

$P \bar{1}$  $C_i^1$  $\bar{1}$ 

Triclinic

No. 2

 $P \bar{1}$ Patterson symmetry  $P \bar{1}$ Origin at  $\bar{1}$ 

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry,  
Coordinates

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

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

## Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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

e, d	$0, 1/2, 0$ (2)
e, c	$1/2, 0, 0$ (2)
e, b	$1/2, 1/2, 1/2$ (2)
e, a	$1/2, 1/2, 0$ (2)
d, c	$1/2, 1/2, 0$ (2)
d, b	$1/2, 0, 1/2$ (2)
d, a	$1/2, 0, 0$ (2)
c, b	$0, 1/2, 1/2$ (2)
c, a	$0, 1/2, 0$ (2)
b, a	$0, 0, 1/2$ (2)