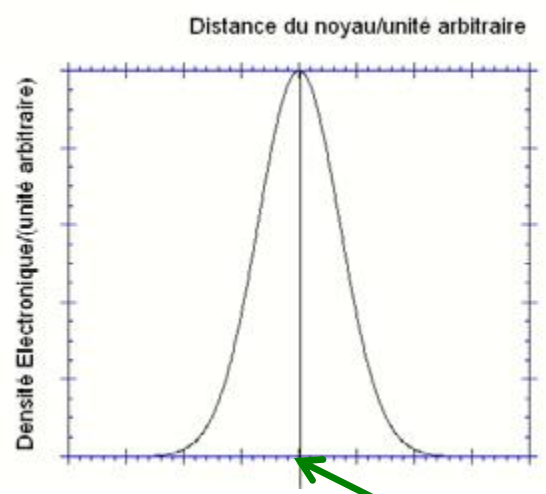
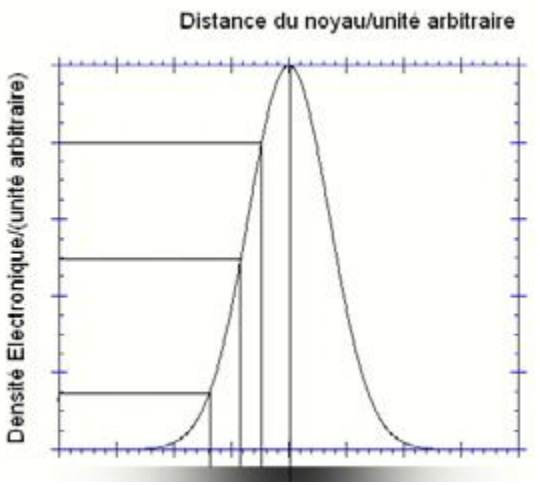
Représentation de la densité électronique autour d'un noyau

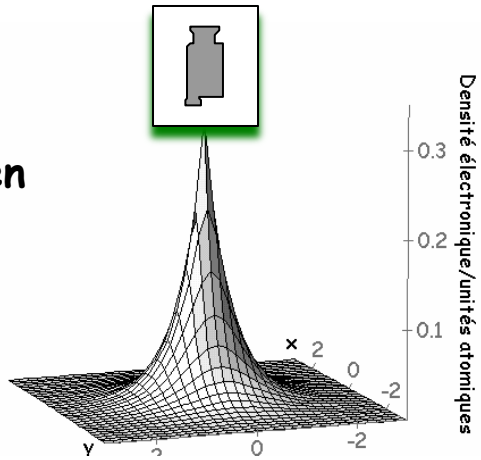


Densité électronique

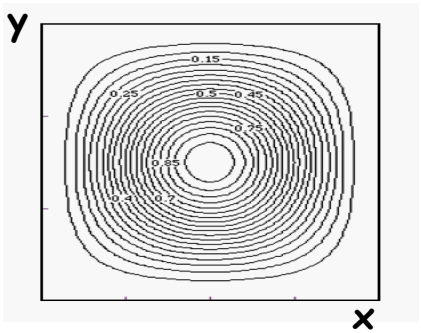


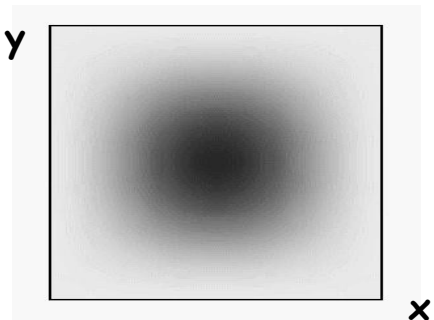
La d. e. peut être représentée par une gamme de gris continue allant du blanc au noir, le noir étant associé à la plus grande valeur de la densité électronique.

une représentation en «perspective»

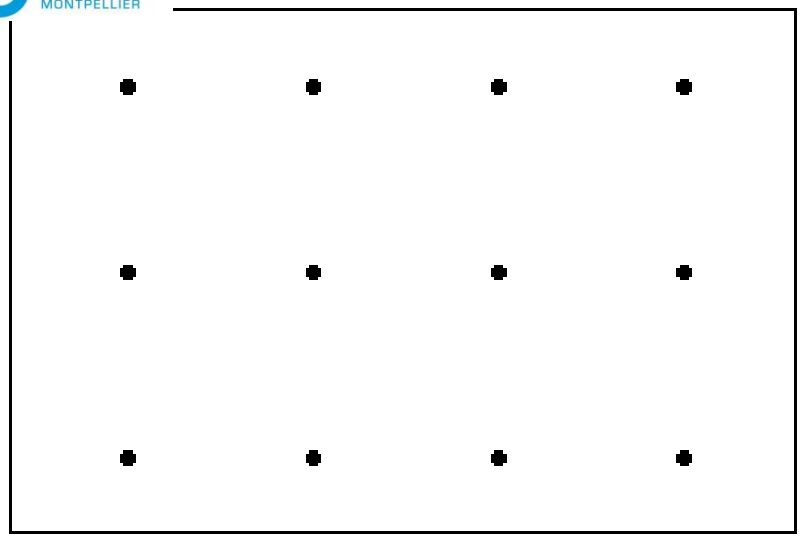


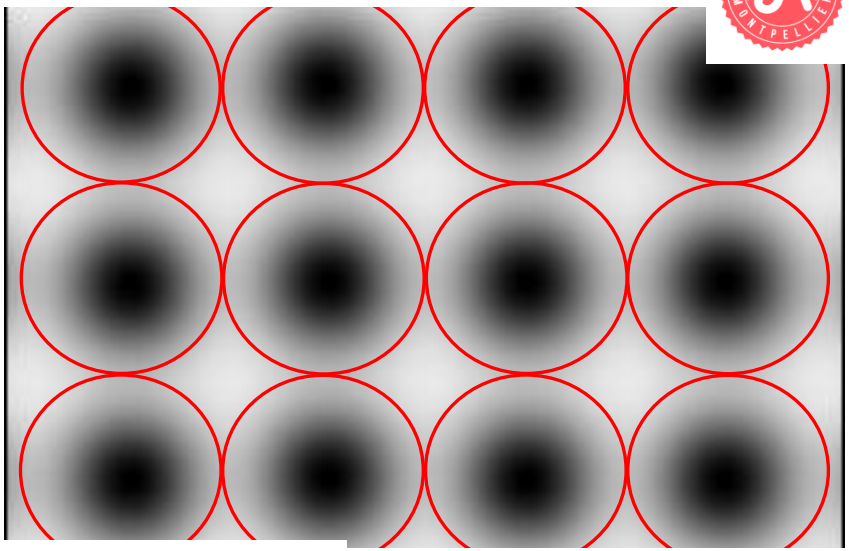
Densité électronique

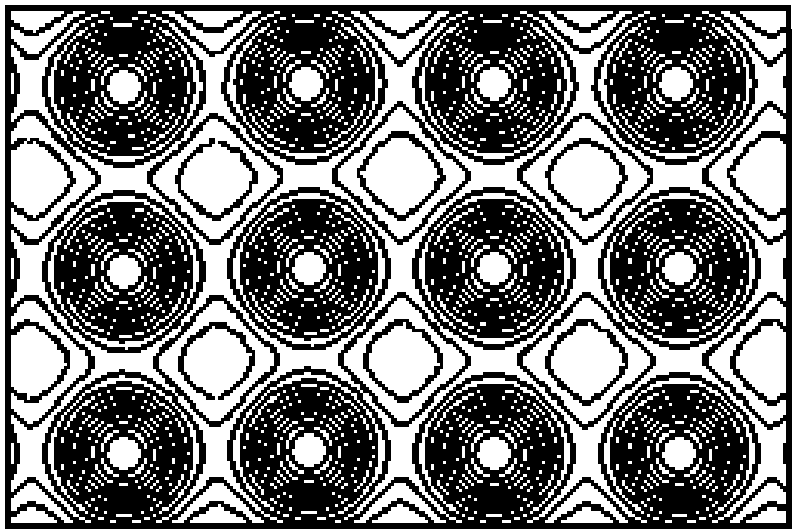


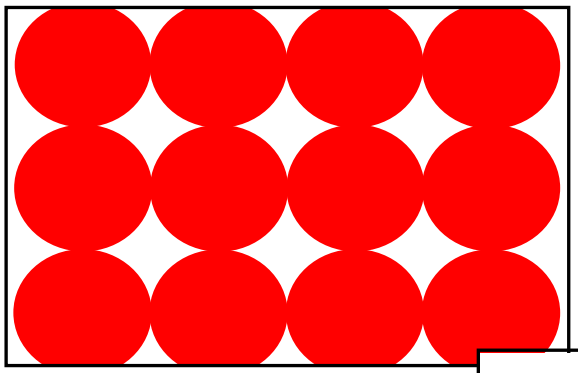


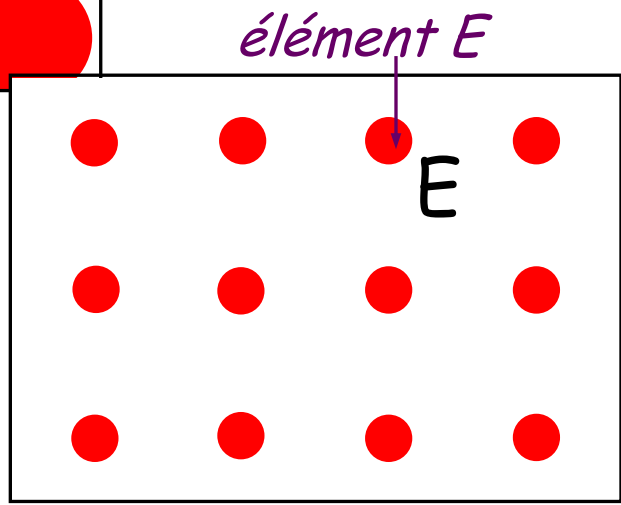
Une autre façon de représenter cette répartition de la densité électronique est d'utiliser la méthode de «dégradé de gris» ou celle des pointillés.





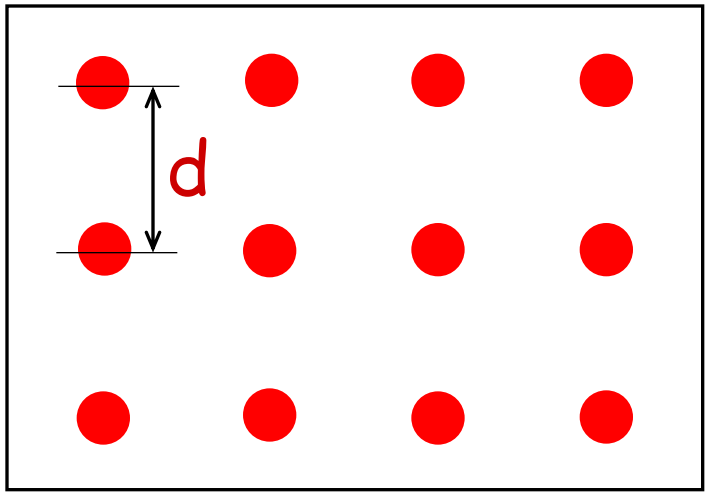




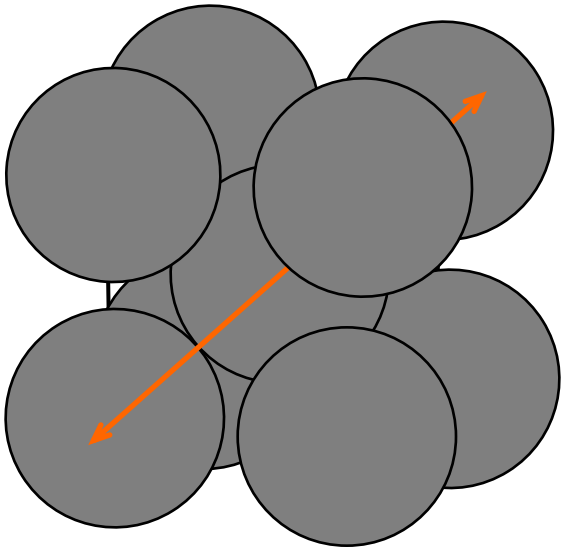

élément E
E

Rayon atomique

Cristal bidimensionnel :

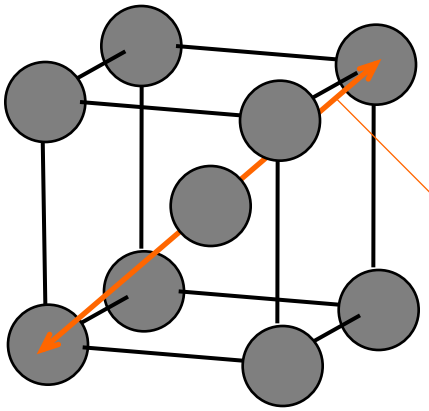


$$r_{at} = \frac{1}{2} \cdot d$$



Système cubique centré (Na, K)

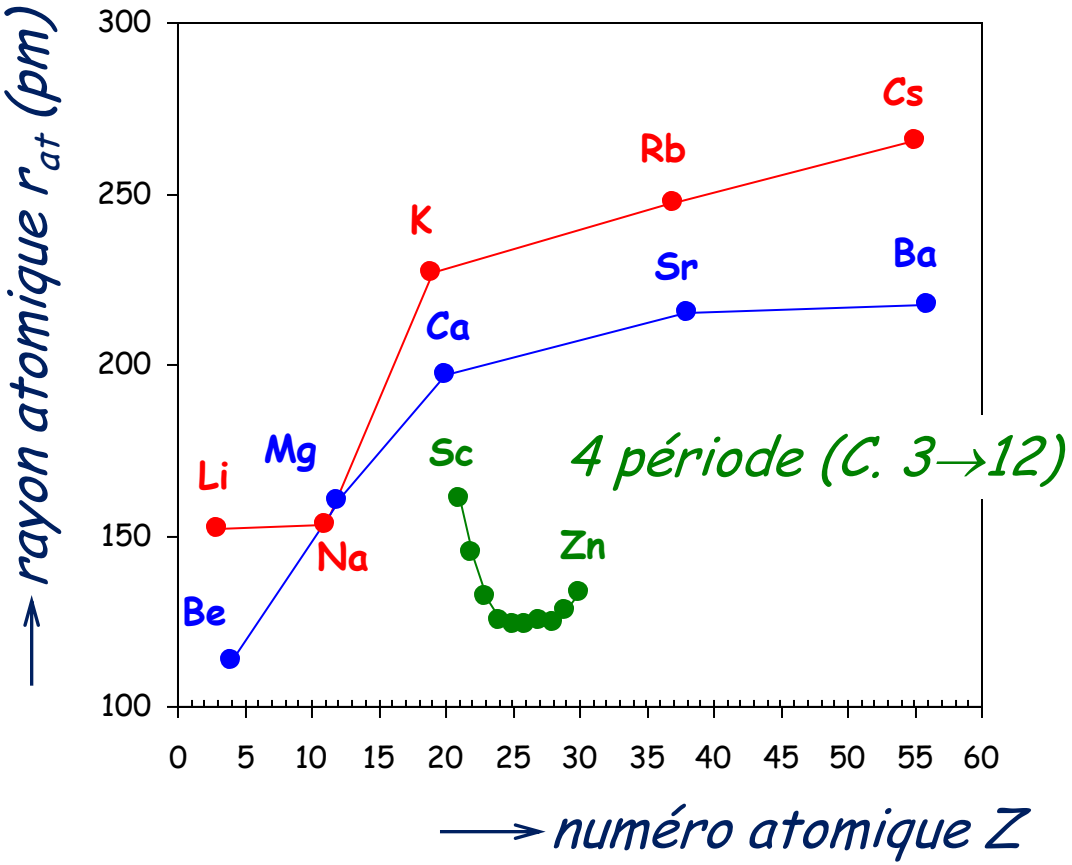
Cristal tridimensionnel :



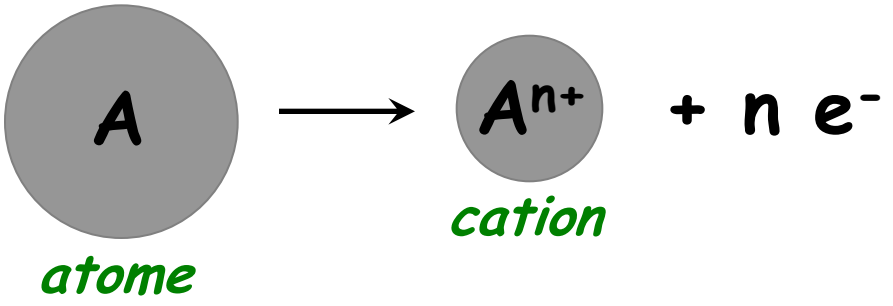
$$r_{at} = \frac{1}{4} \cdot d$$

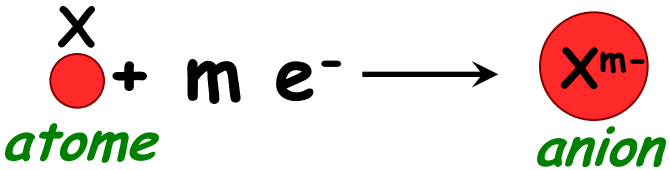
Evolution des rayons atomiques :

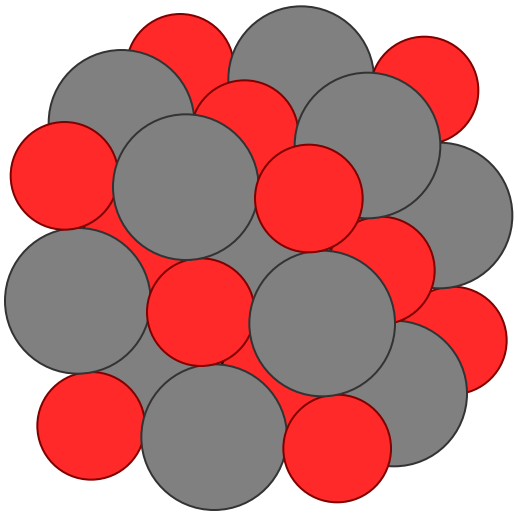
$1\ pm = 10^{-12}\ m = 10^{-3}\ nm$

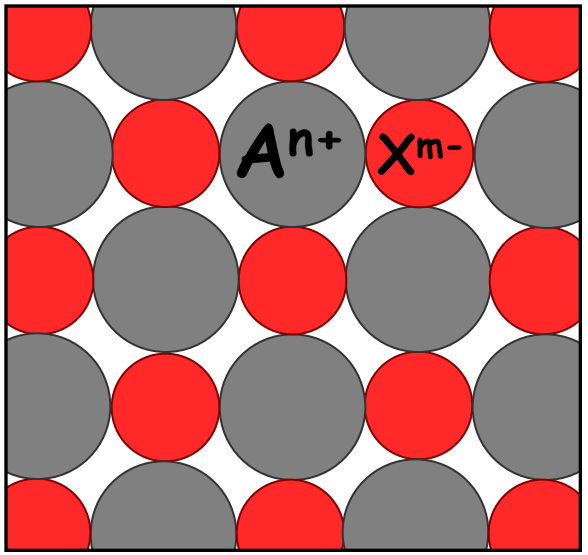


$100\ pm < r_{at} < 300\ pm$



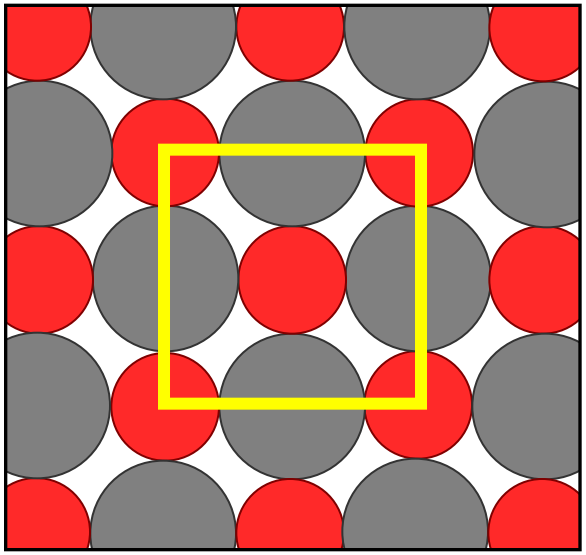


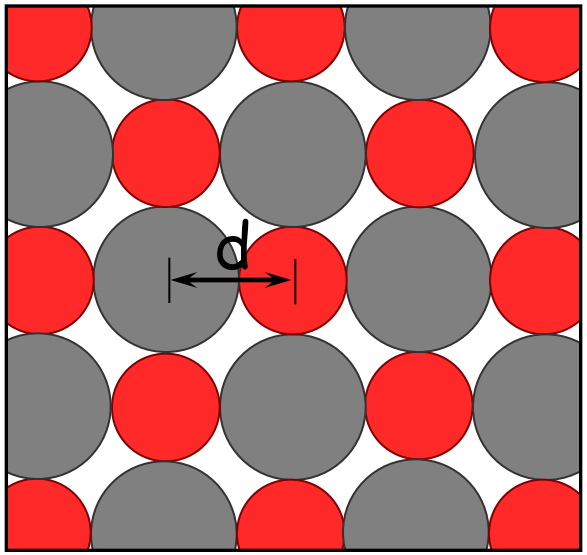




Modèles compacts

$(A^{n+})_p(X^{m-})_q$



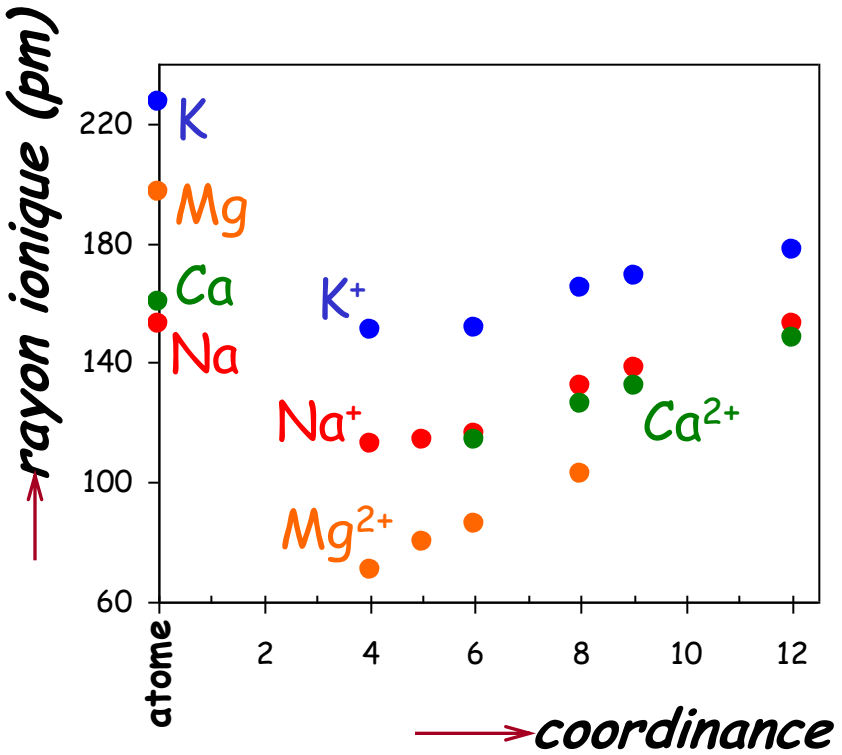


Condition d'électroneutralité

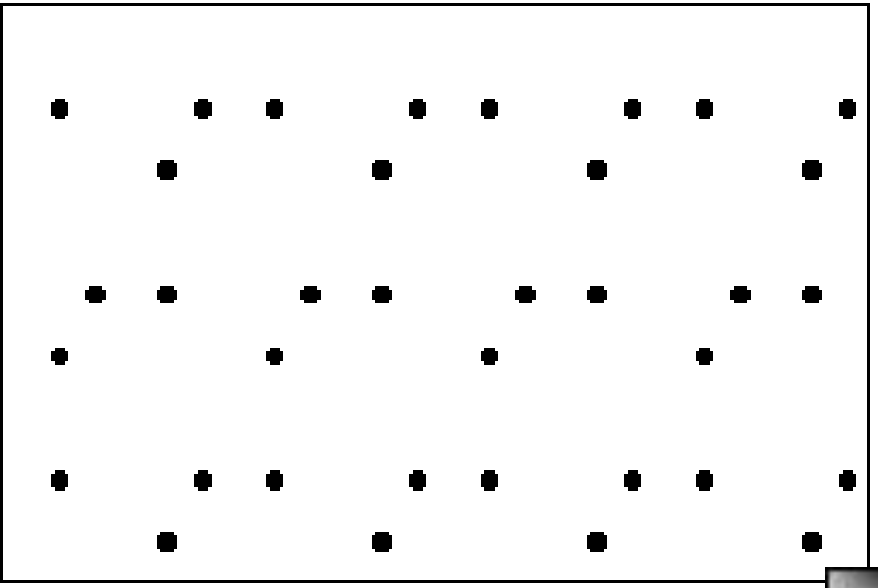
$$n \cdot p = m \cdot q$$

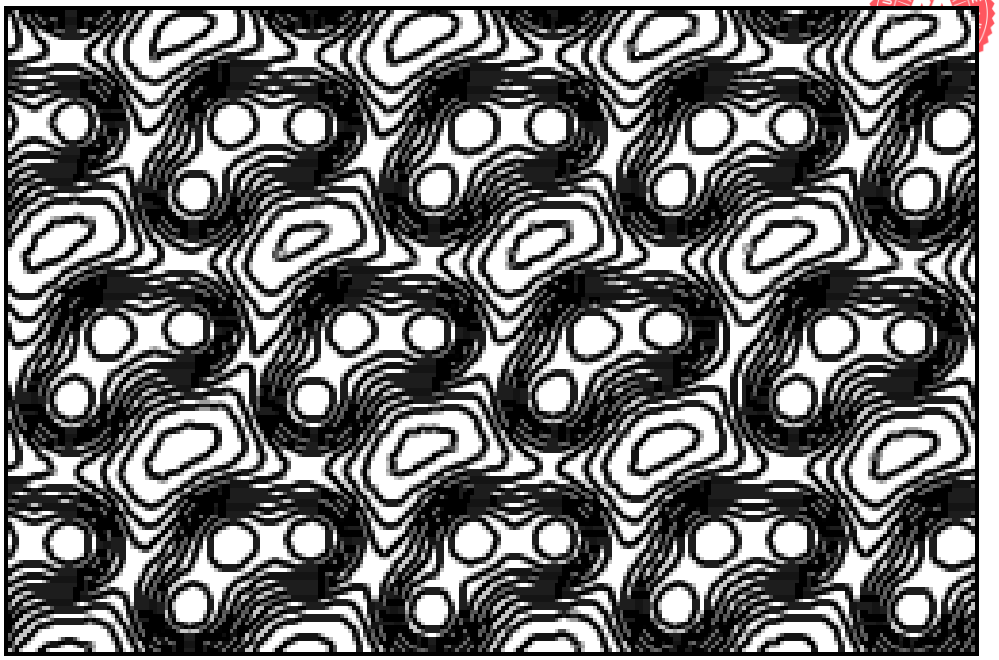
Maille cristalline :

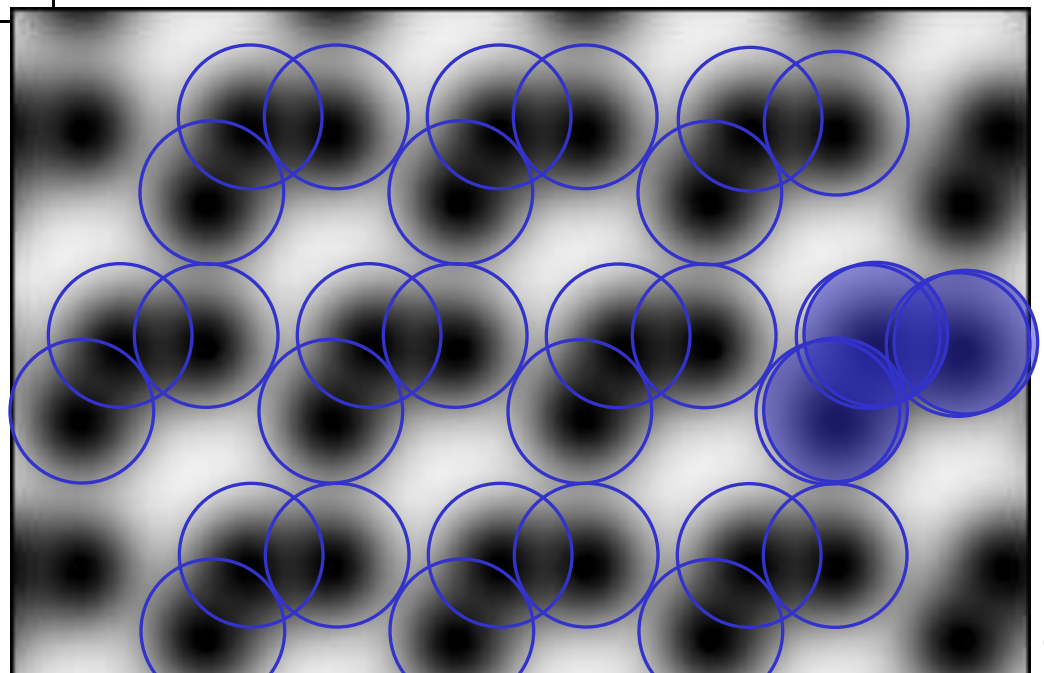
$\{A^{n+} : 1 ; X^{m-} : 1\}$



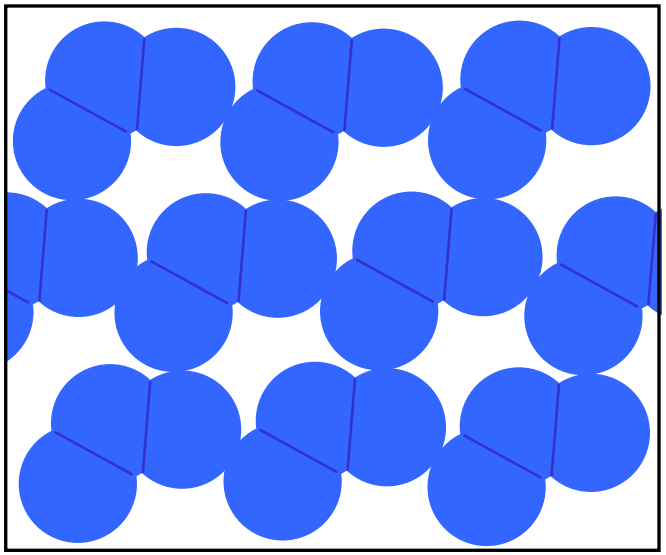
Agrégats d'atomes :







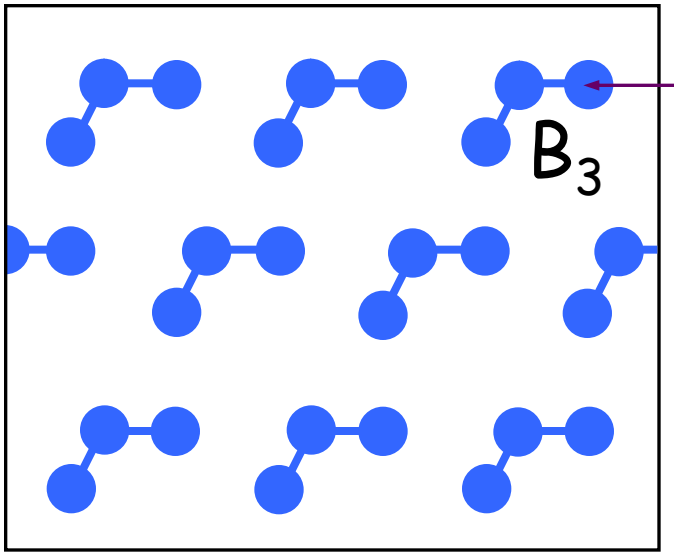
Représentation compacte : les volumes rigides formés par des sphères qui «s'interpénètrent»



Volumes rigides centrés autours de plusieurs noyaux

→ entités moléculaires

Modèle éclaté :

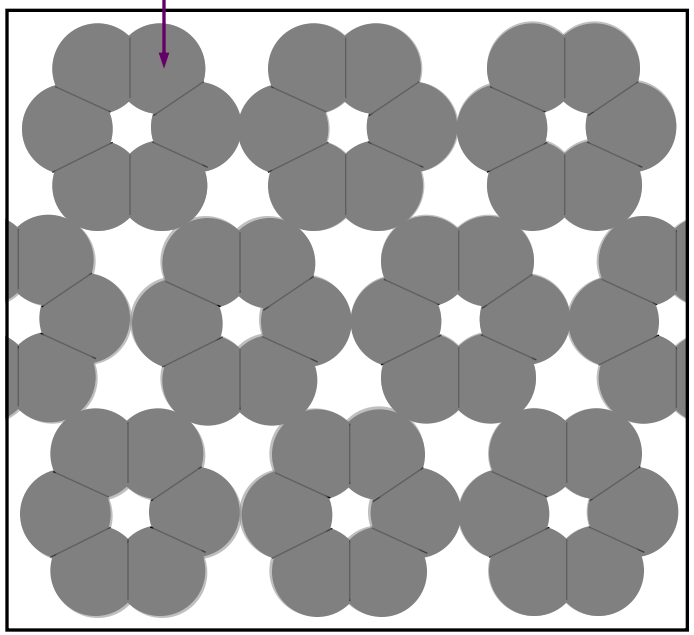


Molécules discrètes :

formées par un nombre fini d'atomes

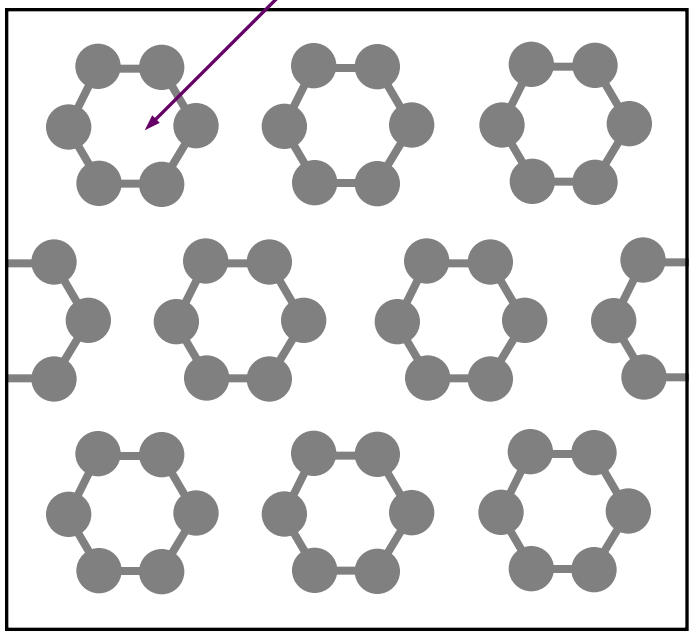
(on les caractérise par leur formule chimique)

élément C



Modèle compact

entité C_6



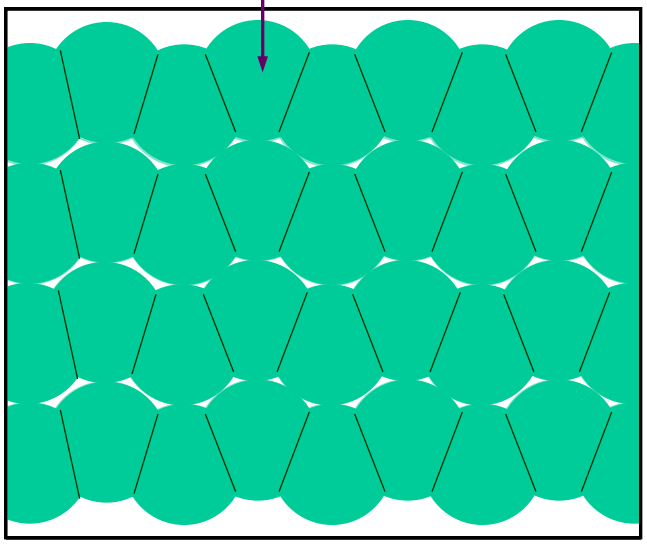
Modèle éclaté

Formule de la substance : C_6

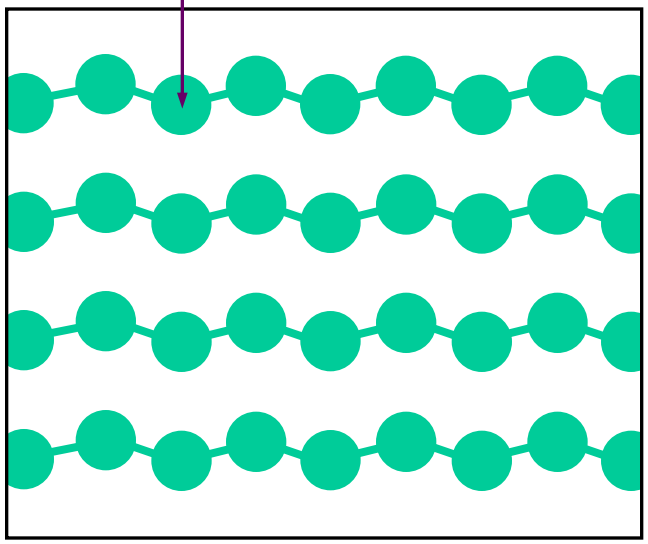
Molécules polymères :

formées par un nombre quasiment infini d'atomes

élément D



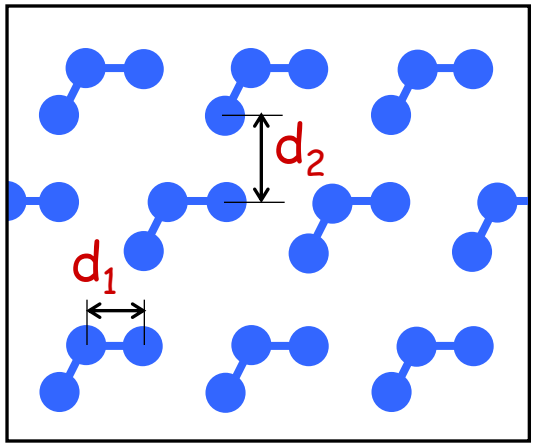
polymère monodimensionnel



Dans un corps simple cristallisé :

Rayon covalent : il est égal à la demi distance entre deux atomes liés entre eux dans une entité moléculaire (molécule)

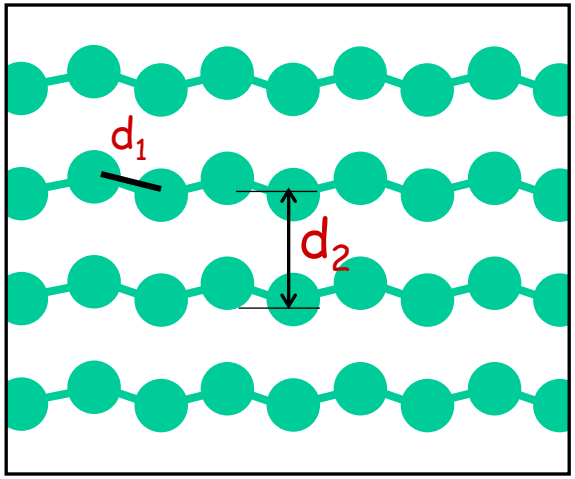
Rayon de van der Waals : il est égal à la demi distance entre deux atomes tangents appartenant à deux molécules différentes



$$r_{cov} = \frac{1}{2} d_1$$

$$r_{vdW} = \frac{1}{2} d_2$$

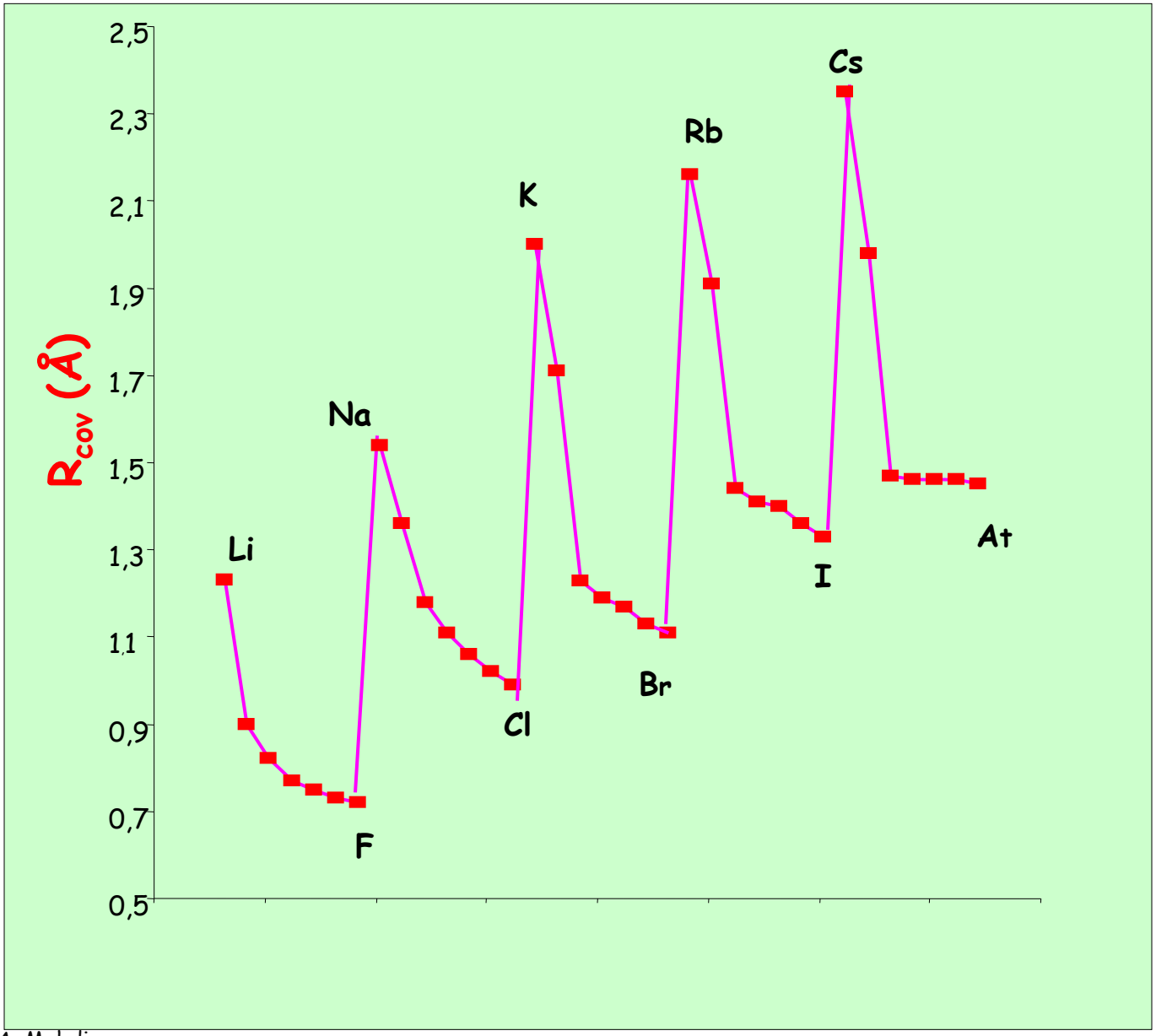
$$r_{cov} < r_{vdW}$$



Rayons covalent et de van der Waals des atomes :

élément	r_{vdW} (pm)	r_{cov} (pm)	*élément*	r_{vdW} (pm)	r_{cov} (pm)
H	120	37	F	147	71
C	170	77	Cl	175	99
N	155	75	P	180	106
O	152	73	S	180	102

Rayons Covalent des éléments s et p

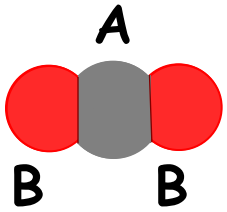


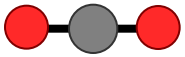
Rayons Cov. (en Å)

Li	1,23	Na	1,54
Be	0,90	Mg	1,36
B	0,82	Al	1,18
C	0,77	Si	1,11
N	0,75	P	1,06
O	0,73	S	1,02
F	0,72	Cl	0,99

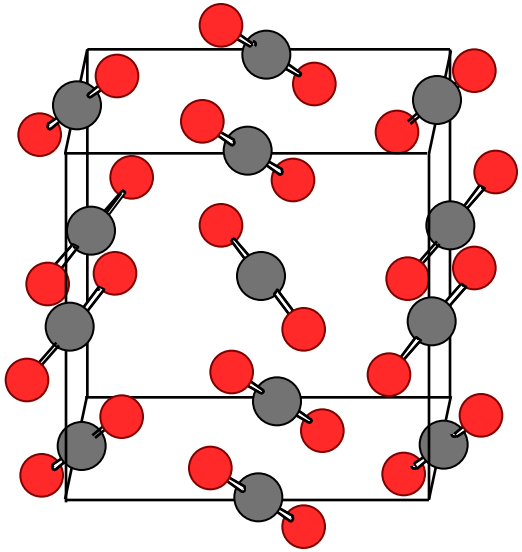
K	2,03	Rb	2,16
Ca	1,74	Sr	1,91
Ga	1,26	In	1,44
Ge	1,22	Sn	1,41
As	1,20	Sb	1,40
Se	1,16	Te	1,36
Br	1,14	I	1,33

Cs	2,35
Ba	1,98
Tl	1,47
Pb	1,46
Bi	1,46
Po	1,46
At	1,45



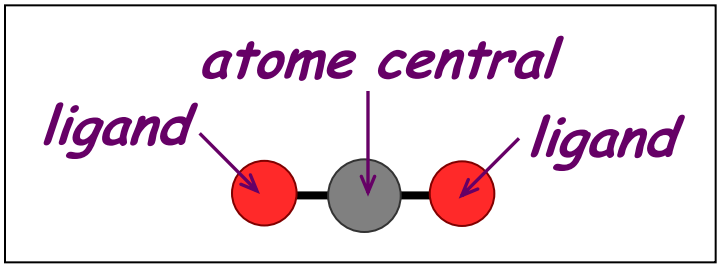


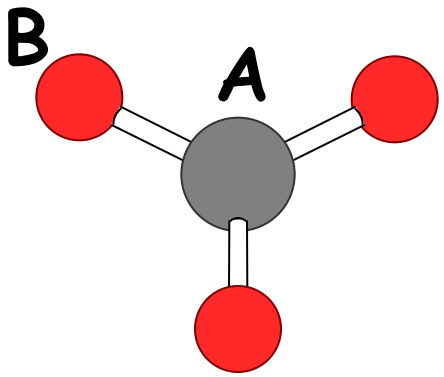
molécule AB_2

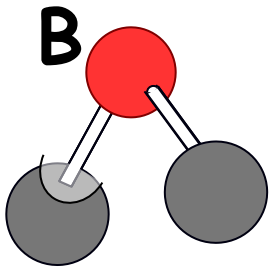


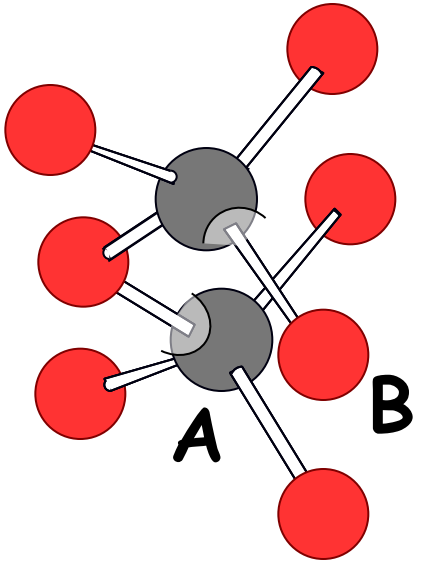
cristal de AB_2

Formule de la substance : AB_2

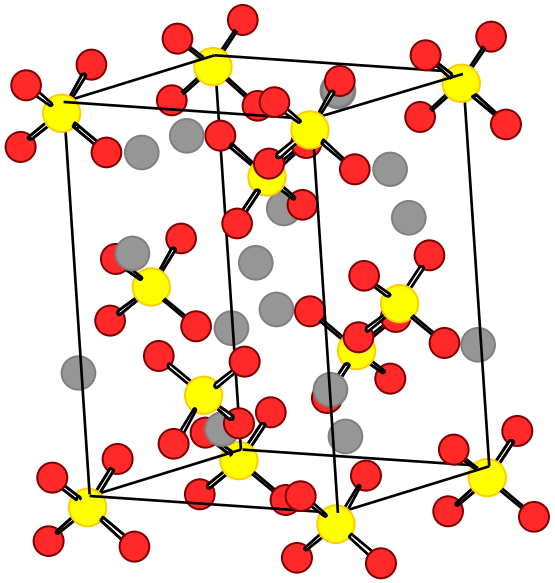


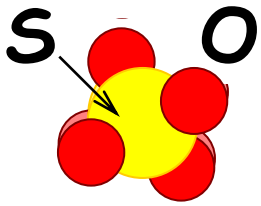






Entités moléculaires chargées (ion moléculaires):



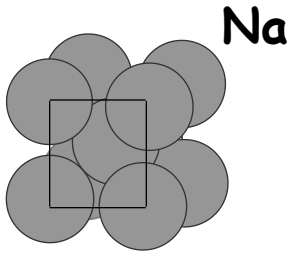


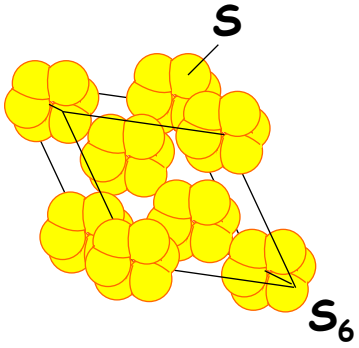
anion moléculaire SO_4^{2-}

cristal de Na_2SO_4

(corps simple)

Formule : Na

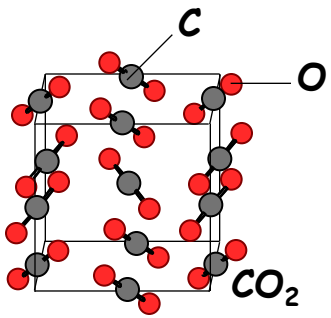


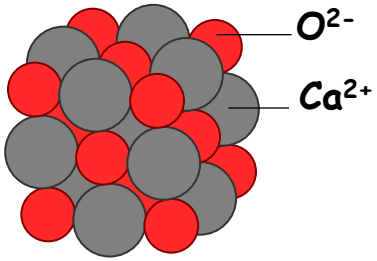


Formule : S_6

(corps composé)

Formule : CO_2



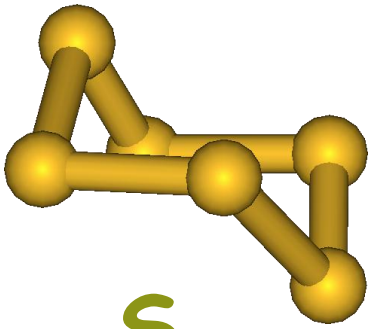


Formule : CaO

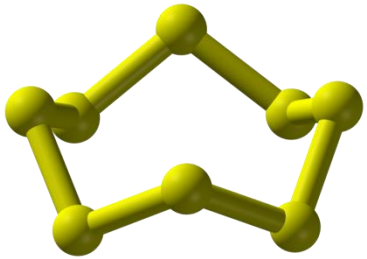
La chaux

$K_2S_2O_8$: $2\times K^+$ *et* $S_2O_8^{2-}$

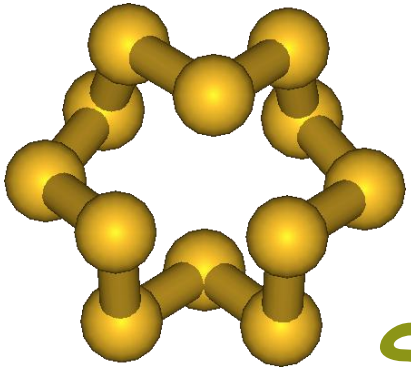
NH_4OH : NH_4^+ *et* OH^-



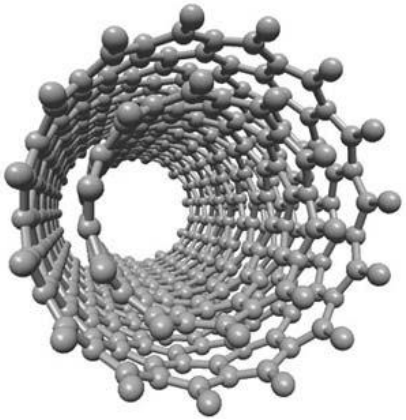
S_6

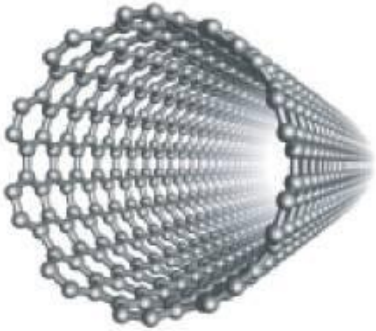


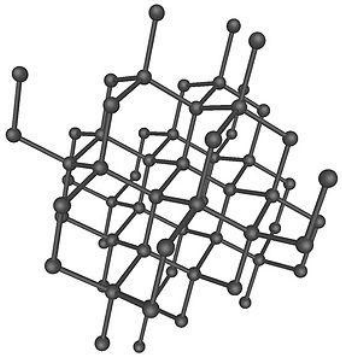
S_8

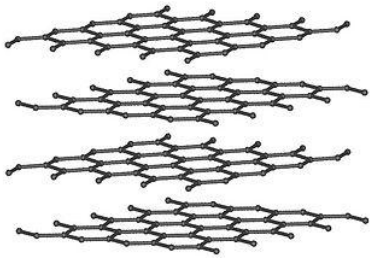


S_{12}



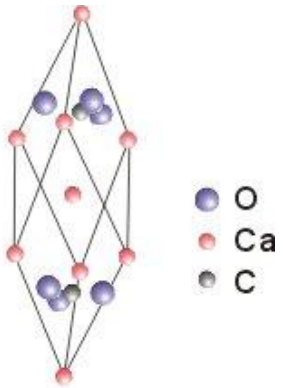


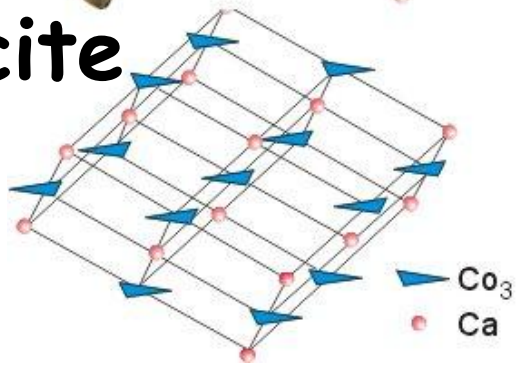




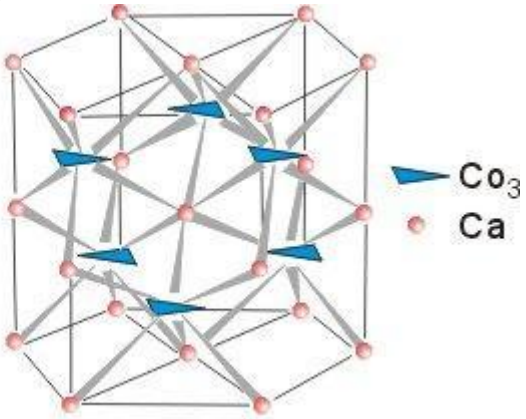
Polymorphisme du carbonate de calcium ($CaCO_3$)

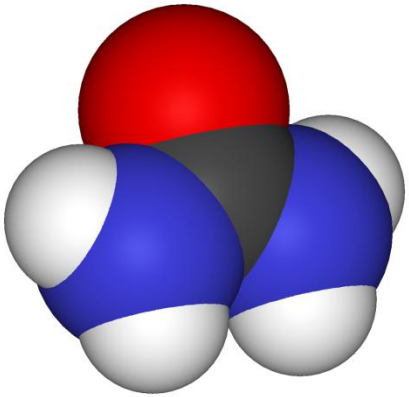
Calcite

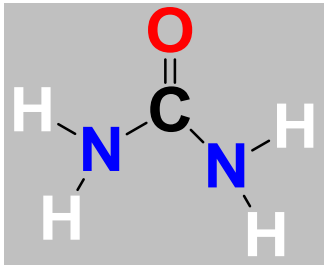




Aragonite







molécule d'urée CON_2H_4