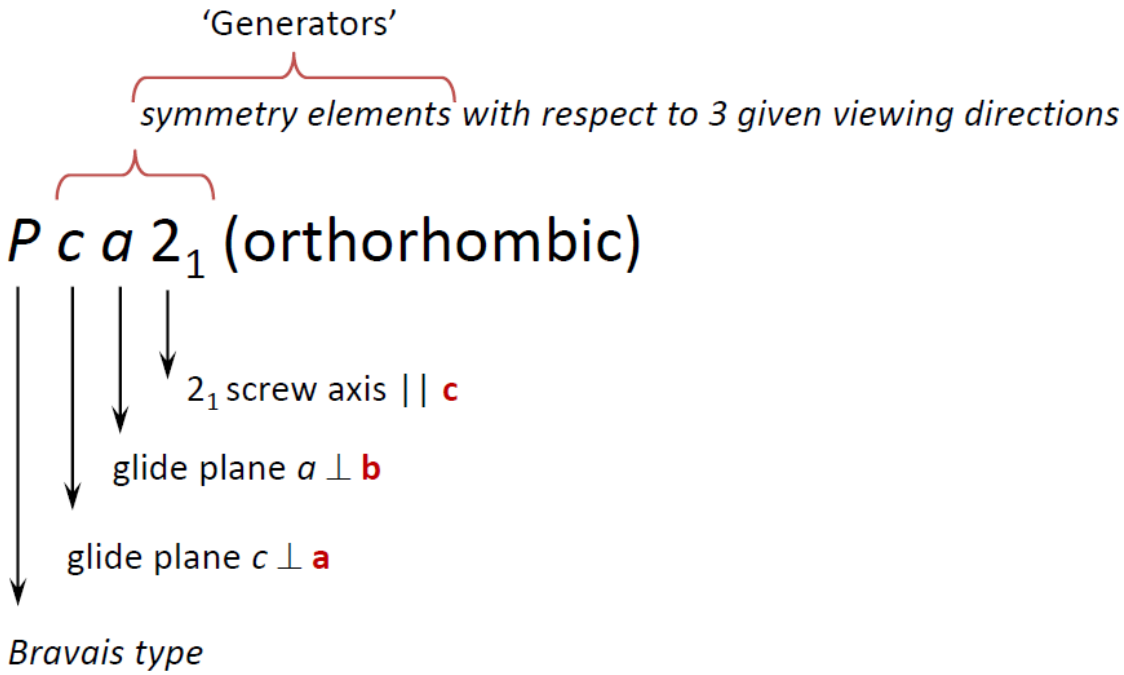
INTRODUÇÃO A CRISTALOGRAFIA APLICADA À DIFRAÇÃO DE ELÉTRONS PARA MATERIAIS SÓLIDOS

Aula 6 – “The International Tables”

Space groups

- Conjunto dos elementos de simetria (e seus respectivas operações), que descrevem por completo o arranjo espacial periódico em 3 dimensões.

- Nomenclatura



Space groups

"Crystallographic viewing directions"

	crystal system	*viewing directions*		
	triclinic	—		
	monoclinic	*b (c)*		
	orthorhombic	*a*	*b*	*c*
a = b	tetragonal	*c*	*a*	[110]
a = b	trigonal	*c*	*a*	[210]
a = b	hexagonal	*c*	*a*	[210]
	cubic	*a*	[111]	[110]

Space Groups

- Vamos estudar um pouco como algumas informações são mostradas nessa tabela.

International Tables for Crystallography
Volume A: Space-group symmetry

Edited by Th. Hahn

Space Groups

- Lista de forma sistemática os 17 plane groups e os 230 space groups.
- Contém os símbolos completos e simplificados dos space groups.
- Contém o nome do sistema cristalino bem como seu crystal class (grupo pontual).
- Contém diagramas das posições dos seus elementos de simetria.
- Contém diagramas das general positions.
- Lista as operações de simetria como transformação de coordenadas.
- Entre muitas outras informações.

Space Groups

- Vamos começar com um exemplo do grupo espacial Pmm2.

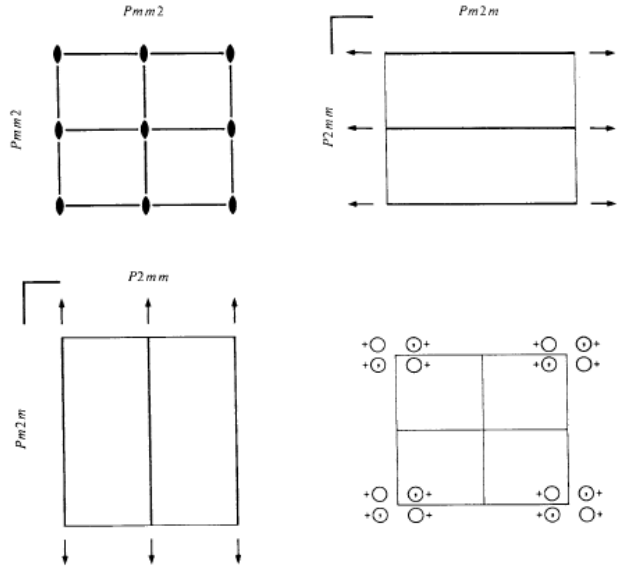
Space Groups

- Pmm2.

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^{1} $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$mm2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$mm2$	$\frac{1}{2},0,z$				
1	b	$mm2$	$0,\frac{1}{2},z$				
1	a	$mm2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0,0,z

Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at x,0,0

Along [010] $p11m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pma2$ ($\mathbf{a}' = 2\mathbf{a}$) (28); [2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2$, 28); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27); [2] $Pmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (26); [2] $Pcm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmc2_1$, 26); [2] $Aem2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (39); [2] $Amm2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (38); [2] $Bme2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Aem2$, 39); [2] $Bmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Amm2$, 38); [2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); [2] $Fmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Minimal non-isomorphic supergroups

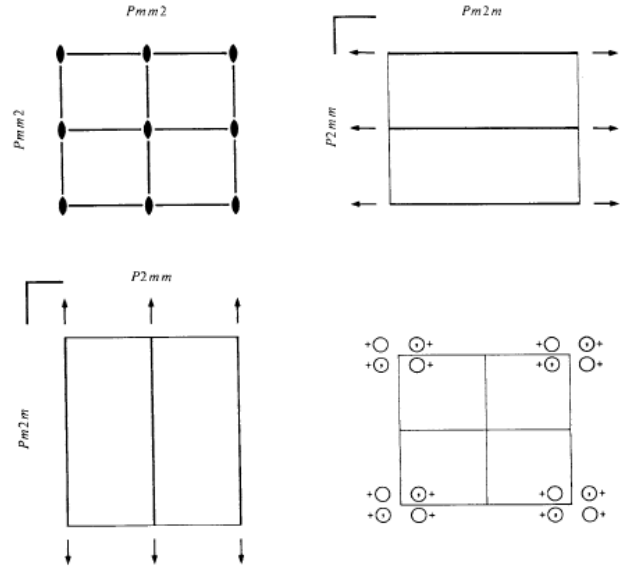
I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

Space Groups

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$	C_{2v}^{1}	$mm2$	Orthorhombic
No. 25	$Pmm2$		Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
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2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$mm2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$mm2$	$\frac{1}{2},0,z$				
1	b	$mm2$	$0,\frac{1}{2},z$				
1	a	$mm2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0,0,z

Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at x,0,0

Along [010] $p11m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0,y,0

Maximal non-isomorphic subgroups

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[2] $P112$ ($P2$, 3) 1; 2

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Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Minimal non-isomorphic supergroups

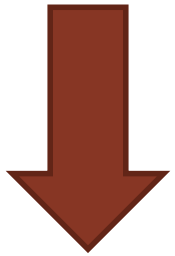
I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

Space Groups

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Schoenflies H.-M.

Short symbol $Pmm2$ *Crystal class* C_{2v}^1 $mm2$ *Crystal system* Orthorhombic

Number No. 25 *Full symbol* $Pmm2$ [Patterson Symmetry $Pmmm$]

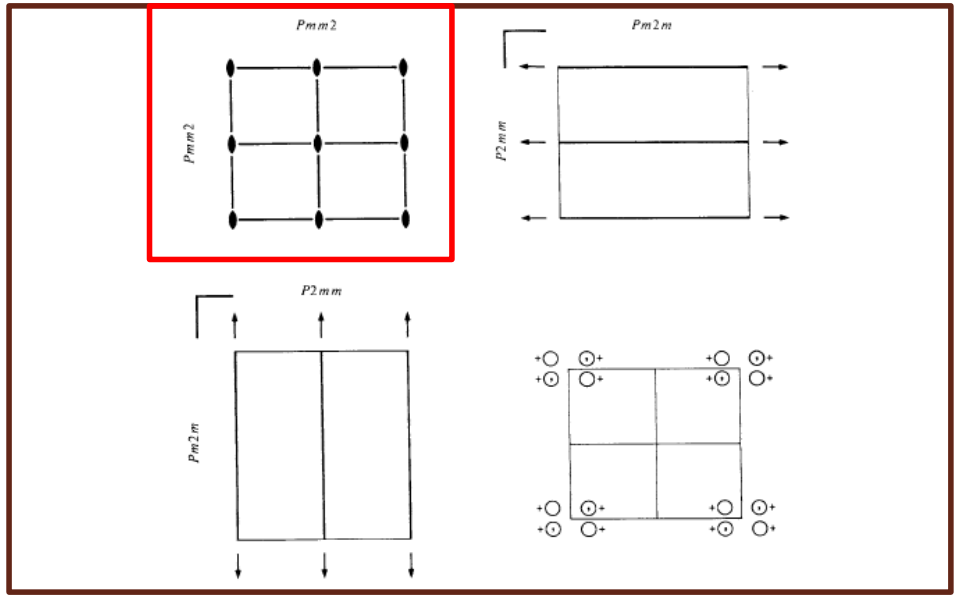
Space Groups

- Pmm

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

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Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
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							Special: no extra conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$mm2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$mm2$	$\frac{1}{2},0,z$				
1	b	$mm2$	$0,\frac{1}{2},z$				
1	a	$mm2$	$0,0,z$				

Symmetry of special projections

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Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at x,0,0

Along [010] $p1 1m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
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Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

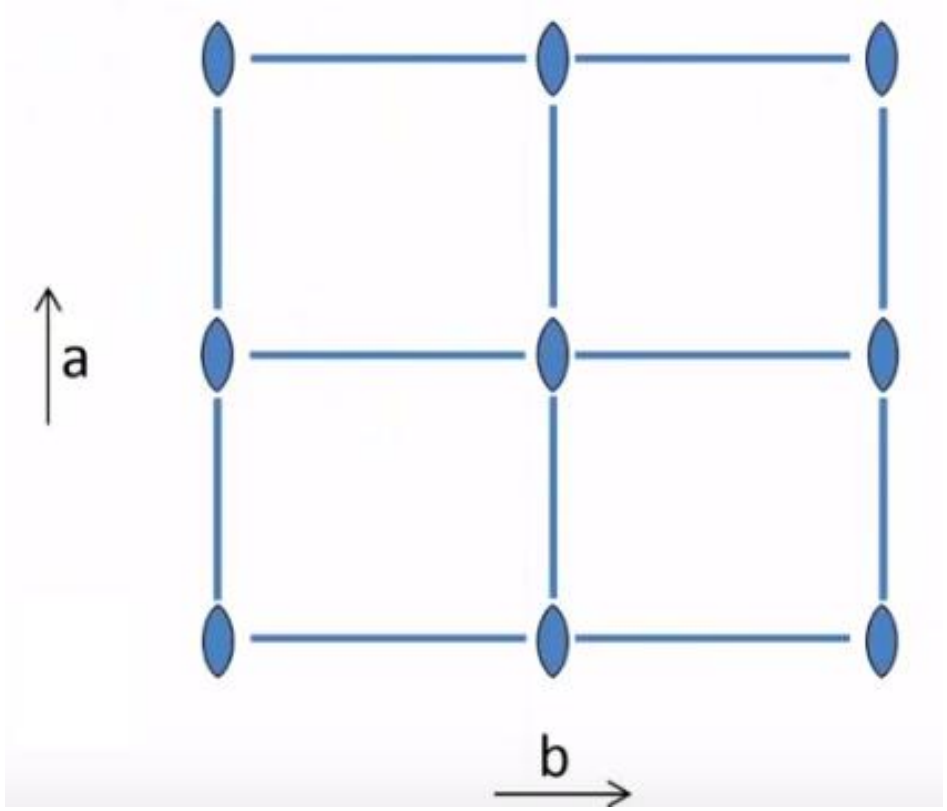
Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

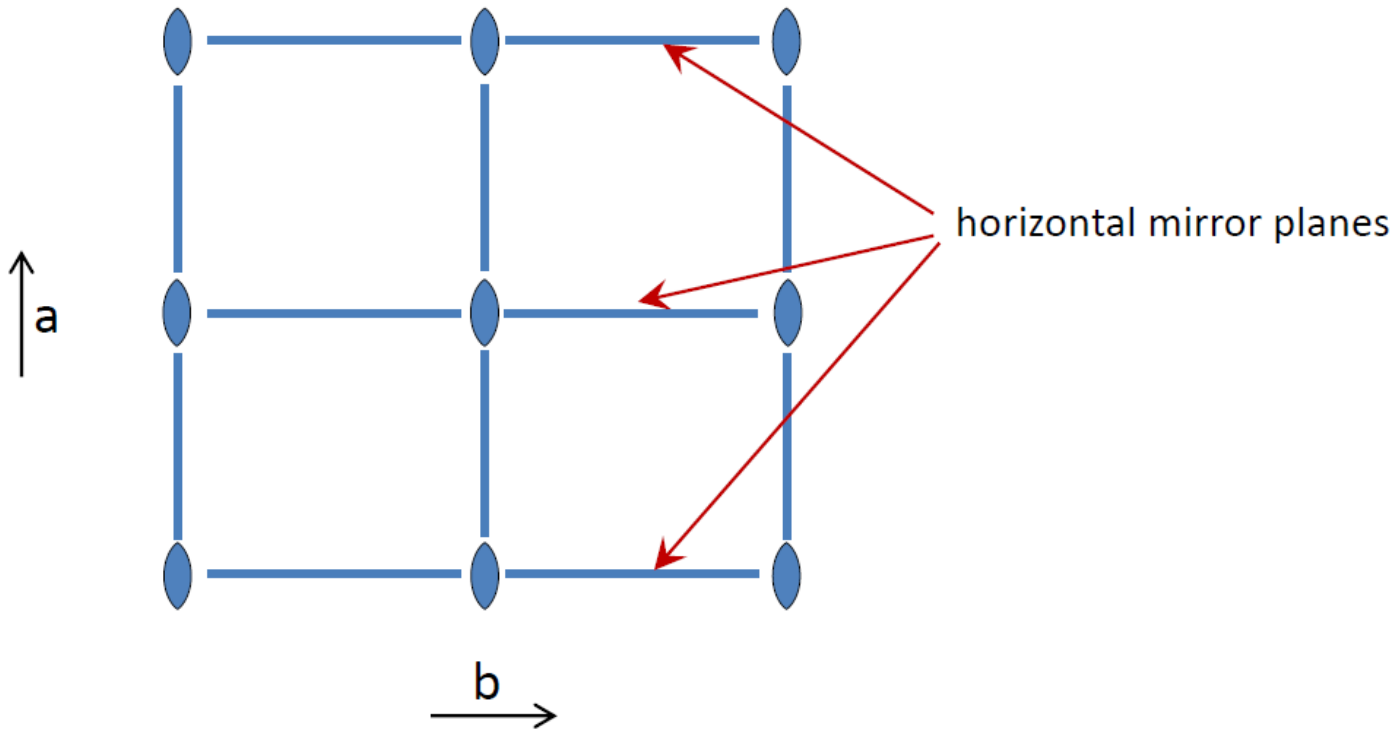
Space Groups

- Diagrama dos elementos de simetria



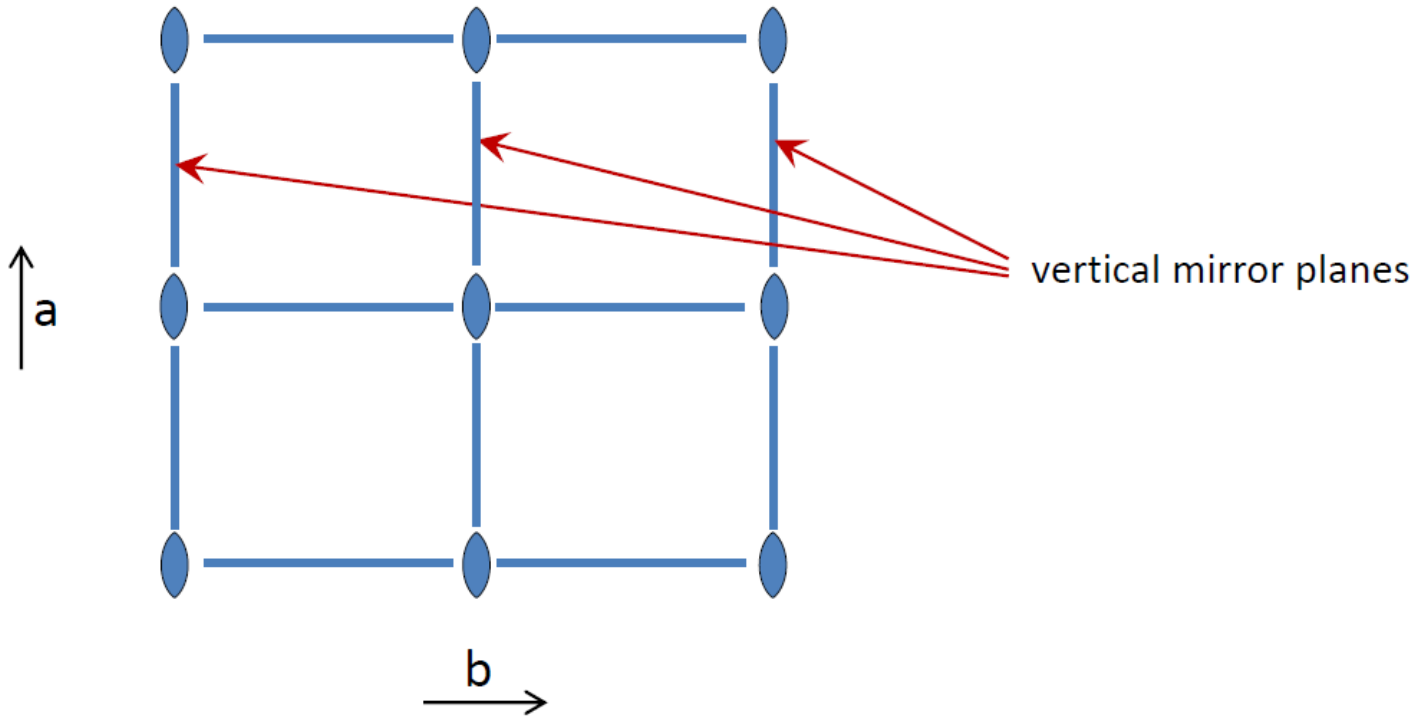
Space Groups

- Diagrama dos elementos de simetria



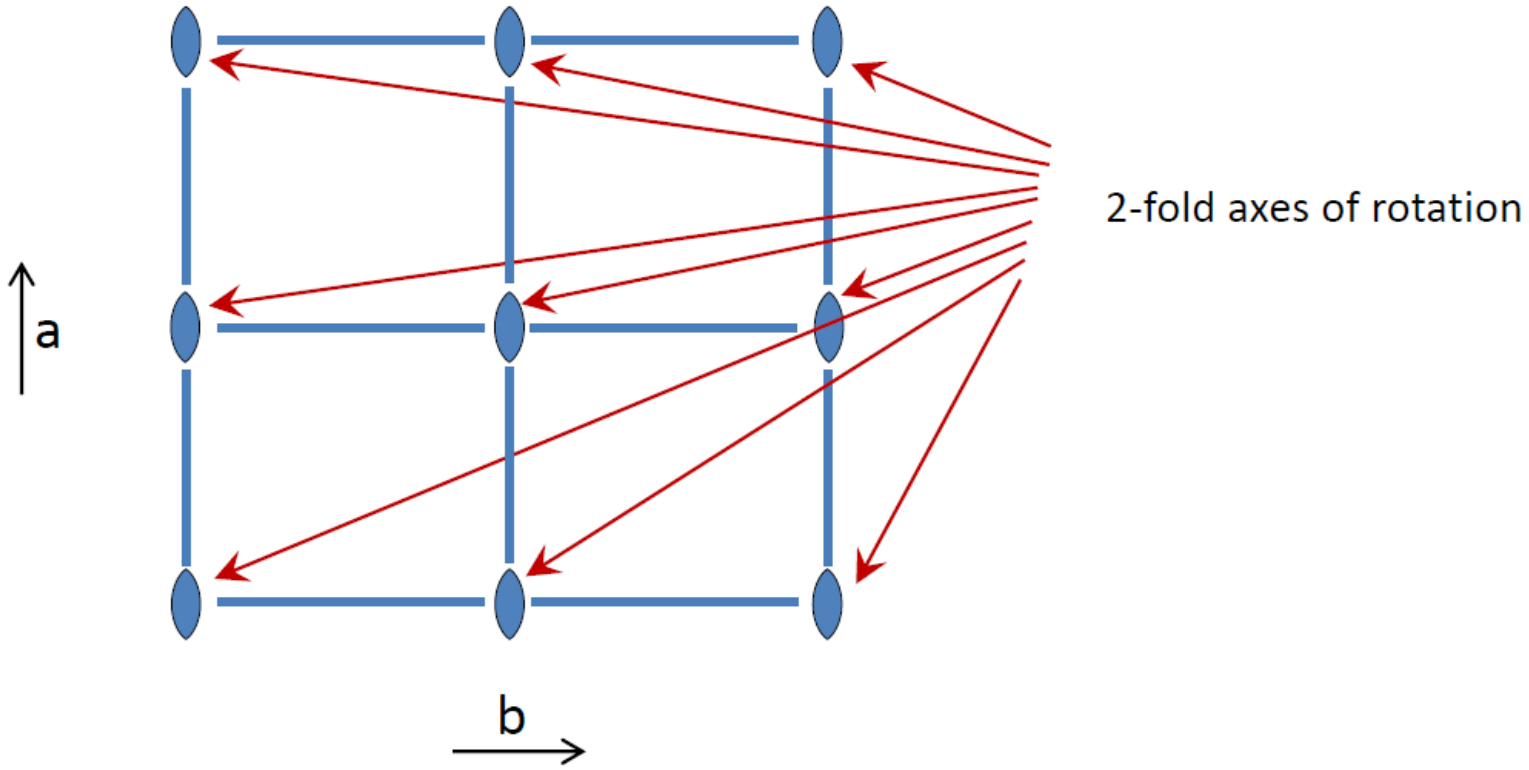
Space Groups

- Diagrama dos elementos de simetria



Space Groups

- Diagrama dos elementos de simetria



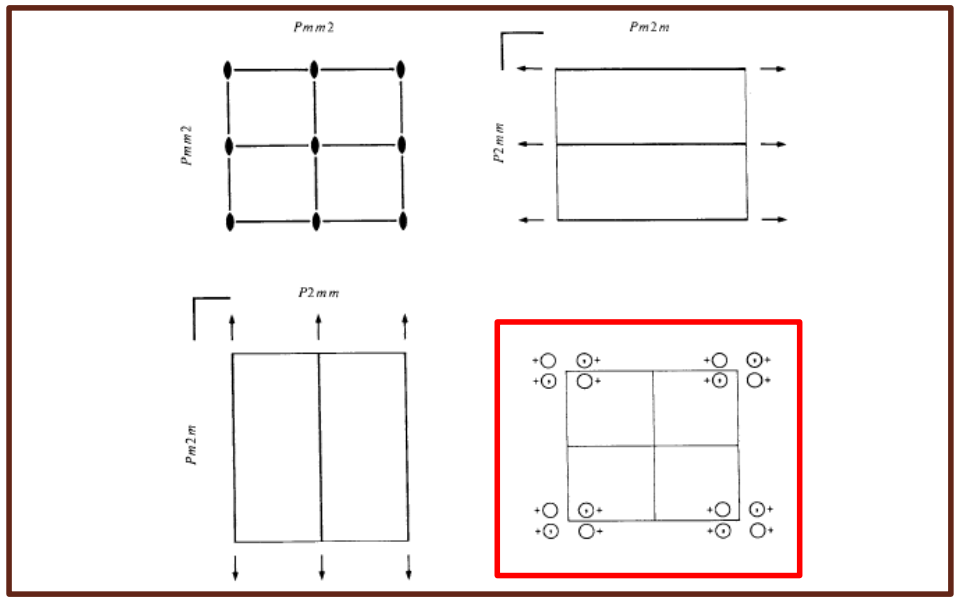
Space Groups

- Pmm

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

CONTINUED No. 25 $Pmm2$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	no conditions
							Special: no extra conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2	g	m . .	0,y,z	0,$\bar{y}$,z			
2	f	. m .	x,$\frac{1}{2}$,z	$\bar{x}$,$\frac{1}{2}$,z			
2	e	. m .	x,0,z	$\bar{x}$,0,z			
1	d	$m\,m\,2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$m\,m\,2$	$\frac{1}{2}$,0,z				
1	b	$m\,m\,2$	0,$\frac{1}{2}$,z				
1	a	$m\,m\,2$	0,0,z				

Symmetry of special projections

Along [001] $p2mm$ **a**′ = **a** **b**′ = **b** Origin at 0,0,z

Along [100] $p1m1$ **a**′ = **b** **b**′ = **c** Origin at x,0,0

Along [010] $p11m$ **a**′ = **c** **b**′ = **a** Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pma2$ (**a**′ = 2**a**) (28); [2] $Pbm2$ (**b**′ = 2**b**) ($Pma2$, 28); [2] $Pcc2$ (**c**′ = 2**c**) (27); [2] $Pmc2_1$ (**c**′ = 2**c**) (26); [2] $Pcm2_1$ (**c**′ = 2**c**) ($Pmc2_1$, 26); [2] $Aem2$ (**b**′ = 2**b**, **c**′ = 2**c**) (39); [2] $Amm2$ (**b**′ = 2**b**, **c**′ = 2**c**) (38); [2] $Bme2$ (**a**′ = 2**a**, **c**′ = 2**c**) ($Aem2$, 39); [2] $Bmm2$ (**a**′ = 2**a**, **c**′ = 2**c**) ($Amm2$, 38); [2] $Cmm2$ (**a**′ = 2**a**, **b**′ = 2**b**) (35); [2] $Fmm2$ (**a**′ = 2**a**, **b**′ = 2**b**, **c**′ = 2**c**) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ (**a**′ = 2**a** or **b**′ = 2**b**) (25); [2] $Pmm2$ (**c**′ = 2**c**) (25)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

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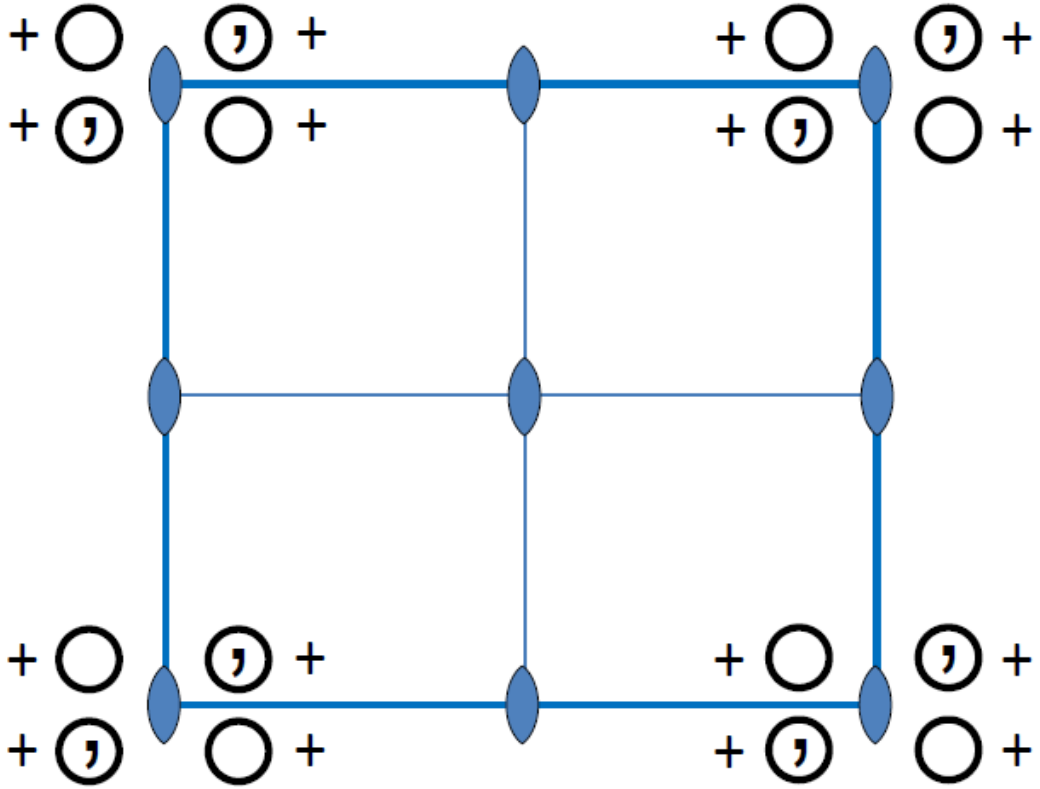
Space Groups

- Diagrama dos “general positions”



Space Groups

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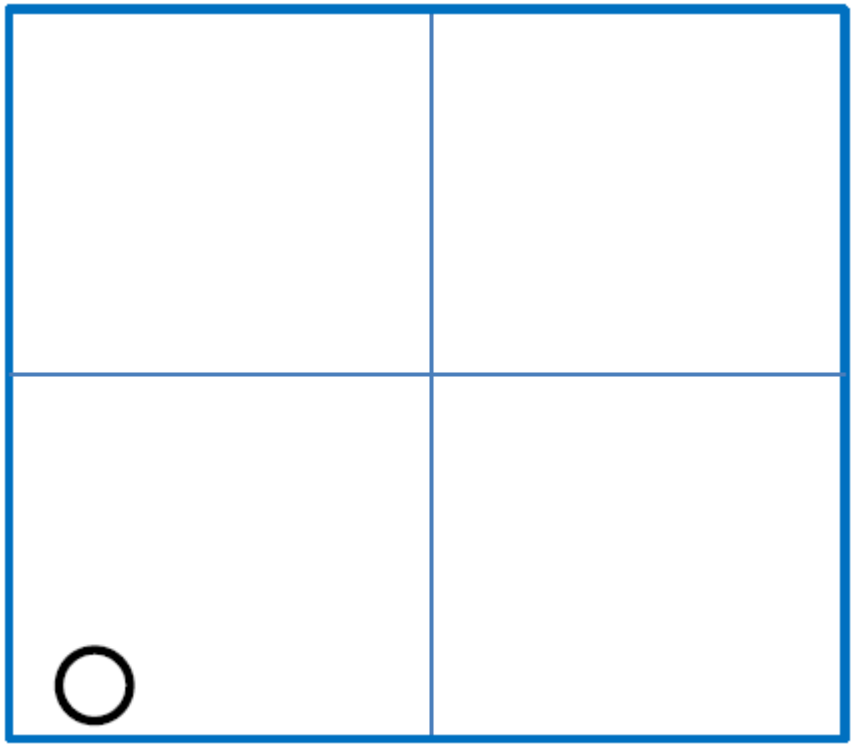

Space Groups

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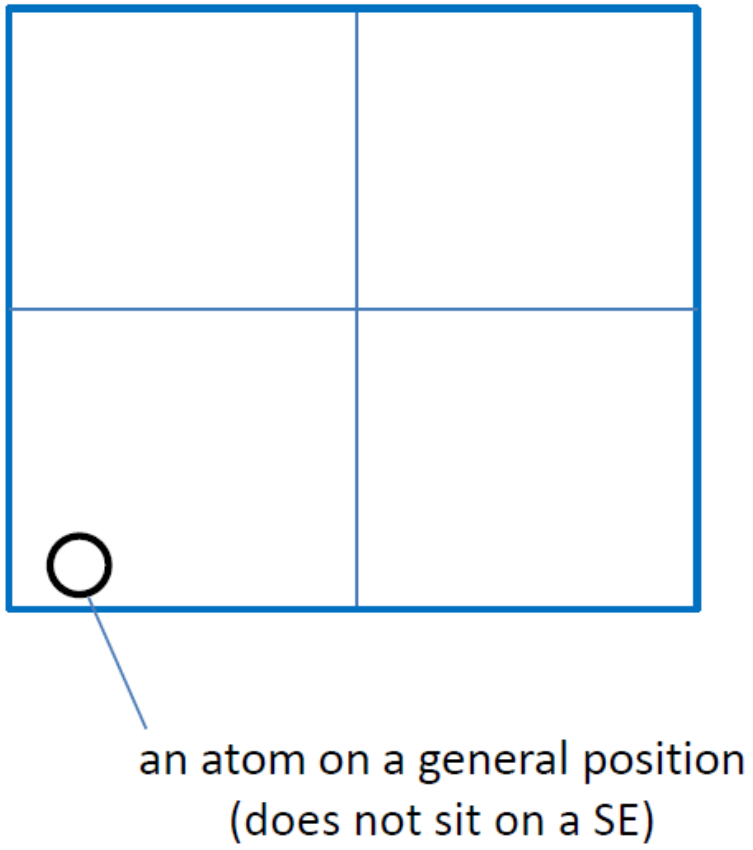

Space Groups

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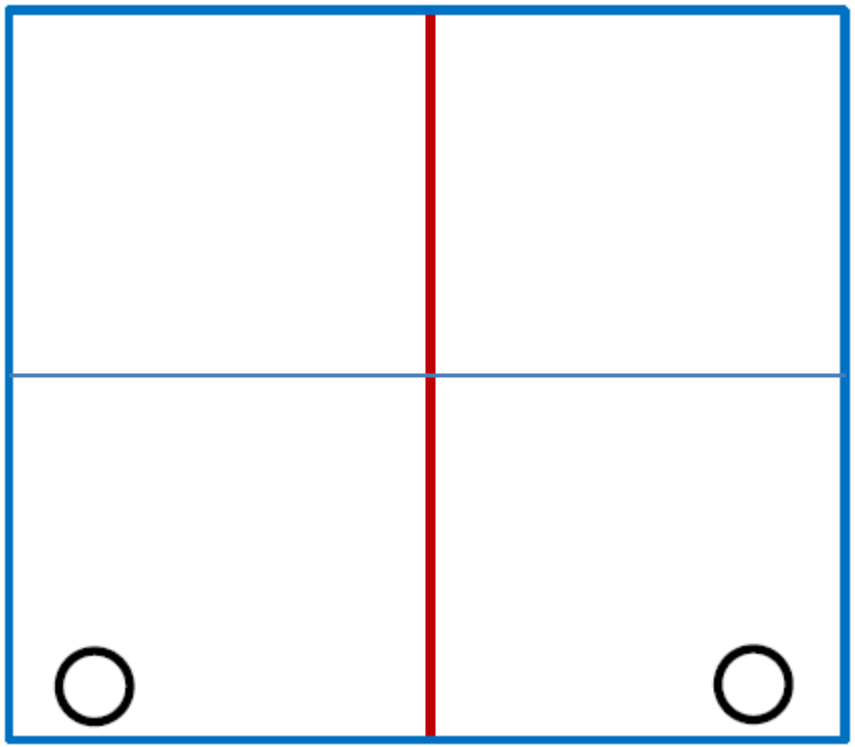

Space Groups

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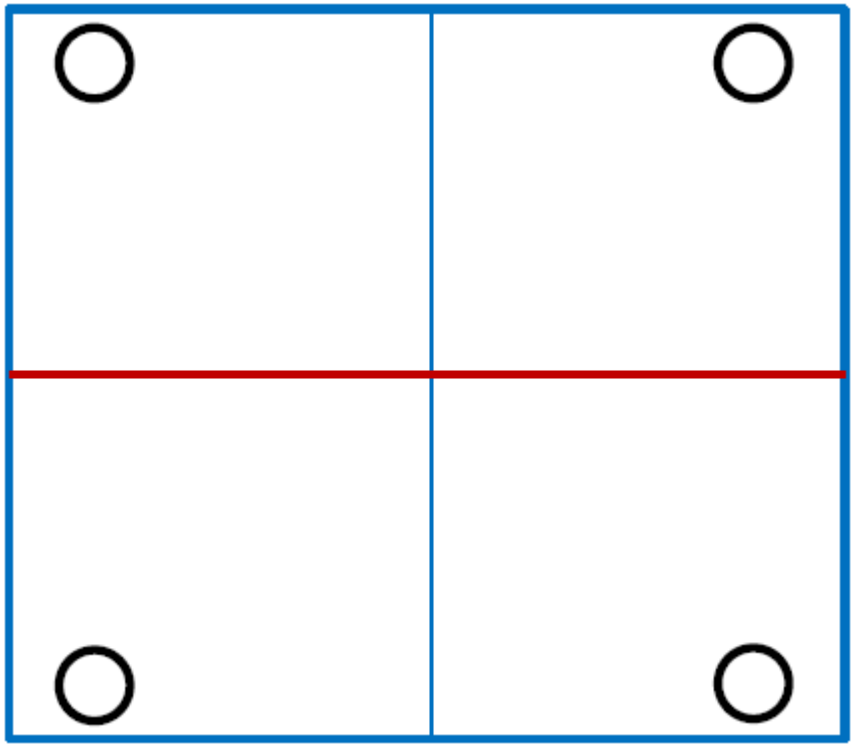

Space Groups

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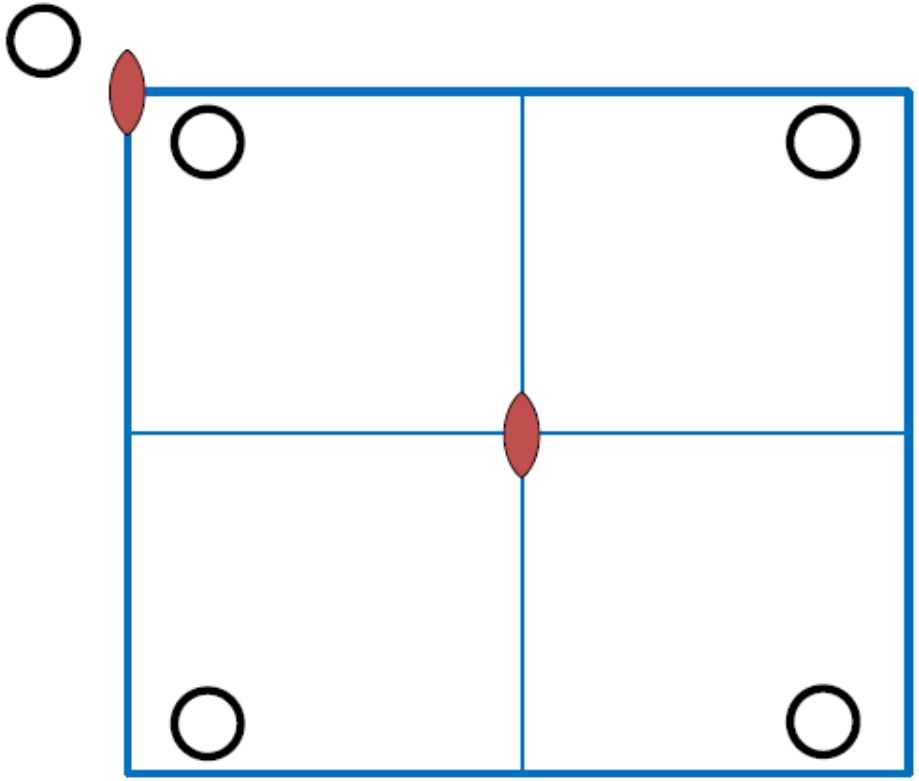

Space Groups

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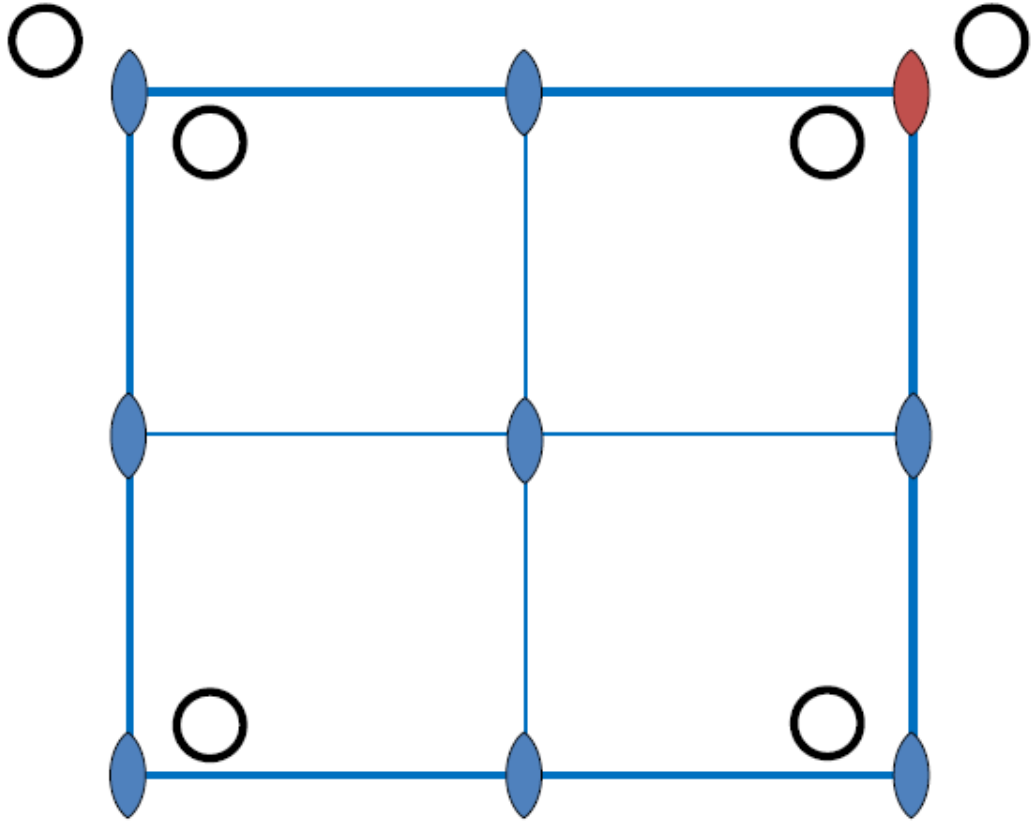
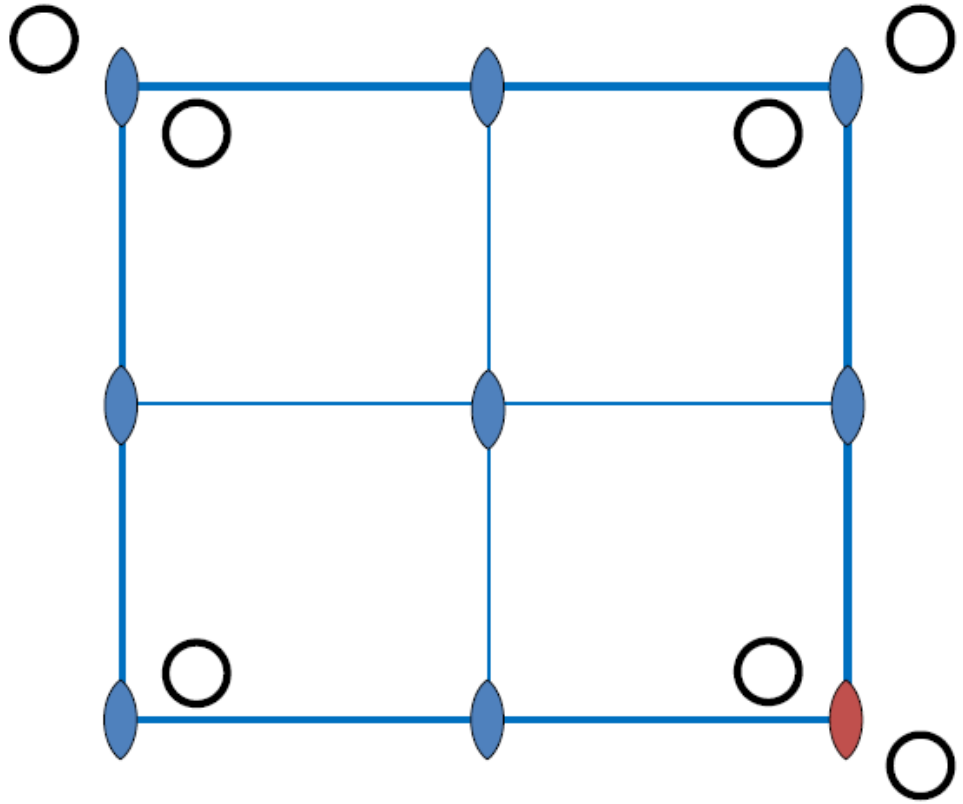


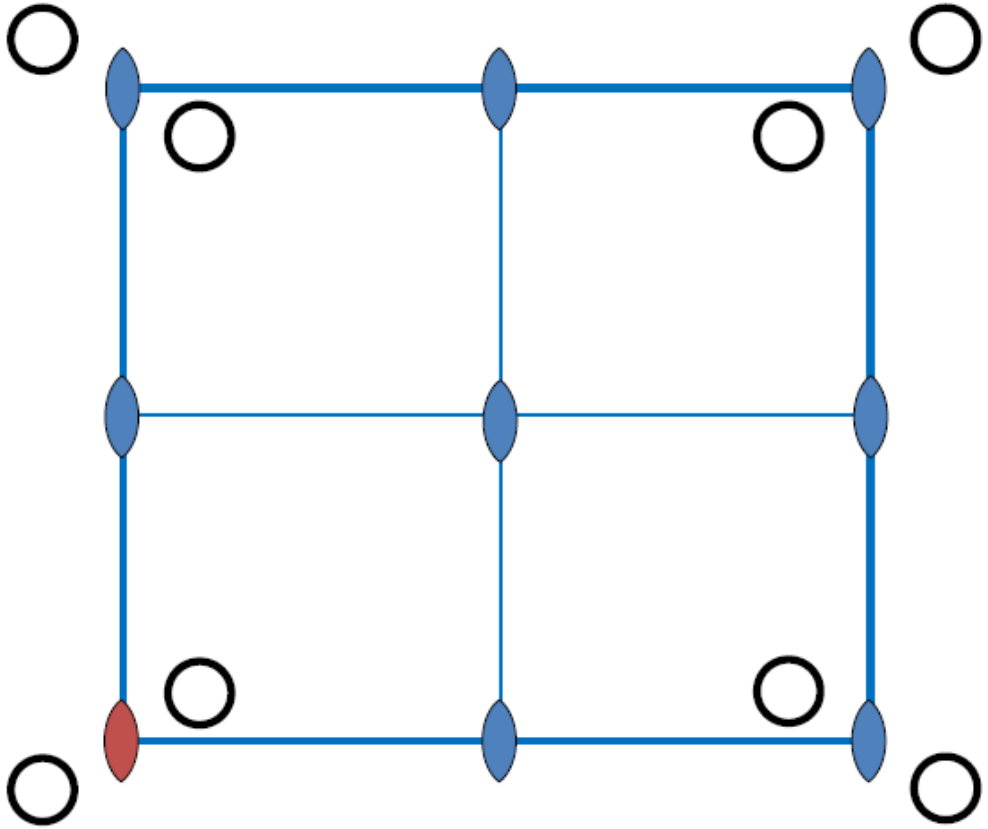
Space Groups

- Diagrama dos “general positions”



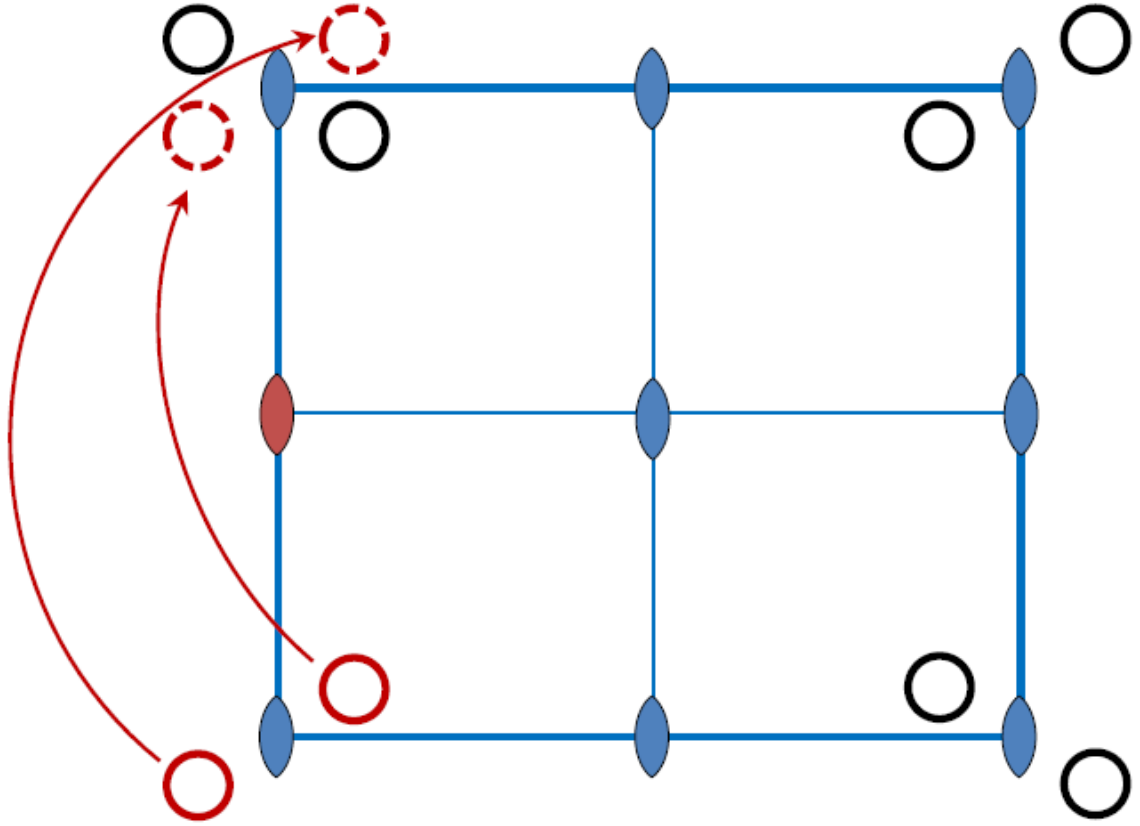
Space Groups

- Diagrama dos “general positions”



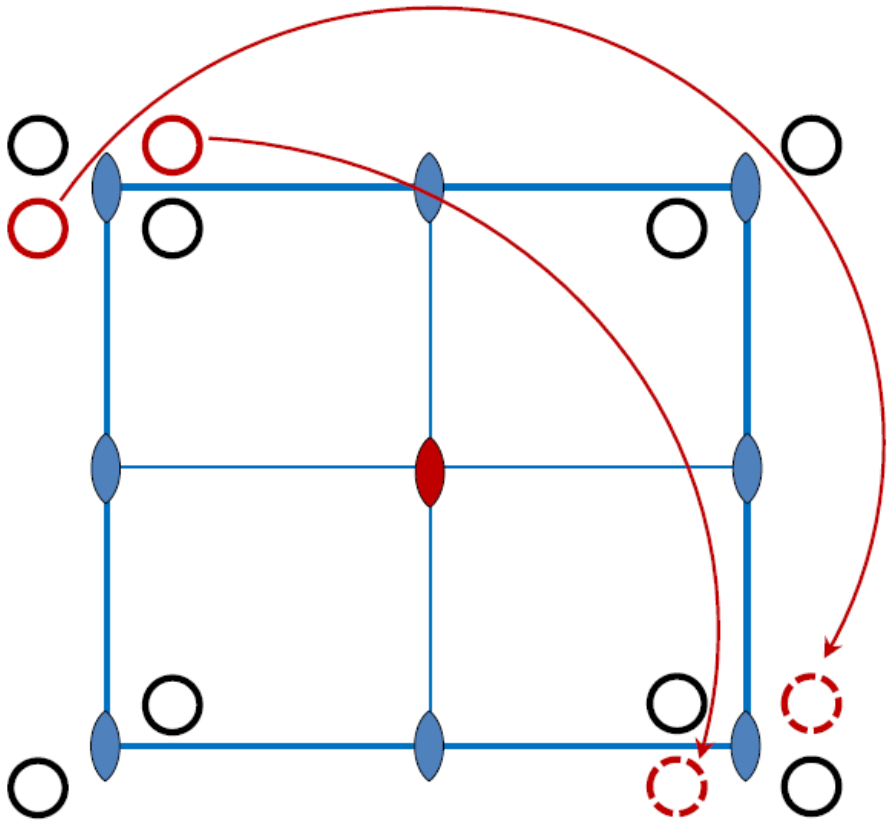
Space Groups

- Diagrama dos “general positions”



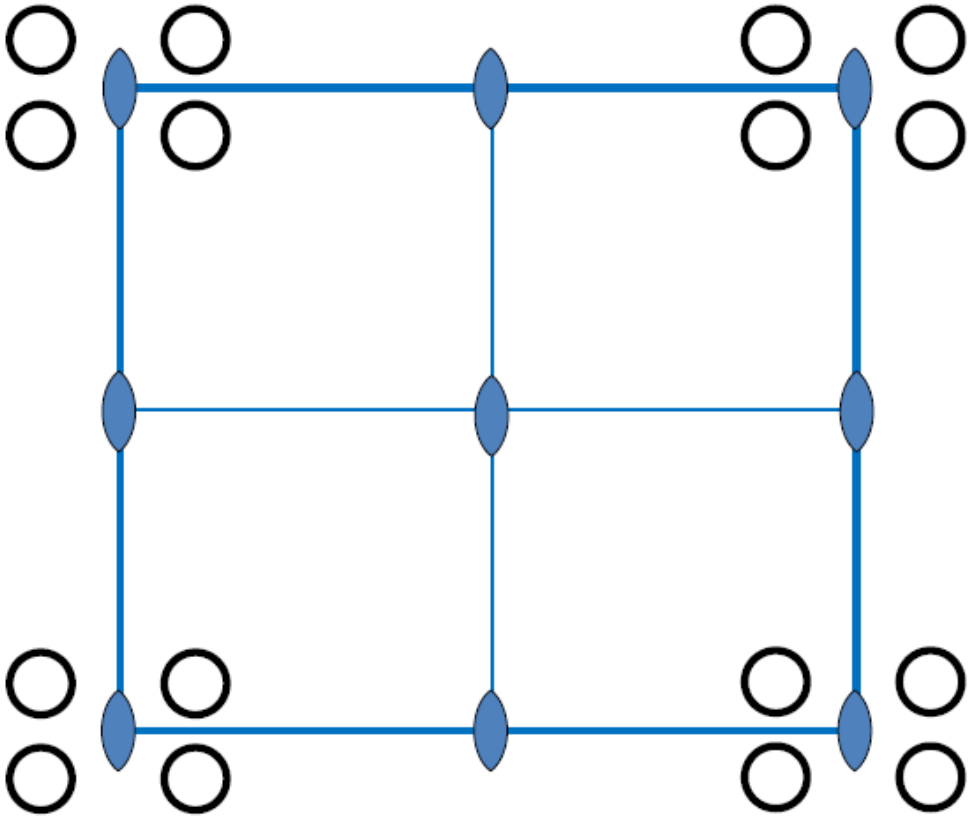
Space Groups

- Diagrama dos “general positions”



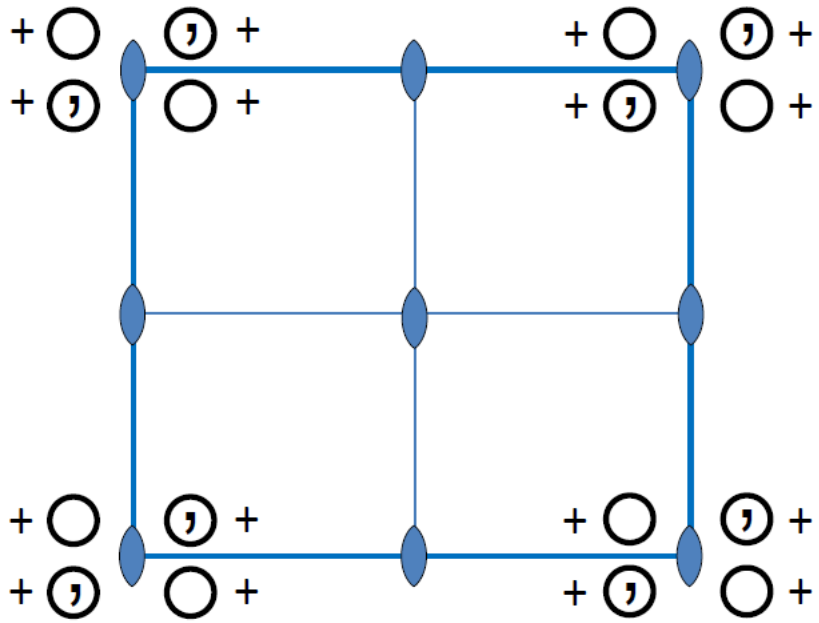
Space Groups

- Diagrama dos “general positions”



Space Groups

- Diagrama dos “general positions”



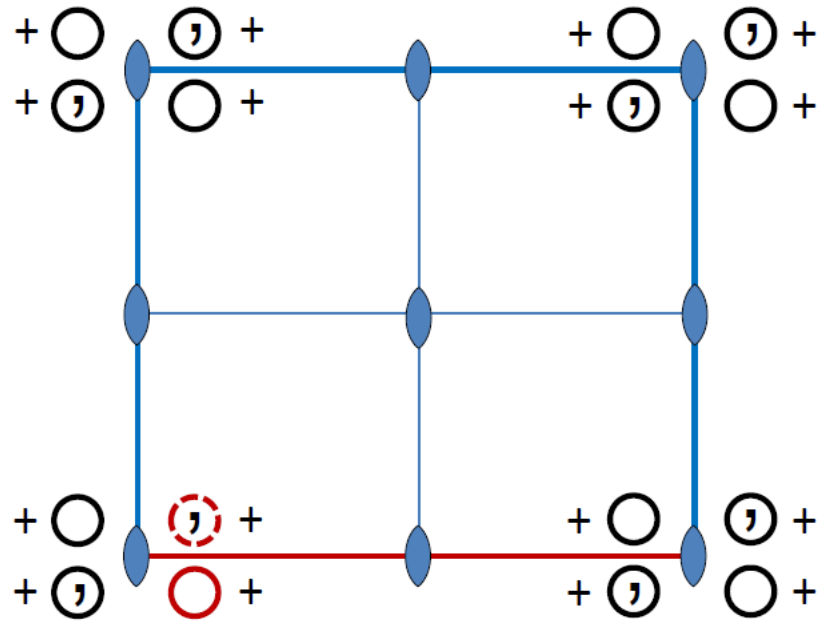
\+

position along the *c*-direction above the projection plane

image and mirror image of chiral objects

Space Groups

- Diagrama dos “general positions”



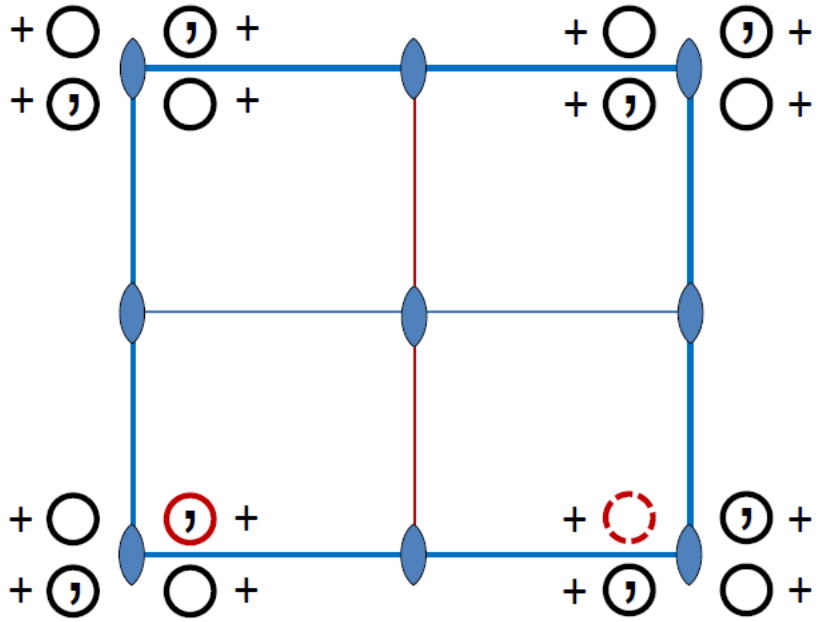
\+

position along the *c*-direction above the projection plane

image and mirror image

Space Groups

- Diagrama dos “general positions”



\+

position along the *c*-direction above the projection plane

image and mirror image

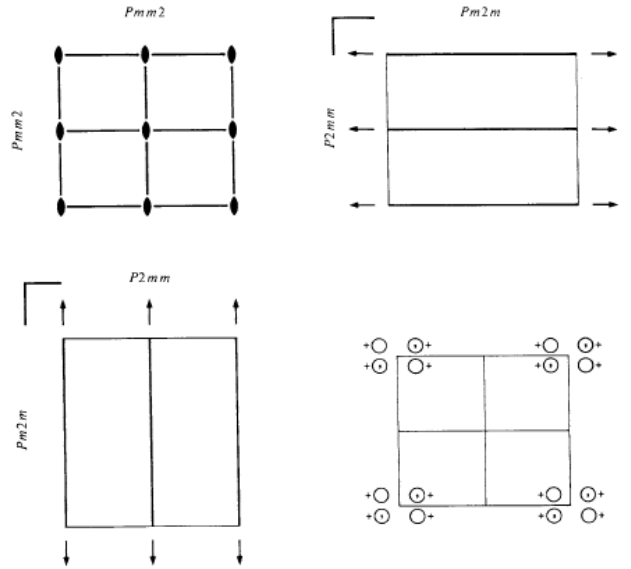
Space Groups

- Pmm

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$mm2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$mm2$	$\frac{1}{2},0,z$				
1	b	$mm2$	$0,\frac{1}{2},z$				
1	a	$mm2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0,0,z

Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at x,0,0

Along [010] $p11m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pma2$ ($\mathbf{a}' = 2\mathbf{a}$) (28); [2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2$, 28); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27); [2] $Pmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (26); [2] $Pcm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmc2_1$, 26); [2] $Aem2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (39); [2] $Amm2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (38); [2] $Bme2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Aem2$, 39); [2] $Bmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Amm2$, 38); [2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); [2] $Fmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

Space Groups

Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

-Origem é tomada em um ponto onde há intersecção de 2 espelhos e um 2-fold axis (para esse grupo espacial).

-Unidade assimétrica: Menor parte do espaço onde a aplicação de todos os elementos de simetria vai preencher todo o restante do espaço vazio.

-Operações de simetria: Incluem as operações de simetria e sua localização na célula unitária.

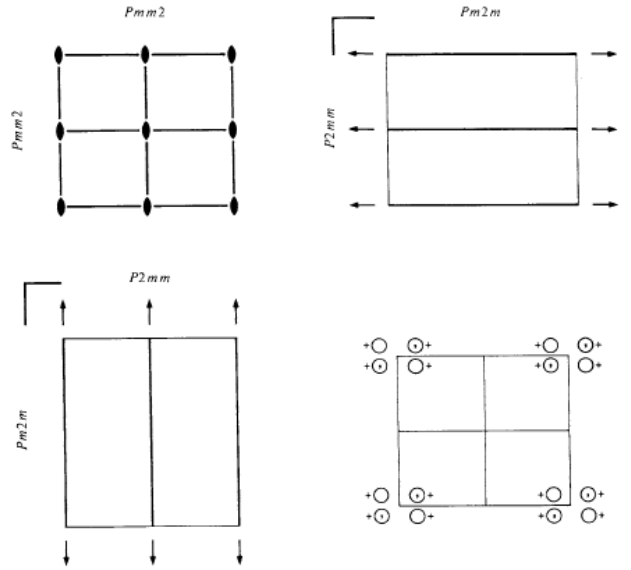
Space Groups

- Pmm

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$mm2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$mm2$	$\frac{1}{2},0,z$				
1	b	$mm2$	$0,\frac{1}{2},z$				
1	a	$mm2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0,0,z

Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at x,0,0

Along [010] $p1 1m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pma2$ ($\mathbf{a}' = 2\mathbf{a}$) (28); [2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2$, 28); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27); [2] $Pmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (26); [2] $Pcm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmc2_1$, 26); [2] $Aem2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (39); [2] $Amm2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (38); [2] $Bme2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Aem2$, 39); [2] $Bmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Amm2$, 38); [2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); [2] $Fmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

Space Groups

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

-Os geradores são os elementos de simetria a partir dos quais todos os outros podem ser gerados por combinações entre elementos de simetria.

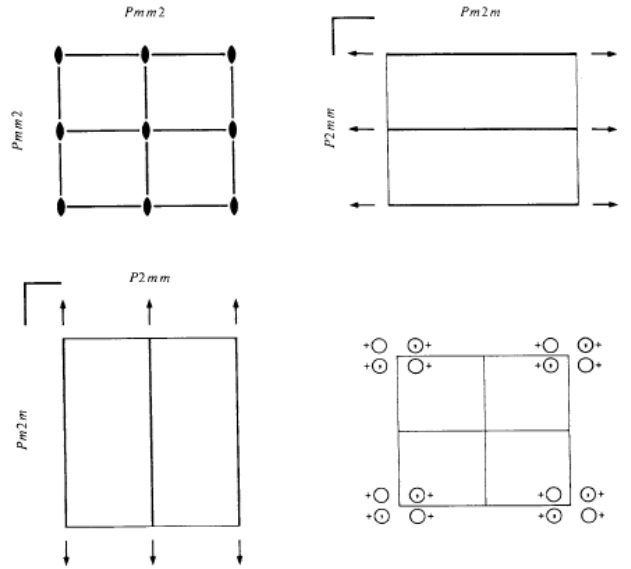
Space Groups

- Pmm

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$mm2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$mm2$	$\frac{1}{2},0,z$				
1	b	$mm2$	$0,\frac{1}{2},z$				
1	a	$mm2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at 0,0,z

Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ Origin at x,0,0

Along [010] $p11m$ $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pma2$ ($\mathbf{a}' = 2\mathbf{a}$) (28); [2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2$, 28); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27); [2] $Pmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (26); [2] $Pcm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmc2_1$, 26); [2] $Aem2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (39); [2] $Amm2$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (38); [2] $Bme2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Aem2$, 39); [2] $Bmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Amm2$, 38); [2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); [2] $Fmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (25); [2] $Pmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (25)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pmmn$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Amm2$, 38); [2] $Imm2$ (44)

Space Groups

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
2	g	m . .	$0,y,z$	$0,\bar{y},z$		
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$		
2	e	. m .	$x,0,z$	$\bar{x},0,z$		
1	d	m m 2	$\frac{1}{2},\frac{1}{2},z$			
1	c	m m 2	$\frac{1}{2},0,z$			
1	b	m m 2	$0,\frac{1}{2},z$			
1	a	m m 2	$0,0,z$			

general positions

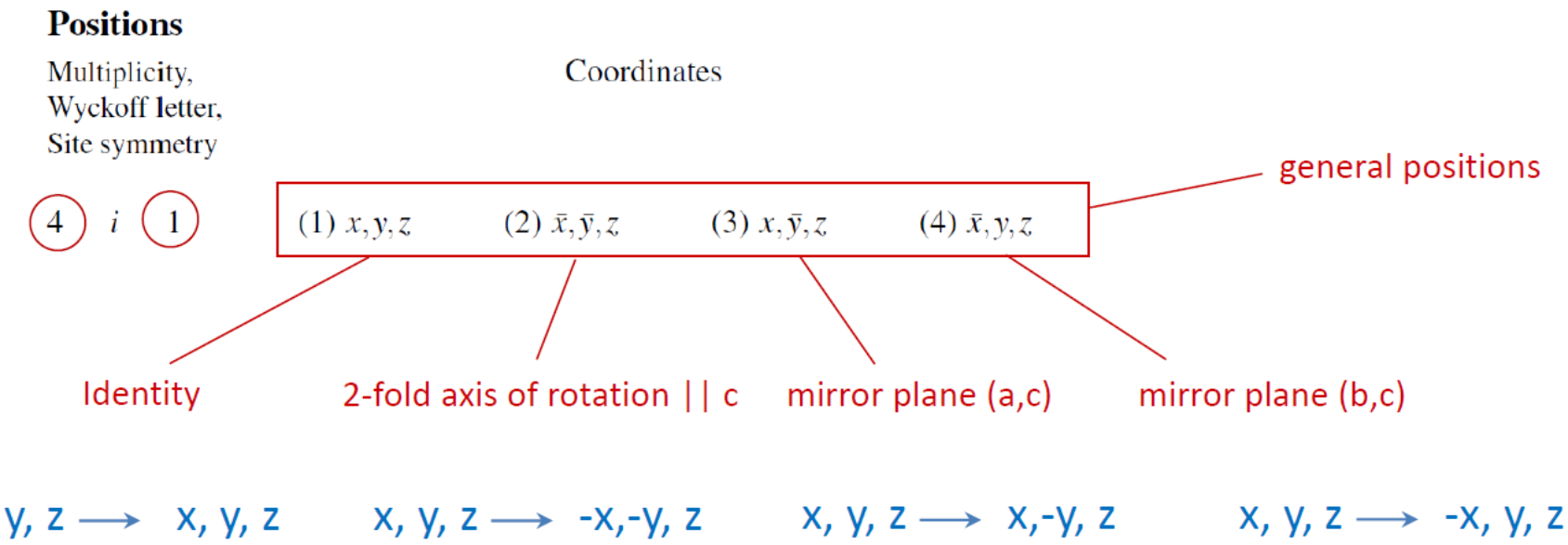
special positions (at SEs!)

Site symmetry (on which SE(s) does this point sit?)

Wyckoff letter (alphabetically)

Multiplicity (= number of equivalent sites/points within the unit cell)

Space Groups



x, y, z ⟶ x, y, z

x, y, z ⟶ -x,-y, z

x, y, z ⟶ x,-y, z

x, y, z ⟶ -x, y, z

Space Groups

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4 *i* 1

(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

general positions

Identity

2-fold axis of rotation || c

mirror plane (a,c)

mirror plane (b,c)

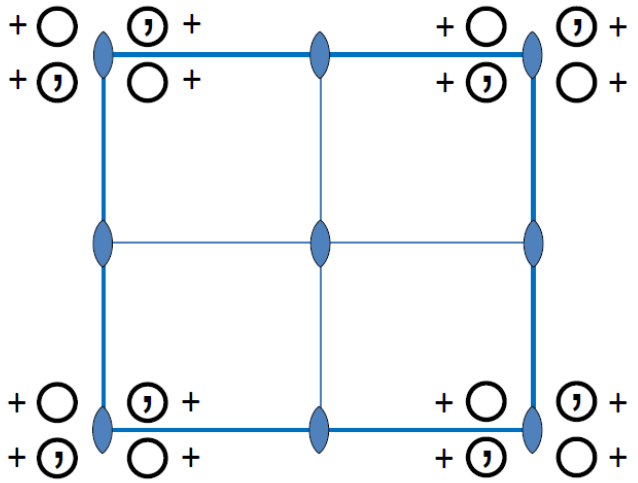
x, y, z ⟶ x, y, z

x, y, z ⟶ -x,-y, z

x, y, z ⟶ x,-y, z

x, y, z ⟶ -x, y, z

4 posições equivalentes dentro da célula unitária



Space Groups

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
2	*h*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
2	*g*	*m* . .	$0,y,z$	$0,\bar{y},z$		
2	*f*	. *m* .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$		
2	*e*	. *m* .	$x,0,z$	$\bar{x},0,z$		
1	*d*	*m m* 2	$\frac{1}{2},\frac{1}{2},z$			
1	*c*	*m m* 2	$\frac{1}{2},0,z$			
1	*b*	*m m* 2	$0,\frac{1}{2},z$			
1	*a*	*m m* 2	$0,0,z$			

general positions

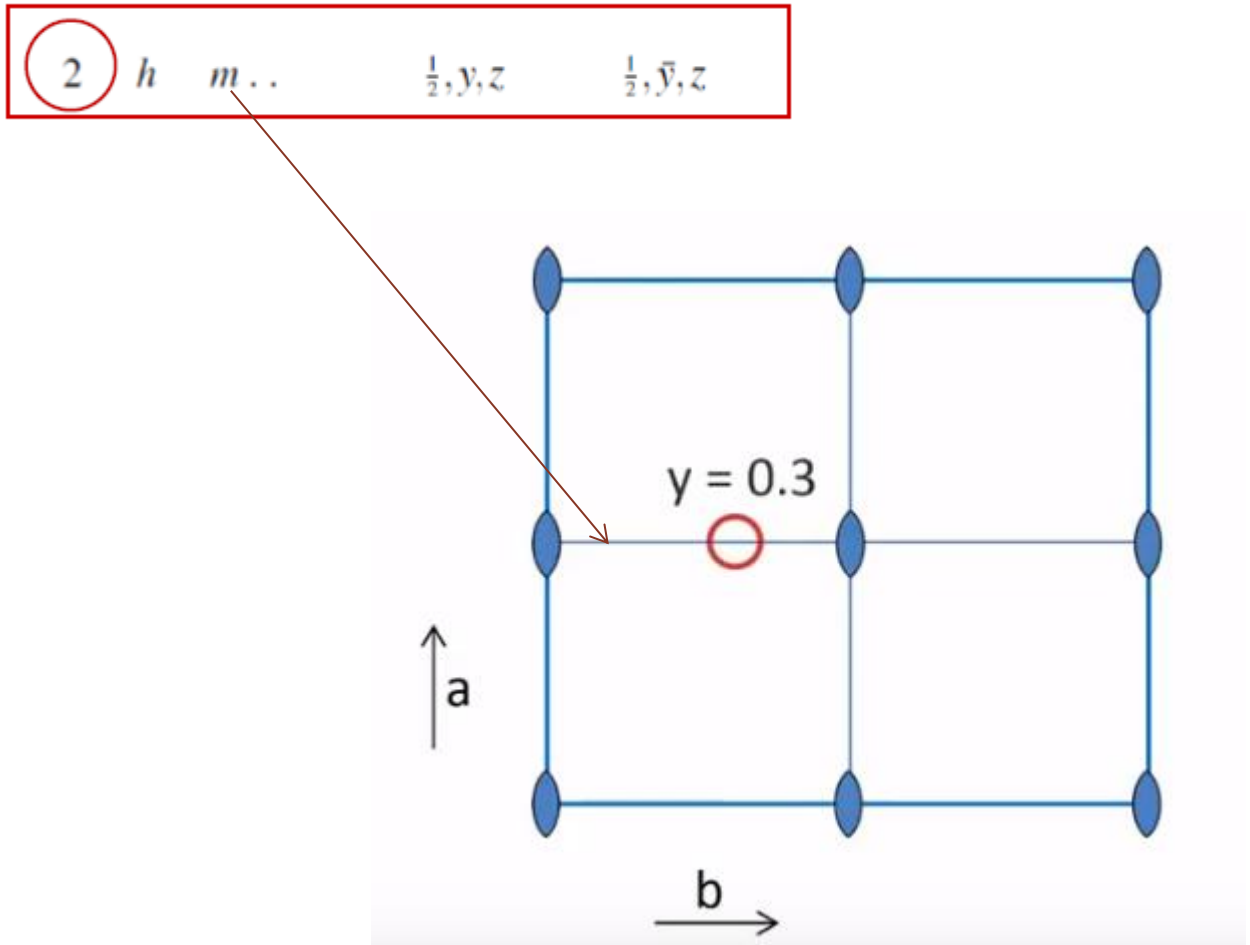
special positions (at SEs!)

Site symmetry (on which SE(s) does this point sit?)

alphabetic

Multiplicity (= number of equivalent sites/points within the unit cell)

Space Groups

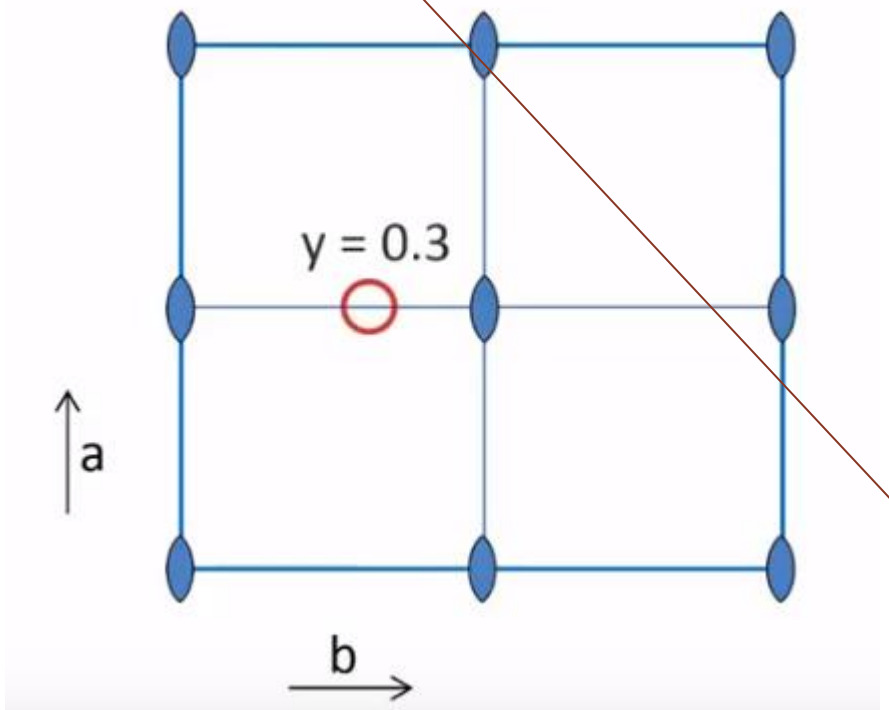


Wyckoff letter h.
Átomo na posição
(1/2,y,z)

Escolhi
(1/2, 0.3, z)

Space Groups

2	*h*	*m* . .	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$



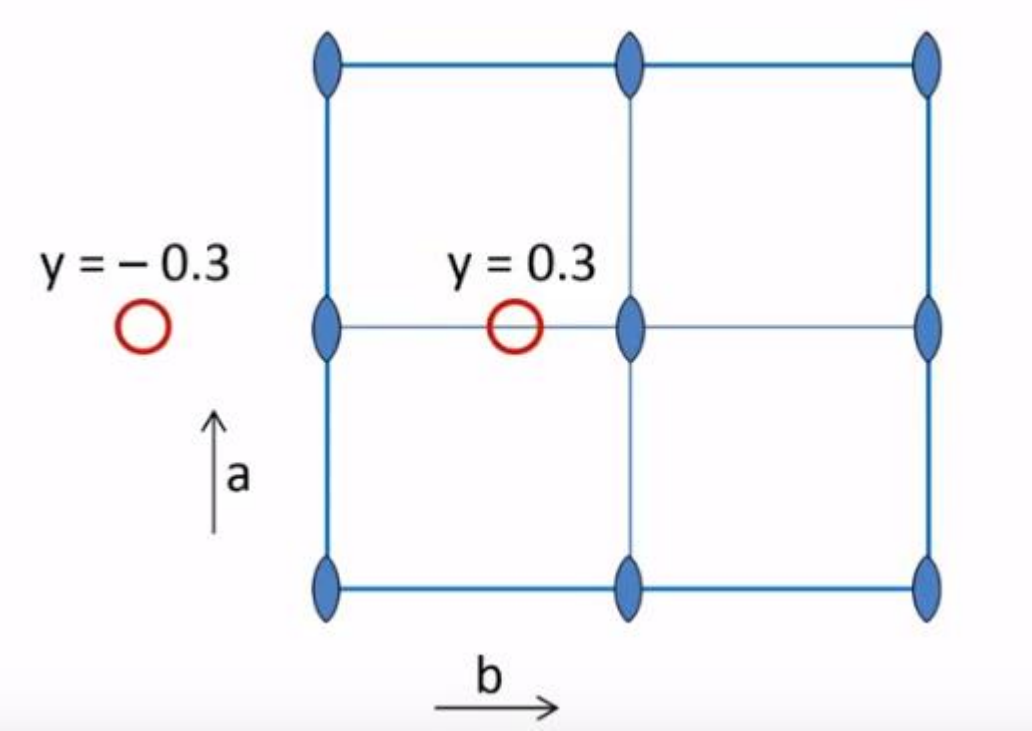
Wyckoff letter h.
Átomo na posição
(1/2,y,z)

Escolhi
(1/2, 0.3, z)

Vai gerar uma posição equivalente em
(1/2, -y, z)

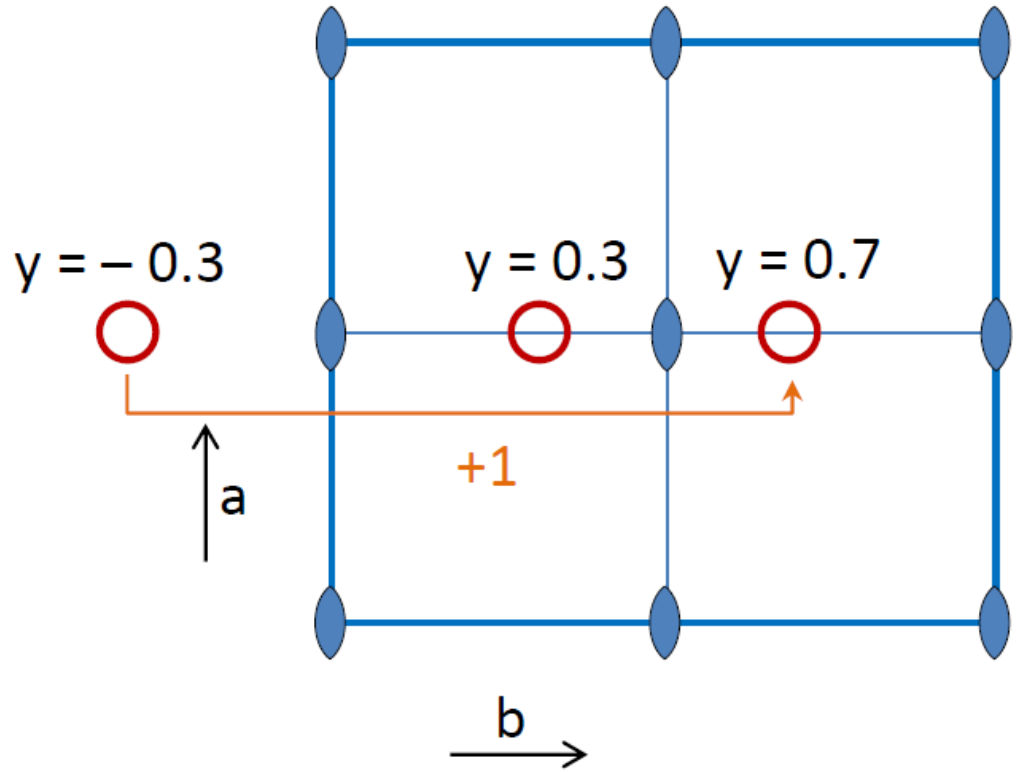
Space Groups

2	*h*	*m* . .	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$



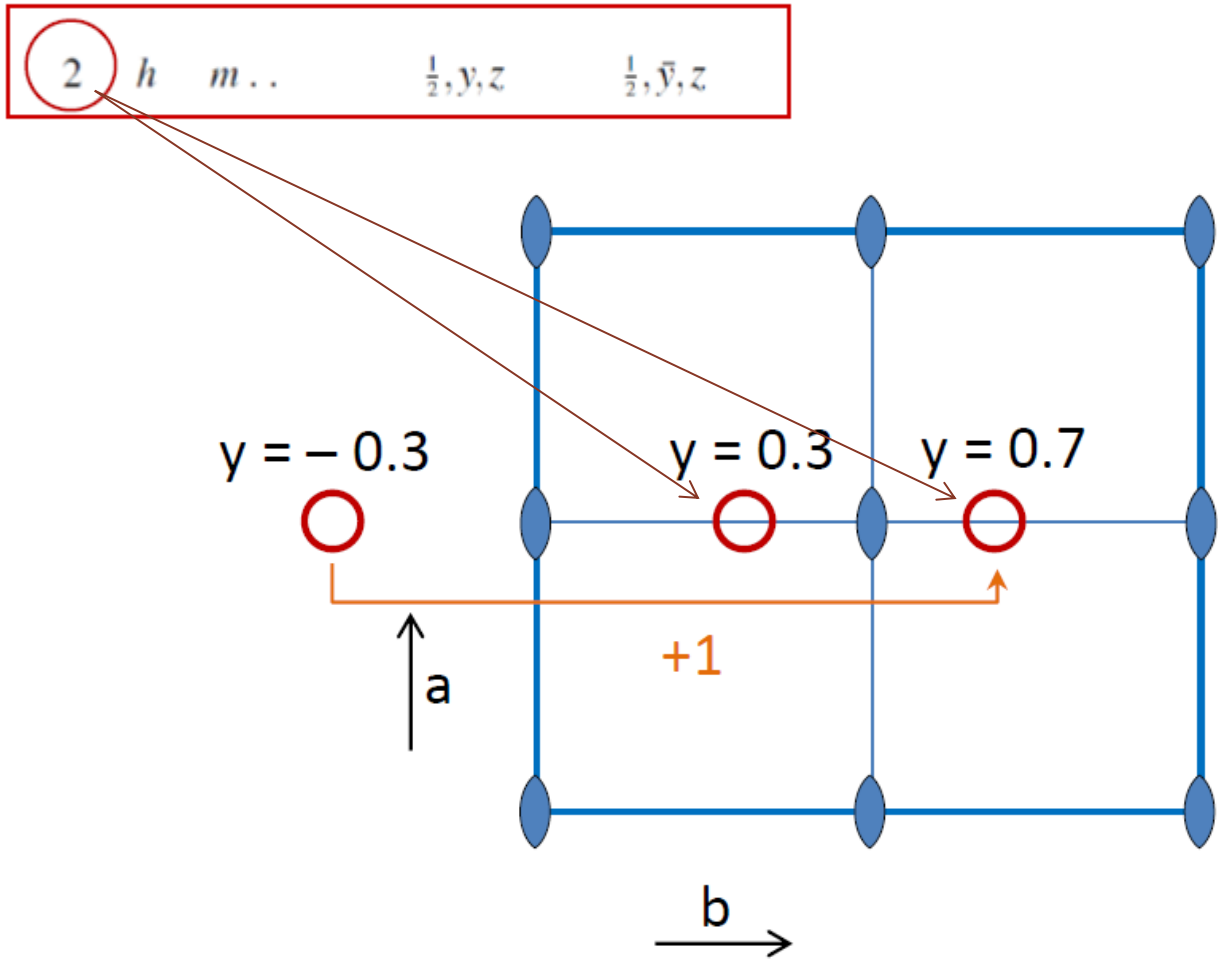
Space Groups

2	*h*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$



Pela simetria de translação posso andar 1 comprimento de célula em b.

Space Groups



Pela simetria de translação posso andar 1 comprimento de célula em b.

Veja que podemos aplicar os outros elementos de simetria mas nenhum outra posição será gerada.

Temos 2 posições equivalentes

Space Groups

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
2	*h*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
2	*g*	*m* . .	$0,y,z$	$0,\bar{y},z$		
2	*f*	. *m* .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$		
2	*e*	. *m* .	$x,0,z$	$\bar{x},0,z$		
1	*d*	*m m* 2	$\frac{1}{2},\frac{1}{2},z$			
1	*c*	*m m* 2	$\frac{1}{2},0,z$			
1	*b*	*m m* 2	$0,\frac{1}{2},z$			
1	*a*	*m m* 2	$0,0,z$			

general positions

special positions (at SEs!)

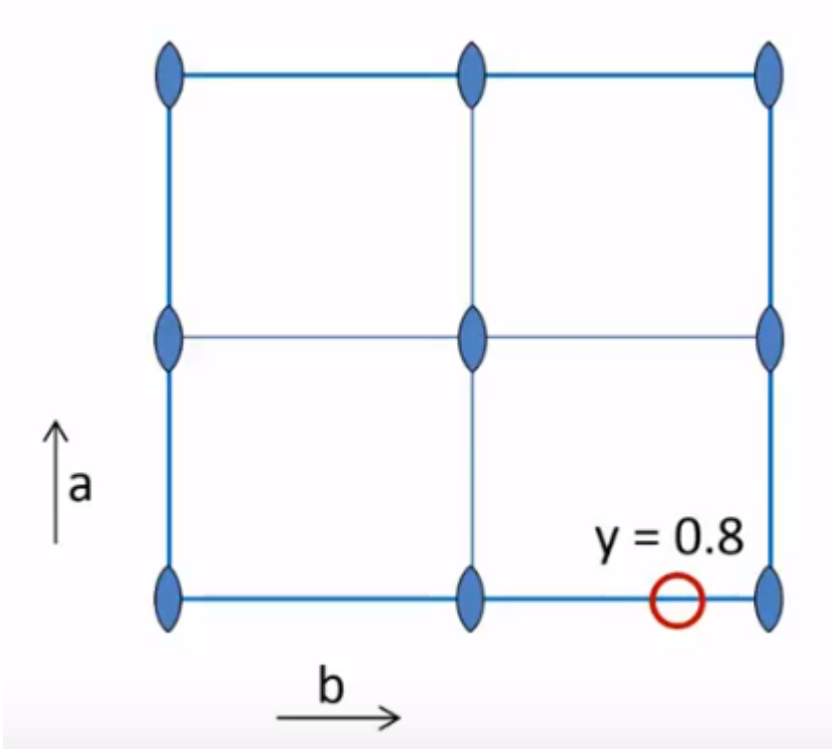
Site symmetry (on which SE(s) does this point sit?)

alphabetic

Multiplicity (= number of equivalent sites/points within the unit cell)

Space Groups

2	*g*	*m* . .	$0,y,z$	$0,\bar{y},z$

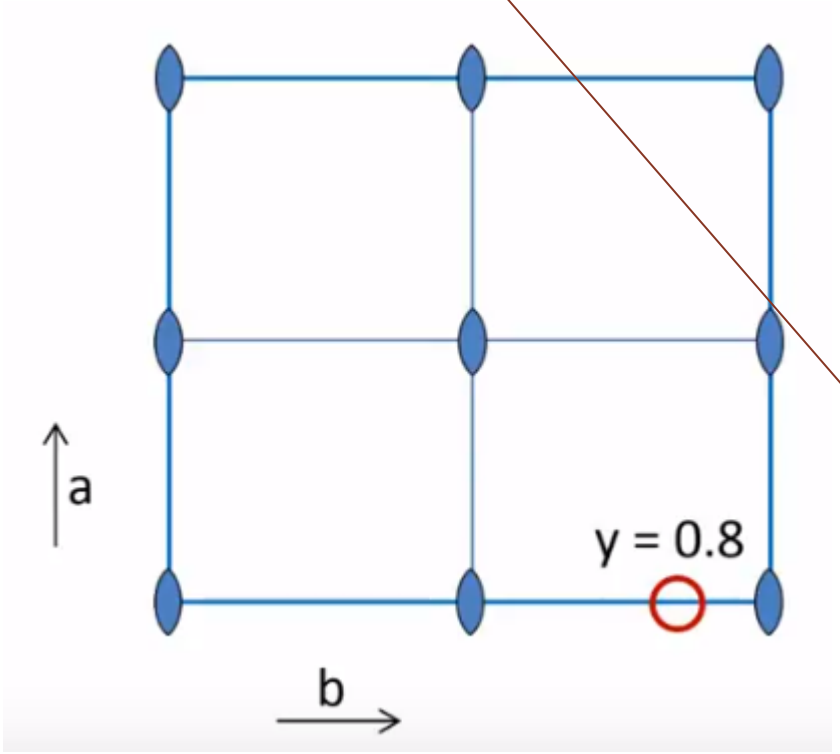


Wyckoff letter g.
Átomo na posição
(0,y,z)

Escolhi
(0, 0.8, z)

Space Groups

2	*g*	*m* . .	0, *y*, *z*	0, $\bar{y}$, *z*



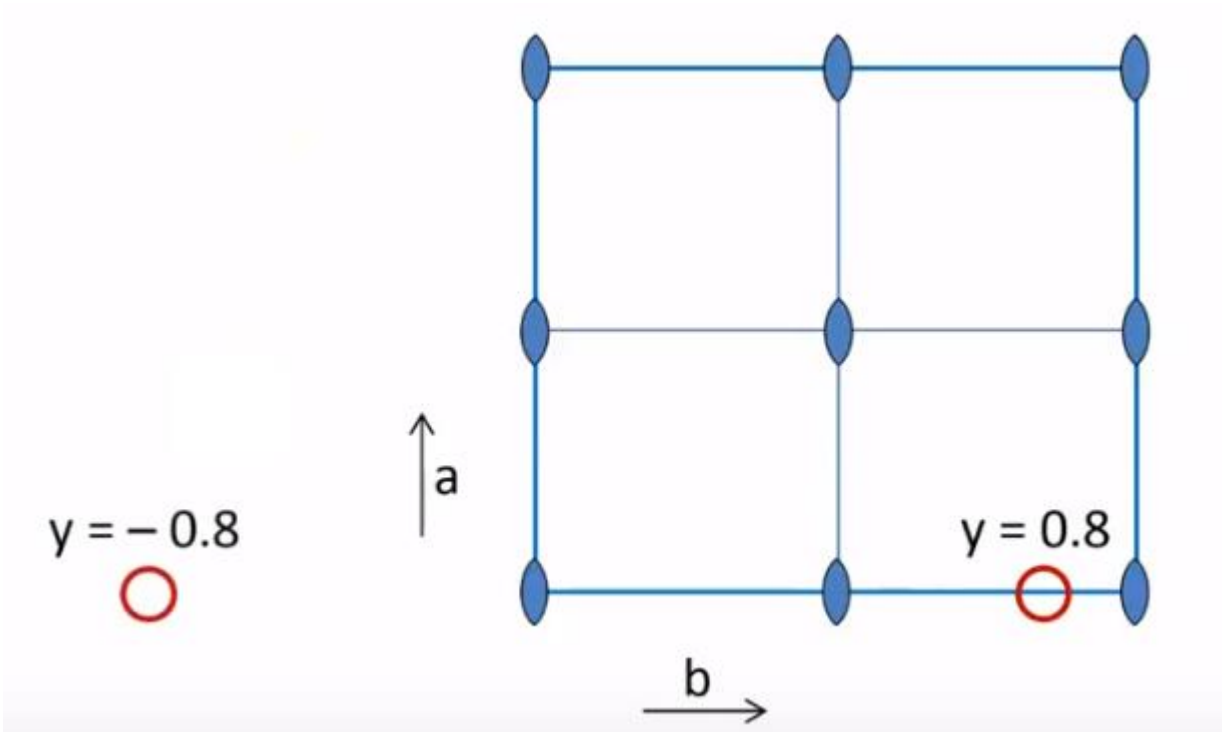
Wyckoff letter g.
Átomo na posição
(0,y,z)

Escolhi
(0, 0.8, z)

Vai gerar uma posição equivalente em:
(0,-0.8,z)

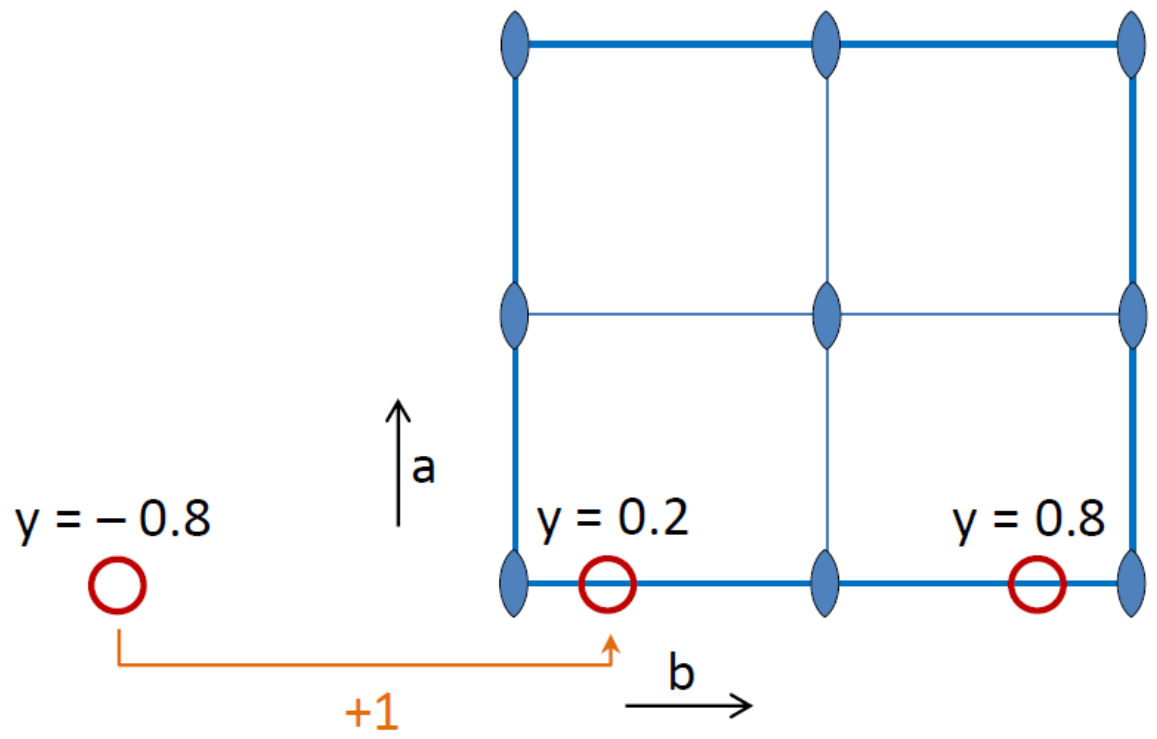
Space Groups

2	g	m . .		$0,y,z$	$0,\bar{y},z$



Space Groups

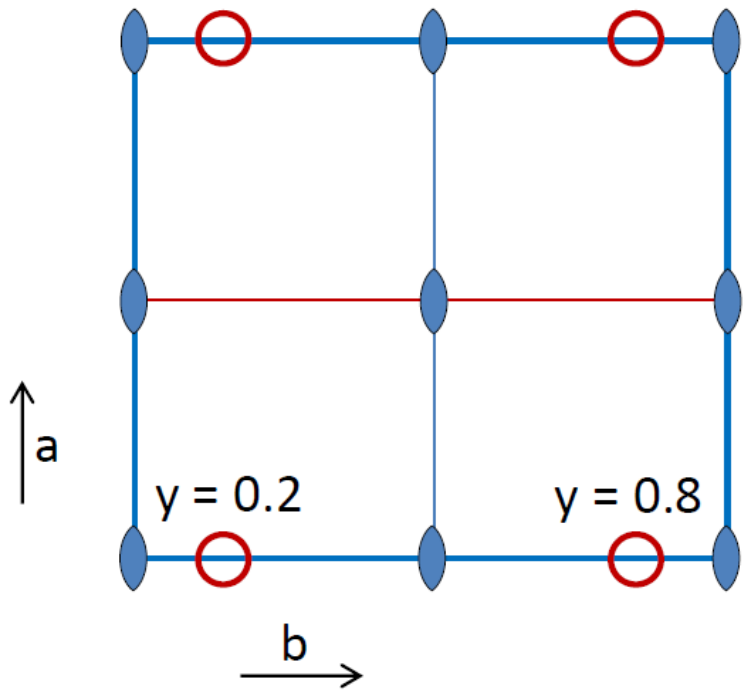
2	*g*	*m* . .	$0,y,z$	$0,\bar{y},z$



Pela simetria de translação posso andar 1 comprimento de célula em b.

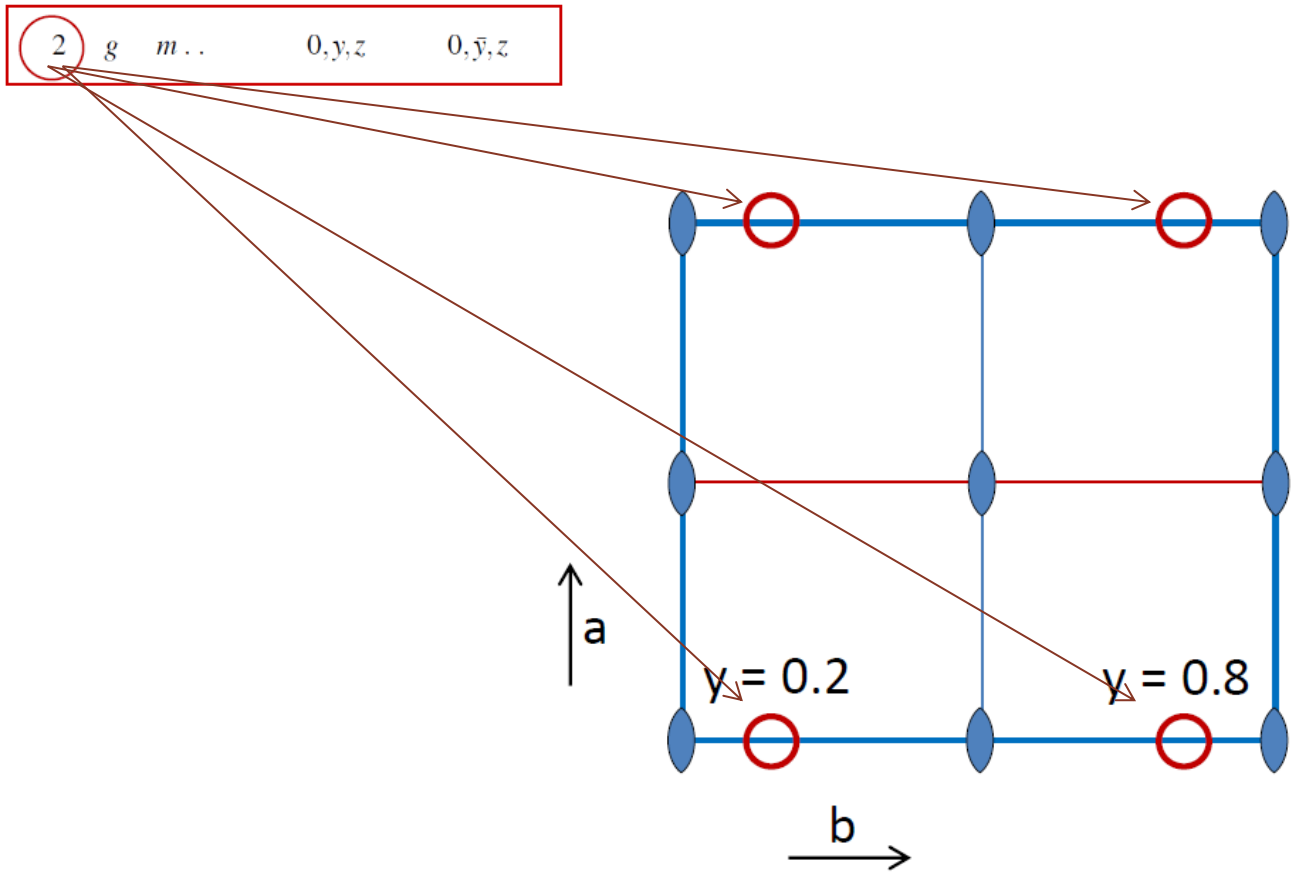
Space Groups

2	*g*	*m* . .	0, *y*, *z*	0, $\bar{y}$, *z*



O espelho localizado em (1/2,y,z) vai gerar outras duas posições equivalentes.

Space Groups



O espelho localizado em (1/2,y,z) vai gerar outras duas posições equivalentes.

Veja que cada átomo colocado está com metade de seu volume dentro da célula, totalizando 2 posições equivalentes.

Space Groups

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
2	*h*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
2	*g*	*m* . .	$0,y,z$	$0,\bar{y},z$		
2	*f*	. *m* .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$		
2	*e*	. *m* .	$x,0,z$	$\bar{x},0,z$		
1	*d*	*m m* 2	$\frac{1}{2},\frac{1}{2},z$			
1	*c*	*m m* 2	$\frac{1}{2},0,z$			
1	*b*	*m m* 2	$0,\frac{1}{2},z$			
1	*a*	*m m* 2	$0,0,z$			

general positions

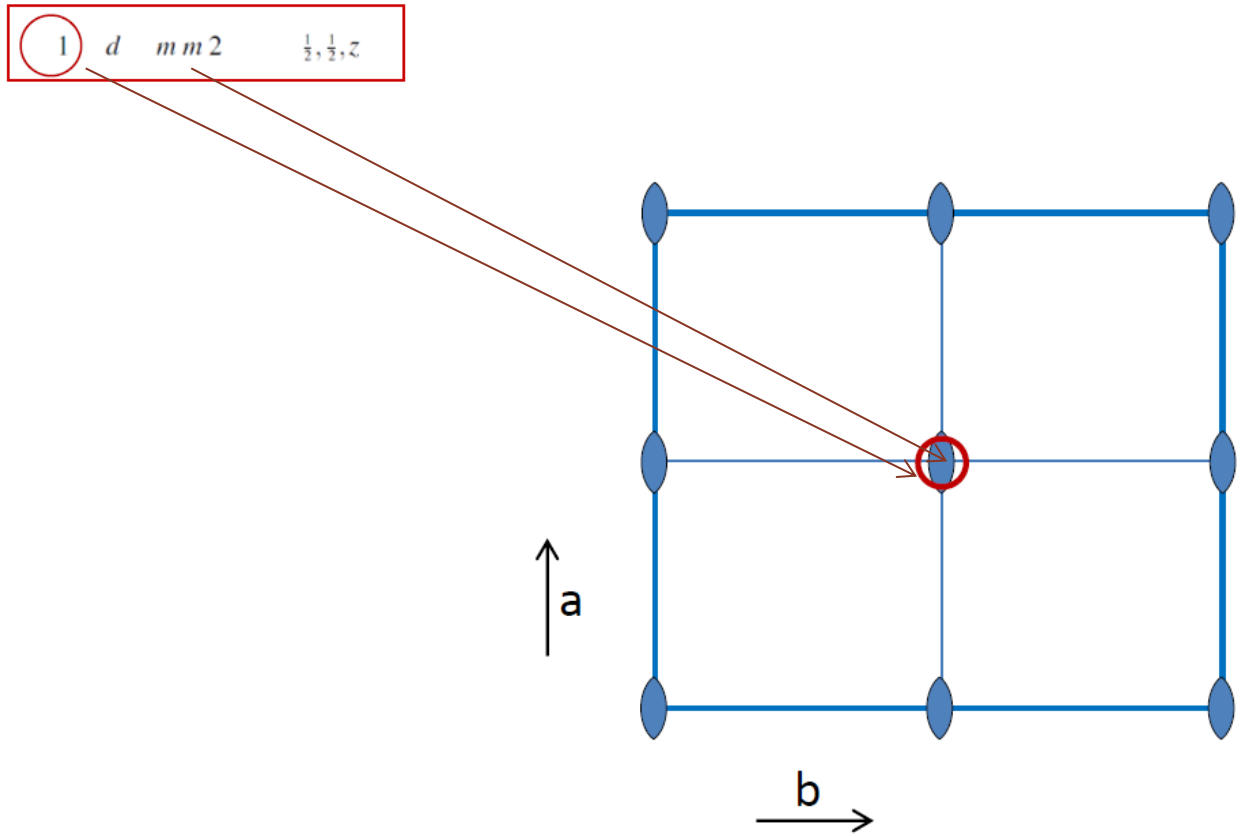
special positions (at SEs!)

Site symmetry (on which SE(s) does this point sit?)

alphabetic

Multiplicity (= number of equivalent sites/points within the unit cell)

Space Groups



Veja que apenas uma posição equivalente é obtida quando se coloca um átomo nessa posição especial “d”.

Space Groups

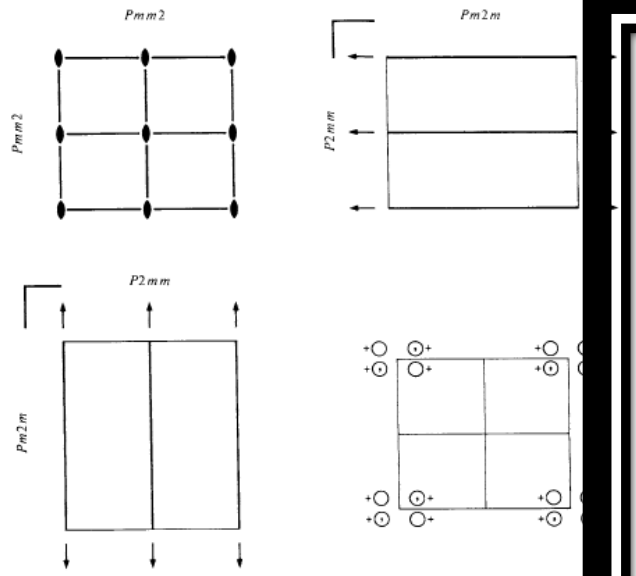
- Pmm

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

Pmm2 C_{2v}^1 *mm2* Orthorhombic

No. 25 *Pmm2*

Patterson symmetry *Pmmm*



Origin on *mm2*

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

Symmetry operations

(1) 1 (2) 2 0,0,*z* (3) *m* *x*,0,*z* (4) *m* 0,*y*,*z*

Generators selected (1); *t*(1,0,0); *t*(0,1,0); *t*(0,0,1); (2); (3)

Reflection conditions

General:

no conditions

Special: no extra conditions

Reflection conditions

General:

no conditions

Special: no extra conditions

Along [010] *p* 1 1 *m*
a′ = **c** **b**′ = **a**
Origin at 0,*y*,0

IIb [2] *Pma2* (**a**′ = 2**a**) (28); [2] *Pbm2* (**b**′ = 2**b**) (*Pma2*, 28); [2] *Pcc2* (**c**′ = 2**c**) (27); [2] *Pmc2*$_1$ (**c**′ = 2**c**) (26); [2] *Pcm2*$_1$ (**c**′ = 2**c**) (*Pmc2*$_1$, 26); [2] *Aem2* (**b**′ = 2**b**, **c**′ = 2**c**) (39); [2] *Amm2* (**b**′ = 2**b**, **c**′ = 2**c**) (38); [2] *Bme2* (**a**′ = 2**a**, **c**′ = 2**c**) (*Aem2*, 39); [2] *Bmm2* (**a**′ = 2**a**, **c**′ = 2**c**) (*Amm2*, 38); [2] *Cmm2* (**a**′ = 2**a**, **b**′ = 2**b**) (35); [2] *Fmm2* (**a**′ = 2**a**, **b**′ = 2**b**, **c**′ = 2**c**) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] *Pmm2* (**a**′ = 2**a** or **b**′ = 2**b**) (25); [2] *Pmm2* (**c**′ = 2**c**) (25)

Minimal non-isomorphic supergroups

I [2] *Pmmm* (47); [2] *Pmma* (51); [2] *Pmmn* (59); [2] *P4mm* (99); [2] *P4*$_2$*mc* (105); [2] *P*$\bar{4}$*m2* (115)

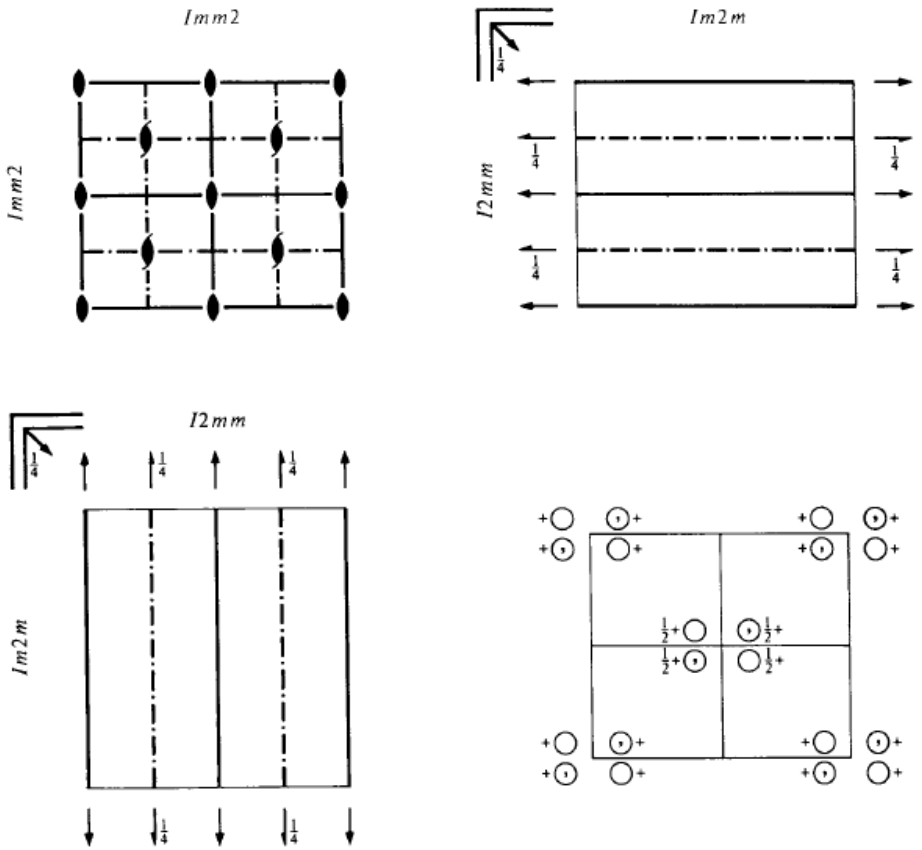
II [2] *Cmm2* (35); [2] *Amm2* (38); [2] *Bmm2* (*Amm2*, 38); [2] *Imm2* (44)

Space Groups

- Outro exemplo: Imm2

$Imm2$ C_{2v}^{20} $mm2$ Orthorhombic

No. 44 $Imm2$ Patterson symmetry $Immm$



Origin on $mm2$

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

Symmetry operations

For $(0,0,0)+$ set

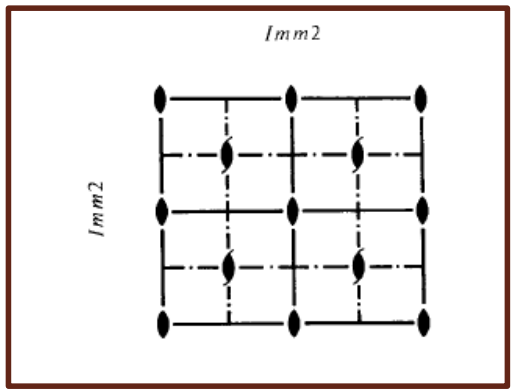
(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

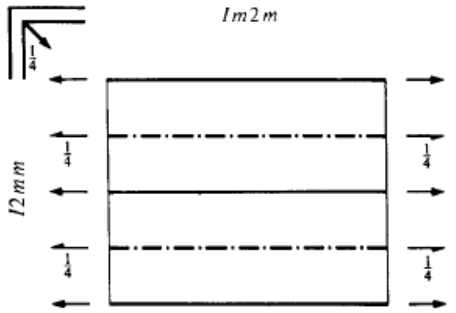
For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

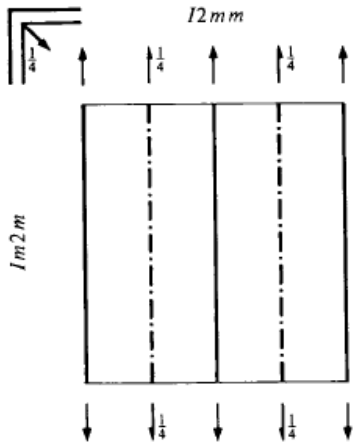
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

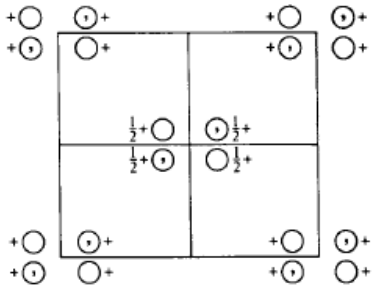
$Imm2$ C_{2v}^{20} $mm2$ Orthorhombic

No. 44 $Imm2$ Patterson symmetry $Immm$









Origin on $mm2$

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

Symmetry operations

For $(0,0,0)+$ set

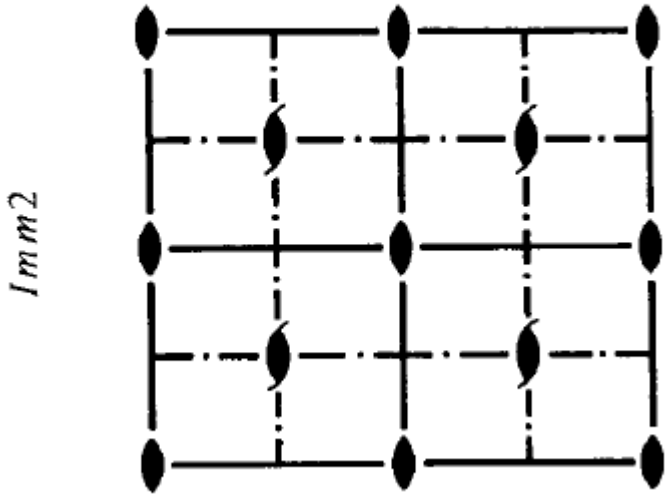
(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Space Groups

$Imm2$



Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

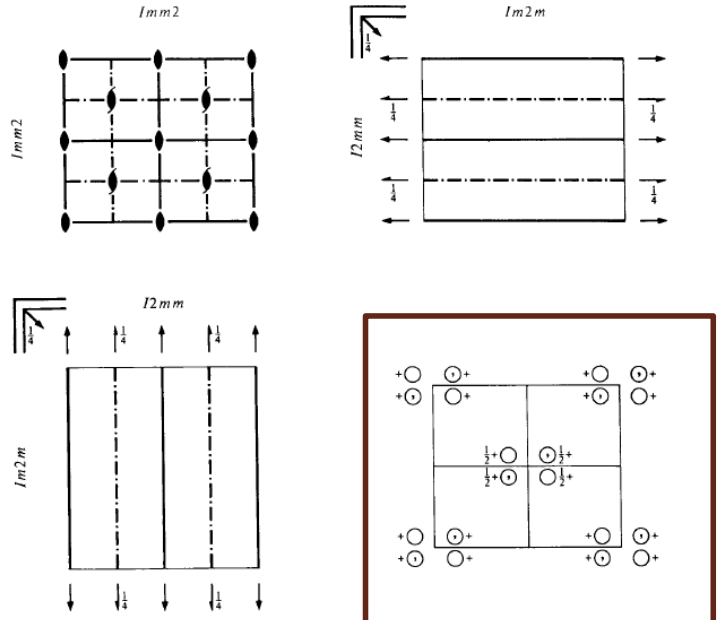
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Space Groups

$Imm2$ C_{2v}^{20} $mm2$ Orthorhombic

No. 44 $Imm2$

Patterson symmetry $Immm$



Origin on $mm2$

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

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

CONTINUED No. 44 $Imm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
				$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
4	d	m . .	$0,y,z$	$0,\bar{y},z$		
4	c	. m .	$x,0,z$	$\bar{x},0,z$		
2	b	$mm2$	$0,\frac{1}{2},z$			
2	a	$mm2$	$0,0,z$			

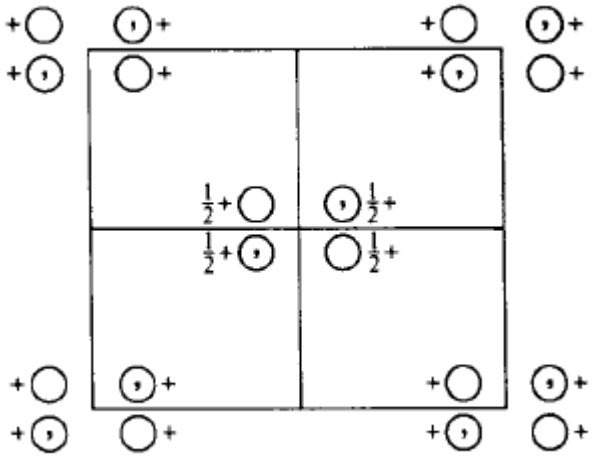
Reflection conditions

General:

hkl : $h+k+l=2n$
$0kl$: $k+l=2n$
$h0l$: $h+l=2n$
$hk0$: $h+k=2n$
$h00$: $h=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

Special: no extra conditions

Space Groups

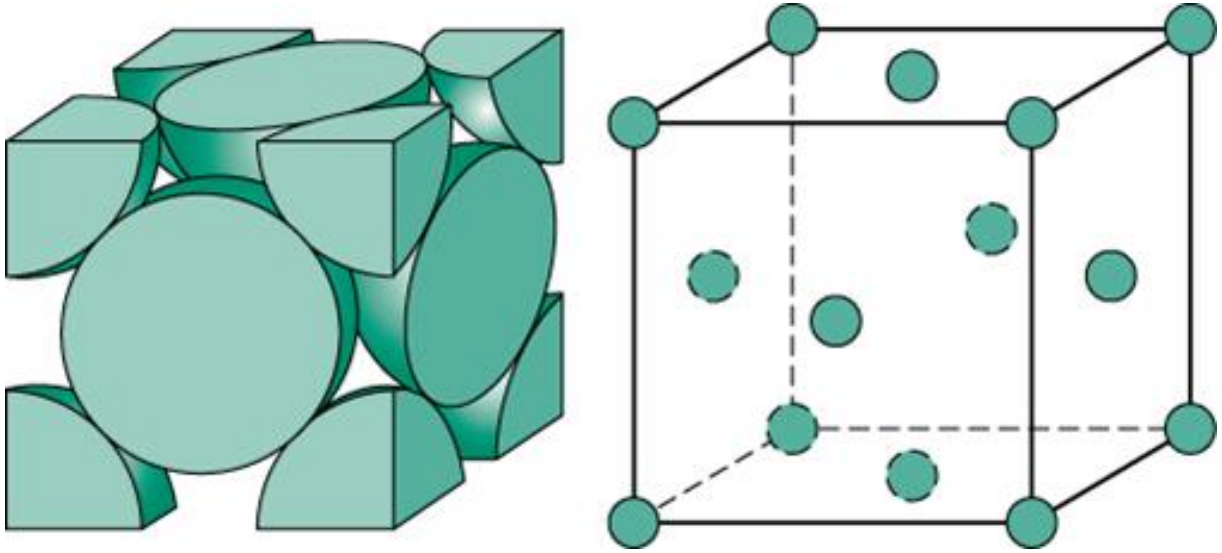


Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
4	d	m . .	$0,y,z$	$0,\bar{y},z$		
4	c	. m .	$x,0,z$	$\bar{x},0,z$		
2	b	$m\,m\,2$	$0,\frac{1}{2},z$			
2	a	$m\,m\,2$	$0,0,z$			

Space Groups

- Outro exemplo: $Fm\bar{3}m$



Estrutura tão simples…..

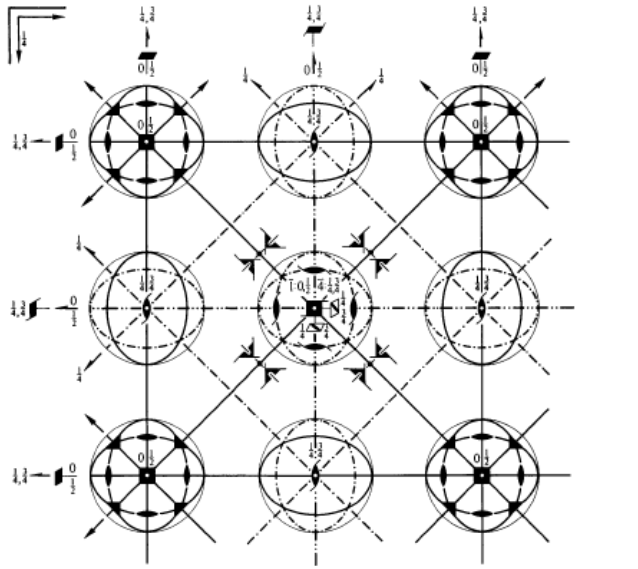
Space Groups

- Outro e

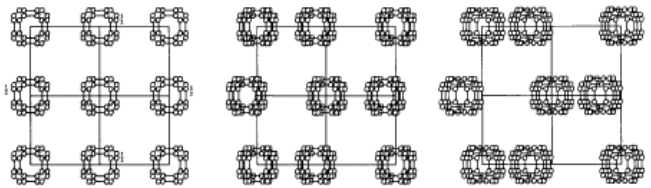
International Tables for Crystallography (2006). Vol. A, Space group 225, pp. 688–691.

$F\,m\,\bar{3}\,m$ O_h^5 $m\bar{3}m$ Cubic

No. 225 $F\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $F\,m\bar{3}m$



Upper left quadrant only



Origin at centre $(m\bar{3}m)$

Asymmetric unit $0\le x\le\frac{1}{4};\quad 0\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{4};\quad y\le\min(x,\frac{1}{2}-x);\quad z\le y$

Vertices $0,0,0\quad\frac{1}{2},0,0\quad\frac{1}{4},\frac{1}{4},0\quad\frac{1}{2},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(*given on page 691*)

Symmetry operations

For (0,0,0)+ set

(1) 1 (2) 2 0,0,*z* (3) 2 0,*y*,0 (4) 2 *x*,0,0
(5) 3⁺ *x*,*x*,*x* (6) 3⁺ *x*,*x*,*x̄* (7) 3⁺ *x*,*x̄*,*x* (8) 3⁺ *x*,*x̄*,*x̄*
(9) 3⁻ *x*,*x*,*x* (10) 3⁻ *x*,*x*,*x̄* (11) 3⁻ *x*,*x̄*,*x* (12) 3⁻ *x*,*x̄*,*x̄*
(13) 2 *x*,*x*,0 (14) 2 *x*,*x̄*,0 (15) 4⁻ 0,0,*z* (16) 4⁺ 0,0,*z*
(17) 4⁻ *x*,0,0 (18) 2 0,*y*,*y* (19) 2 0,*y*,*ȳ* (20) 4⁺ *x*,0,0
(21) 4⁺ 0,*y*,0 (22) 2 *x*,0,*x* (23) 4⁻ 0,*y*,0 (24) 2 *x̄*,0,*x*
(25) $\bar{1}$ 0,0,0 (26) *m* *x*,*y*,0 (27) *m* *x*,0,*z* (28) *m* 0,*y*,*z*
(29) 3⁺ *x*,*x*,*x*; 0,0,0 (30) 3⁺ *x*,*x*,*x̄*; 0,0,0 (31) 3⁺ *x*,*x̄*,*x*; 0,0,0 (32) 3⁺ *x*,*x̄*,*x̄*; 0,0,0
(33) 3⁻ *x*,*x*,*x*; 0,0,0 (34) 3⁻ *x*,*x̄*,*x̄*; 0,0,0 (35) 3⁻ *x̄*,*x*,*x*; 0,0,0 (36) 3⁻ *x̄*,*x*,*x̄*; 0,0,0
(37) *m* *x*,*x*,*z* (38) *m* *x*,*x*,*z* (39) 4̄⁻ 0,0,*z*; 0,0,0 (40) 4̄⁺ 0,0,*z*; 0,0,0
(41) 4̄⁻ *x*,0,0; 0,0,0 (42) *m* *x*,*y*,*y* (43) *m* *x*,*y*,*y* (44) 4̄⁺ *x*,0,0; 0,0,0
(45) 4̄⁺ 0,*y*,0; 0,0,0 (46) *m* *x*,*y*,*x* (47) 4̄⁻ 0,*y*,0; 0,0,0 (48) *m* *x*,*y*,*x*

For $(0,\frac{1}{2},\frac{1}{2})$+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{2}$ (4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x-\frac{1}{4},x$ (6) 3^+ $x,x+\frac{1}{2},\bar{x}$ (7) $3^+(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x}-\frac{1}{4},x$ (8) 3^+ $x,\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x+\frac{1}{4},x$ (10) $3^-(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}$ (11) 3^- $\bar{x}+\frac{1}{2},x+\frac{1}{2},x$ (12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x+\frac{1}{2},\frac{1}{4}$ (14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$ (15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (16) $4^+(0,0,\frac{1}{2})$ $-\frac{1}{4},\frac{1}{4},z$
(17) 4^- $x,\frac{1}{4},0$ (18) $2(0,\frac{1}{4},\frac{1}{4})$ $0,y,y$ (19) 2 $0,y+\frac{1}{2},y$ (20) 4^+ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{4},y,\frac{1}{4}$ (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},\frac{1}{4},x$ (23) $4^-(0,\frac{1}{4},0)$ $-\frac{1}{4},y,\frac{1}{4}$ (24) $2(-\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$ (26) *b* $x,y,\frac{1}{2}$ (27) *c* $x,\frac{1}{4},z$ (28) $n(0,\frac{1}{4},\frac{1}{4})$ $0,y,z$
(29) 3^+ $x,x+\frac{1}{4},x;\ 0,\frac{1}{4},0$ (30) 3^+ $\bar{x}-1,x+\frac{1}{4},x;\ -\frac{1}{4},0,\frac{1}{4}$ (31) 3^+ $x,x+\frac{1}{4},\bar{x};\ 0,\frac{1}{4},0$ (32) 3^+ $x+1,x+\frac{1}{4},x;\ \frac{1}{4},0,\frac{1}{4}$
(33) 3^- $x-\frac{1}{4},x-\frac{1}{4},x;\ 0,0,\frac{1}{2}$ (34) 3^- $x+\frac{1}{4},\bar{x}-\frac{1}{4},x;\ 0,0,\frac{1}{2}$ (35) 3^- $\bar{x}-\frac{1}{4},x+\frac{1}{4},x;\ -\frac{1}{4},\frac{1}{4},0$ (36) 3^- $\bar{x}+\frac{1}{4},x+\frac{1}{4},\bar{x};\ \frac{1}{4},\frac{1}{4},0$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x,z$ (38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$ (39) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) 4^- $x,0,\frac{1}{4};\ 0,0,\frac{1}{4}$ (42) *m* $x,y+\frac{1}{4},y$ (43) $g(0,\frac{1}{4},\frac{1}{4})$ x,y,y (44) $\bar{4}^+$ $x,\frac{1}{4},0;\ 0,\frac{1}{4},0$
(45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (46) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ (47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ (48) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},y,x$

For $(\frac{1}{4},0,\frac{1}{4})$+ set

(1) $t(\frac{1}{4},0,\frac{1}{4})$ (2) $2(0,0,\frac{1}{4})$ $\frac{1}{4},0,z$ (3) 2 $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{4},0,0)$ $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x-\frac{1}{4},x$ (6) $3^+(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $\bar{x}+\frac{1}{4},x+\frac{1}{4},\bar{x}$ (7) 3^+ $x+\frac{1}{4},x-\frac{1}{4},x$ (8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(9) $3^-(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x-\frac{1}{4},x$ (10) 3^- $x+\frac{1}{4},\bar{x},x$ (11) 3^- $\bar{x}+\frac{1}{4},x,x$ (12) $3^-(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $\bar{x}-\frac{1}{4},x+\frac{1}{4},x$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x-\frac{1}{4},\frac{1}{4}$ (14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$ (15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},-\frac{1}{4},z$ (16) $4^+(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{1}{4},\frac{1}{4}$ (18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y-\frac{1}{4},y$ (19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$ (20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{4}$
(21) 4^+ $\frac{1}{4},y,0$ (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,0,x$ (23) 4^- $0,y,\frac{1}{4}$ (24) 2 $\bar{x}+\frac{1}{2},0,x$
(25) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$ (26) *a* $x,y,\frac{1}{4}$ (27) $n(\frac{1}{4},0,\frac{1}{4})$ $x,0,z$ (28) *c* $\frac{1}{4},y,z$
(29) 3^+ $x-\frac{1}{4},x-\frac{1}{4},x;\ 0,0,\frac{1}{2}$ (30) 3^+ $\bar{x}-\frac{1}{4},x+\frac{1}{4},x;\ 0,0,\frac{1}{2}$ (31) 3^+ $x+\frac{1}{4},x+\frac{1}{4},\bar{x};\ \frac{1}{4},\frac{1}{4},0$ (32) 3^+ $x+\frac{1}{4},\bar{x}-\frac{1}{4},x;\ \frac{1}{4},-\frac{1}{4},0$
(33) 3^- $x+\frac{1}{4},x,x;\ \frac{1}{4},0,0$ (34) 3^- $x+\frac{1}{4},x-1,x;\ 0,-\frac{1}{2},\frac{1}{2}$ (35) 3^- $x+\frac{1}{4},x+1,x;\ 0,\frac{1}{2},\frac{1}{2}$ (36) 3^- $\bar{x}+\frac{1}{4},x,x;\ \frac{1}{2},0,0$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x,z$ (38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x,z$ (39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ (40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(41) 4^- $x,-\frac{1}{4},\frac{1}{4};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$ (42) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$ (43) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$ (44) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+$ $0,y,\frac{1}{4};\ 0,0,\frac{1}{4}$ (46) *m* $x+\frac{1}{4},y,x$ (47) $\bar{4}^-$ $\frac{1}{4},y,0;\ \frac{1}{4},0,0$ (48) $g(\frac{1}{4},0,\frac{1}{4})$ x,y,x

For $(\frac{1}{4},\frac{1}{4},0)$+ set

(1) $t(\frac{1}{4},\frac{1}{4},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{4},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{4},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x+\frac{1}{4},x$ (6) 3^+ $x+\frac{1}{4},x,\bar{x}$ (7) 3^+ $\bar{x}+\frac{1}{4},x,x$ (8) $3^+(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},x+\frac{1}{4},x$
(9) $3^-(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x+\frac{1}{4},x$ (10) 3^- $x,x+\frac{1}{2},x$ (11) $3^-(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},x+\frac{1}{2},x$ (12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,0$ (14) 2 $x,\bar{x}+\frac{1}{2},0$ (15) 4^- $\frac{1}{2},0,z$ (16) 4^+ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{1}{4},-\frac{1}{4}$ (18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},y$ (19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$ (20) $4^+(\frac{1}{4},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{4},y,-\frac{1}{4}$ (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},\frac{1}{4},x$ (23) $4^-(0,\frac{1}{4},0)$ $\frac{1}{4},y,\frac{1}{4}$ (24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ (26) $n(\frac{1}{4},\frac{1}{4},0)$ $x,y,0$ (27) *a* $x,\frac{1}{4},z$ (28) *b* $\frac{1}{4},y,z$
(29) 3^+ $x+\frac{1}{4},x,x;\ \frac{1}{4},0,0$ (30) 3^+ $\bar{x}-\frac{1}{4},x+1,x;\ 0,\frac{1}{4},\frac{1}{2}$ (31) 3^+ $x-\frac{1}{4},x+1,x;\ 0,\frac{1}{4},-\frac{1}{2}$ (32) 3^+ $x+\frac{1}{4},x,x;\ \frac{1}{4},0,0$
(33) 3^- $x,x+\frac{1}{4},x;\ 0,\frac{1}{4},0$ (34) 3^- $x+1,x-\frac{1}{4},x;\ \frac{1}{2},0,\frac{1}{2}$ (35) 3^- $x,x+\frac{1}{4},x;\ 0,\frac{1}{4},0$ (36) 3^- $x+1,x-\frac{1}{4},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$
(37) m $x+\frac{1}{4},x,z$ (38) $g(\frac{1}{4},\frac{1}{4},0)$ x,x,z (39) $\bar{4}^-$ $0,\frac{1}{4},z;\ 0,\frac{1}{4},0$ (40) $\bar{4}^+$ $\frac{1}{2},0,z;\ \frac{1}{2},0,0$
(41) 4^- $x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ (42) $g(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},y$ (43) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,y,y (44) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ (46) $g(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ (47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$ (48) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},y,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			h,k,l permutable General:
192 l 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y,x,\bar{z}$ (17) $x,z,\bar{y}$ (21) $z,y,\bar{x}$ (25) $\bar{x},\bar{y},z$ (29) $\bar{z},\bar{x},\bar{y}$ (33) $\bar{y},\bar{z},\bar{x}$ (37) $\bar{y},\bar{x},z$ (41) $\bar{x},\bar{z},y$ (45) $\bar{z},\bar{y},x$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y},\bar{x},\bar{z}$ (18) $\bar{x},z,\bar{y}$ (22) $z,\bar{y},\bar{x}$ (26) $x,\bar{y},\bar{z}$ (30) $\bar{z},x,\bar{y}$ (34) $\bar{y},\bar{z},x$ (38) $\bar{y},x,\bar{z}$ (42) $x,\bar{z},\bar{y}$ (46) $\bar{z},\bar{y},\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y,\bar{x},z$ (19) $\bar{x},\bar{z},y$ (23) $\bar{z},y,x$ (27) $x,\bar{y},z$ (31) $z,x,\bar{y}$ (35) $\bar{y},z,x$ (39) $\bar{y},x,\bar{z}$ (43) x,z,y (47) $z,\bar{y},\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y},x,z$ (20) $x,\bar{z},y$ (24) $\bar{z},\bar{y},\bar{x}$ (28) $\bar{x},y,z$ (32) $z,\bar{x},y$ (36) $y,z,\bar{x}$ (40) $y,\bar{x},z$ (44) $\bar{x},z,\bar{y}$ (48) z,y,x		hkl : $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ hhl : $h+l=2n$ $h00$: $h=2n$
							Special: as above, plus
96 k . . m	x,x,z $z,\bar{x},x$ $\bar{x},x,z$ $\bar{x},\bar{z},\bar{x}$	$\bar{x},\bar{x},z$ $z,x,\bar{x}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{z},x$	$\bar{x},x,\bar{z}$ x,z,x $x,\bar{x},z$ $z,x,\bar{x}$	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$ $\bar{x},x,\bar{z}$ $z,\bar{x},x$	z,x,x $x,\bar{z},\bar{x}$ $x,z,\bar{x}$ $\bar{z},x,x$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$ $\bar{x},z,x$ $\bar{z},\bar{x},\bar{x}$	no extra conditions
96 j m . .	$0,y,z$ $z,0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $z,0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,z,y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},z,0$ $0,z,y$ $z,\bar{y},0$	no extra conditions
48 i m . $m2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$	no extra conditions
48 h m . $m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,y,0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$	no extra conditions
48 g 2 . mm	$x,\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},x,\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $x,\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$ $\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$ $\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{1}{4},\frac{3}{4},x$	hkl : $h=2n$
32 f . 3 m	x,x,x $x,\bar{x},\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			no extra conditions
24 e 4 m . m	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24 d m . mm	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$
8 c $\bar{4}$ 3 m	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$					hkl : $h=2n$
4 b $m\bar{3}$ m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4 a $m\bar{3}$ m	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Construindo arquivos CIF

- Vamos usar o software Vesta.

- Ex: Alumínio

Sistema: Cúbico

Grupo espacial: $Fm\bar{3}m$

Parâmetro de rede a=4,05A

Posição dos átomo: Wyckoff position= “a”