Trigonal $\bar{3}m1$ D_{3d}^{3} $P\,\bar{3}\,m\,1$

Patterson symmetry $P\ \bar{3}\ m\ 1$ $P\ \bar{3}\ 2/m\ 1$ No. 164

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

Positions

Multiplicity, Wyckoff letter, Site symmetry, Coordinates

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

12	j	1	x,y,z; -y,x-y,z; etc.		
			0, 0, 0 (12)	***x+y, -x+2y, 0 (2)***	***x-y, -x+y, 2z (2)***	***y, 2y, 2z (2)***
			2x, x, 2z (2)	***2x, 2y, 2z (1)***	***x-y, x, 2z (2)***	***x+y, x+y, 0 (2)***
			2x-y, 0, 0 (2)	***0, -x+2y, 0 (2)***		
6	i	. *m* .	x,-x,z; x,2x,z; etc.		
			0, 0, 0 (6)	***0, -3x, 0 (2)***	***2x, -2x, 2z (1)***	***-x, -2x, 2z (2)***
6	h	. 2 .	x,0,1/2; 0,x,1/2; etc.		
			0, 0, 0 (6)	***x, -x, 0 (2)***	***2x, 0, 0 (1)***	***x, x, 0 (2)***
6	g	. 2 .	x,0,0; 0,x,0; etc.		
			0, 0, 0 (6)	***x, -x, 0 (2)***	***2x, 0, 0 (1)***	***x, x, 0 (2)***
3	f	. 2/*m* .	1/2,0,1/2; 0,1/2,1/2; etc.		
			0, 0, 0 (3)	***1/2, 1/2, 0 (2)***		
3	e	. 2/*m* .	1/2,0,0; 0,1/2,0; etc.		
			0, 0, 0 (3)	***1/2, 1/2, 0 (2)***		
2	d	3 *m* .	1/3,2/3,z; 2/3,1/3,-z		
			0, 0, 0 (2)	***2/3, 1/3, 2z (1)***		
2	c	3 *m* .	0,0,z; 0,0,-z		
			0, 0, 0 (2)	***0, 0, 2z (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	
j, j	***x1-x2, y1-y2, z1-z2 (2)***		***x1+y2, y1+x2, z1-z2 (2)***
	x1+y2, y1-x2+y2, z1-z2 (2)		***x1+x2-y2, y1-y2, z1-z2 (2)***
	x1+x2-y2, y1+x2, z1-z2 (2)		***x1-x2, y1-x2+y2, z1-z2 (2)***
	x1-y2, y1-x2, z1+z2 (2)	j, i	***x1-x2, y1+x2, z1-z2 (2)***
	x1-x2+y2, y1+y2, z1+z2 (2)		***x1-x2, y1-2x2, z1-z2 (2)***
	x1+x2, y1+x2-y2, z1+z2 (2)		***x1+2x2, y1+x2, z1-z2 (2)***
	x1+x2, y1+y2, z1+z2 (2)		***x1+x2, y1-x2, z1+z2 (2)***
	x1-y2, y1+x2-y2, z1+z2 (2)		***x1-2x2, y1-x2, z1+z2 (2)***
	x1-x2+y2, y1-x2, z1+z2 (2)		***x1+x2, y1+2x2, z1+z2 (2)***

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

		1/3, 2/3, z1+z2 (1)
		1/3, 2/3, -z1+z2 (1)
		1/3, 2/3, -z1-z2 (1)
d,	b	***1/3, 2/3, 1/2+z1 (1)***
		1/3, 2/3, 1/2-z1 (1)
d,	a	***1/3, 2/3, z1 (1)***
		1/3, 2/3, -z1 (1)
c,	c	***0, 0, z1-z2 (2)***
		0, 0, z1+z2 (2)
c,	b	***0, 0, 1/2+z1 (2)***
c,	a	***0, 0, z1 (2)***
b,	a	***0, 0, 1/2 (2)***