

$P 2_1/c$ C_{2h}^5 $2/m$

Monoclinic

No. 14

 $P 1 2_1/c 1$ Patterson symmetry $P 1 2/m 1$ UNIQUE AXIS b , CELL CHOICE 1Origin at $\bar{1}$

Positions

Multiplicity,
Wyckoff letter,
Site symmetry,
Coordinates

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

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

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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