

$I b c a$  $D_{2h}^{27}$  $mmm$ 

Orthorhombic

No. 73

 $I 2_1/b 2_1/c 2_1/a$ Patterson symmetry  $I m m m$ Origin at  $\bar{1}$  at  $c a b$ 

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry,  
Coordinates

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

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

## Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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

e, e      $0, 0, z1-z2$  (8)  
            $0, 1/2, 1/2+z1+z2$  (8)  
            $0, 1/2, z1+z2$  (8)  
            $0, 0, 1/2+z1-z2$  (8)  
 e, d      $3/4, 1/4-y2, z1$  (4)  
            $1/4, 1/4+y2, z1$  (4)  
 e, c      $-x2, 1/4, 3/4+z1$  (4)  
            $x2, 1/4, 1/4+z1$  (4)  
 e, b      $3/4, 0, 3/4+z1$  (8)  
            $1/4, 1/2, 3/4+z1$  (8)  
 e, a      $0, 1/4, z1$  (8)  
            $0, 3/4, 1/2+z1$  (8)  
 d, d      $0, y1-y2, 0$  (8)  
            $0, y1+y2, 1/2$  (8)  
            $1/2, y1+y2, 0$  (8)  
            $1/2, y1-y2, 1/2$  (8)  
 d, c      $1/4-x2, y1, 3/4$  (4)  
            $1/4+x2, y1, 1/4$  (4)  
 d, b      $0, 3/4+y1, 3/4$  (8)  
            $0, 1/4+y1, 1/4$  (8)  
 d, a      $1/4, y1, 0$  (8)  
            $3/4, y1, 1/2$  (8)  
 c, c      $x1-x2, 0, 0$  (8)  
            $1/2+x1+x2, 0, 1/2$  (8)  
            $x1+x2, 0, 1/2$  (8)  
            $1/2+x1-x2, 0, 0$  (8)  
 c, b      $3/4+x1, 3/4, 0$  (8)  
            $3/4+x1, 1/4, 1/2$  (8)  
 c, a      $x1, 0, 1/4$  (8)  
            $1/2+x1, 0, 3/4$  (8)  
 b, a      $1/4, 1/4, 1/4$  (16)