

Orthorhombic

 mmm D_{2h}^{17} $Cmcm$ Patterson symmetry $Cmcm$ $C 2/m 2/c 2_1/m$

No. 63

Origin at centre ($2/m$) at $2/m c 2_1$

Positions

Multiplicity,
Wyckoff letter,
Site symmetry,
Coordinates

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

16	h 1	x,y,z; -x,-y,1/2+z; etc. $0, 0, 0$ (16) $2x, 2y, 2z$ (2)	$2x, 2y, 1/2$ (4) $0, 0, 1/2+2z$ (8)	$2x, 0, 1/2+2z$ (4) $0, 2y, 1/2$ (8)	$0, 2y, 2z$ (4) $2x, 0, 0$ (8)
8	g . . m	x,y,1/4; -x,-y,3/4; etc. $0, 0, 0$ (8)	$2x, 2y, 1/2$ (2)	$2x, 0, 0$ (4)	$0, 2y, 1/2$ (4)
8	f m . .	0,y,z; 0,-y,1/2+z; etc. $0, 0, 0$ (8)	$0, 2y, 1/2$ (4)	$0, 0, 1/2+2z$ (4)	$0, 2y, 2z$ (2)
8	e 2 . .	x,0,0; -x,0,1/2; etc. $0, 0, 0$ (8)	$2x, 0, 1/2$ (4)	$2x, 0, 0$ (4)	$0, 0, 1/2$ (8)
8	d $\bar{1}$	1/4,1/4,0; 3/4,3/4,1/2; etc. $0, 0, 0$ (8)	$1/2, 1/2, 1/2$ (8)	$1/2, 0, 1/2$ (8)	$0, 1/2, 0$ (8)
4	c m 2 m	0,y,1/4; 0,-y,3/4; etc. $0, 0, 0$ (4)	$0, 2y, 1/2$ (2)		
4	b $2/m$. .	0,1/2,0; 0,1/2,1/2; etc. $0, 0, 0$ (4)	$0, 0, 1/2$ (4)		
4	a $2/m$. .	0,0,0; 0,0,1/2; etc. $0, 0, 0$ (4)	$0, 0, 1/2$ (4)		

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

h, h	$x1-x2, y1-y2, z1-z2$ (4) $x1+x2, y1+y2, 1/2+z1-z2$ (4) $x1+x2, y1-y2, 1/2+z1+z2$ (4) $x1-x2, y1+y2, z1+z2$ (4) $x1+x2, y1+y2, z1+z2$ (4) $x1-x2, y1-y2, 1/2+z1+z2$ (4) $x1-x2, y1+y2, 1/2+z1-z2$ (4) $x1+x2, y1-y2, z1-z2$ (4)	h, f	$-x1+x2, -y1-y2, 1/4-z1$ (2) $x1, y1-y2, z1-z2$ (4) $x1, y1+y2, 1/2+z1-z2$ (4) $x1, y1-y2, 1/2+z1+z2$ (4) $x1, y1+y2, z1+z2$ (4)
h, g	$x1-x2, y1-y2, 3/4+z1$ (2) $x1+x2, y1+y2, 1/4+z1$ (2) $x1+x2, y1-y2, 3/4+z1$ (2) $x1-x2, y1+y2, 1/4+z1$ (2) $-x1+x2, -y1+y2, 3/4-z1$ (2) $-x1-x2, -y1-y2, 1/4-z1$ (2) $-x1-x2, -y1+y2, 3/4-z1$ (2)	h, e	$x1-x2, y1, z1$ (4) $x1+x2, y1, 1/2+z1$ (4) $x1+x2, y1, z1$ (4) $x1-x2, y1, 1/2+z1$ (4)
		h, d	$3/4+x1, 3/4+y1, z1$ (4) $1/4+x1, 1/4+y1, 1/2+z1$ (4) $1/4+x1, 3/4+y1, 1/2+z1$ (4) $3/4+x1, 1/4+y1, z1$ (4)
		h, c	$x1, y1-y2, 3/4+z1$ (2) $x1, y1+y2, 1/4+z1$ (2)

	$-x1, -y1+y2, 3/4-z1$ (2)				
	$-x1, -y1-y2, 1/4-z1$ (2)				
h, b	$x1, 1/2+y1, z1$ (4)			e, a	$x1, 0, 0$ (8)
	$x1, 1/2+y1, 1/2+z1$ (4)				$x1, 0, 1/2$ (8)
h, a	$x1, y1, z1$ (4)			d, c	$1/4, 1/4-y2, 3/4$ (4)
	$x1, y1, 1/2+z1$ (4)			d, b	$1/4, 3/4, 0$ (8)
g, g	$x1-x2, y1-y2, 0$ (4)				$1/4, 3/4, 1/2$ (8)
	$x1+x2, y1+y2, 1/2$ (4)			d, a	$1/4, 1/4, 0$ (8)
	$x1+x2, y1-y2, 0$ (4)				$1/4, 1/4, 1/2$ (8)
	$x1-x2, y1+y2, 1/2$ (4)			c, c	$0, y1-y2, 0$ (4)
g, f	$x1, y1-y2, 1/4-z2$ (2)				$0, y1+y2, 1/2$ (4)
	$x1, y1+y2, 3/4-z2$ (2)			c, b	$0, 1/2+y1, 1/4$ (4)
	$-x1, -y1+y2, 1/4+z2$ (2)			c, a	$0, y1, 1/4$ (4)
	$-x1, -y1-y2, 3/4+z2$ (2)			b, a	$0, 1/2, 0$ (8)
g, e	$x1-x2, y1, 1/4$ (4)				$0, 1/2, 1/2$ (8)
	$x1+x2, y1, 3/4$ (4)				
g, d	$3/4+x1, 3/4+y1, 1/4$ (4)				
	$1/4+x1, 3/4+y1, 3/4$ (4)				
g, c	$x1, y1-y2, 0$ (4)				
	$x1, y1+y2, 1/2$ (4)				
g, b	$x1, 1/2+y1, 1/4$ (4)				
g, a	$x1, y1, 1/4$ (4)				
f, f	$0, y1-y2, z1-z2$ (4)				
	$0, y1+y2, 1/2+z1-z2$ (4)				
	$0, y1-y2, 1/2+z1+z2$ (4)				
	$0, y1+y2, z1+z2$ (4)				
f, e	$-x2, y1, z1$ (4)				
	$x2, y1, 1/2+z1$ (4)				
f, d	$3/4, 3/4+y1, z1$ (4)				
	$1/4, 1/4+y1, 1/2+z1$ (4)				
f, c	$0, y1-y2, 3/4+z1$ (2)				
	$0, y1+y2, 1/4+z1$ (2)				
	$0, -y1+y2, 3/4-z1$ (2)				
	$0, -y1-y2, 1/4-z1$ (2)				
f, b	$0, 1/2+y1, z1$ (4)				
	$0, 1/2+y1, 1/2+z1$ (4)				
f, a	$0, y1, z1$ (4)				
	$0, y1, 1/2+z1$ (4)				
e, e	$x1-x2, 0, 0$ (8)				
	$x1+x2, 0, 1/2$ (8)				
	$x1+x2, 0, 0$ (8)				
	$x1-x2, 0, 1/2$ (8)				
e, d	$3/4+x1, 3/4, 0$ (8)				
	$1/4+x1, 1/4, 1/2$ (8)				
e, c	$x1, -y2, 3/4$ (4)				
e, b	$x1, 1/2, 0$ (8)				
	$x1, 1/2, 1/2$ (8)				