

Trigonal

$\bar{3}1m$

D_{3d}^1

$P\bar{3}1m$

Patterson symmetry $P\bar{3}1m$

$P\bar{3}12/m$

No. 162

Origin at centre ($\bar{3}1m$)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry,
Coordinates

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

12	l	1	x,y,z; -y,x-y,z; etc. 0, 0, 0 (12) 0, -x+2y, 2z (2) y, 2y, 0 (2)	x+y, -x+2y, 0 (2) 2x, 2y, 2z (1) 2x, x, 0 (2)	x+y, x+y, 2z (2) x-y, x, 2z (2)	2x-y, 0, 2z (2) x-y, -x+y, 0 (2)
6	k	..m	x,0,z; 0,x,z; etc. 0, 0, 0 (6)	x, -x, 0 (2)	x, x, 2z (2)	2x, 0, 2z (1)
6	j	..2	x,-x,1/2; x,2x,1/2; etc. 0, 0, 0 (6)	0, -3x, 0 (2)	2x, -2x, 0 (1)	2x, x, 0 (2)
6	i	..2	x,-x,0; x,2x,0; etc. 0, 0, 0 (6)	0, -3x, 0 (2)	2x, -2x, 0 (1)	2x, x, 0 (2)
4	h	3..	1/3,2/3,z; 1/3,2/3,-z; etc. 0, 0, 0 (4)	0, 0, 2z (2)	2/3, 1/3, 2z (1)	2/3, 1/3, 0 (2)
3	g	..2/m	1/2,0,1/2; 0,1/2,1/2; etc. 0, 0, 0 (3)	1/2, 1/2, 0 (2)		
3	f	..2/m	1/2,0,0; 0,1/2,0; etc. 0, 0, 0 (3)	1/2, 1/2, 0 (2)		
2	e	3.m	0,0,z; 0,0,-z 0, 0, 0 (2)	0, 0, 2z (1)		
2	d	3.2	1/3,2/3,1/2; 2/3,1/3,1/2 0, 0, 0 (2)	2/3, 1/3, 0 (1)		
2	c	3.2	1/3,2/3,0; 2/3,1/3,0 0, 0, 0 (2)	2/3, 1/3, 0 (1)		
1	b	$\bar{3}.m$	0,0,1/2 0, 0, 0 (1)			
1	a	$\bar{3}.m$	0,0,0 0, 0, 0 (1)			

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

l, l
 $x1-x2, y1-y2, z1-z2 (2)$
 $x1+y2, y1-x2+y2, z1-z2 (2)$
 $x1+x2-y2, y1+x2, z1-z2 (2)$
 $x1+y2, y1+x2, z1+z2 (2)$
 $x1+x2-y2, y1-y2, z1+z2 (2)$

$x1-x2, y1-x2+y2, z1+z2 (2)$
 $x1+x2, y1+y2, z1+z2 (2)$
 $x1-y2, y1+x2-y2, z1+z2 (2)$
 $x1-x2+y2, y1-x2, z1+z2 (2)$
 $x1-y2, y1-x2, z1-z2 (2)$

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

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