

A quick introduction to crystallographic orbits



Didactic material for the MaThCryst schools

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Definitions

A **crystallographic orbit** is the (infinite) set of atoms obtained from a given atom under the action of the symmetry operations of the space group of the crystal.

A **crystal structure** consists of **one or more crystallographic orbits**.

Each crystallographic orbit possesses an **eigensymmetry** that is **equal or higher** than the **space group** that has generated the orbit.

The space group of a crystal structure is the **intersection group** of the groups that correspond to the eigensymmetry of each crystallographic orbit occupied by a type of atom in the crystal structure.

Classification of crystallographic orbits

G = space group of the crystal structure

E = eigensymmetry of the crystallographic orbit

$G = E$: characteristic orbit

$G \langle (t) \rangle^* E$: non-characteristic orbit

$G < E, T(G) < T(E)$: extraordinary orbit

* (t) *translationengleiche* subgroup (same translations, common lattice)

Effects of the crystallographic orbits on the diffraction pattern

Atoms on **characteristic** orbits contribute to the diffraction pattern with the same symmetry as the space group.

Atoms on **non-characteristic** orbits contribute do the diffraction pattern with a symmetry higher than that of the space group.

Atoms on **extraordinary** orbits contribute only to a (reciprocal!) sub-lattice of the diffraction lattice of the crystal structure(**special systematic absences**).

The special systematic absences appear only for a **limited number of cases** in the *International Tables of Crystallography*.

Exercises

(Only the generators of E that are not contained in G are shown in the following slides)

A simple example

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

$P2$

C_2^1

2

Monoclinic

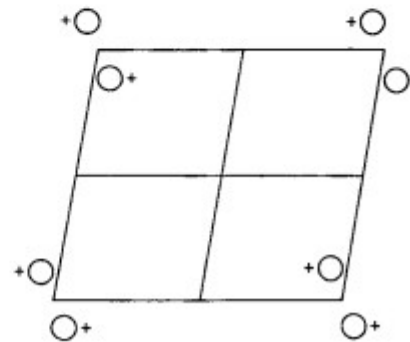
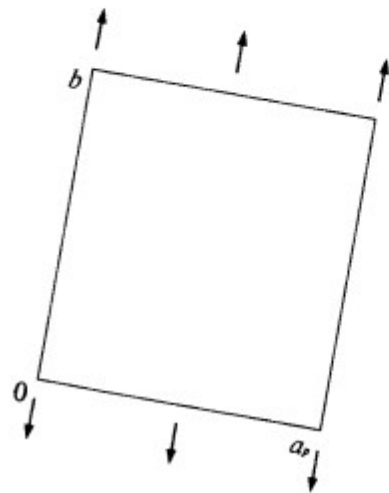
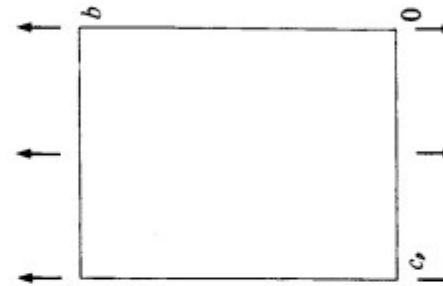
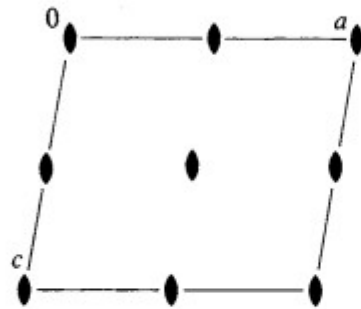
No. 3

$P121$

Patterson symmetry $P12/m1$

UNIQUE AXIS b

Find the
eigensymmetry of
the general orbit



A simple example

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

$P2$

C_2^1

2

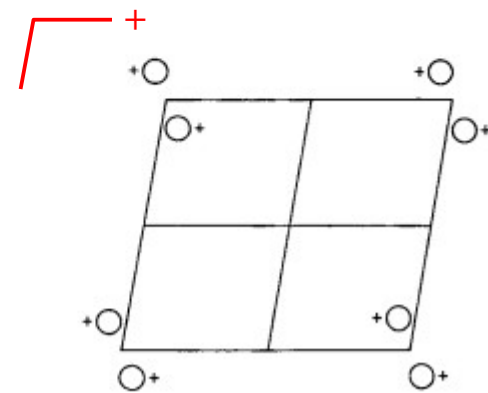
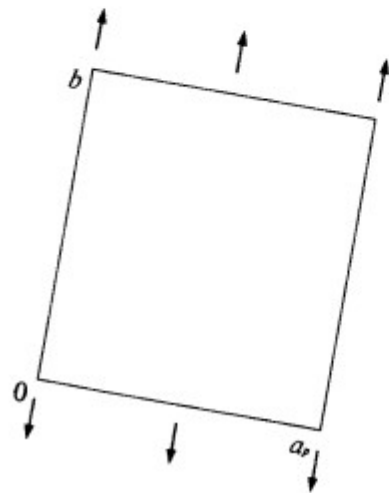
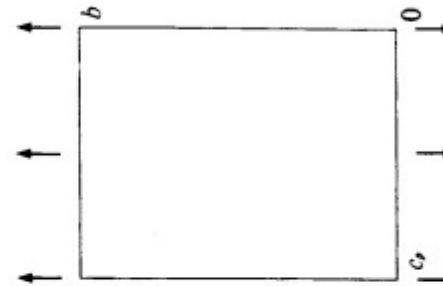
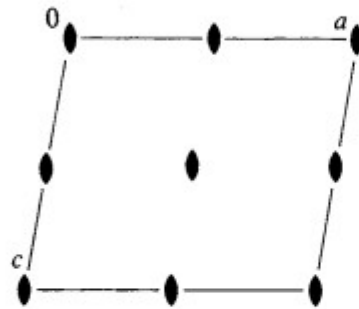
Monoclinic

No. 3

$P121$

Patterson symmetry $P12/m1$

UNIQUE AXIS b



$P2/m, P(111)$

non-caractéristic orbit

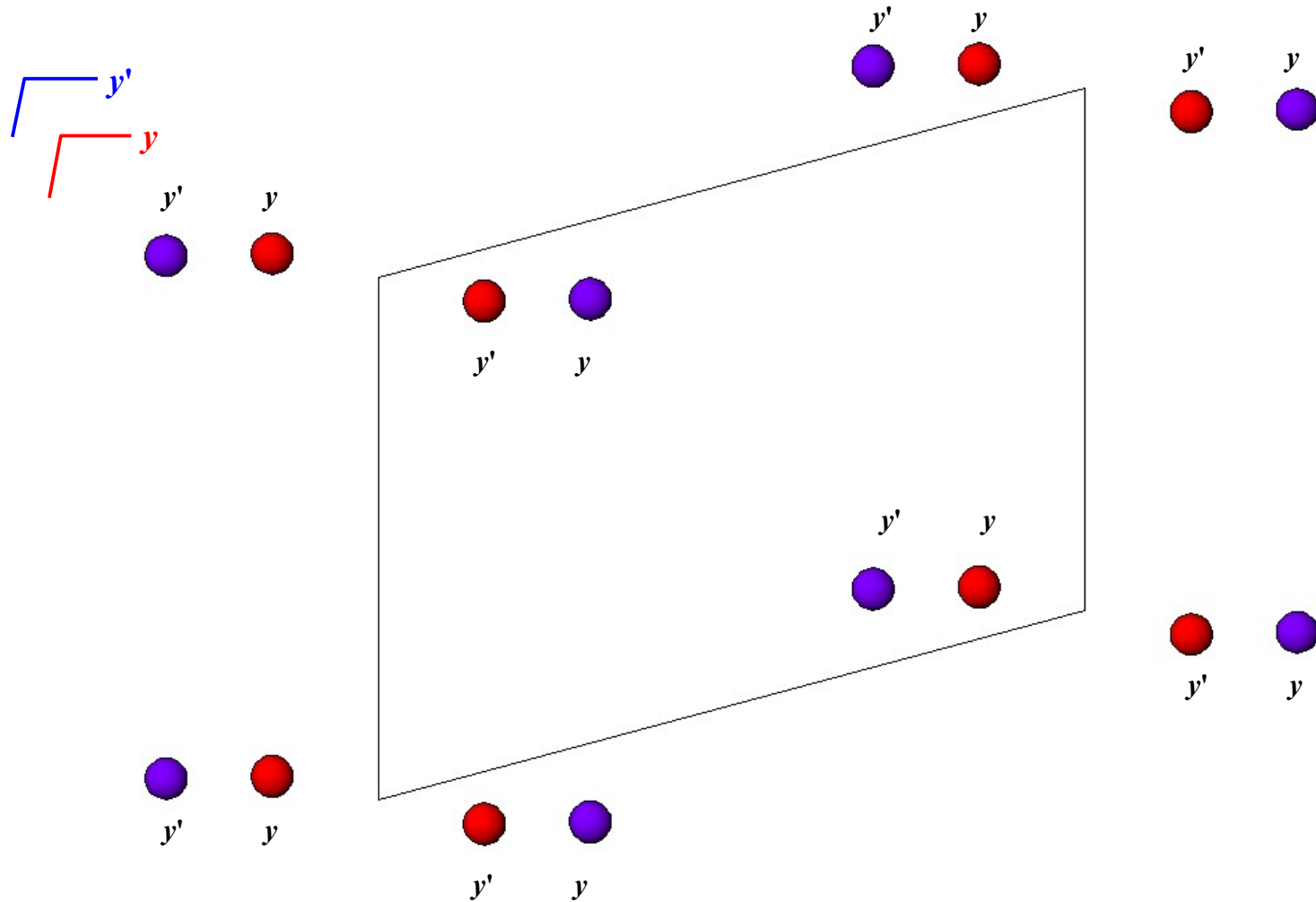
The notion of intersection group

The space group of a crystal structure is the **intersection group** of the groups that correspond to the eigensymmetry of each crystallographic orbit occupied by a type of atom in the crystal structure.

Let's see one example with two general orbits in a space group of type $P2$

Two general orbits in $P2$

$$P2/m, P(111) \cap P2/m, P(111) = P2, P(111)$$



A more complex example

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

$Fmm2$

No. 42

C_{2v}^{18}

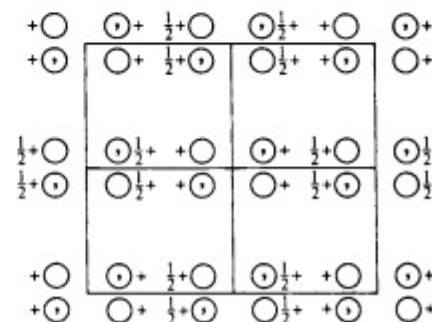
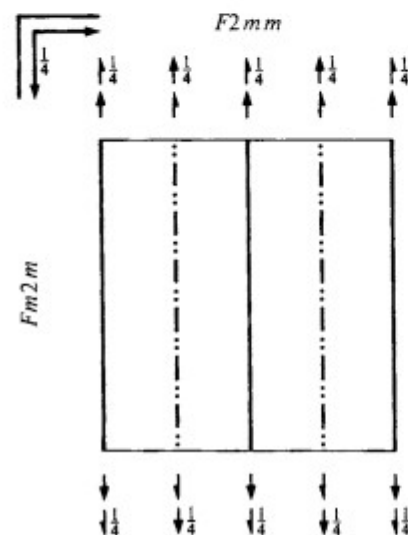
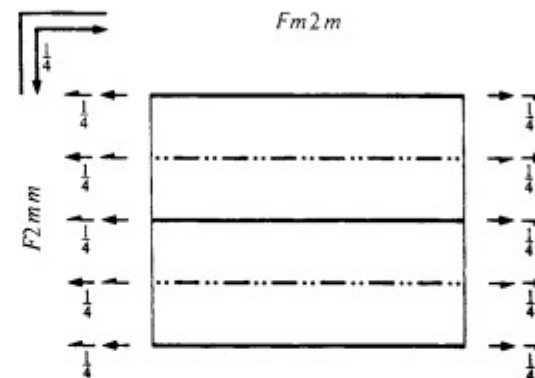
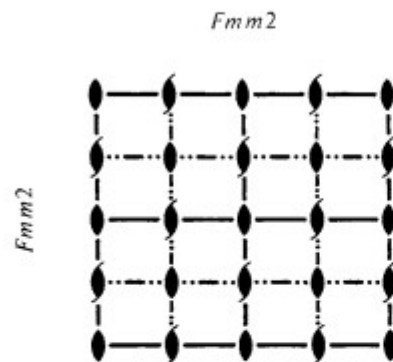
$Fmm2$

$mm2$

Orthorhombic

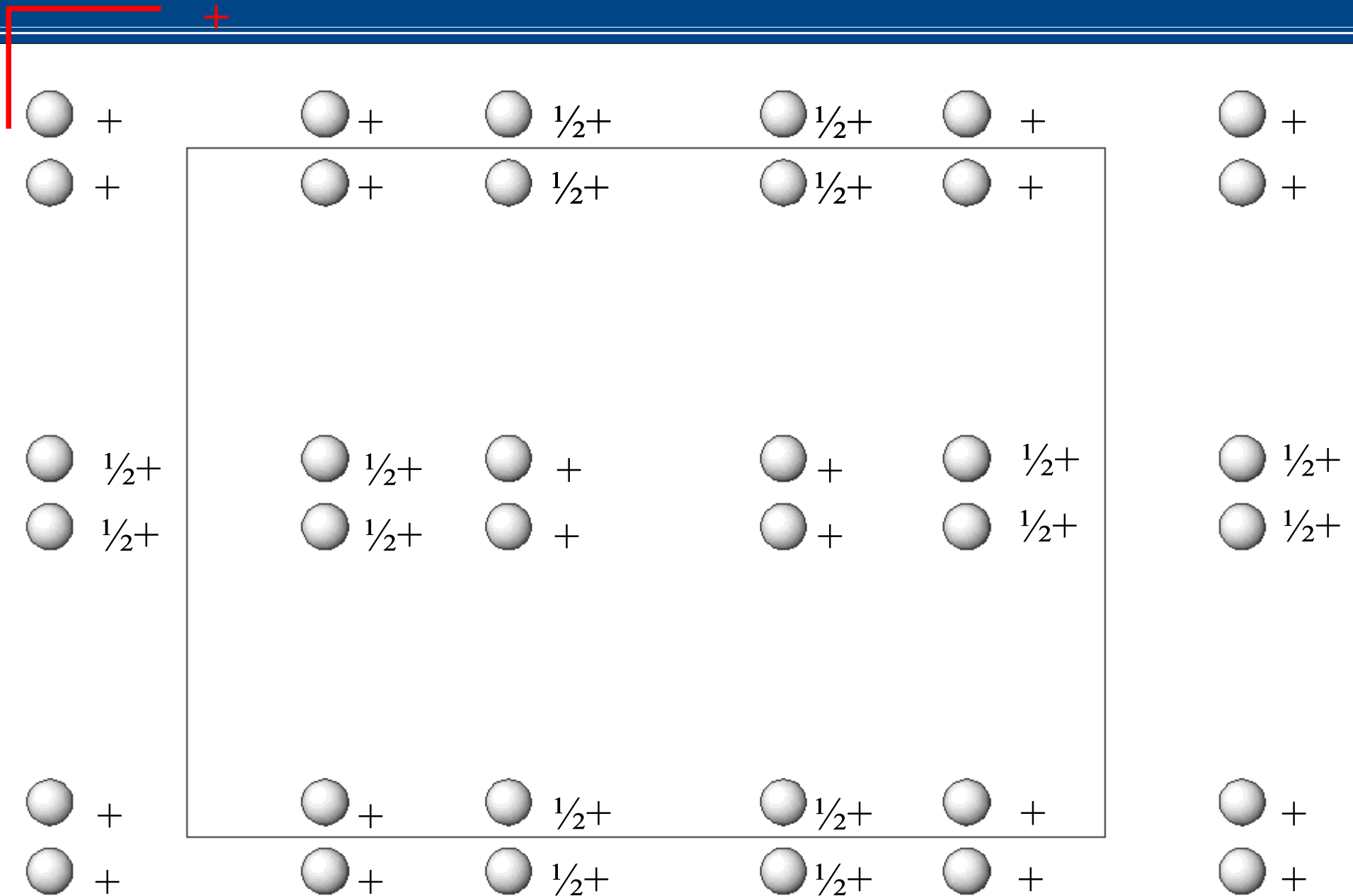
Patterson symmetry $Fmmm$

Analyse
ALL types
of orbits



Fmm2, orbit 16 *e*
 Non-characteristic orbit

Eigensymmetry: *Fmmm*
 Lattice *F(1,1,1)*

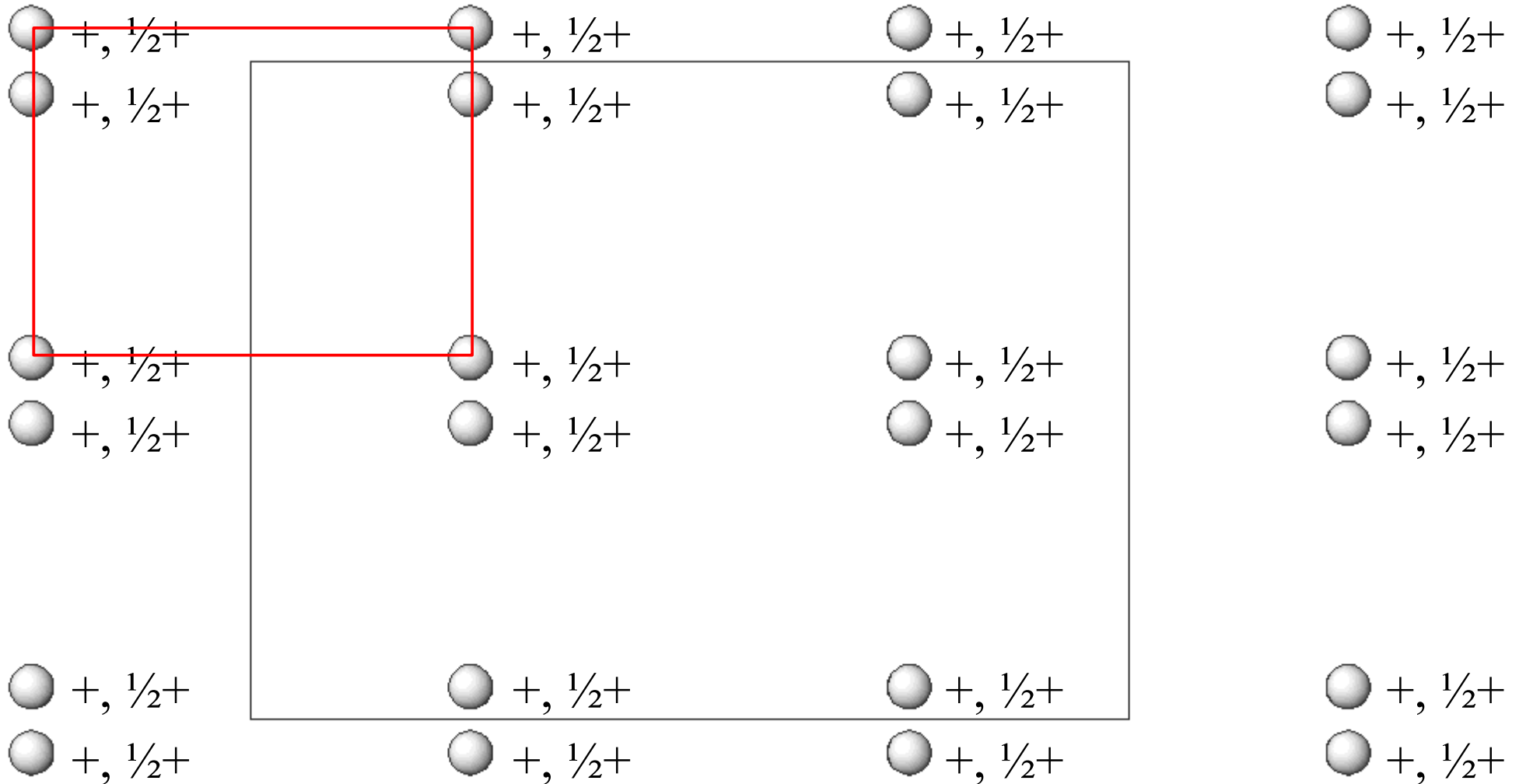


Fmm2, orbit 16 *e*, $y = 1/4$

+

Extraordinary orbit

**Eigensymmetry: *Pmmm*
Lattice $P(1/2, 1/2, 1/2)$**

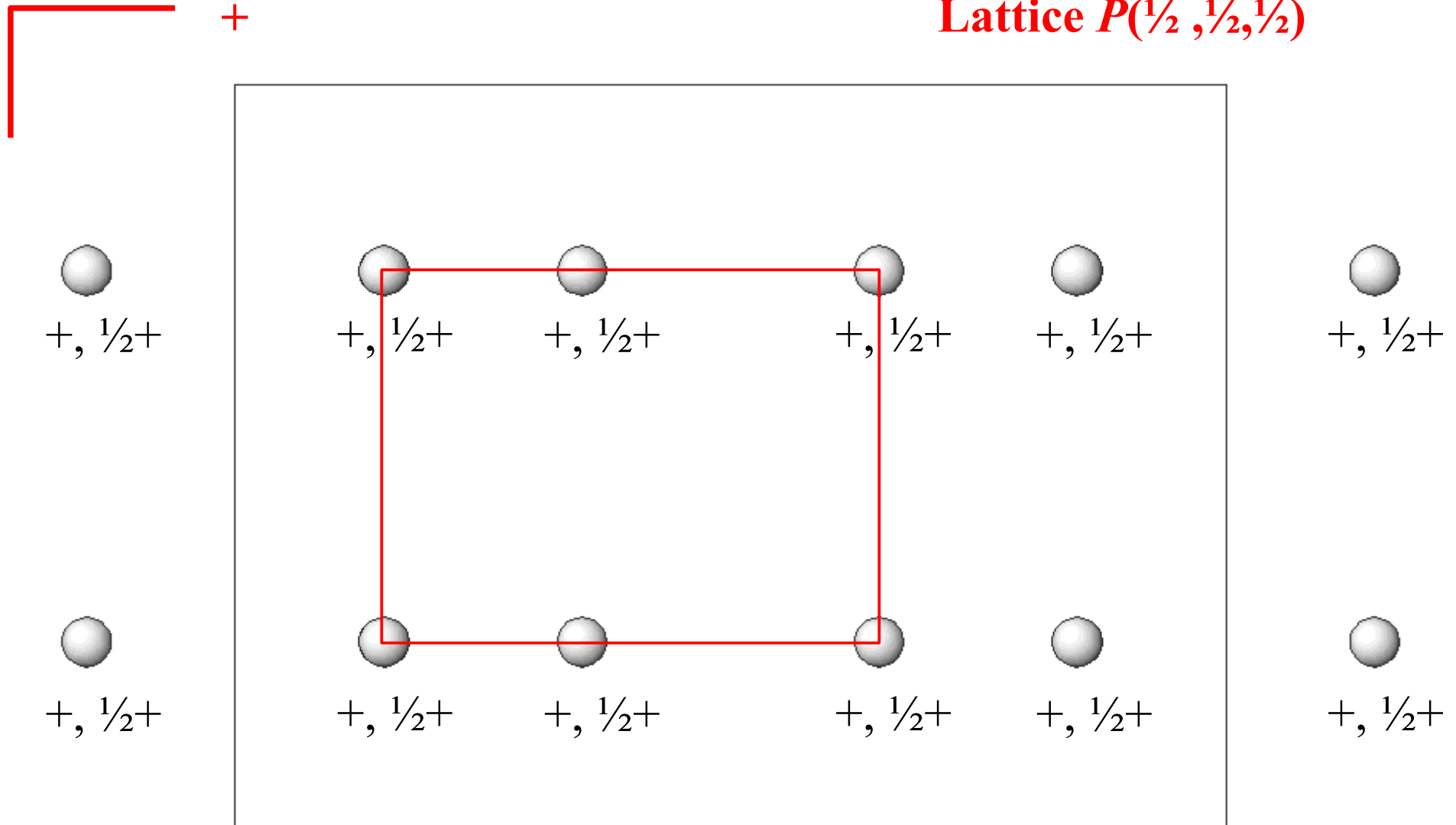


Reflection conditions: $hkl : h, k, l = 2n$

Fmm2, orbit 16 e , $x = 1/4$

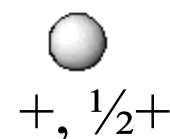
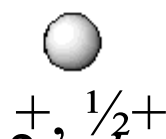
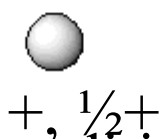
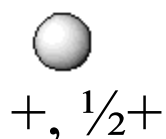
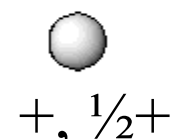
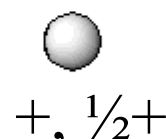
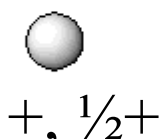
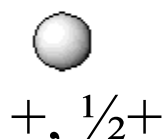
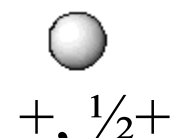
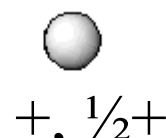
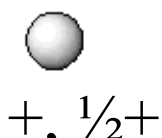
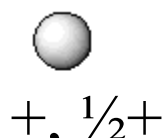
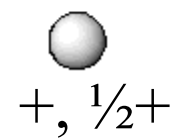
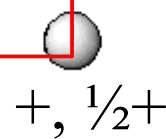
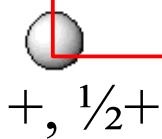
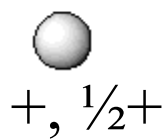
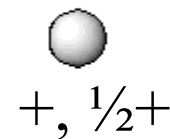
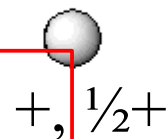
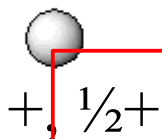
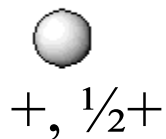
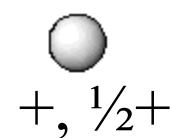
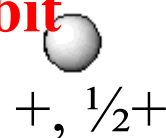
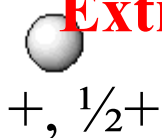
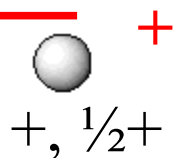
Extraordinary orbit

Eigensymmetry: *Pmmm*
Lattice $P(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$



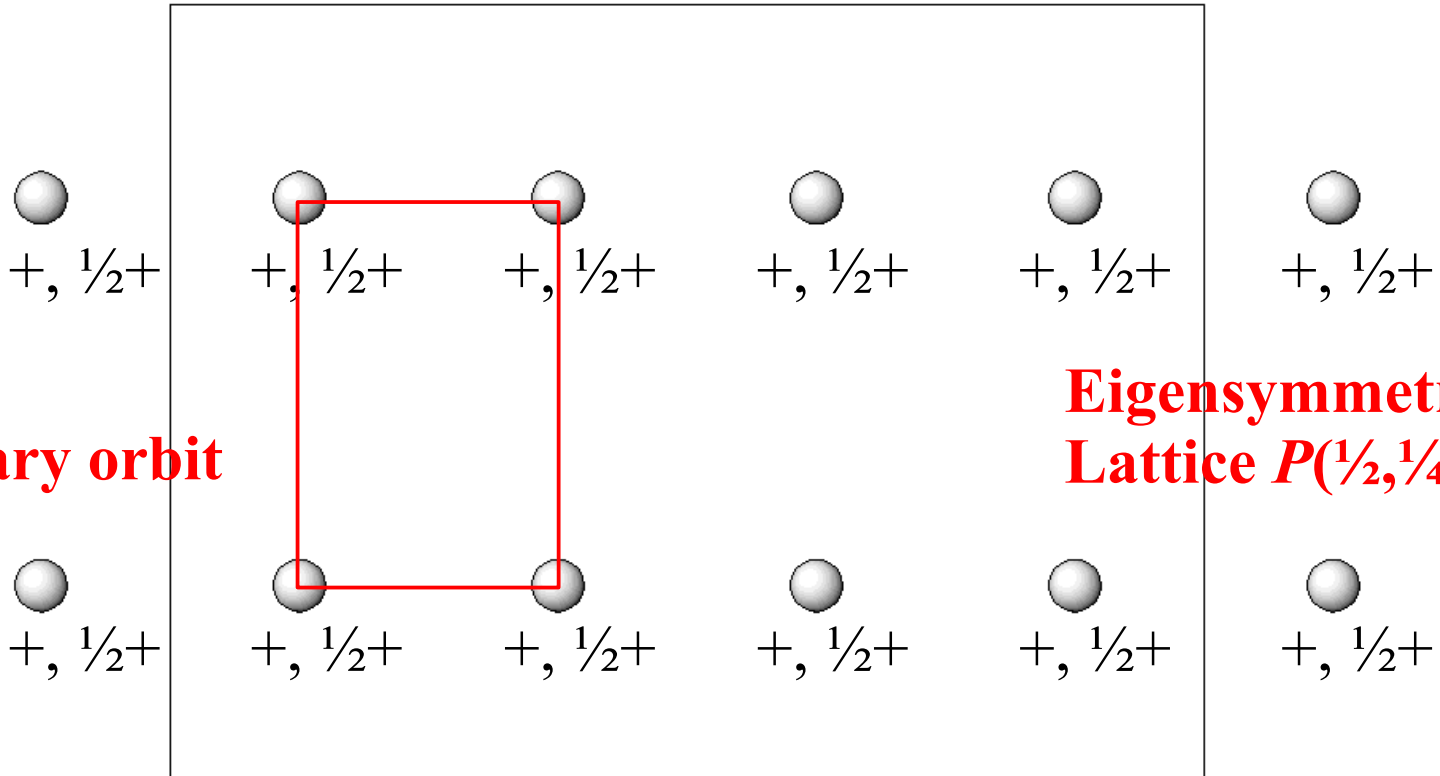
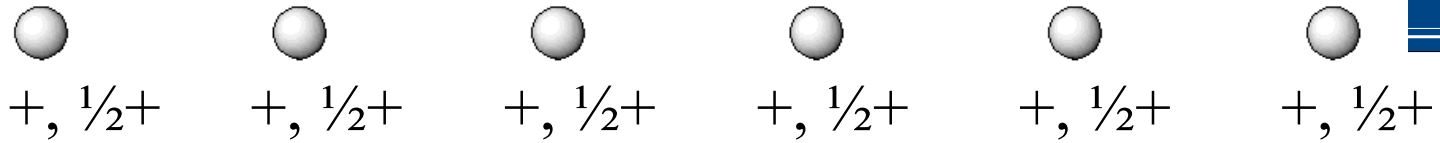
Reflection conditions: $hkl : h, k, l = 2n$

Extraordinary orbit

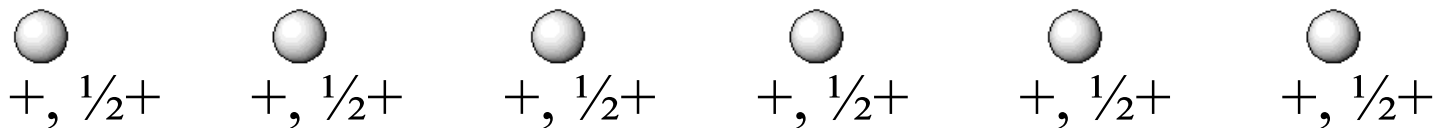


Reflection conditions: $hkl : k, l = 2n, h = 4n$

Fmm2, orbit 16 *e*, $x = 1/4, y = 1/8$



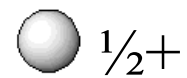
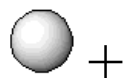
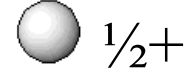
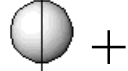
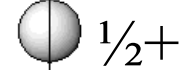
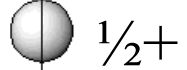
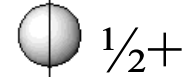
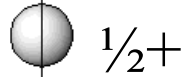
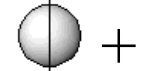
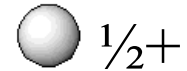
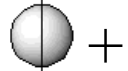
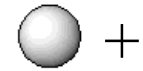
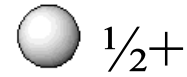
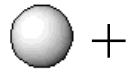
Reflection conditions: $hkl : h, l = 2n, k = 4n$



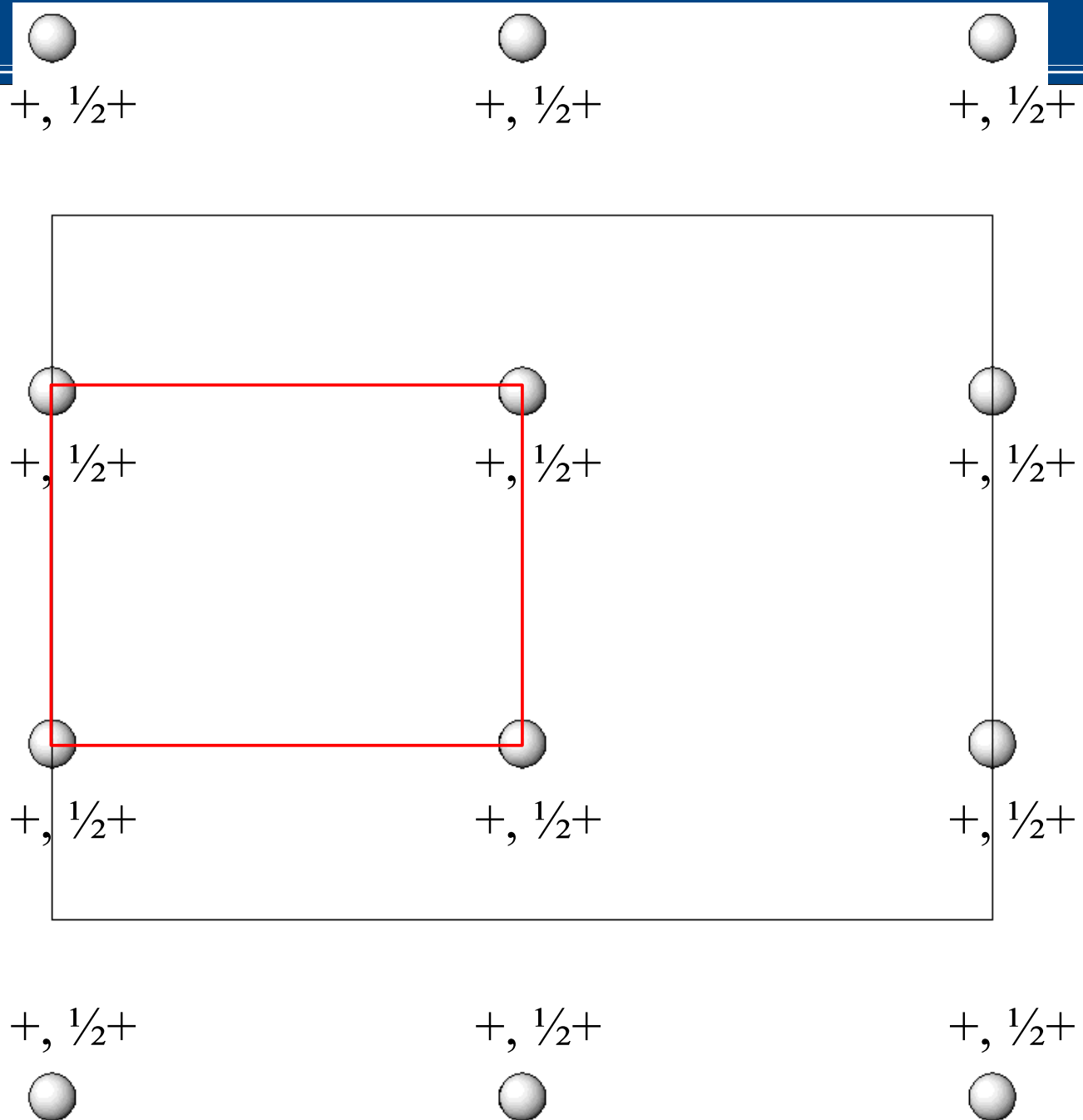
Non-characteristic orbit



+



Eigensymmetry: *Fmmm*
Lattice *F(1,1,1)*



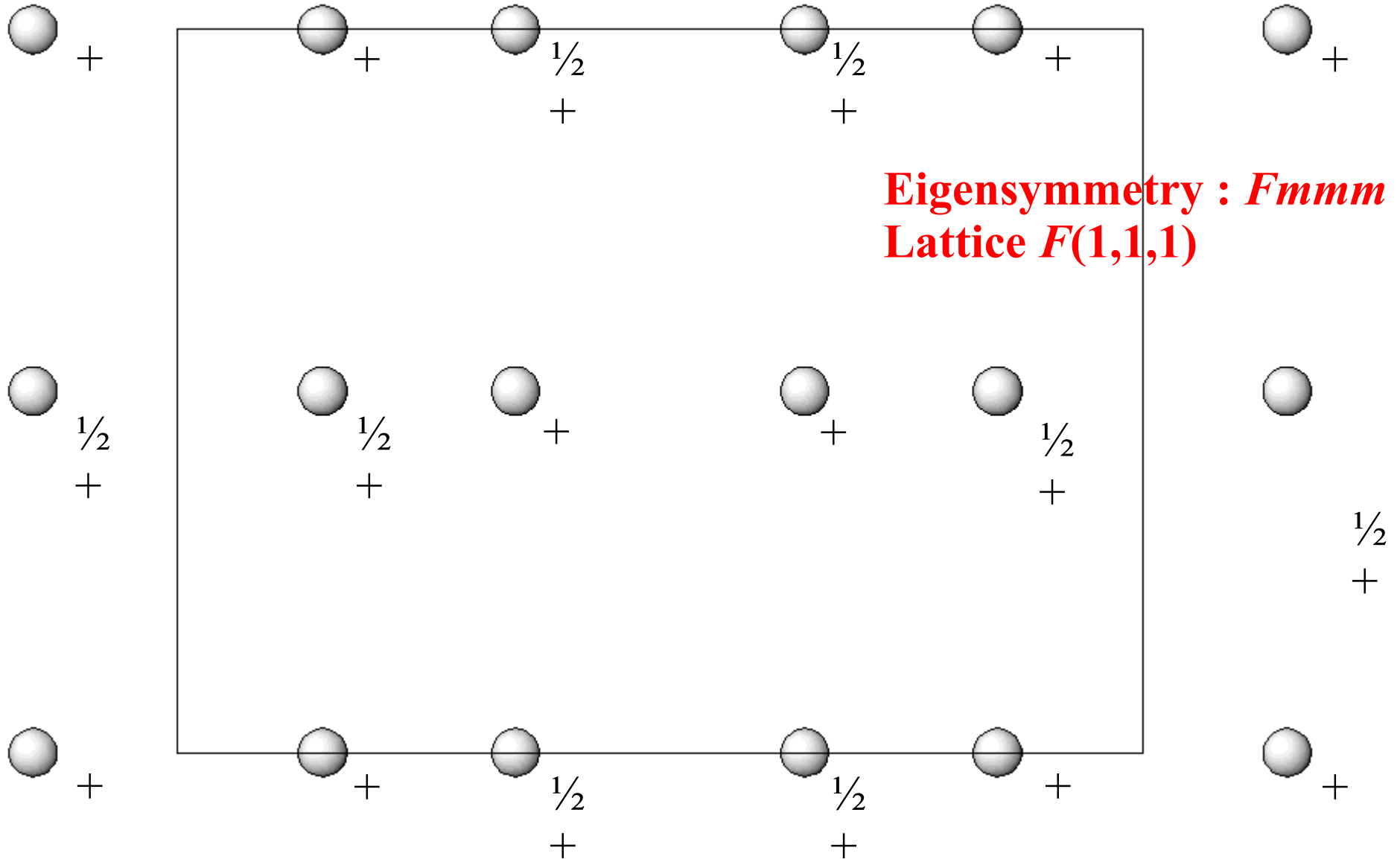
Extraordinary orbit

Eigensymmetry : *Pmmm*
Lattice $P(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

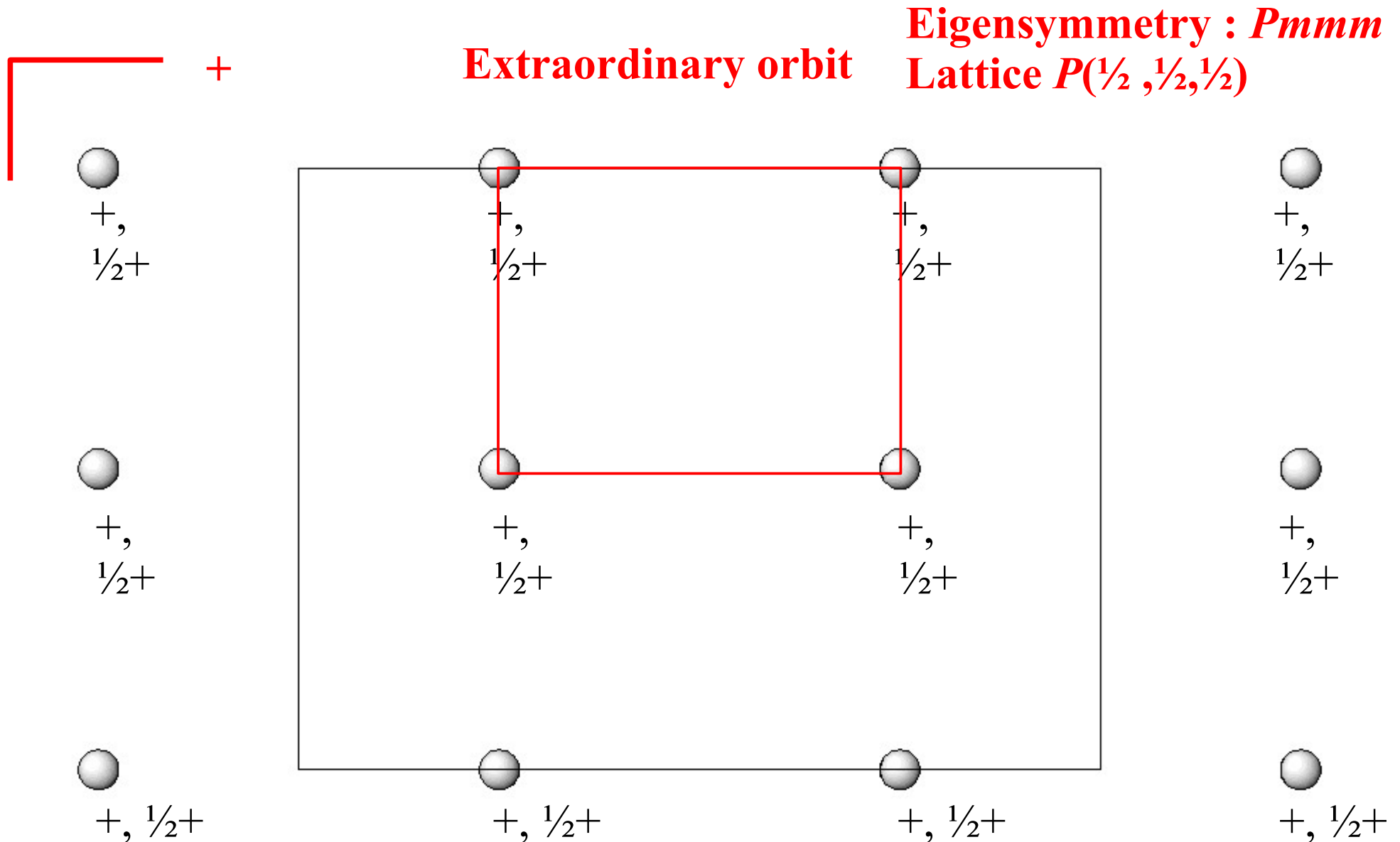
Reflection conditions:
 $hkl : h, k, l = 2n$

Non-characteristic orbit

**Eigensymmetry : *Fmmm*
Lattice *F(1,1,1)***

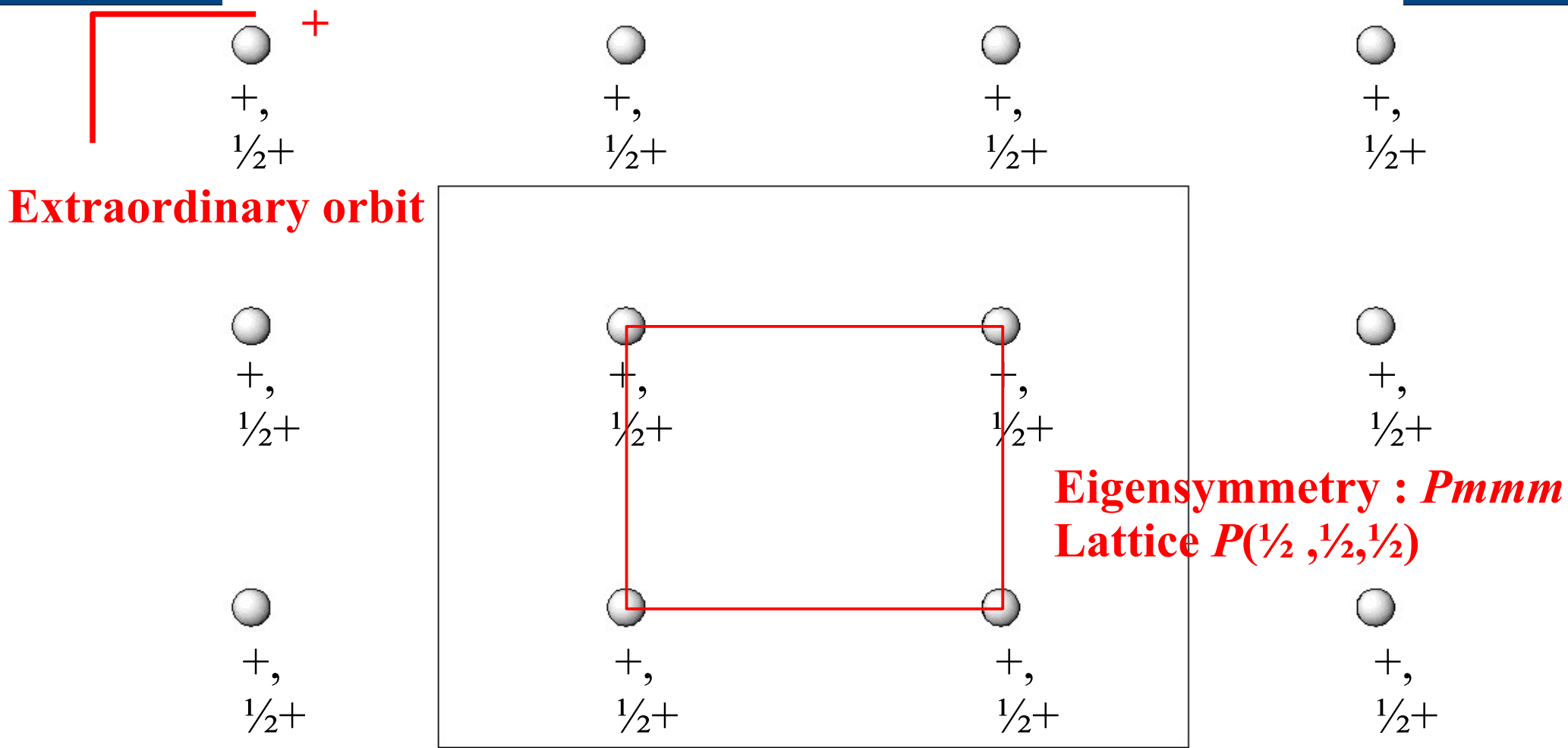


Fmm2, orbit 8 *c*, $y = 1/4$



Reflection conditions: $hkl : h, k, l = 2n$

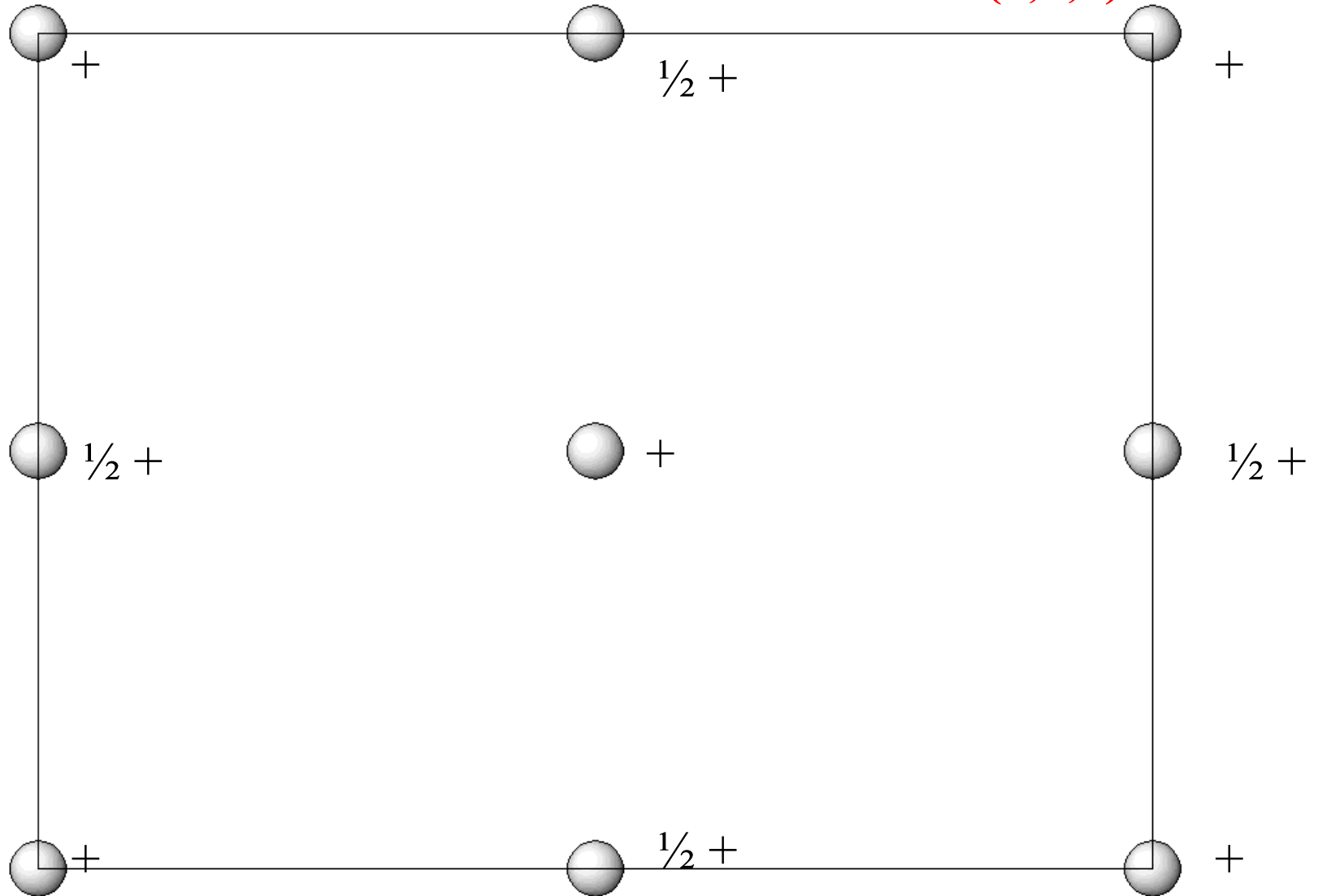
Fmm2, orbit 8 b



Reflection conditions: $hkl : h, k, l = 2n$



Non-characteristic orbit **Eigensymmetry : *Fmmm***
Lattice *F(1,1,1)*



Summary

orbits 16 e , 8 d , 8 c , 4 a	non-characteristic	Eigensymmetry: $Fmmm$ Lattice $F(1,1,1)$
orbit 16 e , $x = 1/4$ or $y = 1/4$ orbit 8 d , $x = 1/4$ or $y = 1/4$ orbit 8 b	extraordinary	Eigensymmetry: $Pmmm$ Lattice $P(1/2, 1/2, 1/2)$
orbit 16 e , $x = 1/8$, $y = 1/4$	extraordinary	Eigensymmetry: $Pmmm$ Lattice $P(1/4, 1/2, 1/2)$
orbit 16 e , $x = 1/4$ and $y = 1/8$	extraordinary	Eigensymmetry: $Pmmm$ Lattice $P(1/2, 1/4, 1/2)$

No characteristic orbit in this type of space group!

Another interesting example

International Tables for Crystallography (2006). Vol. A, Space group 120, pp. 424–425.

$I\bar{4}c2$

No. 120

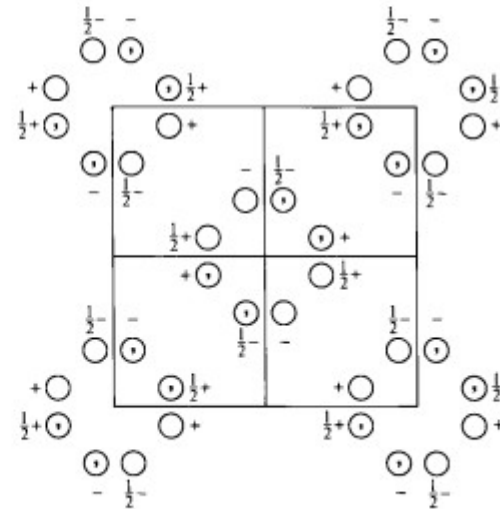
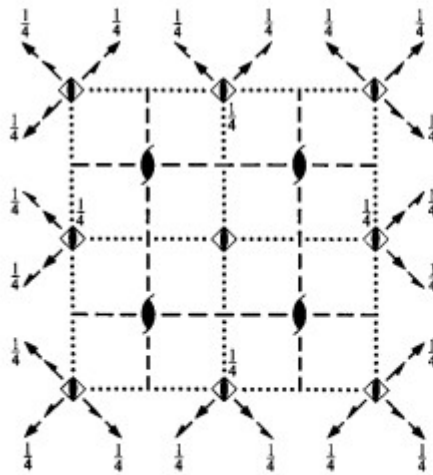
D_{2d}^{10}

$I\bar{4}c2$

$\bar{4}m2$

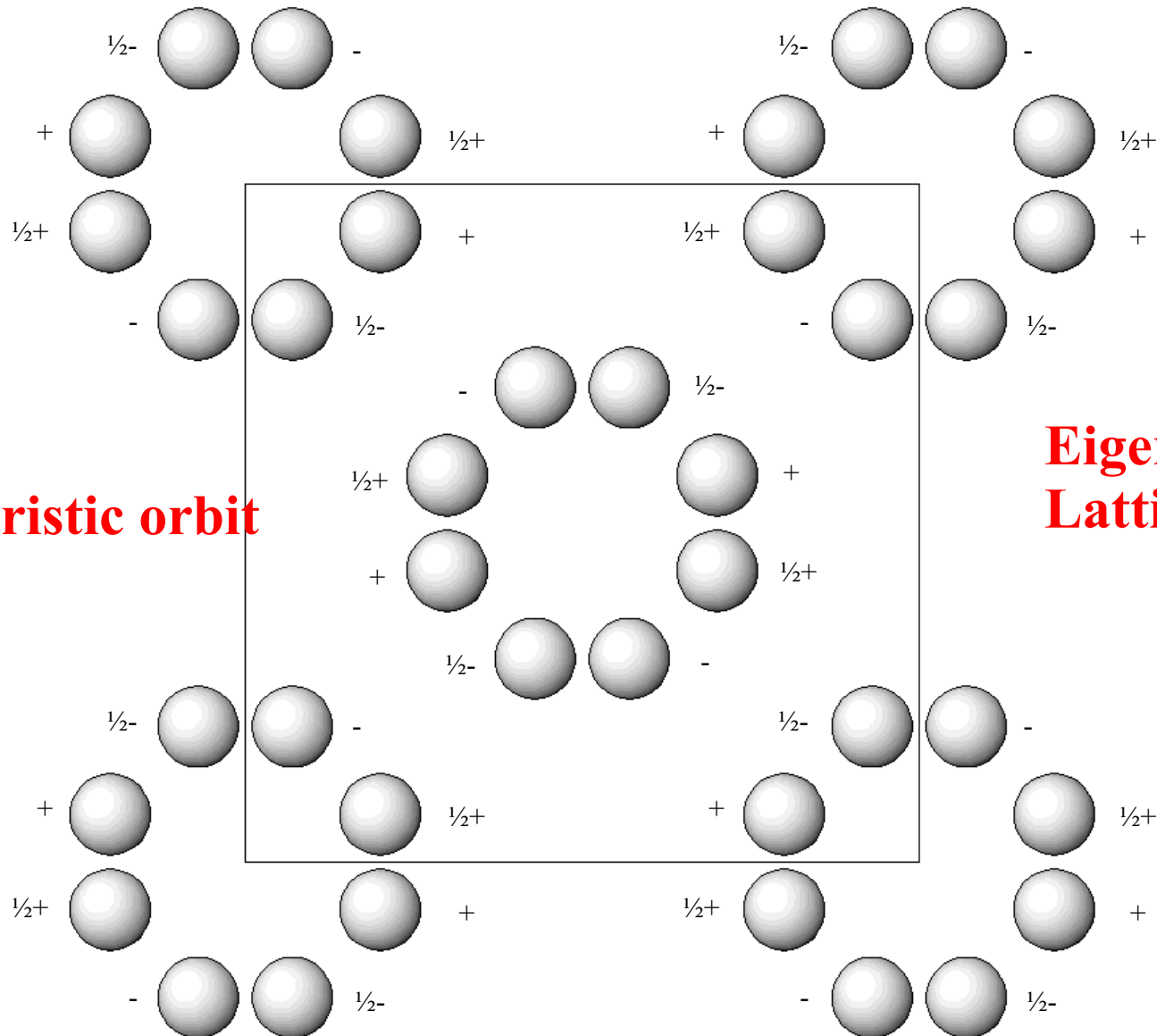
Tetragonal

Patterson symmetry $I4/mmm$



Analysis of some types of orbits

$\bar{I}4c2$ orbit $16i$

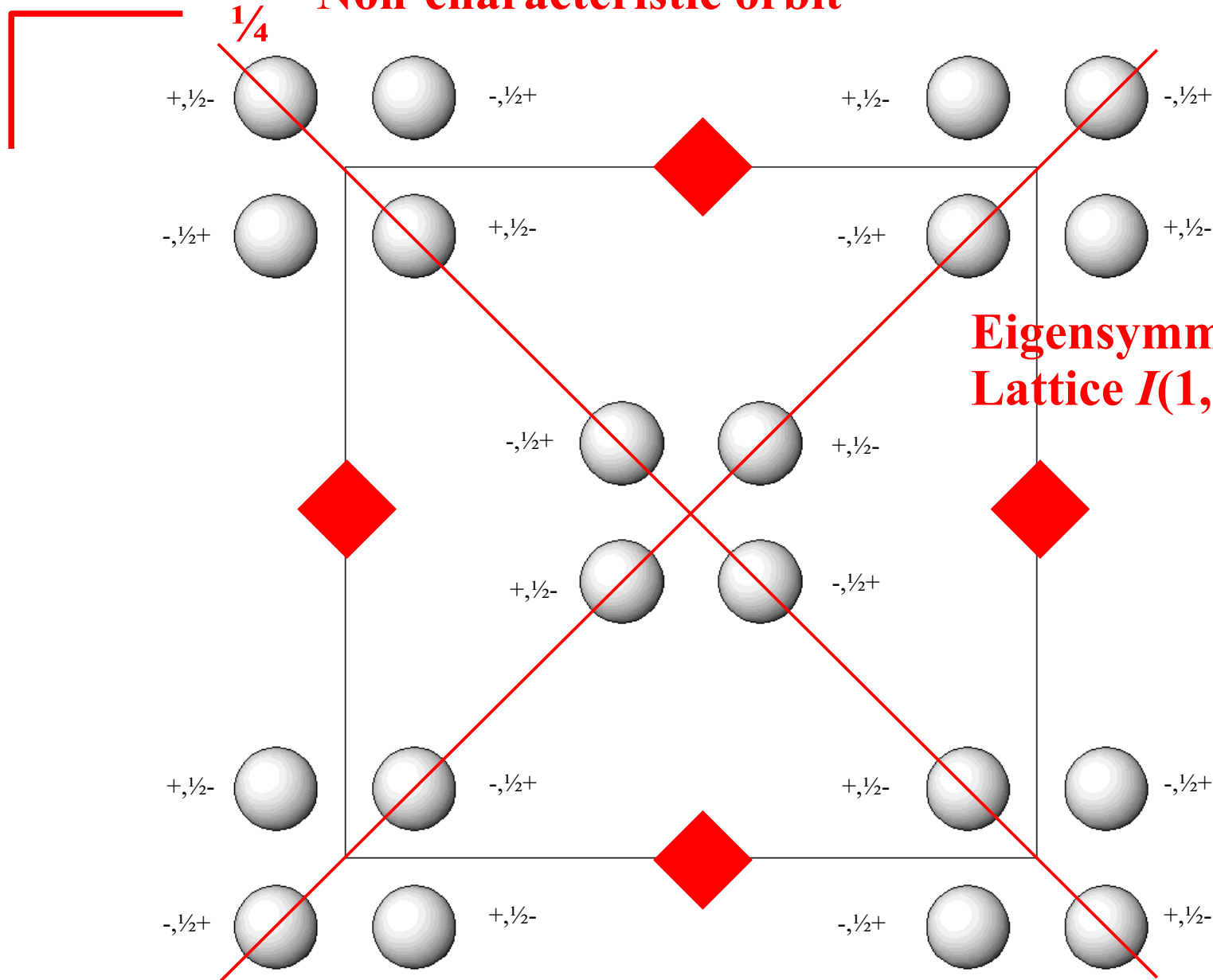


Characteristic orbit

**Eigensymmetry: $\bar{I}4c2$
Lattice $I(1,1,1)$**

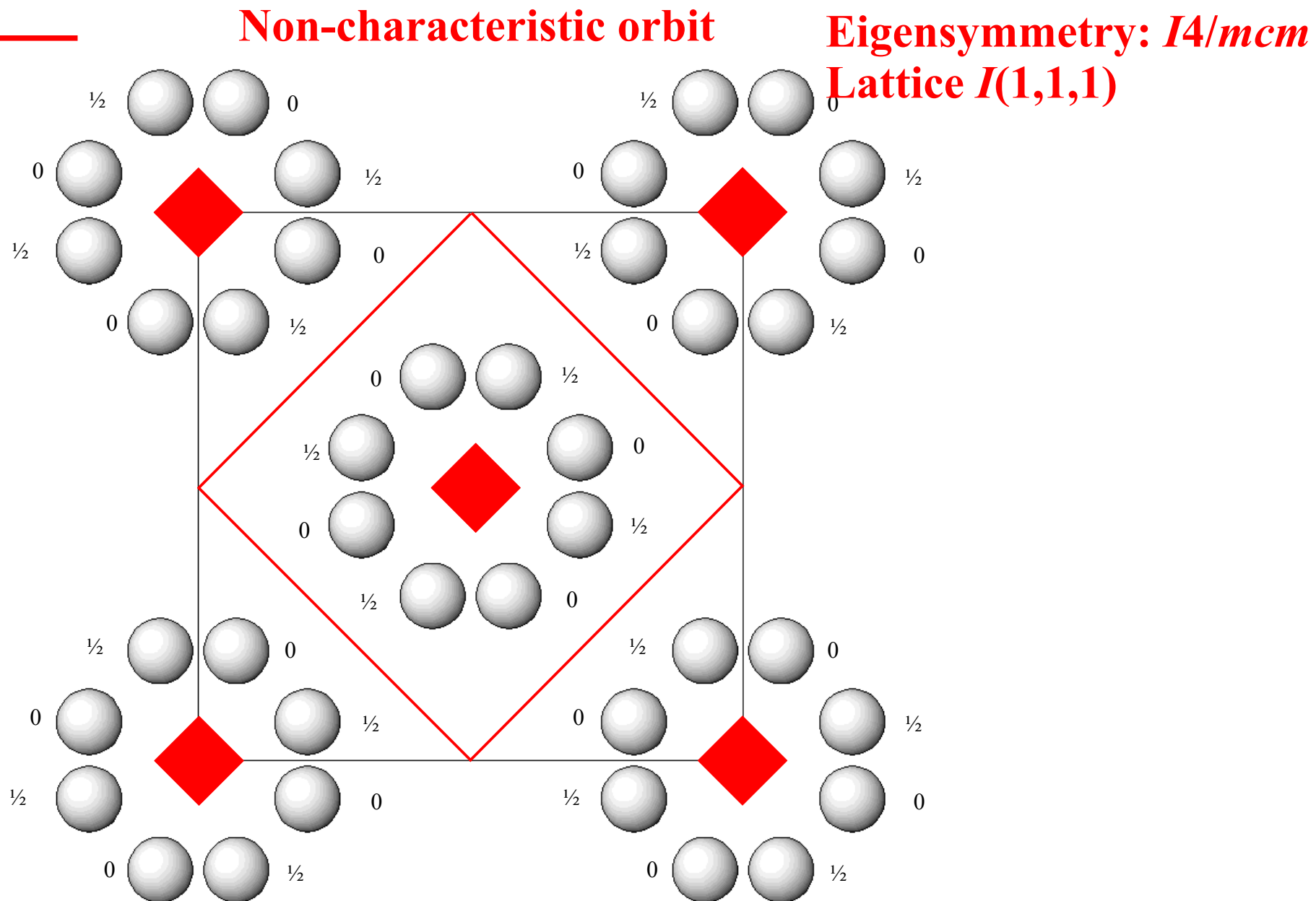
$\bar{I}4c2$ orbit 16 $i, x x z$

Non-characteristic orbit

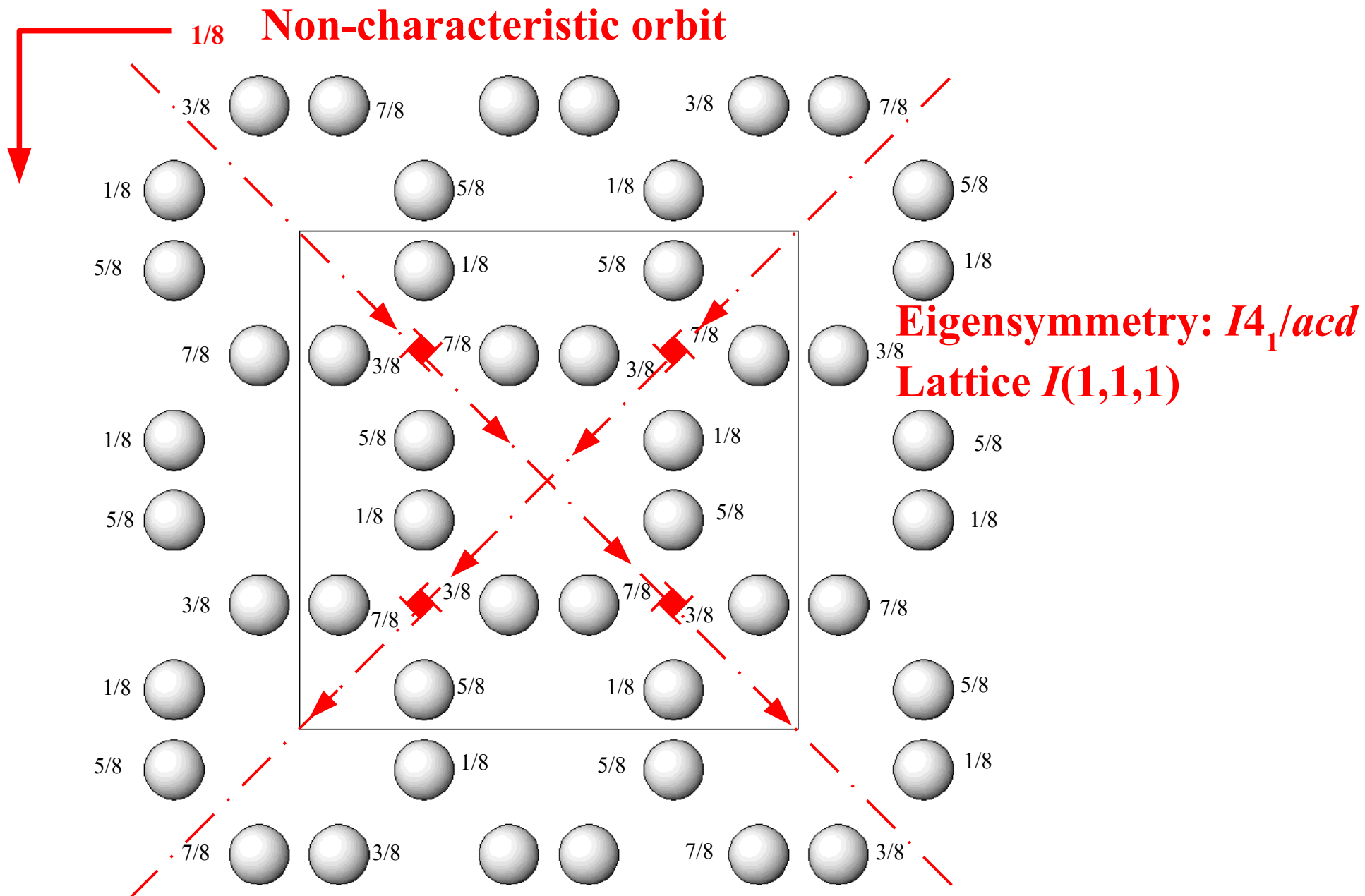


**Eigensymmetry: $I4/mcm$
Lattice $I(1,1,1)$**

$\bar{I}4c2$ orbit 16 $i x y 0$

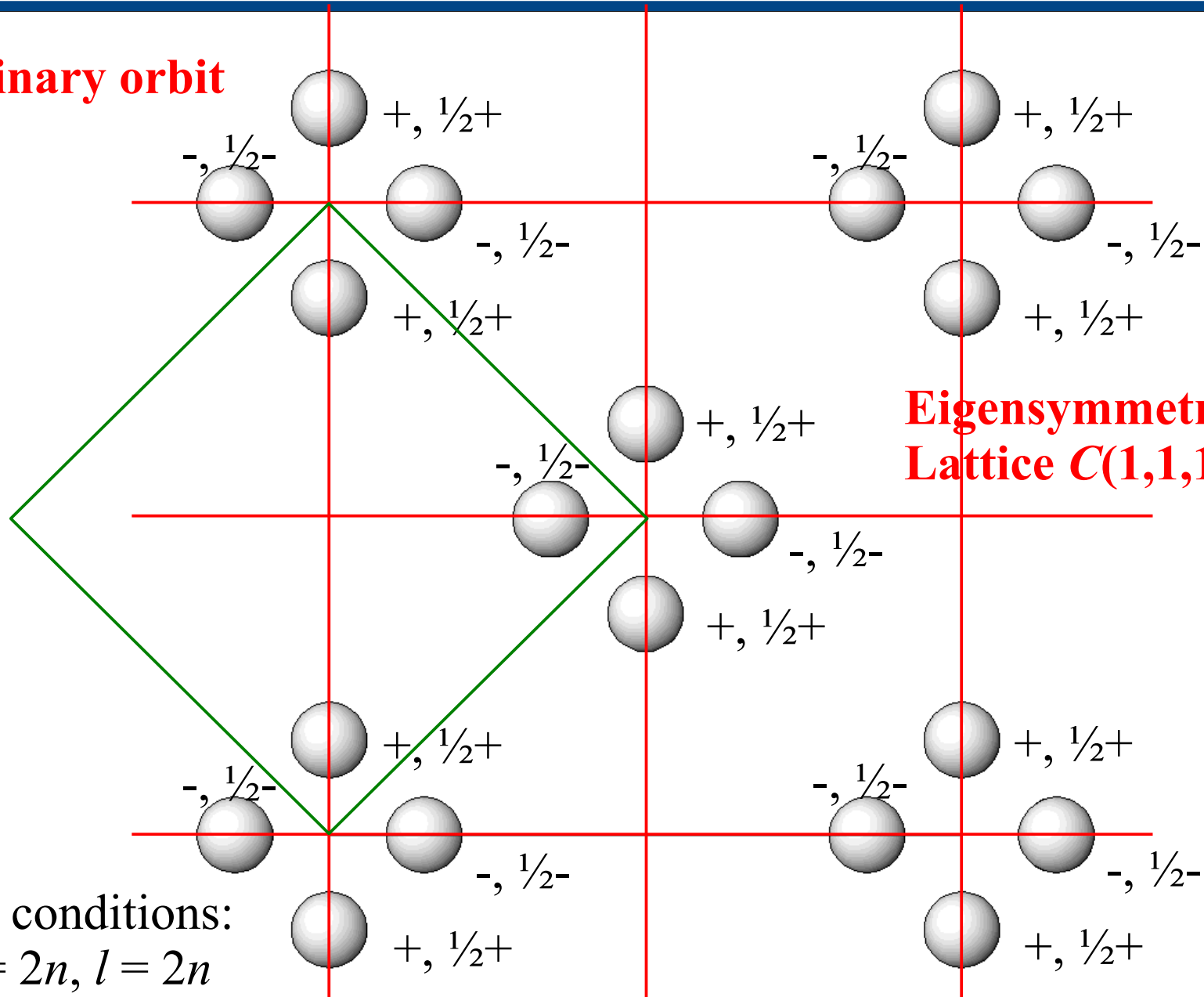


$\bar{I}4c2$ orbit $16 i x 1/4 1/8$



$\bar{I}4c2$ orbit $16 i x 0 z$

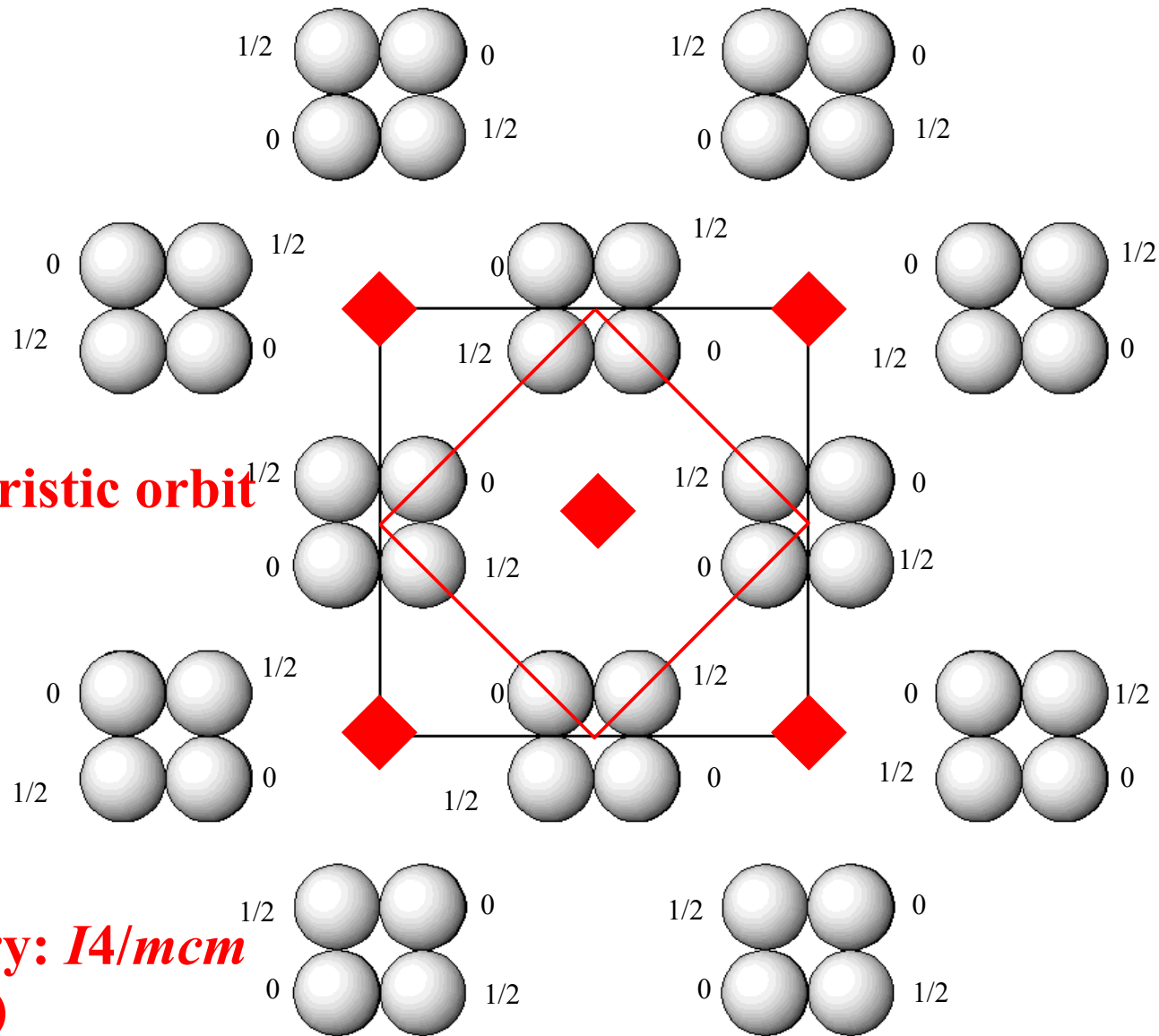
Extraordinary orbit



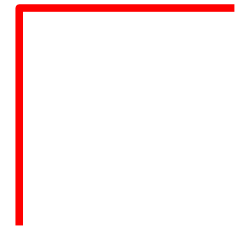
Eigensymmetry: $P\bar{4}m2$
Lattice $C(1,1,1/2)$

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

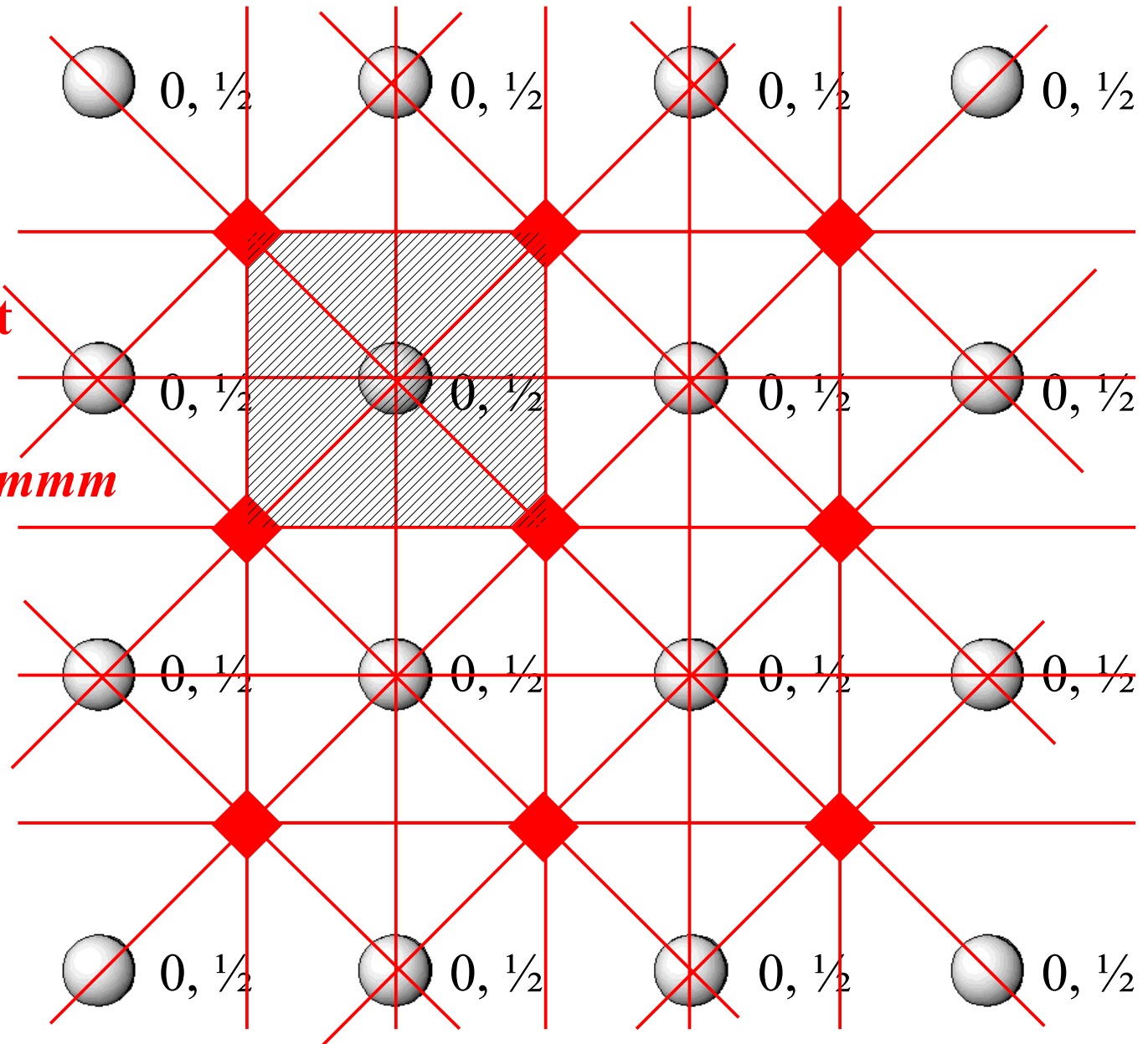
$\bar{I}4c2$ orbit $8h$



$\bar{I}4c2$ orbit $8h, x = 1/4$



Extraordinary orbit



Eigensymmetry: $P4/mmm$
Lattice $P(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Reflection conditions:
 $hkl : h, k, l = 2n$

$I\bar{4}c2$ complete analysis

Space group No.120 $I\bar{4}c2$

Superlattices

SL	Symbol	density	add.gen.
SL 0	I(1,1,1)	1	add.gen.
SL 1	C(1,1,1/2)	2	add.gen. 0,0,1/2
SL 2	C(1,1,1/4)	4	add.gen. 0,0,1/4
SL 3	P(1/2,1/2,1/2)	4	add.gen. 1/2,0,0 0,1/2,0
SL 6	P(1/2,1/2,1/4)	8	add.gen. 1/2,0,0 0,0,1/4
SL 8	C(1/2,1/2,1/2)	8	add.gen. 1/2,0,0 1/4,1/4,0
SL 9	I(1/2,1/2,1/2)	8	add.gen. 1/2,0,0 0,1/2,0 1/4,1/4,1/4

Wyckoff letter non-characteristic crystallographic orbits

Wyckoff letter	SL	Coordinates	Space Group	Coordinates	Space Group
16 i 1	SL 0	x, y, 0	I4/mcm (16k)	x, y, 1/4	I4/mcm (16k)
		x, x, z	I4/mcm (16l)	x, 1/2+x, z	I4/mcm (16l)
		x, 1/4, 1/8	I41/acd (16a)	x, 1/4, 3/8	I41/acd (16a)
	SL 1	x, 0, z	P42m (4n)	x, 0, 0	P4/mmm (4j, k)
		x, 0, 1/4	P4/mmm (4j, k)	x, 0, 1/8	P42/mcm (4i, j)
		x, 0, 3/8	P42/mcm (4i, j)	x, 1/2+x, 1/4	P4/mmm (4l-o)
	SL 3	1/4, 1/4, z	P4/mmm (4l-o)	1/4, 0, z	P4/mmm (2c)
		1/4, 1/4, 1/8	P4/mmm (2g, h)		
		1/4, 0, 0	P4/mmm (1a-d)	1/4, 0, 1/4	P4/mmm (1a-g)
	SL 8	1/4, 0, 0	P4/mmm (1a-d)	1/4, 0, 3/8	I4/mmm (2a, b)
1/4, 0, 1/8		I4/mmm (2a, b)			
8 h 2	SL 0	x, 1/2+x, 0	I4/mcm (8h)		
		1/4, 3/4, 0	P4/mmm (1a-d)		
8 g 2	SL 1	0, 1/2, z	P4/mmm (2g, h)		
		0, 1/2, 1/8	P4/mmm (1a-d)		
8 f 2	SL 1	0, 0, z	P4/mmm (2g, h)		
		0, 0, 1/8	P4/mmm (1a-d)		
8 e 2	SL 0	x, x, 1/4	I4/mcm (8h)		
		1/4, 1/4, 1/4	P4/mmm (1a-d)		
4 d 222	SL 1	0, 1/2, 0	P4/mmm (1a-d)		
4 c 4	SL 1	0, 1/2, 1/4	P4/mmm (1a-d)		
4 b 4	SL 1	0, 0, 0	P4/mmm (1a-d)		
4 a 222	SL 1	0, 0, 1/4	P4/mmm (1a-d)		

An easier example, yet...

International Tables for Crystallography (2006). Vol. A, Space group 55, pp. 282–283.

$Pbam$

No. 55

D_{2h}^9

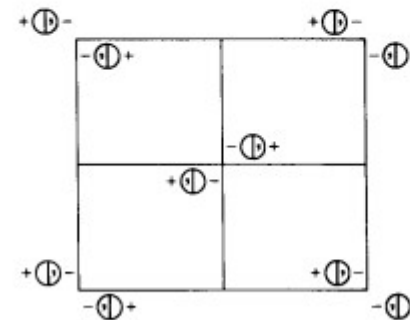
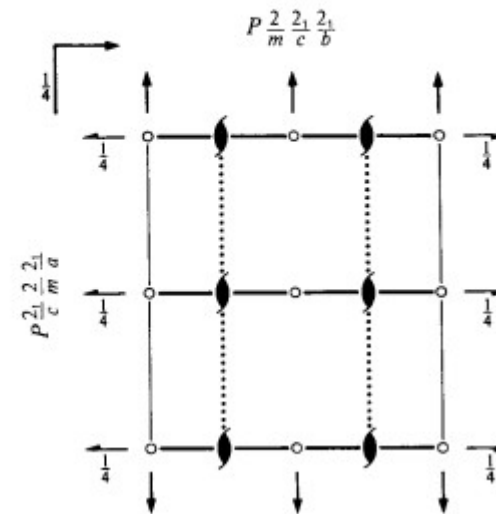
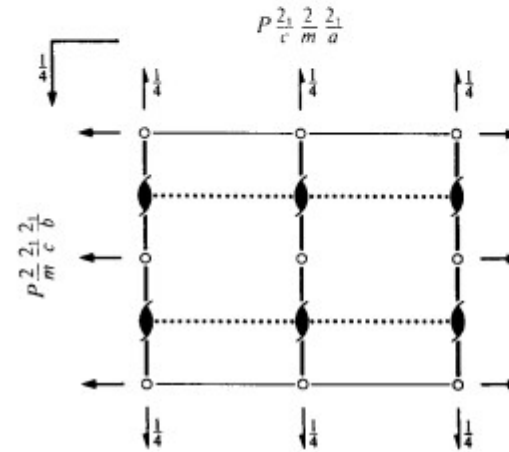
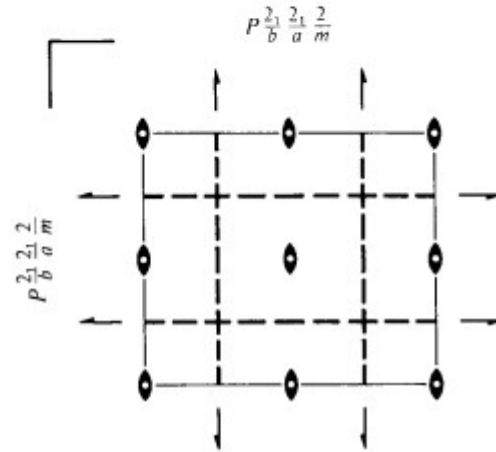
$P 2_1/b 2_1/a 2/m$

mmm

Orthorhombic

Patterson symmetry $Pmmm$

Analyse
ALL the
orbit types



Space group No. 55 Pbam

Superlattices

SL 1	P(1/2, 1, 1)	density	2	add.gen.	1/2, 0, 0
SL 2	P(1, 1/2, 1)	density	2	add.gen.	0, 1/2, 0
SL 3	P(1, 1, 1/2)	density	2	add.gen.	0, 0, 1/2
SL 6	C(1, 1, 1)	density	2	add.gen.	1/2, 1/2, 0
SL 9	P(1/2, 1/2, 1)	density	4	add.gen.	1/2, 0, 0 0, 1/2, 0
SL 10	P(1/2, 1, 1/2)	density	4	add.gen.	1/2, 0, 0 0, 0, 1/2
SL 13	C(1/2, 1, 1)	density	4	add.gen.	1/4, 1/2, 0
SL 16	P(1, 1/2, 1/2)	density	4	add.gen.	0, 1/2, 0 0, 0, 1/2
SL 19	C(1, 1/2, 1)	density	4	add.gen.	1/2, 1/4, 0
SL 24	C(1, 1, 1/2)	density	4	add.gen.	0, 0, 1/2 1/2, 1/2, 0
SL 35	P(1/2, 1/2, 1/2)	density	8	add.gen.	1/2, 0, 0 0, 1/2, 0 0, 0, 1/2
SL 43	C(1/2, 1, 1/2)	density	8	add.gen.	0, 0, 1/2 1/4, 1/2, 0
SL 55	C(1, 1/2, 1/2)	density	8	add.gen.	0, 0, 1/2 1/2, 1/4, 0

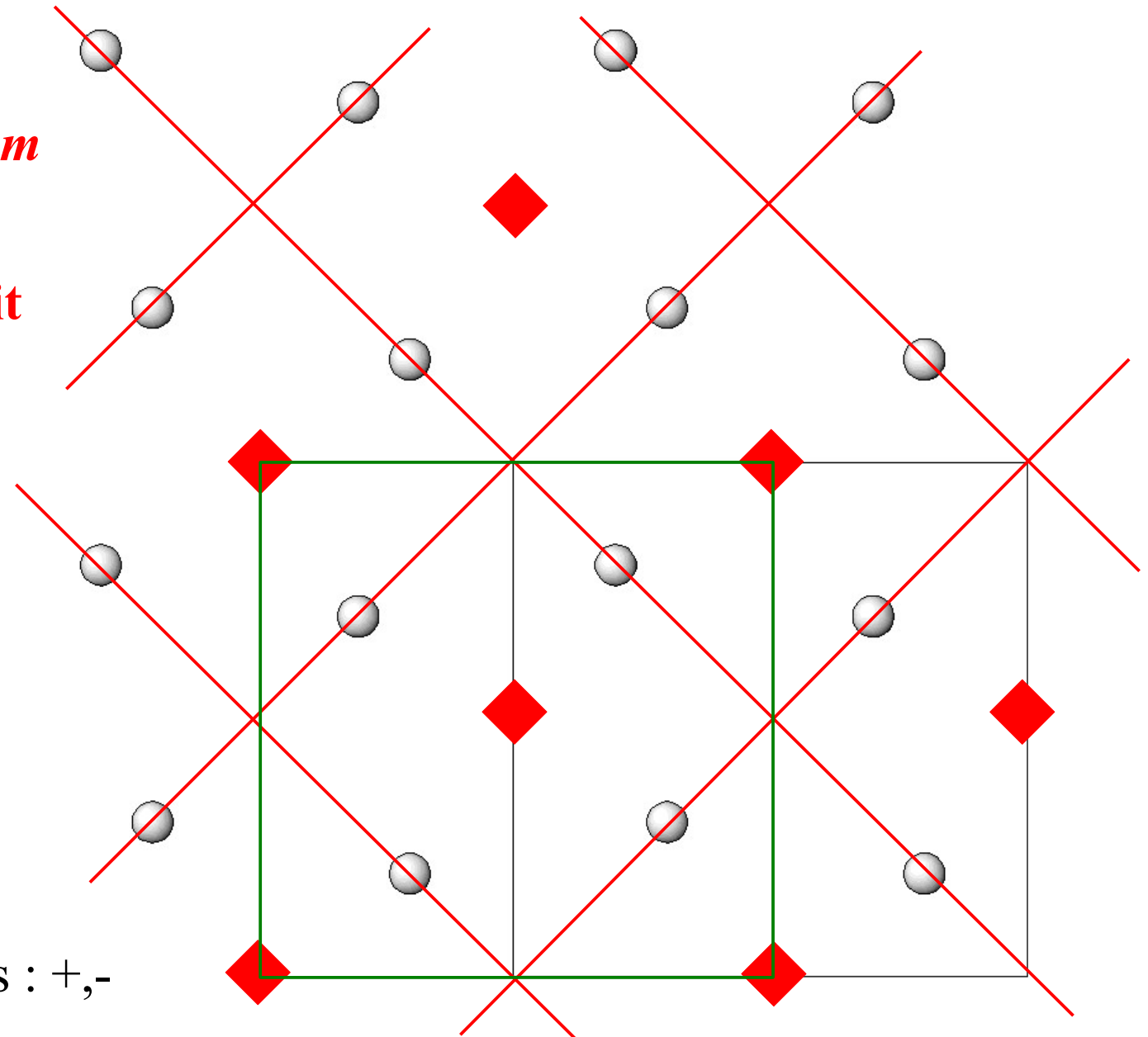
Wyckoff letter non-characteristic crystallographic orbits

8 i 1	SL 1	x, 1/4, z	Pbam (4k)			
	SL 2	1/4, y, z	Pbam (4k)			
	SL 3	x, y, 1/4	Pbam (4g, h)			
	SL 6	x, 0, z	Cmmm (8n, o)	0, y, z	Cmmm (8n, o)	
	SL 9	1/4, 0, z	Pmmm (2i-t)	0, 1/4, z	Pmmm (2i-t)	
		1/4, 1/4, z	Pmmm (2i-t)			
	SL 10	x, 1/4, 1/4	Pbam (2e, f)			
	SL 13	3/8, 1/4, z	Cmmm (4k, l)	1/8, 1/4, z	Cmmm (4k, l)	
	SL 16	1/4, y, 1/4	Pbam (2e, f)			
	SL 19	1/4, 3/8, z	Cmmm (4k, l)	1/4, 1/8, z	Cmmm (4k, l)	
	SL 24	x, 0, 1/4	Cmmm (4g-j)	0, y, 1/4	Cmmm (4g-j)	
	SL 35	1/4, 0, 1/4	Pmmm (1a-h)	0, 1/4, 1/4	Pmmm (1a-h)	
		1/4, 1/4, 1/4	Pmmm (1a-h)			
	SL 43	3/8, 1/4, 1/4	Cmmm (2a-d)	1/8, 1/4, 1/4	Cmmm (2a-d)	
	SL 55	1/4, 3/8, 1/4	Cmmm (2a-d)	1/4, 1/8, 1/4	Cmmm (2a-d)	
4 h m	SL 1	x, 1/4, 1/2	Pbam (2e, f)			
	SL 2	1/4, y, 1/2	Pbam (2e, f)			
	SL 6	x, 0, 1/2	Cmmm (4g-j)	0, y, 1/2	Cmmm (4g-j)	
	SL 9	1/4, 0, 1/2	Pmmm (1a-h)	0, 1/4, 1/2	Pmmm (1a-h)	
		1/4, 1/4, 1/2	Pmmm (1a-h)			
	SL 13	3/8, 1/4, 1/2	Cmmm (2a-d)	1/8, 1/4, 1/2	Cmmm (2a-d)	
	SL 19	1/4, 3/8, 1/2	Cmmm (2a-d)	1/4, 1/8, 1/2	Cmmm (2a-d)	
	4 g m	SL 1	x, 1/4, 0	Pbam (2e, f)		
		SL 2	1/4, y, 0	Pbam (2e, f)		
SL 6		x, 0, 0	Cmmm (4g-j)	0, y, 0	Cmmm (4g-j)	
SL 9		1/4, 0, 0	Pmmm (1a-h)	0, 1/4, 0	Pmmm (1a-h)	
		1/4, 1/4, 0	Pmmm (1a-h)			
SL 13		3/8, 1/4, 0	Cmmm (2a-d)	1/8, 1/4, 0	Cmmm (2a-d)	
SL 19		1/4, 3/8, 0	Cmmm (2a-d)	1/4, 1/8, 0	Cmmm (2a-d)	
4 f 2		SL 6	0, 1/2, z	Cmmm (4k, l)		
		SL 24	0, 1/2, 1/4	Cmmm (2a-d)		
	4 e 2	SL 6	0, 0, z	Cmmm (4k, l)		
SL 24		0, 0, 1/4	Cmmm (2a-d)			
SL 6		0, 1/2, 1/2	Cmmm (2a-d)			
2 d 2/m	SL 6	0, 1/2, 0	Cmmm (2a-d)			
2 c 2/m	SL 6	0, 1/2, 0	Cmmm (2a-d)			
2 b 2/m	SL 6	0, 0, 1/2	Cmmm (2a-d)			
2 a 2/m	SL 6	0, 0, 0	Cmmm (2a-d)			

Something is missing

Eigensymmetry: $P4/mbm$
Lattice $P(1,1,1)$

Non-characteristic orbit



All atoms : +,-

Same data in E^3

- ∞ space groups
- 219 types of affine space groups
- 230 types crystallographic space groups
- 1731 types Wyckoff positions
- 1128 types of Wyckoff sets – Wyckoff positions conjugates under the normalisers
- 402 lattice complexes – crystallographic orbits classified in types

Where to find more information?

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 W and the columns w of crystallographic symmetry operations W depend on the choice of the coordinate system. A suitable choice is essential if W and 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 W matrix

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

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

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

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 $w_j = \mathbf{o}$. Special reasons may justify exceptions from this rule, for example for space groups $I2_12_12_1 \equiv D_2^0$ (No. 24), $P4_332 \equiv O^6$ (No. 212), $P4_132 \equiv O^7$ (No. 213), $I4_132 \equiv O^8$ (No. 214) and $I43d \equiv T_d^6$ (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 $Pnmm \equiv D_{2h}^2$ (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

Where to find more information?

Peter Engel, Takeo Matsumoto,
Gerhard Steinmann, Hans Wondratschek

The Non-characteristic Orbits of the Space Groups

Supplement Issue No. 1

*Zeitschrift für
Kristallographie*

International Journal for Structural, Physical,
and Chemical Aspects of Crystalline Materials

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Space Groups and Lattice Complexes

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Prepared under the auspices of the Commission on International Tables,
International Union of Crystallography, and the Office of Standard
Reference Data, National Bureau of Standards.



U.S. DEPARTMENT OF COMMERCE, Frederick B. Dent, Secretary

NATIONAL BUREAU OF STANDARDS, Richard W. Roberts, Director

Issued May 1973

Where to find more information?

International Tables for Crystallography (2006). Vol. A, Chapter 14.1, pp. 846–847.

14.1. Introduction and definition

BY W. FISCHER AND E. KOCH

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 CaF₂). 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 $P4/mmm$, 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 $\frac{1}{2}(\mathbf{a} + \mathbf{b})$ 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 $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type $P4/mmm$ 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 $P4/mmm$ constitutes a lattice complex. Its point configurations may be derived as described above, but now starting from all space groups $P4/mmm$ 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