$Pmna$ D_{2h}^{7} mmm Orthorhombic

No. 53 $P\ 2/m\ 2/n\ 2_1/a$ Patterson symmetry $P\ m\ m\ m$

Origin at centre (2/*m*) at 2/*m n* 1

Positions

Multiplicity, Wyckoff letter, Site symmetry, Coordinates		Patterson peaks (U, V, W (Multiplicity))			
8 i 1	x,y,z; 1/2-x,-y,1/2+z; etc.				
		0, 0, 0 (8)	***1/2+2x, 2y, 1/2 (2)***	***1/2+2x, 0, 1/2+2z (2)***	***0, 2y, 2z (2)***
		2x, 2y, 2z (1)	***1/2, 0, 1/2+2z (4)***	***1/2, 2y, 1/2 (4)***	***2x, 0, 0 (4)***
4 h *m* . .	0,y,z; 1/2,-y,1/2+z; etc.				
		0, 0, 0 (4)	***1/2, 2y, 1/2 (2)***	***1/2, 0, 1/2+2z (2)***	***0, 2y, 2z (1)***
4 g . 2 .	1/4,y,1/4; 1/4,-y,3/4; etc.				
		0, 0, 0 (4)	***0, 2y, 1/2 (2)***	***1/2, 2y, 1/2 (2)***	***1/2, 0, 0 (4)***
4 f 2 . .	x,1/2,0; 1/2-x,1/2,1/2; etc.				
		0, 0, 0 (4)	***1/2+2x, 0, 1/2 (2)***	***2x, 0, 0 (2)***	***1/2, 0, 1/2 (4)***
4 e 2 . .	x,0,0; 1/2-x,0,1/2; etc.				
		0, 0, 0 (4)	***1/2+2x, 0, 1/2 (2)***	***2x, 0, 0 (2)***	***1/2, 0, 1/2 (4)***
2 d 2/*m* . .	0,1/2,0; 1/2,1/2,1/2				
		0, 0, 0 (2)	***1/2, 0, 1/2 (2)***		
2 c 2/*m* . .	1/2,1/2,0; 0,1/2,1/2				
		0, 0, 0 (2)	***1/2, 0, 1/2 (2)***		
2 b 2/*m* . .	1/2,0,0; 0,0,1/2				
		0, 0, 0 (2)	***1/2, 0, 1/2 (2)***		
2 a 2/*m* . .	0,0,0; 1/2,0,1/2				
		0, 0, 0 (2)	***1/2, 0, 1/2 (2)***		

Vectors between two sets of unique atoms

Wyckoff letters	
i, i	***x1-x2, y1-y2, z1-z2 (2)***
	1/2+x1+x2, y1+y2, 1/2+z1-z2 (2)
	1/2+x1+x2, y1-y2, 1/2+z1+z2 (2)
	x1-x2, y1+y2, z1+z2 (2)
	x1+x2, y1+y2, z1+z2 (2)
	1/2+x1-x2, y1-y2, 1/2+z1+z2 (2)
	1/2+x1-x2, y1+y2, 1/2+z1-z2 (2)
	x1+x2, y1-y2, z1-z2 (2)
i, h	***x1, y1-y2, z1-z2 (2)***
	1/2+x1, y1+y2, 1/2+z1-z2 (2)
	1/2+x1, y1-y2, 1/2+z1+z2 (2)
	x1, y1+y2, z1+z2 (2)
i, g	***3/4+x1, y1-y2, 3/4+z1 (1)***
	3/4+x1, y1+y2, 1/4+z1 (1)
	1/4+x1, y1+y2, 1/4+z1 (1)
	1/4+x1, y1-y2, 3/4+z1 (1)
	3/4-x1, -y1+y2, 3/4-z1 (1)
	3/4-x1, -y1-y2, 1/4-z1 (1)
	1/4-x1, -y1-y2, 1/4-z1 (1)
	1/4-x1, -y1+y2, 3/4-z1 (1)
i, f	***x1-x2, 1/2+y1, z1 (2)***
	1/2+x1+x2, 1/2+y1, 1/2+z1 (2)
	x1+x2, 1/2+y1, z1 (2)
	1/2+x1-x2, 1/2+y1, 1/2+z1 (2)
i, e	***x1-x2, y1, z1 (2)***
	1/2+x1+x2, y1, 1/2+z1 (2)

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