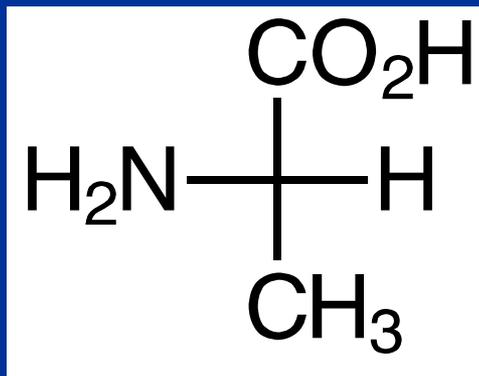
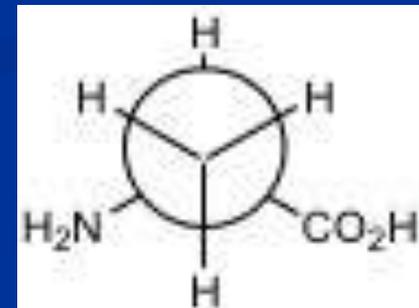
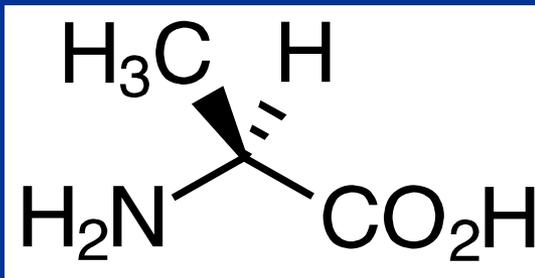
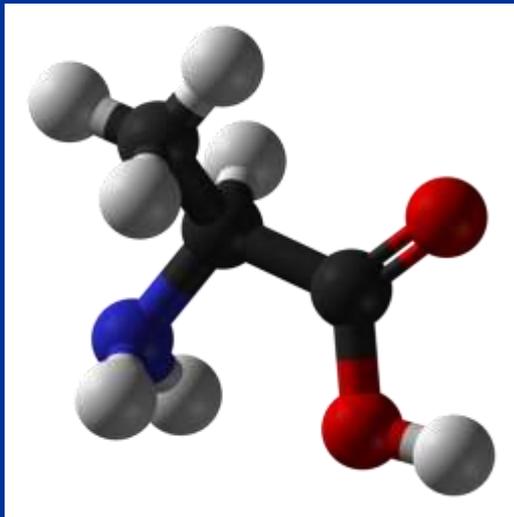


# CO 04

## Savoir représenter les molécules en 3D



# I – Les différents modes de représentation

## 1) La convention de Cram

### ■ Construire avec les modèles

- Méthane

- Ethane

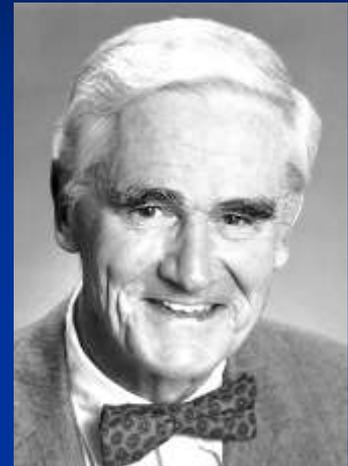
- Propan-1-ol

### ■ Les représenter avec la convention de Cram

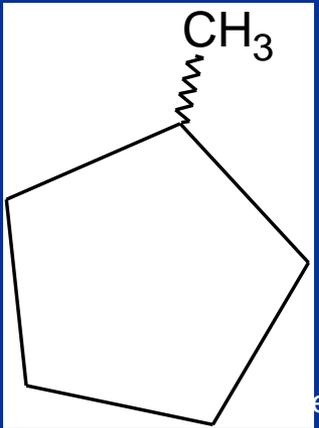
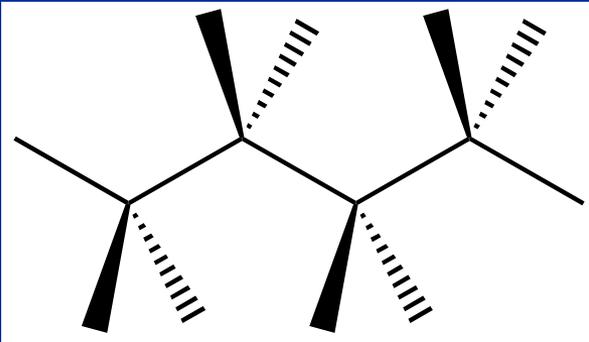
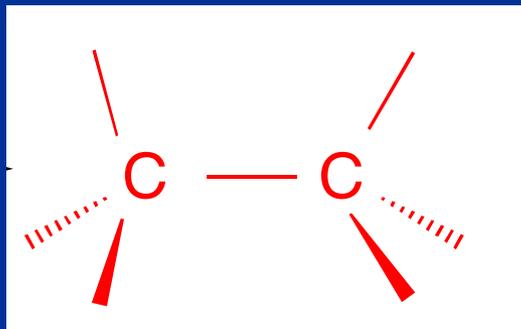
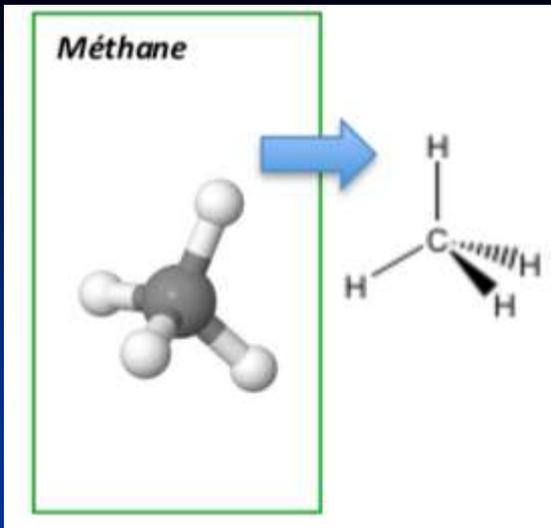
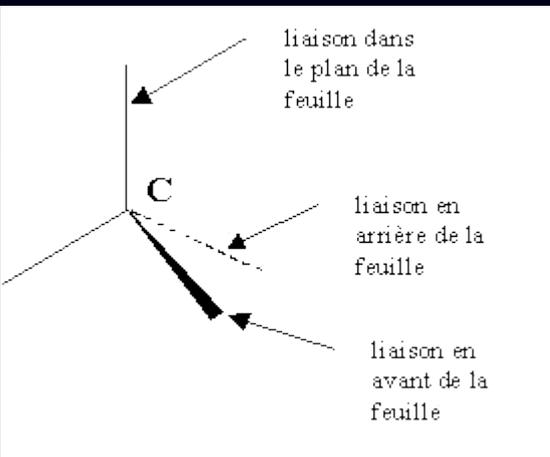
- Liaison dans le plan

- Liaison vers l'avant

- Liaison vers l'arrière

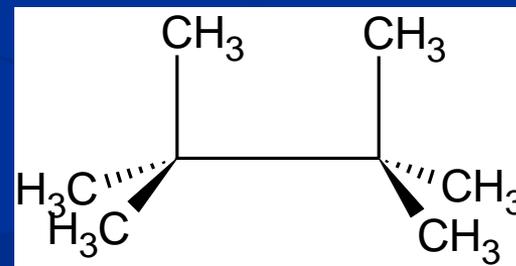
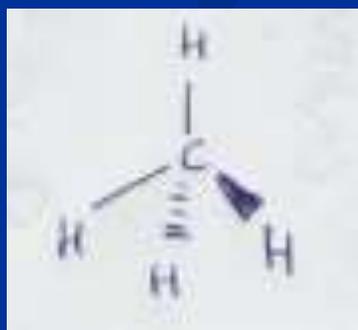
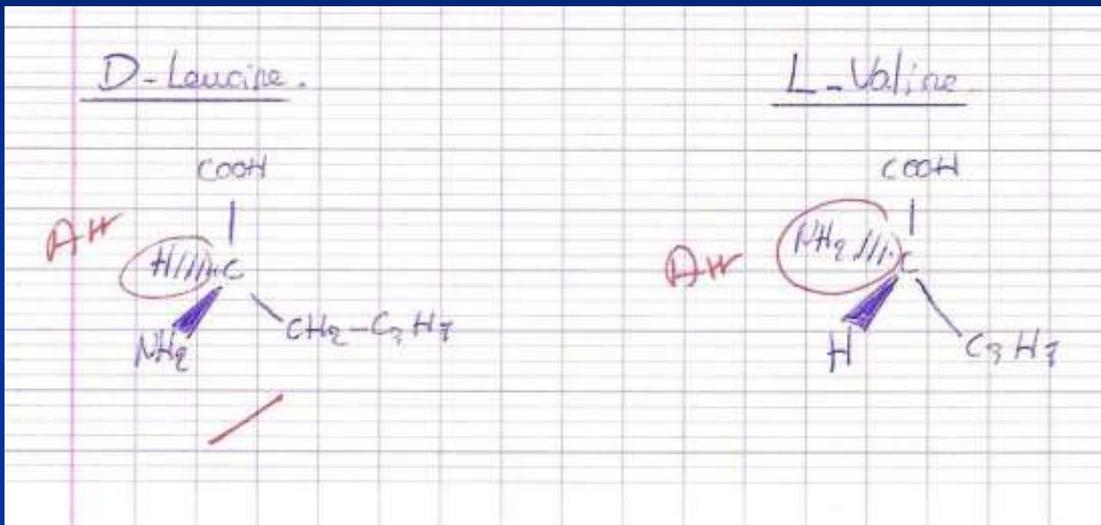
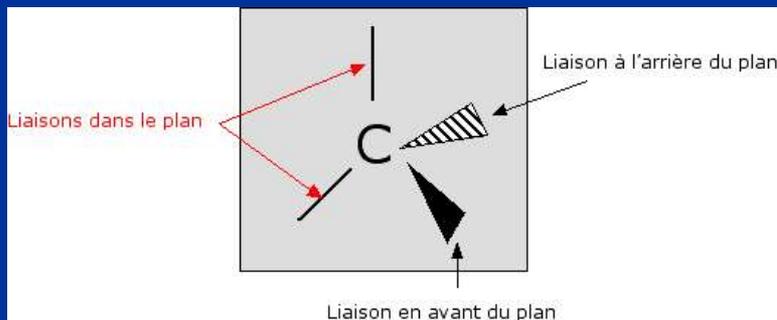
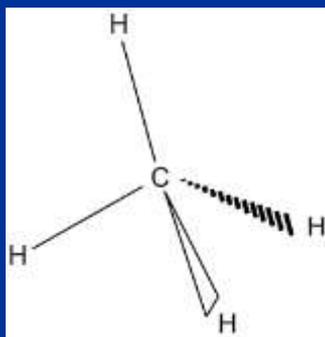
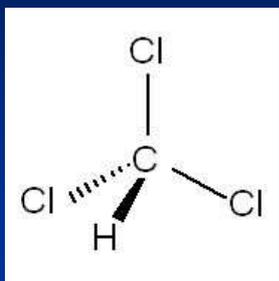


1919 - 2001



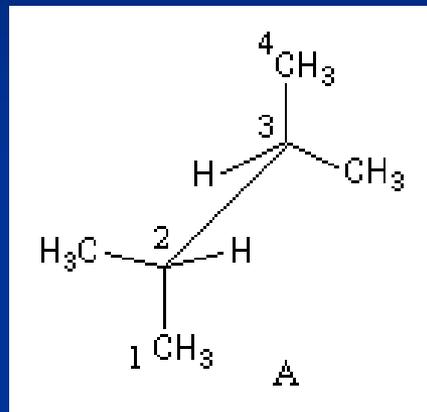
Remarque :

# ■ Erreurs classiques : commenter

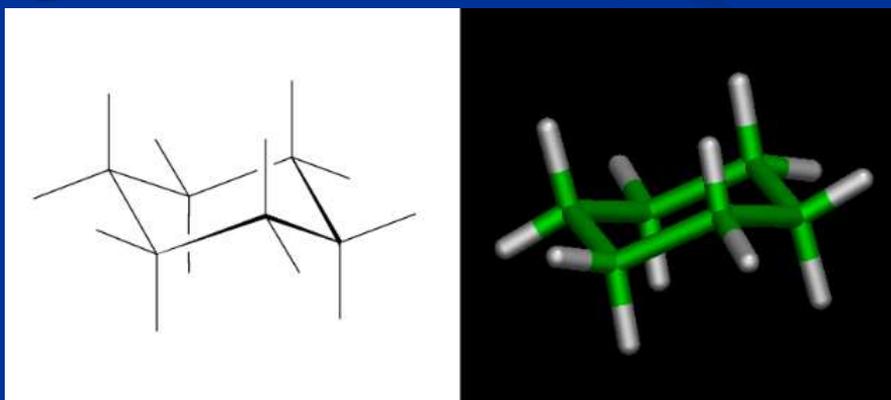


## 2) La perspective cavalière

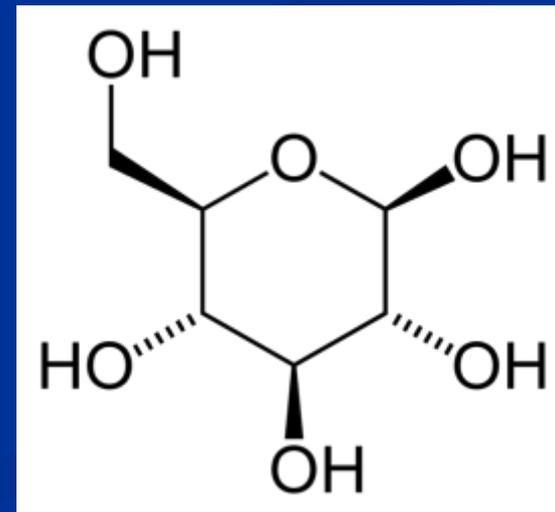
- Représentation en perspective avec un point de fuite à l'infini
- Exemple : l'éthane



- Intérêt : représentation du cyclohexane et de ses dérivés

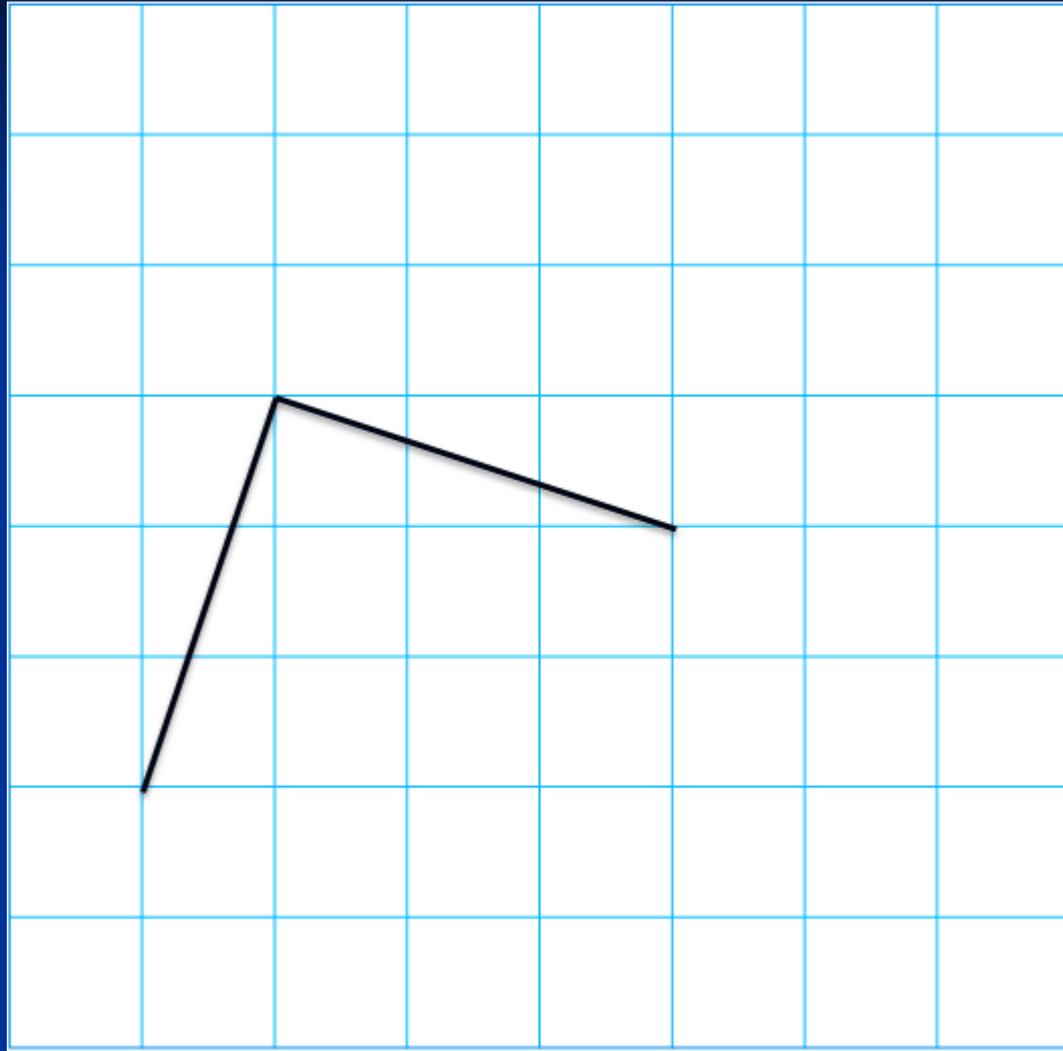


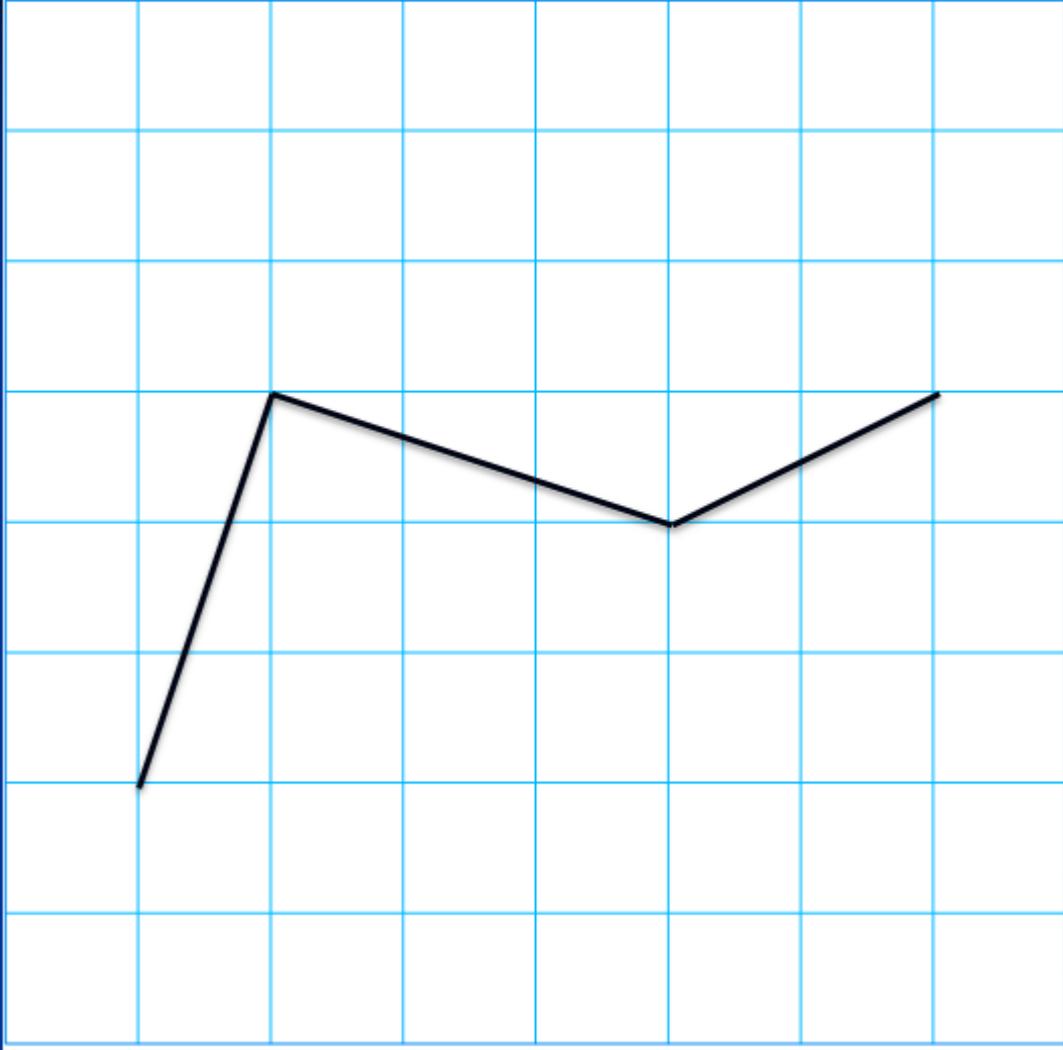
- Savoir représenter un cyclohexane
  - Construction avec le modèle moléculaire
  - Trouver la **conformation** (cf CO 05) la plus stable
- Appliquer ce mode de représentation à la molécule de glucose représentée ici en convention de Cram

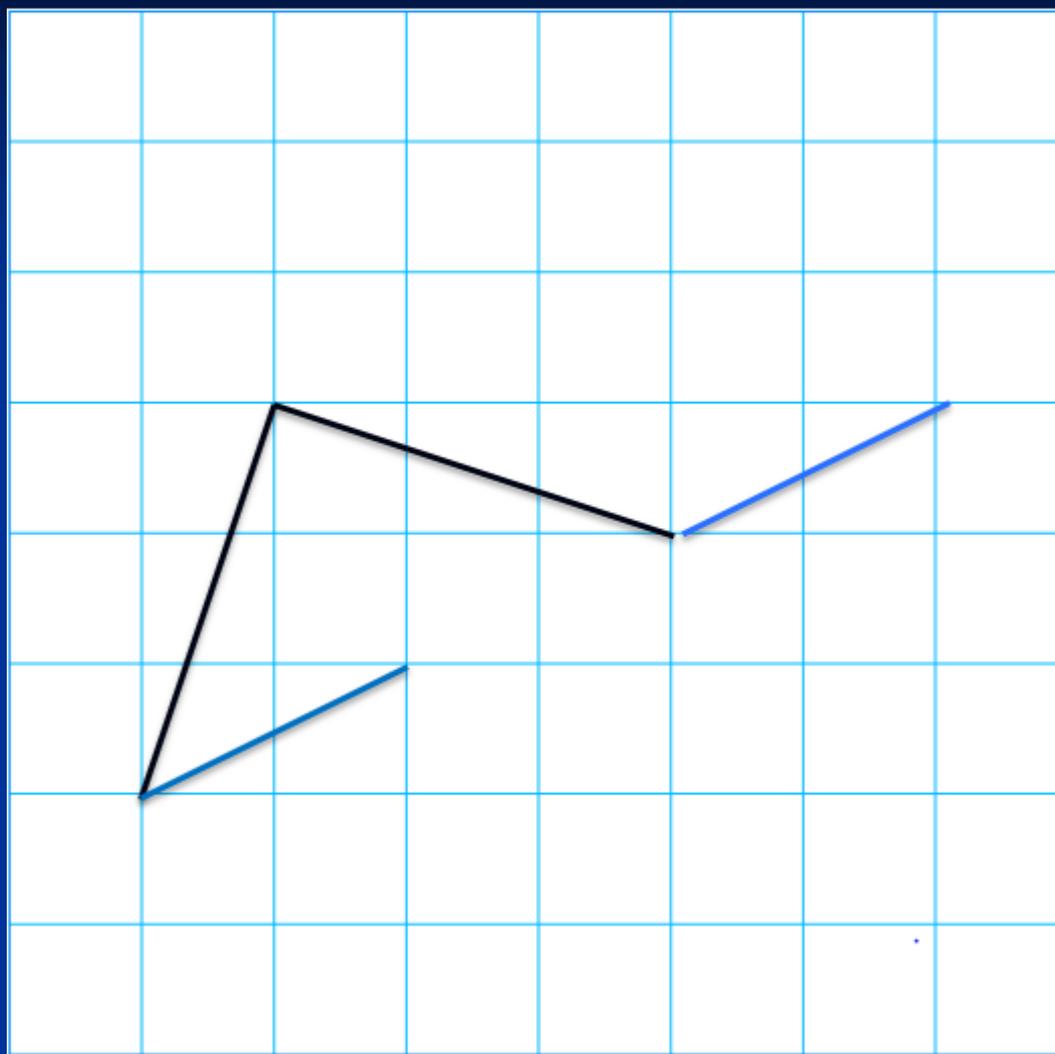




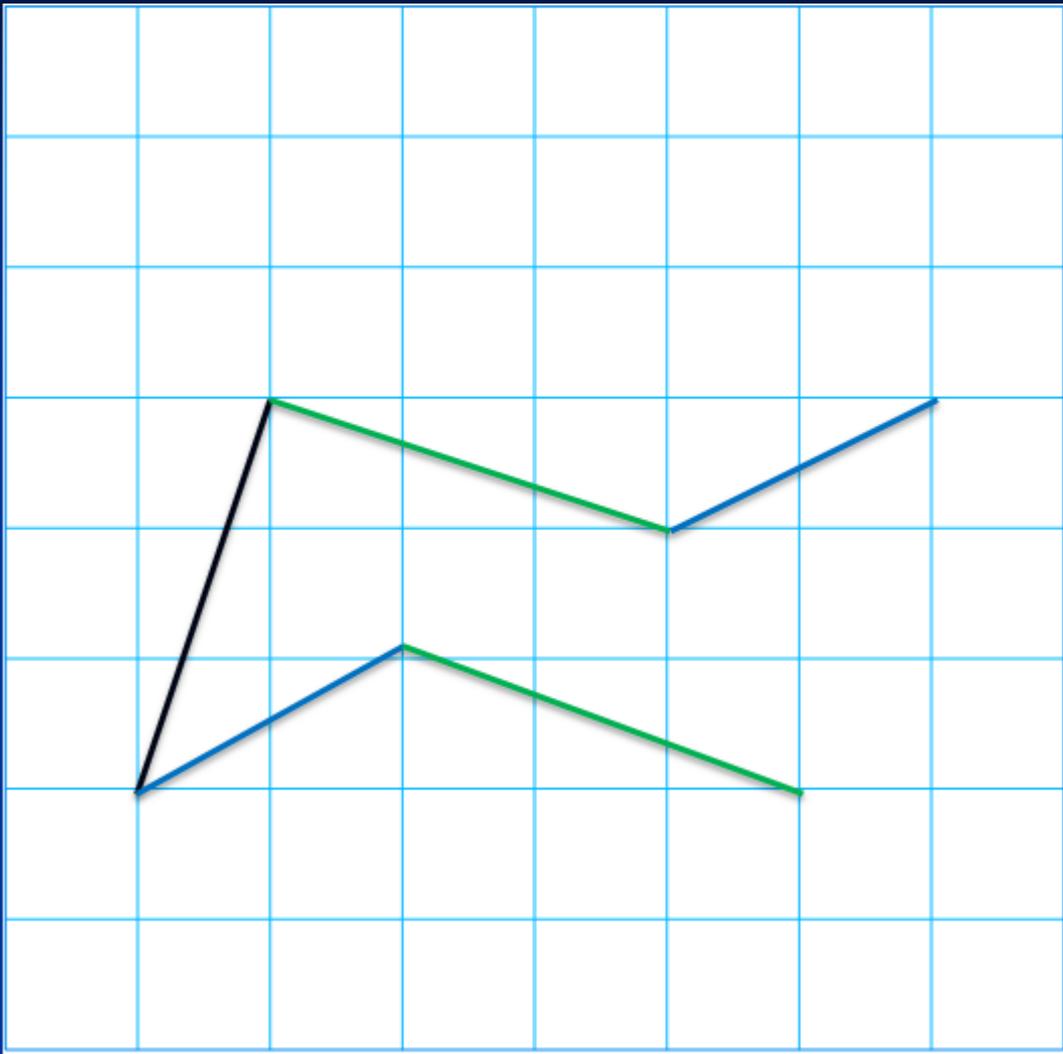


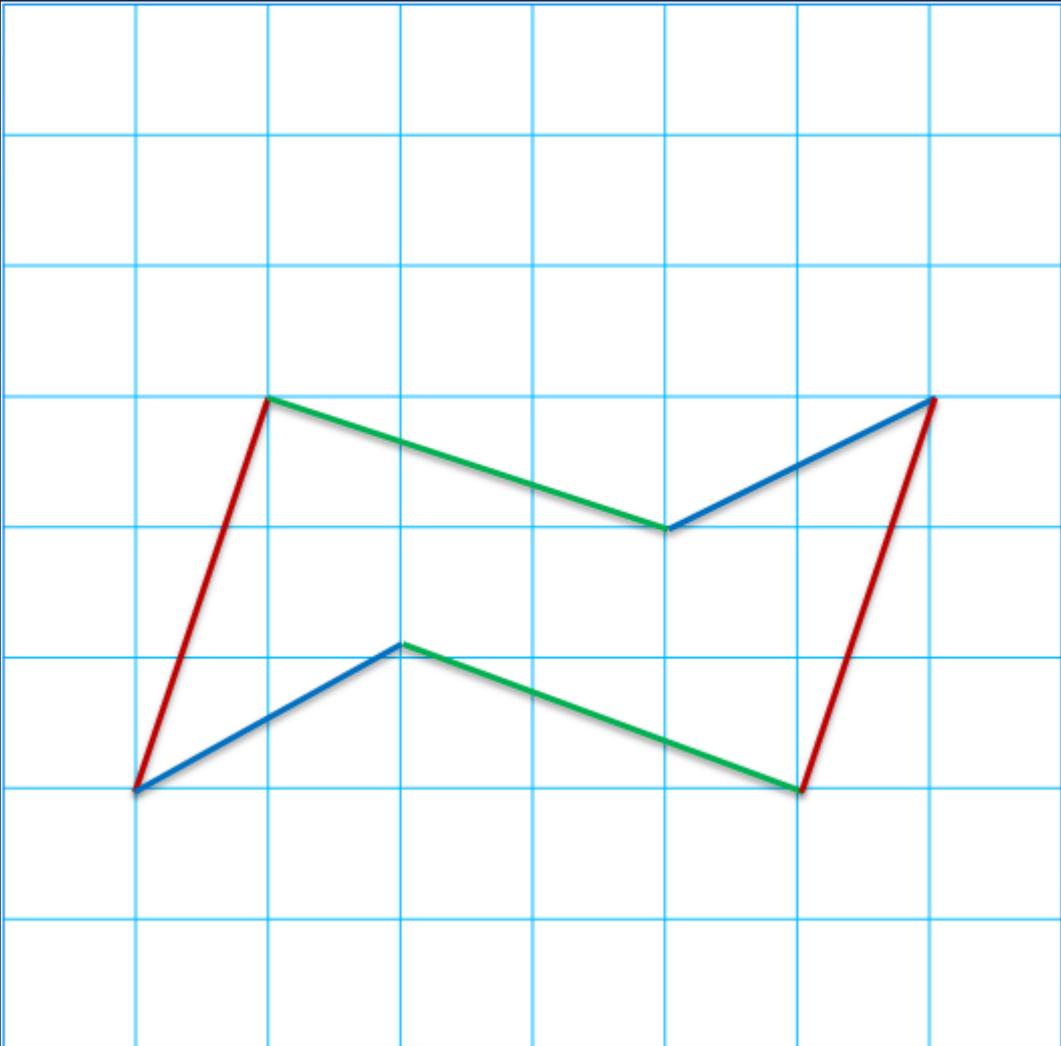


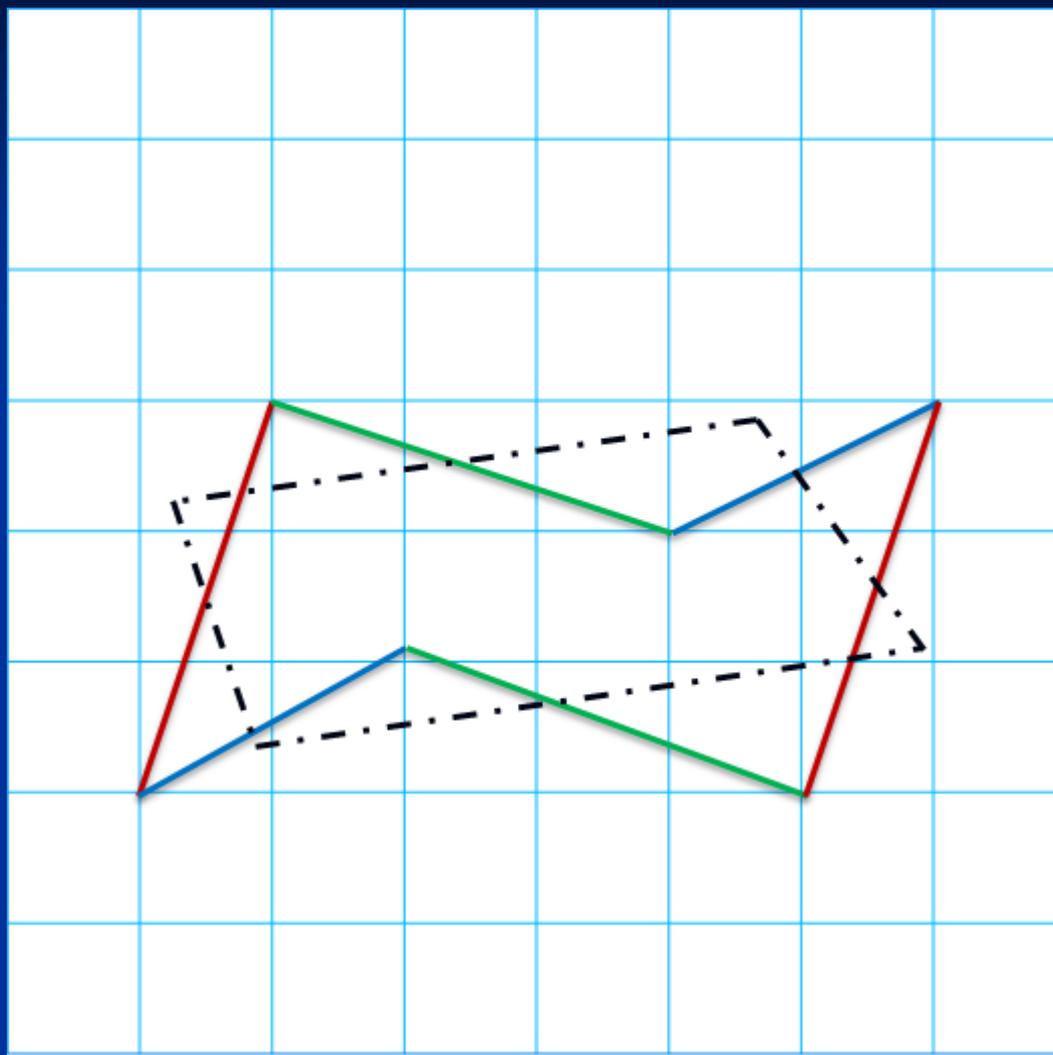




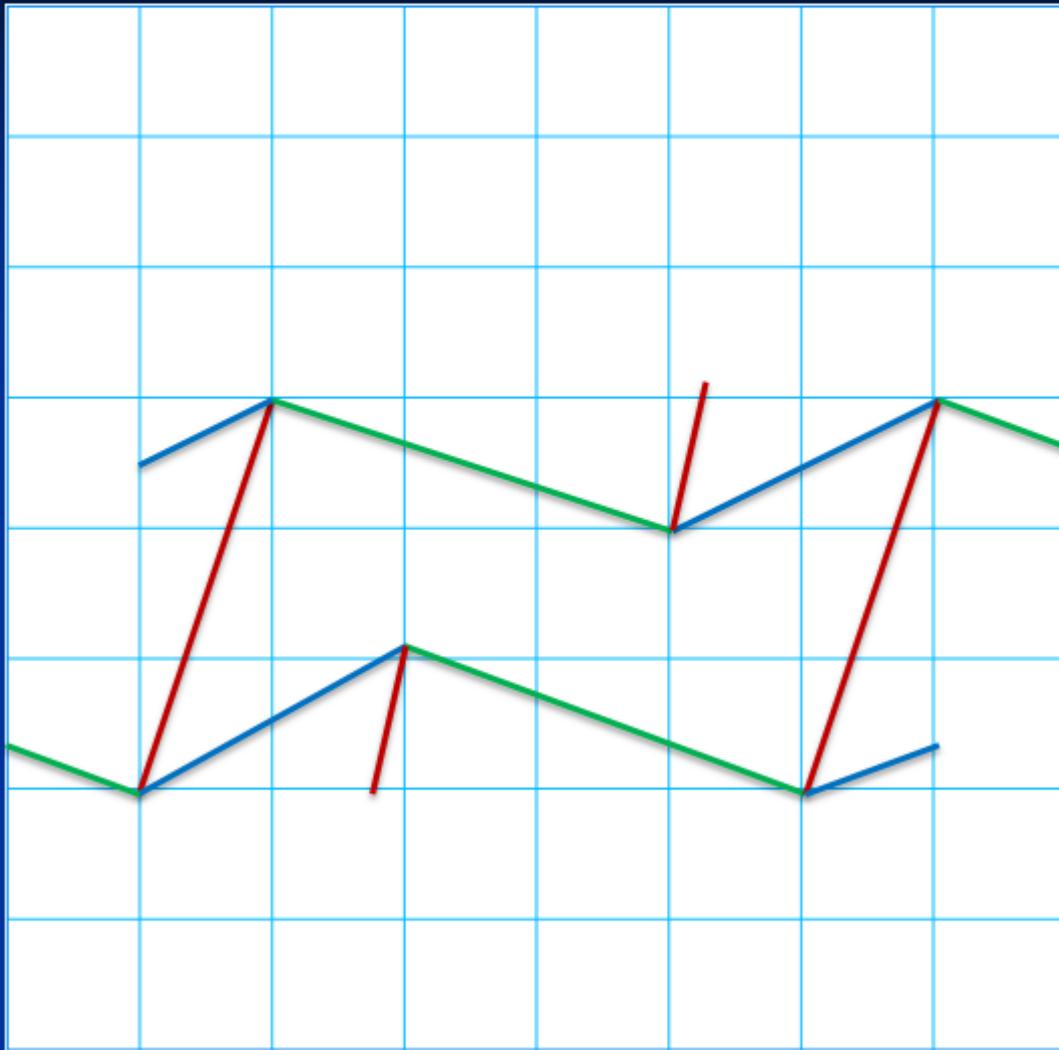
Les côtés opposés sont parallèles



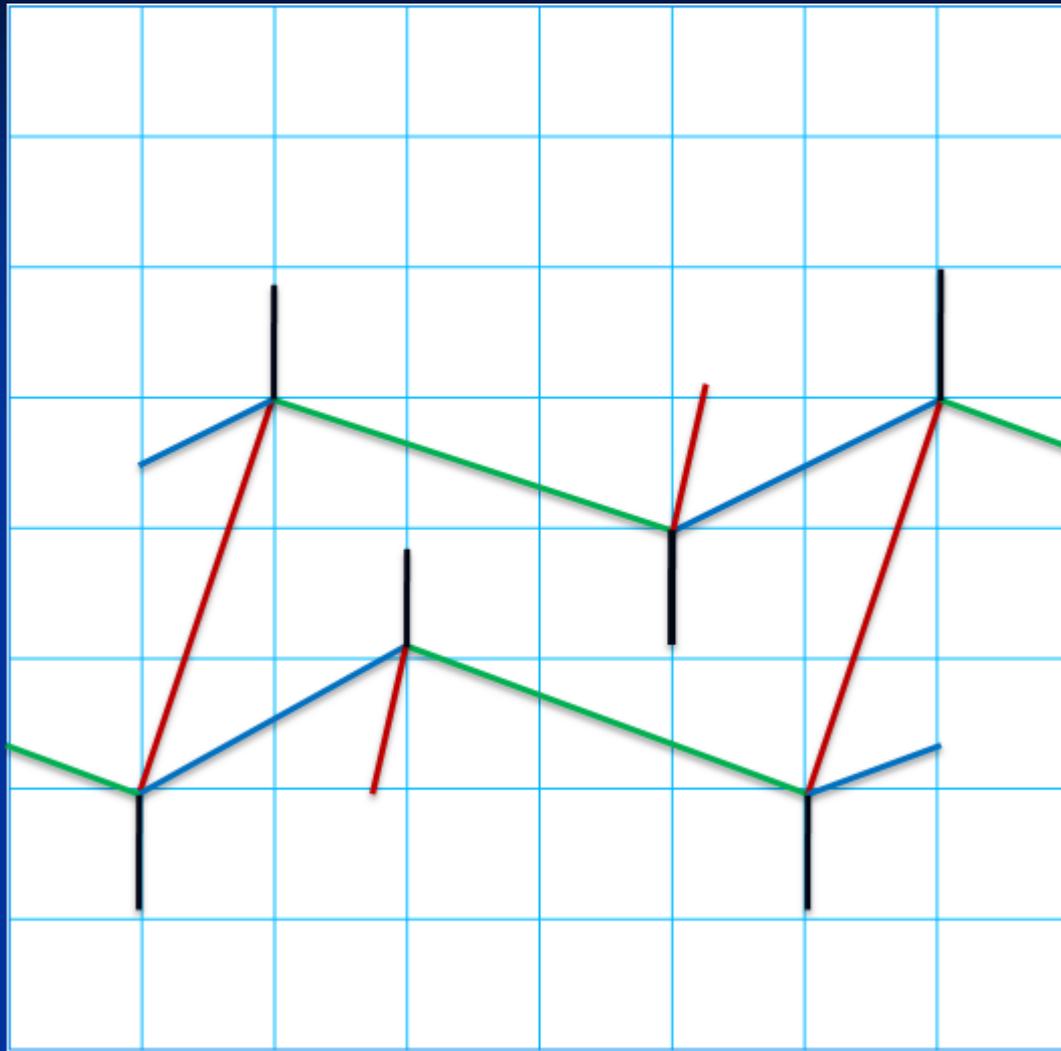




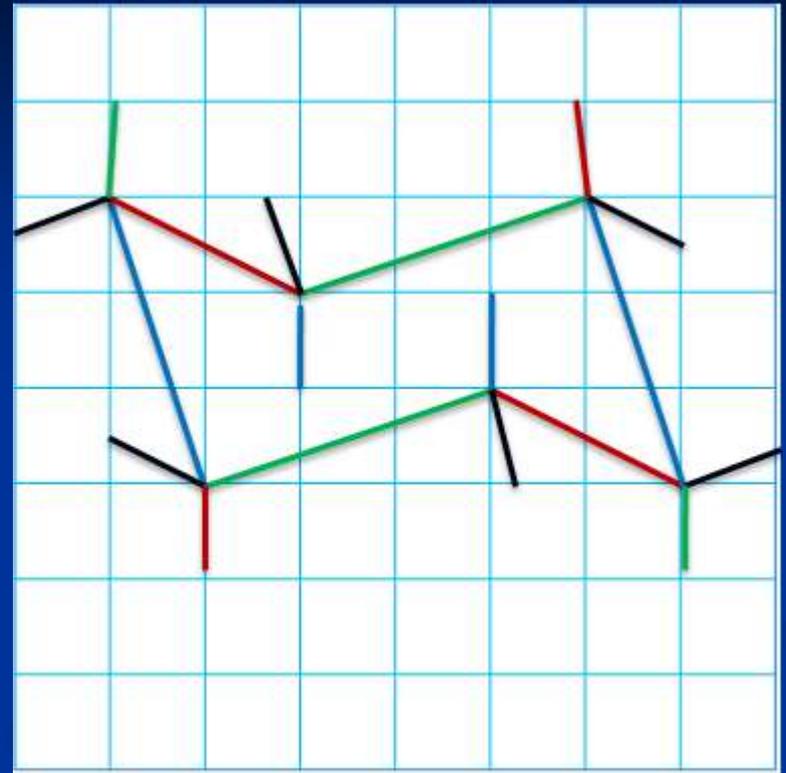
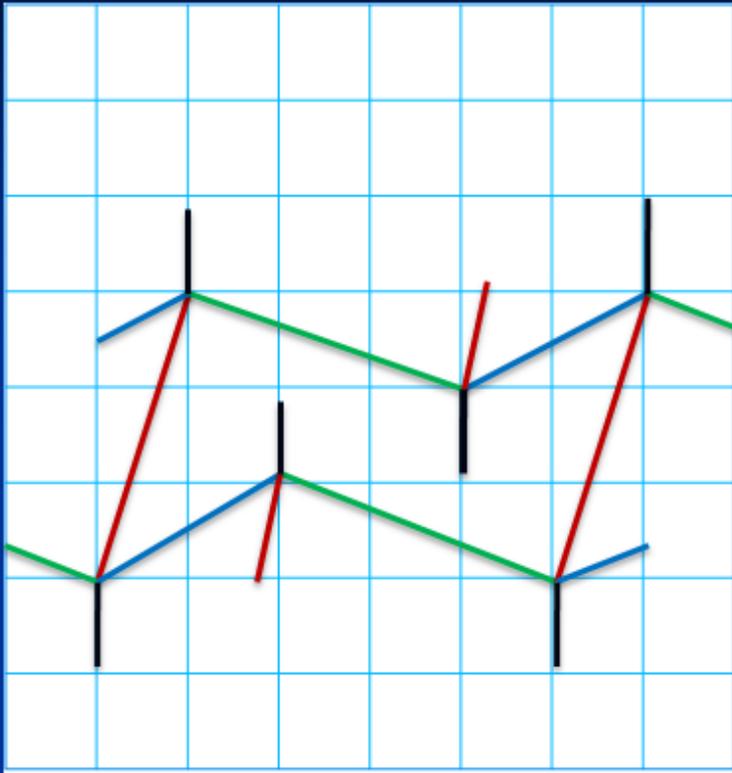
Plan moyen du cycle



Chaque liaison équatoriale est parallèle à un côté situé deux places plus loin



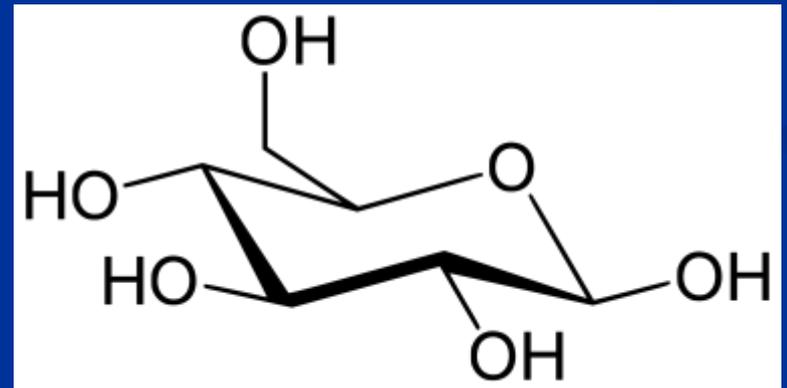
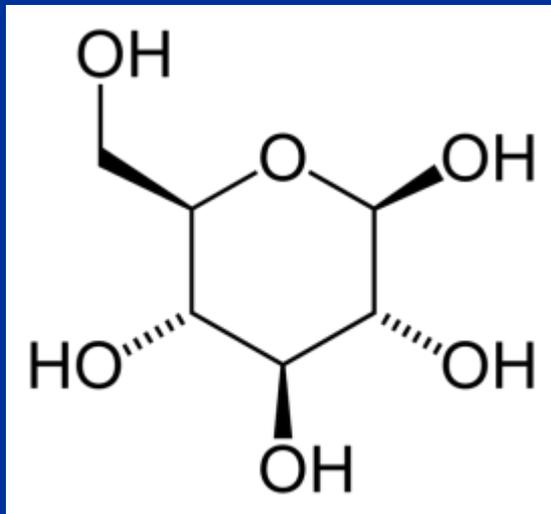
Les liaisons axiales perpendiculaires au plan moyen du cycle.



Equilibre de **conformation** (cf. CO 05) entre les deux formes « chaise »

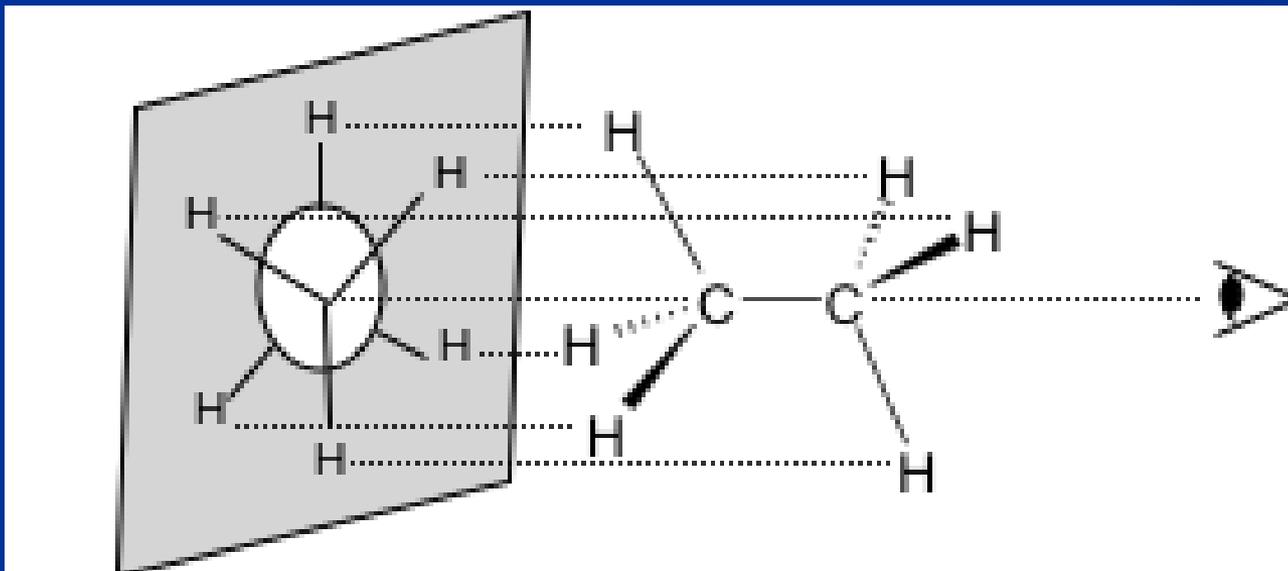
Transformation axial - équatorial

- Application à la molécule de glucose :



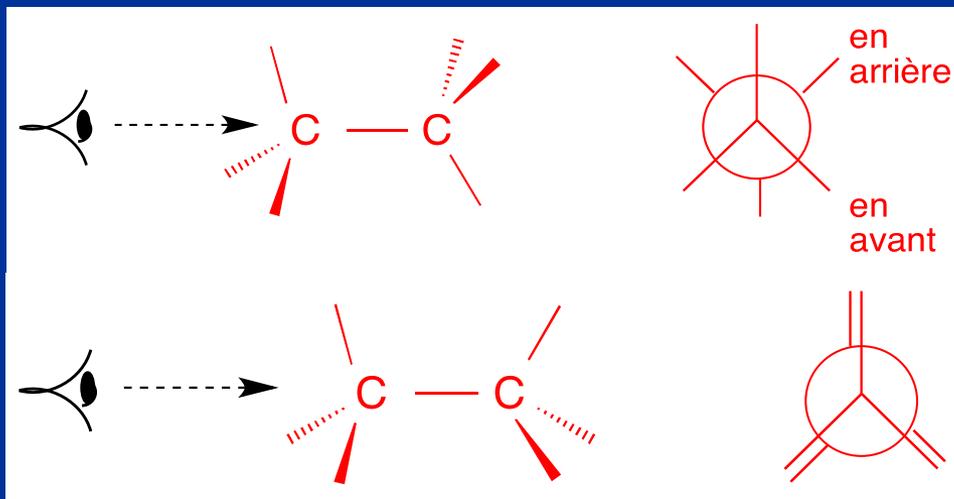
### 3) La projection de Newman

- On regarde la molécule dans l'axe de la liaison entre 2 atomes de carbone voisins
  - On projette dans un plan frontal.
  - L'atome de devant est représenté par un point
  - L'atome de derrière est masqué(cercle).

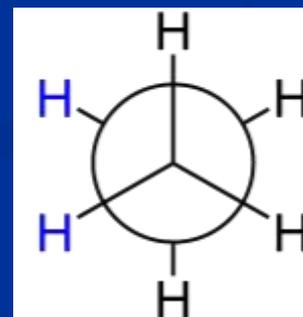


# ■ Libre rotation autour de la liaison C-C

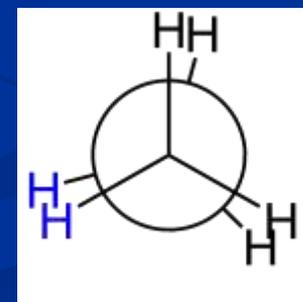
- Plusieurs « conformations » possibles
- Plusieurs représentation de Newman possibles
- 2 particulières : décalée / éclipsée
- Passage de l'une à l'autre : rotation



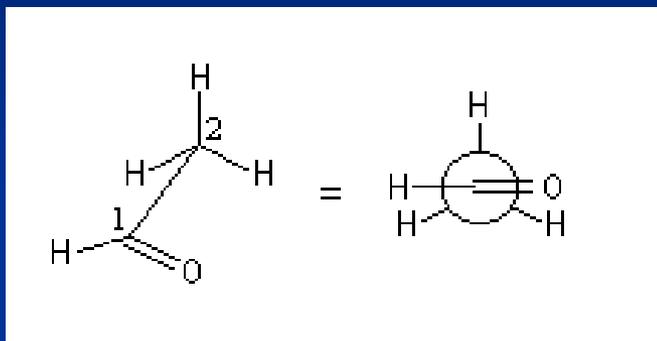
Forme décalée  
ou étoilée



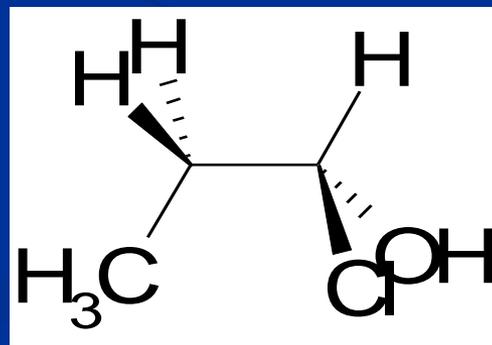
Forme éclipsée



- Il est possible de représenter des alcènes avec ce mode de représentation :

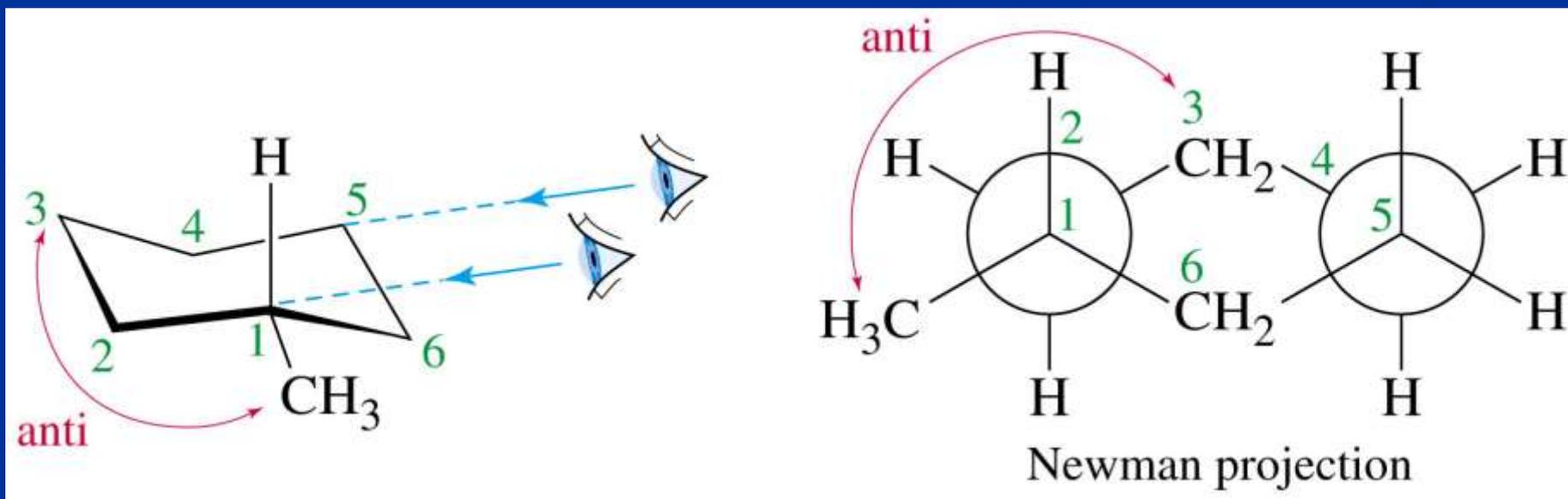


- Pour s'entraîner : représenter cette molécule (nom ?), en projection de Newman, vue de droite et vue de gauche.



# ■ Représentation de Newman pour le cyclohexane et ses dérivés :

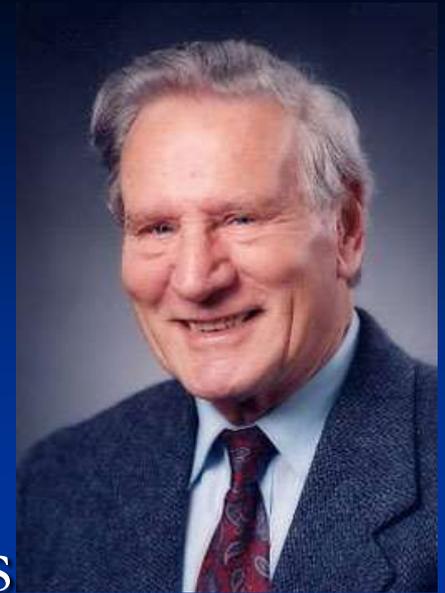
- Choisir deux liaisons
- Faire la représentation pour chacune d'elles
- Les « relier »



# II – La méthode V.S.E.P.R.

Ou méthode de Gillespie (1957)

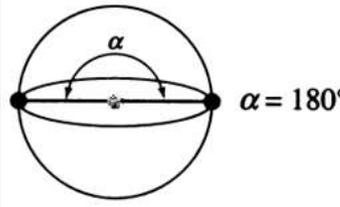
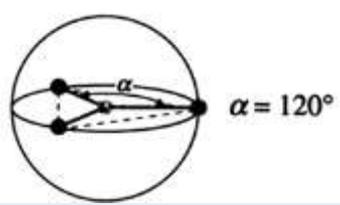
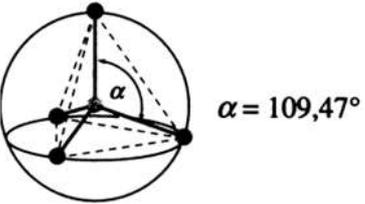
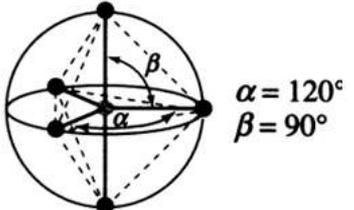
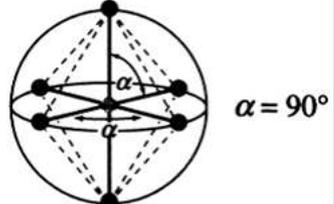
- **V.S.E.P.R : Valence Shell Electron Pair Repulsion** ou répulsion des paires d'électrons de valence.
- Complète la théorie de Lewis
- Modèle purement électrostatique : les doublets liants, non liants, et les électrons célibataires se repoussent et s'éloignent le plus possible les uns des autres



# Méthode pour prévoir les géométries :

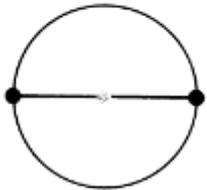
## ■ AX<sub>m</sub>En

- A : atome central
  - X : doublets liants (=substituants)
  - E : doublets non liants
- La géométrie de l'**environnement électronique** autour de A dépend de **m + n**
- La **géométrie moléculaire** dépend de **m et n**

m + n	Géométrie de l'environnement électronique	Représentation
2	Linéaire / Segment	 <p><math>\alpha = 180^\circ</math></p>
3	Triangle équilatéral	 <p><math>\alpha = 120^\circ</math></p>
4	Tétraèdre	 <p><math>\alpha = 109,47^\circ</math></p>
5	Bipyramide trigonale (= à base triangulaire)	 <p><math>\alpha = 120^\circ</math> <math>\beta = 90^\circ</math></p>
6	Octaèdre	 <p><math>\alpha = 90^\circ</math></p>

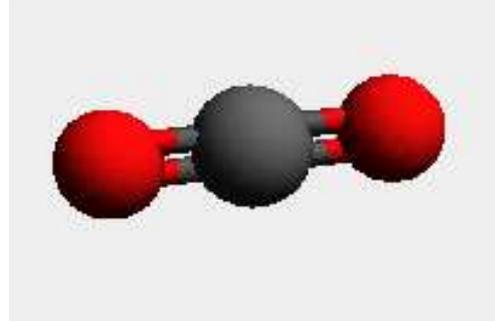
## Différentes géométries moléculaires à connaître :

➤  $m + n = 2$



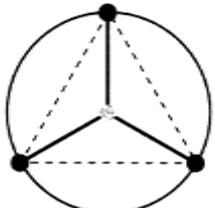
a)  $AX_2E_0$

Exemple :  $CO_2$



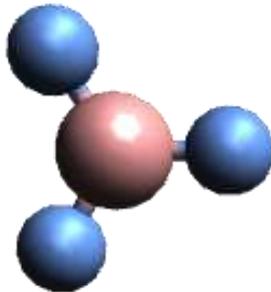
Géométrie moléculaire  
**linéaire**

➤  $m + n = 3$

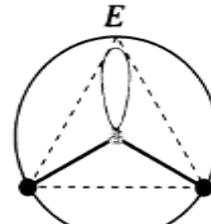


b)  $AX_3E_0$

Ex :  $BF_3$

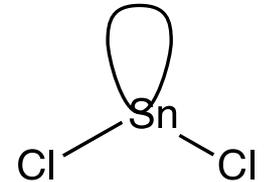
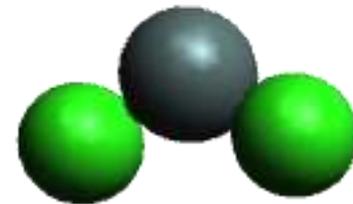


Géométrie moléculaire  
**Trigonale plane**



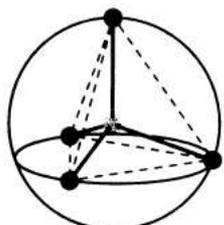
c)  $AX_2E_1$

Ex :  $SnCl_2$



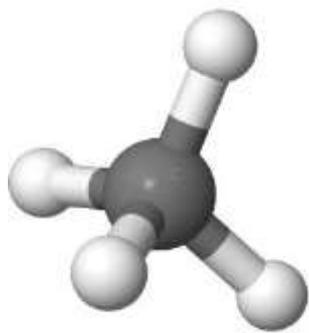
Géométrie moléculaire  
**Coudée**

➤  $m + n = 4$

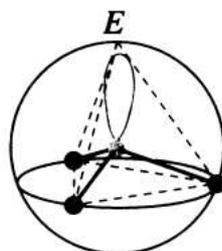


d)  $AX_4E_0$

Ex :  $CH_4$

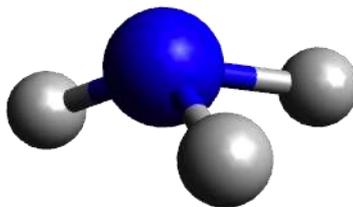


Géométrie moléculaire  
**tétraédrique**

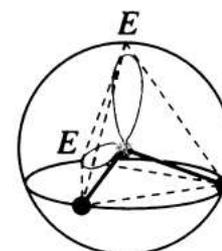


e)  $AX_3E_1$

Ex :  $NH_3$

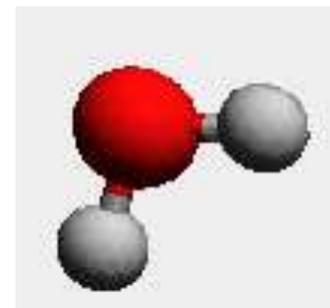


Géométrie moléculaire  
**Pyramidale à base  
triangulaire**



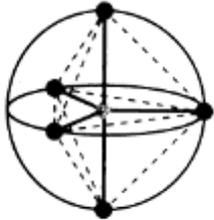
f)  $AX_2E_2$

Ex :  $H_2O$



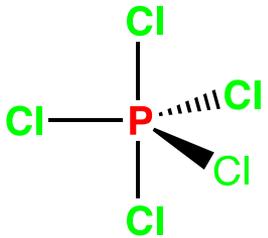
Géométrie moléculaire  
**Coudée**

➤  $m + n = 5$

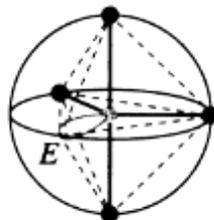


g)  $AX_5E_0$

Exemple :  $PCl_5$

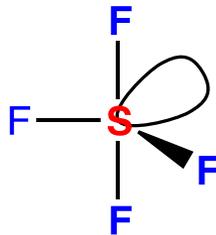


Géométrie  
Moléculaire  
**Bipyramidale à  
base triangulaire**

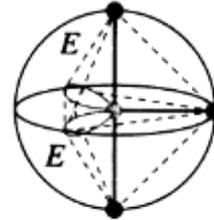


h)  $AX_4E_1$

Exemple :  $SF_4$

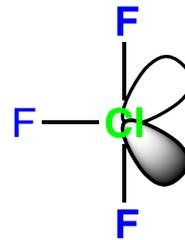


Géométrie  
Moléculaire  
**Tétraédrique  
irrégulière**

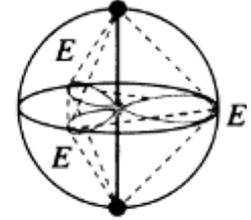


i)  $AX_3E_2$

Exemple :  $ClF_3$

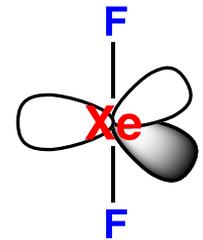


Géométrie  
Moléculaire  
**Plane, en T**



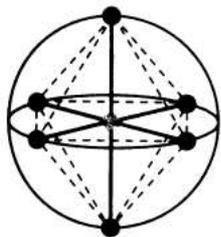
j)  $AX_2E_3$

Exemple :  $XeF_2$



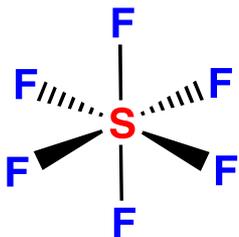
Géométrie  
Moléculaire  
**Linéaire**

➤  $m + n = 6$

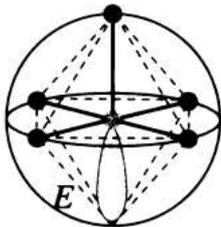


k)  $AX_6E_0$

Exemple :  $SF_6$

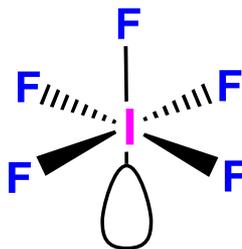


Géométrie  
Moléculaire  
**Octaédrique**

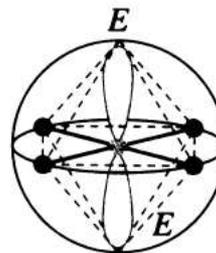


l)  $AX_5E_1$

Exemple :  $IF_4$

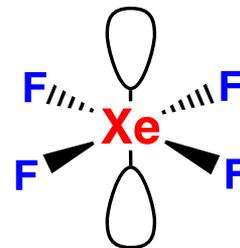


Géométrie  
moléculaire  
**Pyramidale à  
base carrée**



m)  $AX_4E_2$

Exemple :  $XeF_4$



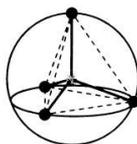
Géométrie  
Moléculaire  
**Plan carré**

## Modification des angles « idéaux »

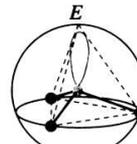
- Présence de doublets non liants :

Exemples : Modification des angles entre les liaisons due à la présence de doublets non liants pour des molécules du type  $AX_mE_n$  avec  $m+n = 4$ .

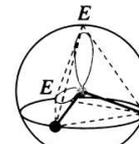
molécule	$CH_4$	$NH_3$	$H_2O$
environnement électronique	$AX_4$	$AX_3E$	$AX_2E_2$
géométrie moléculaire	tétraédrique	pyramidale à base triangulaire	coudée
<i>angle valenciel <math>H\hat{A}H</math></i>	<i><math>109,5^\circ</math></i>	<i><math>107,3^\circ</math></i>	<i><math>104,5^\circ</math></i>



d)  $AX_4E_0$



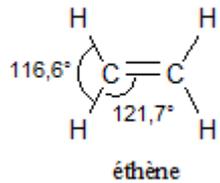
e)  $AX_3E_1$



f)  $AX_2E_2$

**Conclusion ?**

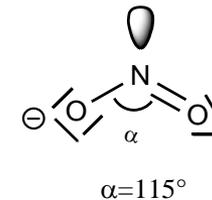
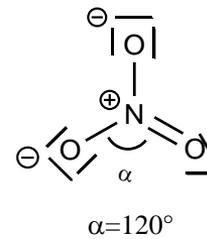
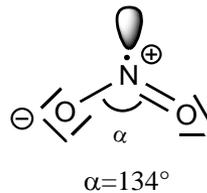
- Liaisons multiples



Conclusion ?

- Présence d'électrons célibataires

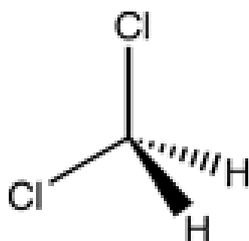
	$\text{NO}_2$	$\text{NO}_3^-$	$\text{NO}_2^-$
Notation	$\text{AX}_2\text{E}_1$	$\text{AX}_3\text{E}_0$	$\text{AX}_2\text{E}_1$
Environnement électronique	triangulaire plan	triangulaire plan	triangulaire plan
Edifice	coudé	triangulaire plan	coudé



Conclusion ?

- Influence de la nature des atomes :

Exemples : Modification des angles entre les liaisons due à l'électronégativité différente des éléments



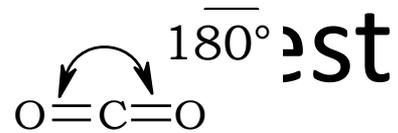
Angle HCCl =  $108,9^\circ < 109,5^\circ$

Cl plus électronégatif, le doublet liant entre C et Cl est en moyenne plus éloigné de l'atome de carbone, donc moins répulsif.

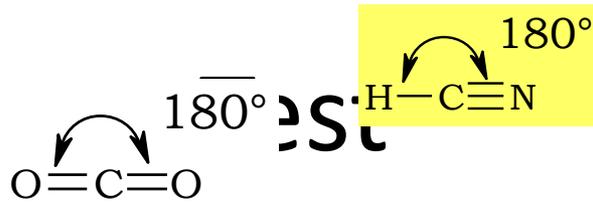
- 
- Plus les interactions répulsives sont grandes, plus les doublets sont éloignés
  - Si les positions autour de A ne sont pas équivalentes ( $m+n=5$  ou  $6$ ), la géométrie la plus stable est celle qui éloigne le plus possible les doublets les plus volumineux.

# Test

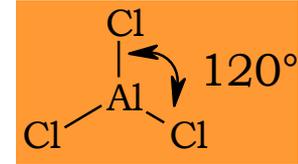
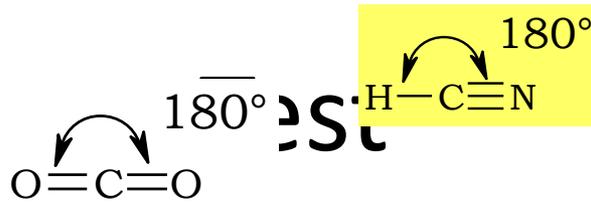
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- Dioxyde de soufre
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- Ion sulfate
- Ammoniac
- Eau
- Pentachlorure de phosphore
- Tétrachlorure de tellure
- Trifluorure de chlore
- Ion triiodure
- Hexafluorure de soufre
- Pentafluorure de brome
- Tétrafluorure de xénon



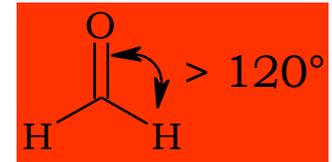
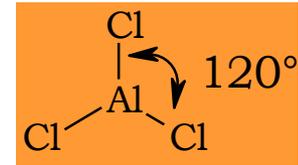
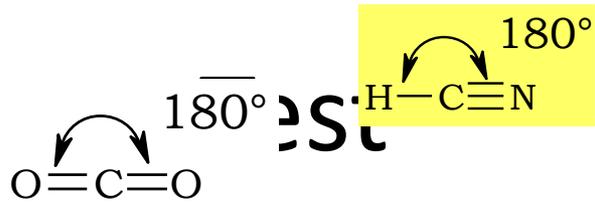
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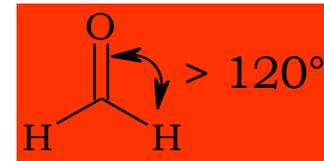
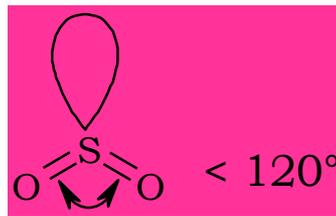
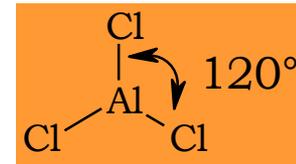
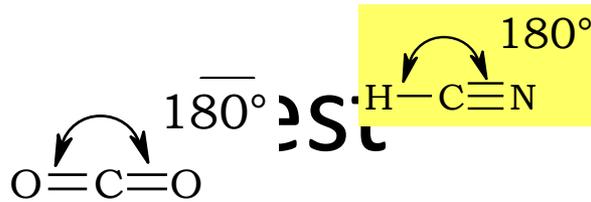
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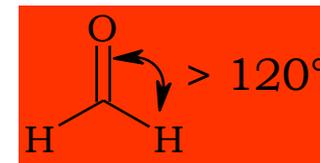
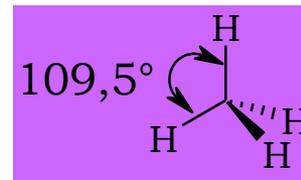
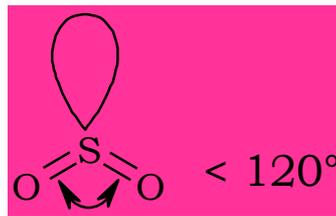
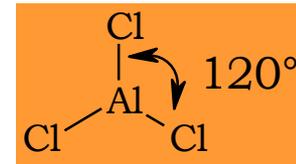
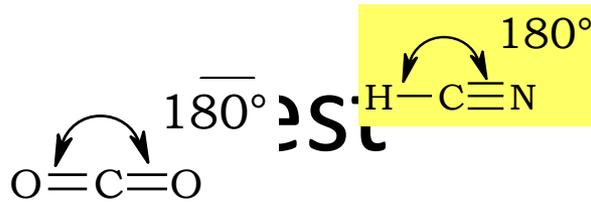
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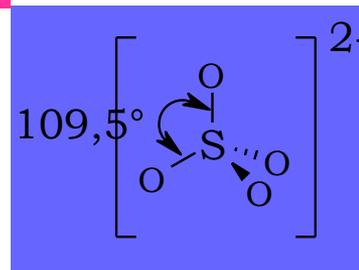
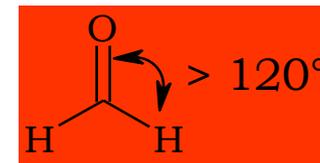
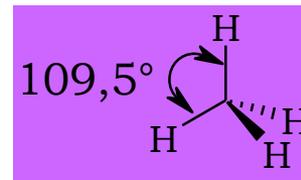
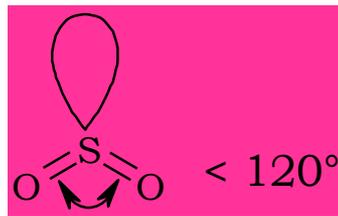
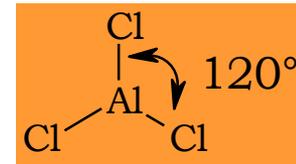
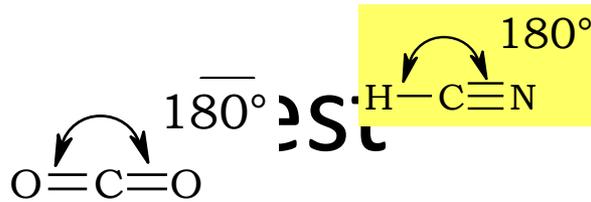
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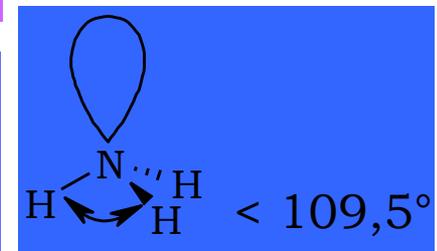
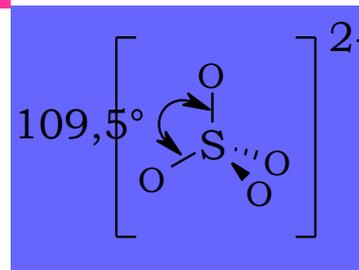
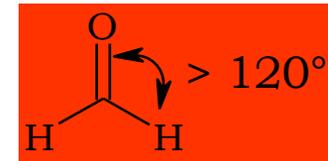
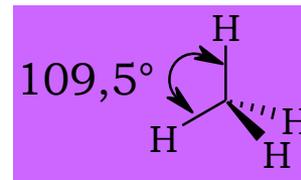
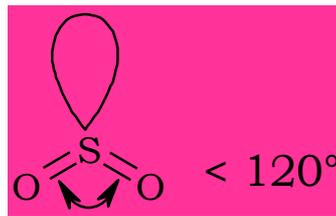
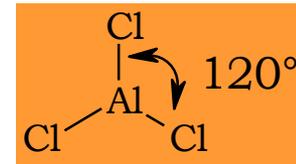
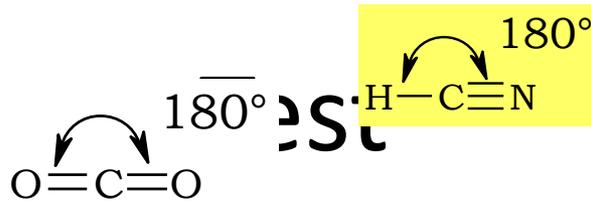
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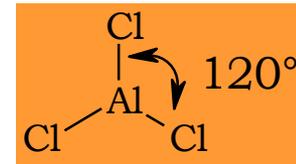
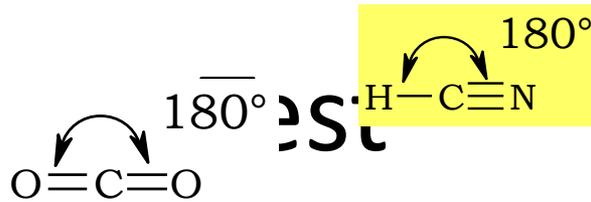
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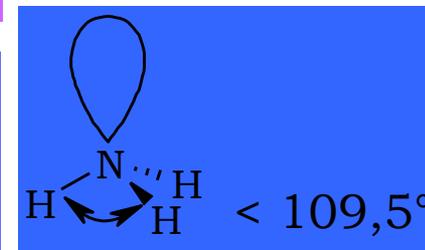
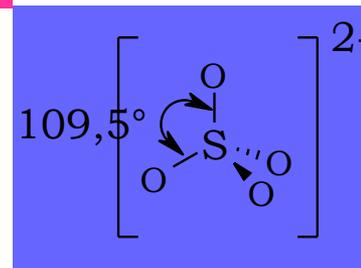
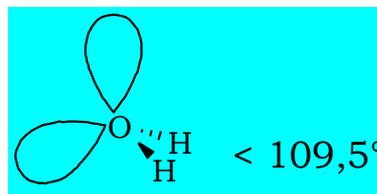
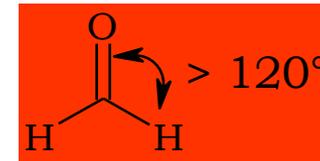
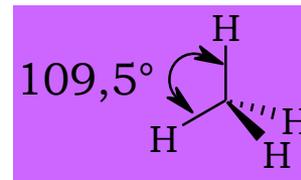
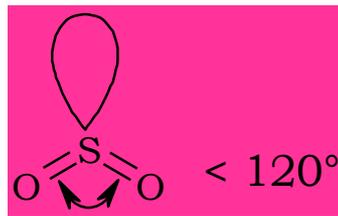
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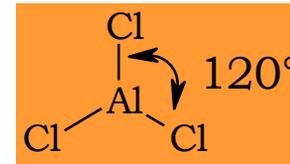
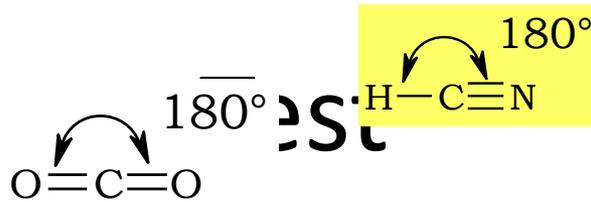


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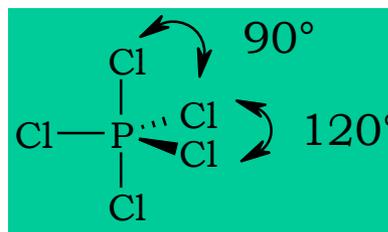
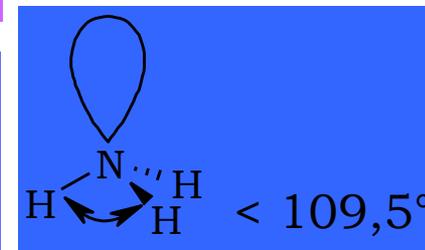
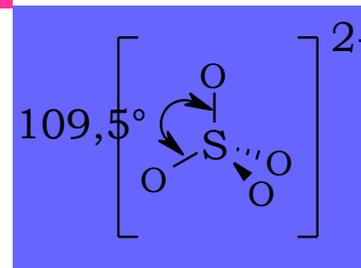
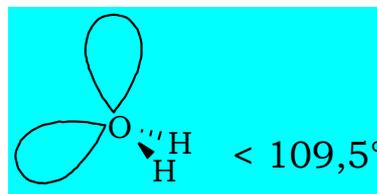
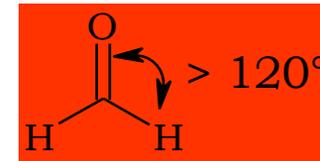
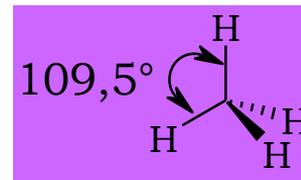
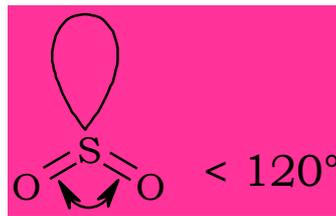


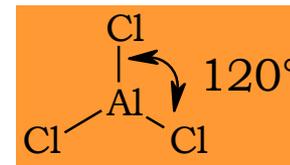
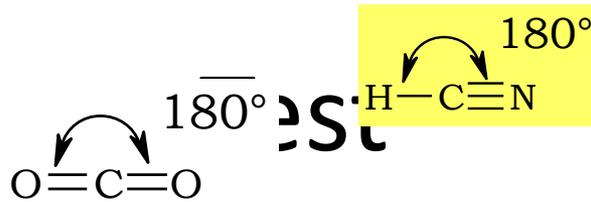
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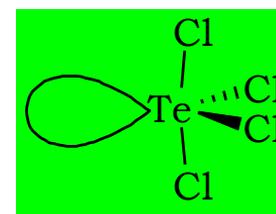
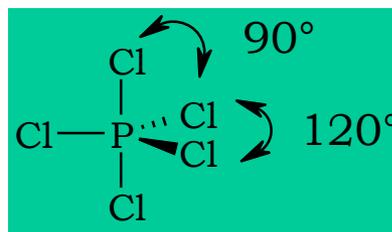
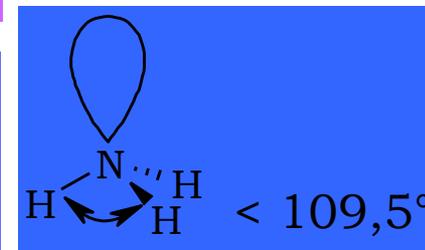
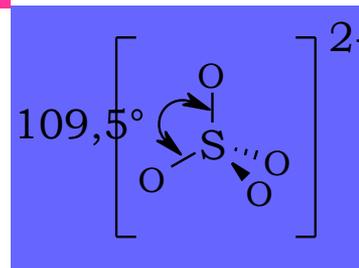
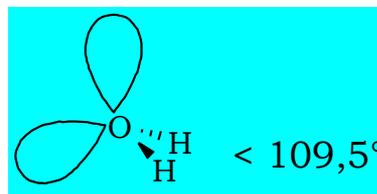
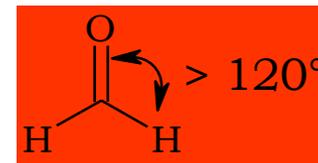
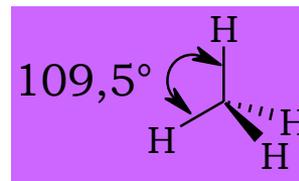
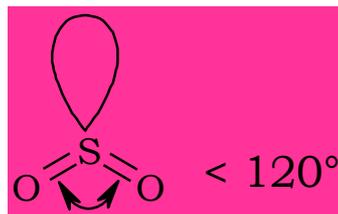


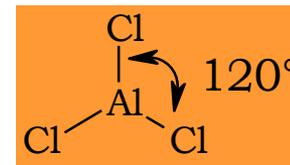
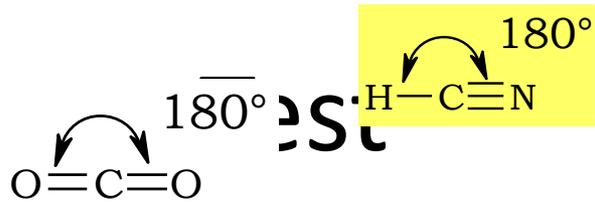
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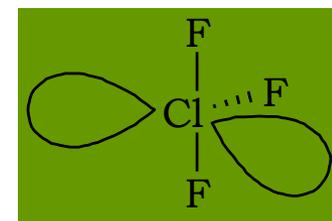
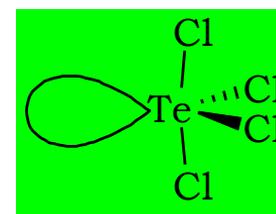
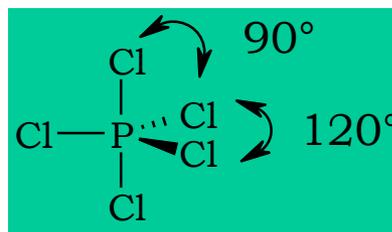
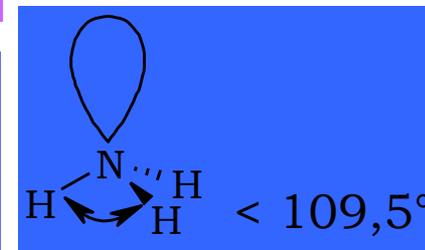
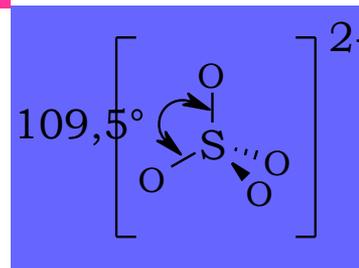
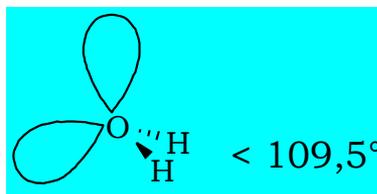
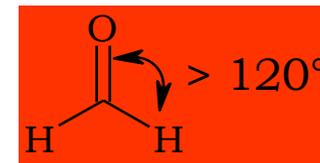
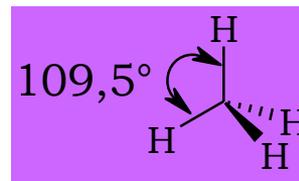
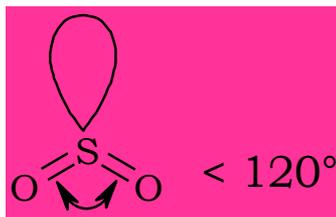


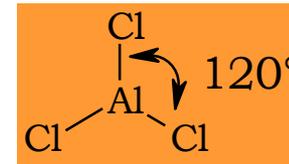
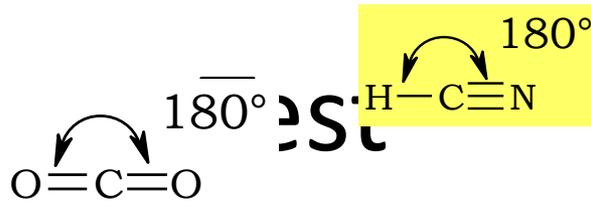
- Dioxyde de carbone
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- Hexafluorure de soufre
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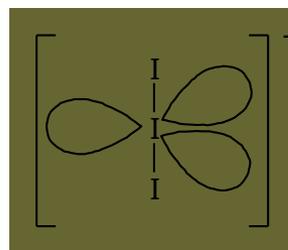
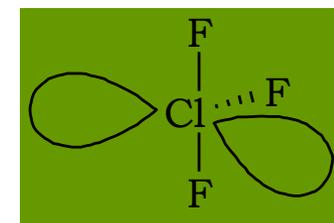
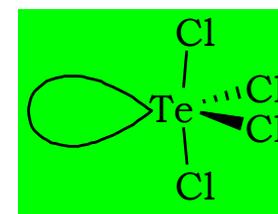
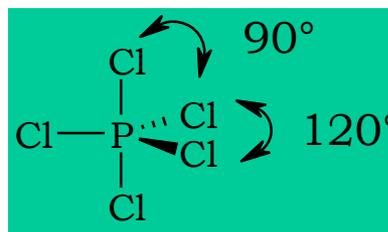
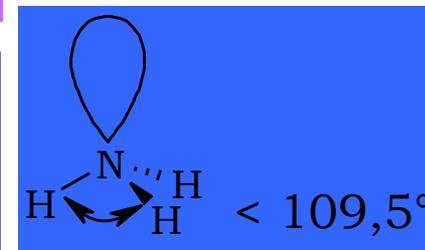
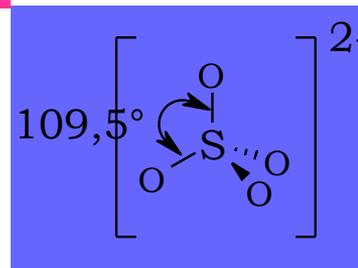
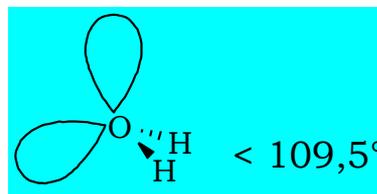
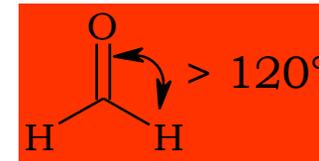
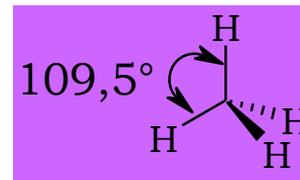
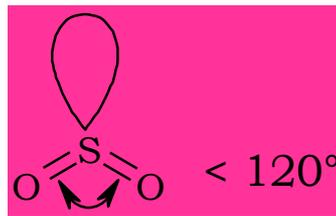


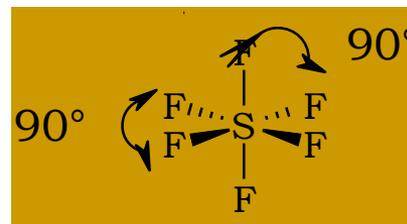
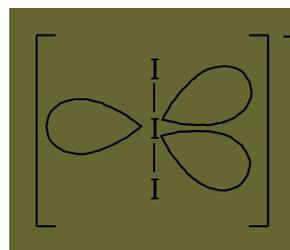
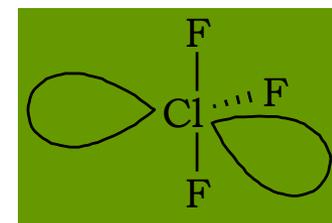
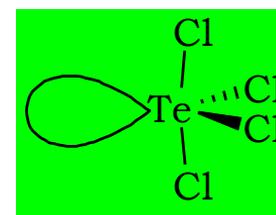
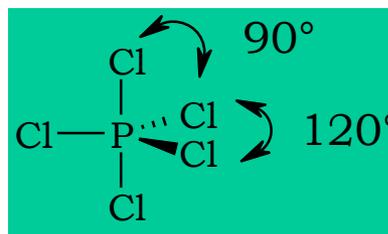
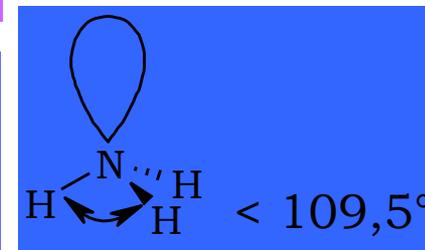
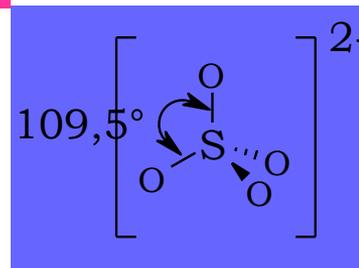
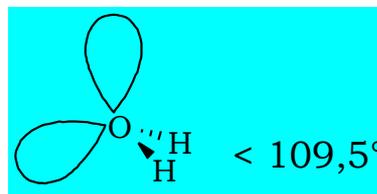
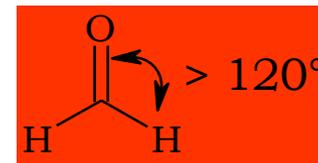
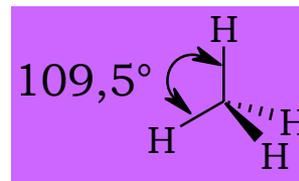
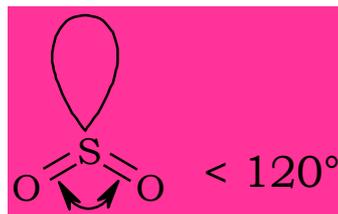
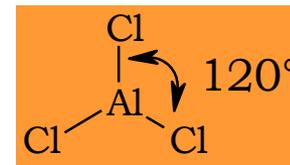
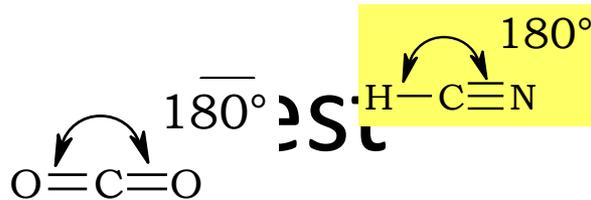
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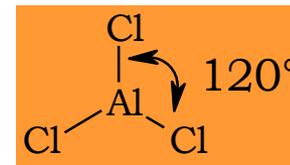
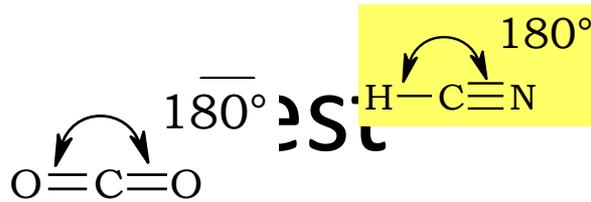


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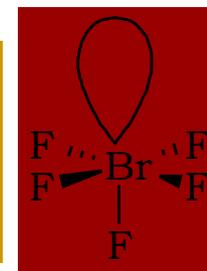
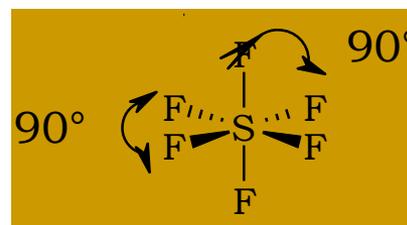
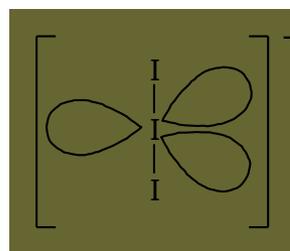
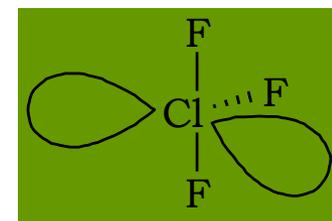
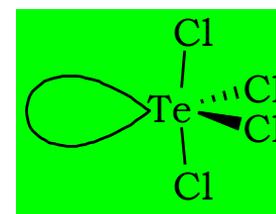
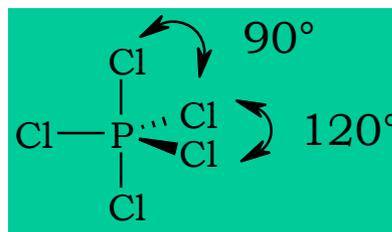
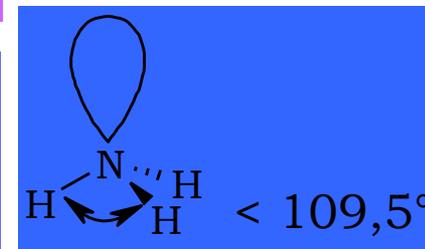
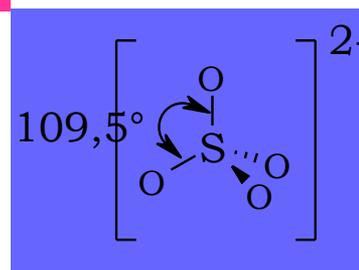
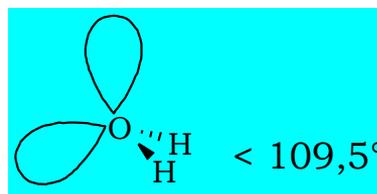
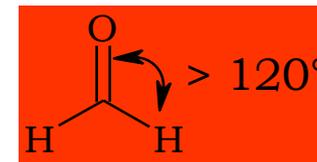
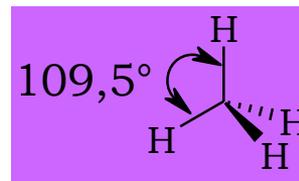
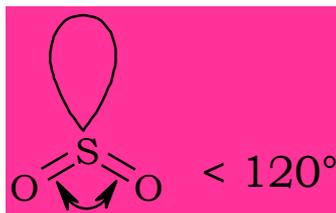


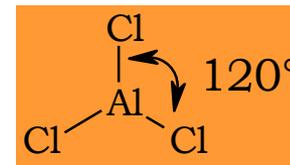
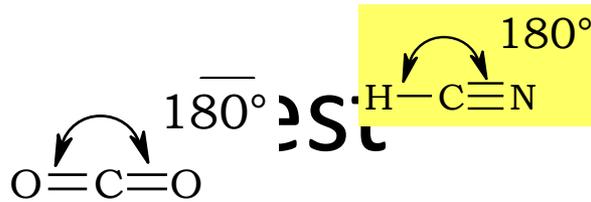


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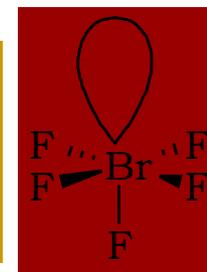
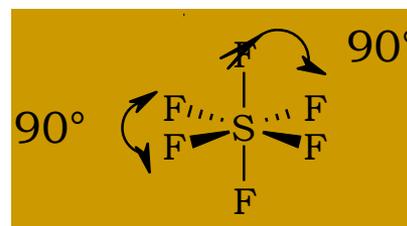
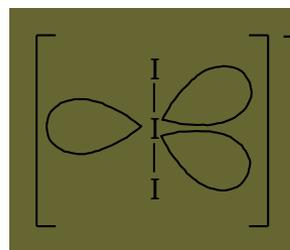
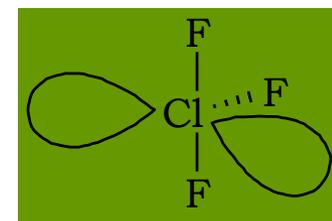
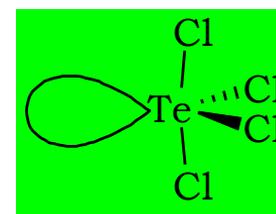
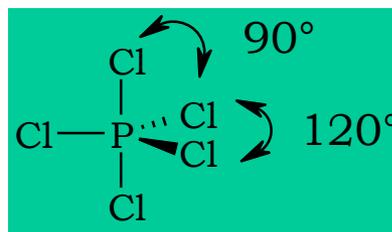
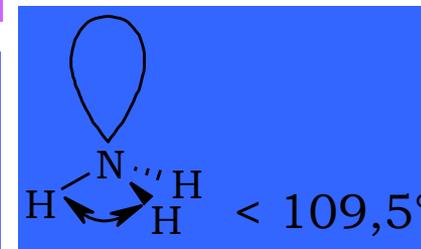
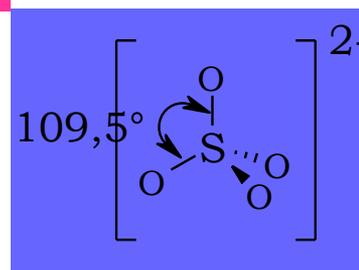
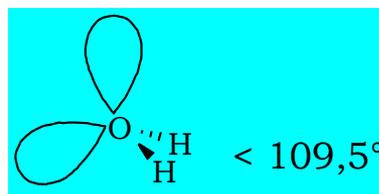
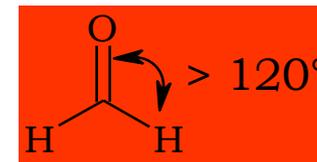
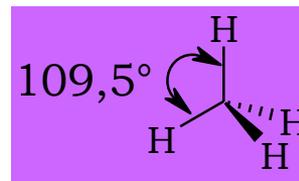
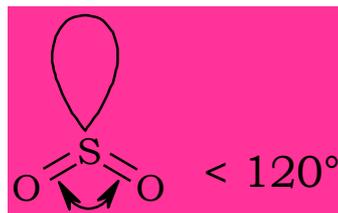


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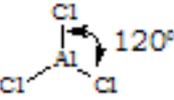
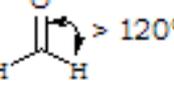
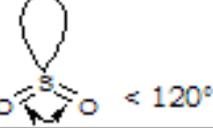
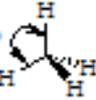
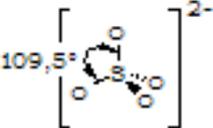
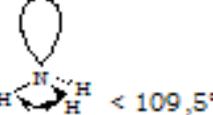
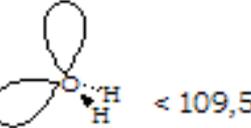


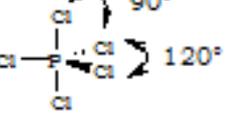
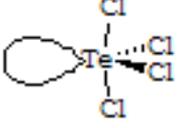
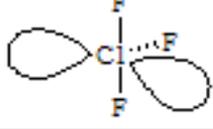
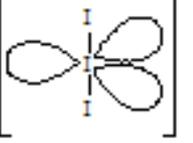
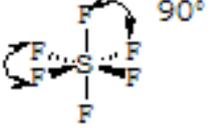
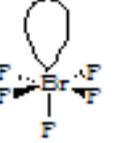
# Relier un chiffre à une lettre

- |                                |    |  |
|--------------------------------|----|--|
| Dioxyde de carbone 1.          | A. | Molécule octaédrique                         |
| Cyanure d'hydrogène 2.         | B. | Système digonal, molécule linéaire           |
| Chlorure d'aluminium 3.        | C. | Tétraèdre non régulier                       |
| Formaldéhyde 4.                | D. | Molécule « en T »                            |
| Dioxyde de soufre 5.           | E. | Molécule coudée                              |
| Méthane 6.                     | F. | Molécule bipyramidale à base triangulaire    |
| Ion sulfate 7.                 | G. | Molécule pyramidale à base triangulaire      |
| Ammoniac 8.                    | H. | Système tétragonal, molécule tétraédrique    |
| Eau 9.                         | I. | Géométrie carrée, plane.                     |
| Pentachlorure de phosphore 10. | J. | Système trigonal plan, molécule triangulaire |
| Tétrachlorure de tellure 11.   | K. | Molécule pyramidale à base carrée            |
| Trifluorure de chlore 12.      | L. | Molécule linéaire                            |
| Ion triiodure 13.              |    |  |
| Hexafluorure de soufre 14.     |    |  |
| Pentafluorure de brome 15.     |    |  |
| Tetrafluorure de xénon 16.     |    |  |

# Réponses

- 1B : C =  $AX_2E_0$
- 2B : C =  $AX_2E_0$
- 3J : Al =  $AX_3E_0$
- 4J : C =  $AX_3E_0$
- 5E : S =  $AX_2E_1$
- 6H : C =  $AX_4E_0$
- 7H : S =  $AX_4E_0$
- 8G : N =  $AX_3E_1$
- 9E : O =  $AX_2E_2$
- 10F : P =  $AX_5E_0$
- 11C : Te =  $AX_4E_1$
- 12D : Cl =  $AX_3E_2$
- 13L : I =  $AX_2E_3$
- 14A : S =  $AX_6E_0$
- 15K : Br =  $AX_5E_1$
- 16I : Xe =  $AX_4E_2$

Géométrie de la molécule	Ordre de grandeur de l'angle de valence	Structure et ordre de grandeur de l'angle de valence de quelques molécules
Système digonal, molécule linéaire	180°	Dioxyde de carbone $180^\circ$  Cyanure d'hydrogène $180^\circ$ 
Système trigonal plan, molécule triangulaire	120°	Chlorure d'aluminium  Formaldéhyde $> 120^\circ$ 
Molécule coudée	< 120°	Dioxyde de soufre 
Système tétraédral, molécule tétraédrique	109°28'	Méthane $109,5^\circ$  Ion sulfate $109,5^\circ$ 
Molécule pyramidale à base triangulaire	< 109°28'	Ammoniac 
Molécule coudée	< 109°28'	Eau 

Géométrie de la molécule	Ordre de grandeur de l'angle de valence	Structure et ordre de grandeur de l'angle de valence de quelques molécules
Molécule bipyramidale à base triangulaire	120° et 90°	Pentachlorure de phosphore $90^\circ$ $120^\circ$ 
Tétraédre non régulier	< 120° et < 90°	Tétrachlorure de tellure 
Molécule « en T »	< 120° et < 90°	Trifluore de chlore 
Molécule linéaire	180°	Ion triiodure 
Molécule octaédrique	90°	Hexafluore de soufre $90^\circ$ $90^\circ$ 
Molécule pyramidale à base carrée	< 90°	Pentafluore de brome 
Géométrie carrée, plane	90°	Tetrafluore de xénon 