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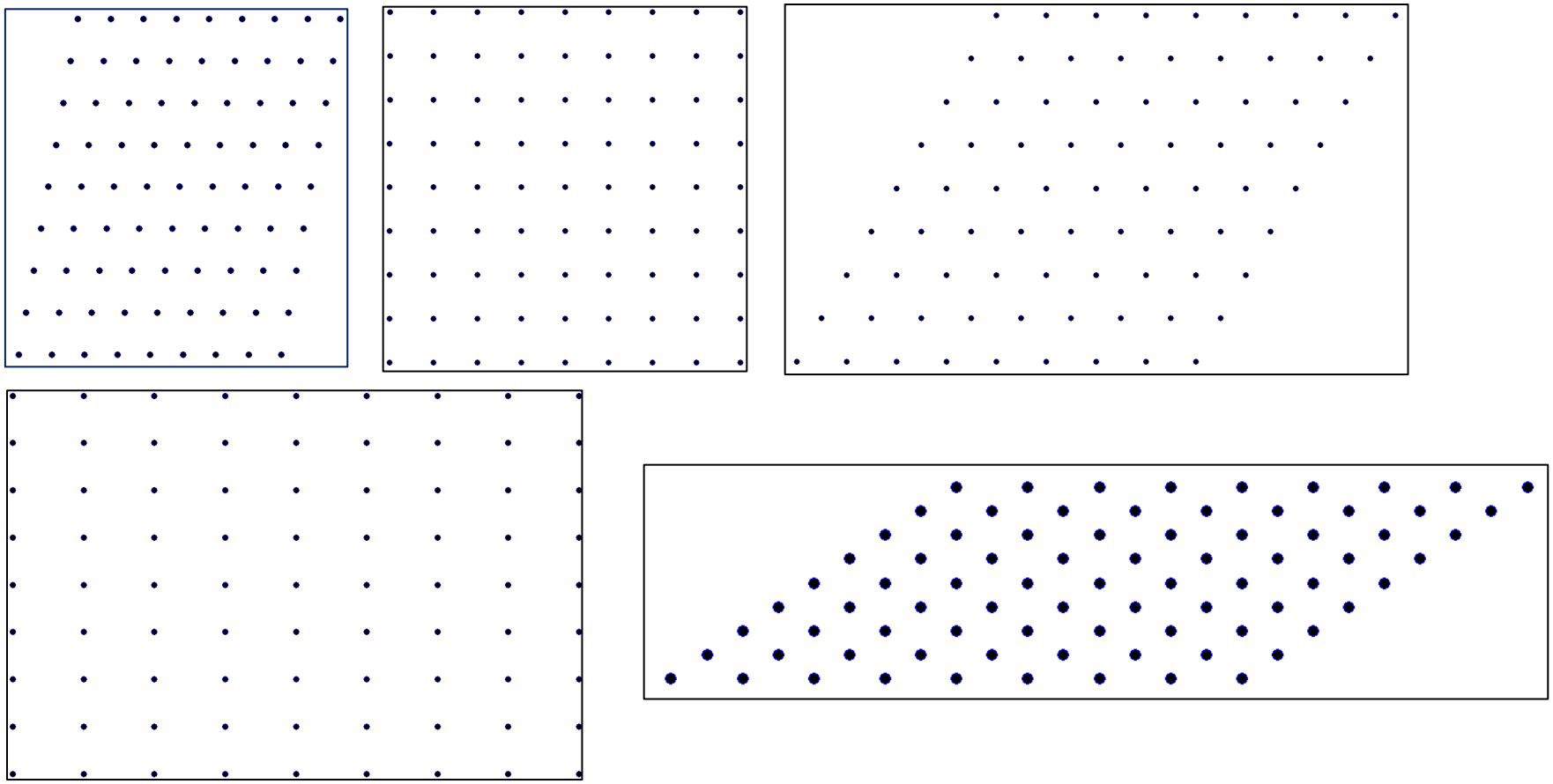
Lecture course on crystallography, 2015

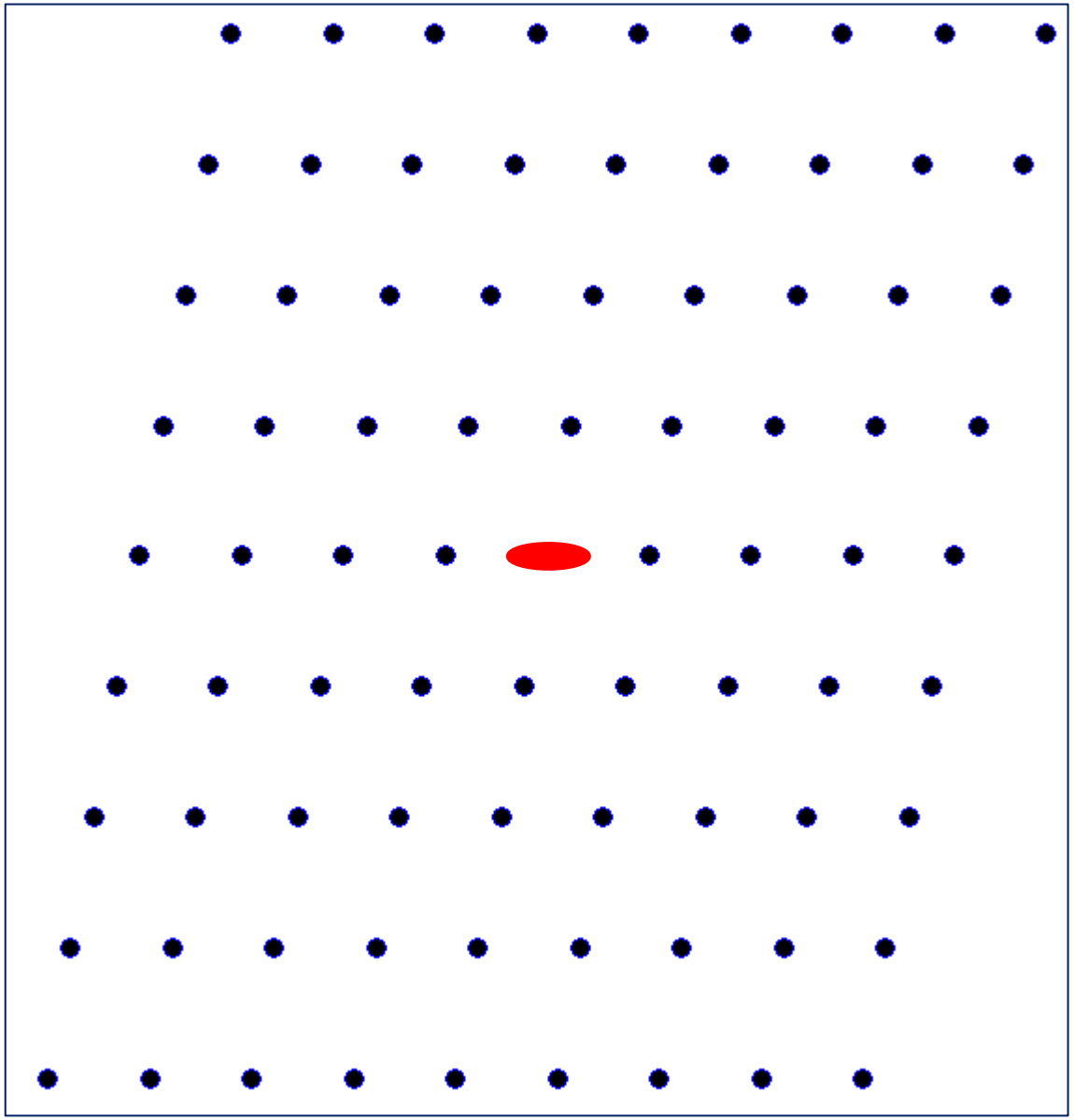
Lecture 6: Bravais types of lattices

Depending on the geometry crystal lattice may sustain different symmetry elements.



According to the symmetry of the LATTICES all CRYSTAL are subdivided into a CRYSTAL SYSTEMS

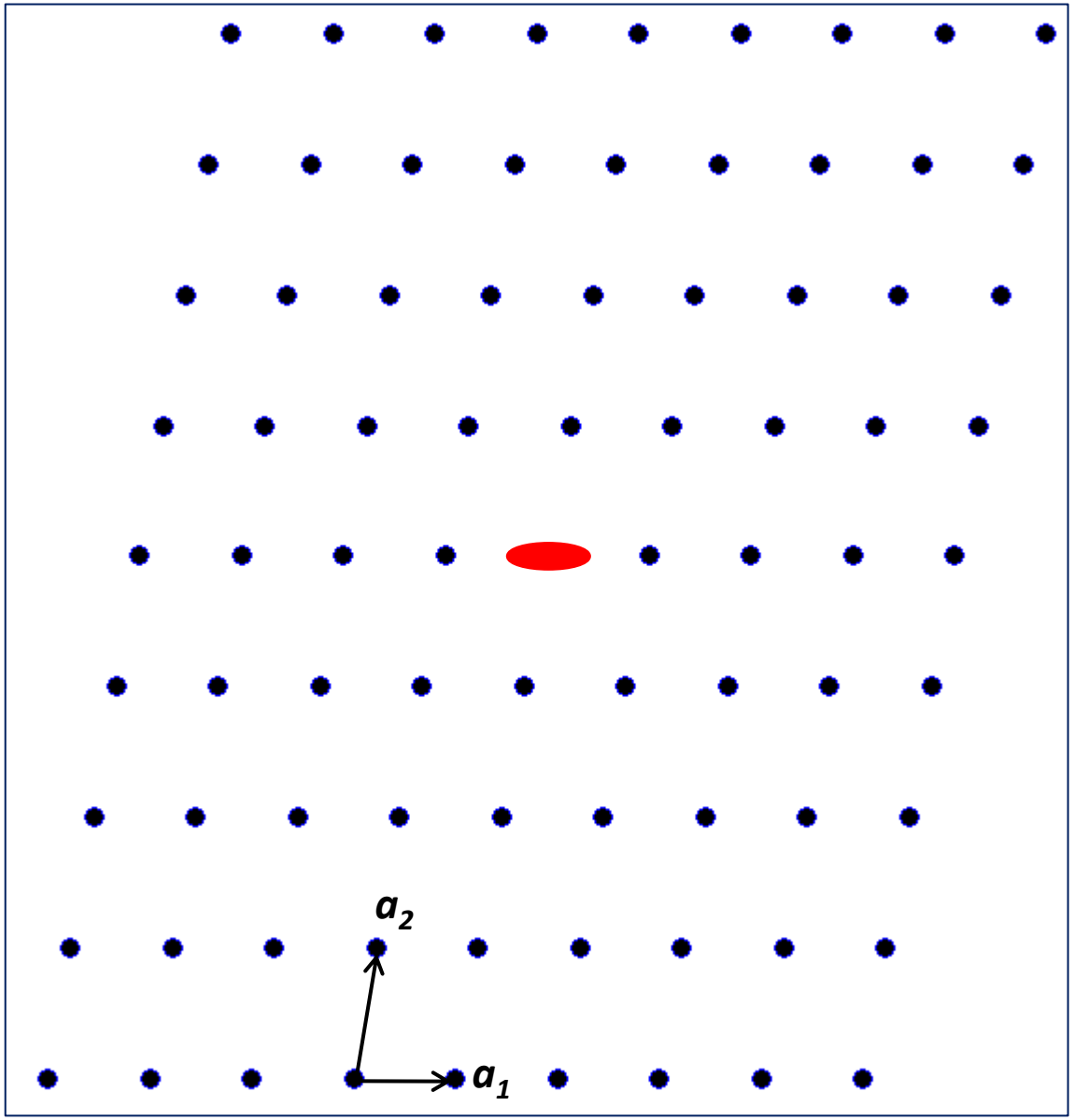
2D Lattice symmetry 1: Oblique



The oblique lattice has 2-fold axis only / centre of inversion .

Note that for two dimensional objects 2-fold axis is equivalent to the centre of inversion

2D Lattice symmetry 1: Oblique. The choice of basis vectors

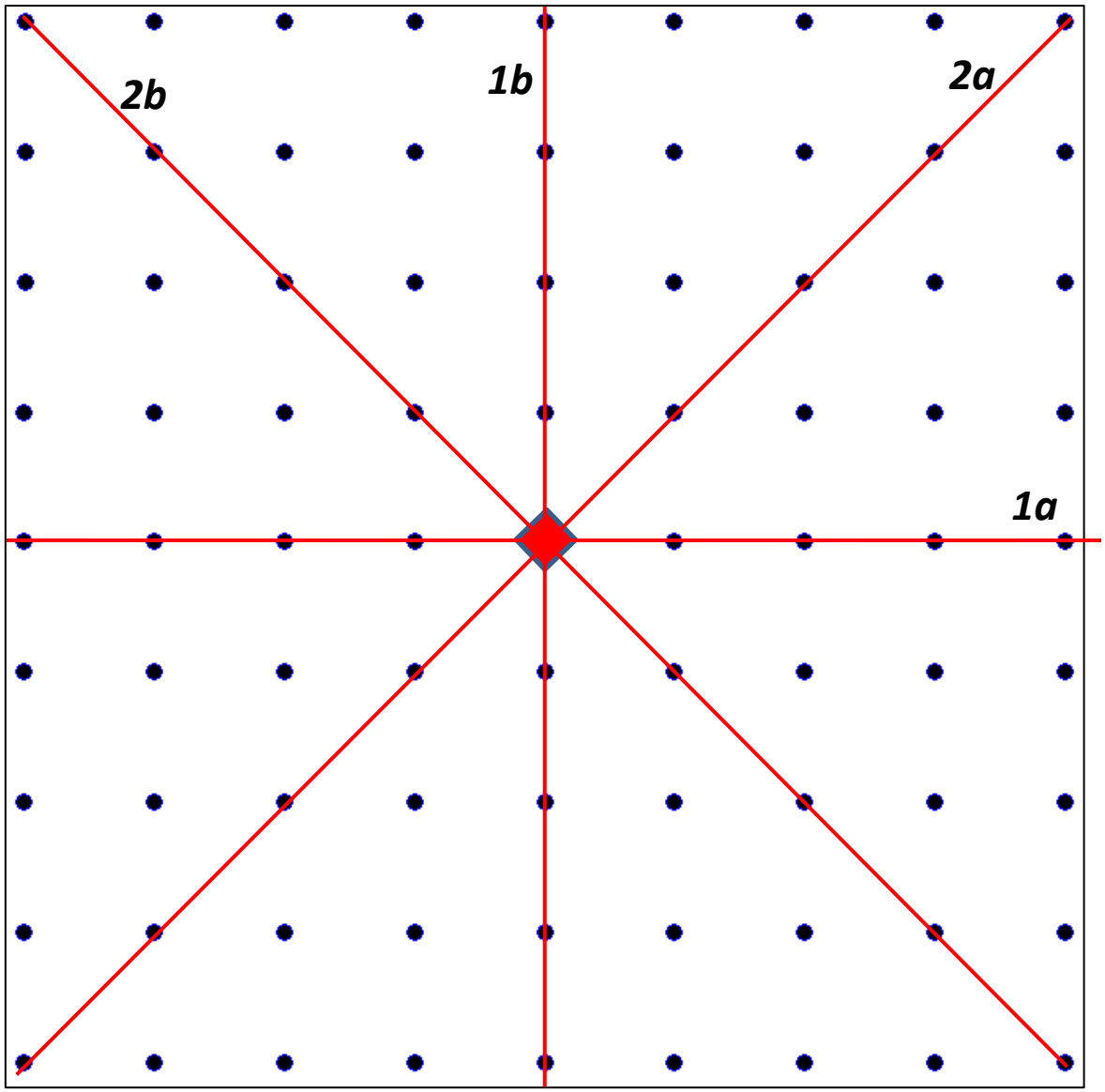


No particular restrictions on the choice of the basis vectors constructing the lattice.

$a \neq b$

$\alpha \neq 90$ deg

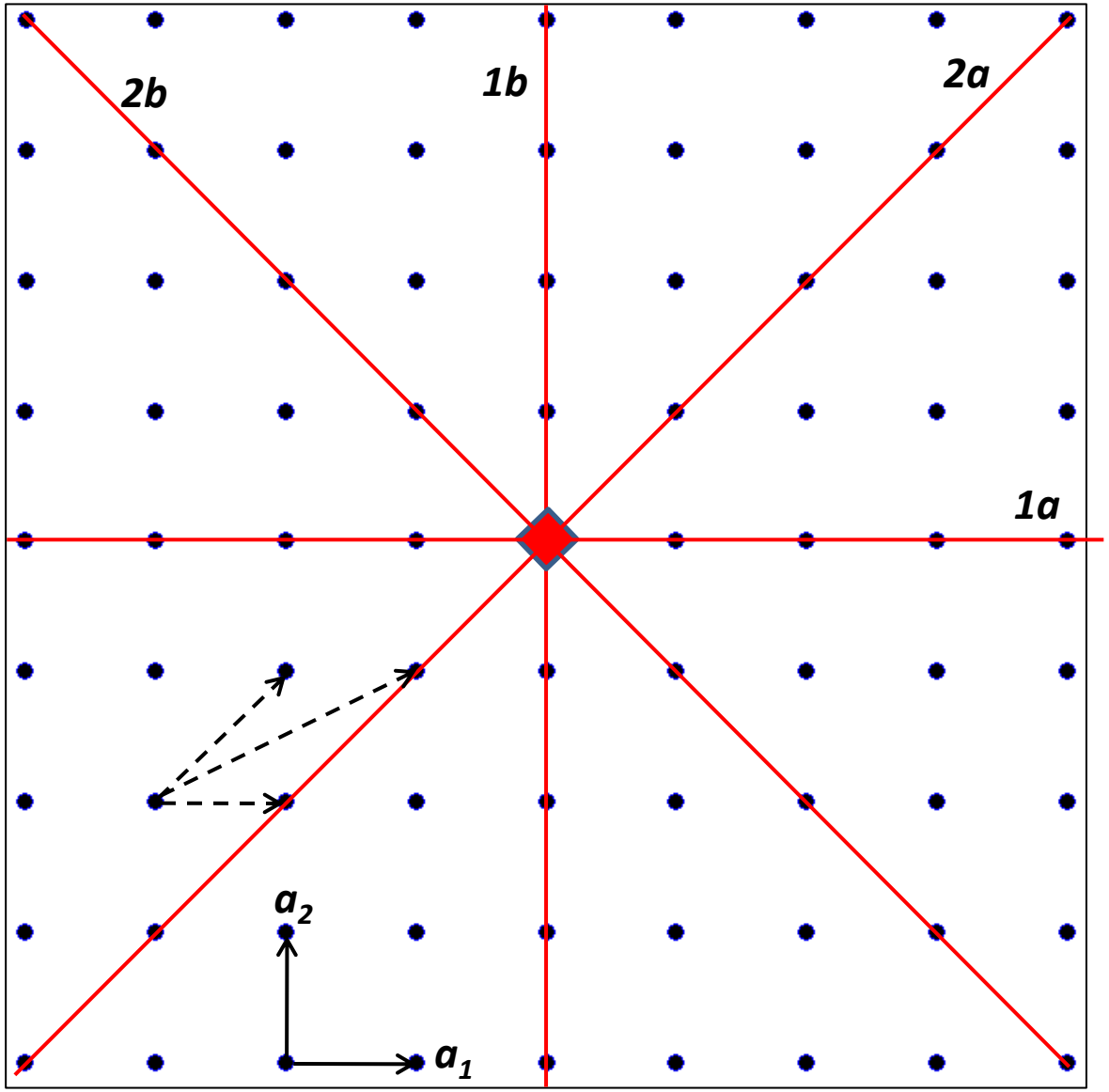
2 D Lattice symmetry 2: Square



The square lattice has

a) 4-fold symmetry axis
b) Mirror plane 1a
c) Mirror plane 1b
d) Mirror plane 2a
e) Mirror plane 2b

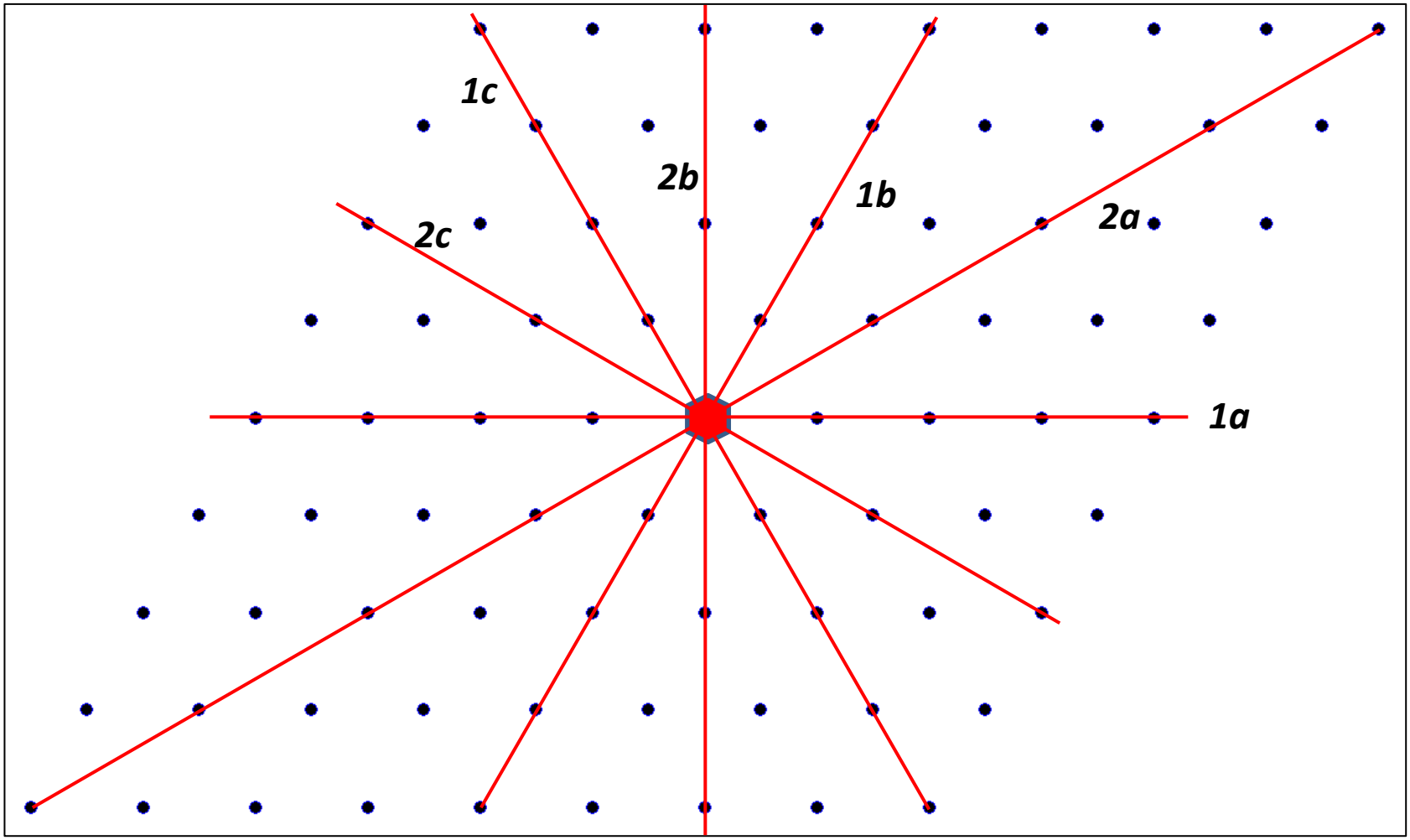
2 D Lattice symmetry 2: Square. The choice of basis



The conventional choice of basis vectors are:
a and b along the mirror planes 1a and 1b
In this case:

a=b, α=90

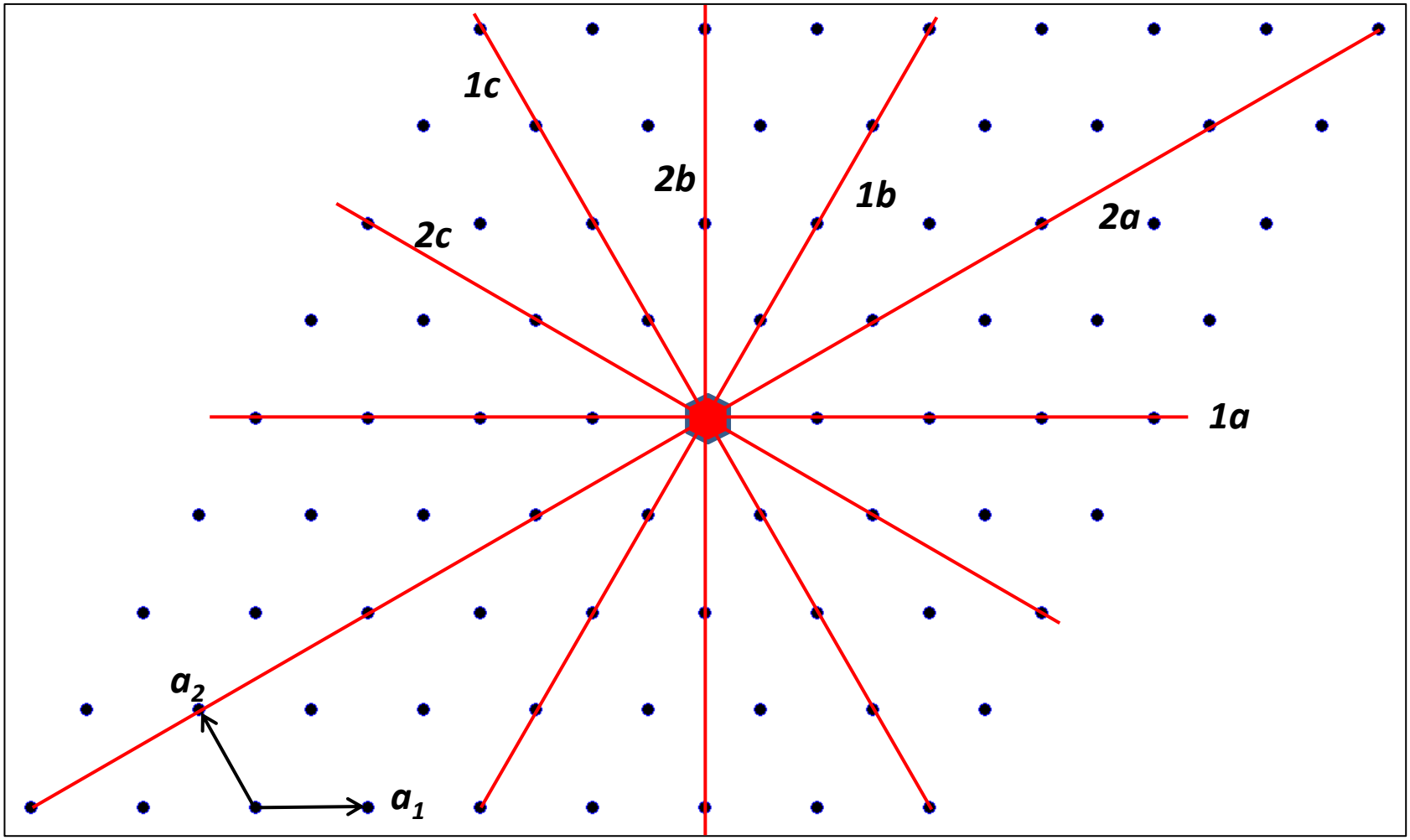
2 D lattice symmetry 3: Hexagonal



a) 6-fold symmetry axis

b) Mirror planes 1a,1b,1c,2a,2b,2c (as shown on the plot)

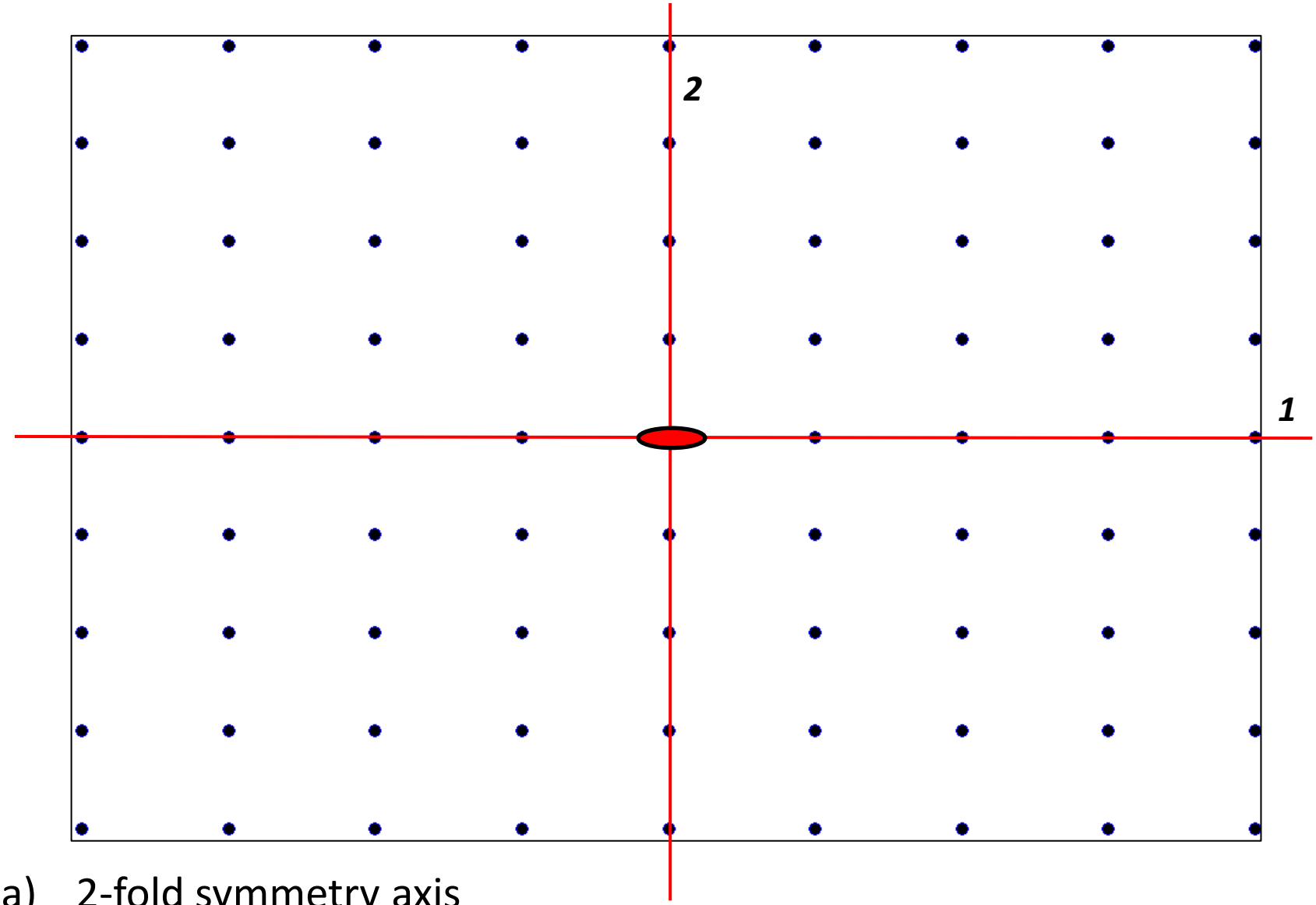
2 D lattice symmetry 3: Hexagonal. The choice of basis



Conventional choice ***a is along mirror plane 1a, b is along mirror plane 1c***

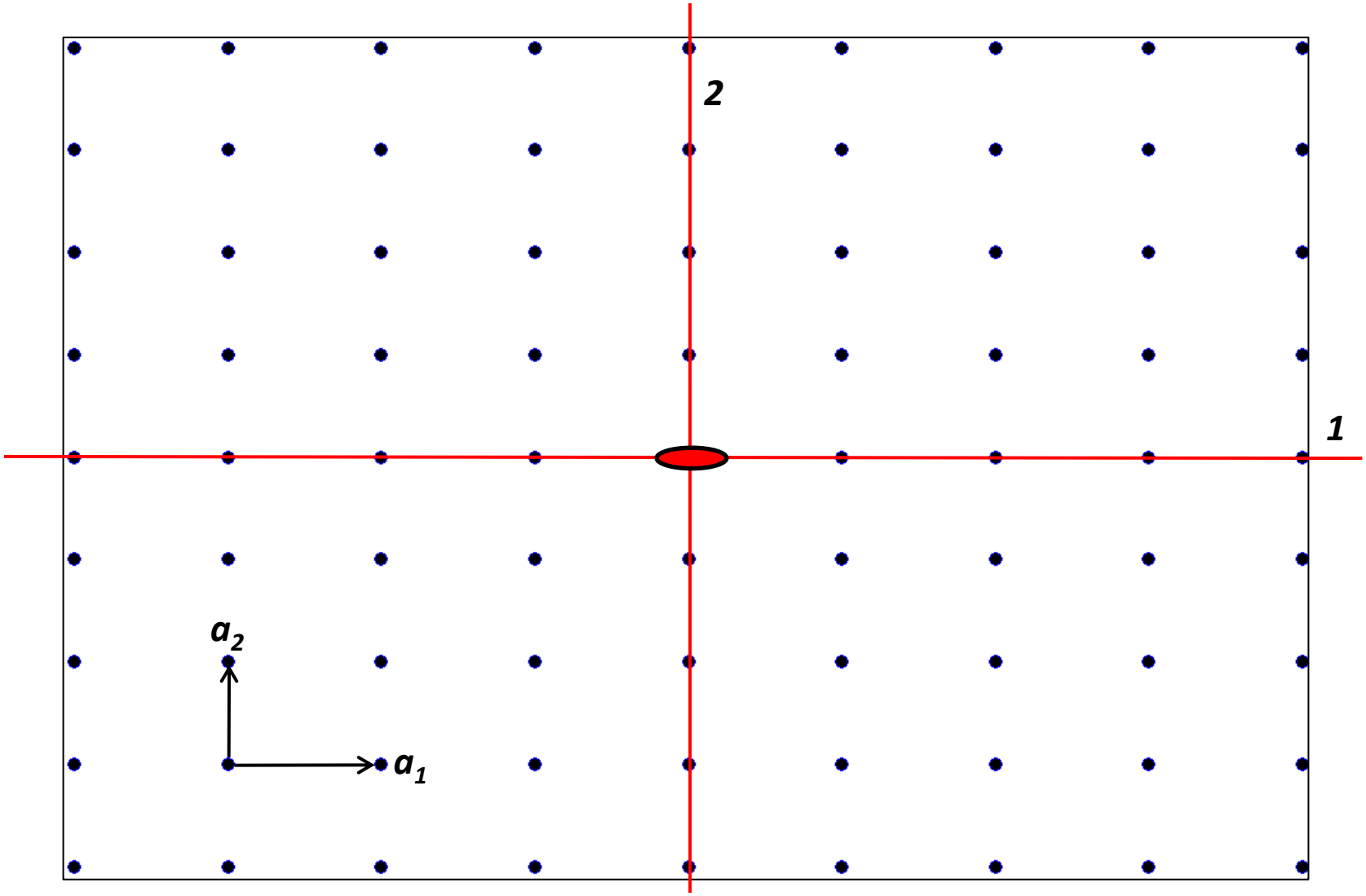
a=b, α=120 deg

2D lattice symmetry 4: Rectangular



a) 2-fold symmetry axis
b) Mirror planes 1 and 2 (see the plot)

2D lattice symmetry 4: Rectangular. The choice of basis

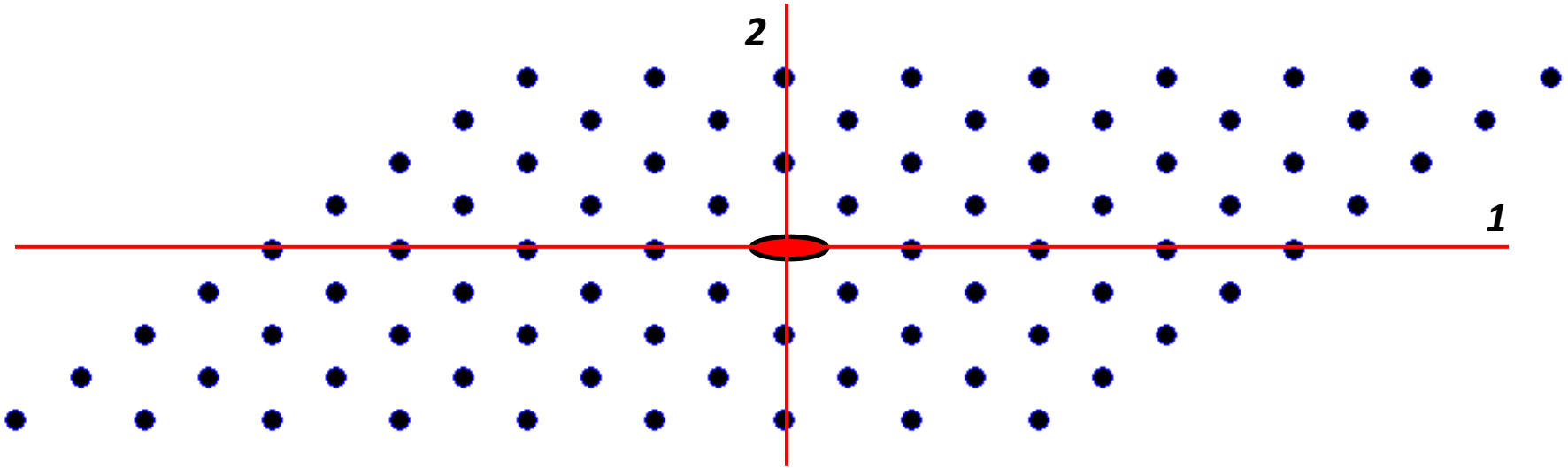


Conventional choice ***a is along mirror plane 1, b is along mirror plane 2***

$a \neq b$, $\alpha=90$

There is possibility to construct the lattice which is different from the one shown on previous page, but has the SAME POINT SYMMETRY:

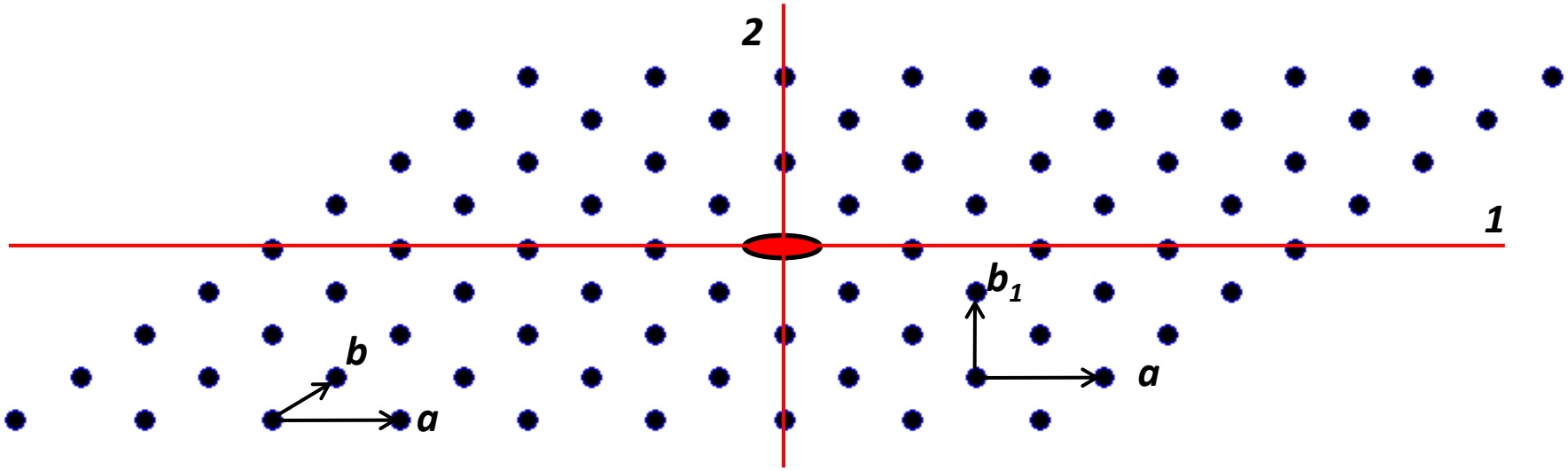
1) 2-fold axis
2) Two mirror plane perpendicular to each other 1 and 2



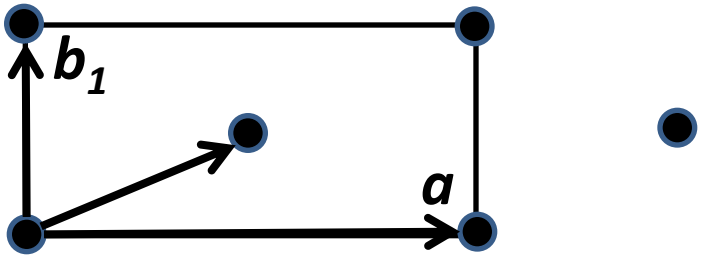
CENTERED RECTANGULAR LATTICE

The basis of this lattice can be chosen as **a** and ***b.*** It is however more convenient to change the basis vectors to ***a*** and b_1 so that they are oriented relative to the symmetry elements as

a is along mirror plane number one, b_1 is long the mirror plane number 2.



Unit cell based on the vectors ***a*** and ***b_1 contains a LATTICE POINT IN THE MIDDLE at the position [1/2, 1/2].***



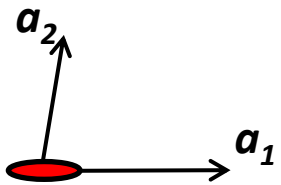
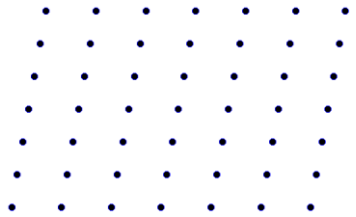
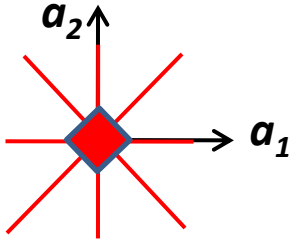
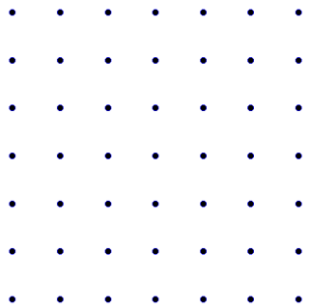
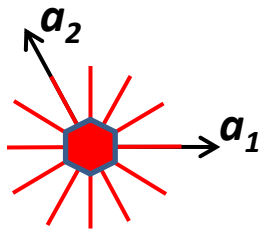
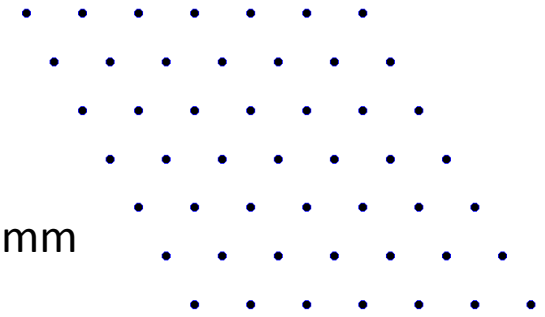
IMPORTANT!!

There are 4 different symmetries of 2D lattice (***oblique***, ***square***, ***hexagonal*** and ***rectangular***). The symmetry of a lattice is referred to as ***CRYSTAL SYSTEM***. So, there are ***4 2D CRYSTAL SYSTEMS.***

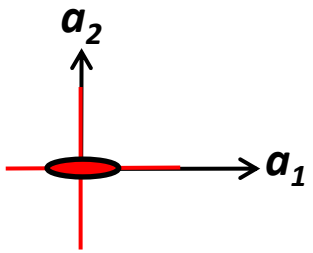
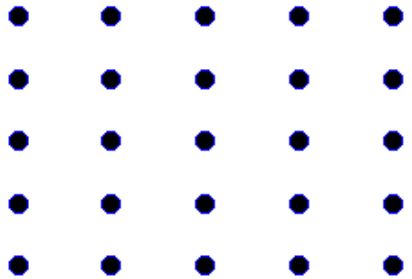
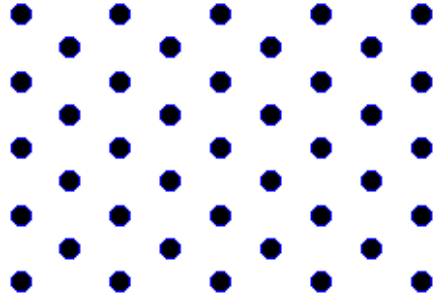
Each CRYSTAL SYSTEM has the ***conventional*** choice of two lattice basis vectors, ***a*** and ***b***, where the orientation of these vectors are specified by the orientation of symmetry elements.

Rectangular CRYSTAL SYSTEM (2 fold axis and 2 mirror planes) is accepted by two different type of lattices. The basis for the unit cell is either primitive (one lattice point per unit cell [0 0]) or centred (two lattice points per unit cell: [0 0] and [1/2 1/2]) unit cell.

CONCLUDING TABLE FOR 2D LATTICES

Crystal system	Basis vectors / Symmetry elements	Lattice constants	Lattice type
1. Oblique		**a ≠ b, α ≠ 90 deg**	p2 
2. Square		**a = b, α = 90 deg**	p4mm 
3. Hexagonal		**a = b, α = 120 deg**	p6mm 

CONCLUDING TABLE FOR 2D LATTICES (cont)

Crystal system	Basis vectors / Symmetry elements	Lattice constants	Lattice type
4. Rectangular		**a ≠ b, α = 90 deg**	pmm2 
			cmm2 

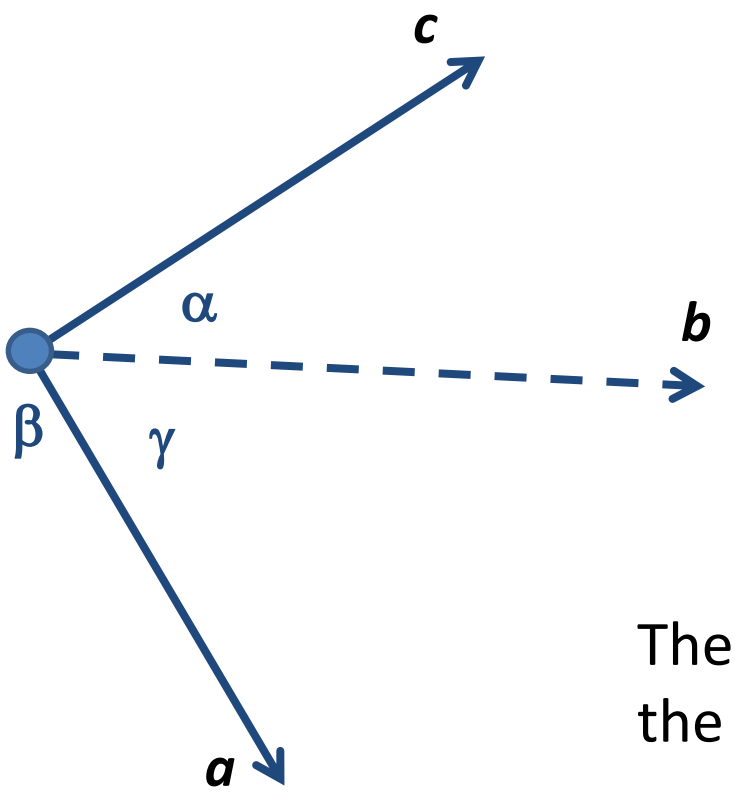
Classification of 3D lattice.

For the case of 3 D lattice there are ***7 different symmetries*** **(crystal systems) and** ***14 different types of lattices*** (compare to 4 symmetries and 5 lattices for the 2D case). The types of lattices were analysed by August Bravais

Auguste Bravais (1811-1863)

Because of this the different types of lattices are referred as Bravais lattices

3D Lattice symmetry 1: Triclinic



The ***triclinic*** lattice has the centre of inversion .

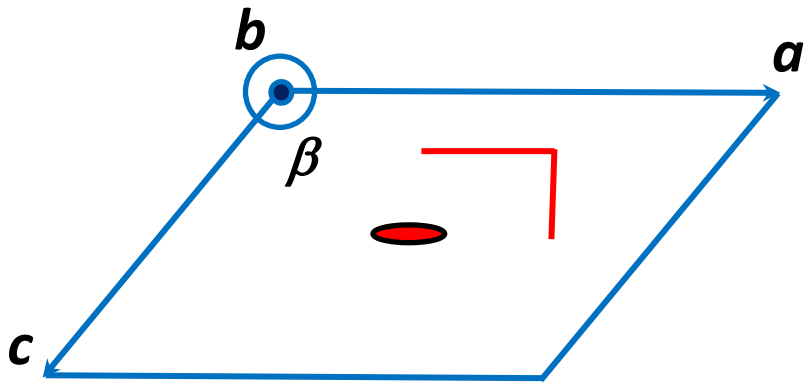
Note that any three dimensional lattice has the centre of inversion as if ***A*** is a lattice point then ***–A*** is also a lattice point

There is no particular restriction on the choice of basis vectors, ***a b*** and ***c***

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90$ deg

3D Lattice symmetry 2: Monoclinic



The ***monoclinic lattice*** has

a) 2-fold axis

b) Mirror plane

Conventional choice of lattice basis vectors is

1) ***b*** is parallel to the 2 fold axis / perpendicular to the mirror plane

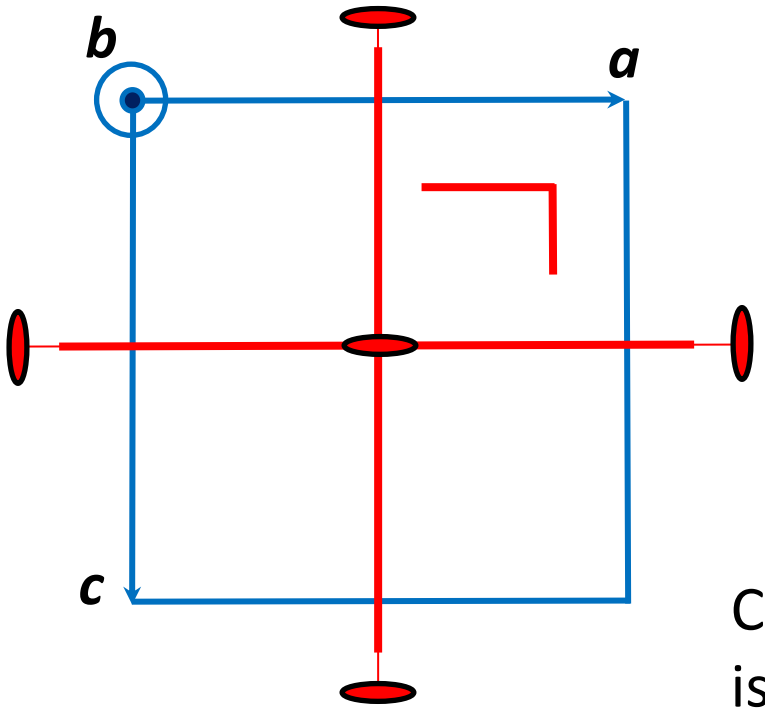
2) ***a and c*** are within a mirror plane

$$a \neq b \neq c$$

$$\alpha = \gamma = 90 \text{ deg} \quad \beta \neq 90 \text{ deg}$$

NB!! 3D *monoclinic* lattice is obtained by stacking 2D *oblique* lattices on the top of each other

3D Lattice symmetry 3: Orthorhombic



The ***orthorhombic*** lattice has

a) 2-fold axis (3 perpendicular to each other)
b) Mirror plane (3 perpendicular to each other)

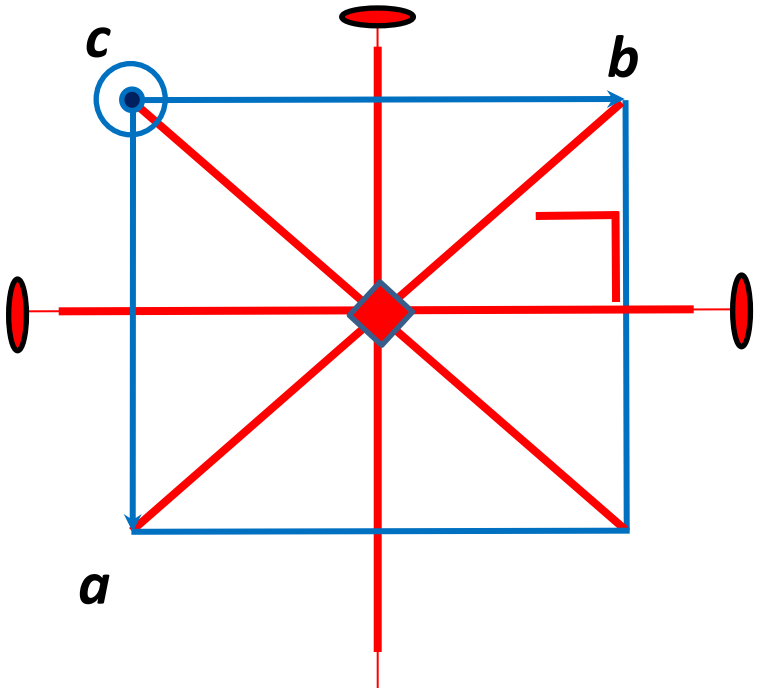
Conventional choice of lattice basis vectors is ***a***, ***b*** and ***c*** are along the directions of the two fold axes

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90 \text{ deg}$$

NB!! 3D *orthorhombic* lattice is obtained by stacking 2D *rectangular* lattices on the top of each other

3D Lattice symmetry 4: Tetragonal



The ***tetragonal*** lattice has

a) 4-fold axis
b) 2-fold axes (2 perpendicular to each other)
c) Mirror plane 1,2,3 parallel to 4 fold axis
d) Mirror plane perpendicular to 4 fold axis

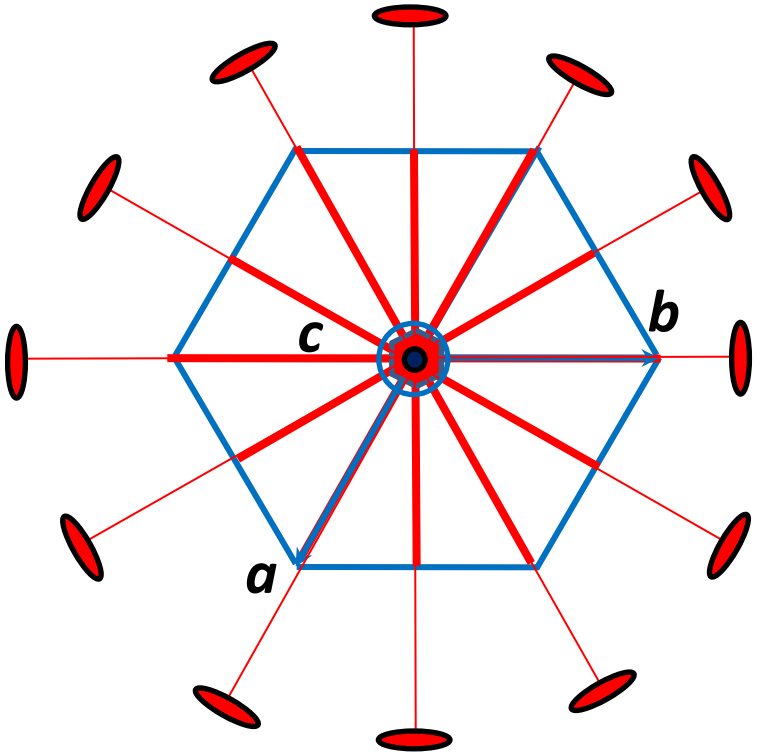
Conventional choice of lattice basis vectors is
c is parallel to the *4* fold axis, ***a*** and ***b*** are parallel to the 2 fold axes

$$a = b \neq c$$

$$\alpha = \beta = \gamma = 90 \text{ deg}$$

NB!! 3D *tetragonal* lattice is obtained by stacking 2D *square* lattices on the top of each other

3D Lattice symmetry 5: Hexagonal



The ***hexagonal*** lattice has

a) 6-fold axis (main)
b) Mirror planes and 2-fold axes as shown on the plot

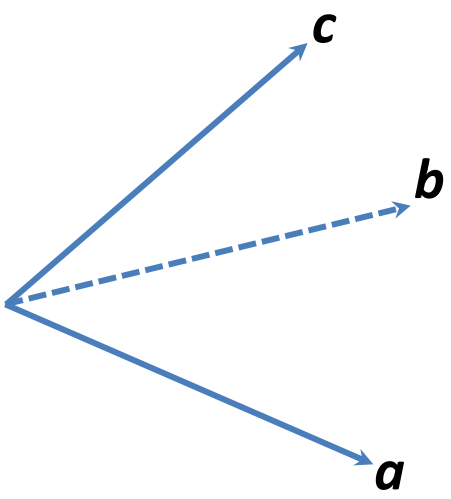
Conventional choice of lattice basis vectors is ***c*** is parallel to the *6* fold axis, ***a*** and ***b*** are chosen according to hexagonal 2 D lattice

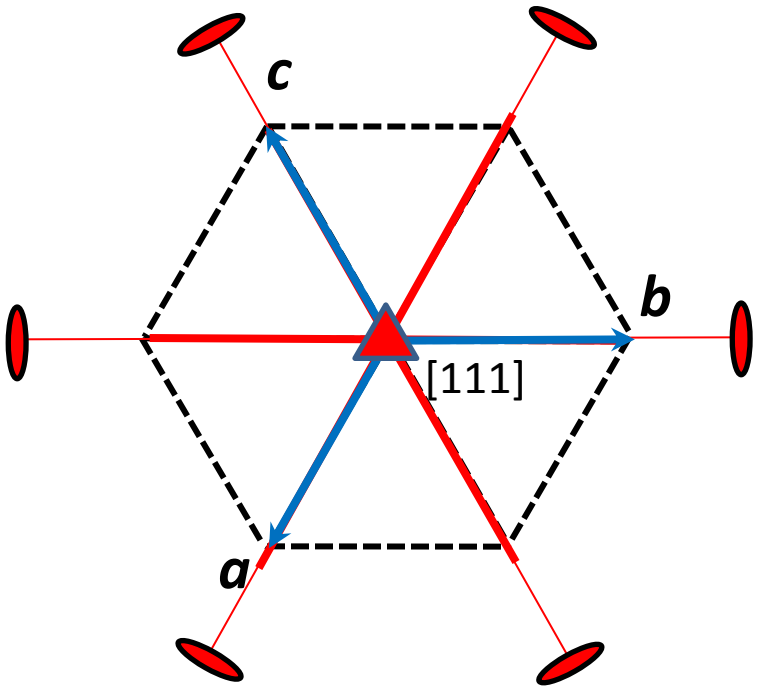
$$a = b \neq c$$

$$\alpha = \beta = 90 \text{ deg } \gamma = 120 \text{ deg}$$

NB!! 3D *hexagonal* lattice is obtained by stacking 2D *hexagonal* lattices on the top of each other

3D Lattice symmetry 6: Trigonal





The ***trigonal*** lattice has

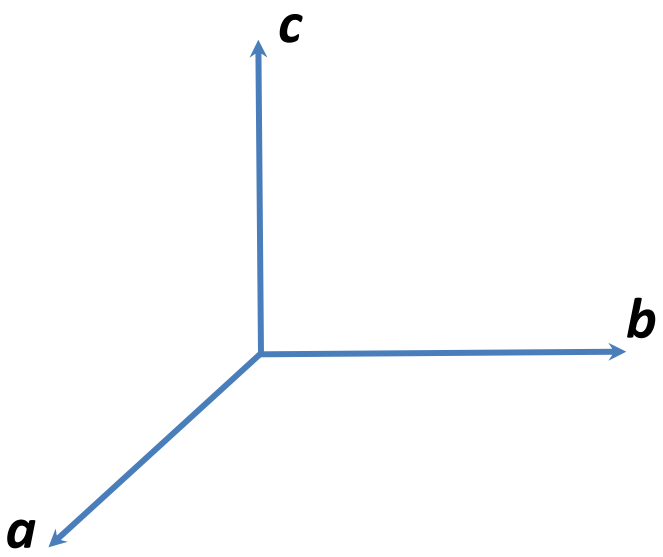
a) Single 3-fold axis

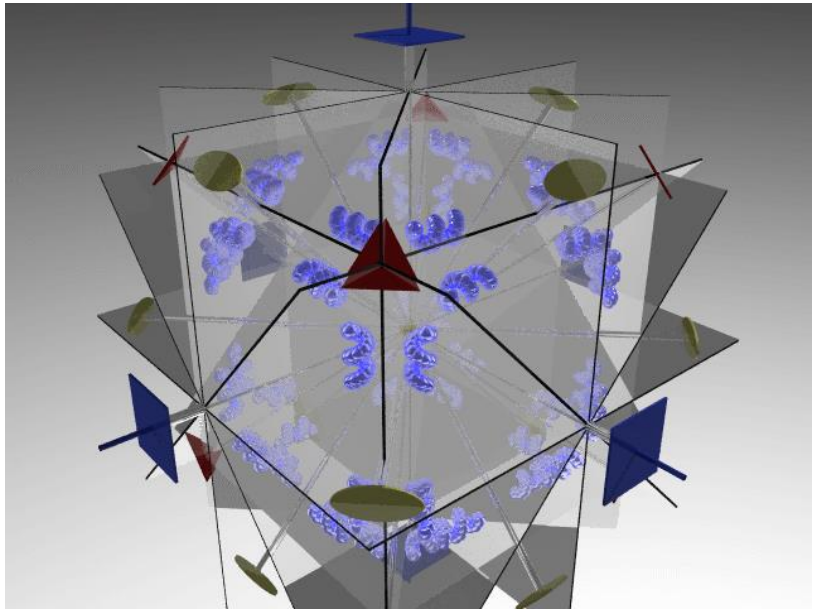
b) Mirror planes and 2-fold axes as shown on the plot

Conventional choice of lattice basis vectors is

a,b and ***c*** are within the mirror planes and [111] is parallel to the 3-fold axis

3D Lattice symmetry 7: Cubic





The ***cubic*** lattice has (symmetry of a cube)

a) 3-fold axis (4 times)

a) All elements of the tetragonal lattice

Conventional choice of lattice basis vectors is

The same as for the tetragonal lattice (a, b and c) are along three orthogonal symmetry directions

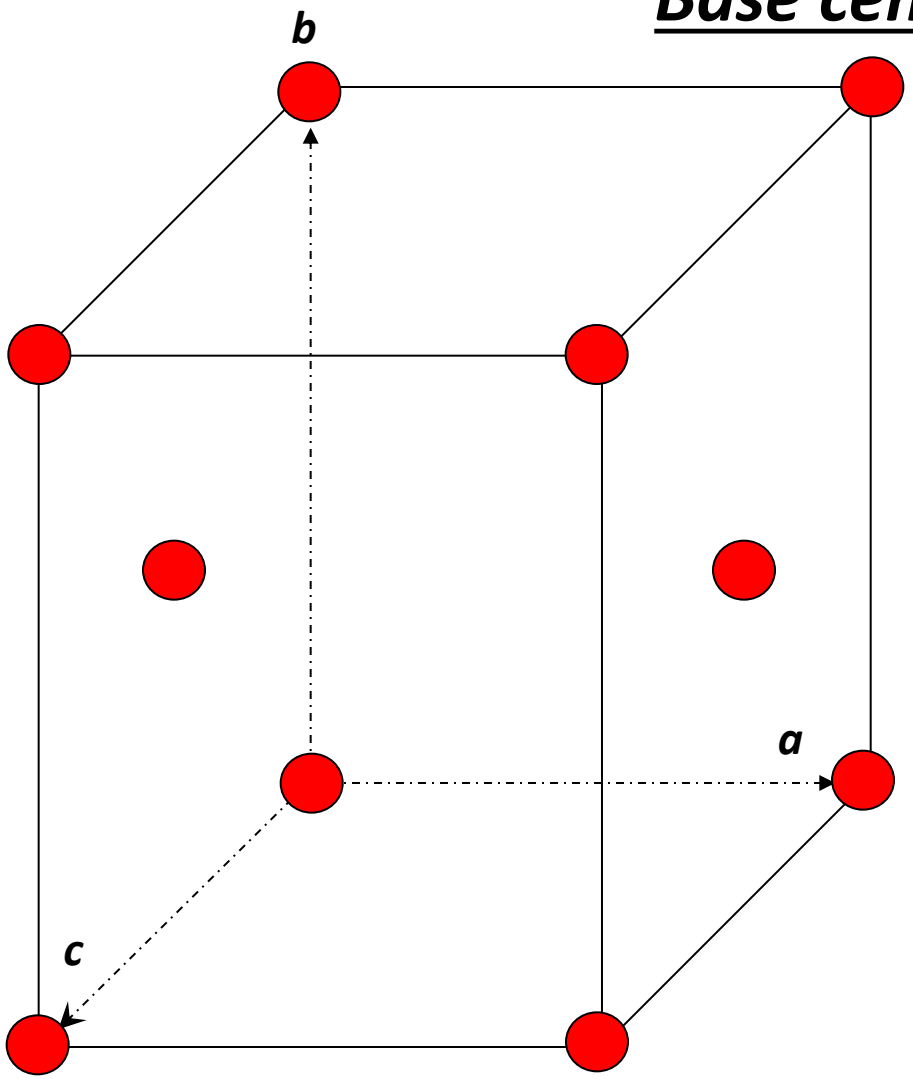
Centering of the unit cell

Some symmetries (in particular ***monoclinic***, ***orthorhombic***, ***tetragonal*** and ***cubic***) can be described by different types of lattice (refer to the rectangular symmetry for the 3D case).

The lattice vectors ***a***, ***b*** and ***c*** chosen according to the conventional rules form the NON-PRIMITIVE UNIT CELL, which has additional lattice points inside. This correspond to the CENTERING OF A UNIT CELL.

For three dimensions all distinct lattices may be described by a few types of centering. It gives 14 3D Bravais lattice.

Base centering (A)



Position of the lattice points

1. [000]
2. [0 1/2 1/2]

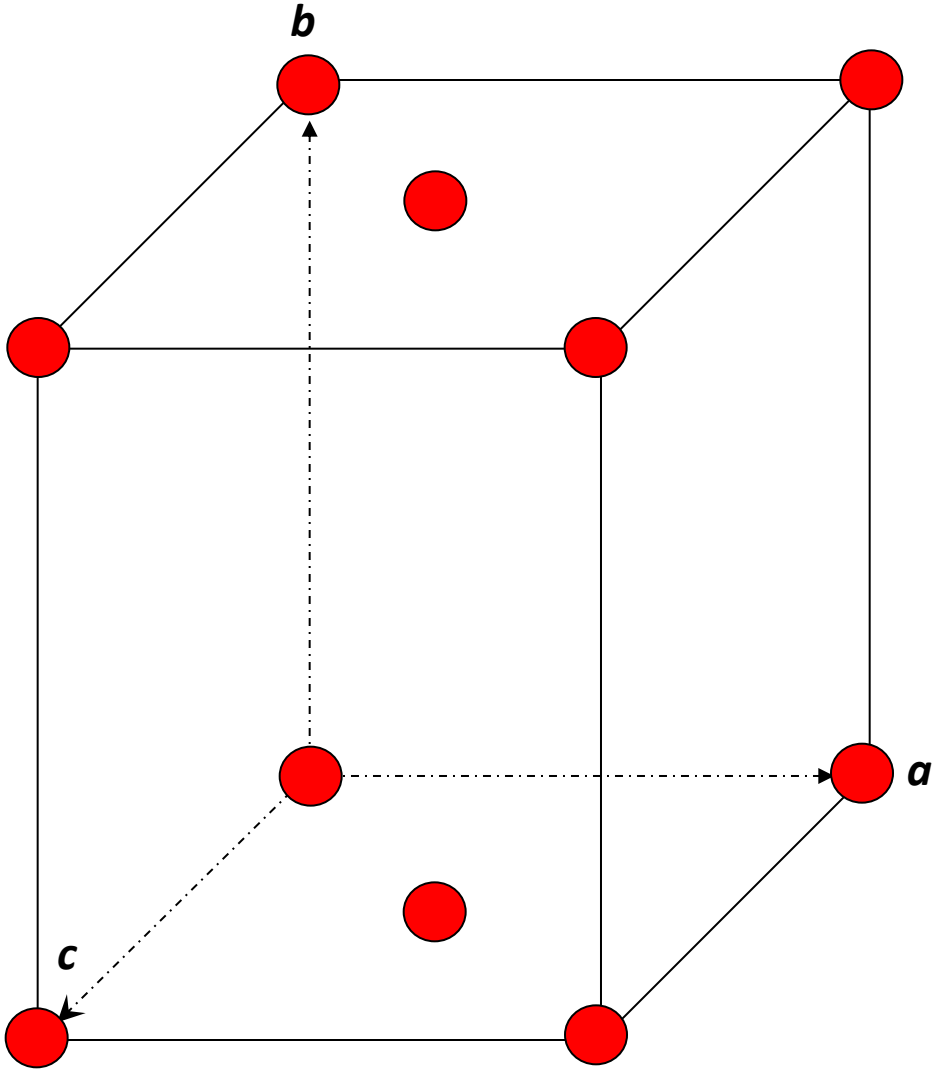
Primitive unit cell

a' = [1,0,0]

b' = [0,1/2,1/2]

c' = [0,-1/2,1/2]

Base centering (B)



Position of the lattice points

1. [000]
2. [1/2 0 1/2]

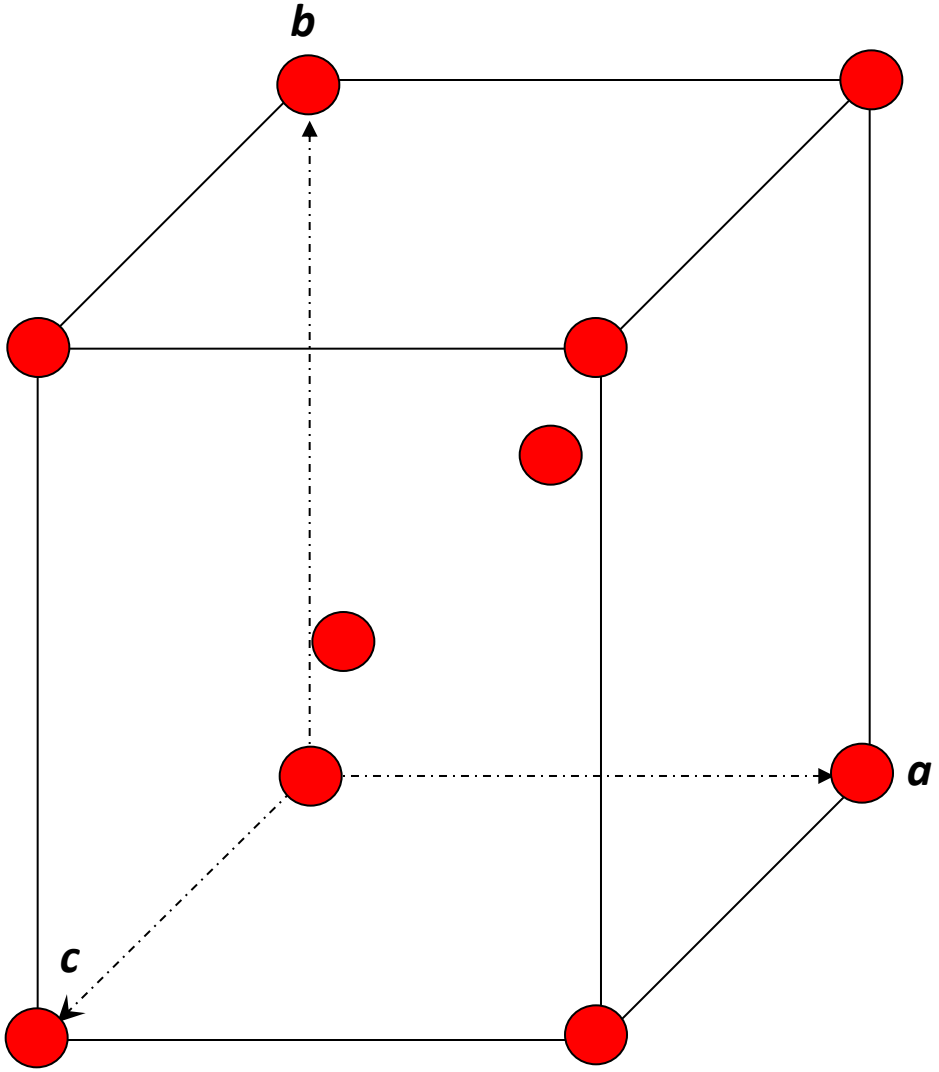
Primitive unit cell

a' = [-1/2,0,1/2]

b' = [0,1,0]

c' = [1/2,0,1/2]

Base centering (C)



Position of the lattice points

1. [000]
2. [1/2 1/2 0]

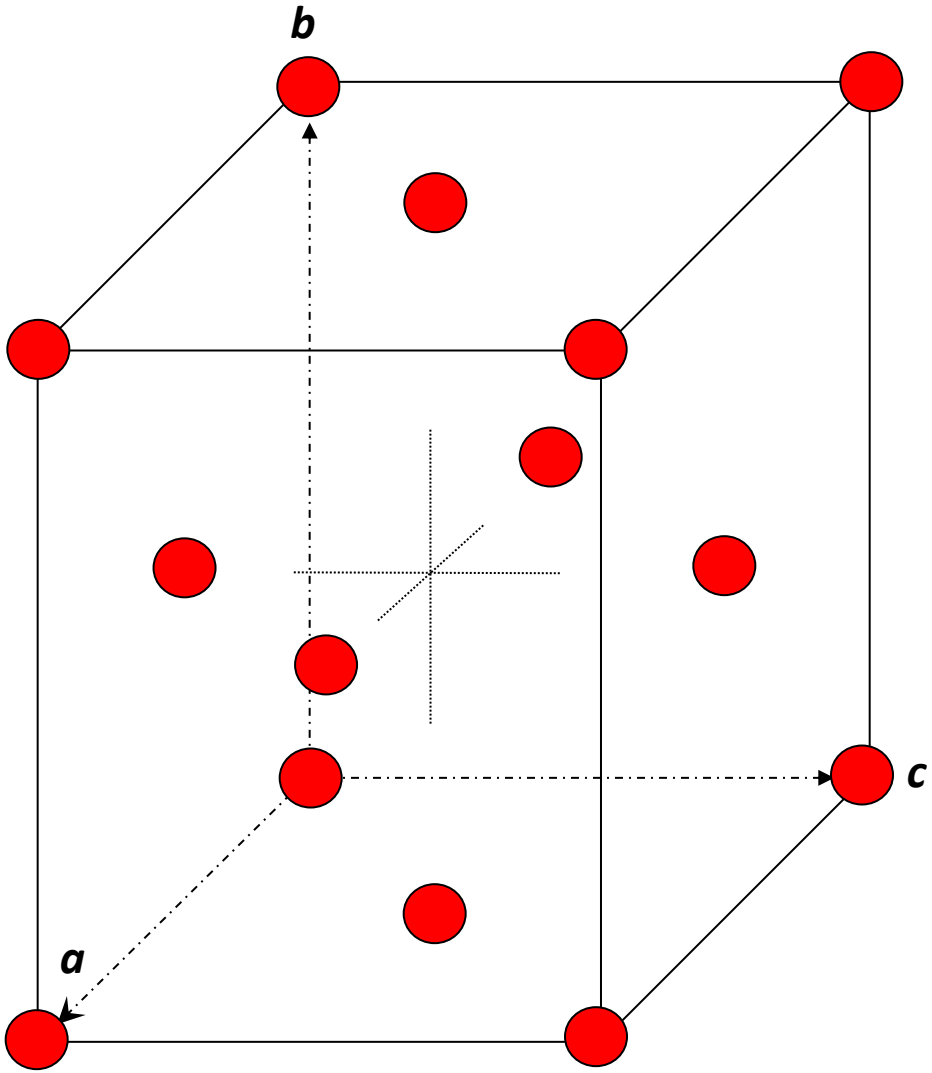
Primitive unit cell

a' = [-1/2,0,1/2]

b' = [0,1,0]

c' = [1/2,0,1/2]

FACE CENTERING (F)



Position of the lattice points

1. [000]
2. [1/2 0 1/2]
3. [1/2 1/2 0]
4. [0 1/2 1/2]

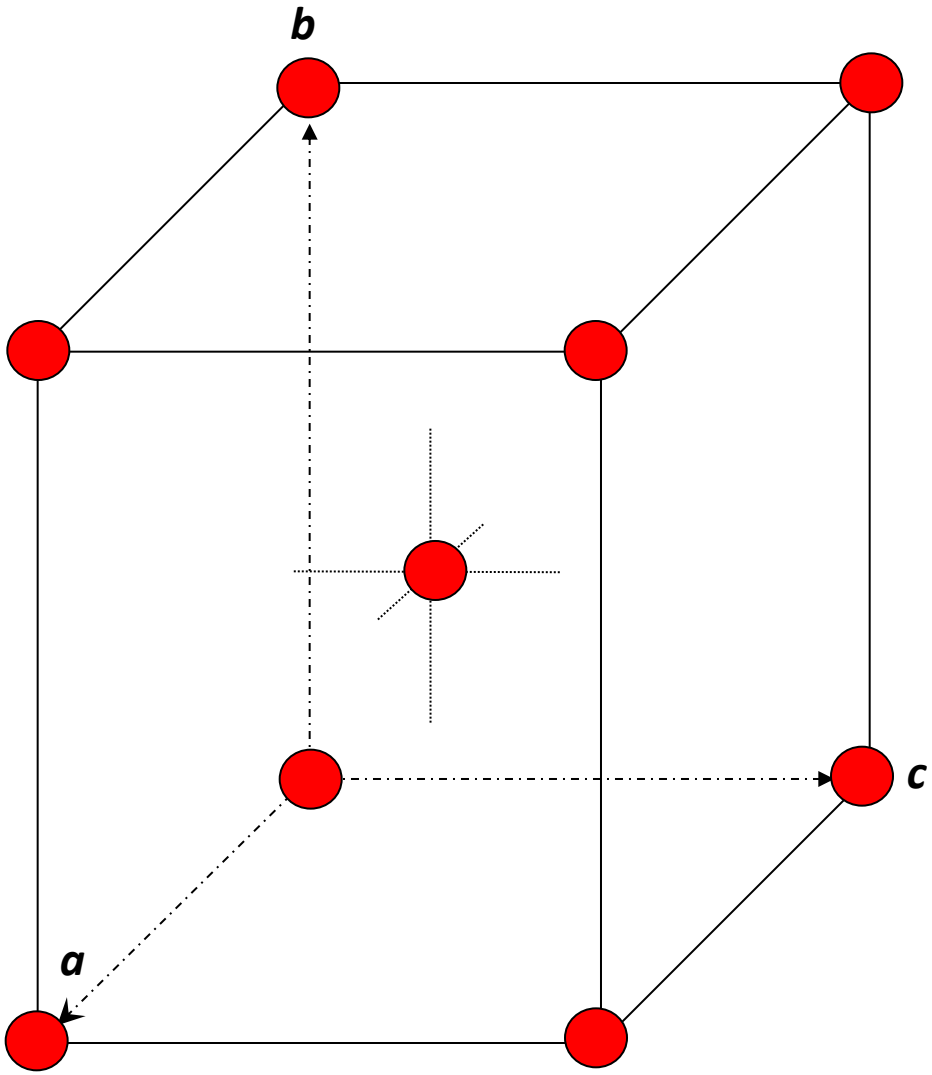
Primitive unit cell

a' = [0 1/2 1/2]

b' = [1/2 0 1/2]

c' = [1/2 1/2 0]

BODY CENTERING (I)



Position of the lattice points

1. [000]
2. [1/2 1/2 1/2]

Primitive unit cell

Find yourself

THEOREM ABOUT BASE CENTERING OF A LATTICE

If the lattice is A and B centred then it is C centered as well

Suppose that the lattice describes the following lattice translations:

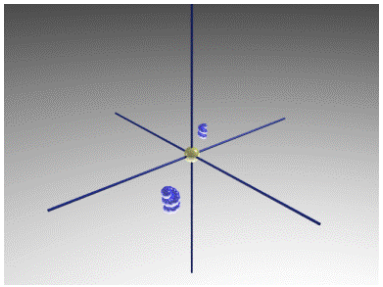
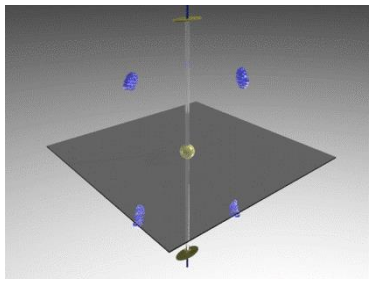
1. ***A_1= [u v w] where u,v, and w are the lattice points***
2. ***A_2 = [0 1/2 1/2] as a result of the A centering***
3. ***A_3 = [1/2 0 1/2] as a result of the B centering***

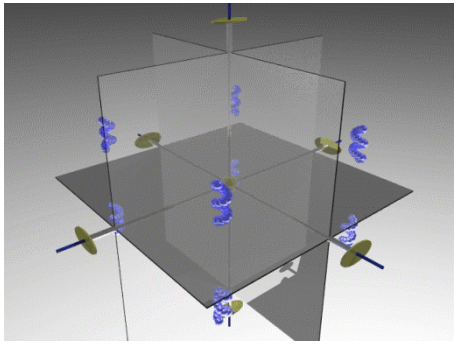
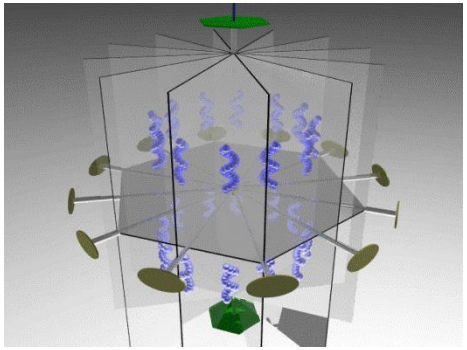
The above lattice translations may be combined in any sequence. For example if A_1 A_2 A_3 are the lattice vectors then A_1+ A_2 –A_3 is a lattice vector as well. Taking the lattice vector A_1 as [100] we get additional translation

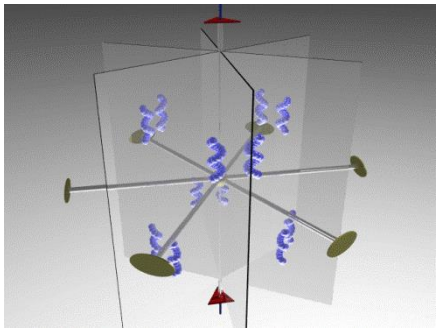
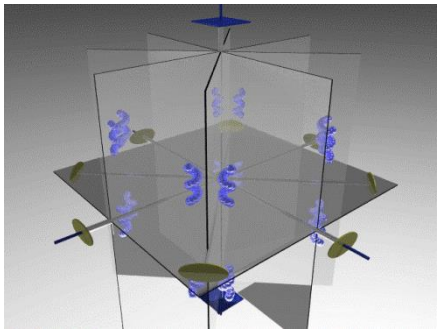
4. ***A_4 = [100] + [0 1/2 1/2] – [1/2 0 1/2] = [1/2 1/2 0] which manifests C centering***

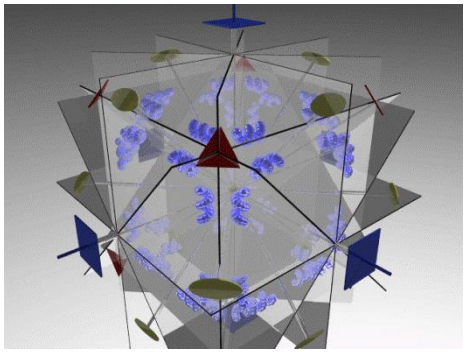
Result: There are no AB, AC or BC centring as they are all equivalent to the F centering

CONCLUDING TABLE FOR 3D LATTICES

Crystal system	Symmetry	Lattice constants	Lattice types
1. Triclinic	Inversion only 	**$a \neq b \neq c$,** **$\alpha \neq \beta \neq \gamma \neq 90$ deg**	1. Primitive (P)
2. Monoclinic	Single 2-fold / single mirror 	**$a \neq b \neq c$,** **$\alpha = \gamma = 90$ deg** **$\beta \neq 90$ deg**	2. Primitive (P) 3. Base centred (C)

Crystal system	Symmetry	Lattice constants	Lattice types
3. Orthorhombic	Three perpendicular mirror planes and 2 fold axes 	**$a \neq b \neq c$,** **$\alpha = \beta = \gamma = 90$ deg**	4. Primitive (P) 5. Base centered (A) 6. Body centered (I) 7. Face centered (F)
4. Hexagonal	6-fold axis plus mirror planes 	**$a = b \neq c$,** **$\alpha = \beta = 90$ deg** **$\gamma = 120$ deg**	8. Primitive (P)

Crystal system	Symmetry	Lattice constants	Lattice types
5. Trigonal	3-fold axis and mirror planes 	**a = b = c,** **$\alpha = \beta = \gamma \neq 90$ deg**	9. Primitive (P)
6. Tetragonal	4-fold axis plus mirror planes 	**a = b ≠ c,** **$\alpha = \beta = \gamma = 90$ deg**	10. Primitive (P) 11. Body centered (I)

Crystal system	Symmetry	Lattice constants	Lattice types
5. Cubic	4 different 3-fold axis and mirror planes 	**a = b = c,** **$\alpha = \beta = \gamma = 90$ deg**	12. Primitive (P) 13. Face centered (F) (face centered cubic) 14. Body centered (I)

Relationships between hexagonal and rhombohedral cell settings

A crystal lattice with 3 fold symmetry axis is usually described by trigonal (rhombohedral) cell setting: $\{\boldsymbol{a_R},\boldsymbol{b_R},\boldsymbol{c_R}\}$ ($a_R=b_R=c_R$, $\alpha_R=\beta_R=\gamma_R$). In this case unit cell is ***primitive,*** i.e. contains ***one*** lattice point

The same lattices (with 3 fold symmetry axis) may be described by hexagonal cell setting: $\{\boldsymbol{a_H},\boldsymbol{b_H},\boldsymbol{c_H}\}$ ($a_H=b_H$, $\alpha_H=\beta_H=90$ deg, $\gamma_H=120$ deg). In this case unit cell is ***non primitive,*** i.e. contains ***three*** lattice points

The transformations between hexagonal and rhombohedral cell basis vectors are given by

$$\begin{cases} \mathbf{a}_H = \mathbf{a}_R - \mathbf{b}_R = [1\bar{1}0]_R \\ \mathbf{b}_H = \mathbf{b}_R - \mathbf{c}_R = [0\bar{1}1]_R \\ \mathbf{c}_H = \mathbf{a}_R + \mathbf{b}_R + \mathbf{c}_R = [111]_R \end{cases}$$

$$\begin{cases} \mathbf{a}_R = 2/3\mathbf{a}_H + 1/3\mathbf{b}_H + 1/3\mathbf{c}_H \\ \mathbf{b}_R = -1/3\mathbf{a}_H + 1/3\mathbf{b}_H + 1/3\mathbf{c}_H \\ \mathbf{c}_R = -1/3\mathbf{a}_H - 2/3\mathbf{b}_H + 1/3\mathbf{c}_H \end{cases}$$

On the illustration below the lattice projection along [001] hexagonal axis is given:

Lattice points in the layer 0 (projection to c_H axis is 0)

Lattice points in the layer 1 (projection to c_H axis is 1/3)

Lattice points in the layer 2 (projection to c_H axis is 2/3)

Relationships between hexagonal and rhombohedral cell settings