

$I4_1/amd$ D_{4h}^{19}

4/mmm

Tetragonal

No. 141

 $I 4_1/a 2/m 2/d$ Patterson symmetry $I 4/m m m$

ORIGIN CHOICE 2

Origin at centre (2/m) at b (2/m, 2₁/n) d , at 0, $-\frac{1}{4}$, $\frac{1}{8}$ from $\bar{4} m 2$ **Positions**Multiplicity,
Wyckoff letter,
Site symmetry,
Coordinates**Patterson peaks (U, V, W (Multiplicity))**

32 i 1	x,y,z; 1/2-x,-y,1/2+z; etc.	$0, 0, 0$ (32)	$1/2+2x, 2y, 1/2$ (4)	$3/4+x+y, 1/4-x+y, 3/4$ (4)
		$1/2+2x, 0, 1/2+2z$ (4)	$0, 2y, 2z$ (4)	$3/4+x-y, 1/4-x+y, 3/4+2z$ (4)
		$3/4+x+y, 3/4+x+y, 1/4+2z$ (4)	$2x, 2y, 2z$ (2)	$1/2, 0, 1/2+2z$ (8)
		$1/4+x-y, 3/4+x+y, 1/4+2z$ (4)	$1/2, 2y, 1/2$ (8)	$2x, 0, 0$ (8)
		$1/4+x+y, 3/4+x+y, 1/4$ (4)	$1/4+x-y, 1/4-x+y, 3/4$ (4)	
16 h . m .	0,y,z; 1/2,-y,1/2+z; etc.	$0, 0, 0$ (16)	$1/2, 2y, 1/2$ (4)	$3/4+y, 1/4+y, 3/4$ (4) $1/2, 0, 1/2+2z$ (4)
		$0, 2y, 2z$ (2)	$3/4-y, 1/4+y, 3/4+2z$ (4)	
16 g . . 2	x,1/4+x,7/8; 1/2-x,3/4-x,3/8; etc.	$0, 0, 0$ (16)	$1/2+2x, 1/2+2x, 1/2$ (4) $2x, 1/2, 3/4$ (4)	$2x, 1/2+2x, 3/4$ (2)
		$1/2, 0, 1/4$ (8)	$0, 2x, 0$ (8)	
16 f . 2 .	x,0,0; 1/2-x,0,1/2; etc.	$0, 0, 0$ (16)	$1/2+2x, 0, 1/2$ (4)	$3/4+x, 1/4-x, 3/4$ (4) $2x, 0, 0$ (4)
		$1/2, 0, 1/2$ (8)	$1/4+x, 3/4+x, 1/4$ (4)	
8 e 2 m m .	0,1/4,z; 0,3/4,1/4+z; etc.	$0, 0, 0$ (8)	$0, 1/2, 3/4$ (4)	$1/2, 0, 1/2+2z$ (2) $1/2, 1/2, 3/4+2z$ (4)
8 d . 2/m .	0,0,1/2; 1/2,0,0; etc.	$0, 0, 0$ (8)	$1/2, 0, 1/2$ (4)	$3/4, 1/4, 3/4$ (4)
8 c . 2/m .	0,0,0; 1/2,0,1/2; etc.	$0, 0, 0$ (8)	$1/2, 0, 1/2$ (4)	$3/4, 1/4, 3/4$ (4)
4 b $\bar{4} m 2$	0,1/4,3/8; 0,3/4,5/8; etc.	$0, 0, 0$ (4)	$0, 1/2, 3/4$ (2)	
4 a $\bar{4} m 2$	0,3/4,1/8; 1/2,3/4,3/8; etc.	$0, 0, 0$ (4)	$1/2, 0, 3/4$ (2)	

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

i, i	$x1-x2, y1-y2, z1-z2$ (4)	$3/4+x1+y2, 3/4+y1+x2, 1/4+z1+z2$ (4)
	$1/2+x1+x2, y1+y2, 1/2+z1-z2$ (4)	$x1+x2, y1+y2, z1+z2$ (4)
	$3/4+x1+y2, 1/4+y1-x2, 3/4+z1-z2$ (4)	$1/2+x1-x2, y1-y2, 1/2+z1+z2$ (4)
	$3/4+x1-y2, 3/4+y1+x2, 1/4+z1-z2$ (4)	$1/4+x1-y2, 3/4+y1+x2, 1/4+z1+z2$ (4)
	$1/2+x1+x2, y1-y2, 1/2+z1+z2$ (4)	$1/4+x1+y2, 1/4+y1-x2, 3/4+z1+z2$ (4)
	$x1-x2, y1+y2, z1+z2$ (4)	$1/2+x1-x2, y1+y2, 1/2+z1-z2$ (4)
	$3/4+x1-y2, 1/4+y1-x2, 3/4+z1+z2$ (4)	$x1+x2, y1-y2, z1-z2$ (4)

ORIGIN CHOICE 2

	$1/4+x1+y2, 3/4+y1+x2, 1/4+z1-z2$ (4)		$1/2, y1+y2, 1/2+z1-z2$ (4)
	$1/4+x1-y2, 1/4+y1-x2, 3/4+z1-z2$ (4)		$3/4+y2, 1/4+y1, 3/4+z1-z2$ (4)
i, h	$x1, y1-y2, z1-z2$ (4)		$1/2, y1-y2, 1/2+z1+z2$ (4)
	$1/2+x1, y1+y2, 1/2+z1-z2$ (4)		$0, y1+y2, z1+z2$ (4)
	$3/4+x1+y2, 1/4+y1, 3/4+z1-z2$ (4)		$3/4-y2, 1/4+y1, 3/4+z1+z2$ (4)
	$3/4+x1-y2, 3/4+y1, 1/4+z1-z2$ (4)	h, g	$-x2, 3/4+y1-x2, 1/8+z1$ (4)
	$1/2+x1, y1-y2, 1/2+z1+z2$ (4)		$1/2+x2, 1/4+y1+x2, 5/8+z1$ (4)
	$x1, y1+y2, z1+z2$ (4)		$x2, 1/4+y1-x2, 7/8+z1$ (4)
	$3/4+x1-y2, 1/4+y1, 3/4+z1+z2$ (4)		$1/2-x2, 3/4+y1+x2, 3/8+z1$ (4)
	$3/4+x1+y2, 3/4+y1, 1/4+z1+z2$ (4)	h, f	$-x2, y1, z1$ (4)
i, g	$x1-x2, 3/4+y1-x2, 1/8+z1$ (4)		$1/2+x2, y1, 1/2+z1$ (4)
	$1/2+x1+x2, 1/4+y1+x2, 5/8+z1$ (4)		$3/4, 1/4+y1-x2, 3/4+z1$ (4)
	$x1+x2, 1/4+y1-x2, 7/8+z1$ (4)		$3/4, 3/4+y1+x2, 1/4+z1$ (4)
	$1/2+x1-x2, 3/4+y1+x2, 3/8+z1$ (4)	h, e	$0, 3/4+y1, z1-z2$ (2)
	$x1+x2, 1/4+y1+x2, 7/8+z1$ (4)		$0, 1/4+y1, 3/4+z1-z2$ (2)
	$1/2+x1-x2, 3/4+y1-x2, 3/8+z1$ (4)		$1/2, 3/4+y1, 1/2+z1+z2$ (2)
	$x1-x2, 3/4+y1+x2, 1/8+z1$ (4)		$1/2, 1/4+y1, 3/4+z1+z2$ (2)
	$1/2+x1+x2, 1/4+y1-x2, 5/8+z1$ (4)		$0, 3/4-y1, -z1+z2$ (2)
i, f	$x1-x2, y1, z1$ (4)		$0, 1/4-y1, 3/4-z1+z2$ (2)
	$1/2+x1+x2, y1, 1/2+z1$ (4)		$1/2, 3/4-y1, 1/2-z1-z2$ (2)
	$3/4+x1, 1/4+y1-x2, 3/4+z1$ (4)		$1/2, 1/4-y1, 3/4-z1-z2$ (2)
	$3/4+x1, 3/4+y1+x2, 1/4+z1$ (4)	h, d	$0, y1, 1/2+z1$ (4)
	$x1+x2, y1, z1$ (4)		$1/2, y1, z1$ (4)
	$1/2+x1-x2, y1, 1/2+z1$ (4)		$3/4, 1/4+y1, 1/4+z1$ (4)
	$1/4+x1, 3/4+y1+x2, 1/4+z1$ (4)	h, c	$0, y1, z1$ (4)
	$1/4+x1, 1/4+y1-x2, 3/4+z1$ (4)		$1/2, y1, 1/2+z1$ (4)
i, e	$x1, 3/4+y1, z1-z2$ (2)		$3/4, 1/4+y1, 3/4+z1$ (4)
	$x1, 1/4+y1, 3/4+z1-z2$ (2)	h, b	$0, 3/4+y1, 5/8+z1$ (4)
	$1/2+x1, 3/4+y1, 1/2+z1+z2$ (2)		$0, 1/4+y1, 3/8+z1$ (4)
	$1/2+x1, 1/4+y1, 3/4+z1+z2$ (2)	h, a	$0, 1/4+y1, 7/8+z1$ (4)
	$-x1, 3/4-y1, -z1+z2$ (2)		$1/2, 1/4+y1, 5/8+z1$ (4)
	$-x1, 1/4-y1, 3/4-z1+z2$ (2)	g, g	$x1-x2, x1-x2, 0$ (8)
	$1/2-x1, 3/4-y1, 1/2-z1-z2$ (2)		$1/2+x1+x2, 1/2+x1+x2, 1/2$ (8)
	$1/2-x1, 1/4-y1, 3/4-z1-z2$ (2)		$x1+x2, 1/2+x1-x2, 3/4$ (4)
i, d	$x1, y1, 1/2+z1$ (4)		$x1+x2, 1/2+x1+x2, 3/4$ (4)
	$1/2+x1, y1, z1$ (4)		$1/2+x1-x2, x1-x2, 1/4$ (4)
	$3/4+x1, 1/4+y1, 1/4+z1$ (4)		$x1-x2, x1+x2, 0$ (8)
	$3/4+x1, 3/4+y1, 3/4+z1$ (4)	g, f	$x1-x2, 1/4+x1, 7/8$ (4)
i, c	$x1, y1, z1$ (4)		$1/2+x1+x2, 1/4+x1, 3/8$ (4)
	$1/2+x1, y1, 1/2+z1$ (4)		$x1+x2, 1/4+x1, 7/8$ (4)
	$3/4+x1, 1/4+y1, 3/4+z1$ (4)		$1/2+x1-x2, 1/4+x1, 3/8$ (4)
	$3/4+x1, 3/4+y1, 1/4+z1$ (4)	g, e	$x1, x1, 7/8-z2$ (4)
i, b	$x1, 3/4+y1, 5/8+z1$ (4)		$x1, 1/2+x1, 5/8-z2$ (2)
	$x1, 1/4+y1, 3/8+z1$ (4)		$-x1, -x1, 7/8+z2$ (4)
i, a	$x1, 1/4+y1, 7/8+z1$ (4)		$-x1, 1/2-x1, 5/8+z2$ (2)
	$1/2+x1, 1/4+y1, 5/8+z1$ (4)	g, d	$x1, 1/4+x1, 3/8$ (4)
h, h	$0, y1-y2, z1-z2$ (4)		$1/2+x1, 1/4+x1, 7/8$ (4)

ORIGIN CHOICE 2

- g, c $x1, 1/4+x1, 7/8$ (4)
 $1/2+x1, 1/4+x1, 3/8$ (4)
- g, b $x1, x1, 1/2$ (8)
 $x1, 1/2+x1, 1/4$ (4)
- g, a $x1, 1/2+x1, 3/4$ (4)
 $1/2+x1, 1/2+x1, 1/2$ (8)
- f, f $x1-x2, 0, 0$ (8)
 $1/2+x1+x2, 0, 1/2$ (8)
 $3/4+x1, 1/4-x2, 3/4$ (4)
 $x1+x2, 0, 0$ (8)
 $1/2+x1-x2, 0, 1/2$ (8)
 $1/4+x1, 3/4+x2, 1/4$ (4)
- f, e $x1, 3/4, -z2$ (4)
 $x1, 1/4, 3/4-z2$ (2)
 $-x1, 1/4, 3/4+z2$ (2)
- f, d $x1, 0, 1/2$ (8)
 $1/2+x1, 0, 0$ (8)
 $3/4+x1, 1/4, 1/4$ (4)
- f, c $x1, 0, 0$ (8)
 $1/2+x1, 0, 1/2$ (8)
 $3/4+x1, 1/4, 3/4$ (4)
- f, b $x1, 3/4, 5/8$ (4)
- f, a $x1, 1/4, 7/8$ (4)
- e, e $0, 0, z1-z2$ (8)
 $0, 1/2, 3/4+z1-z2$ (4)
 $1/2, 0, 1/2+z1+z2$ (4)
 $1/2, 1/2, 3/4+z1+z2$ (4)
 $1/2, 1/2, 3/4-z1-z2$ (4)
- e, d $0, 1/4, 1/2+z1$ (4)
 $3/4, 1/2, 1/4+z1$ (2)
 $3/4, 1/2, 1/4-z1$ (2)
- e, c $0, 1/4, z1$ (4)
 $3/4, 1/2, 3/4+z1$ (2)
 $3/4, 1/2, 3/4-z1$ (2)
- e, b $0, 0, 5/8+z1$ (4)
 $0, 1/2, 3/8+z1$ (2)
 $0, 0, 5/8-z1$ (4)
 $0, 1/2, 3/8-z1$ (2)
- e, a $0, 1/2, 7/8+z1$ (2)
 $1/2, 1/2, 5/8+z1$ (4)
 $0, 1/2, 7/8-z1$ (2)
 $1/2, 1/2, 5/8-z1$ (4)
- d, c $0, 0, 1/2$ (16)
 $1/2, 0, 0$ (8)
 $3/4, 1/4, 1/4$ (8)
- d, b $0, 3/4, 1/8$ (4)
- d, a $0, 1/4, 3/8$ (4)

- c, b $0, 3/4, 5/8$ (4)
- c, a $0, 1/4, 7/8$ (4)
- b, a $0, 1/2, 1/4$ (4)
 $1/2, 1/2, 0$ (8)