

$C2/m$ C_{2h}^3 $2/m$

Monoclinic

No. 12

 $C 1 2/m 1$ Patterson symmetry $C 1 2/m 1$ UNIQUE AXIS b , CELL CHOICE 1Origin at centre ($2/m$)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry,
Coordinates

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

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

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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

UNIQUE AXIS b , CELL CHOICE 1

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