

$P4_2/nbc$

D_{4h}^{11}

$4/mmm$

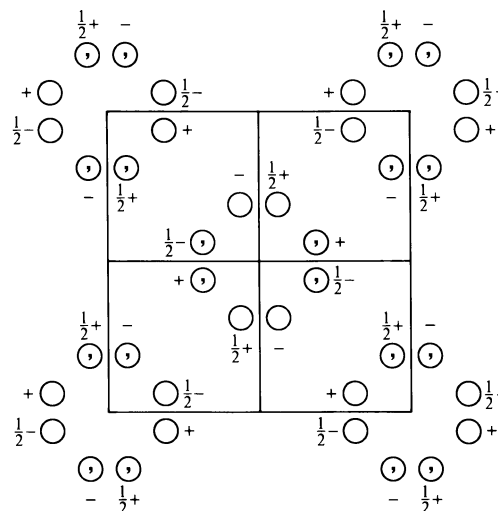
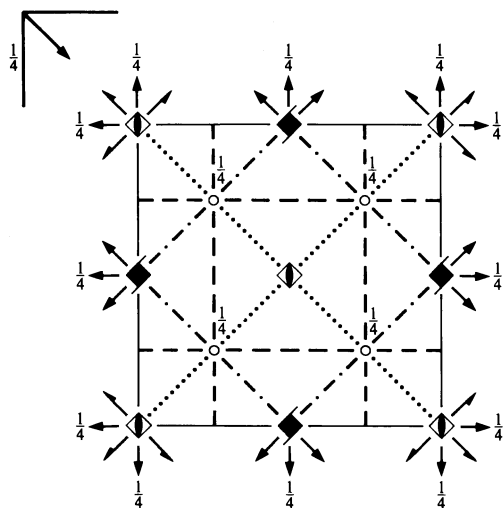
Tetragonal

No. 133

$P 4_2/n 2/b 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}12_1/c$, at $-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$ from $\bar{1}$

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) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (5) 2 $0, y, \frac{1}{4}$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) a $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) c x, \bar{x}, z | (16) c 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
		General:
16 <i>k</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	$hk0 : h + k = 2n$ $0kl : k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
	(2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	
	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	
	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) $y, x, z + \frac{1}{2}$	
		Special: as above, plus
8 <i>j</i> ..2	$x, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$	$hkl : h + k + l = 2n$
	$\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, 0$ $x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, 0$	
8 <i>i</i> .2.	$x, 0, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k = 2n$
	$\bar{x}, 0, \frac{3}{4}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $0, \bar{x}, \frac{1}{4}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $0, x, \frac{1}{4}$	
8 <i>h</i> .2.	$x, 0, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$hkl : h + k = 2n$
	$\bar{x}, 0, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $0, \bar{x}, \frac{3}{4}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $0, x, \frac{3}{4}$	
8 <i>g</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z$ $0, 0, z + \frac{1}{2}$	
8 <i>f</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : h + k, l = 2n$
	$0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	
8 <i>e</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h, k, l = 2n$
	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	
4 <i>d</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$
	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	
4 <i>c</i> 2.22	$0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$	
4 <i>b</i> 222.	$0, 0, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $0, 0, \frac{3}{4}$	
4 <i>a</i> 222.	$0, \frac{1}{2}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k, l = 2n$
	$\frac{1}{2}, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	

Symmetry of special projections

Along [001] $p4mm$

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

Origin at 0, 0, z

Along [100] $p2mm$

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

Origin at $x, 0, \frac{1}{4}$

Along [110] $p2mm$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nbc$ ($\mathbf{c}' = 3\mathbf{c}$) (133); [9] $P4_2/nbc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (133)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

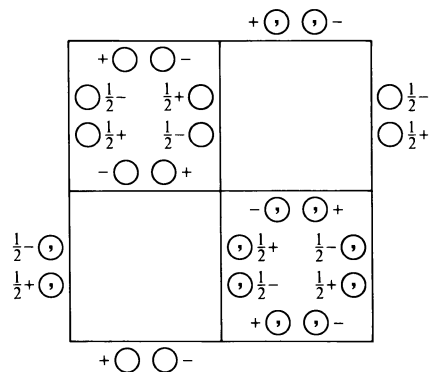
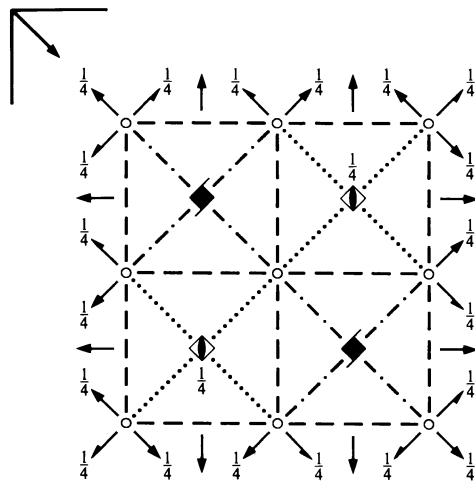
$P4_2/nbc$ D_{4h}^{11} $4/mmm$

Tetragonal

No. 133

 $P 4_2/n 2/b 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $n(b,a)(n,c)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|---------------------------|---|---|---|
| (1) 1 | (2) 2 $\frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ |
| (5) 2 $\frac{1}{4}, y, 0$ | (6) 2 $x, \frac{1}{4}, 0$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ 0, 0, 0 | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) a $x, 0, z$ | (14) b $0, y, z$ | (15) c x, \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	
		General:					
16	k	1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (14) $\bar{x}, y + \frac{1}{2}, z$	(3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $Ok1 : k = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus					
8	j	$\dots 2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k + l = 2n$
8	i	$. 2 .$	$x, \frac{1}{4}, \frac{1}{2}$ $\bar{x}, \frac{3}{4}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{3}{4}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8	h	$. 2 .$	$x, \frac{1}{4}, 0$ $\bar{x}, \frac{3}{4}, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, 0$ $x + \frac{1}{2}, \frac{3}{4}, 0$	$\frac{1}{4}, x, \frac{1}{2}$ $\frac{3}{4}, \bar{x}, \frac{1}{2}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8	g	$2 \dots$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8	f	$2 \dots$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8	e	$\bar{1}$	0, 0, 0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ 0, 0, $\frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k, l = 2n$
4	d	$\bar{4} \dots$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k, l = 2n$
4	c	$2 . 2 2$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
4	b	$2 2 2 .$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4	a	$2 2 2 .$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$

Symmetry of special projections

Along [001] $p4mm$

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

Origin at $\frac{1}{4}, \frac{1}{4}, z$

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 $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIIc [3] $P4_2/nbc$ ($\mathbf{c}' = 3\mathbf{c}$) (133); [9] $P4_2/nbc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (133)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)