

Tetragonal

 $4/mmm$ D_{4h}^{19} $I4_1/amd$ Patterson symmetry $I 4/m m m$ $I 4_1/a 2/m 2/d$

No. 141

ORIGIN CHOICE 1

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

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

Vectors between two sets of unique atoms

Wyckoff letters

Wyckoff letters

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

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

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

