

Monoclinic

 $2/m$  $C_{2h}^6$  $A2/a$ Patterson symmetry  $A 1 1 2/m$  $A 1 1 2/a$ 

No. 15

UNIQUE AXIS  $c$ , CELL CHOICE 1Origin at  $\bar{1}$  on glide plane  $a$ 

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry,  
Coordinates

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

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

## Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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