$R\bar{3}m$ D_{3d}^{5} $\bar{3}m$ Trigonal

No. 166 $R\ \bar{3}\ 2/m$ Patterson symmetry $R\ \bar{3}\ m$

Hexagonal axes

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

Positions

Multiplicity, Wyckoff letter, Site symmetry, Coordinates

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

36	i	1	x,y,z; -y,x-y,z; etc.		
			0, 0, 0 (36)	***x+y, -x+2y, 0 (6)***	***x-y, -x+y, 2z (6)***	***y, 2y, 2z (6)***
			2x, x, 2z (6)	***2x, 2y, 2z (3)***	***x-y, x, 2z (6)***	***x+y, x+y, 0 (6)***
			2x-y, 0, 0 (6)	***0, -x+2y, 0 (6)***		
18	h	. *m*	x,-x,z; x,2x,z; etc.		
			0, 0, 0 (18)	***0, -3x, 0 (6)***	***2x, -2x, 2z (3)***	***-x, -2x, 2z (6)***
18	g	. 2	x,0,1/2; 0,x,1/2; etc.		
			0, 0, 0 (18)	***x, -x, 0 (6)***	***2x, 0, 0 (3)***	***x, x, 0 (6)***
18	f	. 2	x,0,0; 0,x,0; etc.		
			0, 0, 0 (18)	***x, -x, 0 (6)***	***2x, 0, 0 (3)***	***x, x, 0 (6)***
9	e	. 2/*m*	1/2,0,0; 0,1/2,0; etc.		
			0, 0, 0 (9)	***1/2, 1/2, 0 (6)***		
9	d	. 2/*m*	1/2,0,1/2; 0,1/2,1/2; etc.		
			0, 0, 0 (9)	***1/2, 1/2, 0 (6)***		
6	c	3 *m*	0,0,z; 0,0,-z; etc.		
			0, 0, 0 (6)	***0, 0, 2z (3)***		
3	b	$\bar{3}m$	0,0,1/2; etc.		
			0, 0, 0 (3)			
3	a	$\bar{3}m$	0,0,0; etc.		
			0, 0, 0 (3)			

Vectors between two sets of unique atoms

Wyckoff letters		
i,	i	***x1-x2, y1-y2, z1-z2 (6)***
		x1+y2, y1-x2+y2, z1-z2 (6)
		x1+x2-y2, y1+x2, z1-z2 (6)
		x1-y2, y1-x2, z1+z2 (6)
		x1-x2+y2, y1+y2, z1+z2 (6)
		x1+x2, y1+x2-y2, z1+z2 (6)
		x1+x2, y1+y2, z1+z2 (6)
		x1-y2, y1+x2-y2, z1+z2 (6)
		x1-x2+y2, y1-x2, z1+z2 (6)
		x1+y2, y1+x2, z1-z2 (6)
		x1+x2-y2, y1-y2, z1-z2 (6)
		x1-x2, y1-x2+y2, z1-z2 (6)

Wyckoff letters		
i,	h	***x1-x2, y1+x2, z1-z2 (6)***
		x1-x2, y1-2x2, z1-z2 (6)
		x1+2x2, y1+x2, z1-z2 (6)
		x1+x2, y1-x2, z1+z2 (6)
		x1-2x2, y1-x2, z1+z2 (6)
		x1+x2, y1+2x2, z1+z2 (6)
i,	g	***x1-x2, y1, 1/2+z1 (6)***
		x1, y1-x2, 1/2+z1 (6)
		x1+x2, y1+x2, 1/2+z1 (6)
		x1+x2, y1, 1/2+z1 (6)
		x1, y1+x2, 1/2+z1 (6)
		x1-x2, y1-x2, 1/2+z1 (6)

Hexagonal axes

i,	f	***x1-x2, y1, z1 (6)***
		x1, y1-x2, z1 (6)
		x1+x2, y1+x2, z1 (6)
		x1+x2, y1, z1 (6)
		x1, y1+x2, z1 (6)
		x1-x2, y1-x2, z1 (6)
i,	e	***1/2+x1, y1, z1 (6)***
		x1, 1/2+y1, z1 (6)
		1/2+x1, 1/2+y1, z1 (6)
i,	d	***1/2+x1, y1, 1/2+z1 (6)***
		x1, 1/2+y1, 1/2+z1 (6)
		1/2+x1, 1/2+y1, 1/2+z1 (6)
i,	c	***x1, y1, z1-z2 (6)***
		x1, y1, z1+z2 (6)
i,	b	***x1, y1, 1/2+z1 (6)***
i,	a	***x1, y1, z1 (6)***
h,	h	***x1-x2, -x1+x2, z1-z2 (6)***
		x1-x2, -x1-2x2, z1-z2 (6)
		x1+x2, -x1-x2, z1+z2 (6)
		x1-2x2, -x1-x2, z1+z2 (6)
h,	g	***x1-x2, -x1, 1/2+z1 (6)***
		x1, -x1-x2, 1/2+z1 (6)
		x1+x2, -x1+x2, 1/2+z1 (6)
h,	f	***x1-x2, -x1, z1 (6)***
		x1, -x1-x2, z1 (6)
		x1+x2, -x1+x2, z1 (6)
h,	e	***1/2+x1, -x1, z1 (6)***
		1/2+x1, 1/2-x1, z1 (6)
h,	d	***1/2+x1, -x1, 1/2+z1 (6)***
		1/2+x1, 1/2-x1, 1/2+z1 (6)
h,	c	***x1, -x1, z1-z2 (6)***
		x1, -x1, z1+z2 (6)
h,	b	***x1, -x1, 1/2+z1 (6)***
h,	a	***x1, -x1, z1 (6)***
g,	g	***x1-x2, 0, 0 (6)***
		x1, -x2, 0 (6)
		x1+x2, 0, 0 (6)
		x1, x2, 0 (6)
g,	f	***x1-x2, 0, 1/2 (6)***
		x1, -x2, 1/2 (6)
		x1+x2, 0, 1/2 (6)
		x1, x2, 1/2 (6)
g,	e	***1/2+x1, 0, 1/2 (6)***
		x1, 1/2, 1/2 (6)
g,	d	***1/2+x1, 0, 0 (6)***
		x1, 1/2, 0 (6)
g,	c	***x1, 0, 1/2-z2 (6)***
g,	b	***x1, 0, 0 (6)***
g,	a	***x1, 0, 1/2 (6)***
f,	f	***x1-x2, 0, 0 (6)***
		x1, -x2, 0 (6)
		x1+x2, 0, 0 (6)
		x1, x2, 0 (6)
f,	e	***1/2+x1, 0, 0 (6)***
		x1, 1/2, 0 (6)
f,	d	***1/2+x1, 0, 1/2 (6)***
		x1, 1/2, 1/2 (6)
f,	c	***x1, 0, -z2 (6)***
f,	b	***x1, 0, 1/2 (6)***
f,	a	***x1, 0, 0 (6)***
e,	d	***0, 0, 1/2 (18)***
		1/2, 1/2, 1/2 (12)
e,	c	***1/2, 0, -z2 (6)***
e,	b	***1/2, 0, 1/2 (6)***
e,	a	***1/2, 0, 0 (6)***
d,	c	***1/2, 0, 1/2-z2 (6)***
d,	b	***1/2, 0, 0 (6)***
d,	a	***1/2, 0, 1/2 (6)***
c,	c	***0, 0, z1-z2 (6)***
		0, 0, z1+z2 (6)
c,	b	***0, 0, 1/2+z1 (6)***
c,	a	***0, 0, z1 (6)***
b,	a	***0, 0, 1/2 (6)***