Une petite exploration des orbites (*cristallographiques*) dans l'espace (*direct et réciproque*)

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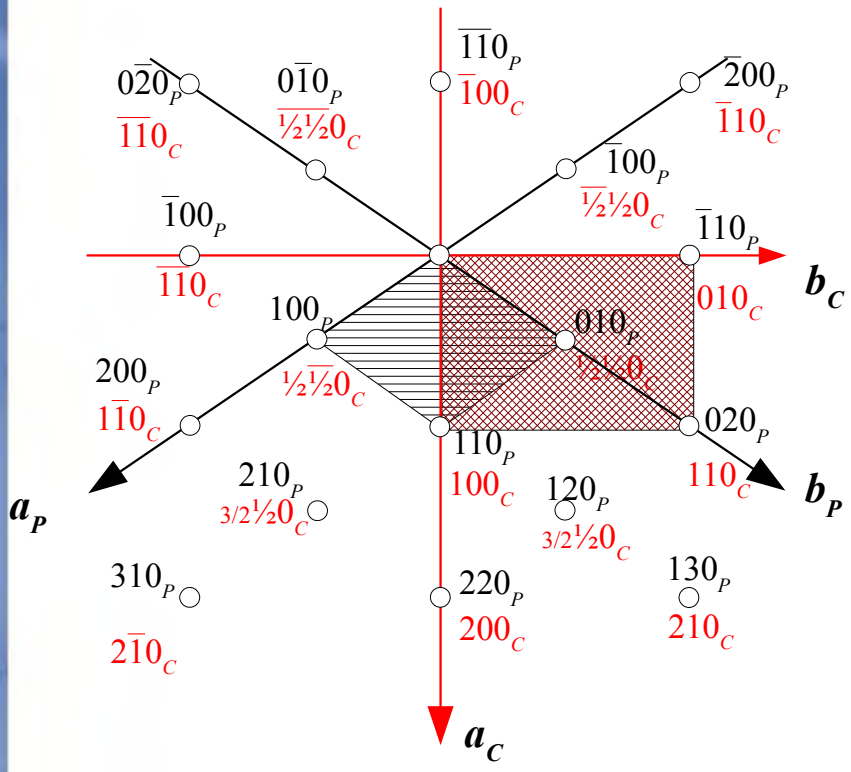
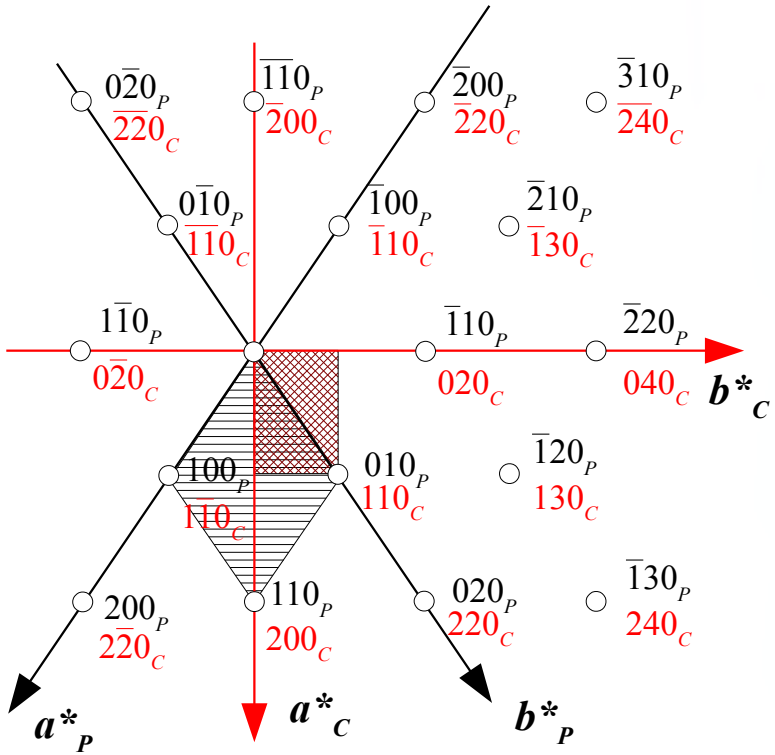
Rappel : dérivation géométrique des absences (« extinctions ») systématiques

Conditions de présence intégrales

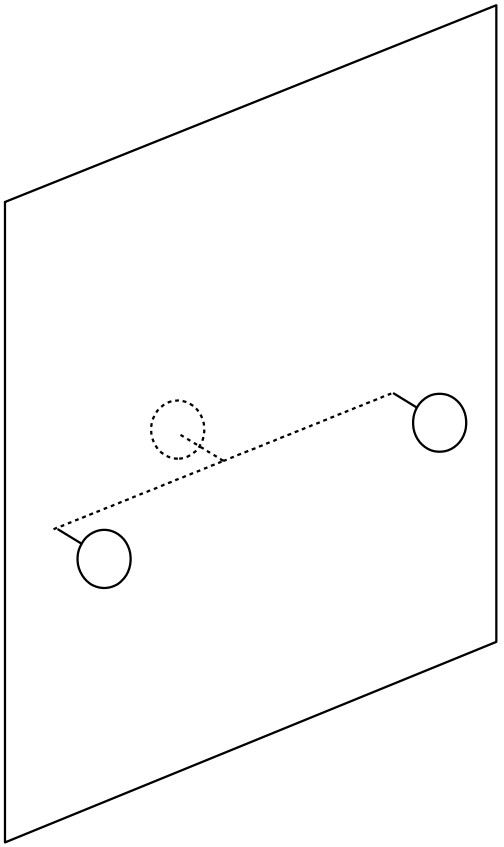
Seulement les nœuds avec *h*+*k* pair existent dans la maille réciproque d'une maille centrée *C*

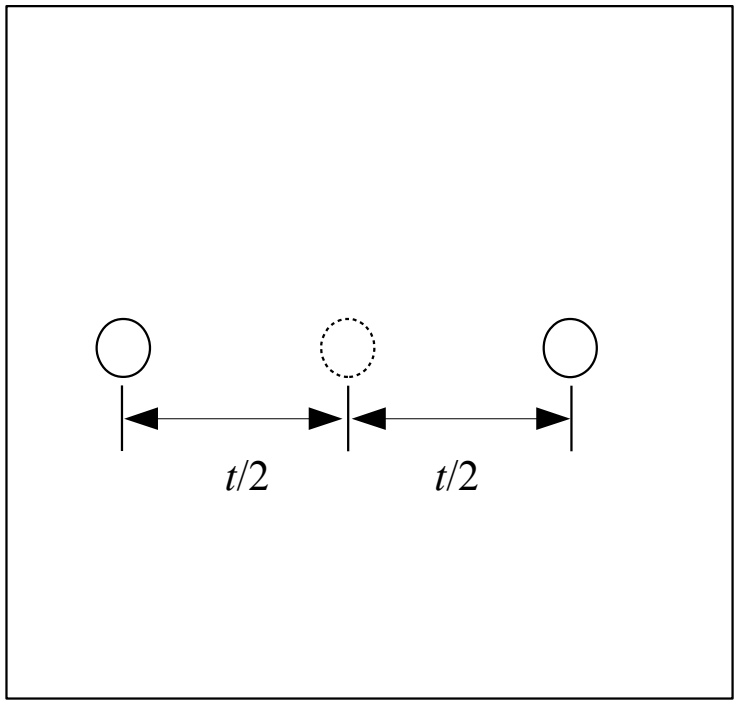
Condition des présence : *hkl* : *h*+*k* = 2*n*

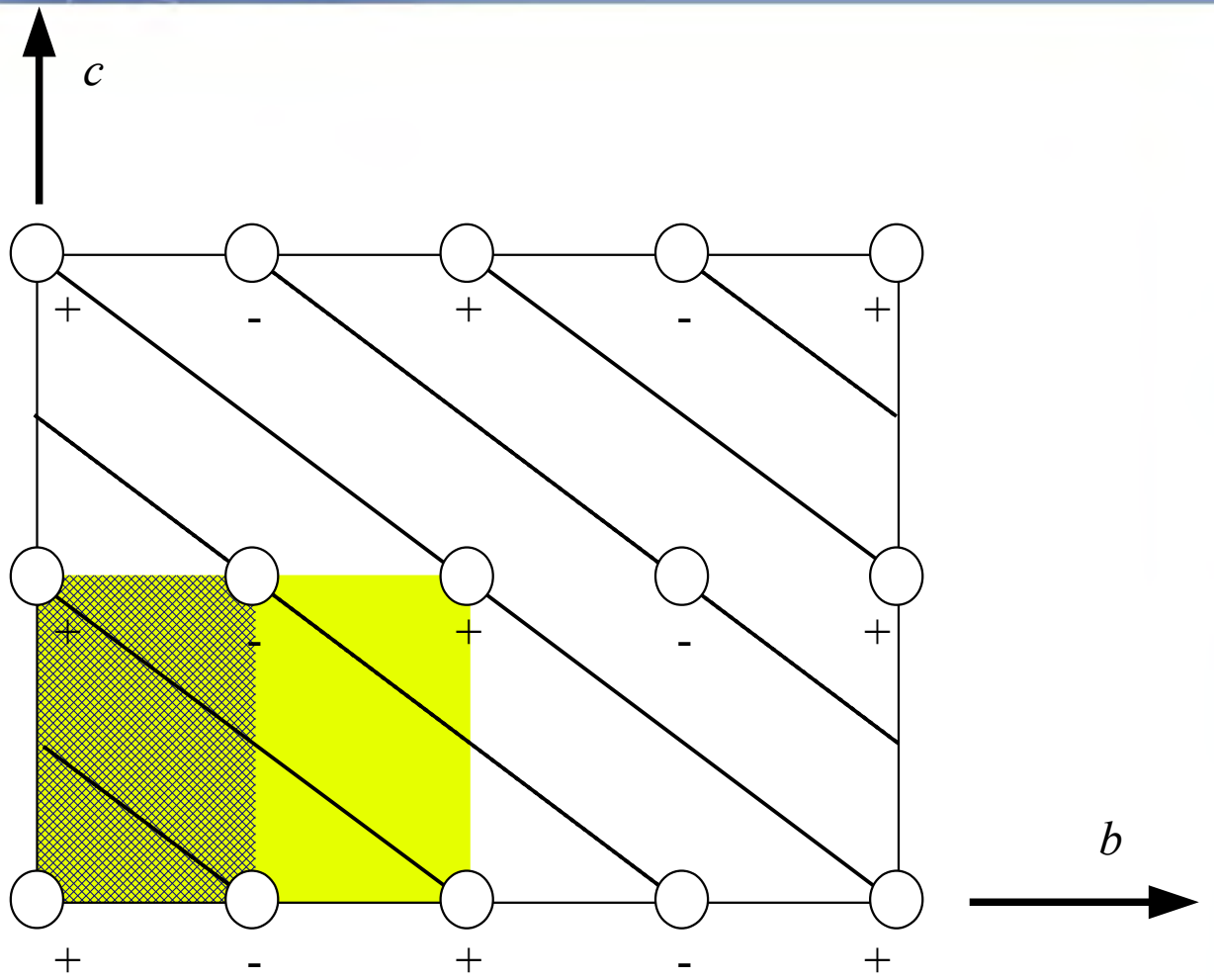




Conditions de présence zonales







Espace direct

La périodicité est réduite de moitié dans la direction *b* direction en projection selon l'axe *a*

Espace réciproque

Périodicité double dans la direction *b** direction sur le plan (0*kl*)*

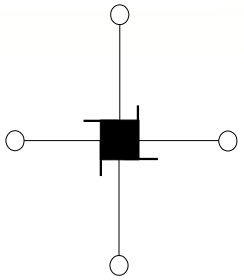
Conditions de présence

0*kl* : *k* = 2*n*

Conditions de présence sériales

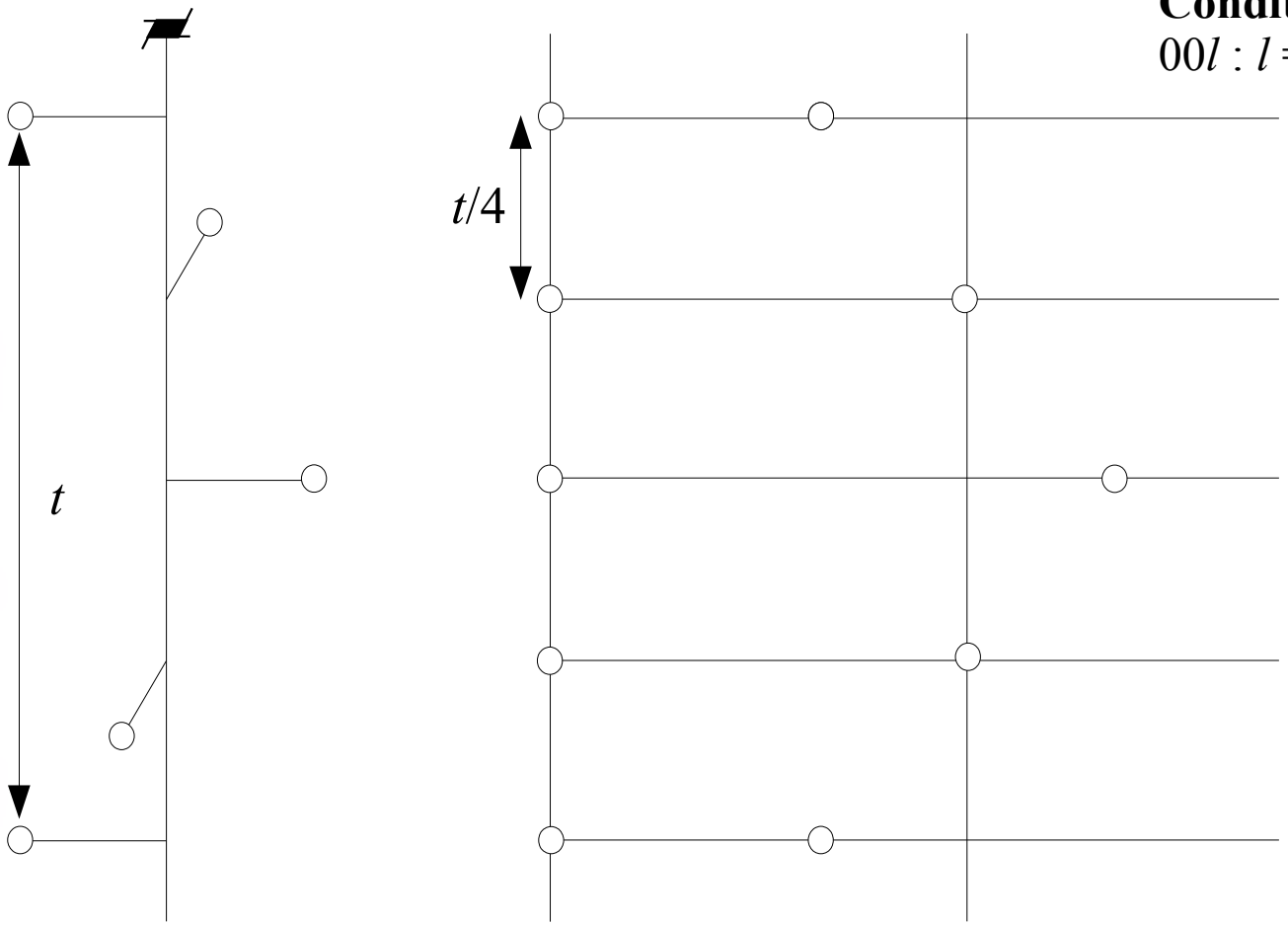
Espace direct

Périodicité réduite à ¼ dans la direction [001]
vue en projection sur l'axe **c**.



Conditions de présence

$00l : l = 4n$



Espace réciproque

Périodicité multiplié par 4 dans la direction [001]*

Définitions

Une orbite cristallographique est l'ensemble (infini) d'atomes obtenus à partir d'un atome donné sous l'action des opérations de symétrie du groupe d'espace du cristal auquel l'atome en question appartient.

Une structure cristalline consiste en une ou plusieurs orbites cristallographiques.

Chaque orbite cristallographique possède une symétrie propre qui est égale ou supérieure au groupe d'espace qui l'a générée.

Le groupe d'espace d'une structure cristalline est le groupe intersection des groupes qui correspondent à la symétrie propre de chaque orbite cristallographique occupée par un type d'atome composant la structure cristalline.

Classification des orbites cristallographiques

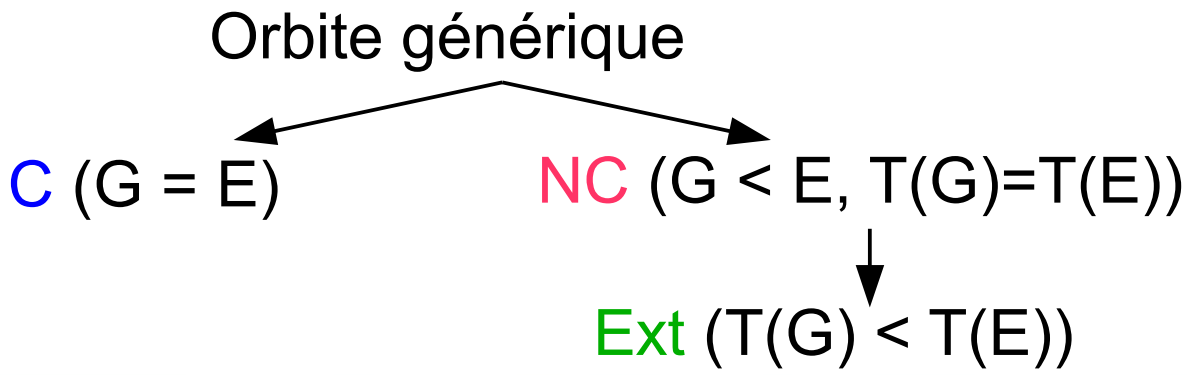
G = groupe d'espace de la structure cristalline

E = symétrie propre de l'orbite cristallographique

G = E : orbite caractéristique

G <(t)* E : orbite non-caractéristique

G < E, T(G) < T(E) : orbite extraordinaire



* (t) sous-groupe *translationengleiche* (mêmes translations, réseau en commun)

Effets des orbites cristallographiques sur les clichés de diffraction

Les atomes sur des orbites caractéristiques contribuent au cliché de diffraction avec une symétrie qui est la même que le groupe d'espace.

Les atomes sur des orbites non-caractéristiques contribuent au cliché de diffraction avec une symétrie supérieure à celle du groupe d'espace.

Les atomes sur des orbites extraordinaires contribuent seulement à un sous-réseau (réciproque!) du réseau de diffraction de la structure cristalline (extinctions systématiques particulières).

Les extinctions systématiques particulières ne sont présentées sur les *Tables Internationales de Cristallographie* que dans un nombre limité de cas.

Exercices

(Seuls les générateurs de E qui ne sont pas contenus en G sont montrés dans les diapositives qui suivent)

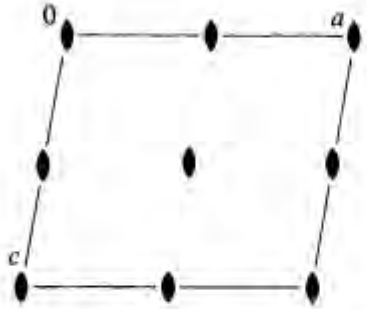
Un exemple banal, mais pas trop

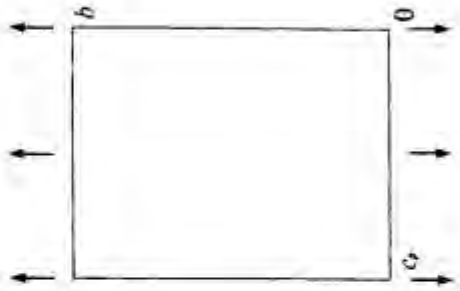
International Tables for Crystallography (2006). Vol. A, Space group 3, pp. 116–119.

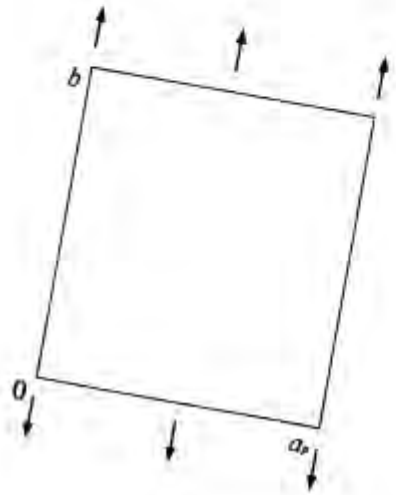
$P2$	C_2^1	2	Monoclinic
No. 3	$P121$		Patterson symmetry $P12/m1$

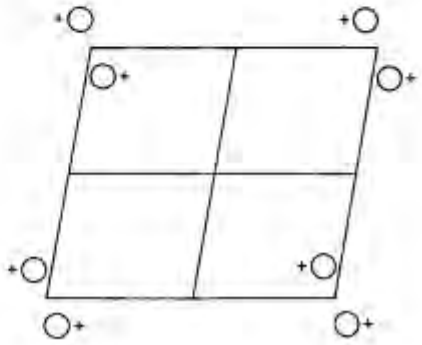
UNIQUE AXIS b

Trouvez la symétrie propre de l'orbite générale









International Tables for Crystallography (2006). Vol. A, Space group 3, pp. 116–119.

$P2$	C_2^1	2	Monoclinic
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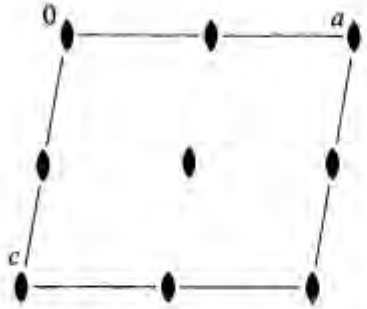
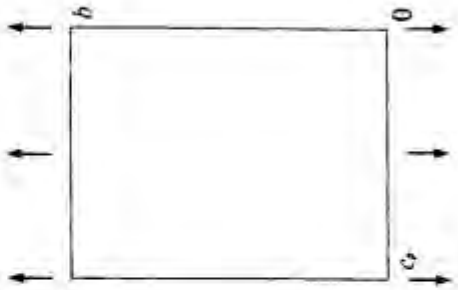
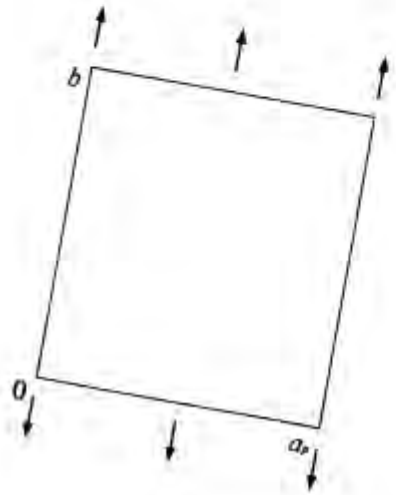
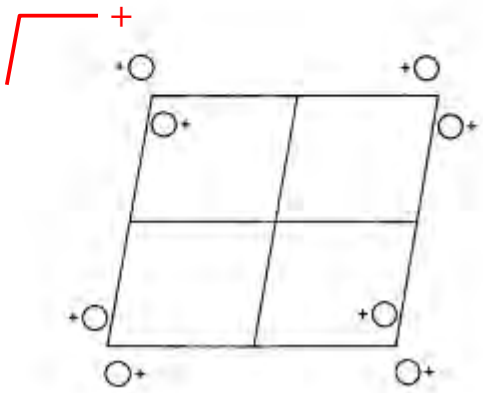
UNIQUE AXIS b









***P*2/*m*, *P*(111)**

orbite non-caractéristique

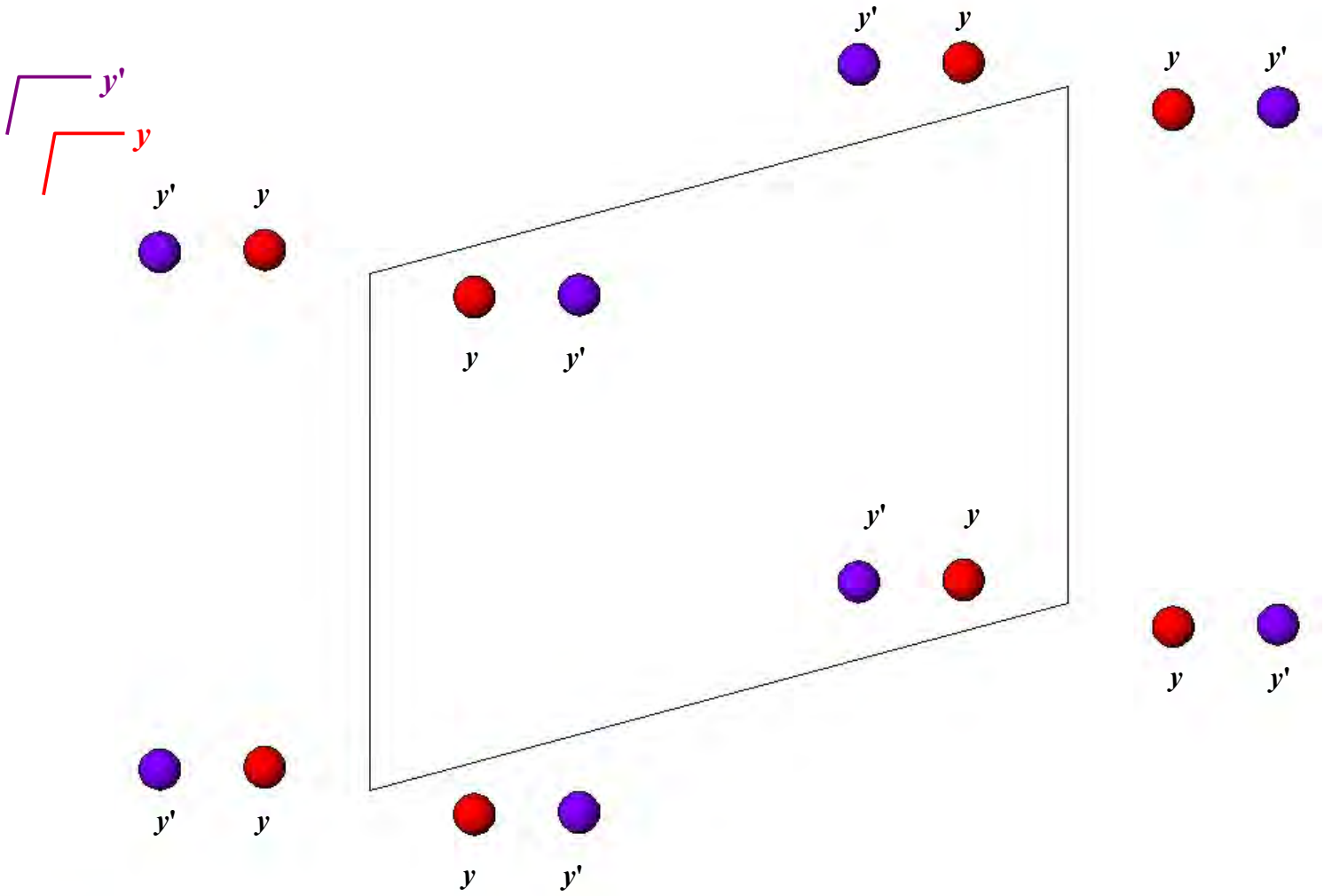
La notion de « groupe intersection »

Le groupe d'espace d'une structure cristalline est le groupe intersection des groupes qui correspondent à la symétrie propre de chaque orbite cristallographique occupée par un type d'atome composant la structure cristalline

Voyons un exemple avec deux orbites générales dans un groupe d'espace de type *P*2

Deux orbites générales en *P*2

***P*2/*m*, *P*(111) ∩ *P*2/*m*, *P*(111) = *P*2, *P*(111)**



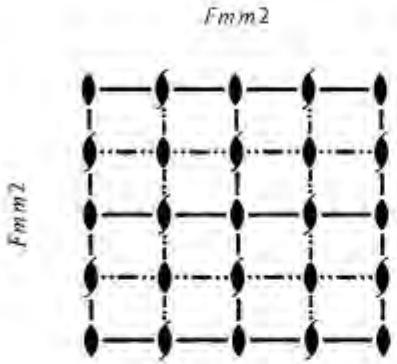
Un exemple un peu moins banal

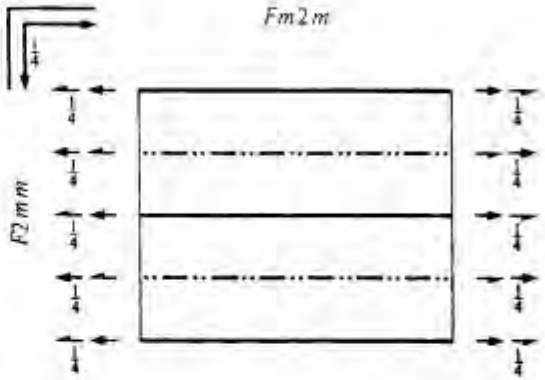
International Tables for Crystallography (2006). Vol. A, Space group 42, pp. 252–253.

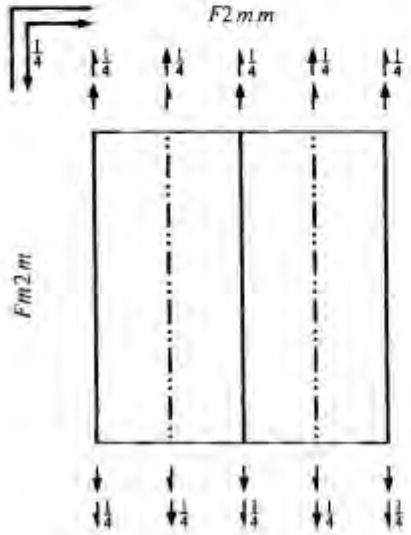
$Fmm2$ C_{2v}^{18} $mm2$ Orthorhombic

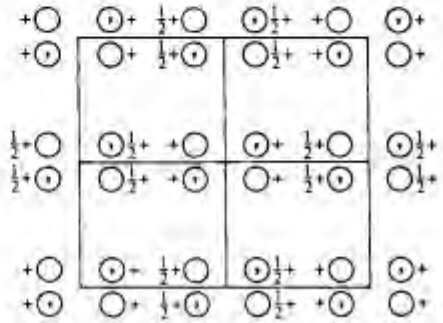
No. 42 $Fmm2$ Patterson symmetry $Fmmm$

Analysez TOUS les types d'orbites

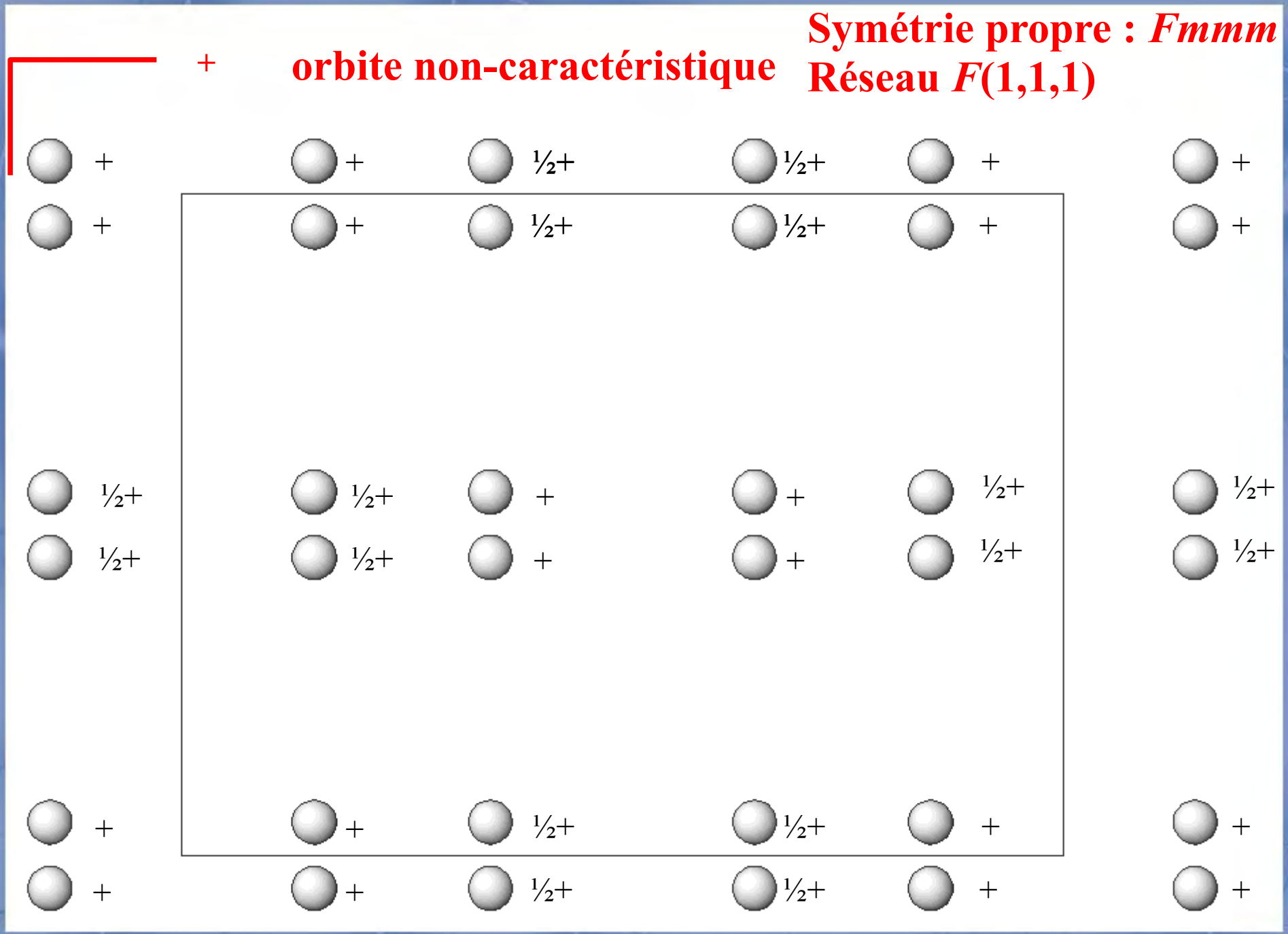








*Fmm*2, orbite 16 *e*

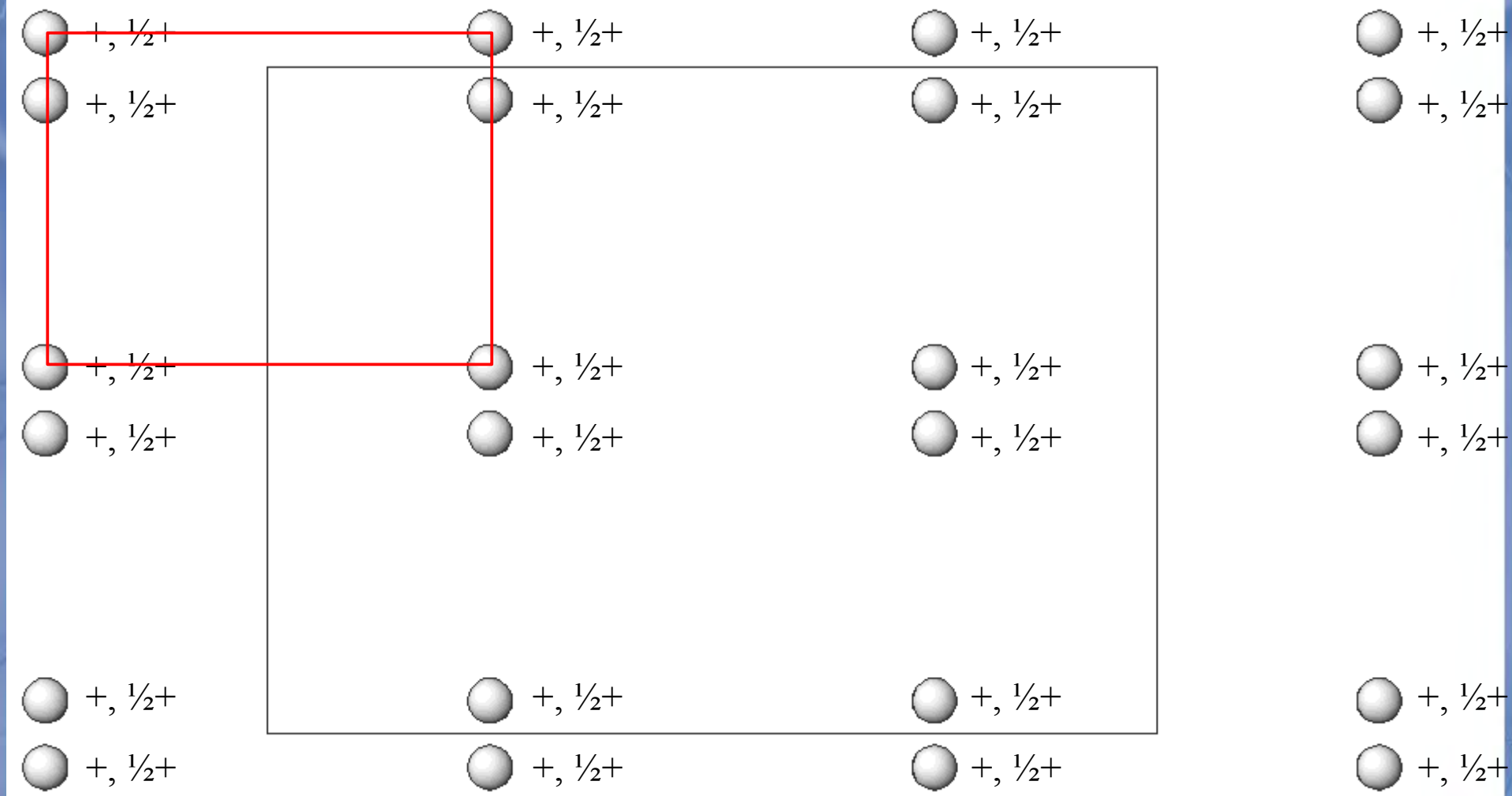


*Fmm*2, orbite 16 *e*, *y* = 1/4

Symétrie propre : *Pmmm*
Réseau *P*(½,½,½)

\+

orbite extraordinaire

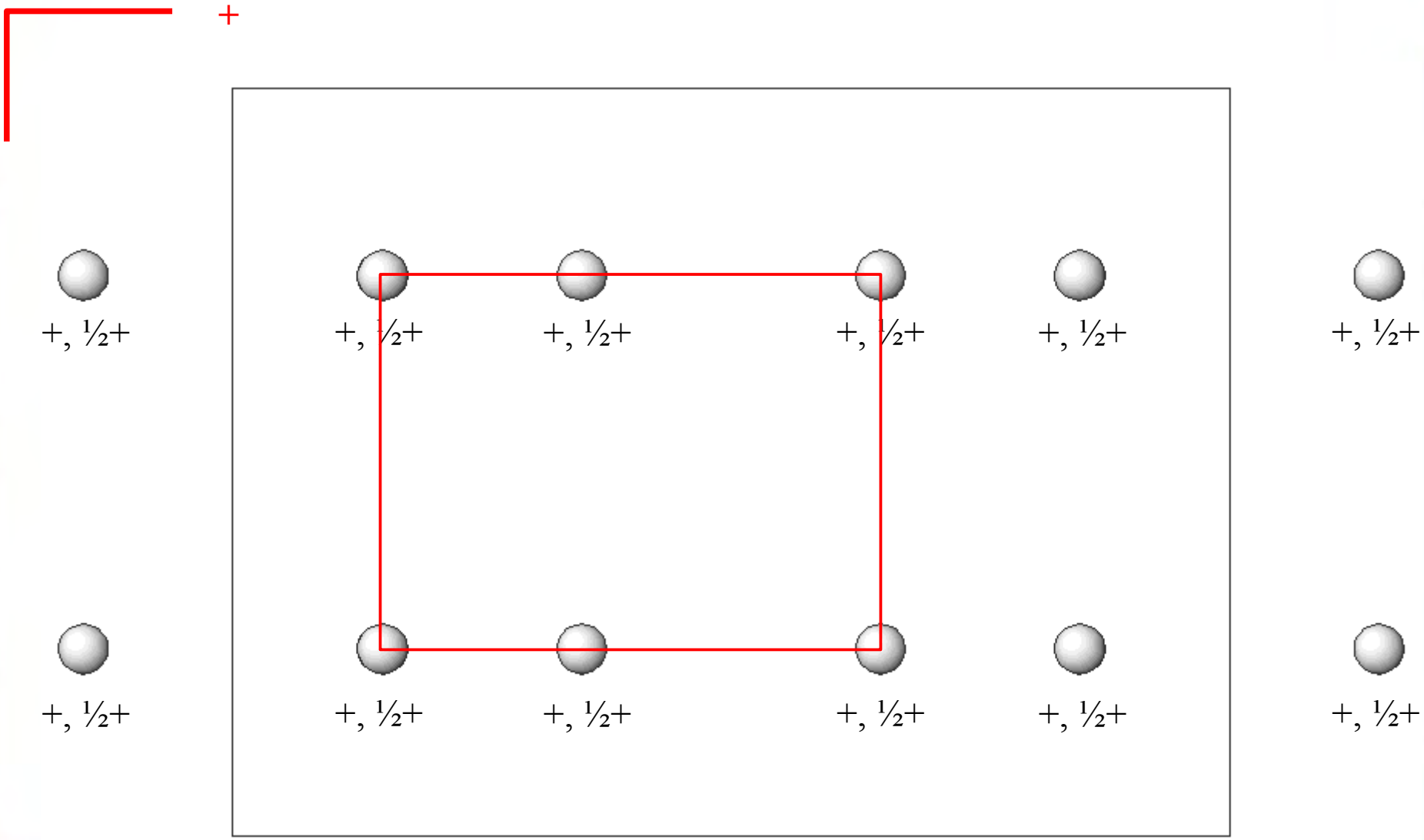


Condition de présence : *hkl* : *h*, *k*, *l* = 2*n*

*Fmm*2, orbite 16 *e*, *x* = 1/4

Symétrie propre : *Pmmm*
Réseau *P*(½,½,½)

orbite extraordinaire

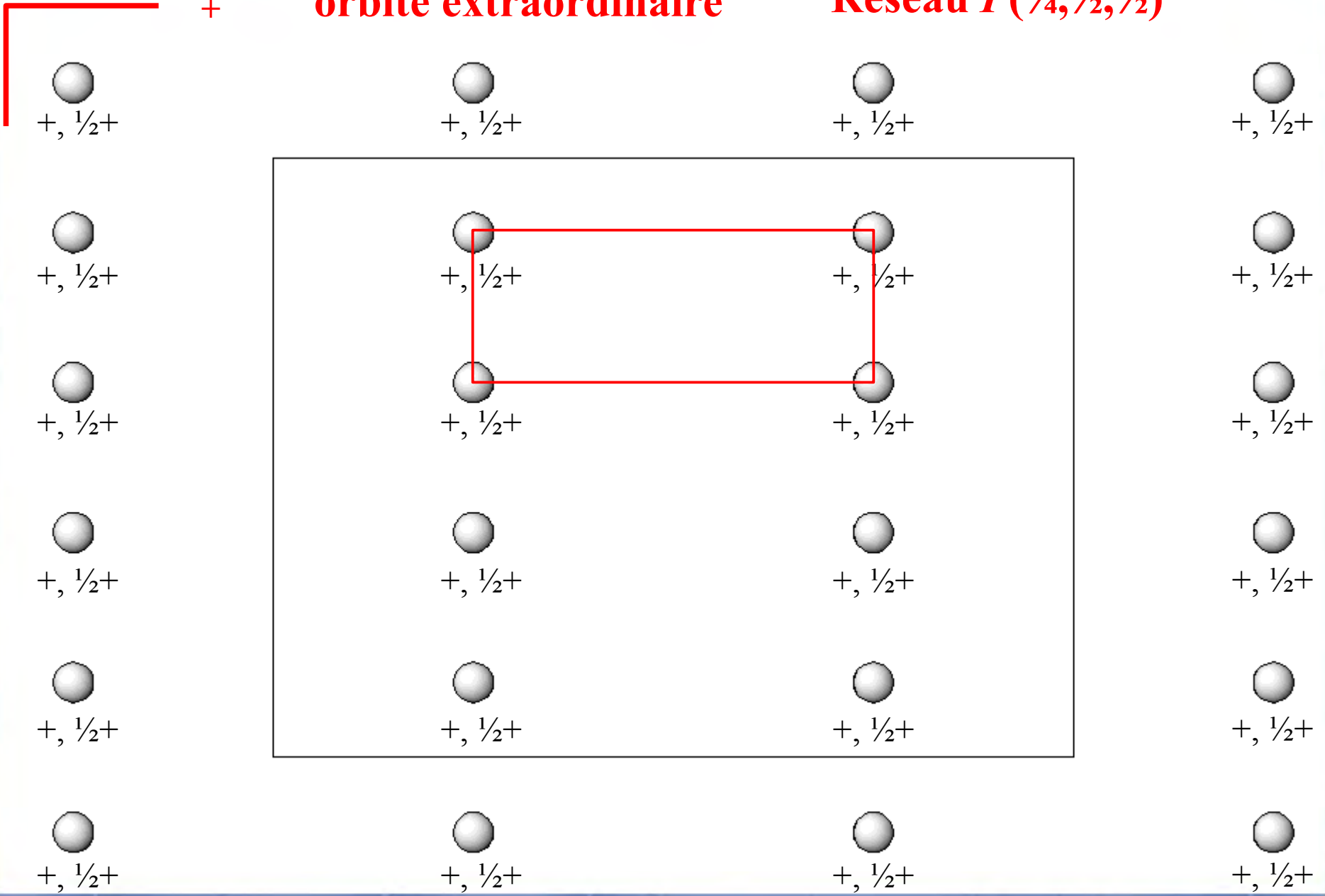


Condition de présence : *hkl* : *h*, *k*, *l* = 2*n*

*Fmm*2, orbite 16 *e*, *x* = 1/8, *y* = 1/4

Symétrie propre : *Pmmm*

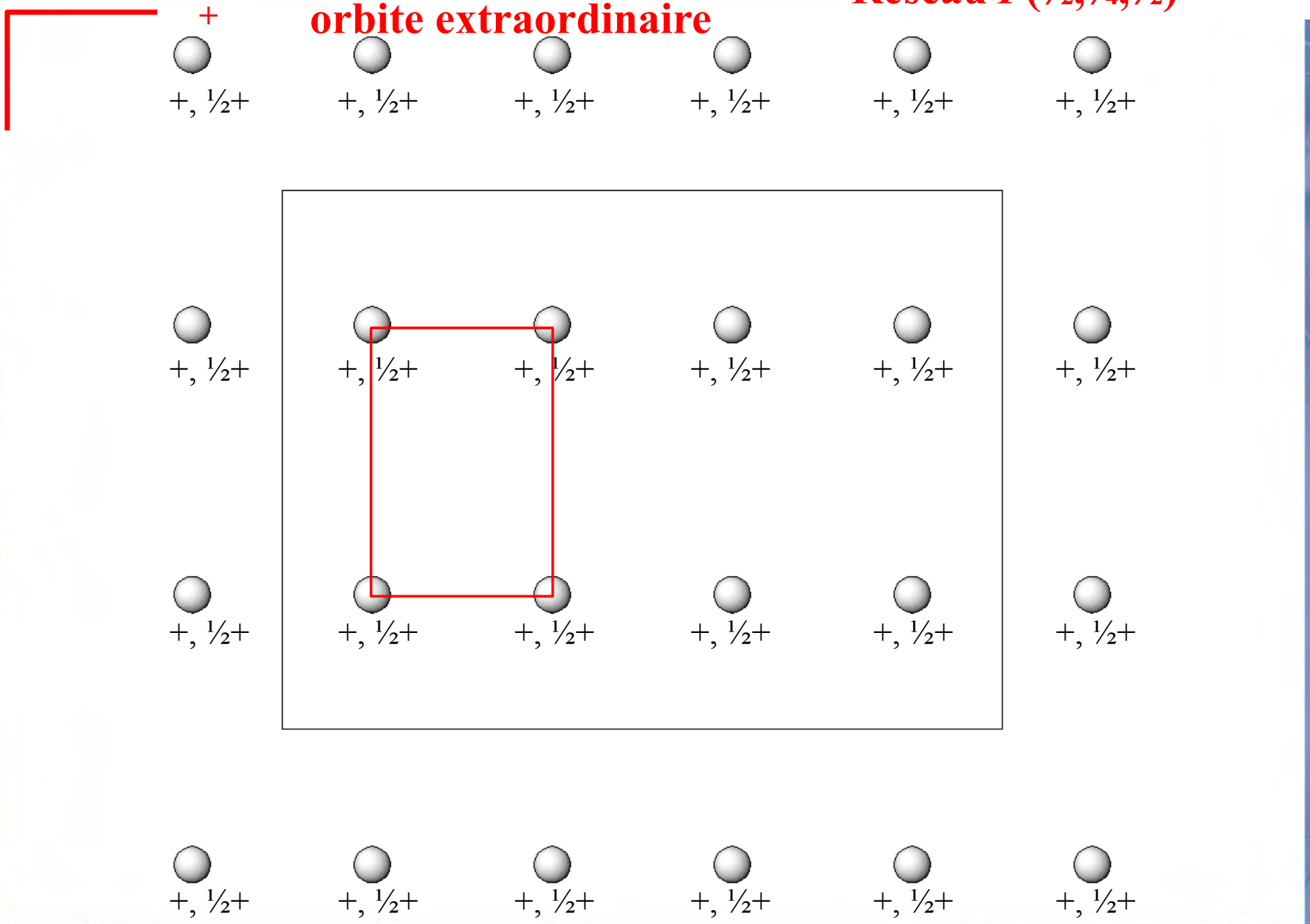
Réseau *P*(¼,½,½)



Condition de présence : *hkl* : *k*, *l* = 2*n*, *h* = 4*n*

*Fmm*2, orbite 16 *e*, *x* = 1/4, *y* = 1/8

Symétrie propre : *Pmmm*
Réseau *P*(½,¼,½)



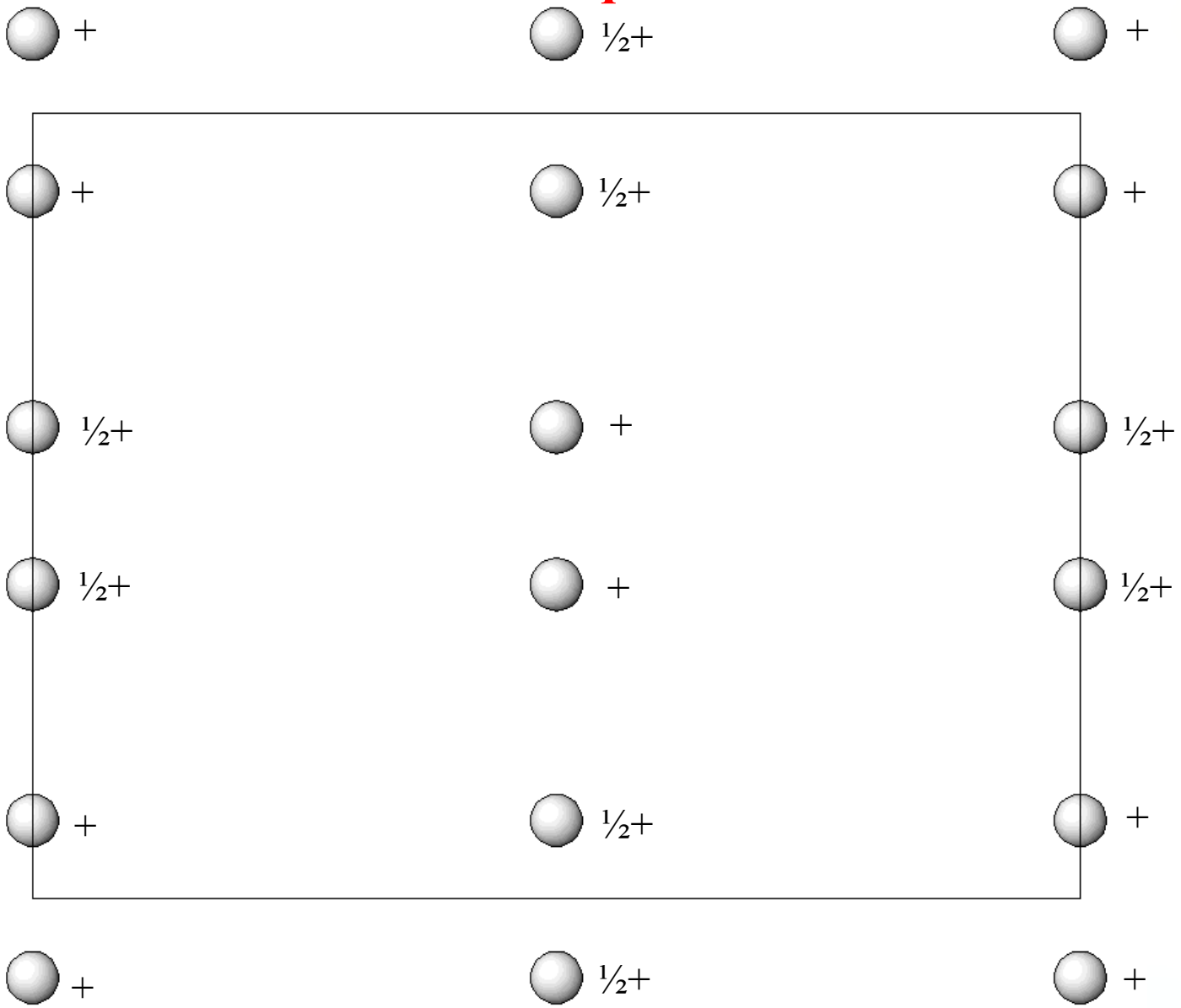
Condition de présence : *hkl* : *h*, *l* = 2*n*, *k*= 4*n*

*Fmm*2, orbite 8 *d*

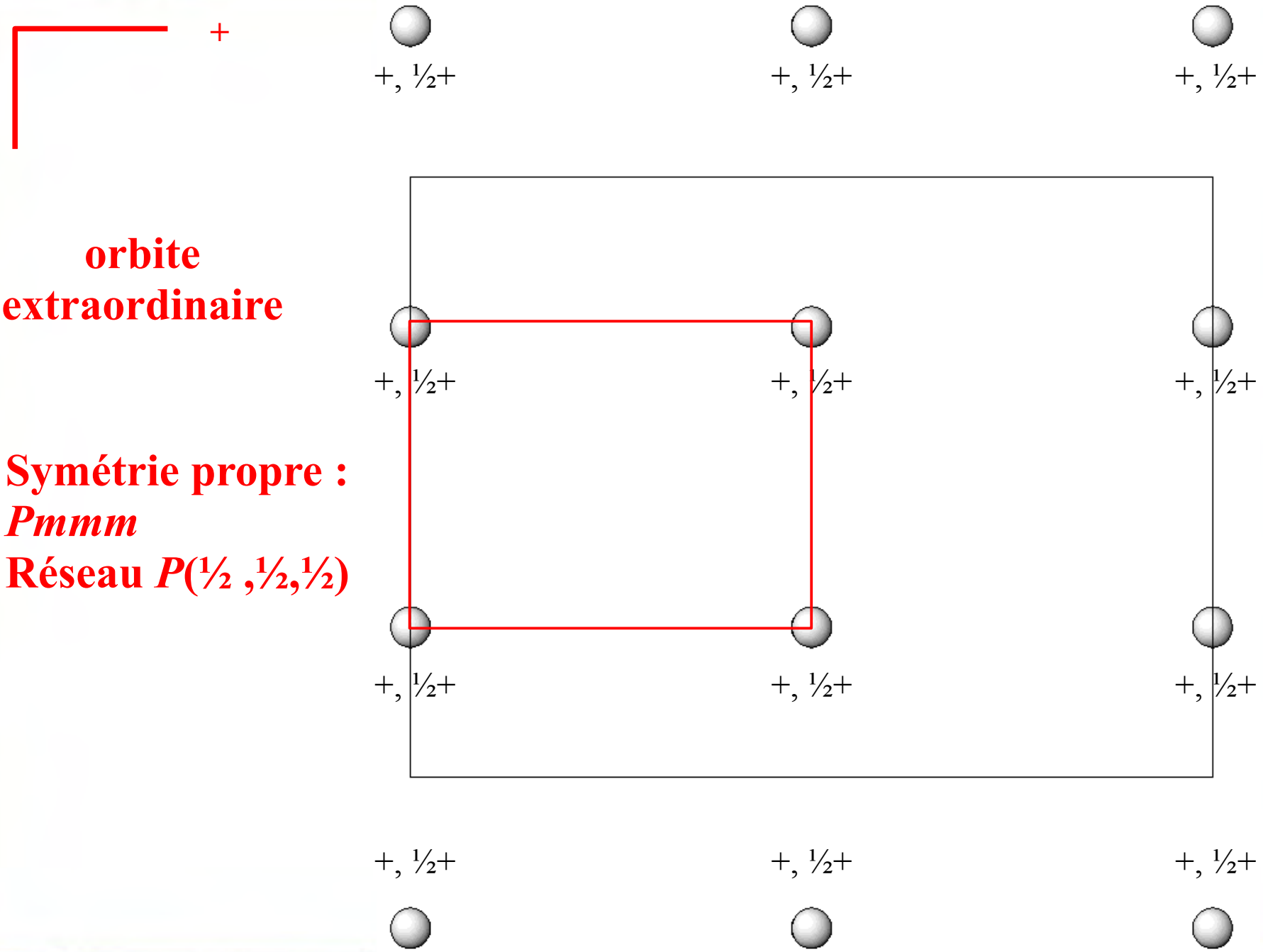
Symétrie propre : *Fmmm*
Réseau *F*(1,1,1)

+

orbite non-caractéristique



*Fmm*2, orbite 8 *d*, *x* = 1/4

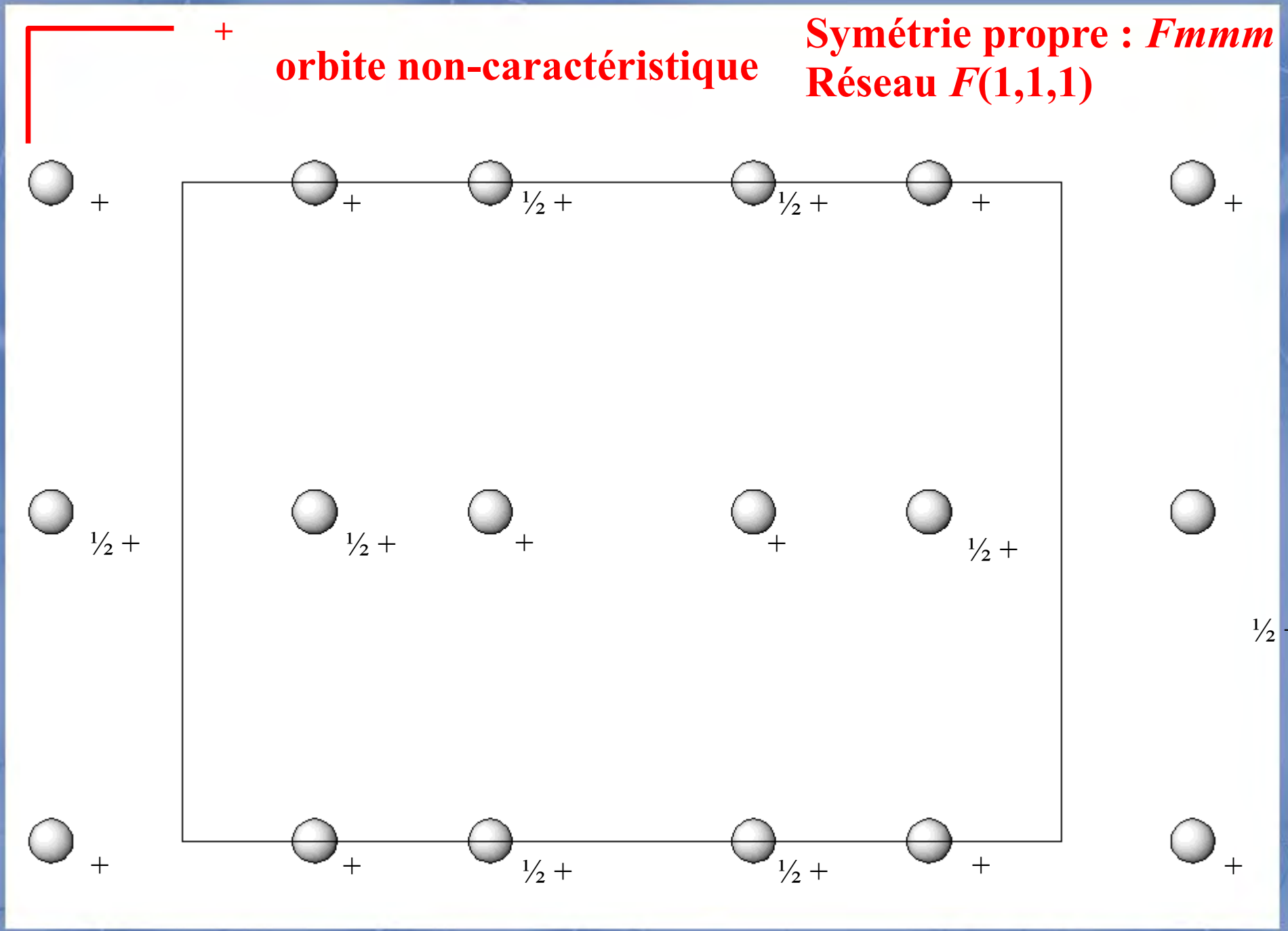


orbite extraordinaire

Symétrie propre :
Pmmm
Réseau *P*(½ ,½,½)

Condition de présence : *hkl* : *h*, *k*, *l* = 2*n*

*Fmm*2, orbite 8 *c*

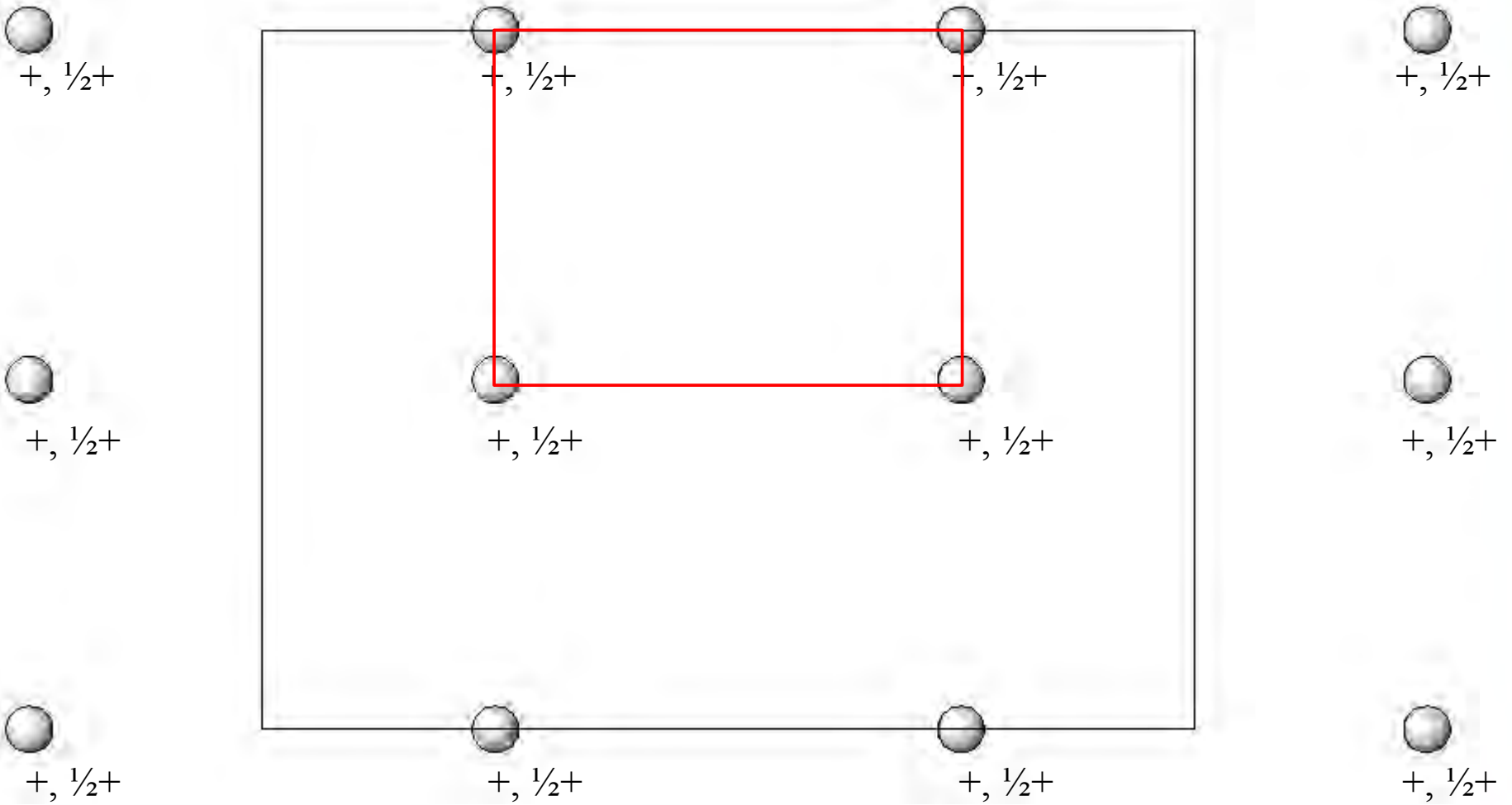


*Fmm*2, orbite 8 *c*, *y* = 1/4

+

orbite extraordinaire

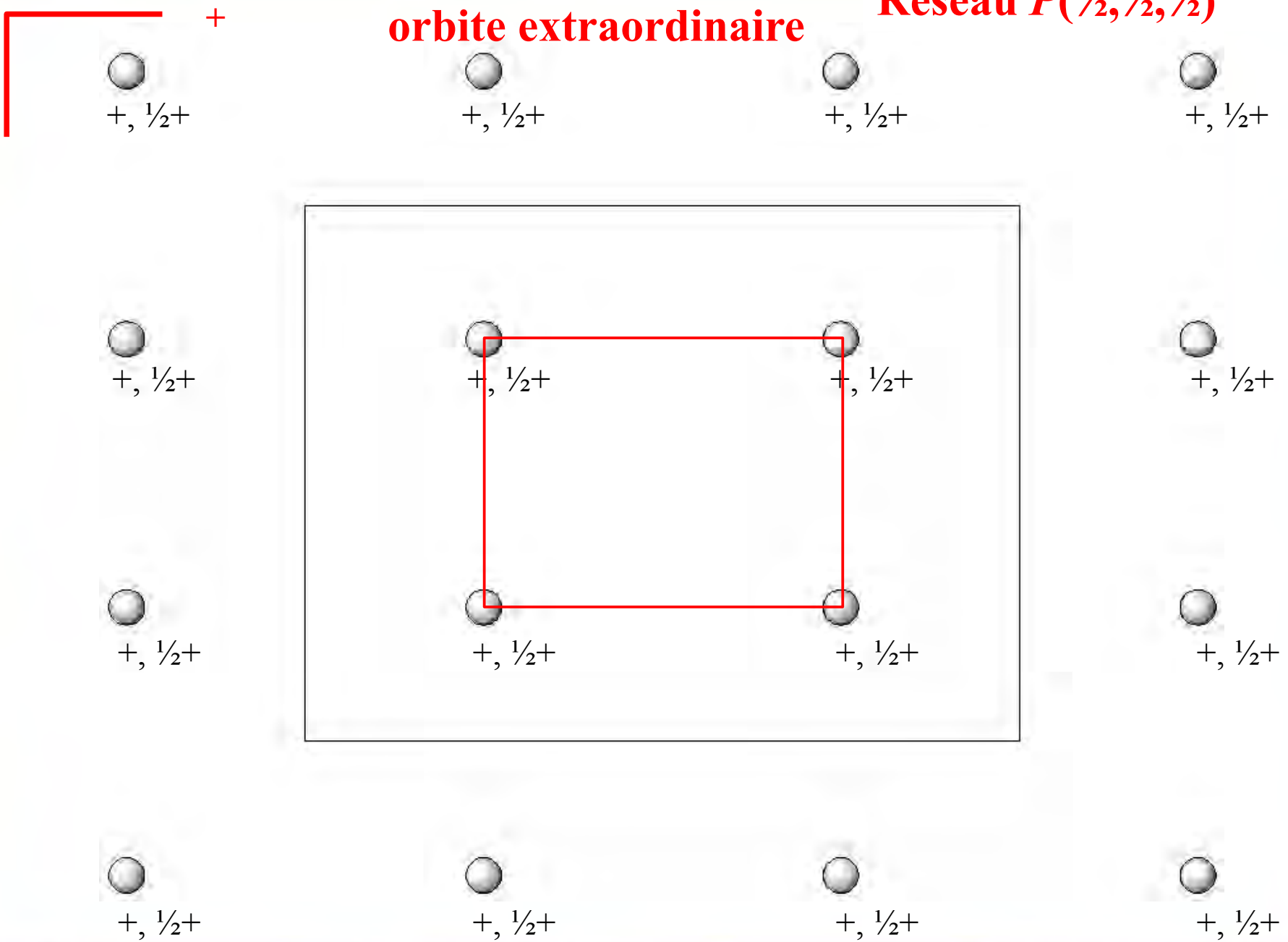
Symétrie propre : *Pmmm*
Réseau *P*(½,½,½)



Condition de présence : *hkl* : *h*, *k*, *l* = 2*n*

*Fmm*2, orbite 8 b

Symétrie propre : *Pmmm*
Réseau *P*(½,½,½)

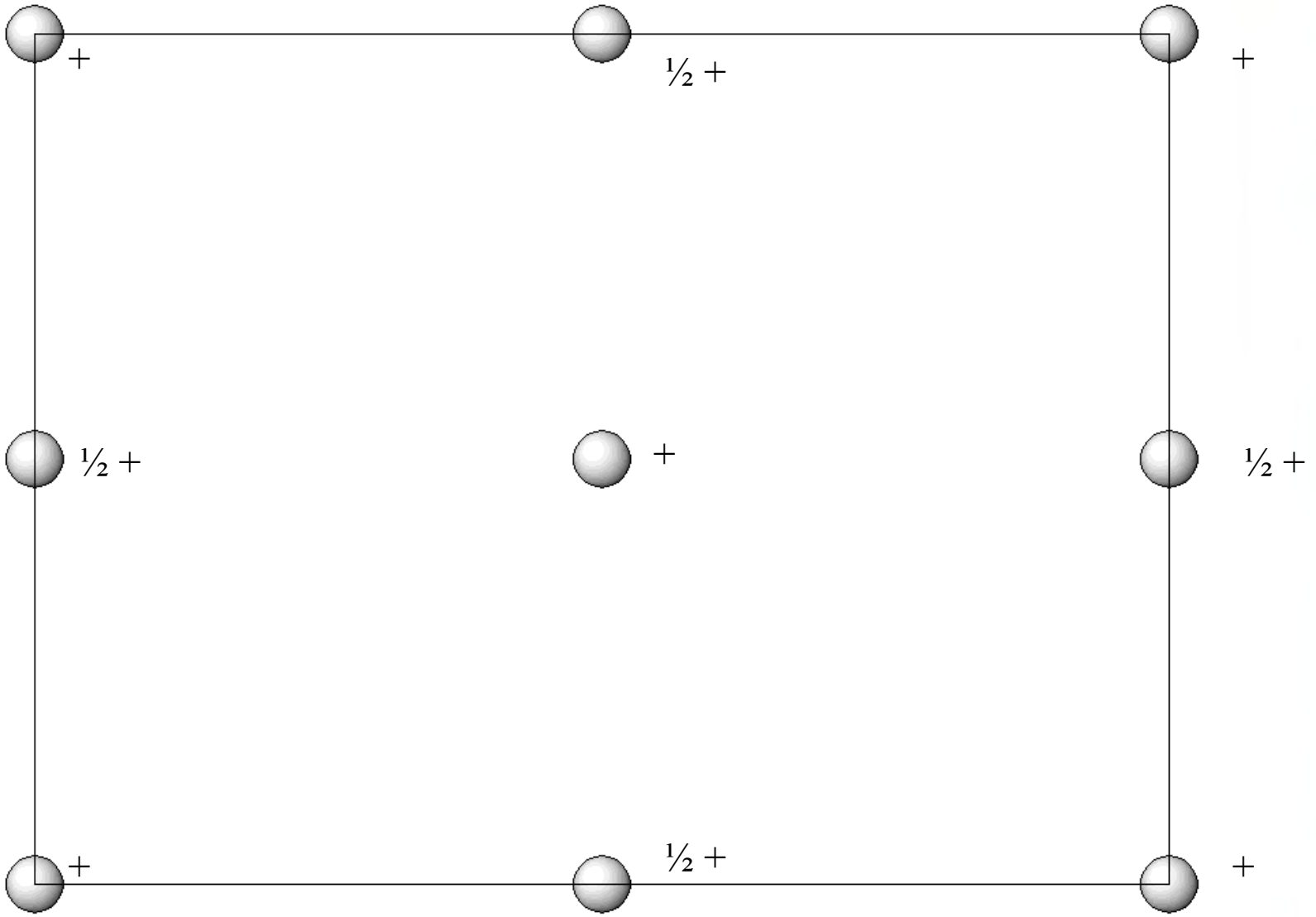


Condition de présence : *hkl* : *h*, *k*, *l* = 2*n*

*Fmm*2, orbite 4 *a*

Symétrie propre : *Fmmm*
Réseau *F*(1,1,1)

orbite non-caractéristique



Résumé

orbites 16 *e*, *8 d*, 8 *c*, 4 *a*	non-caractéristiques	Symétrie propre : *Fmmm* Réseau *F*(1,1,1)
orbite 16 *e*, *x* = 1/4 ou *y* = 1/4 orbite 8 *d*, *x* = 1/4 ou *y* = 1/4 orbite 8 *b*	extraordinaires	Symétrie propre : *Pmmm* Réseau *P*(½ ,½,½)
orbite 16 *e*, *x* = 1/8, *y* = 1/4	extraordinaire	Symétrie propre : *Pmmm* Réseau *P*(¼,½,½)
orbite 16 *e*, *x* = 1/4 et *y* = 1/8	extraordinaire	Symétrie propre : *Pmmm* Réseau *P*(½,¼,½)

Aucune orbite caractéristique dans ce type de groupe d'espace!

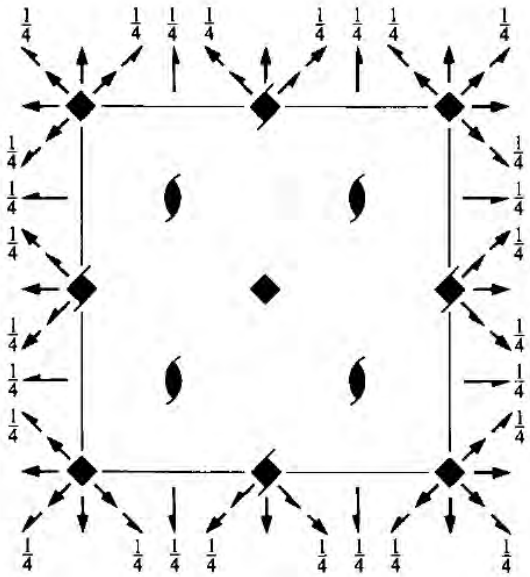
Conclusion plus générale

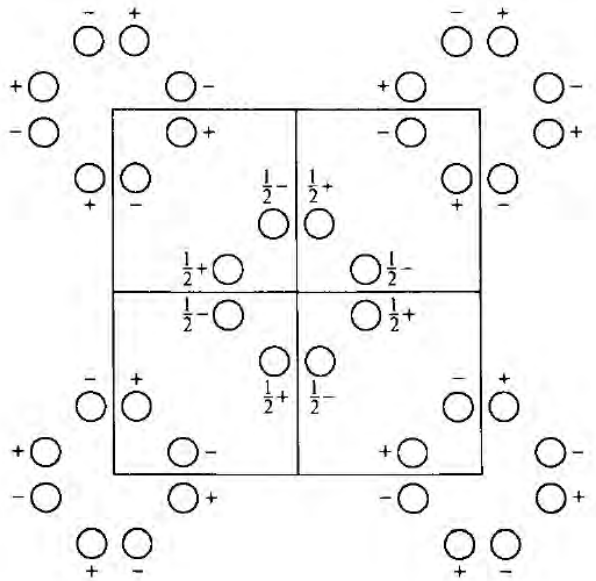
Un groupe d'espace pyroélectrique contient des orbites caractéristiques seulement en présence d'éléments de symétrie avec composante de glissement différente de ½ (miroirs *d*, axes 3_1, 3_2, 4_1, 4_3, 6_1, 6_2, 6_4, 6_5)

Un exemple un peu plus intéressant

International Tables for Crystallography (2006). Vol. A, Space group 97, pp. 378–379.

$I422$	D_4^9	422	Tetragonal
No. 97	$I422$		Patterson symmetry $I4/mmm$



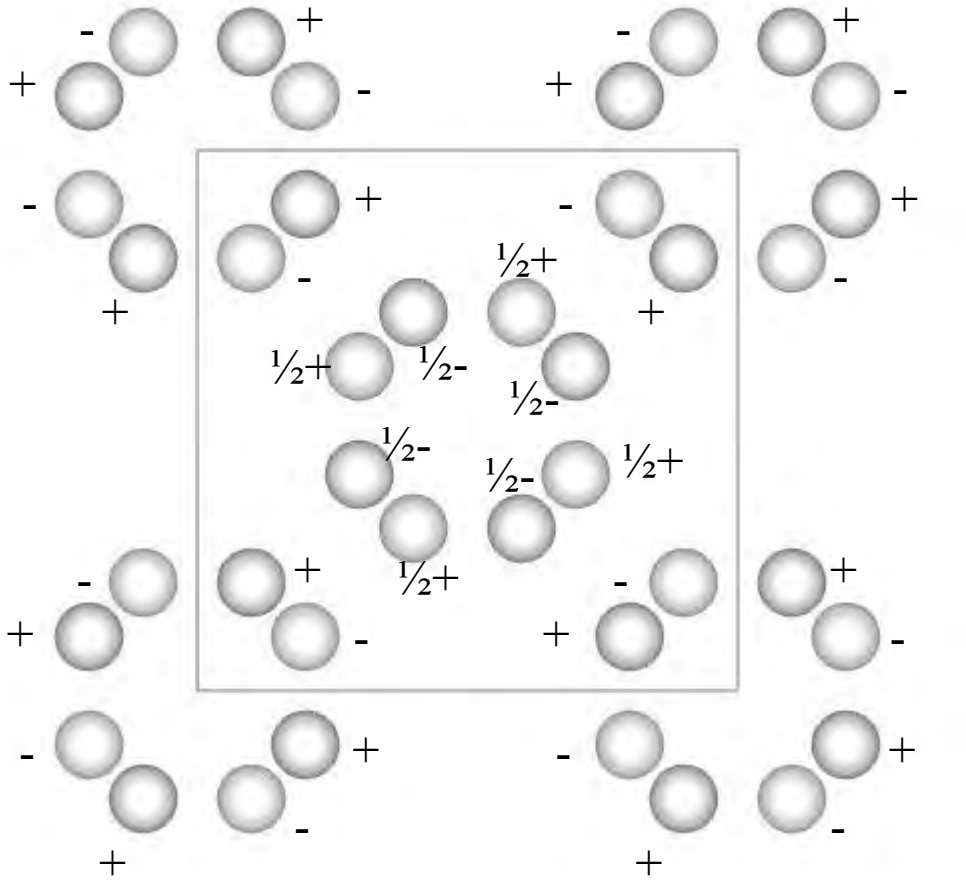


Analyse de quelques type d'orbites

*I*422 orbite 16 *k xyz*

orbite caractéristique

Symétrie propre : *I*422
Réseau *I*(1,1,1)



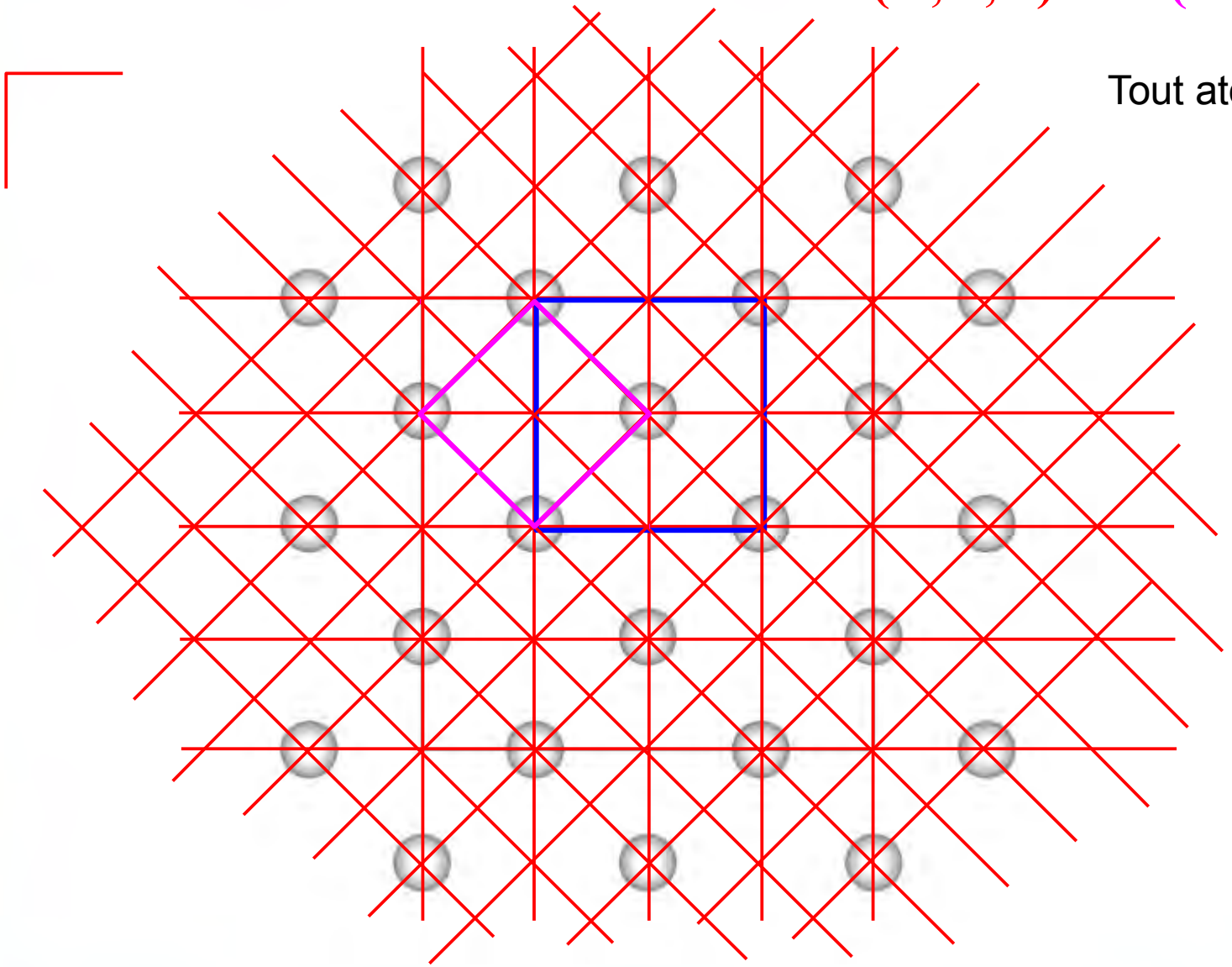
*I*422 orbite 16 *k* ¼ 0 ¼

orbite extraordinaire

Symétrie propre : *P*4/*mmm*

Réseau *C*(½,½,½) → *P*(¼-¼,¼+¼,½)

Tout atome à ¼ et ¾

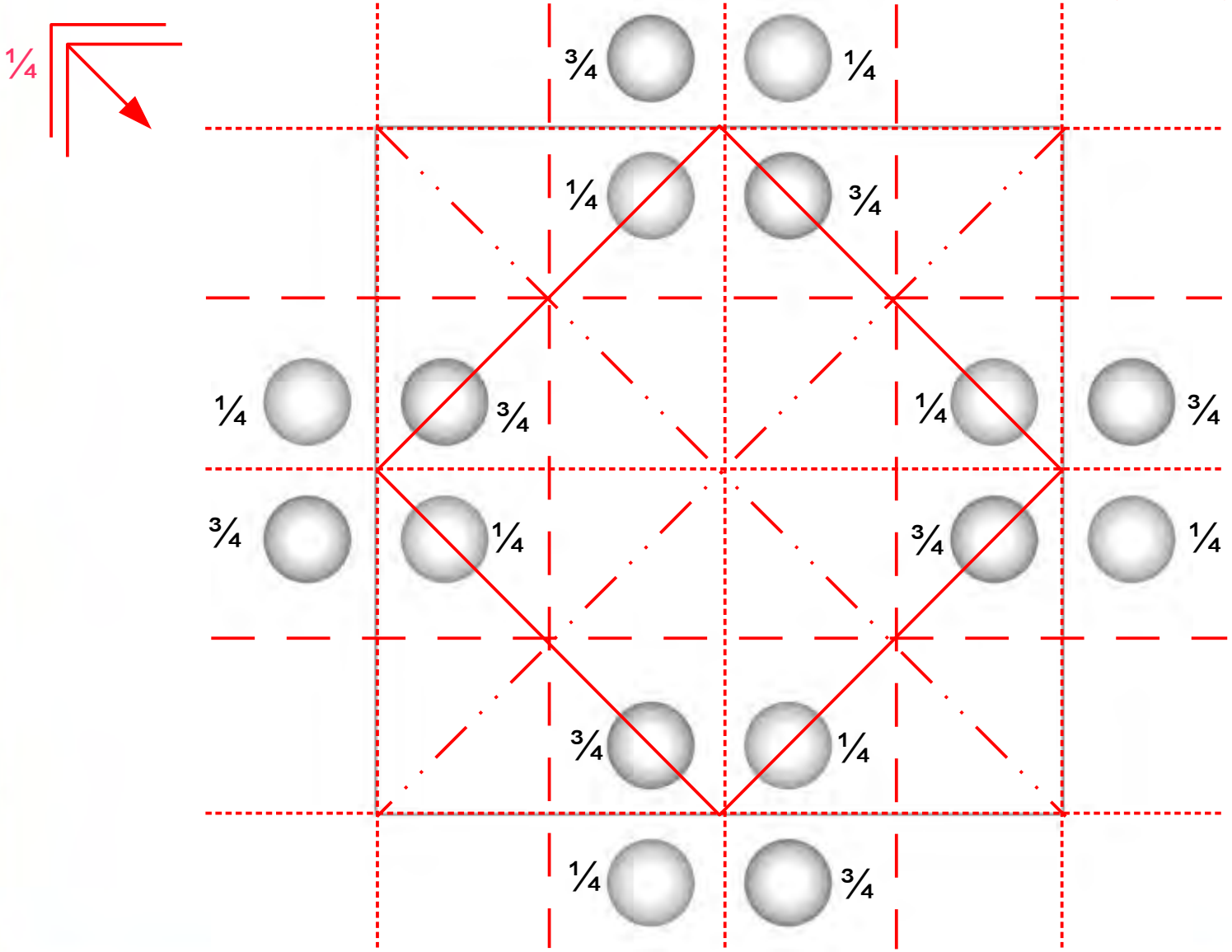


Condition de présence : *hkl* : *h*, *k*, *l* = 2*n*, *h*+*k* = 4*n*

*I*422 orbite 8 *j* *x*+½ *x* ¼

Symétrie propre : *I*4/*mcm*
Réseau *I*(1,1,1)

orbite non-caractéristique



Condition de présence : *h*0*l* : *l* = 2*n* (0*kl* : *l* = 2*n*)

Quelques chiffres en E^3

- ∞ groupes d'espace
- 219 types affines de groupes d'espaces
- 230 types cristallographiques de groupes d'espace
- 1731 types de positions de Wyckoff
- 1128 types de Wyckoff sets – positions de Wyckoff conjuguées sous l'actions de normalisateurs
- 402 lattice complexes – orbites cristallographiques classées par types

Où peux-je trouver plus d'informations?

International Tables for Crystallography (2006). Vol. A, Chapter 8.3, pp. 732–740.

8.3. Special topics on space groups

BY H. WONDRATSCHEK

8.3.1. Coordinate systems in crystallography

The matrices $\boldsymbol{W}$ and the columns $\boldsymbol{w}$ of crystallographic symmetry operations W depend on the choice of the coordinate system. A suitable choice is essential if $\boldsymbol{W}$ and $\boldsymbol{w}$ are to be obtained in a convenient form.

Example

In a space group $I4mm$, the matrix part of a clockwise fourfold rotation around the c axis is described by the $\boldsymbol{W}$ matrix

$$4^-\ 00z: \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

if referred to the *conventional* crystallographic basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. Correspondingly, the matrix

$$m\ 0yz: \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

represents a reflection in a plane parallel to $\mathbf{b}$ and $\mathbf{c}$. These matrices are easy to handle and their geometrical significance is evident. Referred to the *primitive* basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, defined by $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$, the matrices representing the same symmetry operations would be

$$4^-: \begin{pmatrix} 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & -1 & 0 \end{pmatrix}; \quad m: \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix}.$$

These matrices are more complicated to work with, and their geometrical significance is less obvious.

The conventional coordinate systems obey rules concerning the vector bases and the origins.

(i) In all cases, the *conventional* coordinate bases are chosen such that in a number of cases, the symmetry of the space group determines the conventional vector basis uniquely; in other cases, metrical criteria, *e.g.* the length of basis vectors, may be used to define a conventional vector basis.

(ii) The choice of the *conventional origin* in the space-group tables of this volume has been dealt with by Burzlaff & Zimmermann (1980). In general, the origin is a point of highest site symmetry, *i.e.* as many symmetry operations W_j as possible leave the origin fixed, and thus have $\boldsymbol{w}_j = \boldsymbol{o}$. Special reasons may justify exceptions from this rule, for example for space groups $I2_12_12_1 \equiv D_2^9$ (No. 24), $P4_332 \equiv O^6$ (No. 212), $P4_132 \equiv O^7$ (No. 213), $I4_132 \equiv O^8$ (No. 214) and $I\bar{4}3d \equiv T_d^6$ (No. 220); *cf.* Section 2.2.7. If in a centrosymmetric space group a centre of inversion is not a point of highest site symmetry, the space group is described twice, first with the origin in a point of highest site symmetry, and second with the origin in a centre of inversion, *e.g.* at 222 and at $\bar{1}$ for space group $Pnnn \equiv D_{2h}^2$ (No. 48); *cf.* Section 2.2.1.* For space groups with low site symmetries, the origin is chosen so as to minimize the number of nonzero coefficients of the w_j, *e.g.* on a twofold screw axis for space group $P2_1 \equiv C_2^2$ (No. 4).

A change of the coordinate system, *i.e.* referring the crystal pattern and its symmetry operations W to a new coordinate system, results in new coordinates x' and new matrices W'; *cf.* Section 5.1.3.

8.3.2. (Wyckoff) positions, site symmetries and crystallographic orbits

The concept of *positions* and their *site symmetries* is fundamental for the determination and description of crystal structures. Let, for instance, $P\bar{1}$ be the space group of a crystal structure with tetrahedral AX_4 and triangular BY_3 groups. Then the atoms A and B cannot be located at centres of inversion, as the symmetry of tetrahedra and triangles is incompatible with site symmetry $\bar{1}$. If the space group is $P2/m$, again the points with site symmetry $2/m$ cannot be the loci of A or B, but points with site symmetries 2, m or

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Space Groups and Lattice Complexes

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14.1. Introduction and definition

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14.1.1. Introduction

In crystal structures belonging to different structure types and showing different space-group symmetries, the relative locations of symmetrically equivalent atoms nevertheless may be the same (*e.g.* Cl in CsCl and F in CaF_2). The concept of *lattice complexes* can be used to reveal relationships between crystal structures even if they belong to different space-group types.

14.1.2. Definition

The term *lattice complex* (*Gitterkomplex*) had originally been created by P. Niggli (1919), but it was not used by him with an unambiguous meaning. Later on, Hermann (1935) modified and specified the concept of lattice complexes, but the rigorous definition used here was proposed much later by Fischer & Koch (1974) [*cf.* also Koch & Fischer (1978)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at the same time.

To introduce the concept of lattice complexes, relationships between point configurations are regarded.

> The set of all points that are symmetrically equivalent to a given one with respect to a certain space group is called a *point configuration* (*cf.* also crystallographic orbit; Section 8.3.2).

In each space group, there exist infinitely many point configurations. Given a coordinate system, they may be obtained by varying the coordinates x, y, z of a starting point and by calculating all symmetrically equivalent points.

Point configurations refer to the arrangements of atoms in crystal structures. They are analogous to the crystal forms in crystal morphology, where a crystal form is a set of symmetrically

onto each other the site-symmetry groups of the points from the point configurations of the corresponding Wyckoff sets.

According to (i), (ii) and (iii), a lattice complex* is defined as follows:

> A *lattice complex* is the set of all point configurations that may be generated within one type of Wyckoff set.

Example

Take, in a particular space group of type $P4/nmm$, the Wyckoff position $4l$ $x00$. The points of each corresponding point configuration form squares that replace the points of the tetragonal primitive lattice referring to Wyckoff position $1a$. For all conceivable point configurations of $4l$, the squares have the same orientation, but their edges have different lengths. Congruent arrangements of squares but shifted by $\frac{1}{2}\mathbf{c}$ or by $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ give the point configurations of the Wyckoff positions $4m$, $4n$ and $4o$, respectively, in the same space group. The four Wyckoff positions $4l$ to $4o$, all with site symmetry $m2m.$, make up a Wyckoff set (*cf.* Table 14.2.3.2). They are mapped onto each other, for example, by the translations $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type $P4/nmm$ is mapped onto another space group of the same type, the Wyckoff set $4l$ to $4o$ as a whole is transformed to $4l$ to $4o$. The individual Wyckoff positions may be interchanged, however. The set of all point configurations from the Wyckoff positions $4l$ to $4o$ of all space groups of type $P4/nmm$ constitutes a lattice complex. Its point configurations may be derived as described above, but now starting from all space groups $P4/nmm$ with all conceivable lengths and orientations of the basis vectors instead of starting from just a particular group. Accordingly, the point configurations may differ in their orientation, in the size of their squares and in the distances

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Non characteristic orbits for Space Groups

Non characteristic orbits for Space Groups

For a given Wyckoff position NONCHAR calculates its *eigensymmetry* group as well as the *non-chararacteristic* orbits.

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