

Tetragonal

 $4/mmm$  $D_{4h}^{13}$  $P4_2/mbc$ Patterson symmetry  $P4/m m m$  $P4_2/m 2_1/b 2/c$ 

No. 135

Origin at centre ( $2/m$ ) at  $4_2/m 1 n$ 

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry,  
Coordinates

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

16	i	1	x,y,z; -x,-y,z; etc.				
			$0, 0, 0$ (16)	$2x, 2y, 0$ (2)		$x+y, -x+y, 1/2$ (4)	
			$1/2+2x, 1/2, 2z$ (2)	$1/2, 1/2+2y, 2z$ (2)		$1/2+x-y, 1/2-x+y, 1/2+2z$ (2)	
			$1/2+x+y, 1/2+x+y, 1/2+2z$ (2)	$2x, 2y, 2z$ (1)		$0, 0, 2z$ (8)	
			$x-y, x+y, 1/2+2z$ (2)	$1/2, 1/2+2y, 0$ (4)		$1/2+2x, 1/2, 0$ (4)	
			$1/2+x+y, 1/2+x+y, 1/2$ (4)	$1/2+x-y, 1/2-x+y, 1/2$ (4)			
8	h	$m..$	x,y,0; -x,-y,0; etc.				
			$0, 0, 0$ (8)	$2x, 2y, 0$ (1)		$x+y, -x+y, 1/2$ (2)	
			$1/2+2x, 1/2, 0$ (2)	$1/2, 1/2+2y, 0$ (2)		$1/2+x-y, 1/2-x+y, 1/2$ (2)	
			$1/2+x+y, 1/2+x+y, 1/2$ (2)				
8	g	$..2$	x,1/2+x,1/4; -x,1/2-x,1/4; etc.				
			$0, 0, 0$ (8)	$2x, 2x, 0$ (2)	$1/2+2x, 1/2, 1/2$ (4)	$2x, 2x, 1/2$ (2)	
			$0, 0, 1/2$ (8)	$1/2, 1/2+2x, 0$ (4)			
8	f	$2..$	0,1/2,z; 1/2,0,1/2+z; etc.				
			$0, 0, 0$ (8)	$1/2, 1/2, 1/2$ (8)	$1/2, 1/2, 2z$ (4)	$0, 0, 1/2+2z$ (4)	
			$0, 0, 2z$ (4)	$1/2, 1/2, 1/2+2z$ (4)	$1/2, 1/2, 0$ (8)	$0, 0, 1/2$ (8)	
8	e	$2..$	0,0,z; 0,0,1/2+z; etc.				
			$0, 0, 0$ (8)	$0, 0, 1/2$ (8)	$1/2, 1/2, 2z$ (4)	$1/2, 1/2, 1/2+2z$ (4)	
			$0, 0, 2z$ (4)	$0, 0, 1/2+2z$ (4)	$1/2, 1/2, 0$ (8)	$1/2, 1/2, 1/2$ (8)	
4	d	$2.22$	0,1/2,1/4; 1/2,0,3/4; etc.				
			$0, 0, 0$ (4)	$1/2, 1/2, 1/2$ (4)	$0, 0, 1/2$ (4)	$1/2, 1/2, 0$ (4)	
4	c	$2/m..$	0,1/2,0; 1/2,0,1/2; etc.				
			$0, 0, 0$ (4)	$1/2, 1/2, 1/2$ (4)	$1/2, 1/2, 0$ (4)	$0, 0, 1/2$ (4)	
4	b	$\bar{4}..$	0,0,1/4; 0,0,3/4; etc.				
			$0, 0, 0$ (4)	$0, 0, 1/2$ (4)	$1/2, 1/2, 1/2$ (4)	$1/2, 1/2, 0$ (4)	
4	a	$2/m..$	0,0,0; 0,0,1/2; etc.				
			$0, 0, 0$ (4)	$0, 0, 1/2$ (4)	$1/2, 1/2, 0$ (4)	$1/2, 1/2, 1/2$ (4)	

## Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

i, i	$x1-x2, y1-y2, z1-z2$ (2)	$1/2+x1-x2, 1/2+y1+y2, z1+z2$ (2)
	$x1+x2, y1+y2, z1-z2$ (2)	$1/2+x1-y2, 1/2+y1-x2, 1/2+z1+z2$ (2)
	$x1+y2, y1-x2, 1/2+z1-z2$ (2)	$1/2+x1+y2, 1/2+y1+x2, 1/2+z1+z2$ (2)
	$x1-y2, y1+x2, 1/2+z1-z2$ (2)	$x1+x2, y1+y2, z1+z2$ (2)
	$1/2+x1+x2, 1/2+y1-y2, z1+z2$ (2)	$x1-x2, y1-y2, z1+z2$ (2)

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

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