

Tetragonal

422

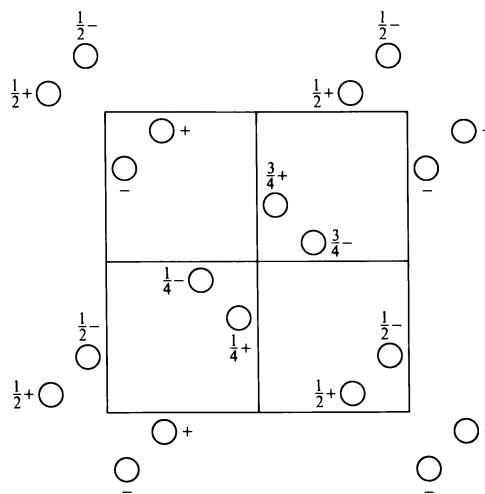
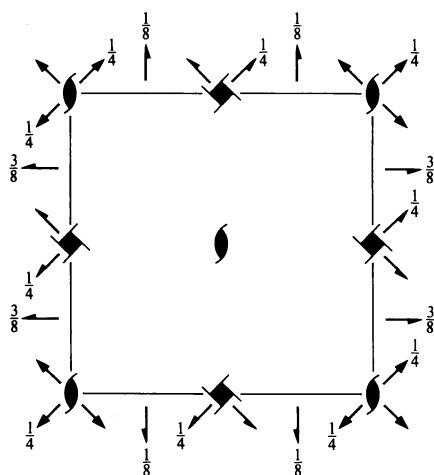
D_4^8

$P4_3 2_1 2$

Patterson symmetry $P4/mmm$

$P4_3 2_1 2$

No. 96



Origin on $2[110]$ at $2, 1(1, 2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

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

General:

- 00*l*: $l = 4n$
- h*00: $h = 2n$

Special: as above, plus

- | | | | | | | |
|---|----------|------|-----------|---------------------------------|---|---|
| 4 | <i>a</i> | .. 2 | $x, x, 0$ | $\bar{x}, \bar{x}, \frac{1}{2}$ | $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ | $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
|---|----------|------|-----------|---------------------------------|---|---|

- 0*kl*: $l = 2n + 1$
or $2k + l = 4n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

Along [100] $p2gg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{4}, \frac{1}{8}$

Along [110] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$