

$P4_222$

D_4^5

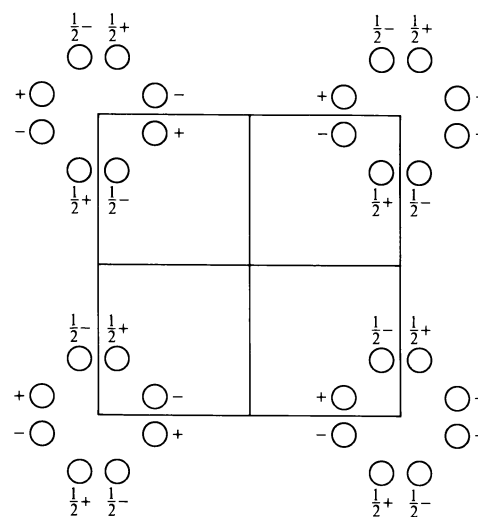
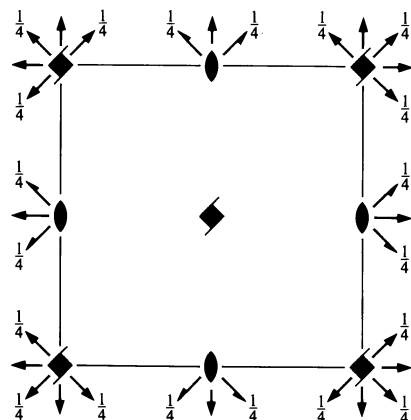
422

Tetragonal

No. 93

$P4_222$

Patterson symmetry $P4/mmm$



Origin at 222 at $4_2 2 1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|-----------------|-----------------|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $0, 0, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $0, 0, z$ |
| (5) 2 $0, y, 0$ | (6) 2 $x, 0, 0$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
8	<i>p</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z}	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z}	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	General: $00l: l = 2n$ Special: as above, plus $0kl: l = 2n$ $0kl: l = 2n$ $hhl: l = 2n$ $hhl: l = 2n$ $hhl: l = 2n$ $hhl: l = 2n$ $hkl: h + k + l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$ $hkl: h + k + l = 2n$ $hkl: h + k + l = 2n$ $hkl: l = 2n$ $hkl: l = 2n$
4	<i>o</i> . . 2	$x, x, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, x, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$	$0kl: l = 2n$
4	<i>n</i> . . 2	$x, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, x, \frac{3}{4}$	$x, \bar{x}, \frac{3}{4}$	$0kl: l = 2n$
4	<i>m</i> . 2 .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$hhl: l = 2n$
4	<i>l</i> . 2 .	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, 0$	$0, \bar{x}, 0$	$hhl: l = 2n$
4	<i>k</i> . 2 .	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$hhl: l = 2n$
4	<i>j</i> . 2 .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	$hhl: l = 2n$
4	<i>i</i> 2 . .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>h</i> 2 . .	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl: l = 2n$
4	<i>g</i> 2 . .	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$hkl: l = 2n$
2	<i>f</i> 2 . 22	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl: l = 2n$
2	<i>e</i> 2 . 22	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl: l = 2n$
2	<i>d</i> 2 2 2 .	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl: h + k + l = 2n$
2	<i>c</i> 2 2 2 .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h + k + l = 2n$
2	<i>b</i> 2 2 2 .	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: l = 2n$
2	<i>a</i> 2 2 2 .	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl: l = 2n$

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, \frac{1}{4}$