e, c  $2/3, 1/3, 3/4+z1$  (2)  
 $1/3, 2/3, 1/4+z1$  (2)
- e, b  $0, 0, 3/4+z1$  (4)  
 $0, 0, 1/4+z1$  (4)
- e, a  $0, 0, z1$  (4)  
 $0, 0, 1/2+z1$  (4)
- d, c  $0, 0, 1/2$  (4)  
 $2/3, 1/3, 0$  (2)
- d, b  $1/3, 2/3, 1/2$  (2)  
 $1/3, 2/3, 0$  (2)
- d, a  $1/3, 2/3, 3/4$  (2)
- c, b  $1/3, 2/3, 0$  (2)  
 $1/3, 2/3, 1/2$  (2)
- c, a  $1/3, 2/3, 1/4$  (2)
- b, a  $0, 0, 1/4$  (4)