

$P4_2/mbc$

D_{4h}^{13}

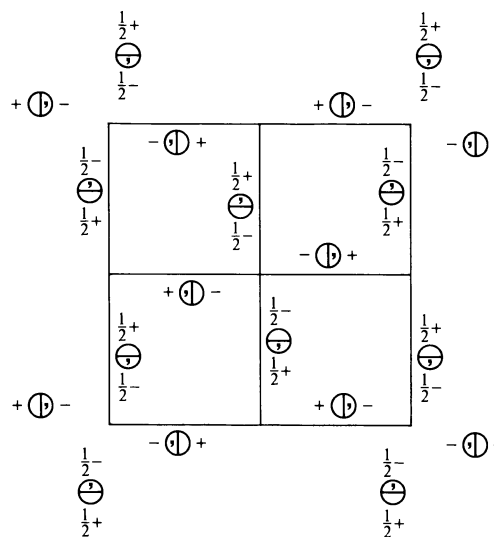
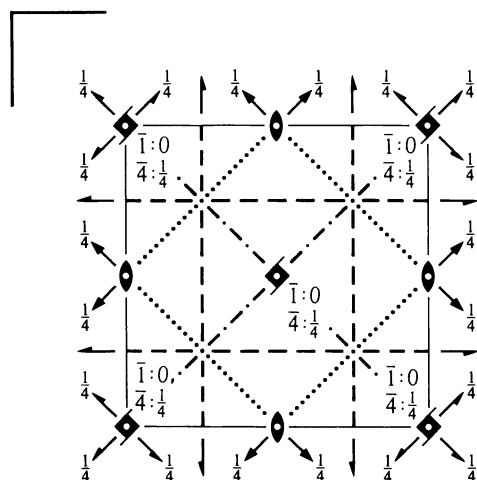
$4/mmm$

Tetragonal

No. 135

$P 4_2/m 2_1/b 2/c$

Patterson symmetry $P4/mmm$



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

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

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) $2 (0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$ | (6) $2 (\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, 0$ | (7) $2 (\frac{1}{2}, \frac{1}{2}, 0) \ x, x, \frac{1}{4}$ | (8) $2 \ x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1} \ 0, 0, 0$ | (10) $m \ x, y, 0$ | (11) $\bar{4}^+ \ 0, 0, z; \ 0, 0, \frac{1}{4}$ | (12) $\bar{4}^- \ 0, 0, z; \ 0, 0, \frac{1}{4}$ |
| (13) $a \ x, \frac{1}{4}, z$ | (14) $b \ \frac{1}{4}, y, z$ | (15) $c \ x + \frac{1}{2}, \bar{x}, z$ | (16) $n (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \ x, x, z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

16	<i>i</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) $\bar{y}, x, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$
			(5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) x, y, \bar{z}	(11) $y, \bar{x}, \bar{z} + \frac{1}{2}$	(12) $\bar{y}, x, \bar{z} + \frac{1}{2}$
			(13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$

General:

$Ok_l: k = 2n$

$hhl: l = 2n$

$00l: l = 2n$

$h00: h = 2n$

Special: as above, plus

no extra conditions

8	<i>h</i>	$m..$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$
			$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	$y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$

8	<i>g</i>	$..2$	$x, x + \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{3}{4}$
			$\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$x, x + \frac{1}{2}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{1}{4}$

$hkl: l = 2n$

8	<i>f</i>	$2..$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$
			$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z + \frac{1}{2}$

$hkl: h + k, l = 2n$

8	<i>e</i>	$2..$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$
			$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$

$hkl: h + k, l = 2n$

4	<i>d</i>	2.22	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$
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$hkl: h + k, l = 2n$

4	<i>c</i>	$2/m..$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
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$hkl: h + k, l = 2n$

4	<i>b</i>	$\bar{4}..$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$
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$hkl: h + k, l = 2n$

4	<i>a</i>	$2/m..$	$0, 0, 0$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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$hkl: h + k, l = 2n$

Symmetry of special projectionsAlong [001] $p4gm$

$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$ Along [100] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$ Along [110] $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, x, 0$