

$Pa\bar{3}$  $T_h^6$  $m\bar{3}$ 

Cubic

No. 205

 $P 2_1/a \bar{3}$ Patterson symmetry  $P m \bar{3}$ Origin at centre ( $\bar{3}$ )

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry,  
Coordinates

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

24	d	1	x,y,z; 1/2-x,-y,1/2+z; etc. <b>0, 0, 0 (24)</b> <b>1/2, 1/2+2y, 2z (2)</b> <b>1/2+x+z, x+y, 1/2-y+z (2)</b> <b>1/2, 0, 1/2+2z (4)</b> <b>x+z, x+y, y+z (2)</b> <b>x-z, 1/2+x+y, 1/2-y+z (2)</b>	<b>1/2+2x, 2y, 1/2 (2)</b> <b>x-z, -x+y, -y+z (2)</b> <b>x+z, 1/2-x+y, 1/2+y+z (2)</b> <b>0, 1/2+2y, 1/2 (4)</b> <b>1/2+x+z, 1/2-x+y, -y+z (2)</b>	<b>2x, 1/2, 1/2+2z (2)</b> <b>1/2+x-z, 1/2+x+y, y+z (2)</b> <b>2x, 2y, 2z (1)</b> <b>1/2+2x, 1/2, 0 (4)</b> <b>1/2+x-z, -x+y, 1/2+y+z (2)</b>
8	c	. 3 .	x,x,x; 1/2-x,-x,1/2+x; etc. <b>0, 0, 0 (8)</b> <b>1/2, 0, 1/2+2x (4)</b>	<b>1/2+2x, 2x, 1/2 (2)</b>	<b>2x, 2x, 2x (1)</b>
4	b	. $\bar{3}$ .	1/2,1/2,1/2; 0,1/2,0; etc. <b>0, 0, 0 (4)</b>	<b>1/2, 0, 1/2 (4)</b>	
4	a	. $\bar{3}$ .	0,0,0; 1/2,0,1/2; etc. <b>0, 0, 0 (4)</b>	<b>1/2, 0, 1/2 (4)</b>	

## Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

d,	d	<b>x1-x2, y1-y2, z1-z2 (2)</b> <b>1/2+x1+x2, y1+y2, 1/2+z1-z2 (2)</b> <b>x1+x2, 1/2+y1-y2, 1/2+z1+z2 (2)</b> <b>1/2+x1-x2, 1/2+y1+y2, z1+z2 (2)</b> <b>x1-z2, y1-x2, z1-y2 (2)</b> <b>1/2+x1-z2, 1/2+y1+x2, z1+y2 (2)</b> <b>1/2+x1+z2, y1+x2, 1/2+z1-y2 (2)</b> <b>x1+z2, 1/2+y1-x2, 1/2+z1+y2 (2)</b> <b>x1-y2, y1-z2, z1-x2 (2)</b> <b>x1+y2, 1/2+y1-z2, 1/2+z1+x2 (2)</b> <b>1/2+x1-y2, 1/2+y1+z2, z1+x2 (2)</b> <b>1/2+x1+y2, y1+z2, 1/2+z1-x2 (2)</b> <b>x1+x2, y1+y2, z1+z2 (2)</b> <b>1/2+x1-x2, y1-y2, 1/2+z1+z2 (2)</b> <b>x1-x2, 1/2+y1+y2, 1/2+z1-z2 (2)</b> <b>1/2+x1+x2, 1/2+y1-y2, z1-z2 (2)</b> <b>x1+z2, y1+x2, z1+y2 (2)</b> <b>1/2+x1+z2, 1/2+y1-x2, z1-y2 (2)</b> <b>1/2+x1-z2, y1-x2, 1/2+z1+y2 (2)</b>		
d,	c	<b>x1-x2, y1-x2, z1-x2 (2)</b> <b>1/2+x1+x2, y1+x2, 1/2+z1-x2 (2)</b> <b>x1+x2, 1/2+y1-x2, 1/2+z1+x2 (2)</b> <b>1/2+x1-x2, 1/2+y1+x2, z1+x2 (2)</b> <b>x1+x2, y1+x2, z1+x2 (2)</b> <b>1/2+x1-x2, y1-x2, 1/2+z1+x2 (2)</b> <b>x1-x2, 1/2+y1+x2, 1/2+z1-x2 (2)</b> <b>1/2+x1+x2, 1/2+y1-x2, z1-x2 (2)</b>		
d,	b	<b>1/2+x1, 1/2+y1, 1/2+z1 (2)</b> <b>x1, 1/2+y1, z1 (2)</b> <b>1/2+x1, y1, z1 (2)</b> <b>x1, y1, 1/2+z1 (2)</b>		
d,	a	<b>x1, y1, z1 (2)</b> <b>1/2+x1, y1, 1/2+z1 (2)</b>		

- $x1, 1/2+y1, 1/2+z1$  (2)  
 $1/2+x1, 1/2+y1, z1$  (2)  
 c, c  $x1-x2, x1-x2, x1-x2$  (2)  
 $1/2+x1+x2, x1+x2, 1/2+x1-x2$  (2)  
 $x1+x2, x1+x2, x1+x2$  (2)  
 $1/2+x1-x2, x1-x2, 1/2+x1+x2$  (2)  
 c, b  $1/2+x1, 1/2+x1, 1/2+x1$  (2)  
 $x1, 1/2+x1, x1$  (2)  
 c, a  $x1, x1, x1$  (2)  
 $1/2+x1, x1, 1/2+x1$  (2)  
 b, a  $1/2, 1/2, 1/2$  (8)  
 $0, 1/2, 0$  (8)