

$Pnma$ D_{2h}^{16} mmm

Orthorhombic

No. 62

 $P 2_1/n 2_1/m 2_1/a$ Patterson symmetry $P m m m$ Origin at $\bar{1}$ on $1 2_1 1$

Positions

Multiplicity,
Wyckoff letter,
Site symmetry,
Coordinates

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

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

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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