Quelques rappels sur la maille Hexagonale Compacte

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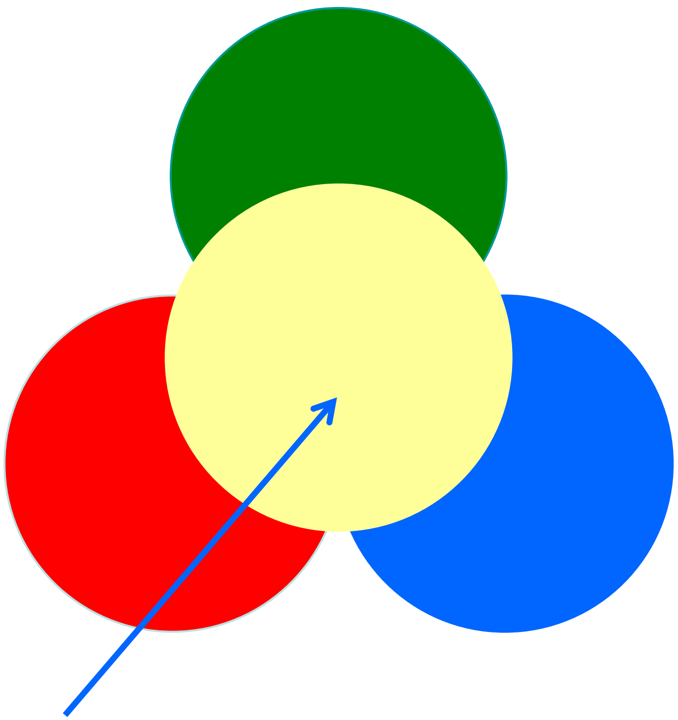
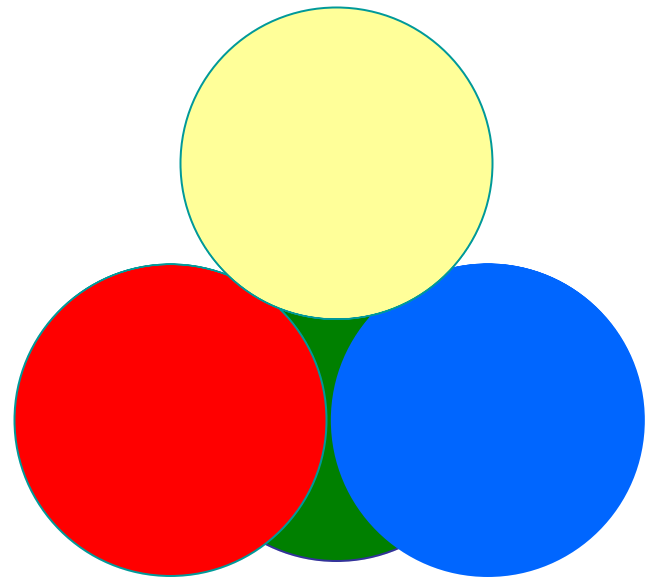
Comment est formé un empilement compact ?

Motif de base

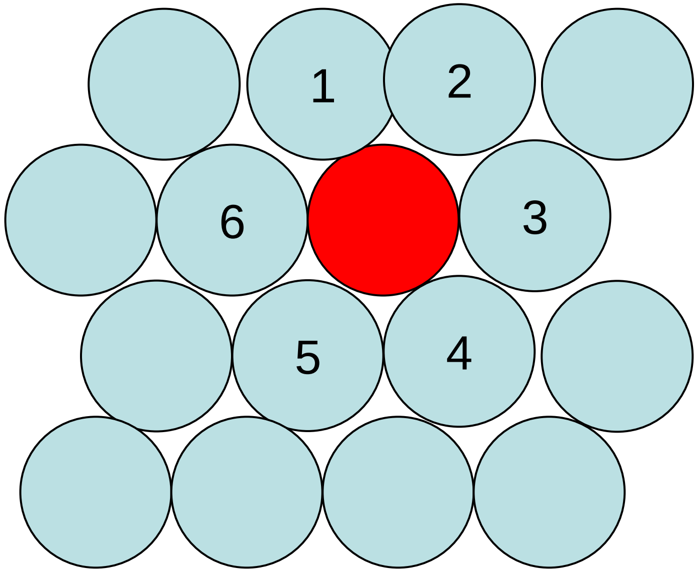


Atome au dessus

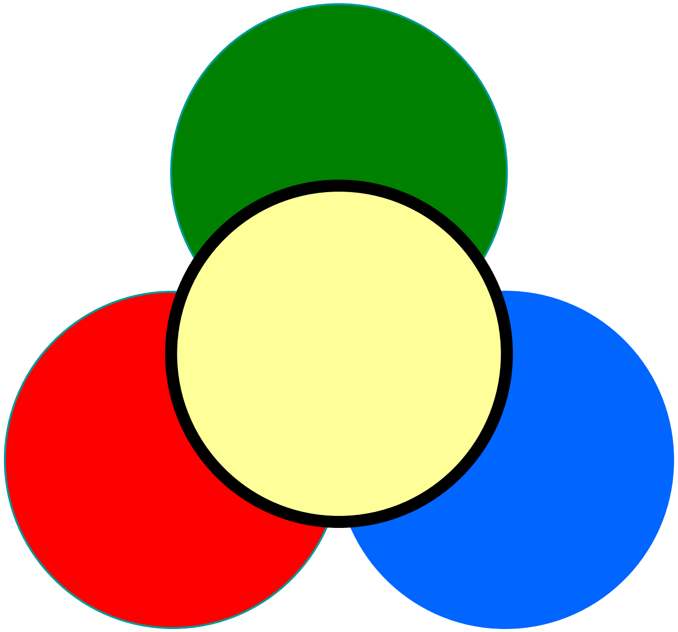


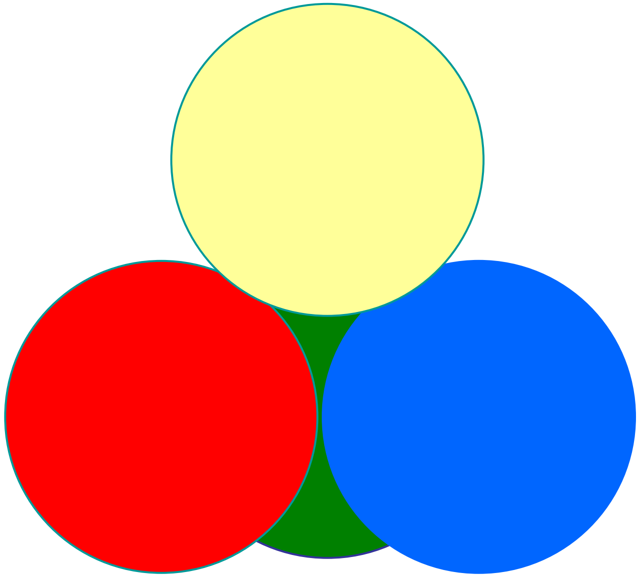
Vue de profil

Empilement de sphères



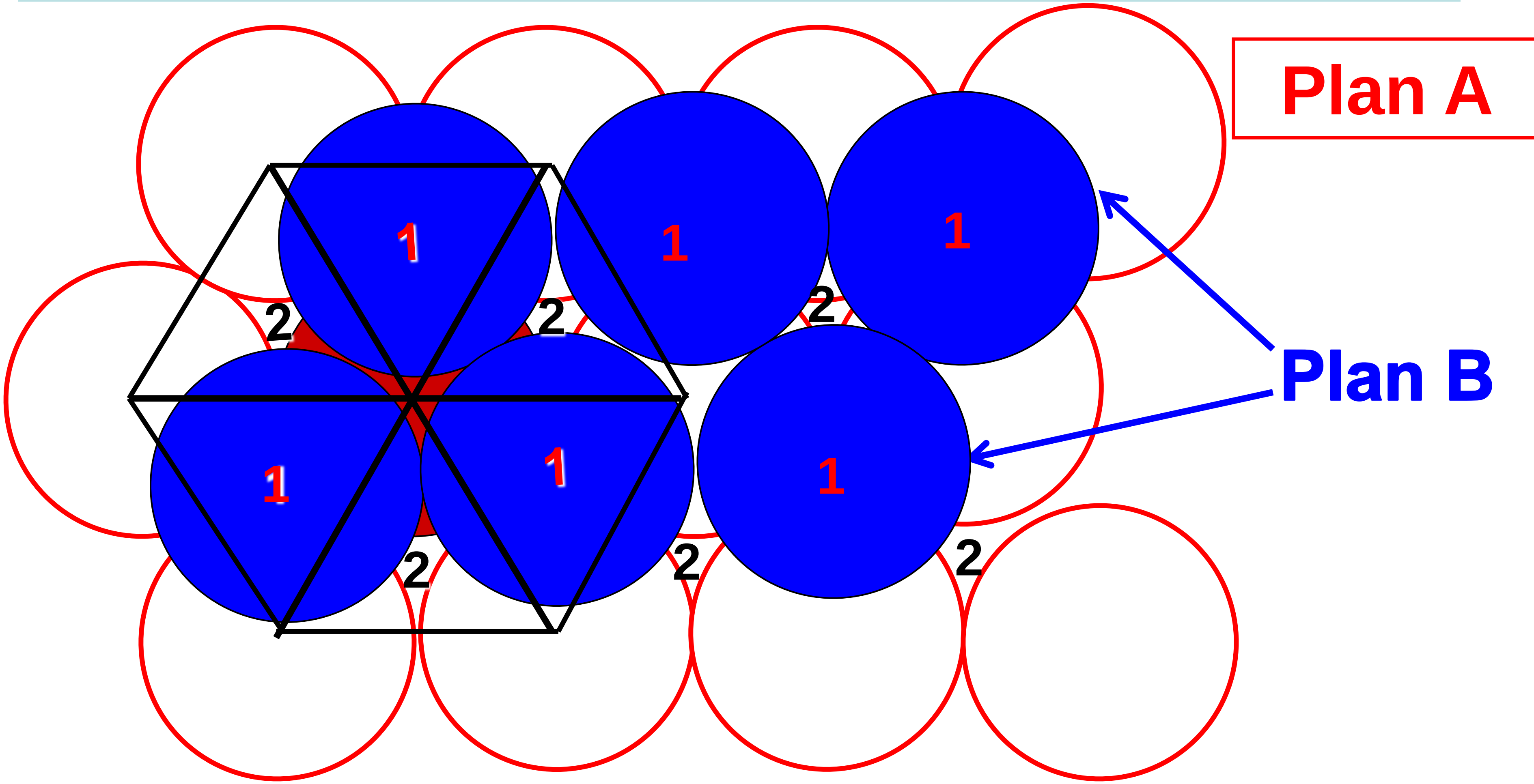
Empilement de sphères





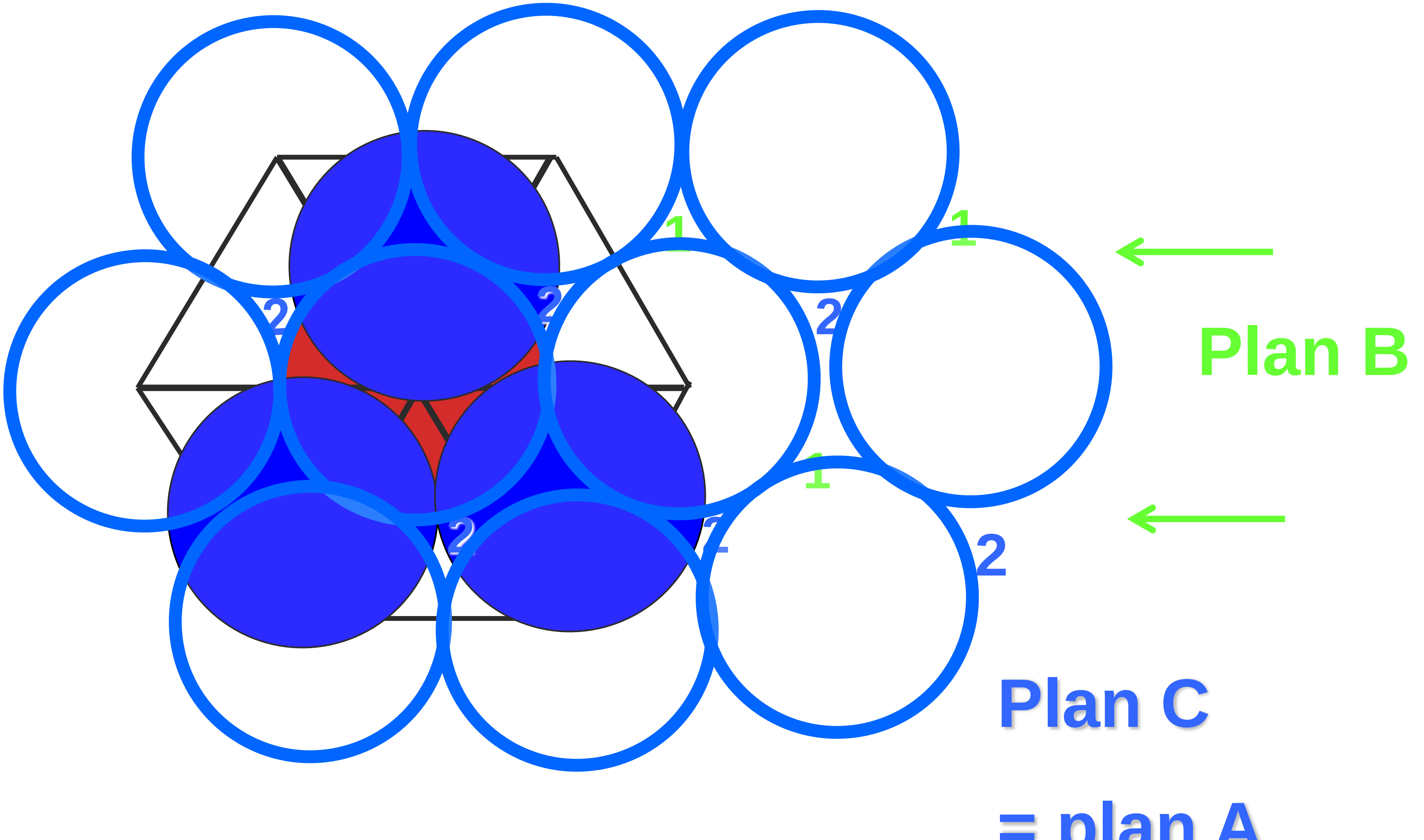
2- Succession

des deux premiers Plans compacts A et B



2- Troisième plan compact C :

deux possibilités : la première est

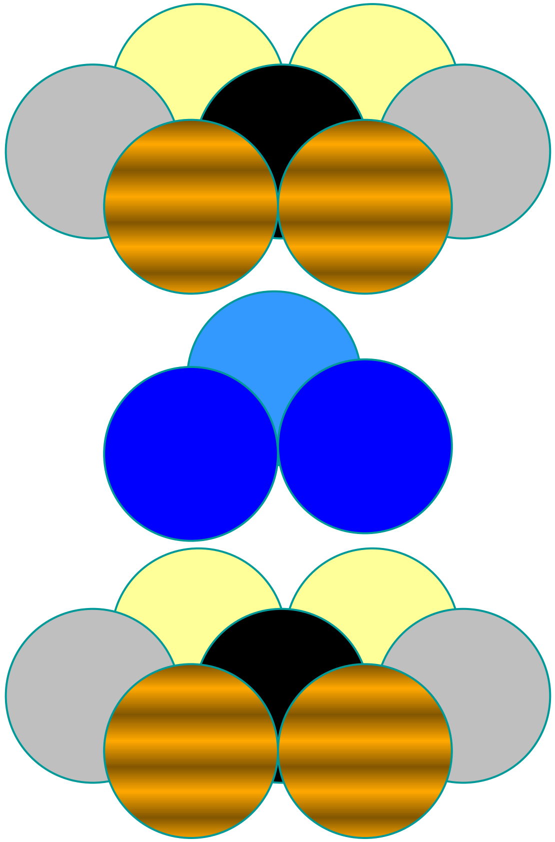


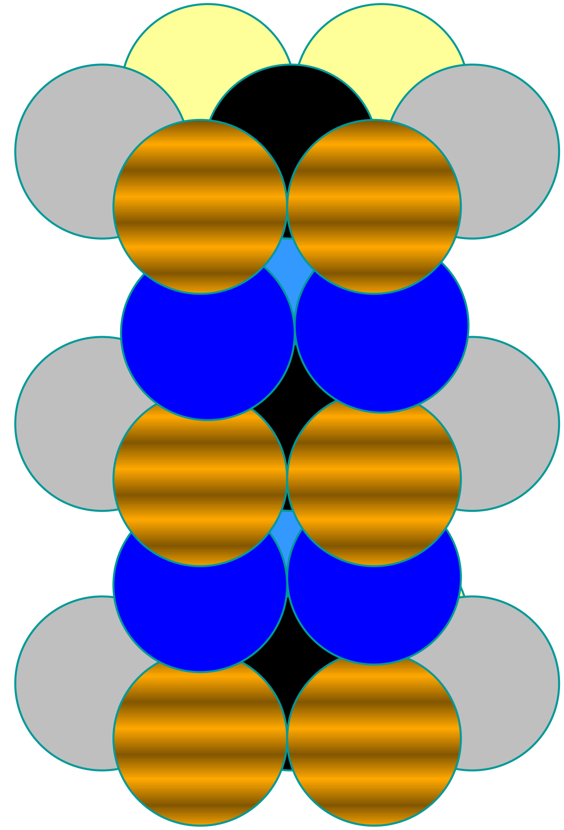
Maille hexagonale compacte HC

Plan C = A

Plan B

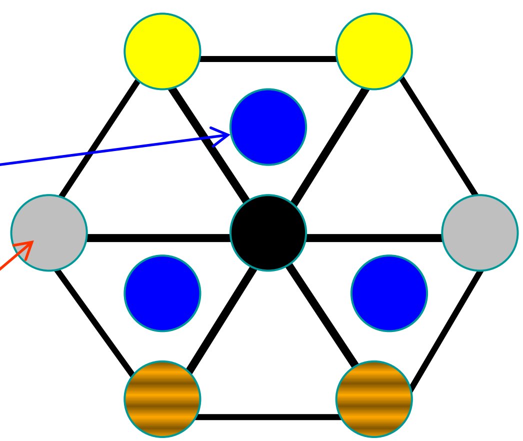
Plan A





Plan B

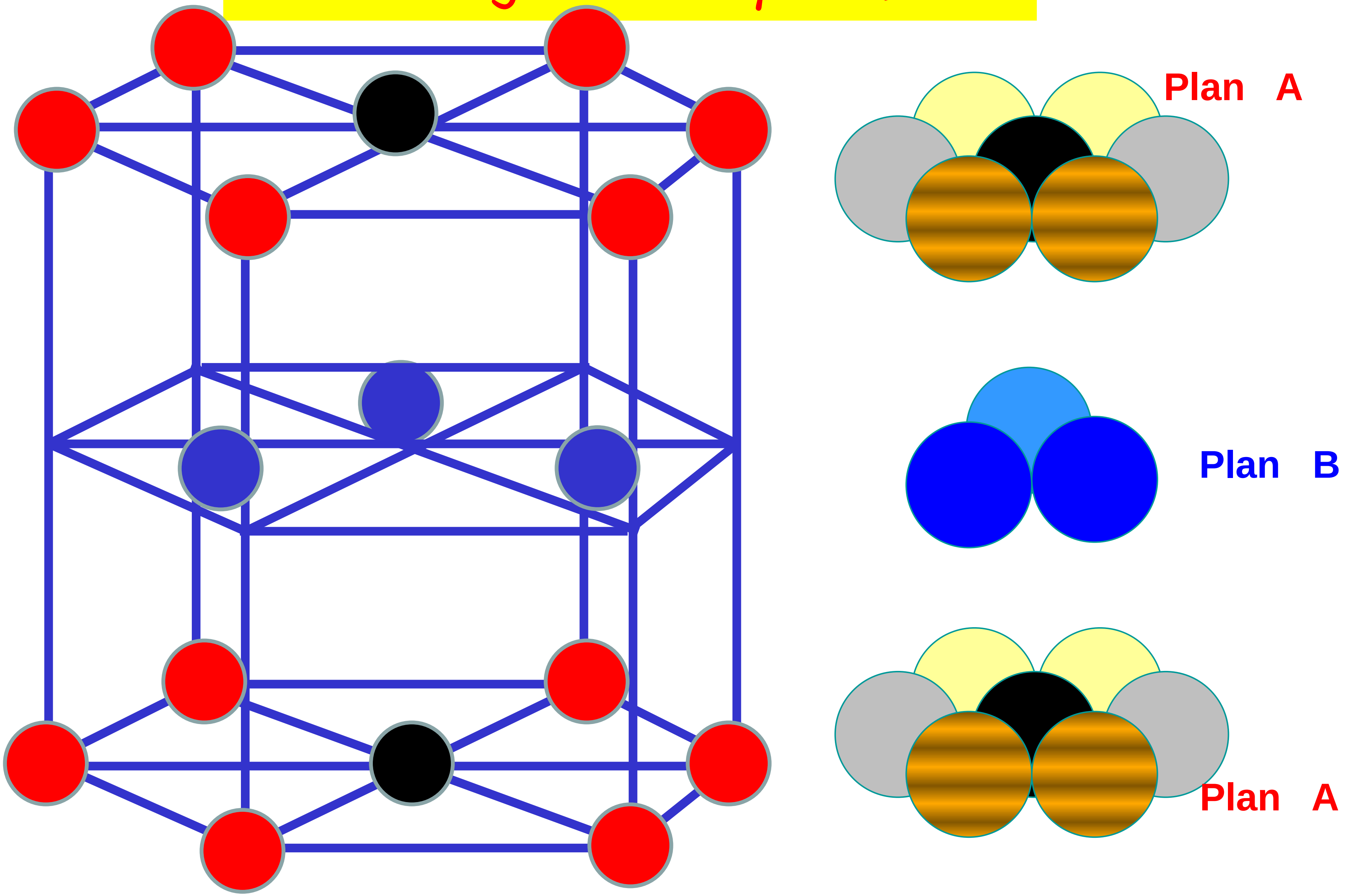
Plan A



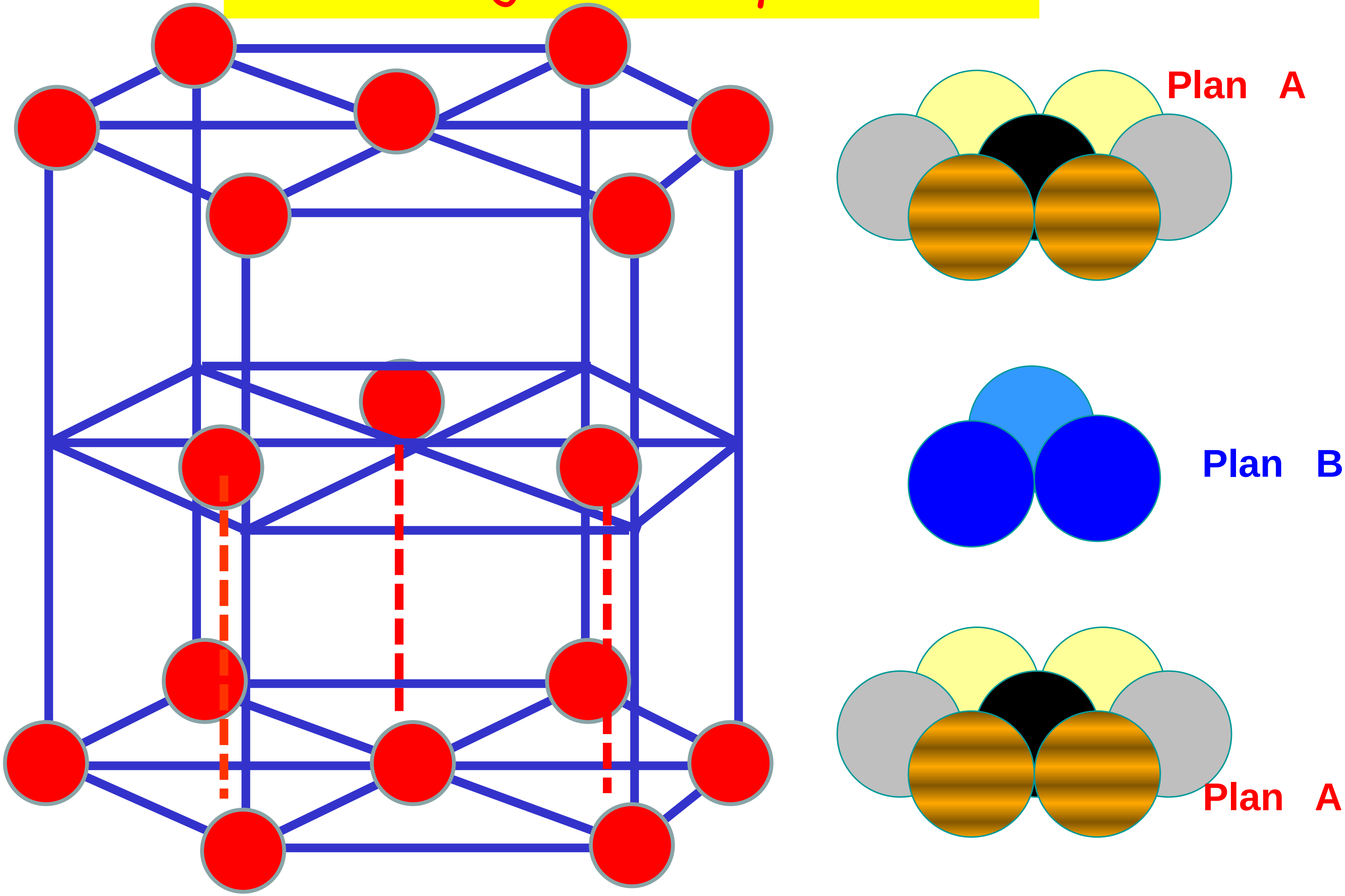
Succession des plans

A B A B A B …….

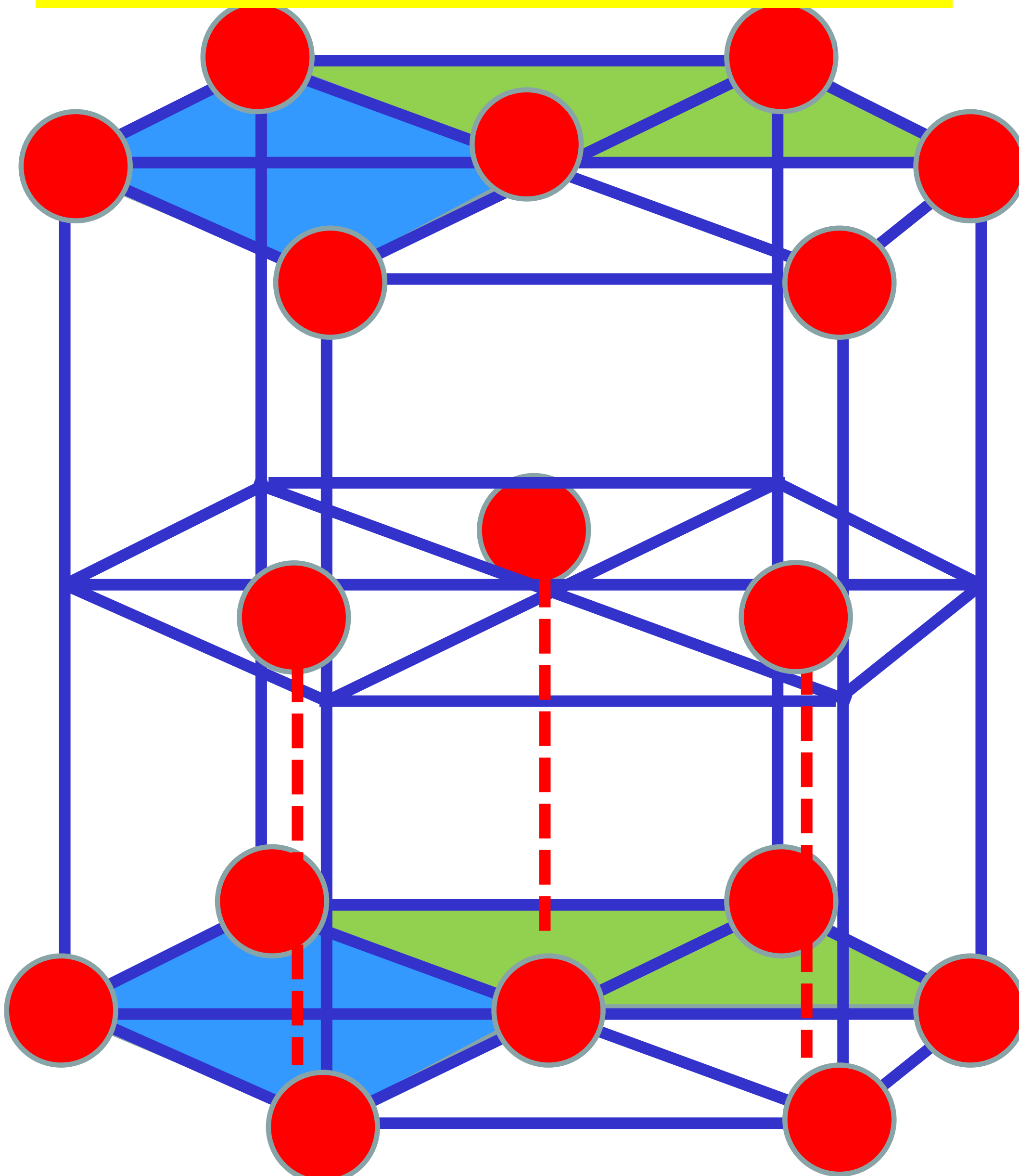
Maille hexagonale compacte, HC



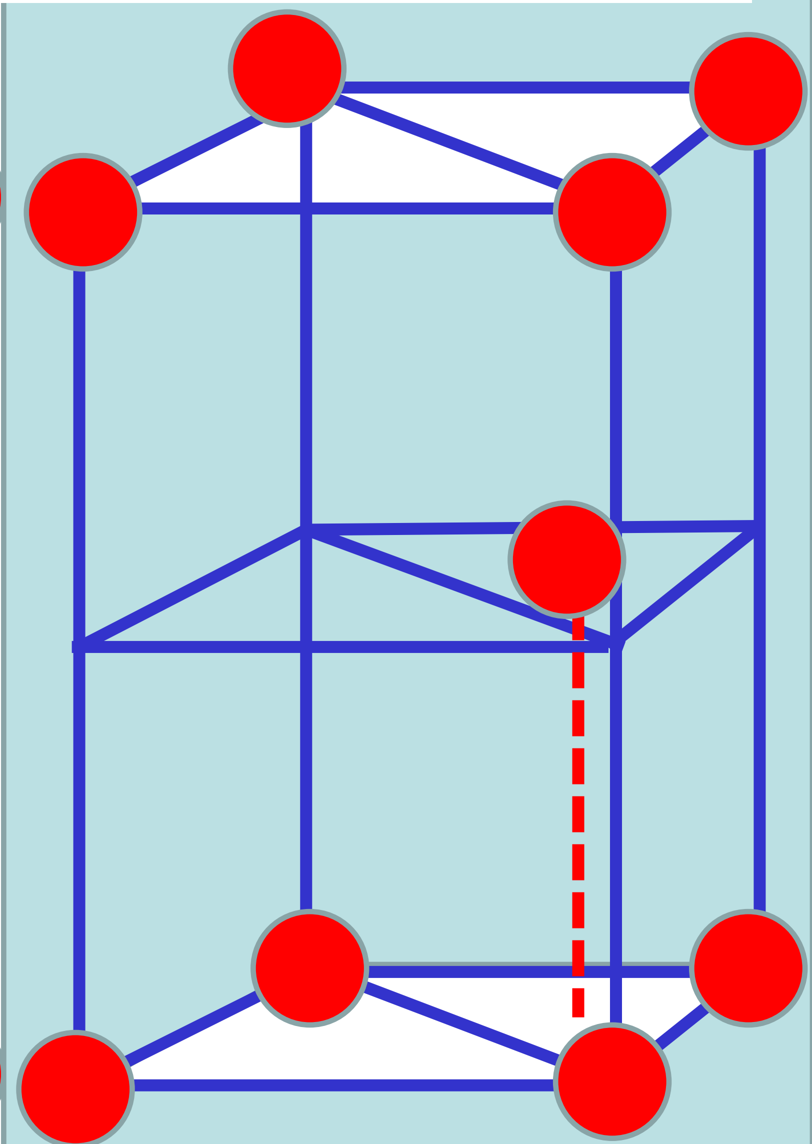
Maille hexagonale compacte, HC



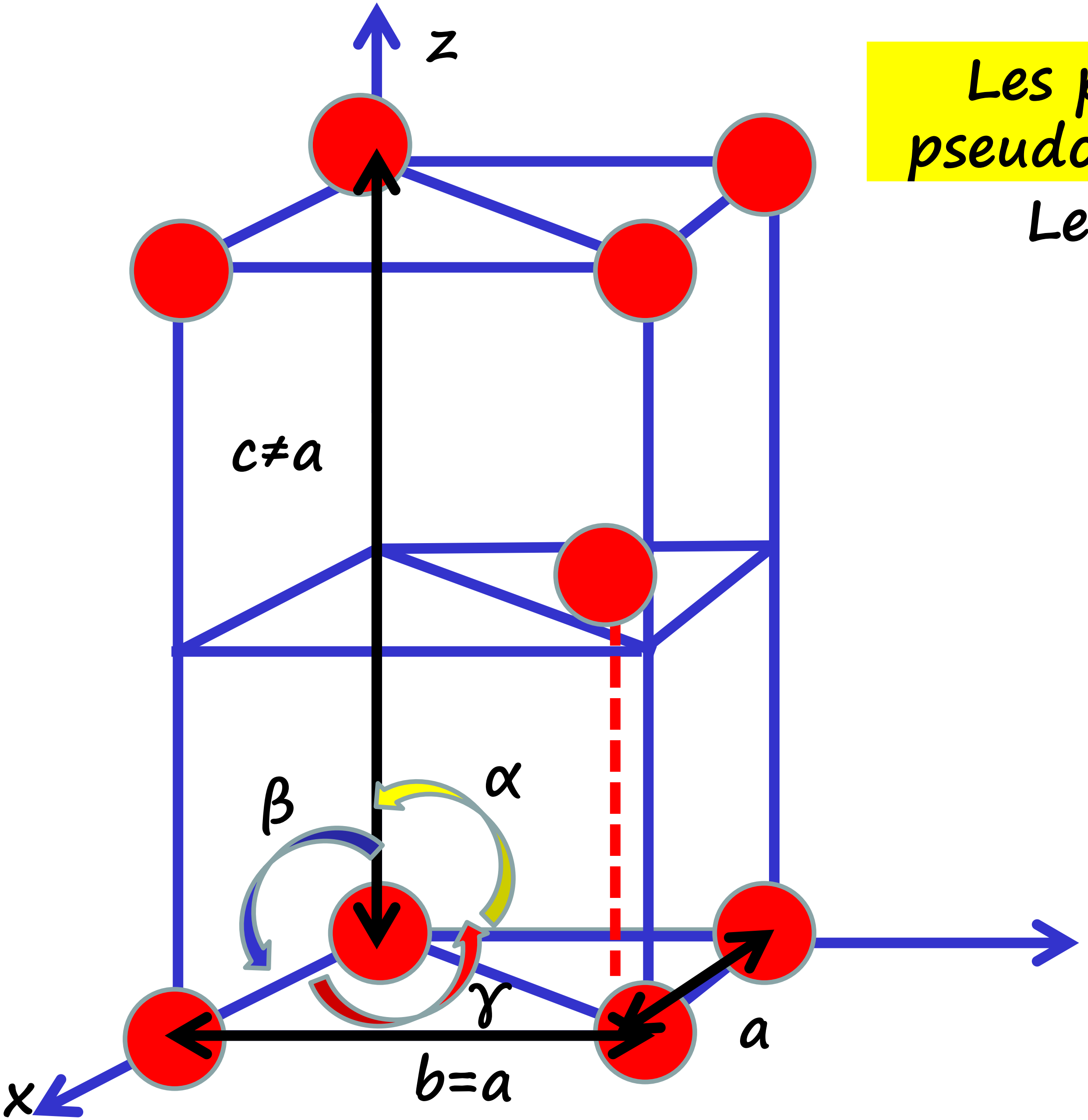
Maille hexagonale compacte, HC



Pseudo maille = 1/3 de la Maille HC



Pseudo maille HC



Les paramètres de la pseudo maille hexagonale

Les paramètres :

a

b = a

c≠a

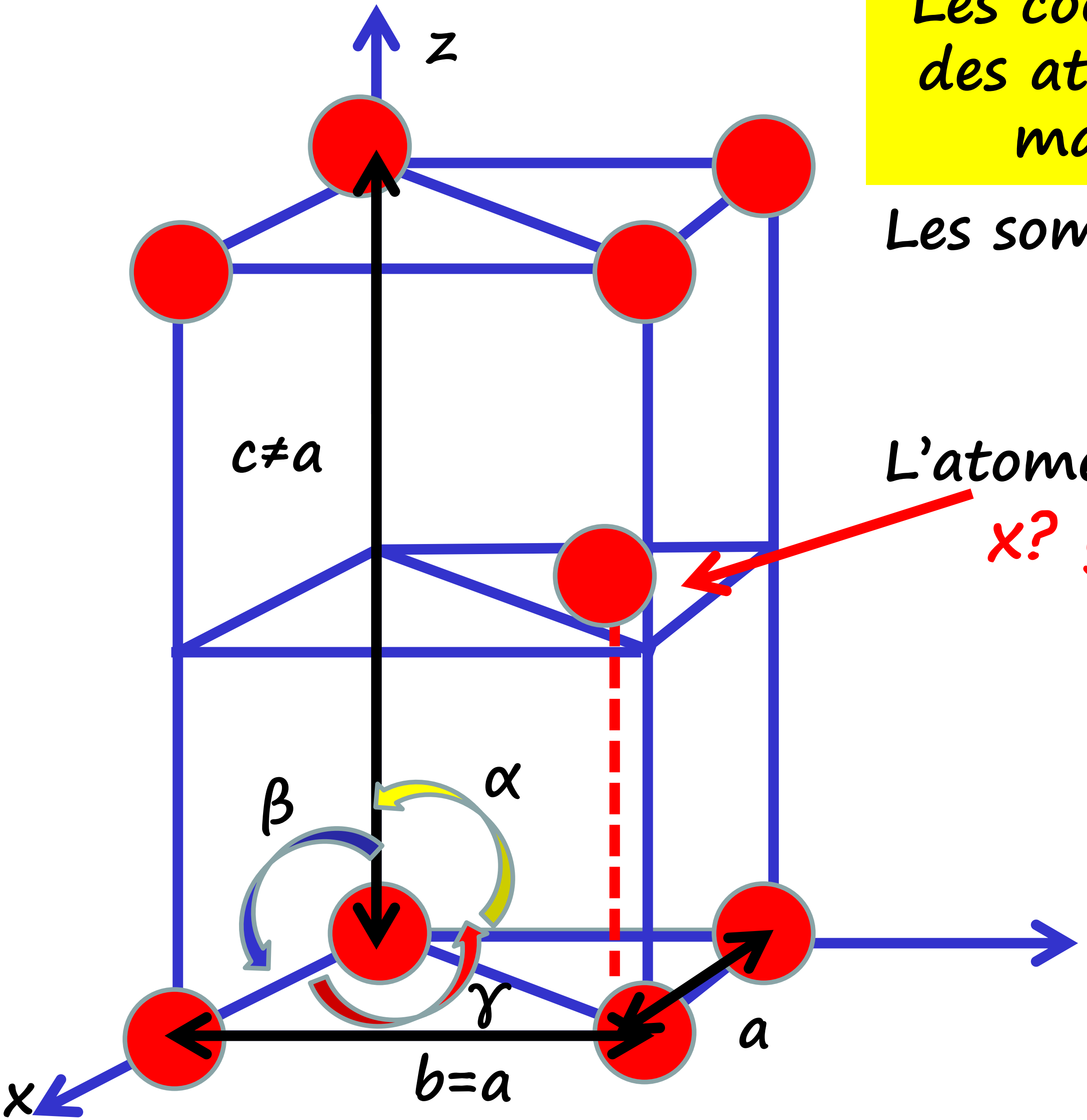
et 3 angles :

$\alpha = 90°$

$\beta = 90°$

$\gamma = 120°$

Pseudo maille HC



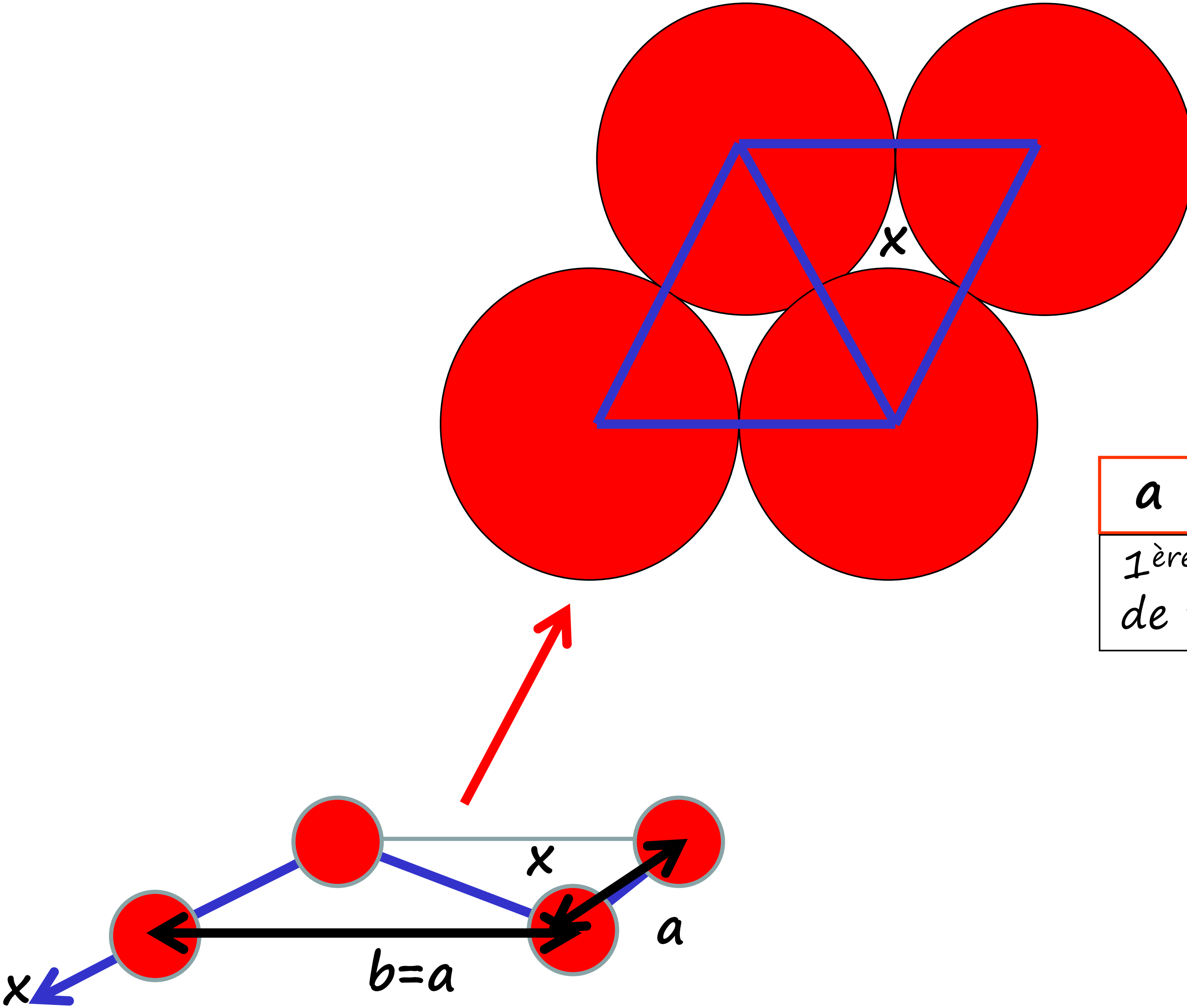
Les coordonnées réduites des atomes de la pseudo maille hexagonale

Les sommets :

(0, 0, 0)

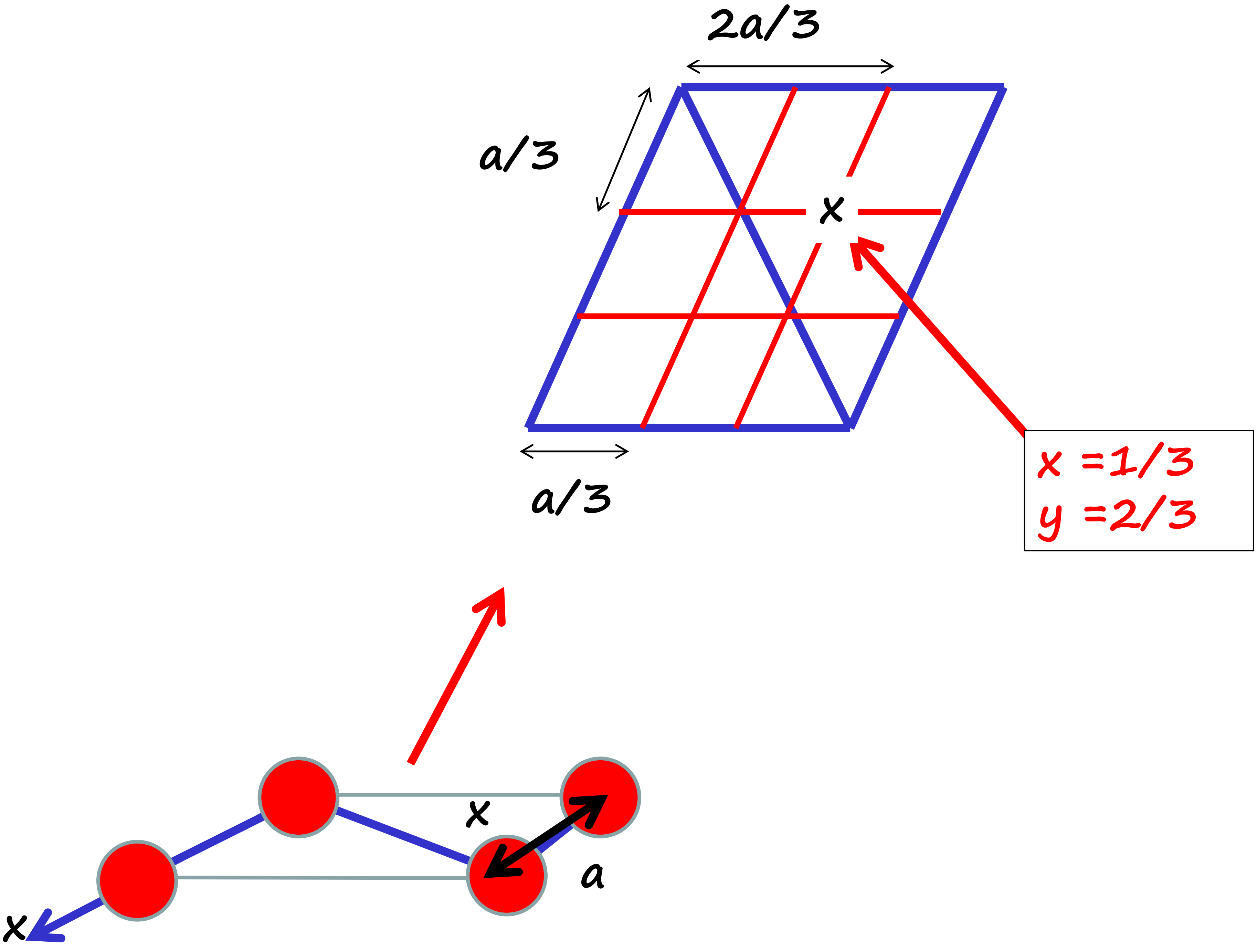
L'atome interne, z= ½

x? y?

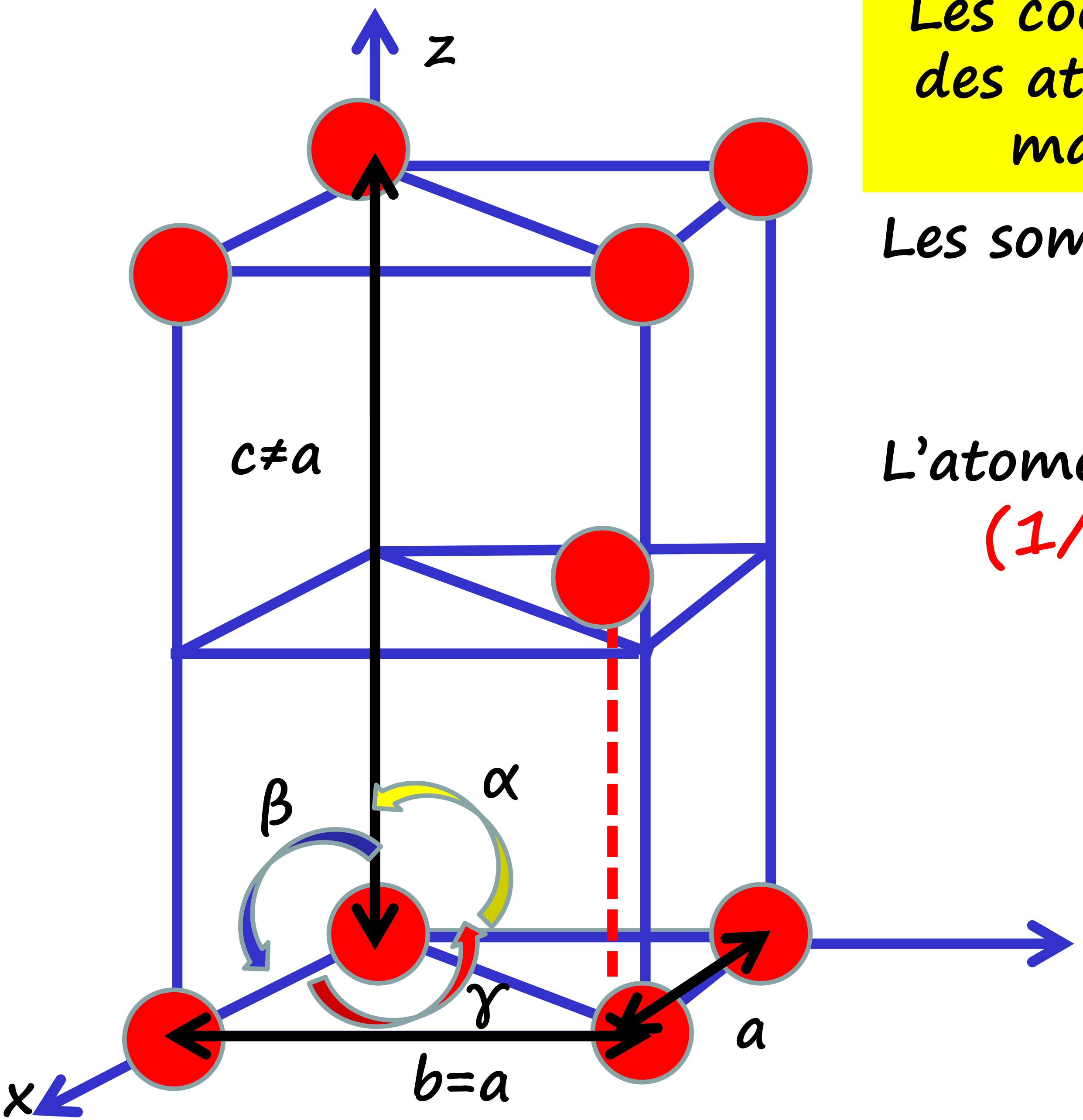


a = 2.R

$1^{ère}$ relation de tangence


2a/3
a/3
x
a/3
x =1/3
y =2/3
x
a
x

Pseudo maille HC



Les coordonnées réduites des atomes de la pseudo maille hexagonale

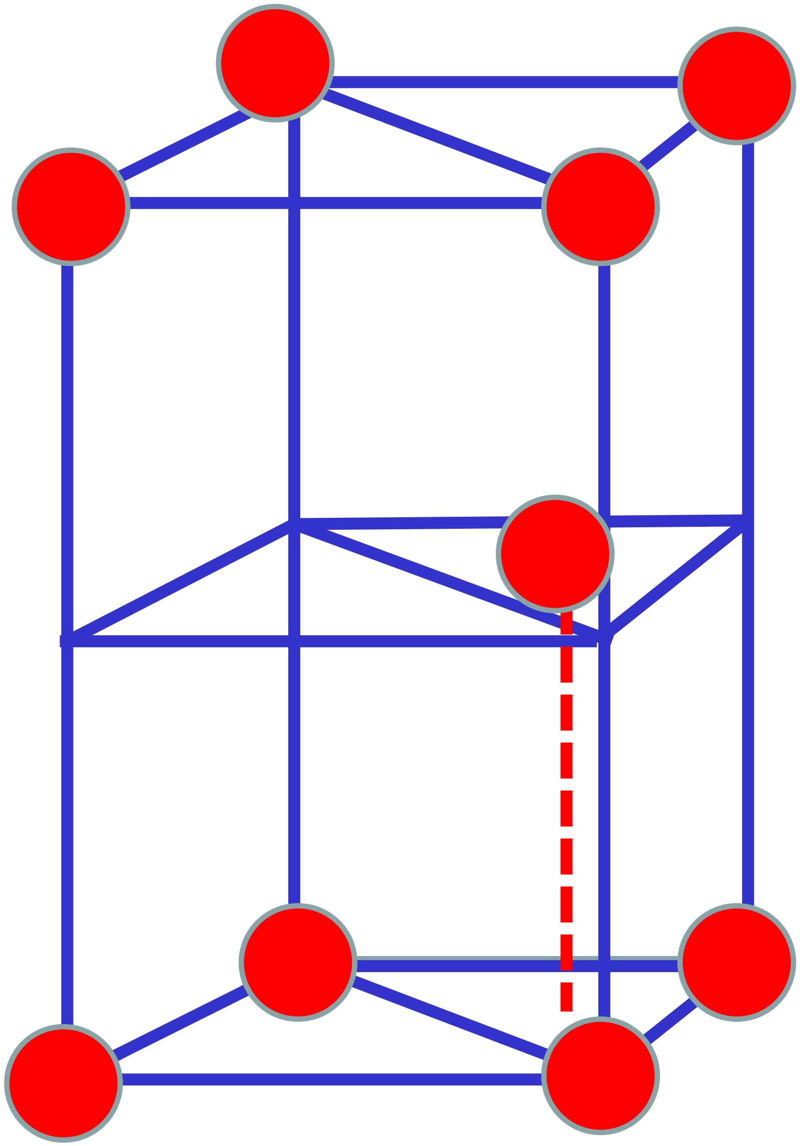
Les sommets :

(0, 0, 0)

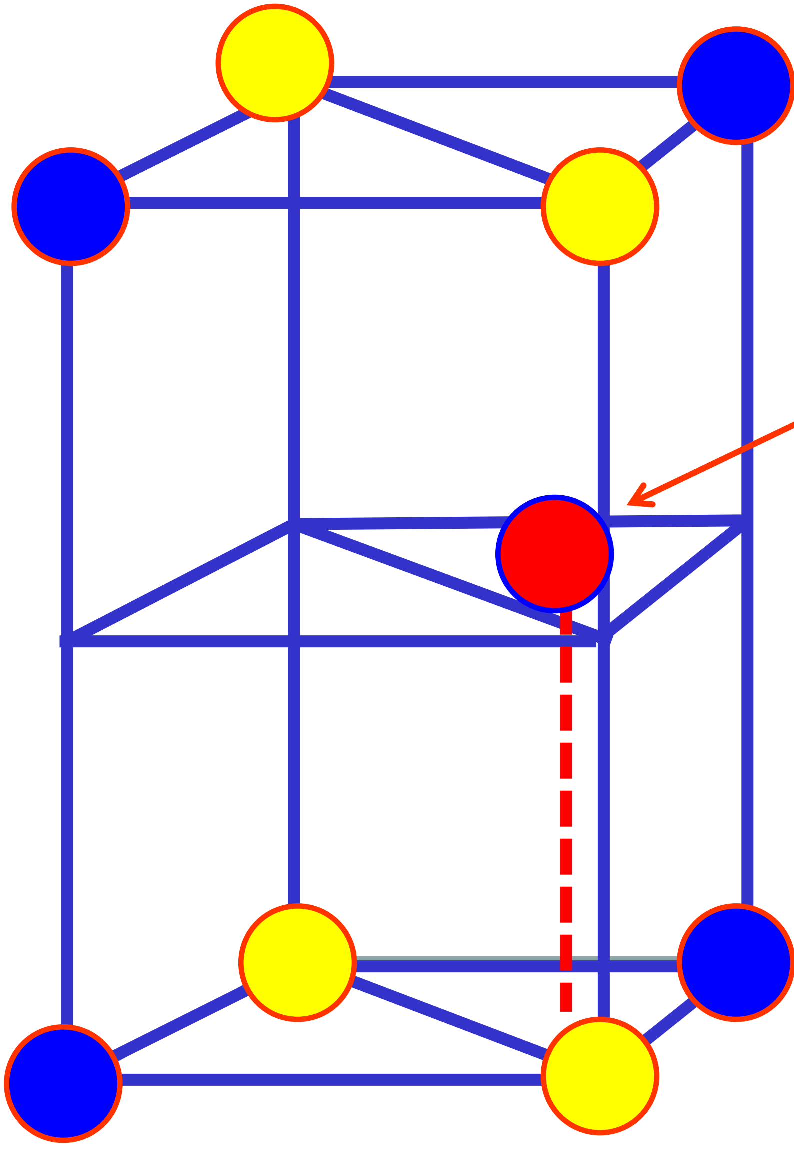
L'atome interne,

(1/3, 2/3, 1/2)

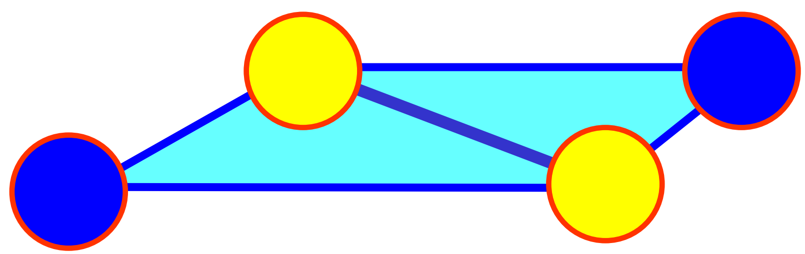
pseudo maille hexagonale

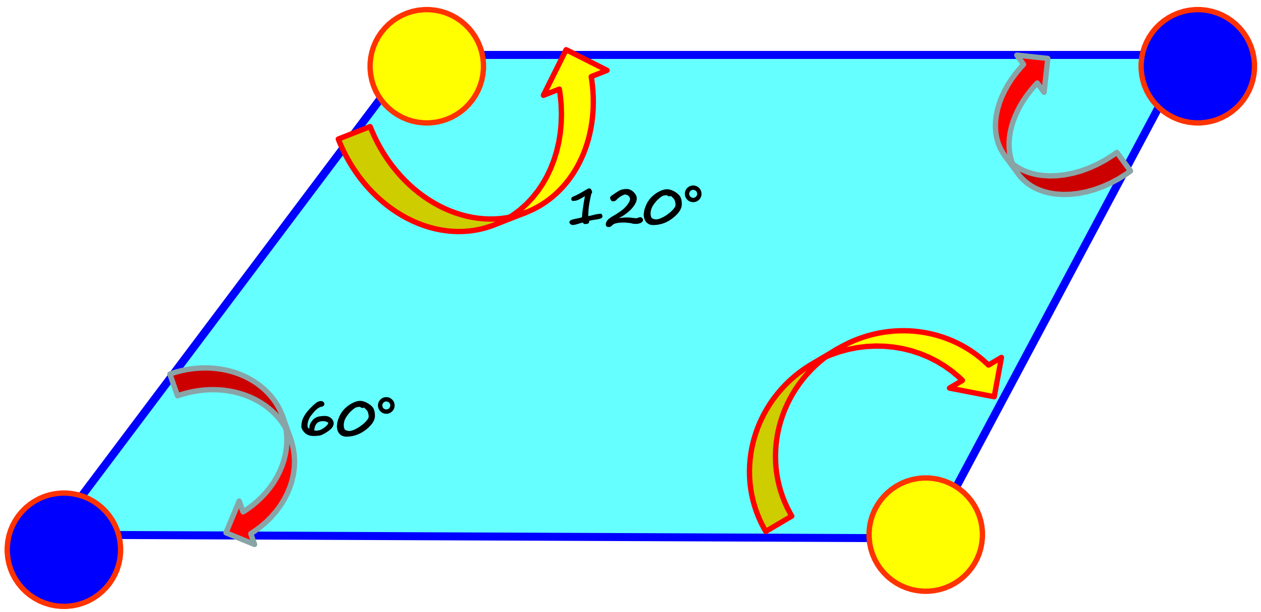


pseudo maille hexagonale

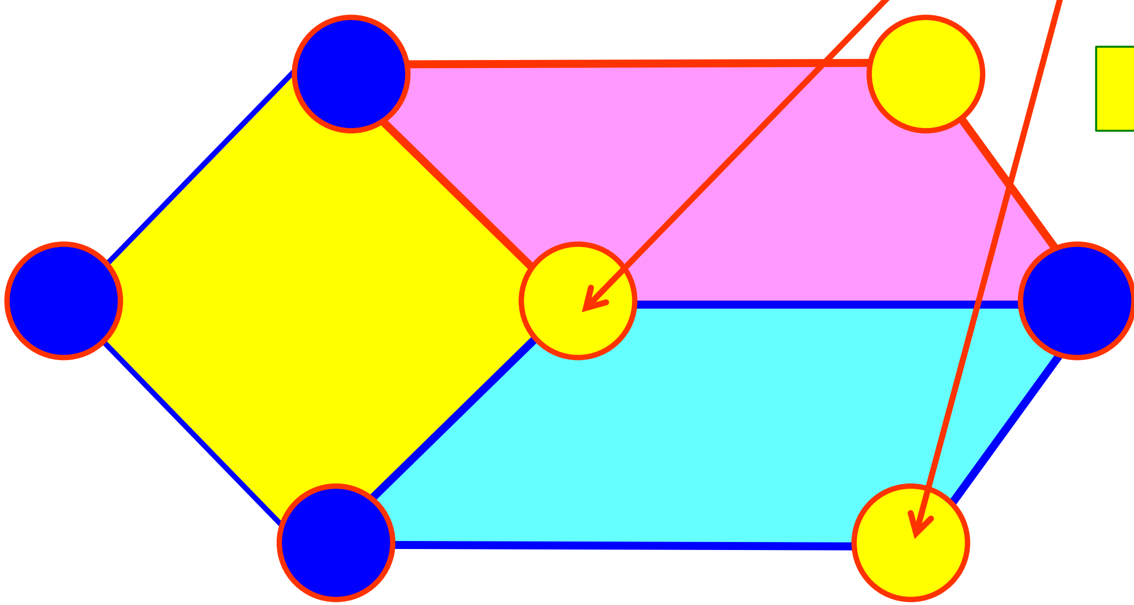


L'atome interne rouge appartient
à 1 pseudo maille




120°
60°

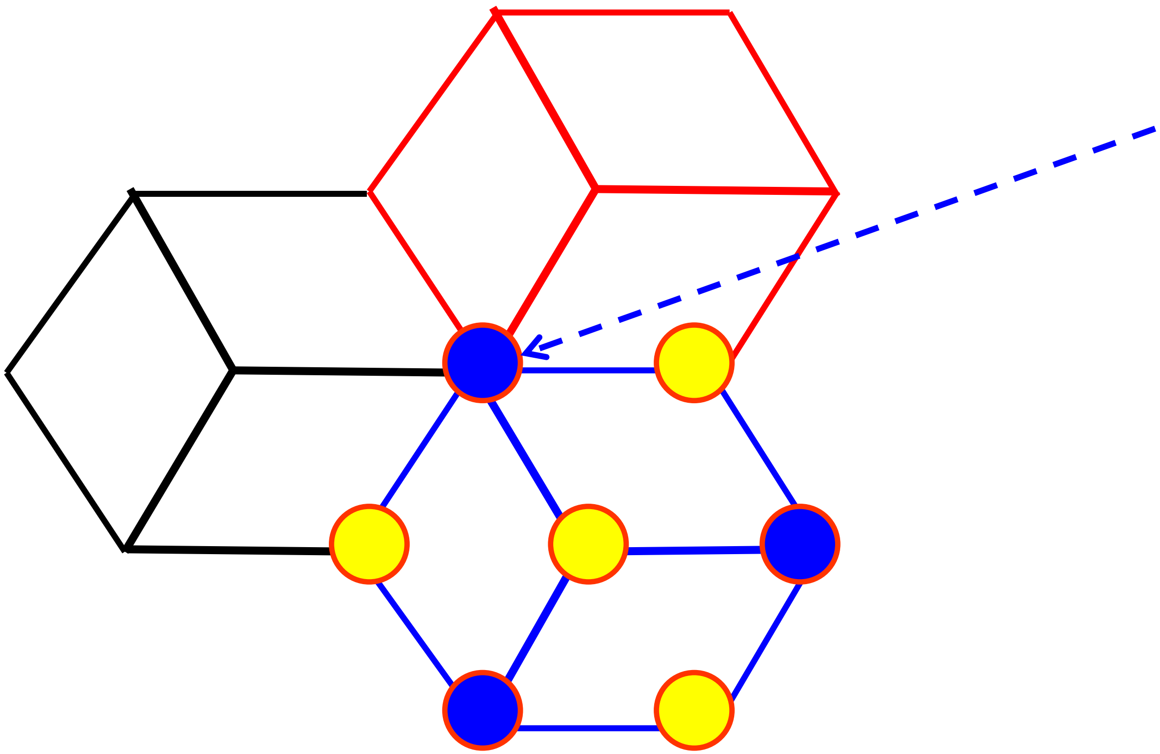
pseudo maille hexagonale



Ces sommets jaunes (120°C) appartiennent à 6 pseudo mailles
3 en bas + 3 en haut

Donc 4 x 1/6

pseudo maille hexagonale

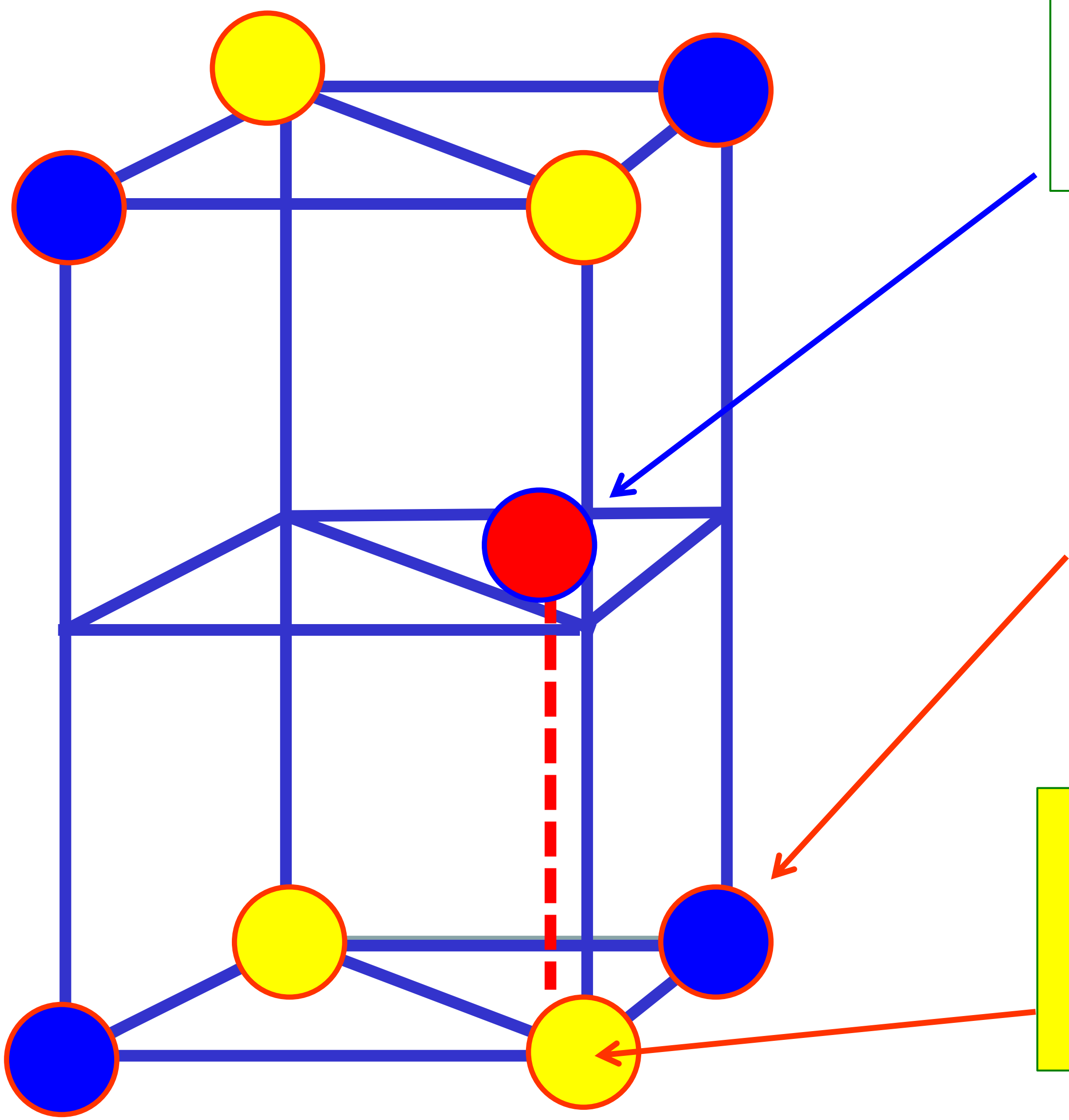


Ces sommets bleus (60°C) appartiennent à 12 pseudo mailles

6 en bas + 6 en haut

Donc 4 x 1/12

pseudo maille hexagonale



L'atome interne rouge appartient à 1 pseudo maille

Donc 1 x 1

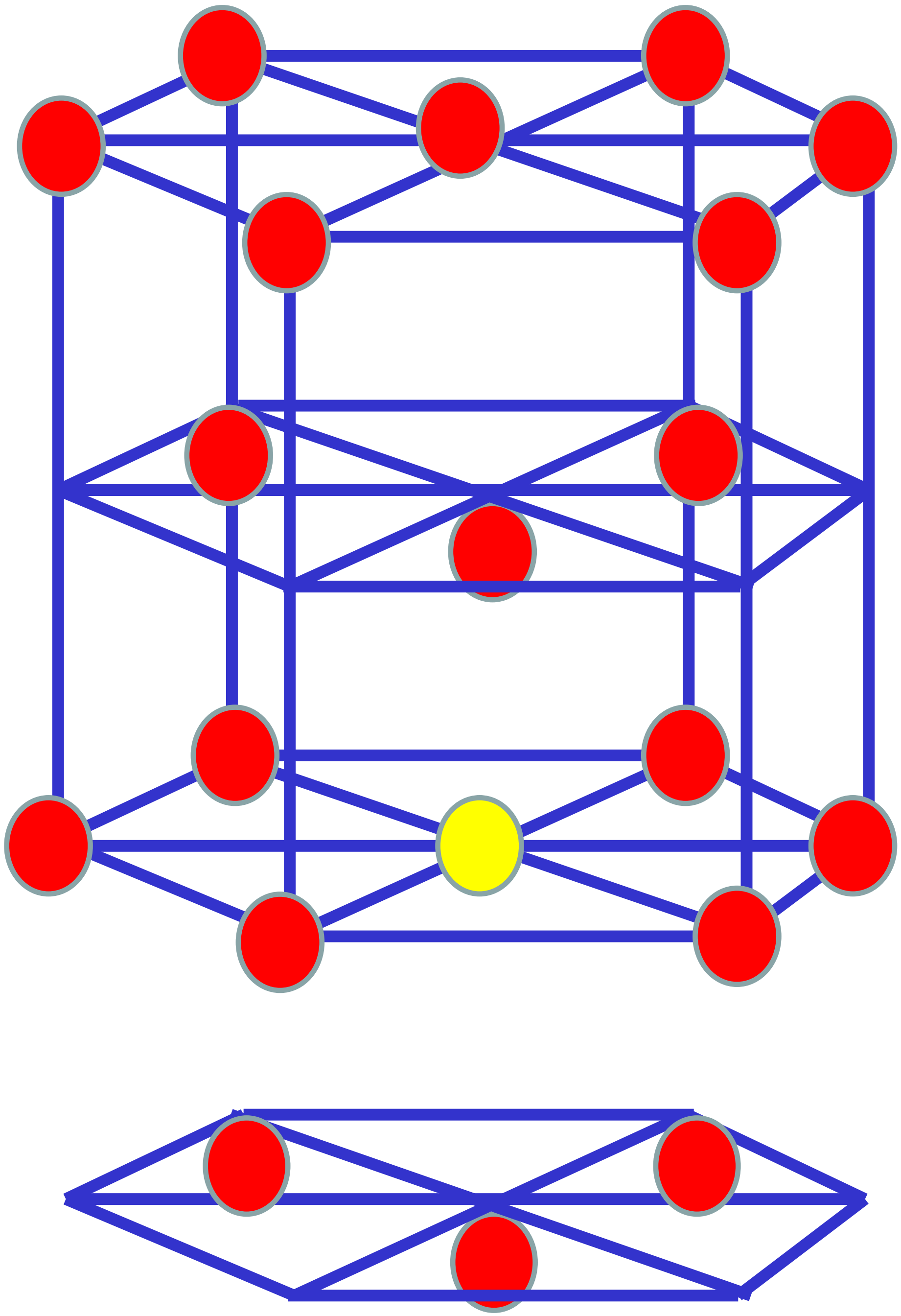
4 atomes aux sommets bleus (60°C) appartiennent à 12 pseudo mailles

Donc 4 x 1/12

4 atomes aux sommets jaunes (120°C) appartiennent à 6 pseudo mailles

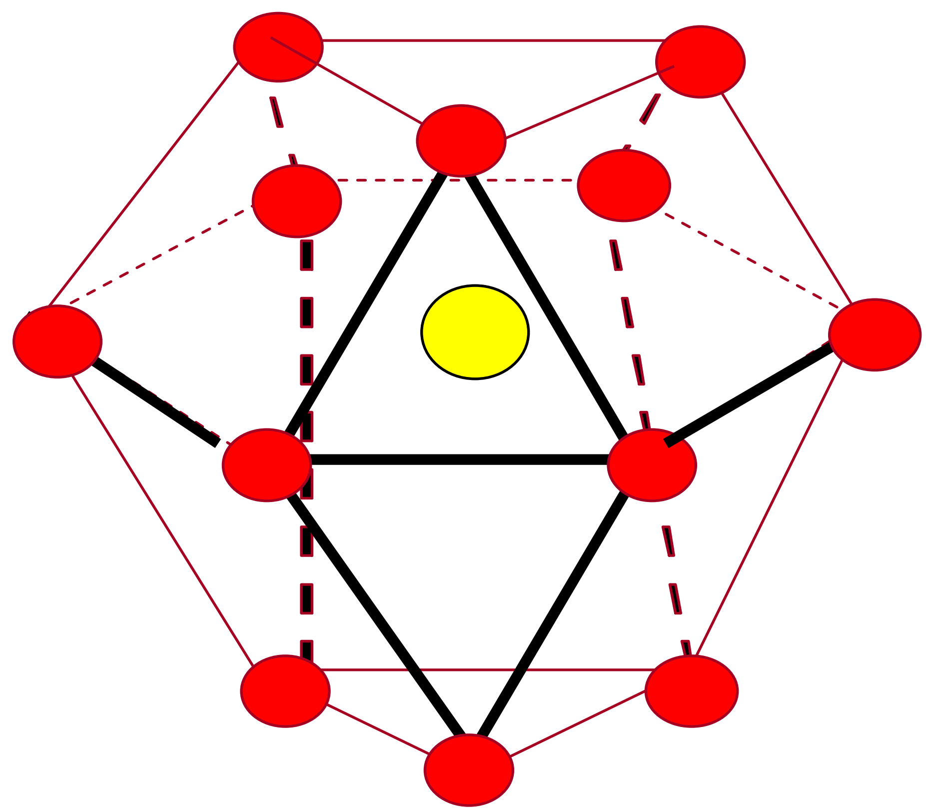
Donc 4 x 1/6

Au total : $n = 1 + (4 \times 1/6) + (4 \times 1/12) = 2$

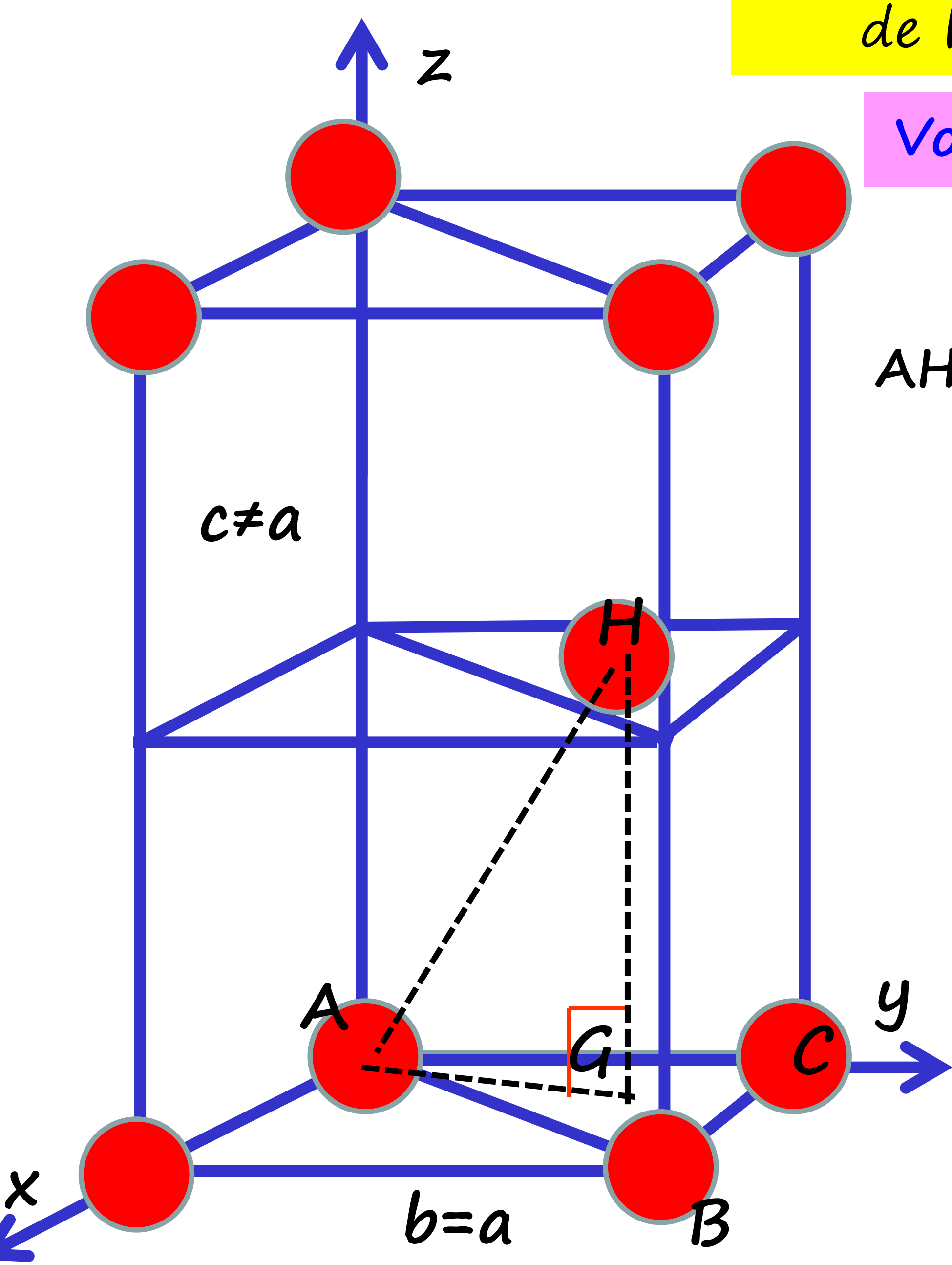


chaque atome a
12 voisins tangents situés
à la distance *a*

Coord (Hex. Comp.) = 12



Pseudo maille HC



Les coord. réd. des atomes de la ps.maille hex.	(0, 0, 0) (1/3, 2/3, ½)

Volume $_{\text{ps. maille hex.}}$ = $a^2 . c . \sin 120°$

Exprimer $c = f(a)$

$AH = BH = CH = AB = BC = CA = a$

Le point G est le centre de gravité du triangle équilatéral ABC

$AG = a / \sqrt{3} = a\sqrt{3} / 3$

Le triangle est rectangle AGH au point G

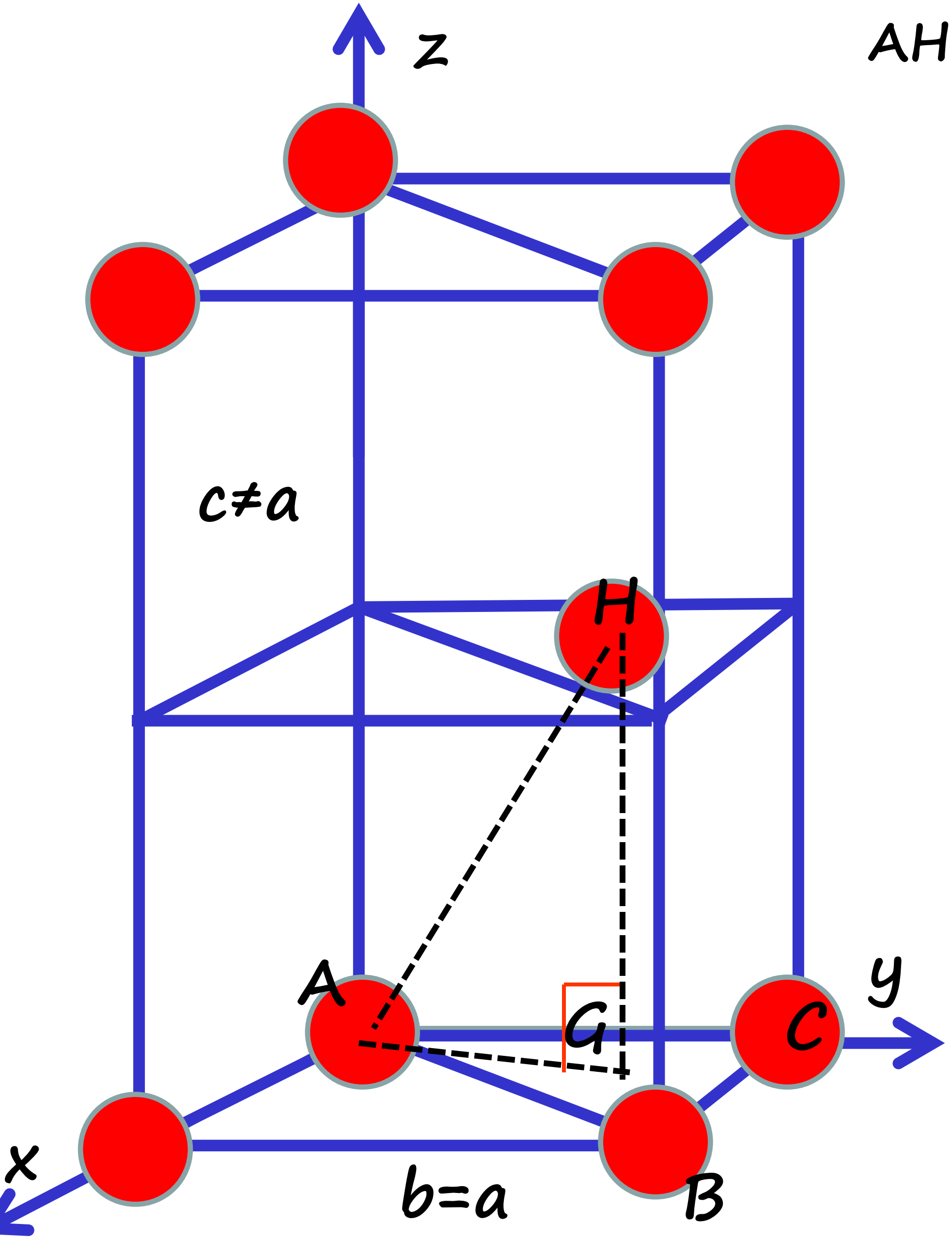
$AG^2 + GH^2 = AH^2$

or $GH = c/2$

$a^2/3 + c^2/4 = a^2$

$$c = \sqrt{\frac{8}{3}} \cdot a$$

Pseudo maille HC



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or $GH = c/2$

$a^2/3 + c^2/4 = a^2$

$$c = \sqrt{\frac{8}{3}} \cdot a$$

Le rapport c/a de la maille hex. Comp. est

une cte = $c/a = \sqrt{8/3} = 1{,}633$, qui permet de savoir

Si l'empilement est compact ou non.

Compacité ou taux de remplissage τ :

Compacité $$\tau = \frac{n \,.\, \text{Volume(1atome)}}{\text{Volume(1 maille)}}$$

n : nombre d'atomes par maille

Compacité ou taux de remplissage τ :

Compacité $\tau = \dfrac{n \,.\, \text{Volume(1atome)}}{\text{Volume(1 maille)}}$

Avec
n atomes/maille

Pseudo maille HC n = 2 atomes/ pseudo maille

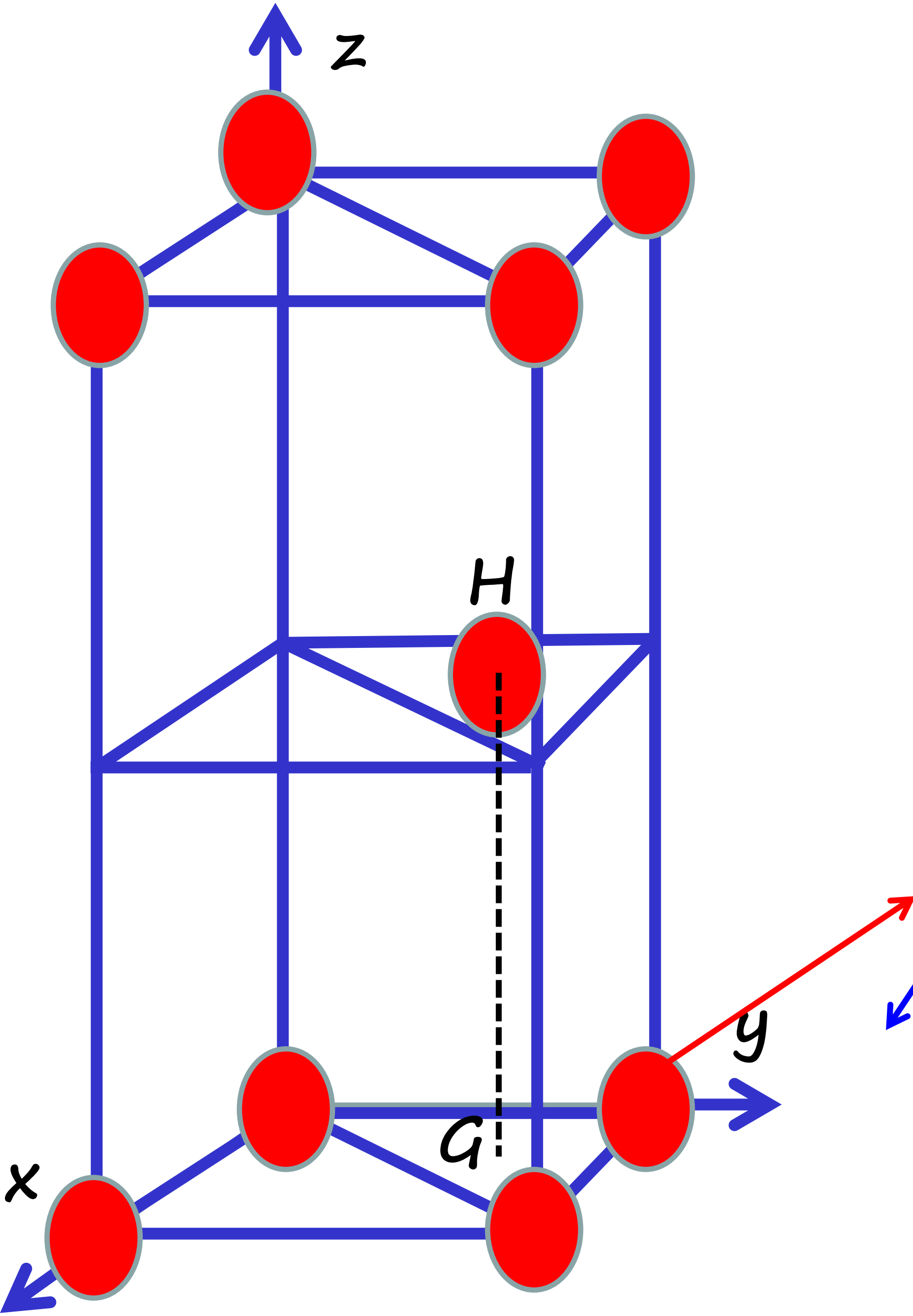
Relation de tangence : **2R = a**

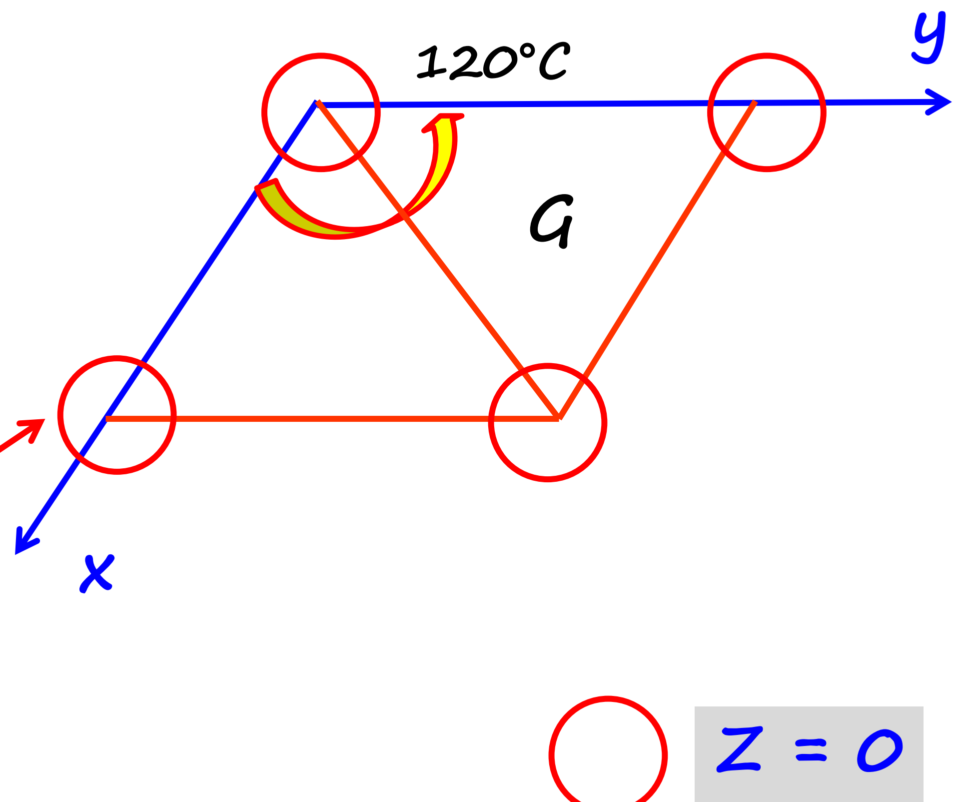
D'où la relation :

$$\tau = \frac{2 \,.\, (4/3)\, \pi\, R^3}{a^2 .\, c \,.\, \sin 120°} = \frac{2 \,.\, (4/3)\, \pi\, (a/2)^3}{a^2 .\, c \,.\, \sin 120°} = 0{,}74$$

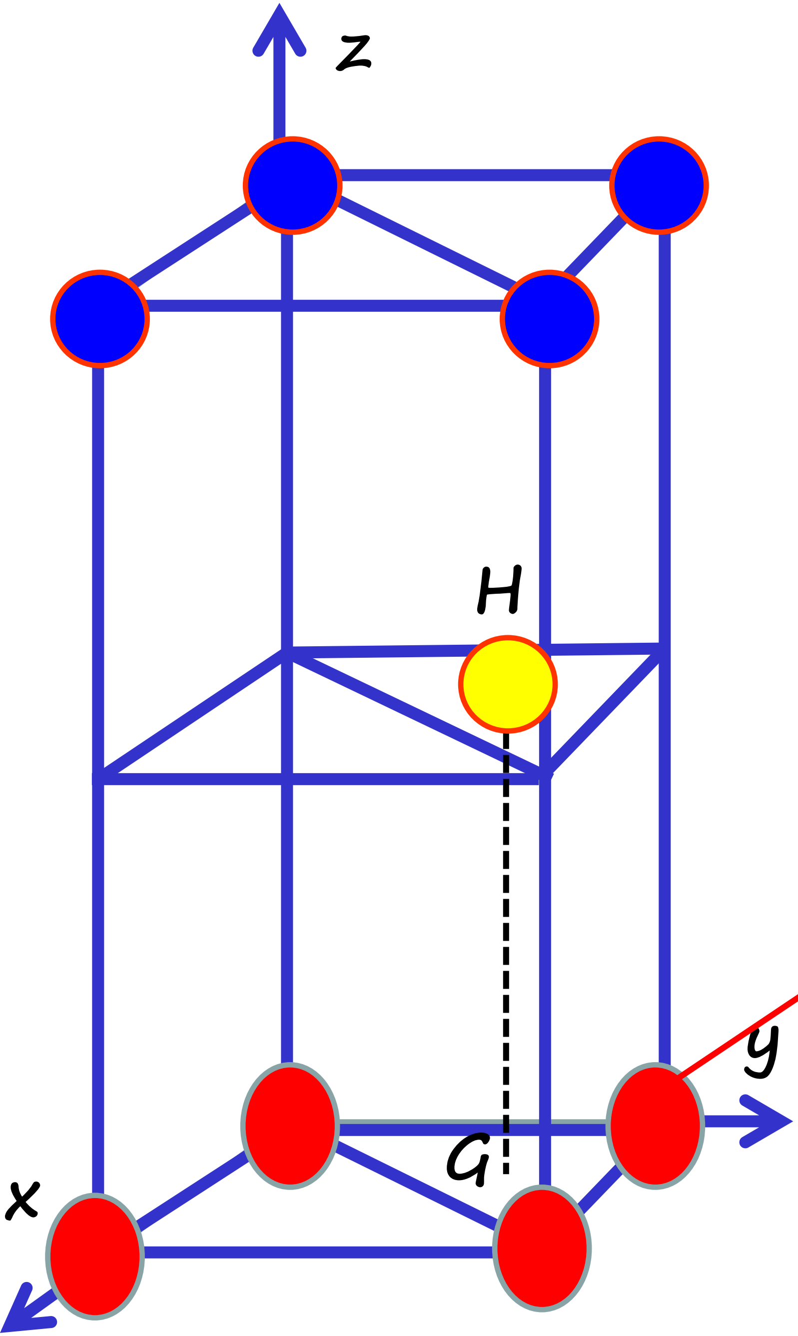
$$c = \sqrt{\frac{8}{3}} \,.\, a$$

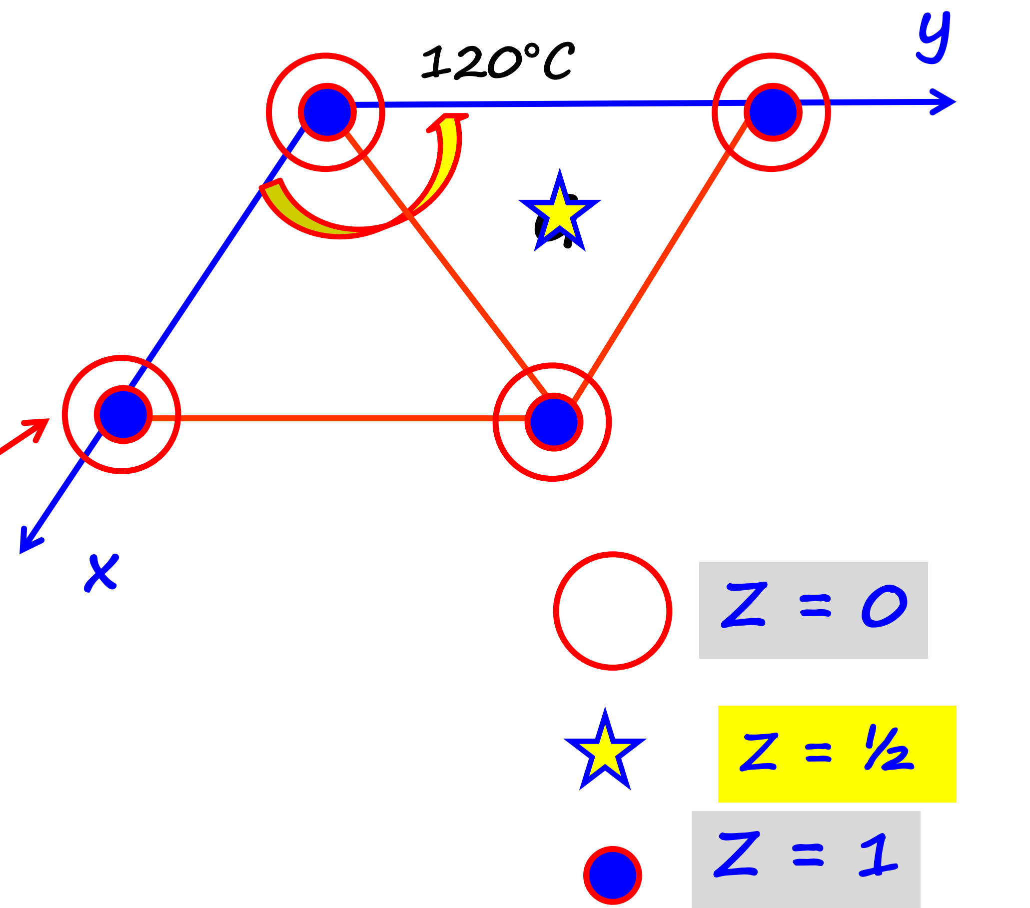
Pseudo maille HC





Projection de la Pseudo maille HC sur le plan (xOy)





Projection de la Pseudo maille HC sur le plan (xOy)