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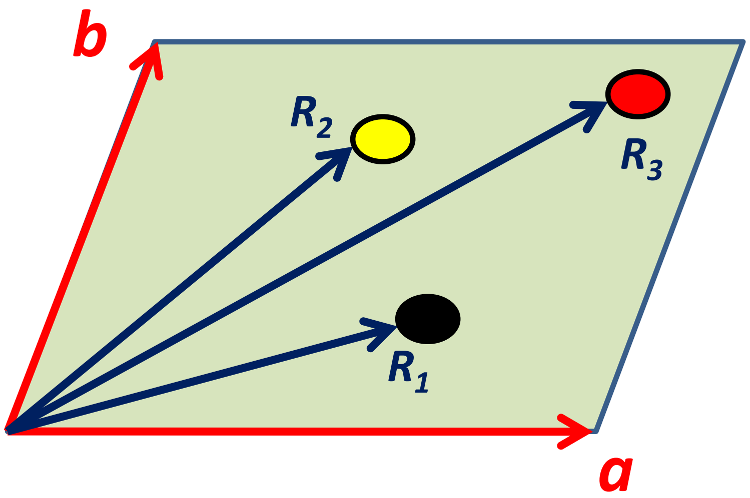
UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Lecture course on crystallography, 2015

Lecture 9: Space groups and International Tables for Crystallography

UNIT CELL and ATOMIC POSITIONS



Consider a crystal lattice. According to its Bravais type we chose the conventional pair (triple) of basis vectors: ***a***,***b*** and ***c.*** The crystallographic unit cell is defined by putting atoms, molecules, etc to the sites, ***R_1 , R_2 ,…, R_n inside the parallelogram based on the vectors a, b and c.*** The site of each and every atom in the unit cell is given by the *fraction atomic positions, x, y and z.*

$$\boldsymbol{R} = x\boldsymbol{a} + y\boldsymbol{b} + z\boldsymbol{c},$$

$$\text{with } 0 \le x < 1,\ 0 \le y < 1,\ 0 \le z < 1$$

The lattice translations are applied to each atomic positions, i.e. if there is an atom with the coordinate [x,y,z] then there is also an atom with the coordinates [x+u, y+v, z+w]. Translation [uvw] is regarded as symmetry operation

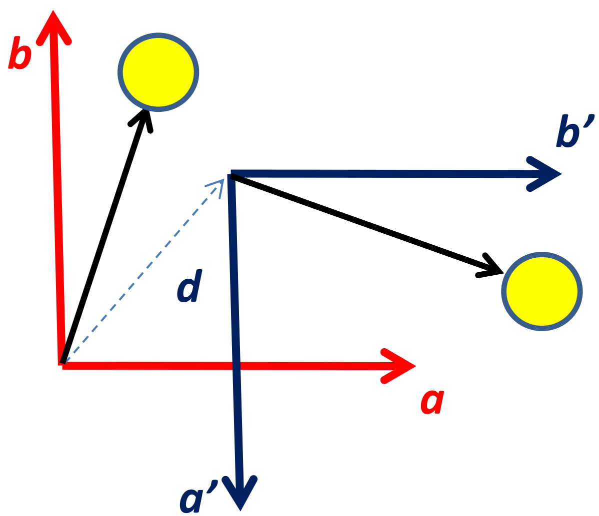
CRYSTALLOGRAPHIC SPACE GROUP IS THE COMPLETE DESCRIPTION OF THE SYMMETRY OF CRYSTAL STRUCTURES. THE ***GROUPS*** ARE COMPILED FROM THE FOLLOWING SYMMETRY OPERATIONS:

1. Lattice translation $\boldsymbol{A_{uvw} = u\,a + v\,b + w\,c}$***. Defines crystal system and type of the Bravais lattice***

2. Further point symmetry and space symmetry operations accepted by the chosen crystal systems.

- ***Rotation***
- ***Reflection***
- ***Inversion***
- ***Rotoinversion***
- ***Glide planes***
- ***Screw axes***

Matrix representation for symmetry operation



Any symmetry operation can be presented by the rotation matrix and displacement vector. Suppose the lattice is built on the basis vectors ***a***, ***b*** and ***c*** and the position of atoms are given by the fractional coordinates [xyz] so that ***R*** = x***a***+y***b***+z***c***. If we apply the movement related to the particular symmetry operation, the vectors a, b and c are transformed into a’, b’ and c’ and the origin is displaced by the vector ***d***. ***The position of symmetry equivalent atom is***

$$\boldsymbol{R'} = x\,\boldsymbol{a'} + y\,\boldsymbol{b'} + z\,\boldsymbol{c'} + \boldsymbol{d} = x_1\,\boldsymbol{a} + y_1\,\boldsymbol{b} + z_1\,\boldsymbol{c}$$

$$\begin{cases} \mathbf{a}' = S_{11}\mathbf{a} + S_{21}\mathbf{b} + S_{31}\mathbf{c} \\ \mathbf{b}' = S_{12}\mathbf{a} + S_{22}\mathbf{b} + S_{32}\mathbf{c} \\ \mathbf{c}' = S_{13}\mathbf{a} + S_{23}\mathbf{b} + S_{33}\mathbf{c} \\ \mathbf{d} = d_1\,\mathbf{a} + d_2\,\mathbf{b} + d_3\,\mathbf{c} \end{cases} \longrightarrow \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}$$

Rotation matrix ***Displacement vector***

Combination of symmetry operations in terms of matrices

Symmetry operation 1: $\{\boldsymbol{S_1}, \boldsymbol{d_1}\}$ $\qquad \boldsymbol{R}_1 = \boldsymbol{S}_1 R_0 + \boldsymbol{d}_1$

Symmetry operation 2: $\{\boldsymbol{S_2}, \boldsymbol{d_2}\}$ $\qquad \boldsymbol{R}_2 = \boldsymbol{S}_2 R_0 + \boldsymbol{d}_2$

Symmetry operation 3: $\{\boldsymbol{S_1}, \boldsymbol{d_1}\}$ -> $\{\boldsymbol{S_2}, \boldsymbol{d_2}\}$

$$\boldsymbol{R_2} = \boldsymbol{S_2}\, \boldsymbol{R_1} + \boldsymbol{d_2} \quad = \boldsymbol{S_2}\, \boldsymbol{S_1}\, \boldsymbol{R_0} + \boldsymbol{S_2}\, \boldsymbol{d_1} + \boldsymbol{d_2}$$

The combination of symmetry operation is represented by the rotation matrix $\boldsymbol{S_2}\, \boldsymbol{S_1}$ and displacement vector $\boldsymbol{S_2}\, \boldsymbol{d_1} + \boldsymbol{d_2}$

THE PRINCIPLE OF SPACE GROUP FORMATION IS SIMILAR TO THAT FOR THE POINT GROUP.

CRYSTAL LATTICE (THE SPACE SYMMETRY GROUP OF A CRYSTAL LATTICE)

TAKING OUT A SYMMETRY ELEMENT

Making sure that this symmetry element is not restored by the combination of the remaining symmetry elements

Getting a space symmetry group for a crystal

Space groups in 2D and 3D space

There are 17 2D (planar) space groups and 230 3D space groups. For the first time the space groups were described by Russian crystallographer E.S Fedorov

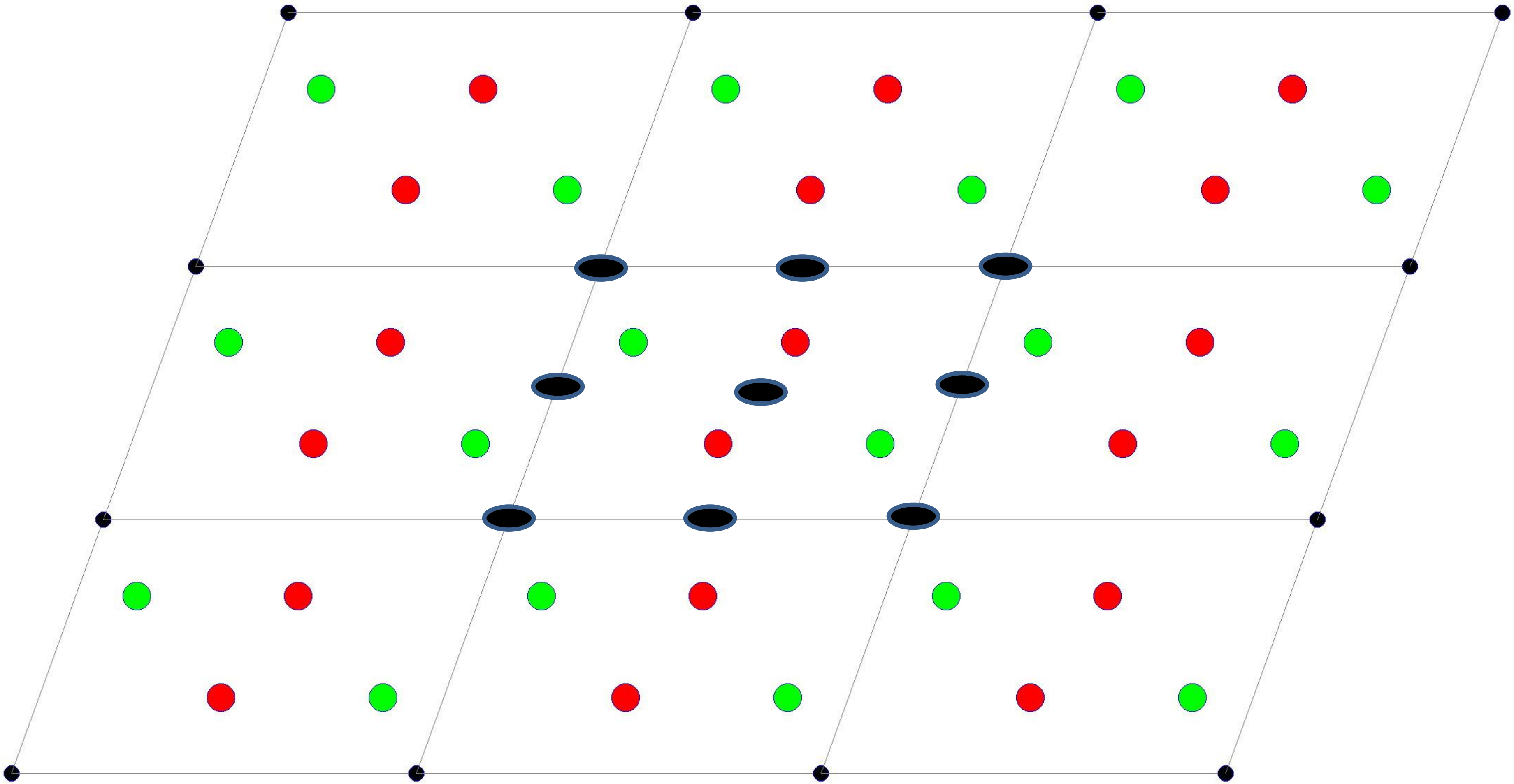
E.S. Fedorov (1853-1919)

Each of the space groups has the own name (space group symbol). As an example

$P2_1$, Fd3m, Cm, Cc, C2, I4bm, ...

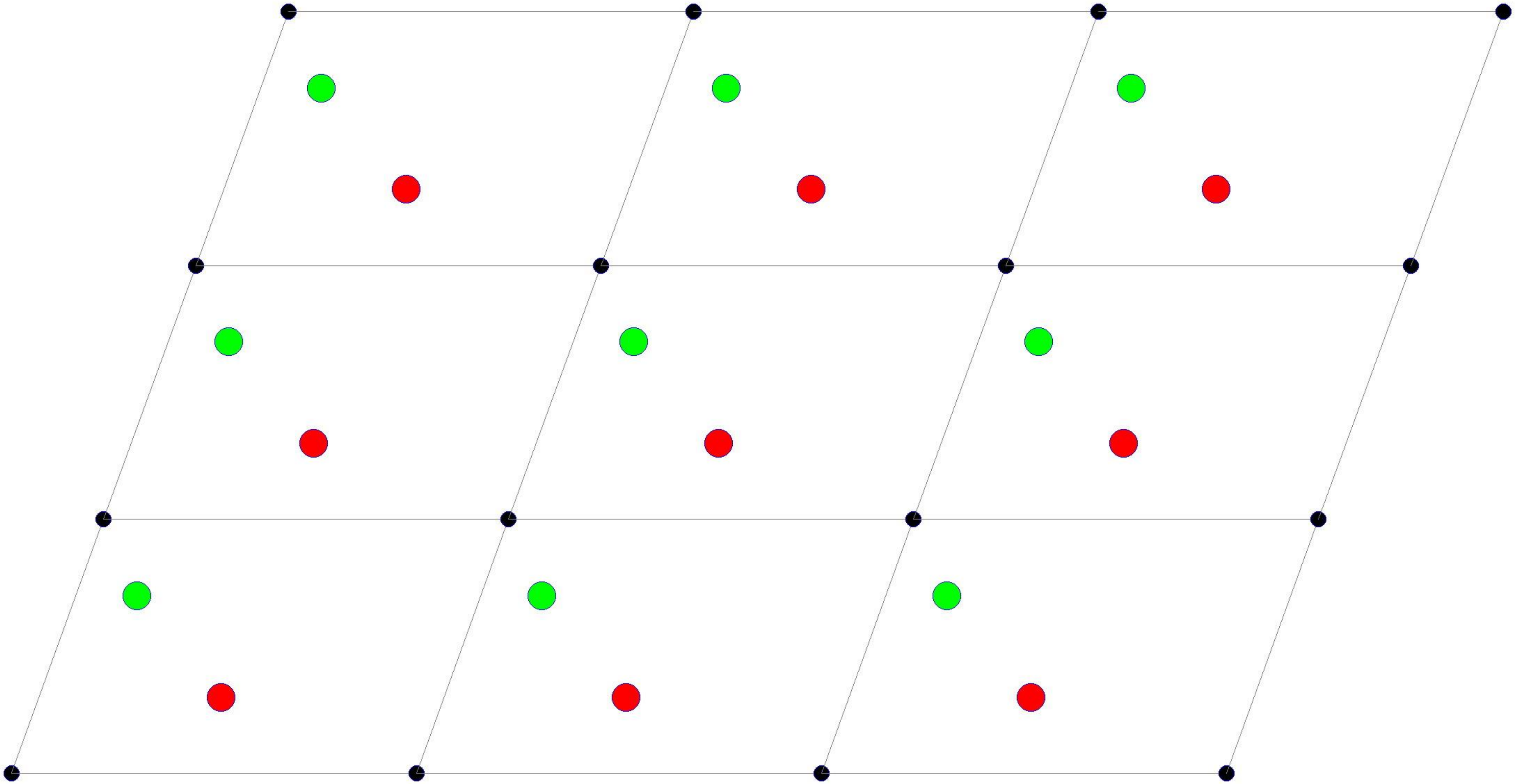
We will start with the planar space groups.

OBLIQUE : p2



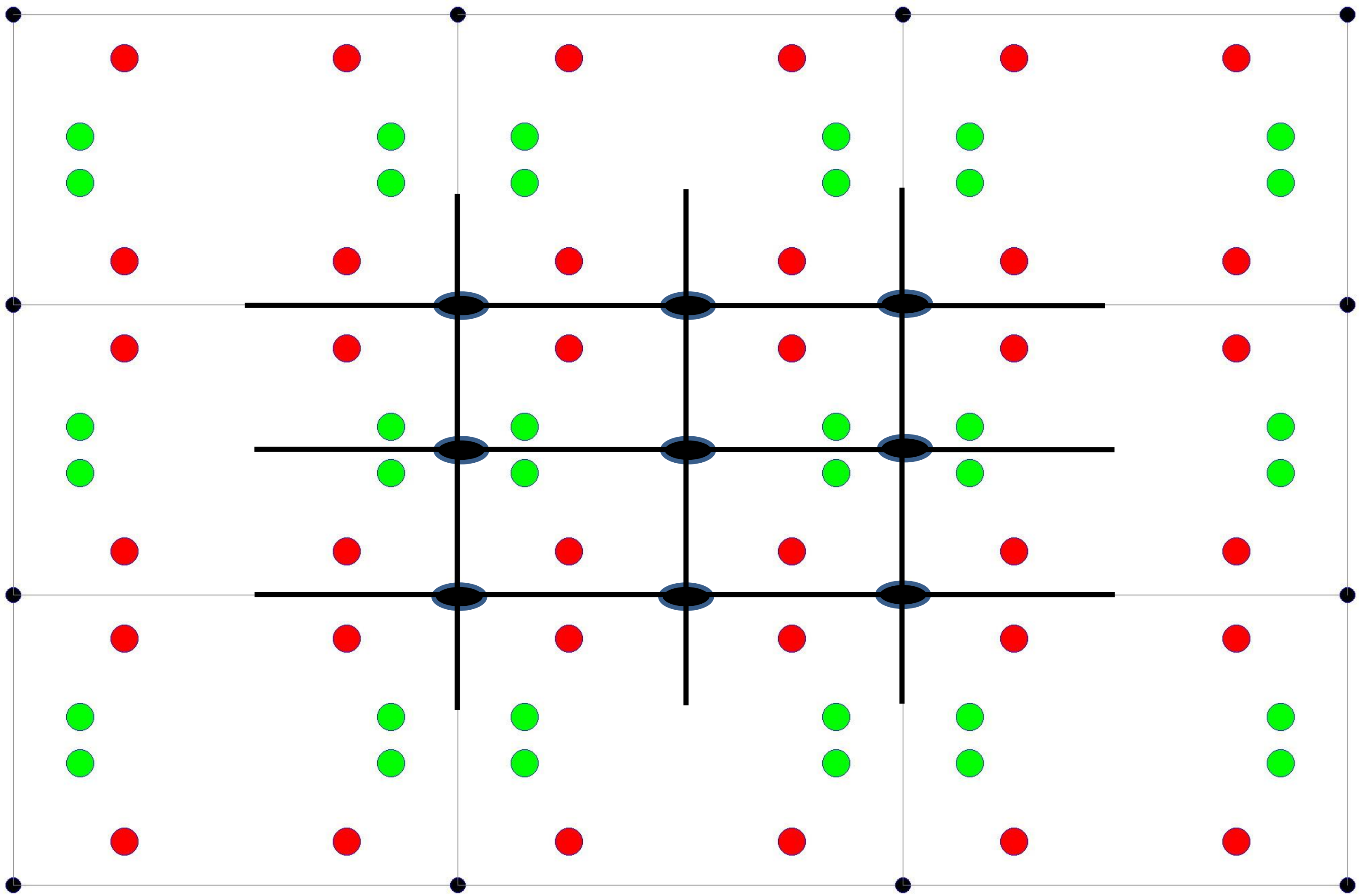
1) x,y; 2) -x,-y

OBLIQUE p1



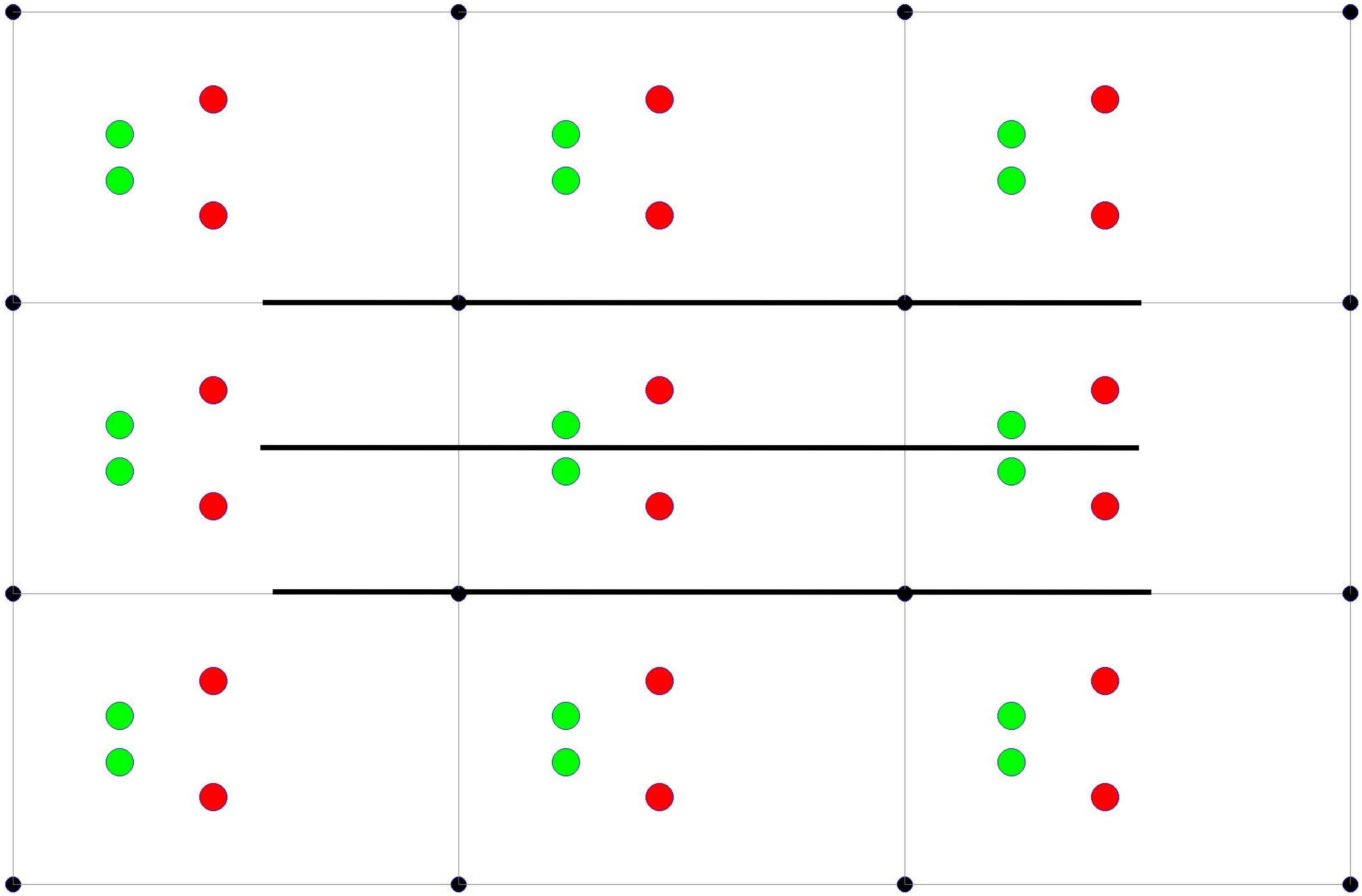
1) x,y

RECTANGULAR p2mm



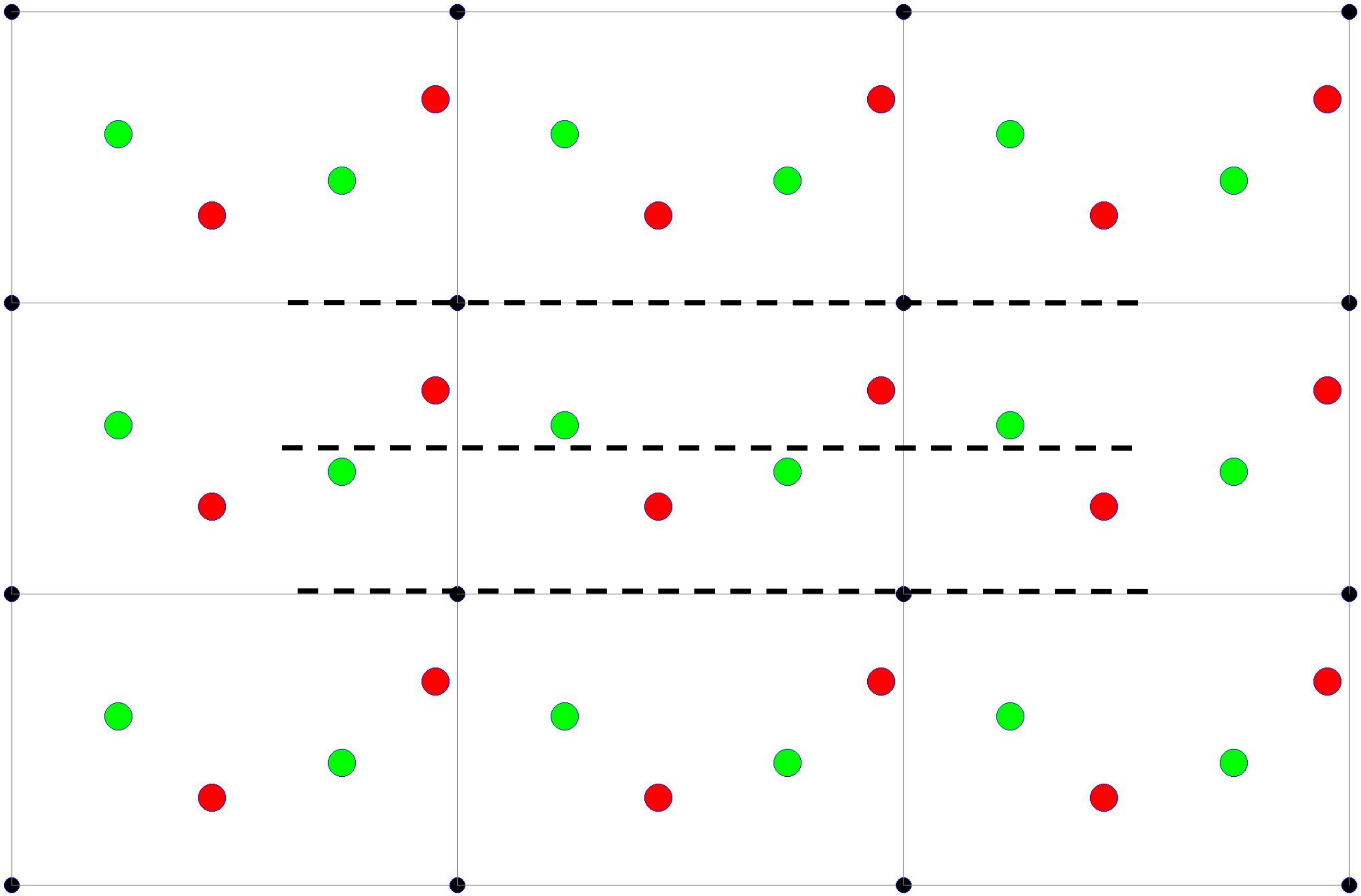
1) x y   2) x -y   3) -x y   4) -x -y

RECTANGULAR pm



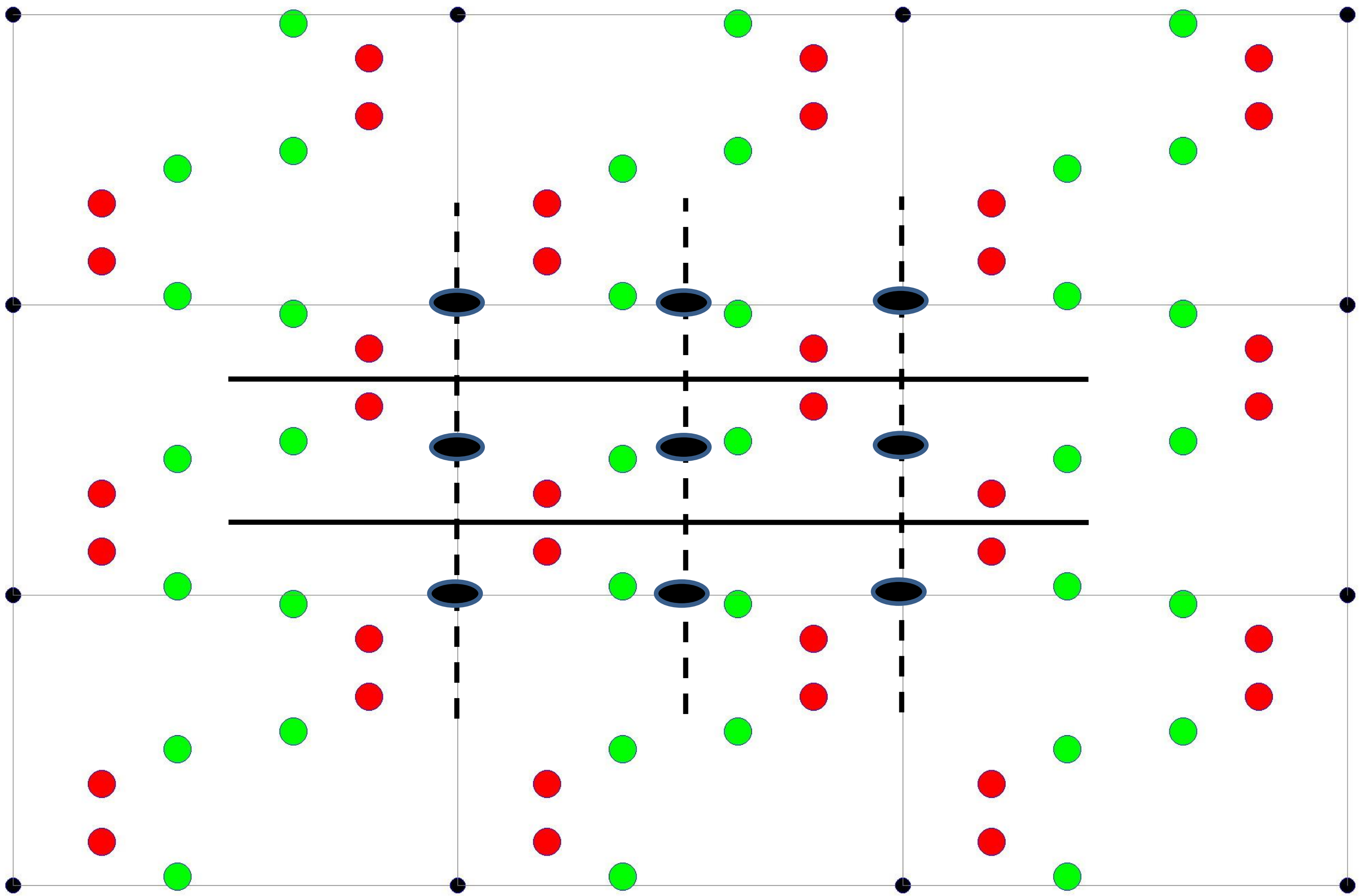
1) x y 2) x -y

RECTANGULAR pg



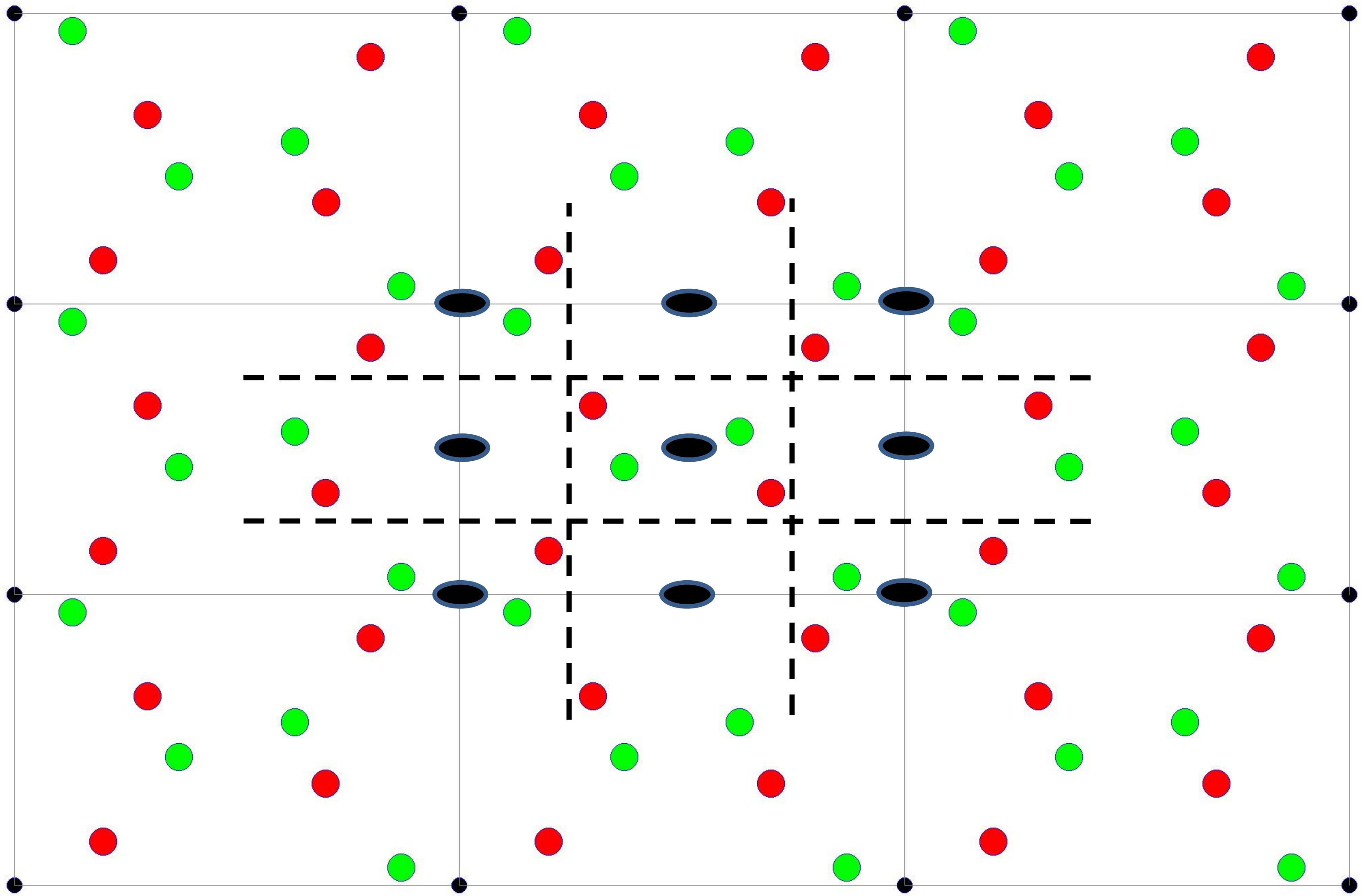
1) x y 2) x+1/2 -y

RECTANGULAR p2mg



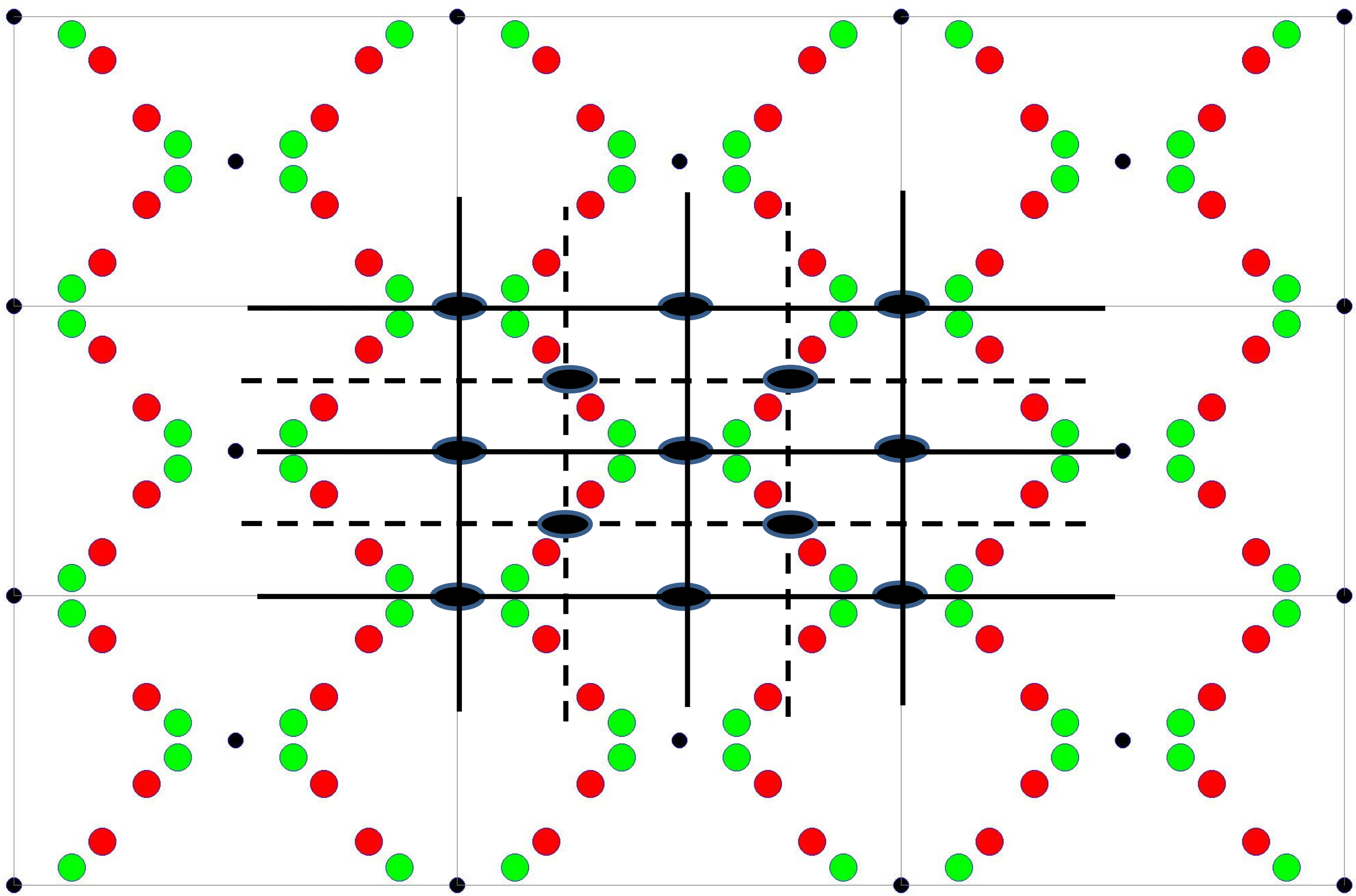
1) x y   2) -x -y   3) x -y+1/2   4) -x y+1/2

RECTANGULAR p2gg



1) x y 2) -x -y 3) -x+1/2 y+1/2 4) x+1/2 -y+1/2

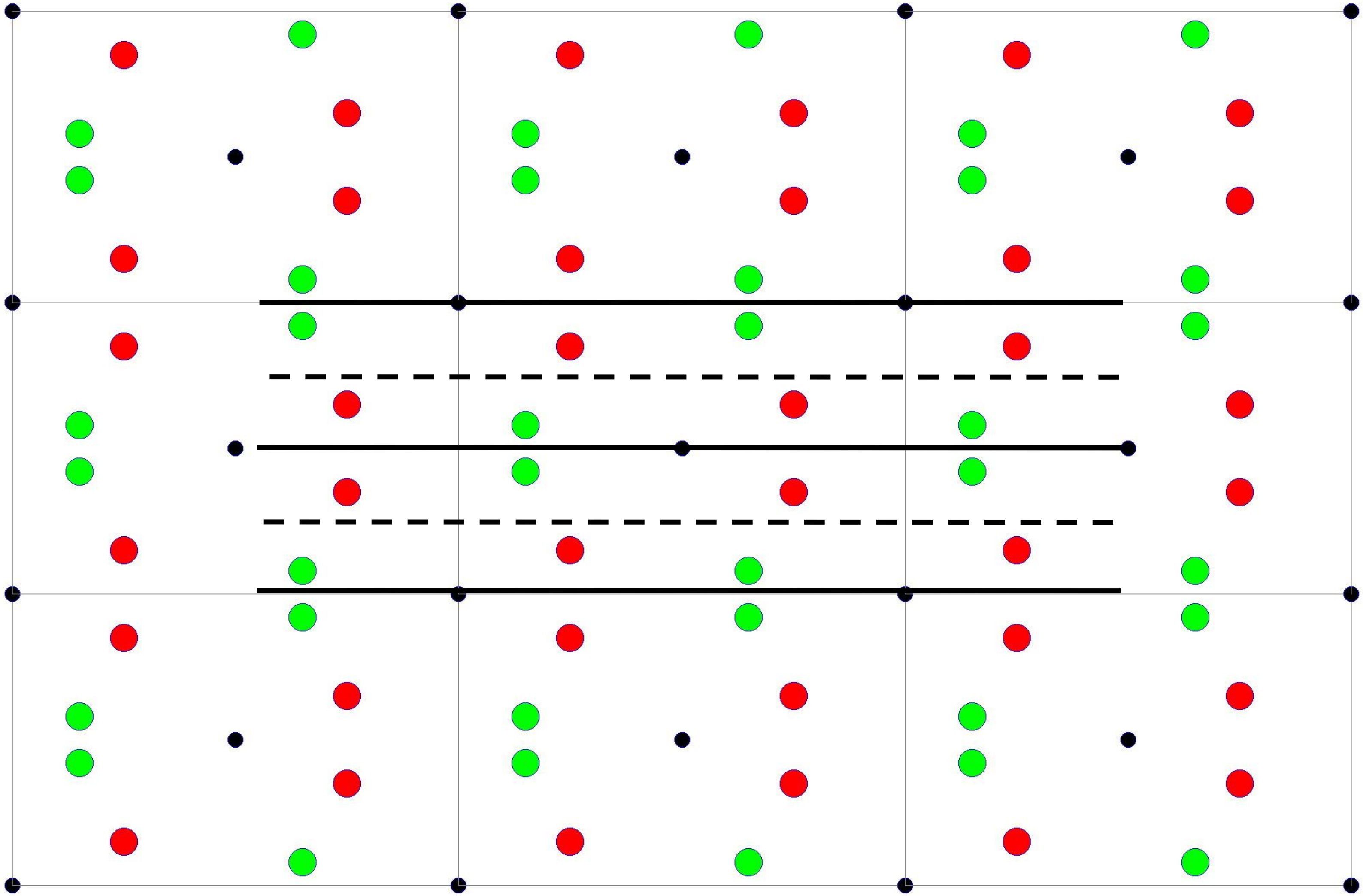
RECTANGULAR c2mm



1) x y 2) x -y 3) -x y 4) -x –y

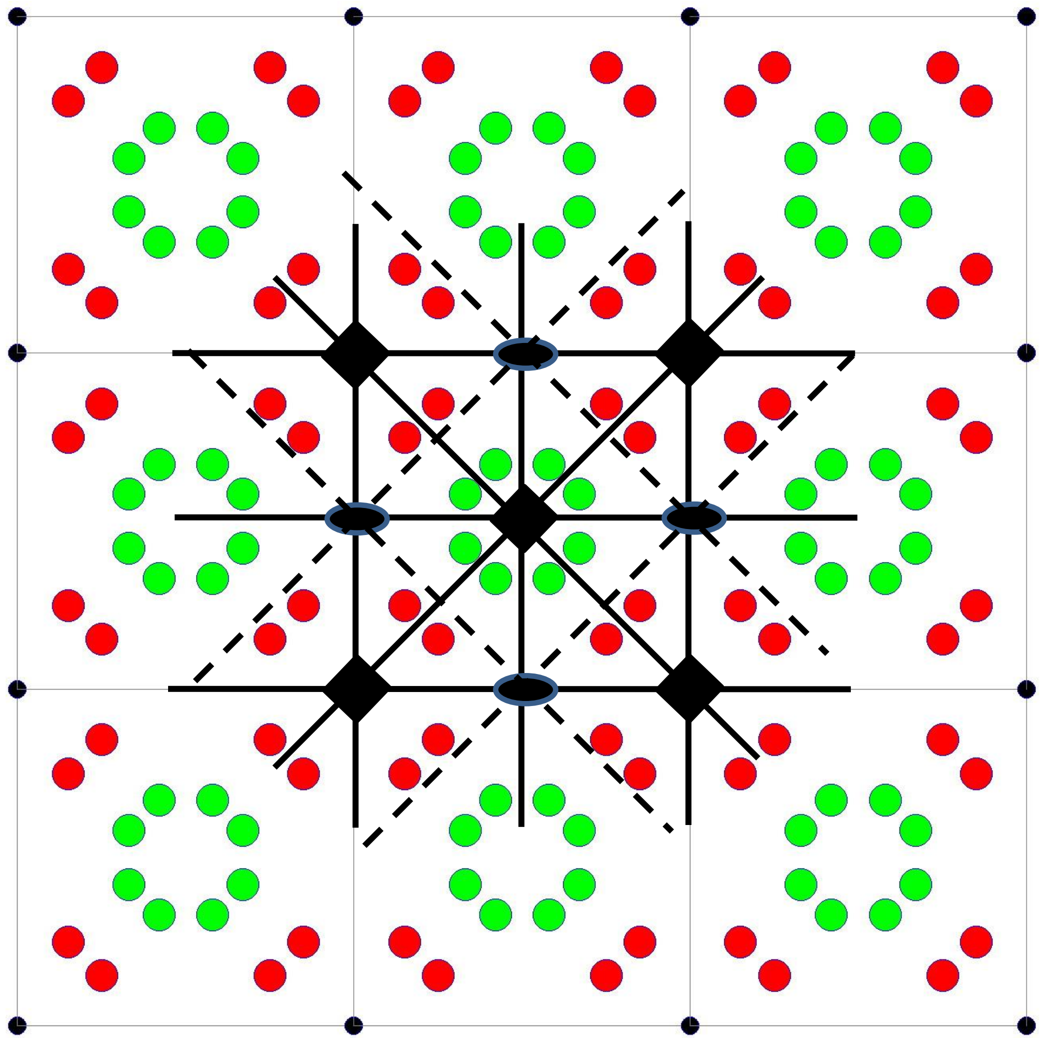
5) x+1/2 y+1/2 6) x+1/2 -y+1/2 7) -x+1/2 y+1/2 8) –x+1/2 –y+1/2

RECTANGULAR cm



1) x y 2) x -y 3) x+1/2 y+1/2 4) x+1/2 -y+1/2

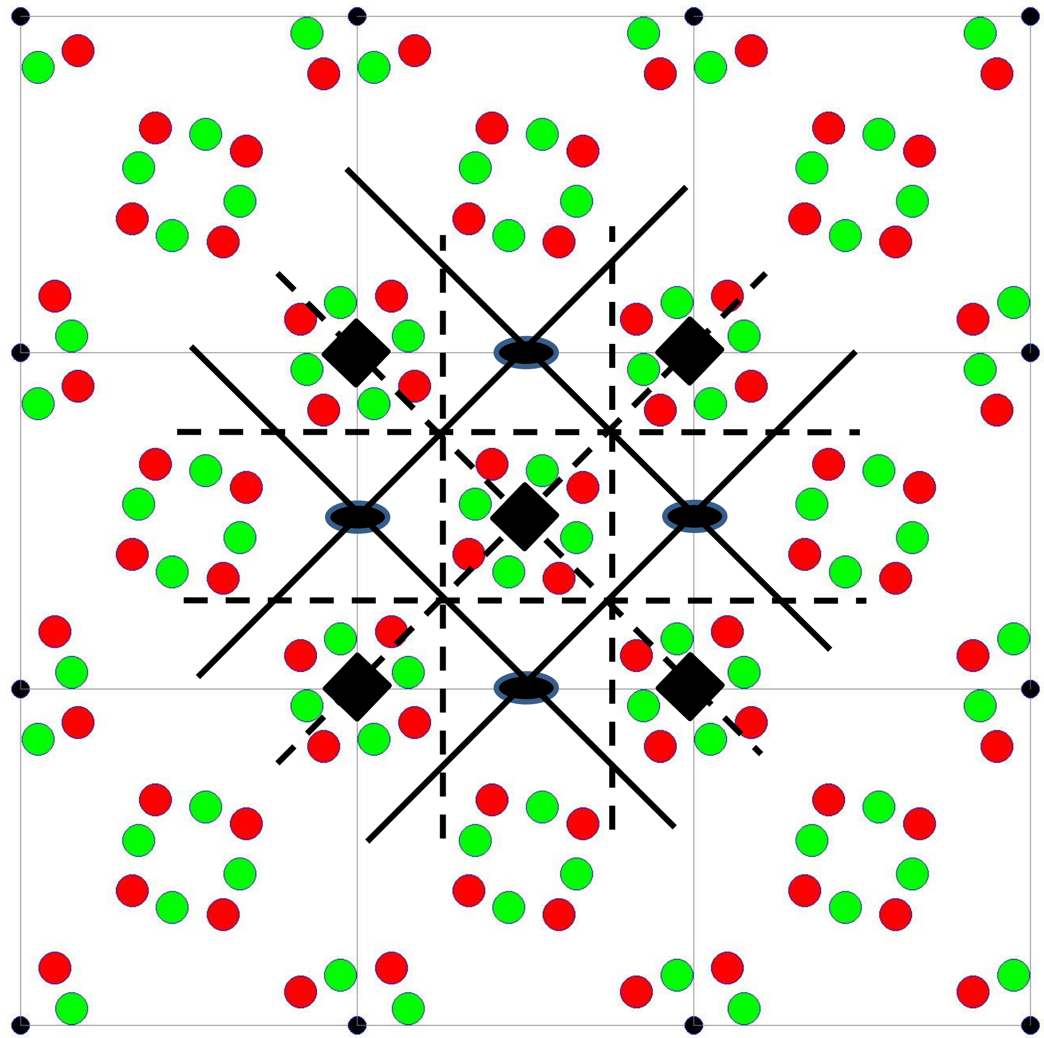
SQUARE p4mm



1) x y 2) -x -y 3) -y x 4) y -x

5) -x y 6) x -y 7) y x 8) -y -x

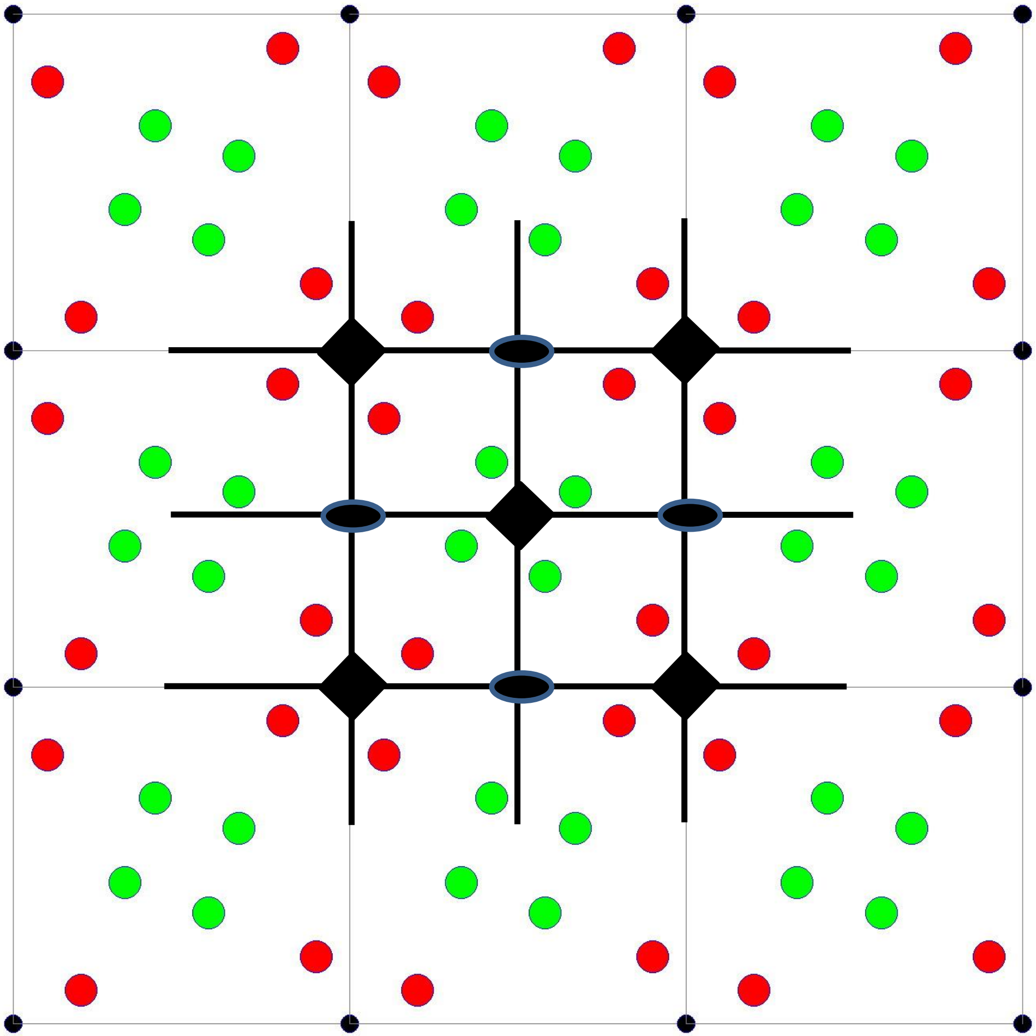
SQUARE p4gm



1) x y   2) -x -y   3) -y x   4) y -x

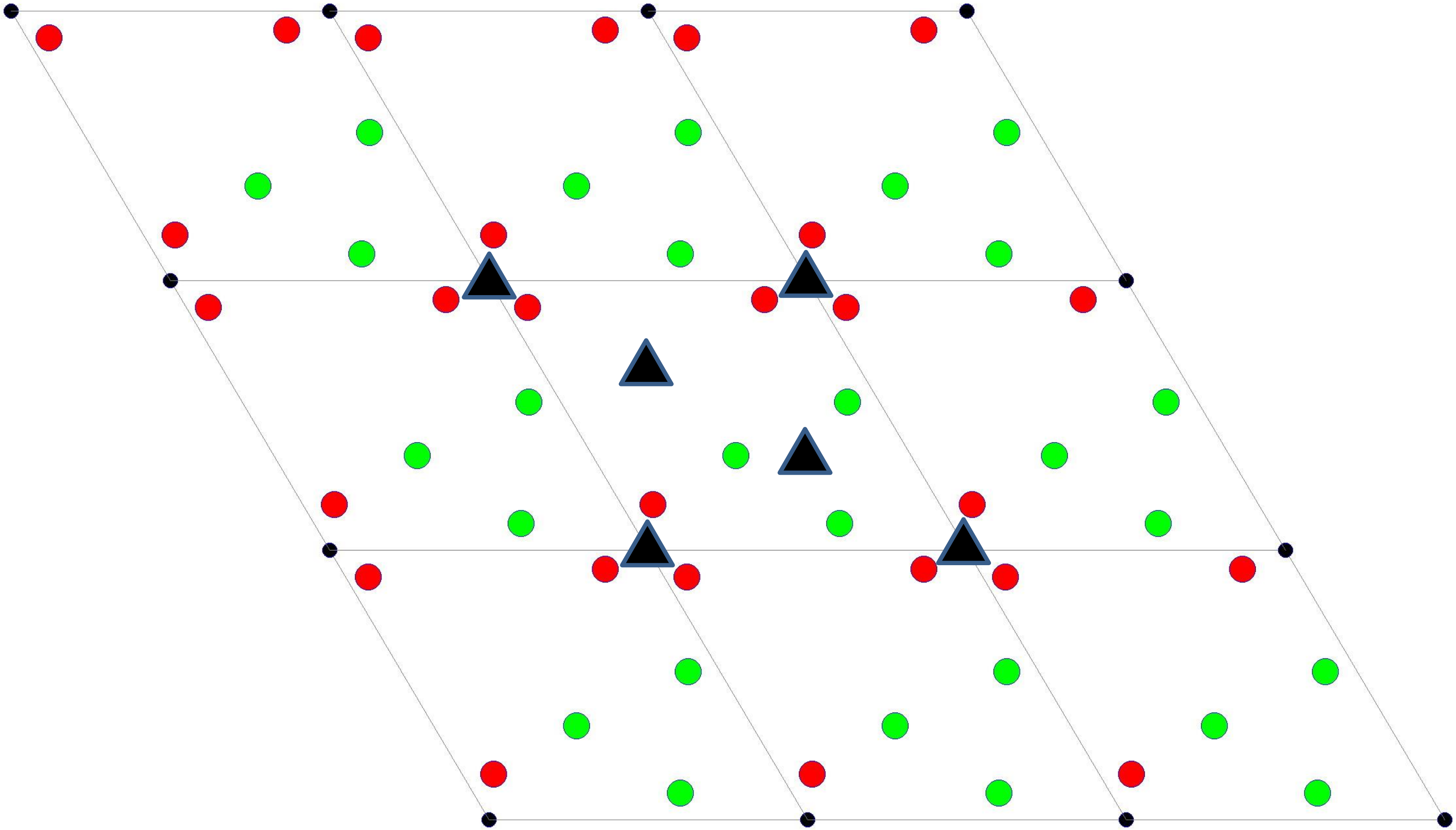
5) -x+1/2 y+1/2   6) x+1/2 –y+1/2   7) y+1/2 x+1/2   8) -y+1/2 -x+1/2

SQUARE p4



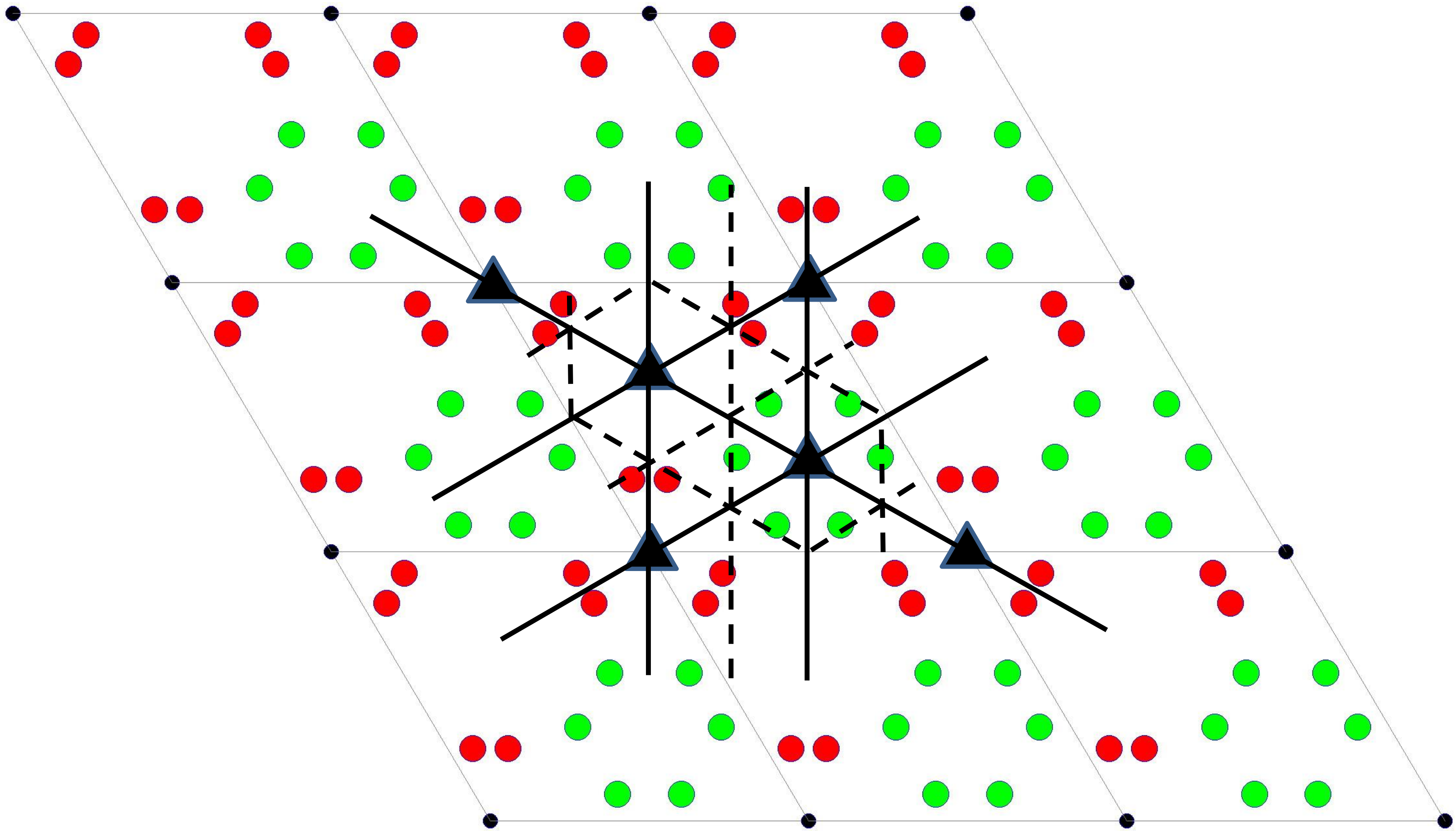
1) x y   2) -x -y   3) -y x   4) y -x

HEXAGONAL: p3



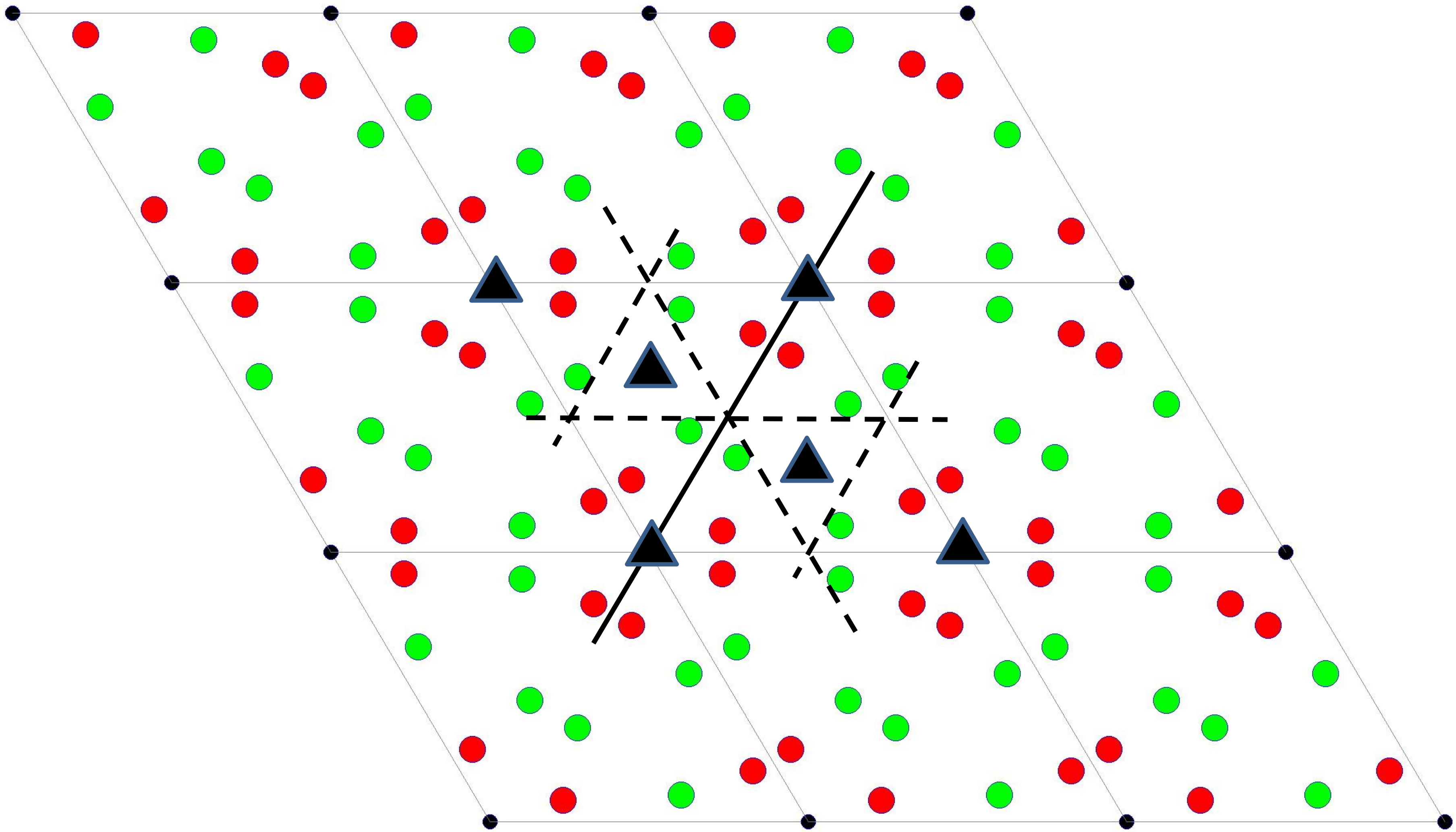
1) x y   2) -y x-y   3) -x+y -x

HEXAGONAL p3m1



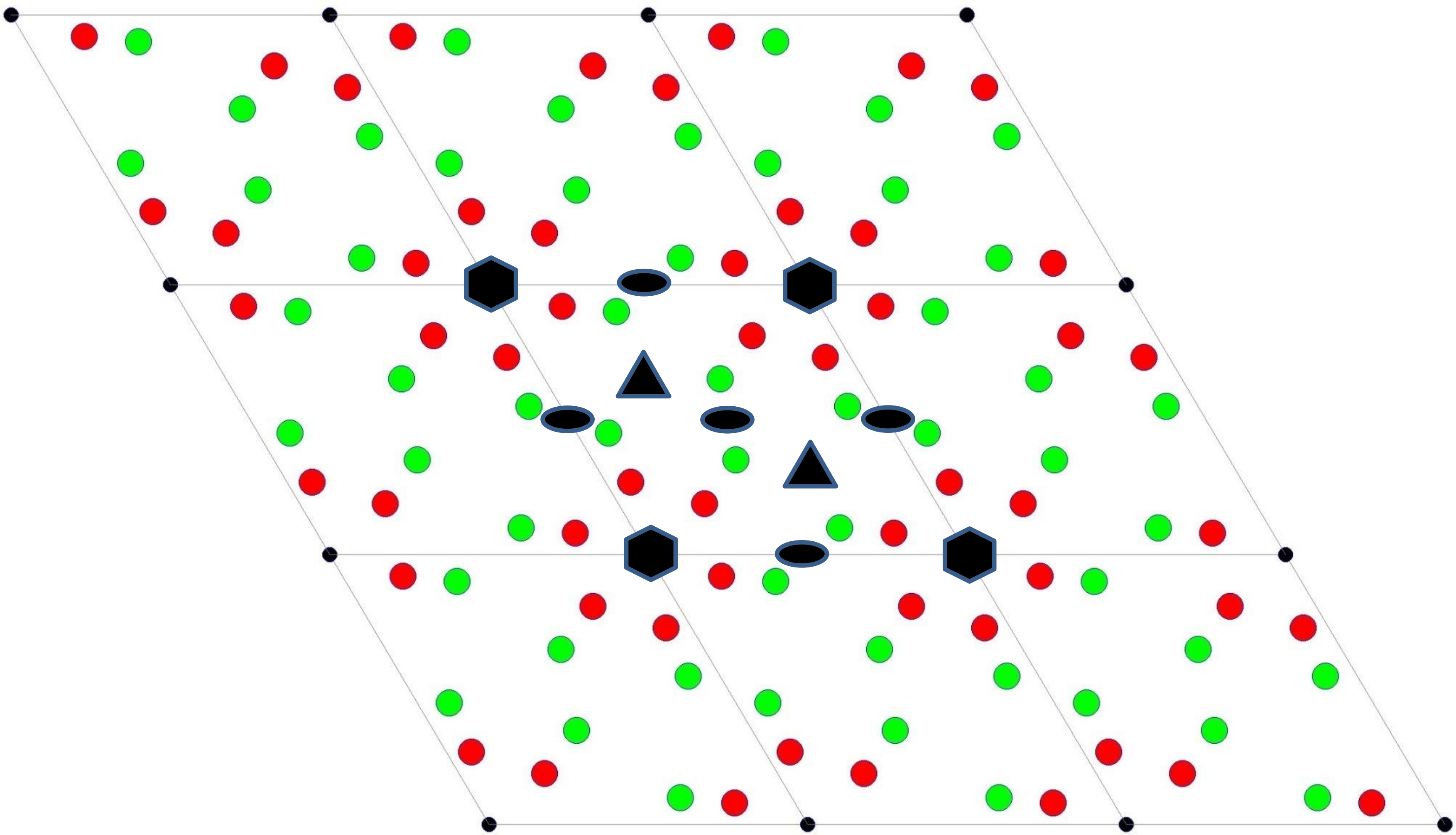
1) x y 2) -y x-y 3) -x+y -x 4)-y -x 5) -x +y y 6) x x-y

HEXAGONAL p31m



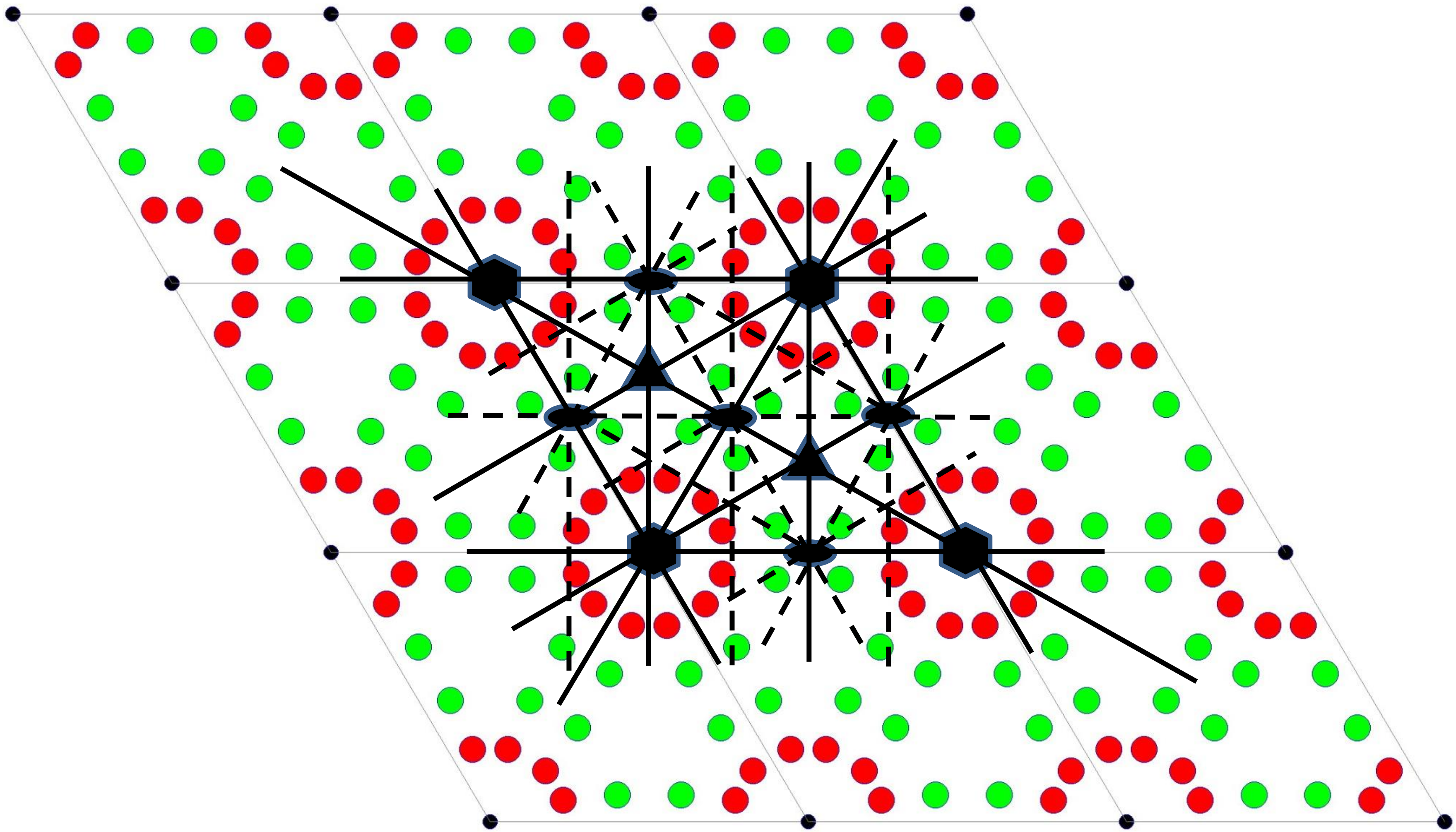
1) x y 2) -y x-y 3) -x+y -x 4)y x 5) x -y -y 6) -x -x+y

HEXAGONAL p6



1) x y 2) -y x-y 3) -x+y -x 4)-x -y 5) y –x+y 6) x-y x

HEXAGONAL p6mm

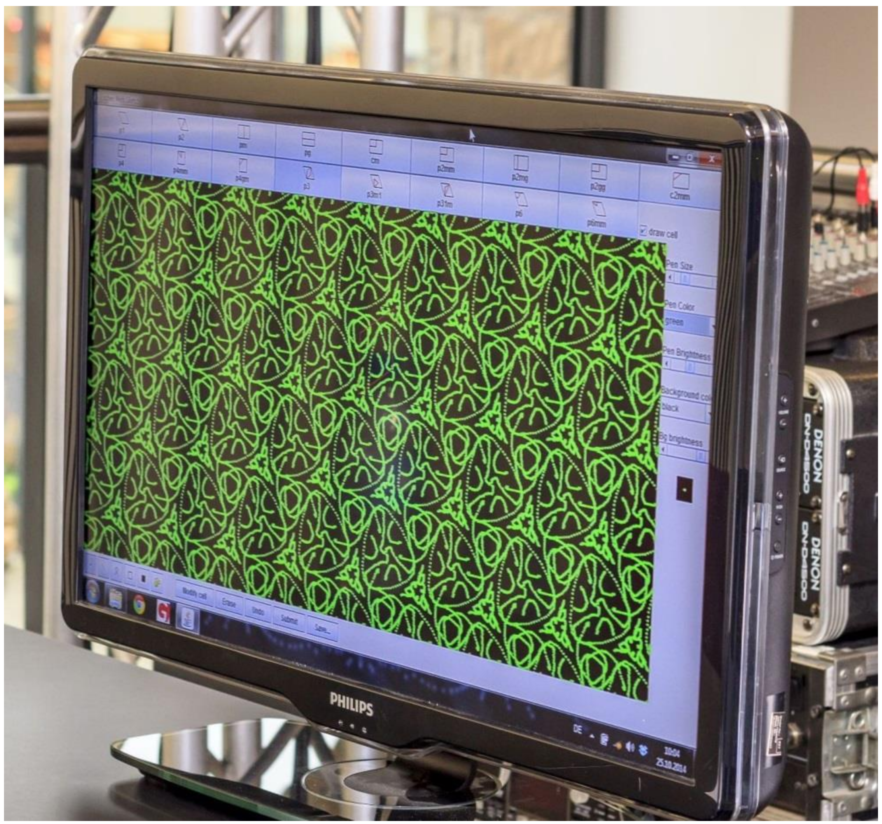


1) x y 2) -y x-y 3) -x+y -x 4)-x -y 5) y -x+y 6) x-y x
7)-y -x 8)-x+y -y 9) x x-y 10) y x 11)x-y -y 12)-x -x+y

Escher Web Sketch

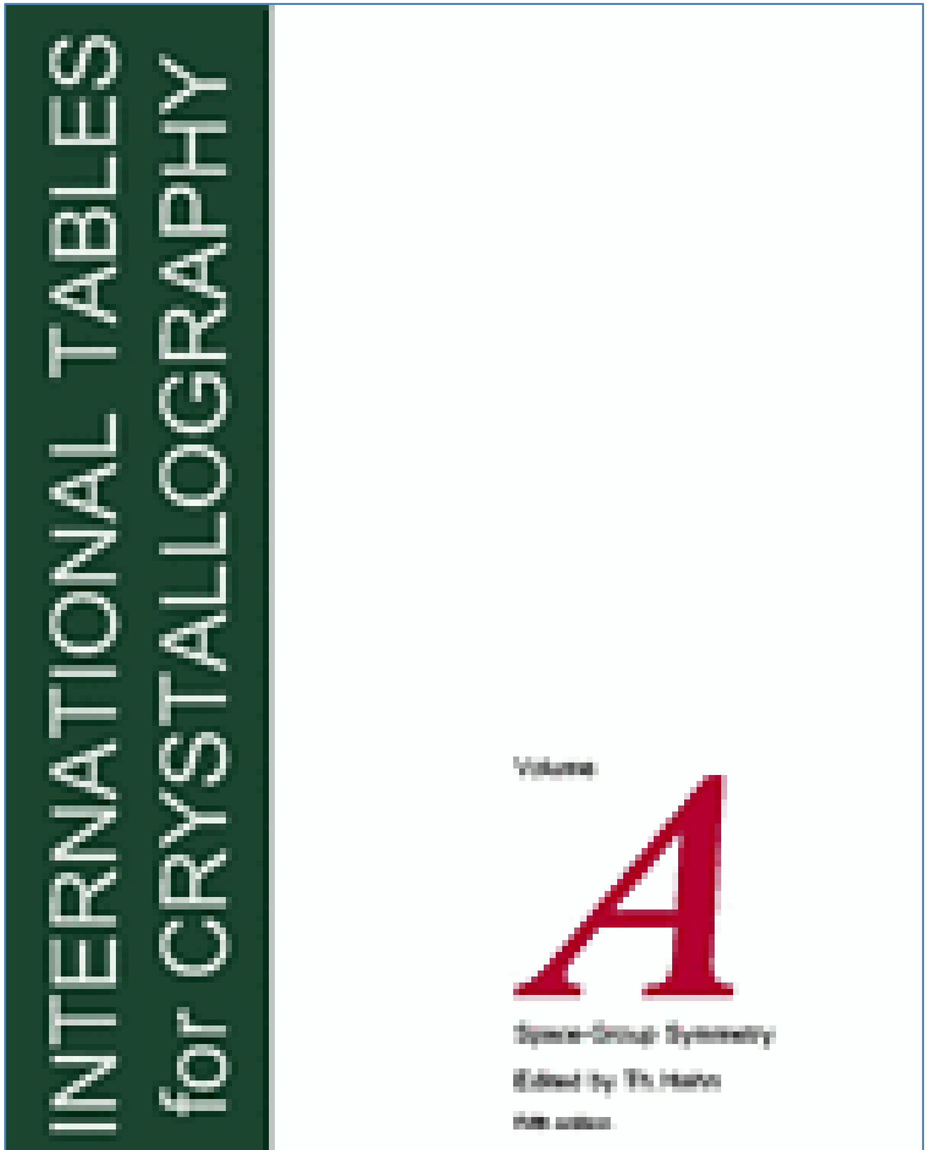
By: Nicolas Schoeni, Wes Hardaker and Gervais Chapuis
At: The Swiss Federal Institute of Technology (EPFL), Switzerland

http://escher.epfl.ch/escher/



NB! I recommend you to download Escher.jar file and run it locally from you computer

SPACE GROUPS IN 3D



International tables
for crystallography
VOLUME A

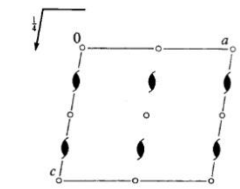
Sample page of the International Tables Volume A ($P2_1/c$)

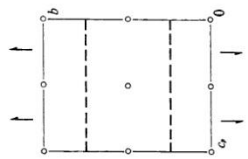
International Tables for Crystallography (2006). Vol. A, Space group 14, pp. 184–191.

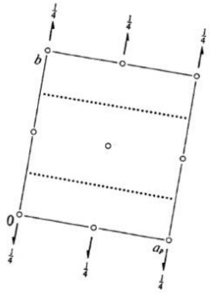
$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

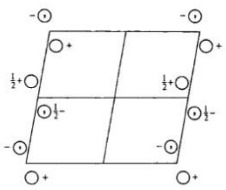
No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1









Origin at $\bar{1}$

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

Symmetry operations

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

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
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a}, \mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

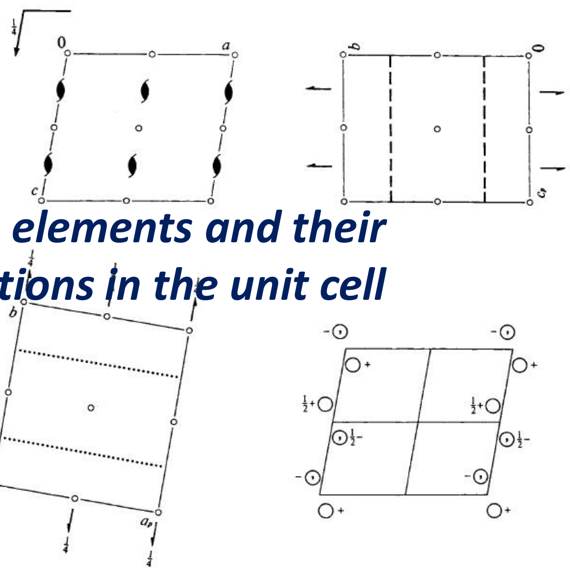
International Tables for Crystallography (2006). Vol. A, Space group 14, pp. 184–191.

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

SG symbol and number   ***Point group***   ***Crystal system***

No. 14 $P\,1\,2_1/c\,1$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1



Unit cell in different projections

Symmetry elements and their positions in the unit cell

Origin at $\bar{1}$

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

Asymmetric unit of the unit cell

Symmetry operations

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

How to identify the space group from the experiment (see next lecture)

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

Positions

Positions inside a unit cell

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

General positions

Point symmetry group of the position

Special positions

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

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Minimal non-isomorphic supergroups

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Another source of information about space groups: Bilbao crystallographic server

http://www.cryst.ehu.es/

bilbao crystallographic server

UPV EHU

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations

Group - Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions