

CHM

E 1 : STRUCTURE ATOMIQUE

- Nucléide : $m \approx Z + A$ (3000 en total)
- Isotopes : $m \approx Z$ mais $N \neq$.
- Masse atomique $\approx A$ une
- Masse molaire atomique = $\frac{\text{masse atomique}}{NA} \times 10^3 = \frac{A}{NA} \times 10^3$ g.mol⁻¹

Charge réduite : $q' = \frac{q}{e}$.

La mole : nbr NA atomes carbone C₆¹² ds 12 g.

$$1 \text{ u} = \frac{1}{NA} \text{ g} = \frac{10^{-3}}{NA} \text{ kg}$$

$$M_{\text{atm}}^X = 12 \times \frac{M_{\text{nucl}}^X}{M_{\text{nucl}}^{\text{C}_6^{12}}}$$

Abondance relative : $M = \sum_i n_i \cdot m_i$

SPECTRE ATOMIQUE espèces hydrogénoides.

- TH maxwell : OEM vs temporelle $\xrightarrow{\text{chp électrique}}$ $\xleftarrow{\text{chp magnétique}}$

$$\lambda = \frac{1}{f} = c \cdot T = \frac{c}{v} = \frac{1}{\bar{v}}$$

$$1 \text{ cm}^{-1} = 10^2 \text{ m}^{-1}$$

$$\bar{v}_{\text{cm}^{-1}} = \frac{10^7}{\lambda_{\text{nm}}}$$

(1)

III théorie quanta & effet photoélectrique

Efft photo Elg: extrac^o / éjic^o électrons
 lux incident $v_i > v_0$: semi + PE.

TH corpusculaire lux : E lux pas répartie uniformément.

$$E = h \nu = h c \cdot \sigma = \frac{hc}{\lambda} = hc \cdot \bar{\nu}$$

W: travail extrac^o.

$$h \cdot \nu_i = W + \frac{1}{2} m_e \cdot v^2$$

$$W = h \cdot \nu_0 = \frac{hc}{\lambda_0}$$

$$v = \sqrt{\frac{2 E}{m_e} (v_f - v_0)}$$

Absorption & Emission photon

$$h \nu = |E_2 - E_{\text{fundant}}|$$

$$\Gamma = \frac{1}{\lambda} = Rn \left(\frac{1}{m^2} - \frac{1}{M^2} \right)$$

TH Bohr: uniq^e électron, se déplace n orbite circulaire
 attenue à \oplus supposée immobile.

$$r = r_m = \frac{e_0 \cdot h^2}{\pi \cdot m^2} \cdot \frac{n^2}{z}$$

$$n = \frac{N}{N_A} = \frac{m}{M} = C \cdot V = \frac{V}{V_m}$$

⚠ moléculas \neq atomes.

C3: Modèle quantique Atome

\rightarrow Lim méca classiq.

\hookrightarrow Modèle quantiq: proba présence.

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

Relat' incertitude Heisenberg: $\Delta x \cdot \Delta p \geq \frac{\hbar}{4\pi m}$

Equa onde: Ψ ; Ψ : \mathcal{D} sign. f. physiq

$$\Psi^2 = \frac{dp}{dv}, \int_v^\infty \frac{dp}{dv} = 1 \int \Psi^2$$

④ \leftrightarrow

$$a_0 = 0,529 \text{ \AA}$$

$$R_H = 1,096 \cdot 10^7 \text{ m}^{-1}$$

$$E_1^H = -13,6 \text{ eV}$$

$$E_m = E_1^H \times \frac{Z^2}{m^2}$$

$$x_m = a_0 \cdot \frac{m^2}{Z^2}$$

$$\sigma = \frac{1}{\lambda} = R_H \cdot Z^2 \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

$$\Delta E = E_1^H \cdot Z^2 \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

③ → INVERSION
③ ↗

$$\left\{ \begin{array}{l} \sum_i a_i = 1 \\ m = \sum_i a_i \times m_i \end{array} \right.$$

a_i abundance relative

(TD)

III. ATOME

III. 1. Eq^o Schrödinger (ES)

$$\Psi(x, \theta, \phi) = \underbrace{R(x)}_{\text{partie radiale}} \cdot \underbrace{\Theta(\theta)}_{\text{partie angulaire}} \cdot \Phi(\phi)$$

Résumé (ES): 3 m^ors quantiques

- || m: quantum principal : $m \in \mathbb{N}$
- || l: qtm azimuthal : $0 \leq l \leq (n-1)$
- || m_l : qtm magnétique : $-l \leq m_l \leq l$.

n	E_n	l	m_l (OA)	Etat quantique	m_s
1	-13,6	0	0	1s [1L]	$+\frac{1}{2}; -\frac{1}{2}$
2	-3,4	0	0	2s [1L]	$+\frac{1}{2}; -\frac{1}{2}$
		1	-1; 0; 1	2p [1 1 1]	$+\frac{1}{2} -\frac{1}{2} +\frac{1}{2} -\frac{1}{2} +\frac{1}{2} -\frac{1}{2}$
3	-1,51	0	0	3s [1L]	:
		1	-1; 0; 1	3p [1 1 1]	:
		2	-2; -1; 0; 1; 2	3d [1 1 1 1]	:
		0	0	4s	:
4	-0,85	1	-1; 0; 1	4p	:
		2	-2; -1; 0; 1; 2	4d	:
		3	-3; -2; -1; 0; 1; 2; 3	4f	:

|| n détermine n° couche électroniq
 l -- " type ss-cche

|| m_l " " m^ors OA. $l=0: s/l=1: p/l=2: d/l=3: f$.

IV

STRUCTURES ATOMIQUES

IV.1. OA 1s

$$\Psi_{1s}(r, \theta, \varphi) = \left(\frac{Z}{a_0}\right)^{3/2} \cdot \frac{1}{\sqrt{\pi}} \cdot e^{\frac{-Zr}{a_0}}$$

↪ ne dépend pas de θ ni φ : symétrique sphérique.

⚠ Étude f ↗ maxima $\Psi' = 0$
minima

Densité volumique proba présence:

↪ proba trouver e^- à distance donnée.

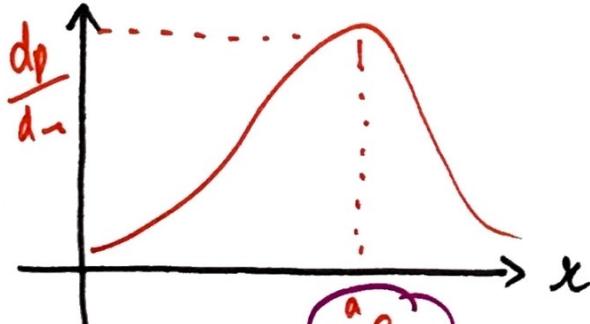
Densité radiale proba présence: $\frac{dp}{dr}$

↪ proba trouver e^- ds élé volume dV compris \leftrightarrow 2 sphères rayons r & $r+dr$

$$\frac{dp}{dr} = \Psi^2 \text{ puis } V = \frac{4}{3}\pi r^3 \Rightarrow \frac{dV}{dr} = 4\pi r^2$$

$$\hookrightarrow \frac{dp}{dr} = \Psi^2 \cdot dV = \Psi^2 \cdot 4\pi r^2 \cdot dr$$

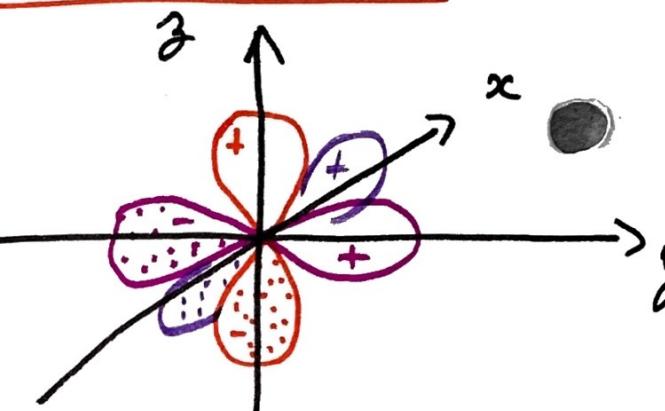
$$\Rightarrow \boxed{\frac{dp}{dr} = \Psi^2 \cdot 4\pi r^2}$$



abscisse r_0 MAXIMUM

IV.2. OA 2p

IV.2. OA 2p



IV/MEV spin : m_s

↪ expér Stern & Gerlach.

$$m_s = +\frac{1}{2} \text{ ou } m_s = -\frac{1}{2}$$

ET4 Configuration Electronique

II Config élec & Règles constru

I.1. Diag E atomes polyélectriques

Énergie (s) < Énergie (p) < Énergie (d)

I.2. Quatre règles

R1 : Aufbau

Si atome E fond.
e⁻ occupent minx
Énergie + bras.

~~2=2~~ He : 1s² ≠ He* : 1s¹ 2s⁰ 2p¹.

R2 : Exclusion Pauli

Deux e⁻ ne peuvent avoir 4 mts quantiques identiques

R3 Régle Hund

Plus e⁻ acceptent avec m énergie, spin e⁻ existent non appariés

R4

Ex 4

Atome q吸收 radiat \Rightarrow Absorp⁺ photon.

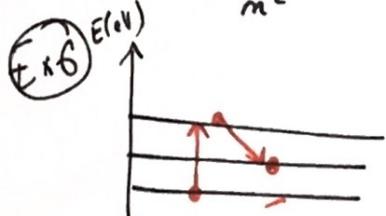
Ionisat⁺ = transis⁺ de $n=1$ à $n=+\infty$.

$$E(\text{eV}) = 1240 / 91,2 \text{ (nm)} = 13,6 \text{ eV}.$$

$$\bullet E_f = -13,6 + 11,3 = -2,32 \rightarrow \text{pas entier niveau } n$$

$$\text{ou } E_n = \frac{-13,6}{n^2} \Leftrightarrow n = \sqrt{\frac{-13,6}{-2,3}} = 2,4 \neq \text{entier}$$

aucune absorpt⁺ possible.



$$E_1 + \frac{1240}{\lambda_1} - \frac{1240}{\lambda_2} = -13,6 + \frac{1240}{91,21} - \frac{1240}{1879} = -1,51$$

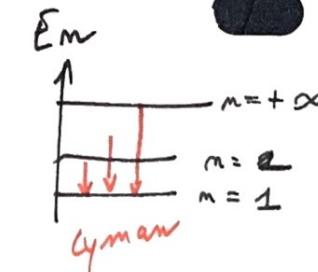
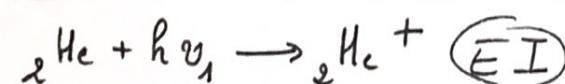
$$\lambda_1: \text{Absorbtion} \quad E_n = \sqrt{\frac{-13,6}{-1,51}} = 3$$

\Rightarrow impossible que $\lambda_2 < \lambda_1$ cad Émission > Énergie absorbée.

+ grande longueur d'onde \Rightarrow petit no^o énergie

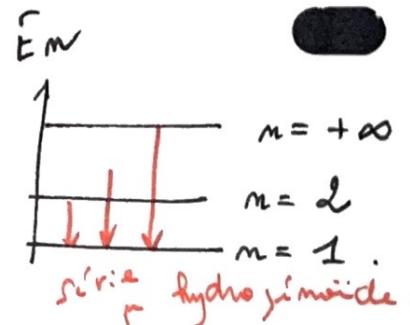
$$\lambda_{nm} = \frac{1}{Z^2 \cdot R_H \left(\frac{1}{n^2} - \frac{1}{m^2} \right)} \quad \text{et } n < m.$$

EI : retrait un SEUL électron SUCCESSIVEMENT.



Si m_i & m_j idntq

$$\frac{1}{\lambda_{\text{Hyd}}} = Z^2 \cdot \frac{1}{\lambda_H}$$



μ H & hydrogénide.

$$\Rightarrow Z = \sqrt{\frac{1/\lambda_{\text{Hyd}}}{1/\lambda_H}} = \boxed{9} \quad \text{Be}^{3+}$$

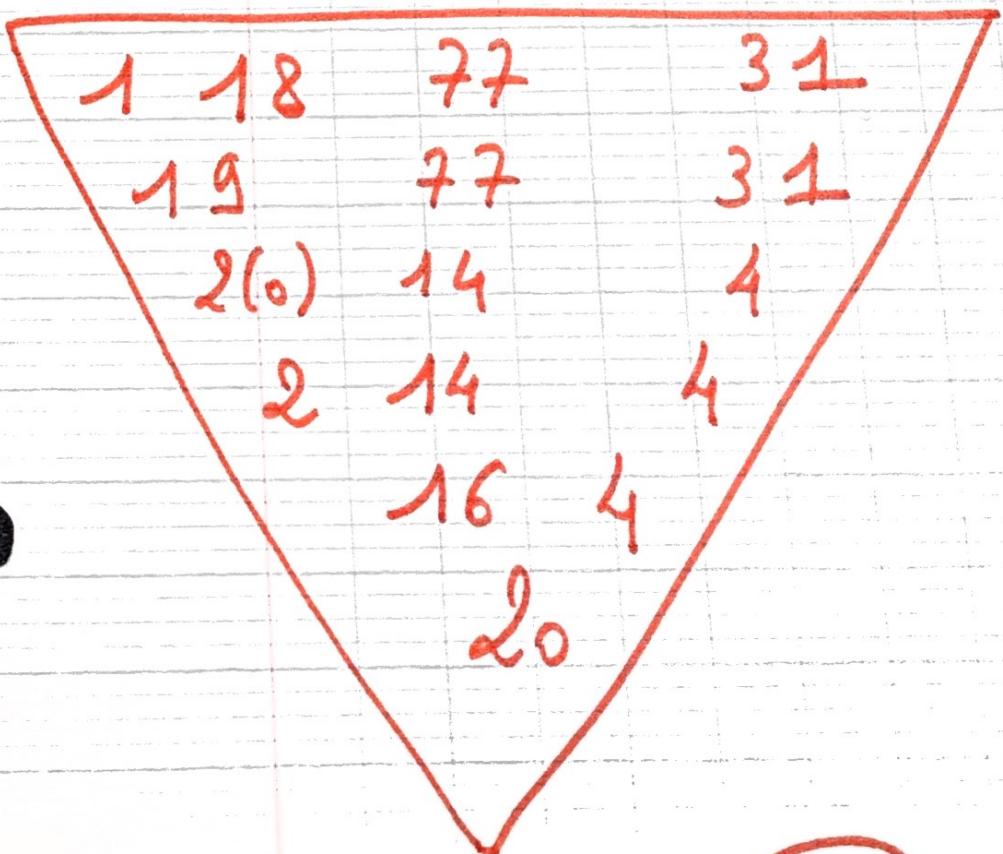
$$\left\{ \begin{array}{l} \sum_i a_i = 1 \\ m = \sum_i a_i \times m_i \end{array} \right.$$

$\sum a_i$
abond
rela

$\lambda(m)$

$$-11 \quad -9 \quad -7 \quad -7 \quad -3 \quad -1$$

γ	x	v	v	IR	μ^0	0
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(TD)

TD.3

Modèle ondulatoire atomique

- 1 particule quantique, on \Leftrightarrow une onde q "guide particule".

$$\lambda = \frac{h}{P} = \frac{h}{m v}$$

cette onde n'est pas PEM, elle ne \rightarrow pas NRJ.

Ex 1 E_C : énergie cinétique $\Rightarrow \lambda$ de Broglie

$$x = \frac{h}{m_p \cdot v} = \frac{h}{m_p \cdot \sqrt{\frac{2 \cdot E_C}{m_p}}} = \frac{h}{\sqrt{2 E_C \cdot m_p}} \approx 1,08 \cdot 10^{-12} \text{ m}$$

$\Delta E_C = 700 \text{ eV} \rightarrow 1,12 \cdot 10^{-16} \text{ J.}$

Ex 2 Principe d'incertitude de Heisenberg

$$\underbrace{\Delta x \cdot \Delta p_x}_{\text{J.s.m}^{-1}} \geq \frac{\hbar}{2} \Leftrightarrow \Delta x \cdot \Delta v_x \geq \frac{\hbar}{4\pi m}$$

$$\Delta p_x = 2,63 \cdot 10^{-22} \text{ J.s.m}^{-1} \quad (1 \text{ J} = 1 \text{ kg} \cdot \text{m}^2 \cdot \text{s}^{-2})$$

$$(v_a = 0,1 c_0)$$

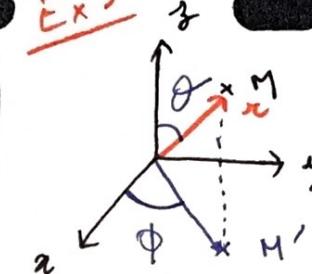
$$\Delta v_x = \frac{\Delta p_x}{m_e} = \frac{2,63 \cdot 10^{-22}}{9,11 \cdot 10^{-31}} \approx 2,9 \cdot 10^8 \text{ m.s}^{-1}$$

$$\Delta v_x = 10 v_a !!! \Rightarrow \text{Aucune précis}^{\circ} \text{e} \text{ de valeur } v_x.$$

(MC) objet $> 10^{-9} - 10^{-8} \text{ m}$

(MQ) objet $< 10^{-9} - 10^{-8} \text{ m}$.

Ex 3

Coord sphériques : x, θ, ϕ .

- $x \in [0, +\infty[$
- $\theta \in [0, \pi]$
- $\phi \in [0, 2\pi]$

$$\Psi_{2p_z}(x, \theta, \phi) = \left(\frac{Z}{a_0}\right)^{3/2} \cdot \frac{1}{4\sqrt{2\pi}} \cdot \frac{Zx}{a_0} \cdot \exp\left(-\frac{Zx}{a_0}\right) \cdot \cos\theta$$

↑ pie radiale $f_{x>0}$

↑ pie angulaire $f_{\theta, \phi}$.

- 1) Ψ_{2p_z} est indép. angle ϕ .
 ↳ m̄ valeur pour $\phi \in [0, 2\pi]$.
- 2) Symétrie révolue p à axe O_z .

- 2) Ψ_{2p_z} est f cosθ. $\rightarrow 0 \leq \theta \leq \pi \rightarrow -1 \leq \cos\theta \leq +1$

si $\theta \in [0, \frac{\pi}{2}] \rightarrow \cos\theta \oplus$ dc $\Psi_{2p_z} \oplus$

si $\theta \in [\frac{\pi}{2}, \pi] \rightarrow \cos\theta \ominus$ dc $\Psi_{2p_z} \ominus$

dc plan xOy symétrie.

Ex H, Z=1 $\Rightarrow \Psi_{2p_z}(x, \theta, \phi) = \left(\frac{1}{a_0}\right)^{3/2} \cdot \frac{1}{4\sqrt{2\pi}} \cdot \frac{x}{a_0} \cdot e^{-\frac{x}{a_0}} \cdot \cos\theta$

$$\Psi_{2p_z}(x, \theta, \phi) = A \cdot x \cdot e^{-\frac{x}{a_0}} \cdot \cos\theta.$$

- 3) Densité volumiq proba présence :

$$R(x, \theta) = |\Psi_{2p_z}(x, \theta=0)|^2$$

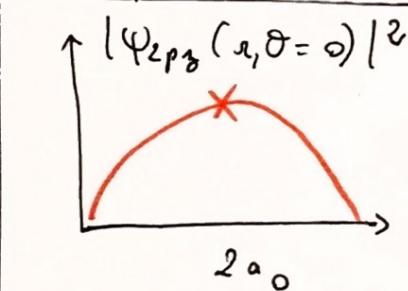
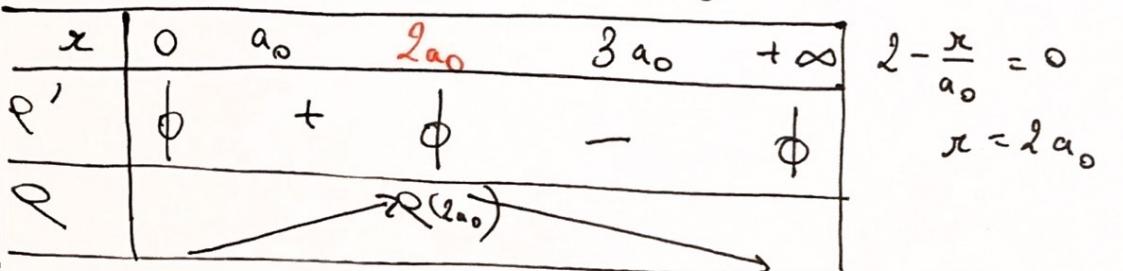
Si long. axe $O_z \Rightarrow \theta=0$

$$R(x, \theta=0) = |\Psi_{2p_3}(x, \theta=0)|^2 = A^2 \cdot x^2 \cdot \left(e^{-\frac{x}{a_0}}\right) \cdot \cos^2(0)$$

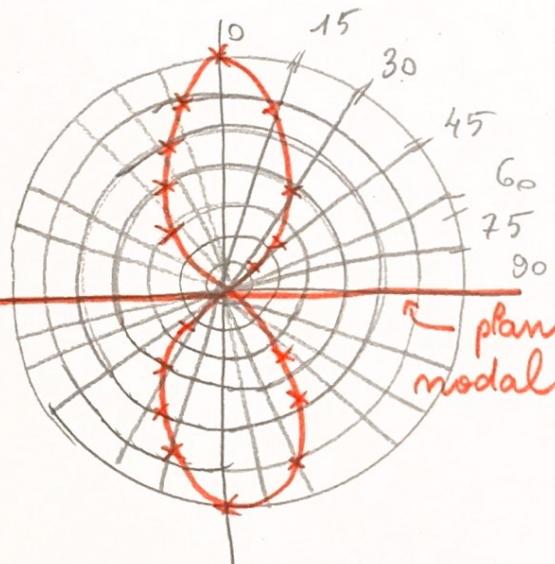
$$R(x, \theta=0) = \underbrace{A^2 \cdot x^2}_{\text{u}} \cdot \underbrace{e^{-\frac{x}{a_0}}}_{\text{v}}.$$

$$R'(x, \theta=0) = 2A^2 x \cdot e^{-\frac{x}{a_0}} + \left(-\frac{1}{a_0}\right) \cdot e^{-\frac{x}{a_0}} \cdot A^2 x^2$$

$$R'(x, \theta=0) = A^2 x e\left(\frac{-x}{a_0}\right) \left[2 - \frac{1}{a_0} \times x \right]$$



θ	$\cos^2 \theta$	Graph pol r
0	1	20
15	0,933	18,66
30	0,75	15
45	0,50	10
60	0,25	5
75	0,167	3,33
90	0	0



Courbe d'«densité» \Rightarrow densité
 \Rightarrow valeur r $\Rightarrow R(x_{\max}, \theta) = 3 \cdot \cos^2 \theta$.

$$E = h\nu = \frac{hc}{\lambda} / \text{Brégaglie} = \lambda = \frac{\hbar}{P} = \frac{\hbar}{mV}$$

$$\Delta E = Z^2 \cdot E_1^4 \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

$$\nabla = \frac{1}{\lambda} = Z^2 \cdot R_H \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

$$1u = \frac{1}{M_A} g = \frac{10^{-3}}{M_A} \text{ kg}$$

$$E(\text{eV}) = \frac{1240}{\lambda(\text{nm})}$$

$$r_n = a_0 \cdot \frac{m^2}{Z^2}$$

$$E_m = E_1^4 \cdot \frac{Z^2}{m^2}$$

$$W = h\nu_0 \quad \& \quad h\nu_i = W + \frac{1}{2} m e V^2$$

$$M^X (\text{cma}) = \frac{M^X \text{néeille}}{M^{C_6} \text{néeille}} \quad \left| \quad m = \frac{N}{N_A} = \frac{m}{M} = \frac{V}{V_m} = C.V \right.$$

$$\sum_i a_i = 1$$

$$m = \sum a_i \times m_i$$

$$E_{\text{incidente}} = W + E_C$$

$$v = \sqrt{\frac{2E_C}{m}}$$

+ grande $\lambda \Rightarrow + \text{petite } r \gg E.$

$$\begin{array}{ccccccc} 1 & 9 & 7 & 3 & 1 & & \lambda \\ 2 & 1 & 4 & 3 & 1 & & \\ 16 & 4 & & & & & \\ 30 & & & & & & \end{array}$$

$$1 \text{ cm}^{-1} = 10^2 \text{ m}^{-1}$$

$$a_0 = 0,529 \text{ \AA}$$

$$R_H = 1,096 \cdot 10^{-7} \text{ m}$$

$$E_1^4 = -13,6 \text{ eV}$$

$$\frac{L_B}{D_p}$$

$$\dots \rightarrow \infty$$

$$E_f = E_i + E_{\text{photon abs}}$$

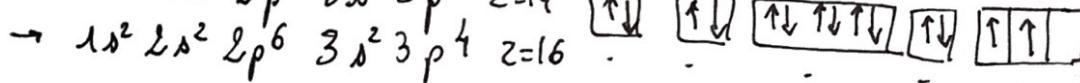
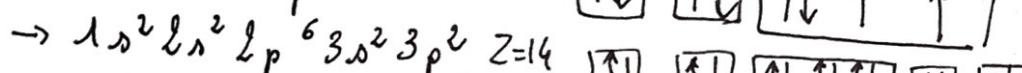
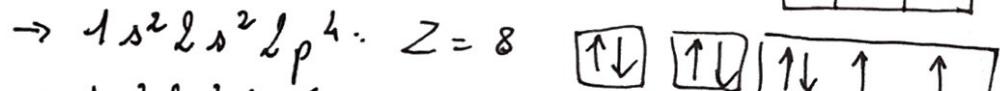
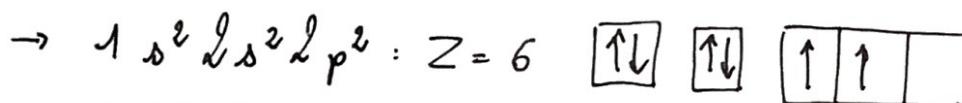
$$\text{si } E_f > E_i$$

\Rightarrow perte ionisante en libérant E_C

$$I_{\text{ionisa}} = t_{\text{transis}} \frac{m=+\infty}{m=1}$$

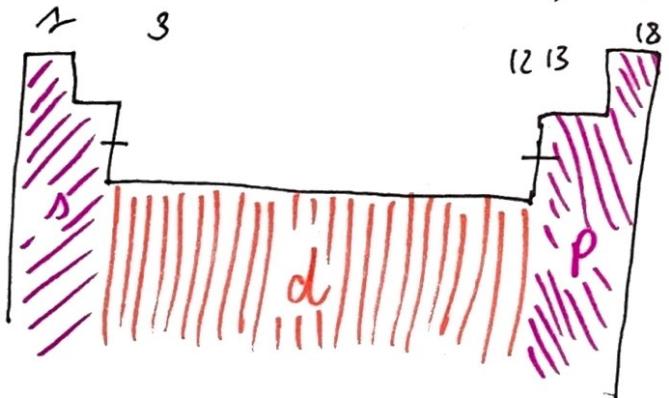
- $\cdot 53 \text{ B} : 1s^2 2s^2 2p^1 \rightarrow n=2 \Rightarrow 2^{\circ} \text{ période}$
 $3e^- \text{ de valence} + \text{bloc d} \rightarrow c^{1n} 13$
- $\cdot 53 \text{ I} : [\text{Kx}] 5s^2 4d^{10} 5p^5 \rightarrow n=5 \Rightarrow 5^{\circ} \text{ période}$
- $\cdot 27 \text{ Co} : [\text{Ar}] 4s^2 3d^7 \rightarrow n=4 \Rightarrow 4^{\circ} \text{ période}$
 $g e^- \text{ valence dc bloc d colonne g}$

X : moins $18 e^-$; $2 e^-$ célibat Rs



\hat{m} groupe sélénum : $16 : p^{18-2} = p^4$

\hat{m} période sodium: $n=3 \Rightarrow X: [\text{Ne}] 3s^2 3p^4$



TD.5

Th. Slater

$$Z_i^* = Z - \sum_j \tau_{ij} \quad E_{nl} = \frac{-13,6 \cdot Z^2}{n^2} \quad r_{n,l} = a_0 \cdot \frac{n^2}{Z^*}$$

1 Cl : $1s^2 2s^2 2p^6 3s^2 3p^5$

$$Z_{1s}^* = 17 - 1 \times 0,3 = 16,7 \quad Z_{2s2p}^* = 17 - 7 \times 0,35 - 2 \times 0,85 = 12,85$$

$$Z_{3s3p}^* = 17 - 6 \times 0,35 - 8 \times 0,85 - 2 \times 1 = 6,1$$

$$E_{1s} = -13,6 \left(\frac{16,7}{1} \right)^2 = -3792,9 \text{ eV} \quad | \quad E_{2s2p} = -13,6 \left(\frac{12,85}{2} \right)^2 = -561,4 \text{ eV}$$

$$E_{3s3p} = -13,6 \left(\frac{6,1}{3} \right)^2 = -56,23 \text{ eV}$$

$$E_{\text{tot}}(\text{Cl}) = 2E_{1s} + 8E_{2s2p} + 8E_{3s3p}$$

$$E_{\text{tot}}(\text{Cl}) = -12470,77 \text{ eV}$$

$$r_{1s} = 0,53 \times \frac{1^2}{16,7} = 3,17 \cdot 10^{-2} \text{ \AA} \quad ; \quad r_{2s2p} = 0,165 \text{ \AA} \quad ; \quad r_{3s3p} = 0,782 \text{ \AA}$$

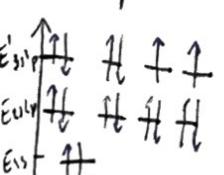
Valeur théorique : $1,988 \text{ \AA}$: dista \leftrightarrow 2 Cl $\rightarrow r_{\text{exp}} = 0,994 \text{ \AA}$

Rayon 1 seul atome Cl : $r_{3s3p} = 0,782 \text{ \AA}$

Calcul erreur incertitude $\leftrightarrow r_{\text{th}} \& r_{\text{exp}}$

Cl⁺ : $1s^2 2s^2 2p^6 3s^2 3p^4$

$$E'_{3s3p} = -13,6 \left(\frac{6,45}{3} \right)^2 = -62,9 \text{ eV} \quad \text{avec } Z'_{3s3p} = 17 - 5 \times 0,35 - 8 \times 0,85 - 2 \times 1$$



Énergie
Imisac

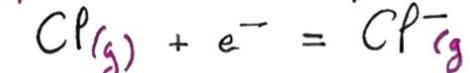
$$\boxed{\text{Enréaction} = E_{\text{produit}} - E_{\text{réactif}}}$$

$$EI_1 = E_{\text{tot}}(\text{Cl}^+) - E_{\text{tot}}(\text{Cl})$$

$$EI_1 = 19 \text{ eV}$$

2 AE

Affinité électronique : Atome qui capte un e^- .



$$AE = E_{\text{produit}} - E_{\text{réactif}} = E_{\text{tot}}(\text{Cl}^-) - E_{\text{tot}}(\text{Cl})$$

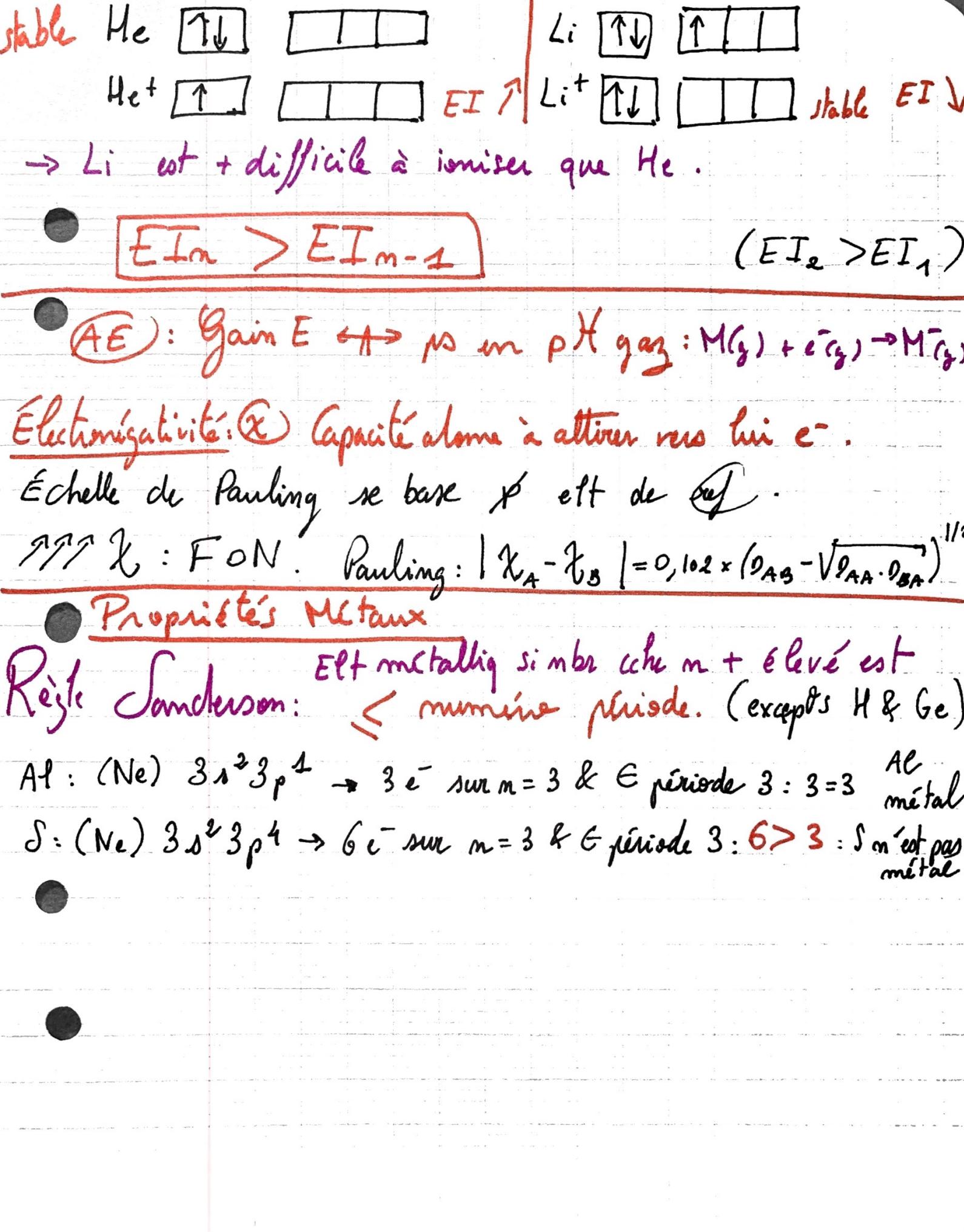
$$AE = 2E_1 + 8E_2 + 8E'_3 - (2E_1 + 8E_2 + 7E_3)$$

$$AE = 8E'_3 - 7E_3 = -6,07 \text{ eV}$$

3 Première Potentiel Ionisant $\Leftrightarrow EI$

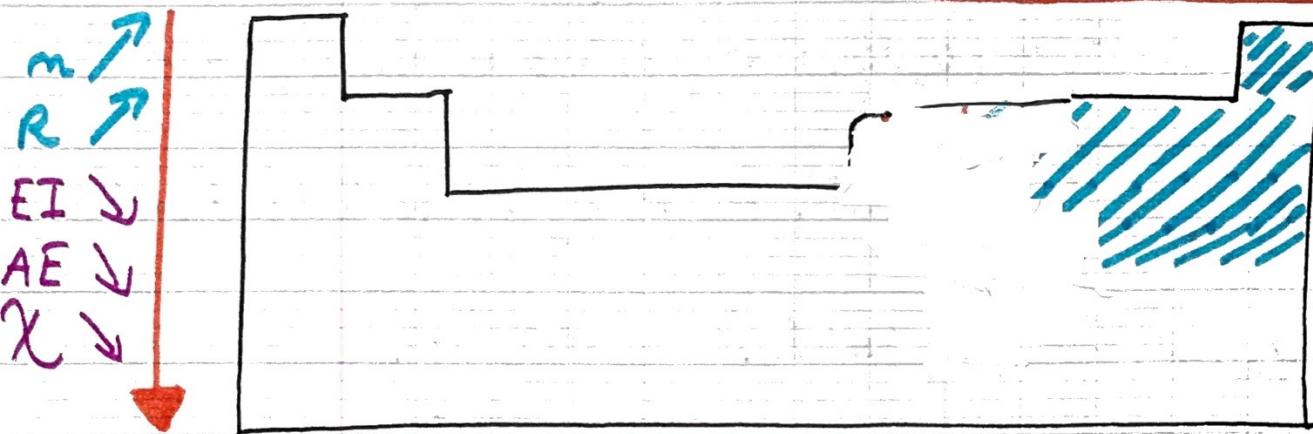


$$dP_a = 6,022 \cdot 10^{23} \text{ mol}^{-1}$$



C6 : Propriétés Éléments

$Z \uparrow, Z^* \uparrow, EI \uparrow, AE \uparrow, \chi \uparrow, R \downarrow$



- $Z^* \geq 0,65$ de colonnes en colonnes.

III. 3. Cas Rayons Ioniques

cation: arracher e^- : $\downarrow \Sigma$ anion: ajoute e^- : $\uparrow \Sigma$
 $Z^* \uparrow$ $Z^* \downarrow$.

$$x(M^{n+}) < \dots < x(M^{3+}) < \dots < x(M)$$

$$x(M) < \dots < x(M^{2-}) < \dots < x(M^{n-})$$

IV. Évolut. énergie 1° ionisat.

EI E nécess^{re} pr ARRACHER e^- à l'attrac^{teur} de son n

EI : évolut. inverse de R .

Atomes dt dernière M^{-cche} est remplie et réempie gagn^t en STABILITÉ.
 → leur EI est + forte qu'attendue.

C2 : Liaison chimiq: modèle empiriq

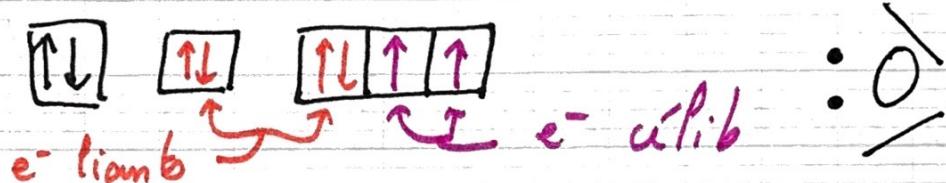
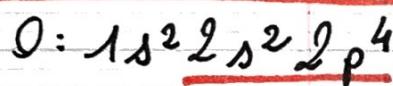
I / Représentat^o S^{ce} électroniq molécules

I.1. Liaison chimiq ?

Liaison Chimiq : résulte int^os coulombiens stab \leftrightarrow 2 ato_g.

► forme^s liaison covalente : stabilisat système.

I.2. [M] Lewis



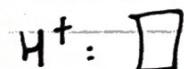
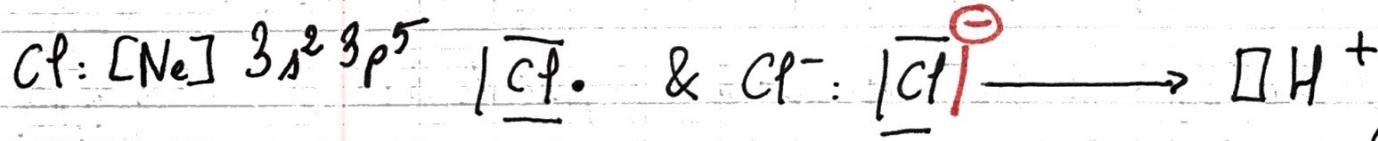
Rq: C* à état fondamental n'est pas tétravalent.

Valence : nbr liaisons q atome est dansⁱ pt former de molécule

Valce = 1: monovalent ; 2: bivalent ; 3: trivalent ; 4: tétravalent

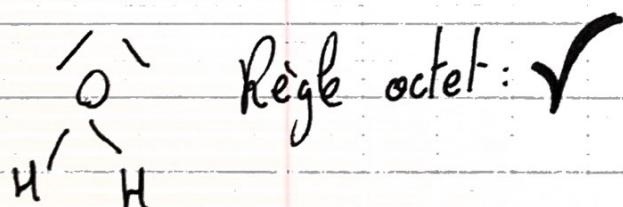
Liaison covalente : mise en commun doublet e⁻ : $A + B \rightarrow A - B$

Lias. covalente dative ou coordinat : $A + \square B \rightarrow A - B$



lacune électrig

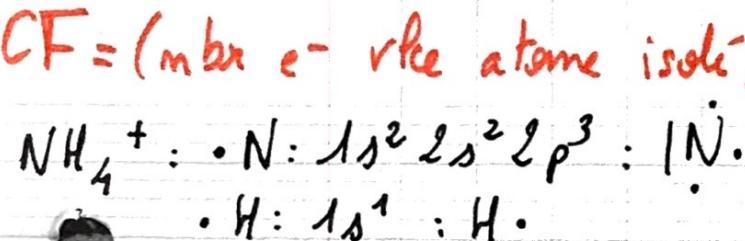
Règle octet: Atomes doivent être entourés 8 e⁻ au total (le⁻ pr He)



Règle octet: ✓

Charge Formelle (CF) atome

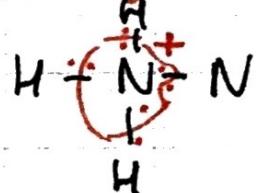
vale entourant cet
atome isolé) - (nbr e⁻ atome de molécule)



$\text{nbr e}^- \text{ vla total} = \sum \text{e}^- \text{ vla chq atome} - \text{charge}$
 $= 5 + 4 \times 1 - 1 = 8$

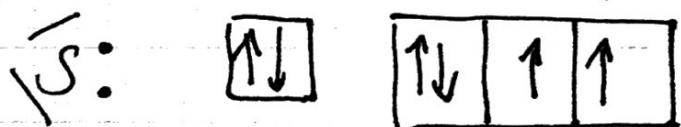
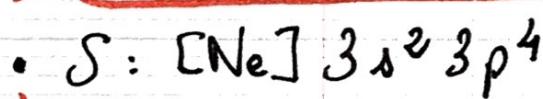
$\text{CF}(\text{N}) = 5 - 4 = 1 \Rightarrow \text{de charge} \oplus \text{sur N}.$

$\text{CF}(\text{H}) = 1 - 1 = 0$

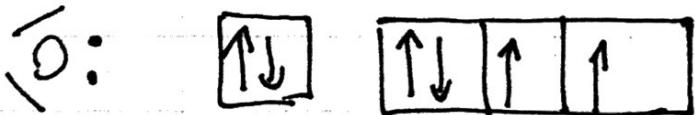
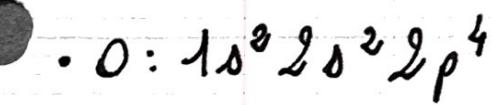


M obtenu à Lewis

@ SO_4^{2-}

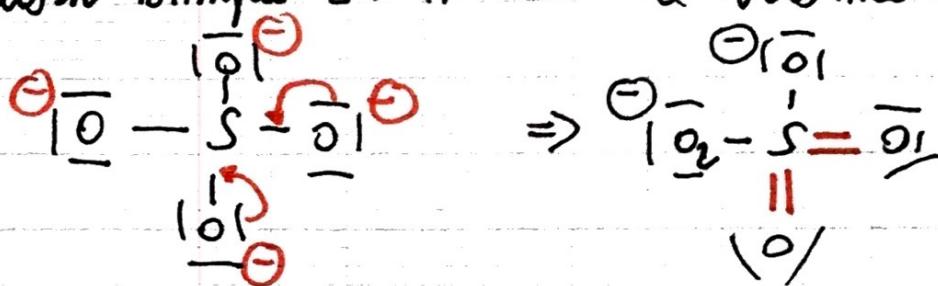


1)



2) nbr total e⁻ vla = $6 + 4 \times 6 - (-2) = 32$ e⁻ vla (16 dblt)

3) Liaison simple \leftrightarrow Atm. liée & voisins



$\text{CF}^{(s)}_{\text{O}} 6 - 6 = 0 \quad \& \quad \text{CF}(\text{O}_1) = 6 - 6 = 0 \quad \text{CF}(\text{O}_2) = 6 - 7 = -1$

Degré oxydat: @ $O: 1s^2 2s^2 2p^4$:

- 1) $+2e^- \rightarrow$ config Ne: - **II** (N.O.)
- 2) $-4e^- \rightarrow$ config He: + **IV** (N.O.)

Mésomérie: écriture ss plus f^{ms} (Lewis)

Hybride de résonance: molécule réelle est moy f^{ms} mésomériques.

M VSEPR : Valence Shell Electron Pairs Repulsion

$A X_m E_n$

mbt dbts non-liaants

mbt liaisons

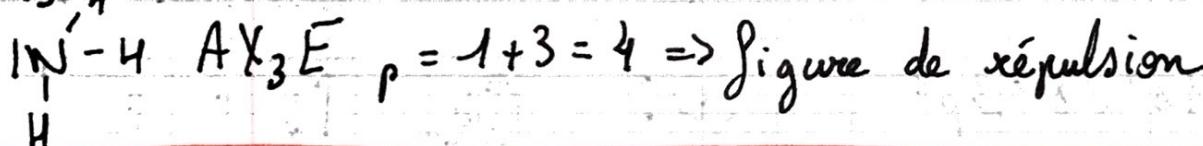
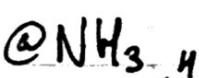


Figure répulsion: géo spatiale adaptée par dbts liaints & non liaints.

$$P = n + m$$

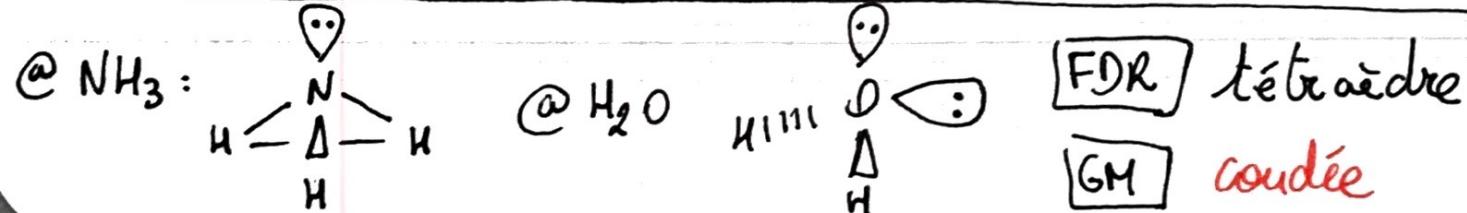
S^{∞} Lewis $\rightarrow F^{\infty}$ VSEPR \rightarrow Figure répul \rightarrow Géo moléculaire

$p=2$ (linéaire 180°) / $P=3$: $\begin{array}{c} \text{N} \\ | \\ \text{H} \end{array} 120^\circ / p=4$: tétraèdre: $109,5^\circ$

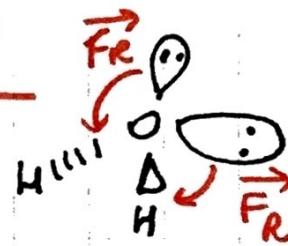
$p=5$ (Bipyramide base triangulaire: $120^\circ, 90^\circ, 180^\circ$) / $P=6$: octaèdre $90^\circ, 180^\circ$

• ϕ dbts. n'autour A: **FDR = GM** (géo moléculaire)

• GM déduit emplacement dbts liants du FDR



Facteurs influençants GM



→ Infle dbt non liant
(ou e⁻ célib)

→ Infle ≠ e χ : DL \downarrow qd $\chi \uparrow$.

NB: DNL pas impliqué ds liaison dc + répulsif.

→ Infle liaisons (\vec{F}_R (liaison dble) $\gg \vec{F}'_R$ (liaison simple))

$\mu = q \cdot d$ direct $\vec{\mu}$: du plus électrogt. au moins électrogt.

$q = f \cdot e$ • $\vec{\mu}$ en C.m ou D (Debye) $1D = 3,33 \cdot 10^{-30} \text{ C.m}$

% $I_{AB} = 100 \cdot \frac{\mu}{ed} = 100f$]: Ionicité liaison

$$\vec{\mu}_{\text{tot}} = \sum_i \vec{\mu}_i$$

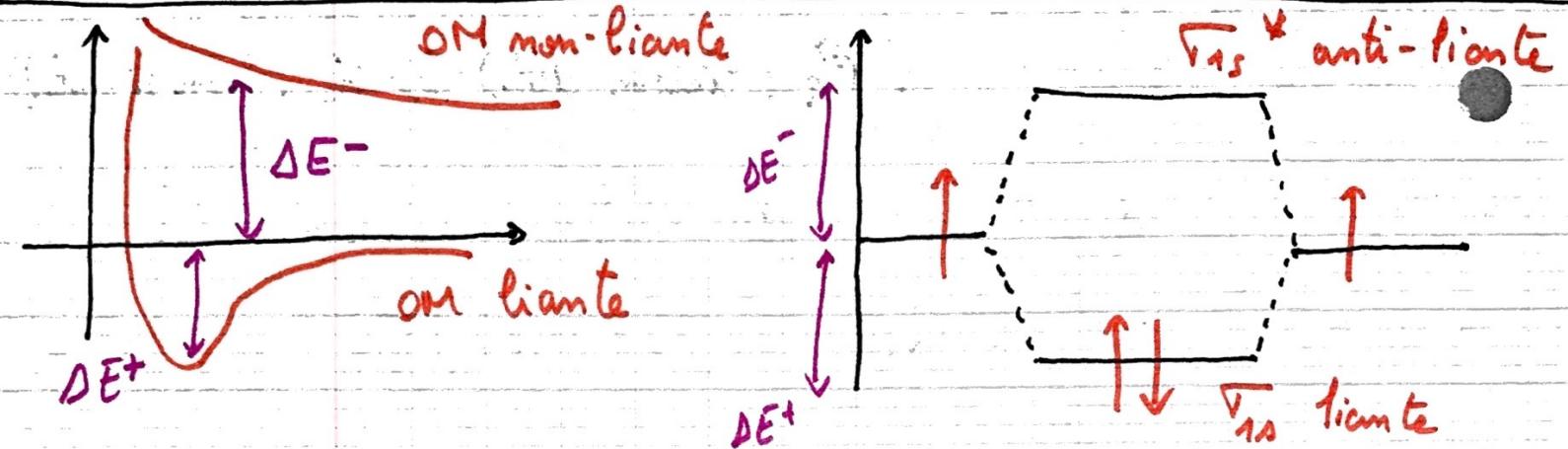
$$@ \vec{\mu}_{H_2O} = 2 \vec{\mu}_{OH} \cdot \cos\left(\frac{\alpha}{2}\right)$$

C8: quantiq liaison chimiq : OM

Diamagnétiq: $\uparrow\downarrow$ / Paramagnétiq: $\uparrow\uparrow$ m̂ sens chp magnétiq

quantiq liaison chimiq: recvr + OA.

$$\Psi_i = \sum_j c_{ij} \cdot \Psi_j \quad (\text{psi: OM e}^- / c: \text{coeff Emiss}/ \Psi: \text{OA}).$$



Indice de liaison:

$$m_p = \frac{1}{2} (n - n^*)$$

nbr e- OM liante

OM mp

- OM liante: n̄m̄ - t 2OA m̄ signe.

- OM ml: n̄t. 2OA ≠ s signes.

(R axial: τ / R lat: π).

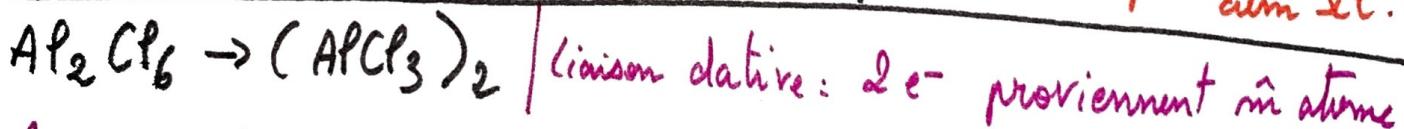
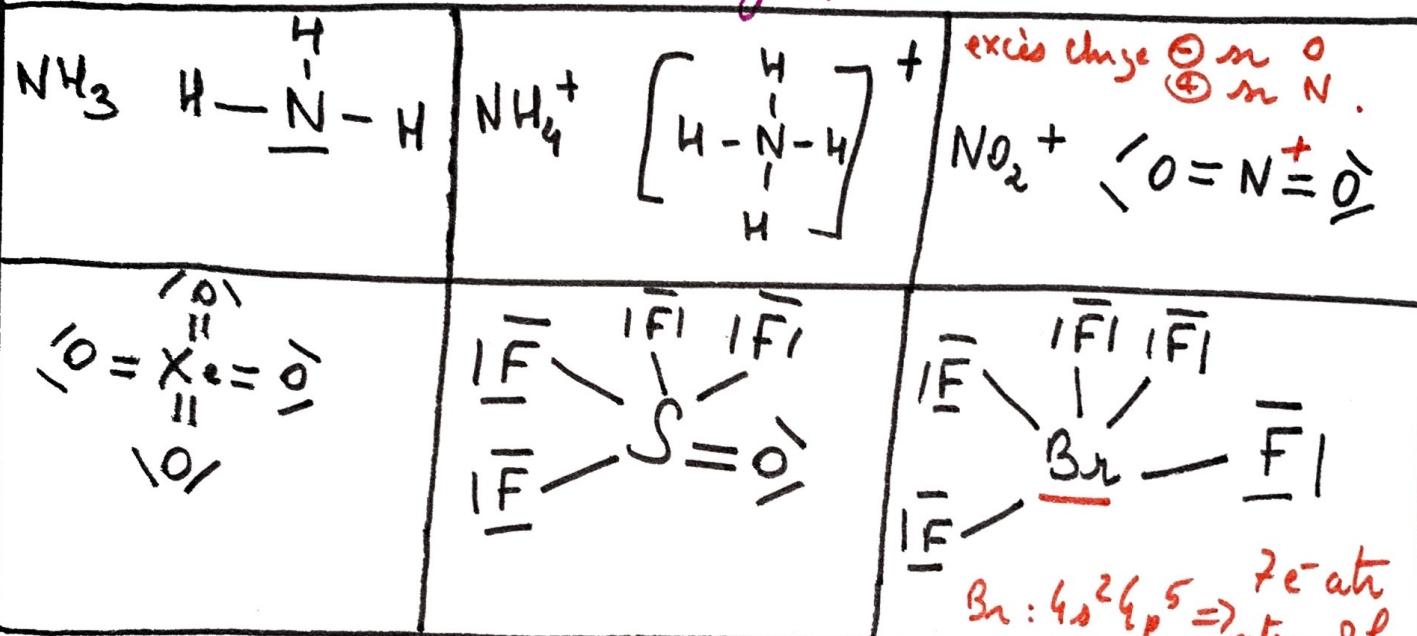
TD 7

Liaison covalente: modèle empirique.

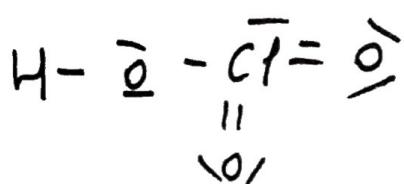
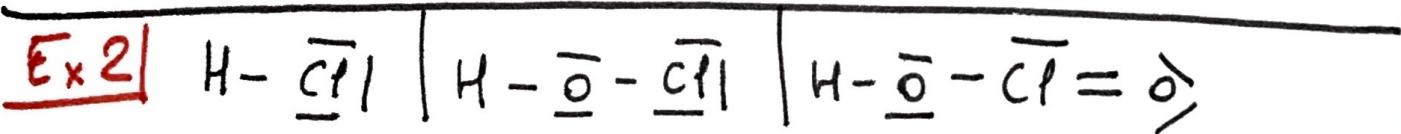
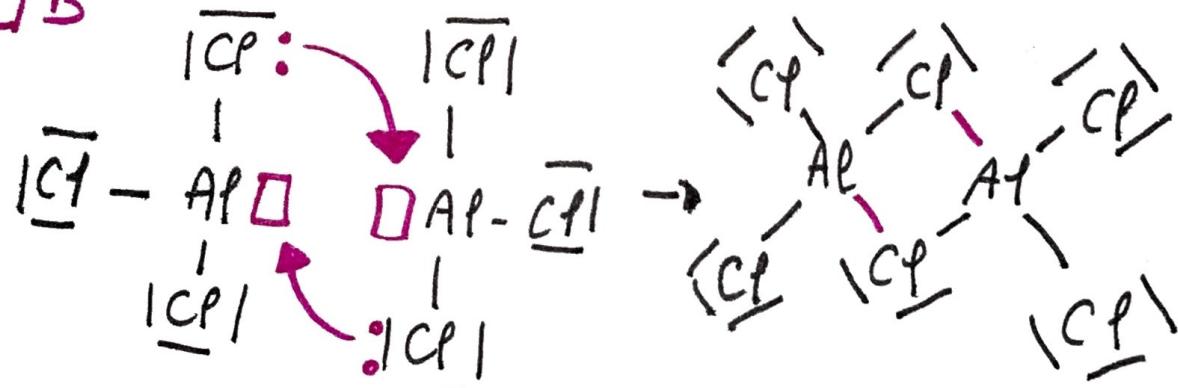
Liaison forte: partage en commun de e^- parmi chacun des atomes.



Atome central: moins électronegatif.



A: B

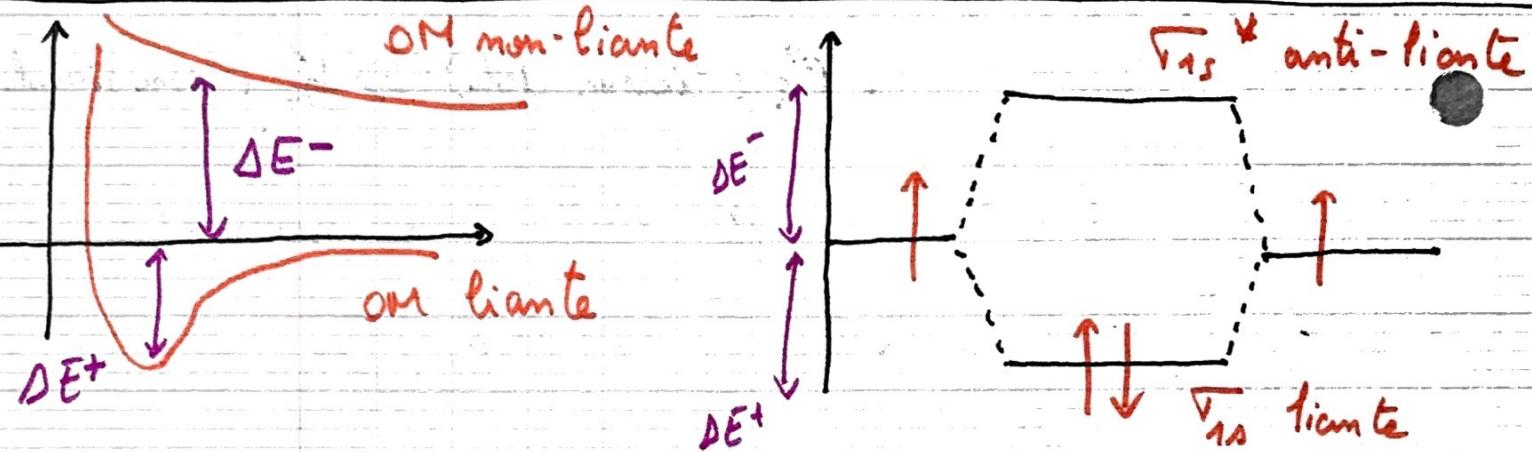


C8: **M** quantiq liaison chimiq : OM

Diamagnétiq: $\uparrow\downarrow$ / Paramagnétiq: $\uparrow\uparrow$ m̂ sens chp magnétiq

M quantiq liaison chimiq: recouvert OA.

$$\Psi_i = \sum c_{ij} \cdot \Psi_j \quad (\text{psi: OM e- / c: coeff Emiss/ } \Psi: \text{OA})$$



Indice de liaison:

$$m_p = \frac{1}{2} (n - n^*)$$

nbr e- OM liante

OM mp

• OM liante: nem - t 2OA m̂ signe.

• OM ml: n^t. 2OA \neq s signes.

(R axial: σ / R lat: π).

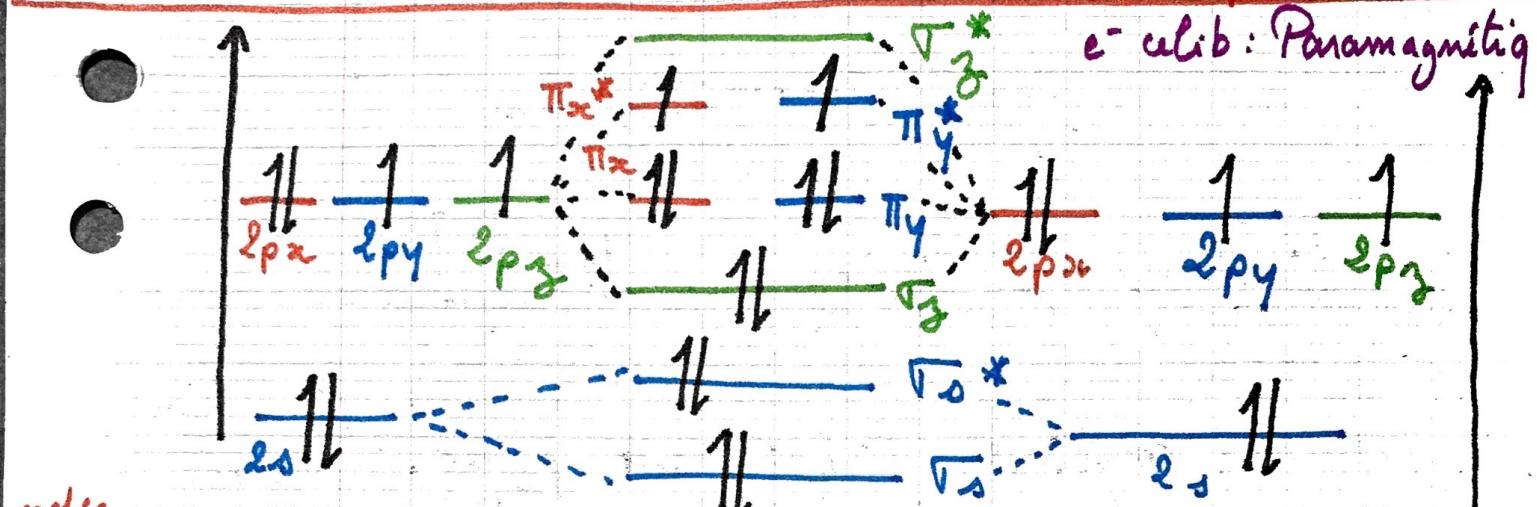
	0	0	$1s + 1s$
σ	∞	∞	$2p_x + 2p_y$
σ^*	0	0	$1s - 1s$
	∞	∞	$2p_x - 2p_y$
π	8	8	$2p_x + 2p_z$
	0	0	$2p_y + 2p_z$

π^*	8	8	$2p_x - 2p_z$
	0	0	$2p_y - 2p_z$
NL	0	8	$1s + 2p_z$

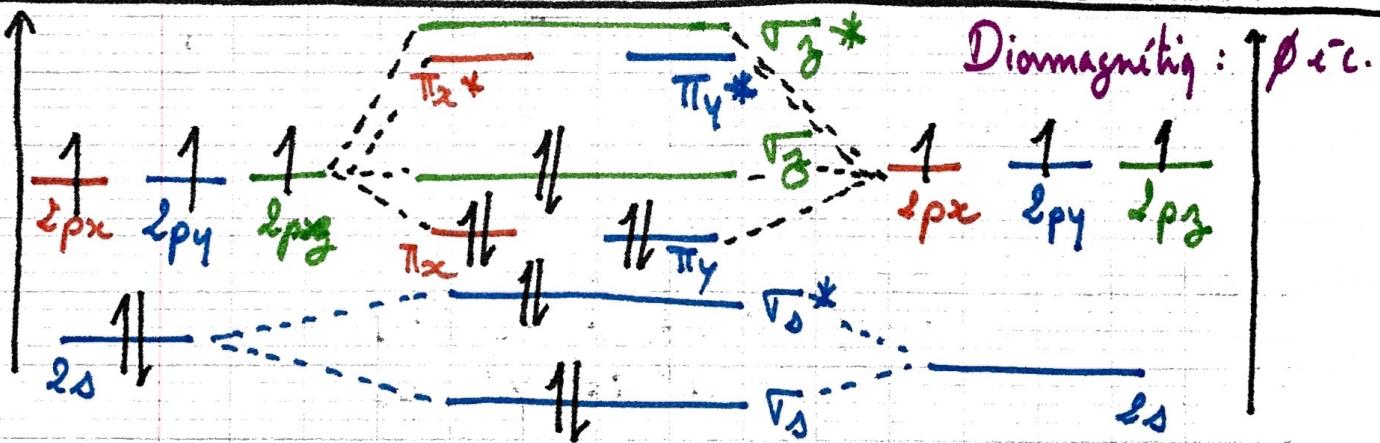
Règles de remplissage

→ Règle Pauli : OM ne doit pas avoir + 2 e⁻.

→ Règle Hund : 1 e⁻ ds chq OM m^l E tant q possible.

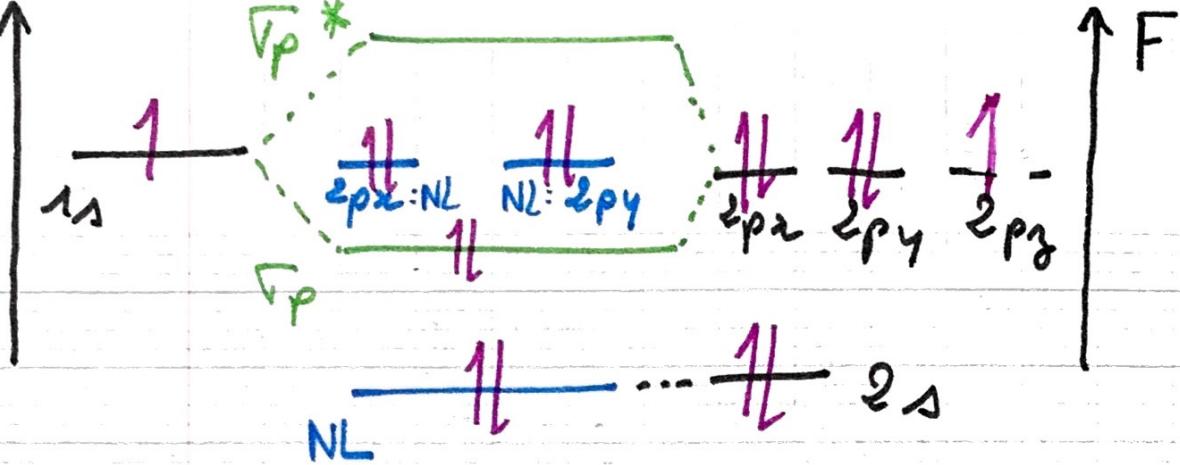


^{molée}
Itération : $m_f = \frac{1}{2} [n_{\text{liante}} - n_{\text{non-liante}}] = \frac{1}{2} [8 - 4] = 2 \quad (O=O)$



⚠ INVERSION σ_3 & π_x, π_y .

molécule N₂ : $(\sigma_3)^2 (\sigma_3^*)^2 (\pi_x)^2 (\pi_y)^2 (\sigma_3)^2$.

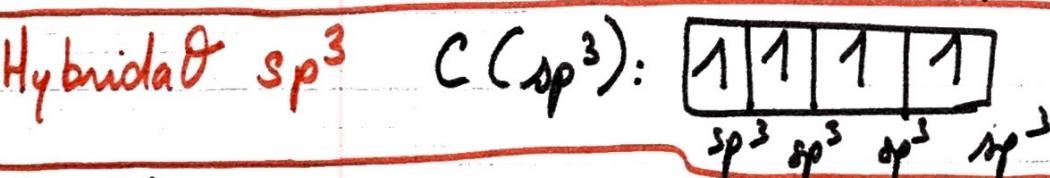
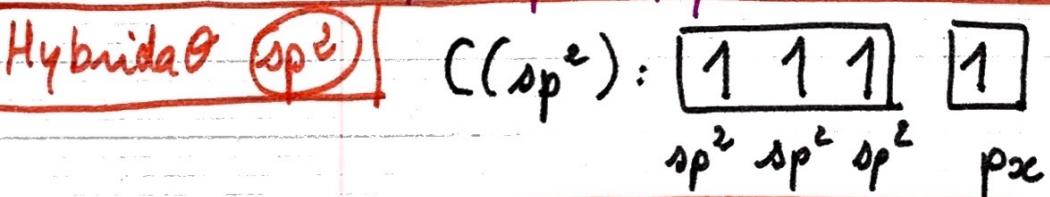
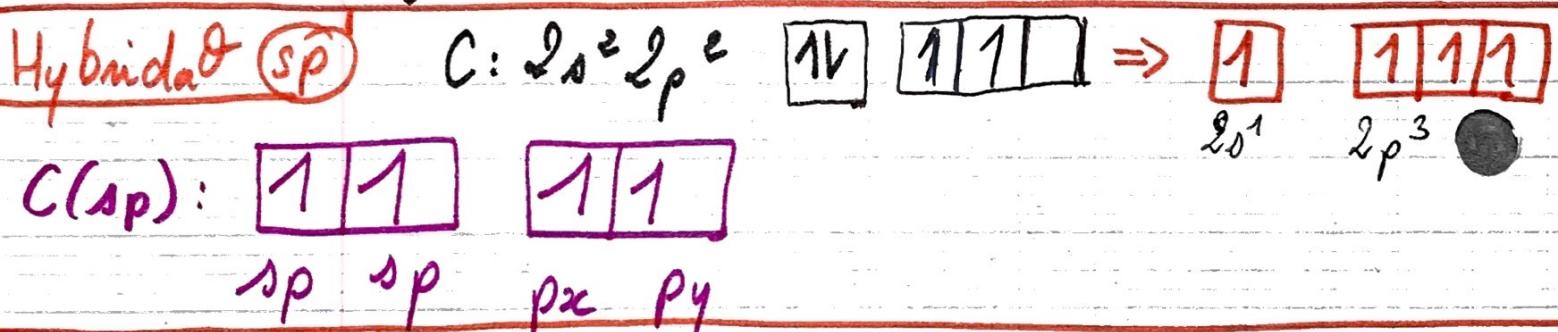


$$m_f = \frac{1}{2}(2-0) = 1 \text{ liaison} \quad H - \overline{F}$$

III / Hybridation Orbitales Atomiques

• **Hybridation**: combiner linéaire OA pures.
 (nouvelles OA hybrides doivent rendre GM).

(O hybrides :
 agpt axiaux)

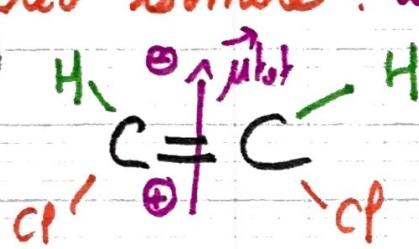


H ⁰	OA connis	OA pure mnh. (H)	FDR	FF brutes
sp	s, p_z^*	p_x, p_y^*	linéaire	AX_2
sp^2	s, p_y, p_z^*	p_x^*	trig ² plane	$AX_3, AX_2 E$
sp^3	s, p_x, p_y, p_z	—	tri tétraédrique	$AX_4, AX_3 E, AX_2 E_2$
sp^{3d}			BET	
sp^{3d^2}			BBC	

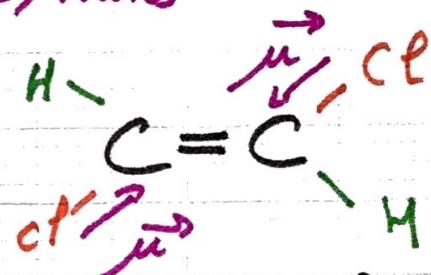
Cg : Isomérie & Représentation spatiale moléculaire

- Isomères : même FF brute peut \Leftrightarrow plans FF semi-diff.
- FF constitutionnelles : même FF b. MS FF sd \neq | • FF positionnelles
 - FF chaîne : nbr carbones \neq s | • FF fonction.

Stereo-isomère : cis (Z) | (E) trans



$$\mu = 1,89 \text{ D} \\ T_{eb} = 60^\circ\text{C}$$



$$\mu = 0 \text{ D} \\ T_{eb} = 48^\circ\text{C}$$

C10 : Interactions faibles $\approx \text{kJ.mol}^{-1}$

- liaisons covalentes : liaisons fortes

\vec{F} Keesom \leftrightarrow 2 molécules polaires (dipôle-dipôle)

\vec{F} Debye \leftrightarrow mol polaire / mol non polaire (dipôle-dipôle induit)

\vec{F} London \leftrightarrow 2 molécules non polaires (moment dipol^{instan})

→ Keesom lié à intensité μ .

→ Debye : $\vec{\mu}_{\text{induit}} = \omega \cdot \vec{E}$ (\uparrow si $\mu(A) \uparrow$)

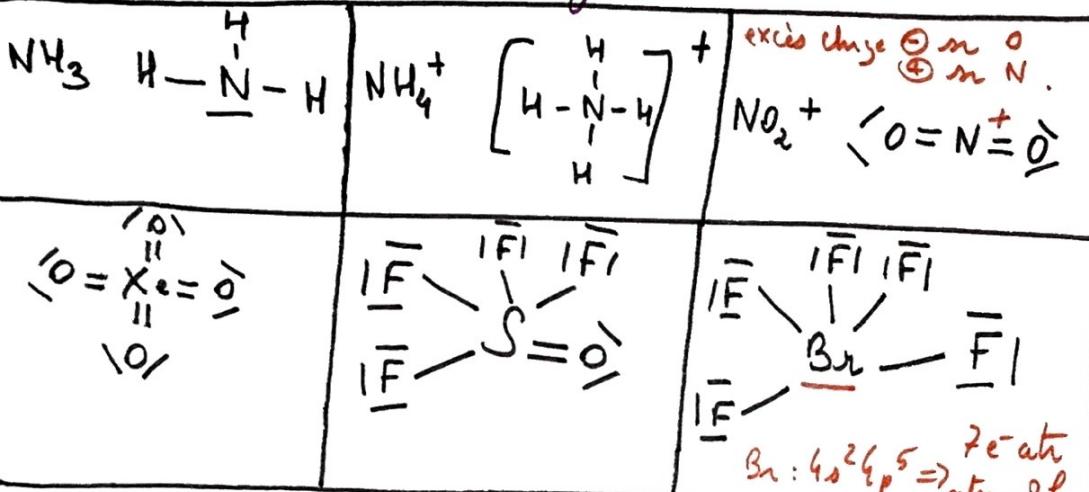
→ London : $F_{LD} \uparrow$ qd masse moléculaire \uparrow . jamais NULLE

TD 7 Liaison covalente: modèle empirique.

Liaison forte: mis en commun de e^- parmi chacun des atomes.

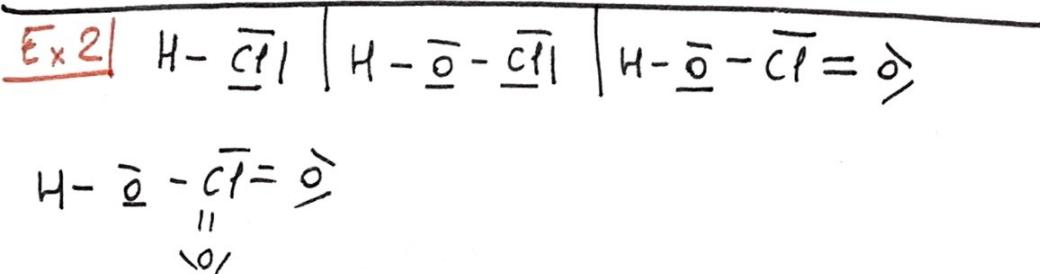
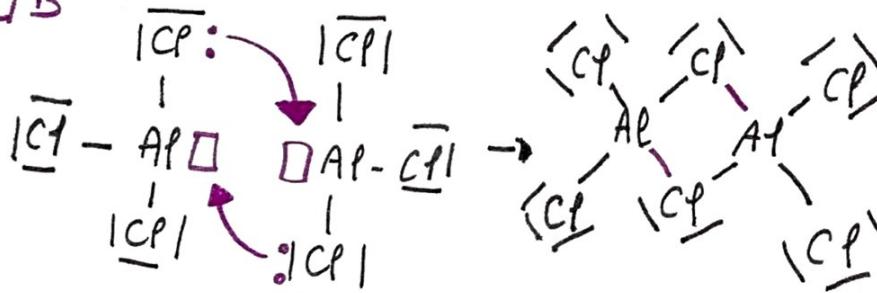


Atome central: moins électronégatif.

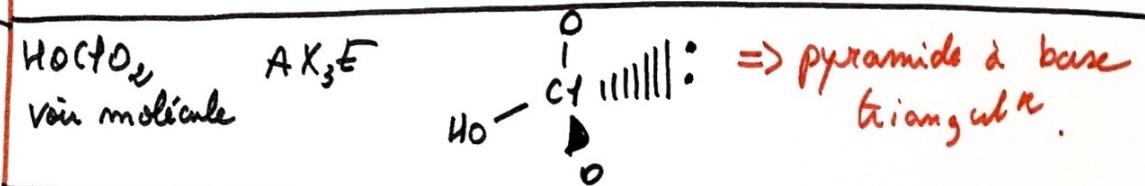
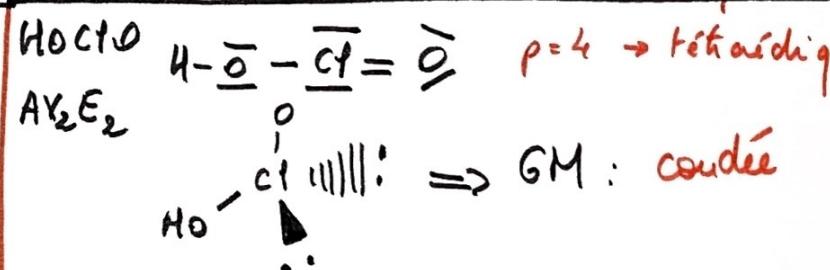
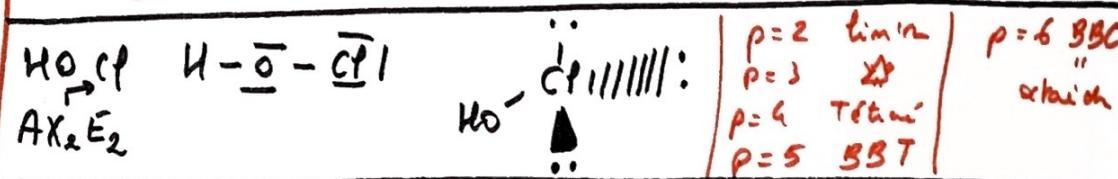


$Al_2Cl_6 \rightarrow (AlCl_3)_2$ | liaison dative: 2 e^- proviennent d'un atome

A: B



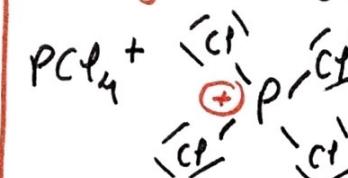
3) GM B méthode VSEPR
 $(CP): AX_3E_3$ H-CP $\begin{matrix} X \rightarrow \text{nbr atomes + proches} \\ E \rightarrow \text{nbr dits NL.} \end{matrix}$



Ex 3 | P: $[Ne] 3s^2 3p^3 \rightarrow$ Vlce max 5.

PCl_n probables? or CP: monovalent

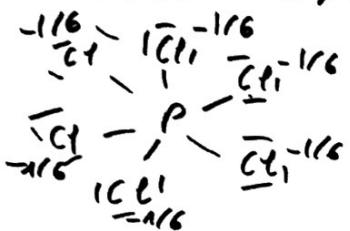
PCl_3 & PCl_5 + probables.



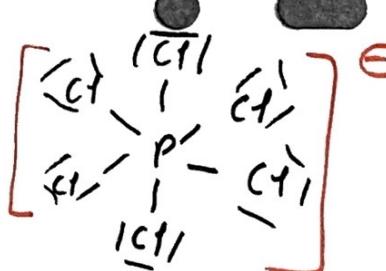
$f(Cl) > f(P) \Rightarrow \oplus \text{ sur P.}$ de excès charge

Suite Ex 3.

VSEPR \rightarrow (P): AX_6

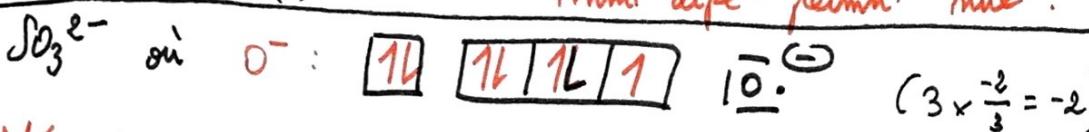
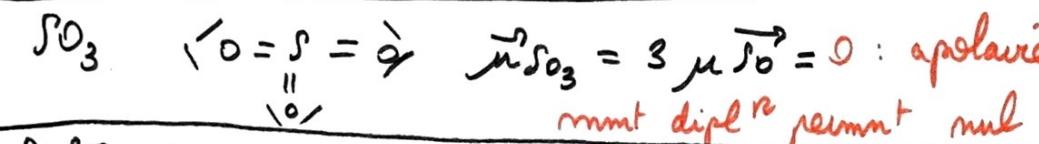
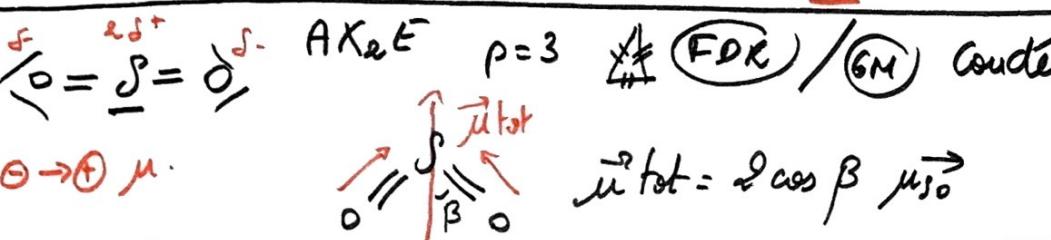


AX_6 : BBC (Octaèdre)

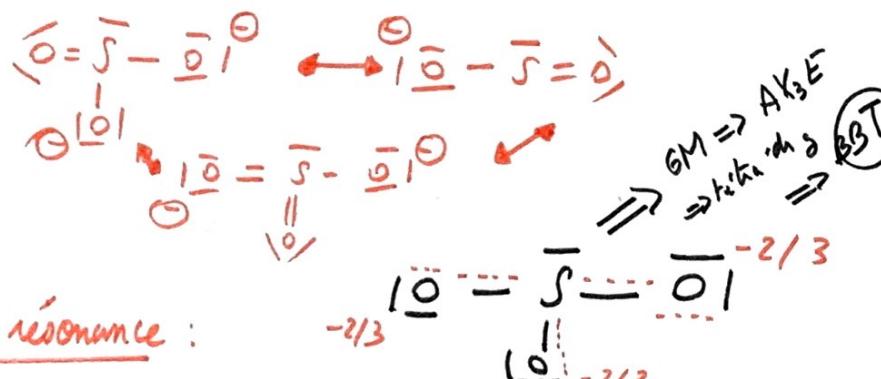


Ex 4! $S: [Ne] 3s^2 3p^4 \rightarrow V_{\text{Max}} 6 \text{ liaisons.}$

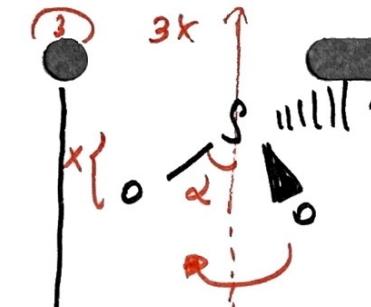
Degré oxydant $\left\{ \begin{array}{l} \text{min: } +2e^{-} \Rightarrow \text{Al: D.O. = -II} \\ \text{max: } -4e^{-} \Rightarrow \text{Ne: D.O. = +VI} \end{array} \right.$



Mésomères

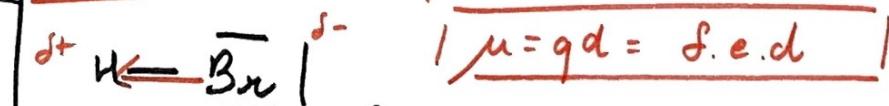


Hybride de résonance :



$$\vec{\mu}_{\text{tot}} = 3 \cos \alpha \vec{\mu}_{S_0}$$

Ex 5 | Moment dipolaire & ionicité



$$\chi_H < \chi_{Br}$$

$$f = \frac{\mu}{ed} \approx 0,136 \quad +0,136 \quad H - \overline{Br}^- \quad -0,136$$

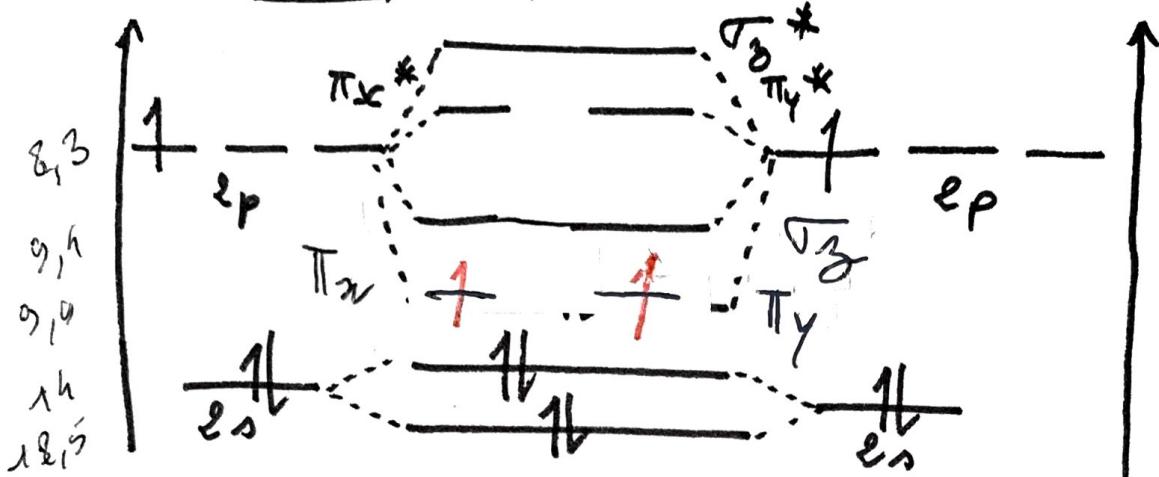
Ionicité : $f \times 100 : 13,5\%$

TD-8-

$B_2: 1s^2 \underline{2s^2 2p^1}$

$B_2: 6 e^-$ r�as

paramagn.



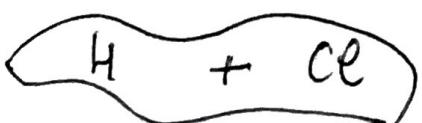
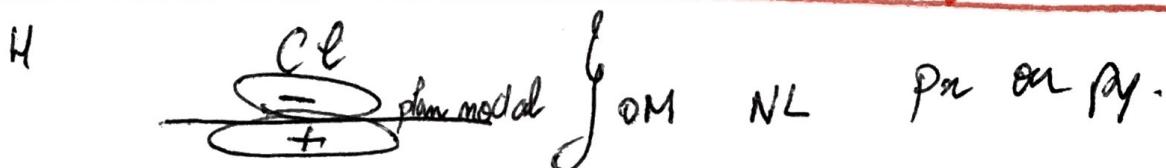
INVERSION(σ_z) $\leftrightarrow (\pi_x)(\pi_y)$ jusqu'à N.

$$OL: \frac{1}{2} [\text{nbr } e^- \text{ liant} - \text{nbr } e^- \text{ anti-liant}] = \frac{1}{2} [4 - 2] = 1 \xrightarrow{\text{à}} 1 \text{ liaison}$$

$\rightarrow n E_{\text{photon}} > 9,4 \text{ eV} \Rightarrow$ ionisat molécule : $B_2 + h\nu = B_2^+ + e^-$

$\rightarrow \lambda = 2,48 \mu m \Leftrightarrow 0,5 \text{ eV}$ or $-9,1 + 9,9 = +0,5 \text{ eV} \Rightarrow B_2^*$ excited.

+ OL \rightarrow + LL \downarrow (longueur liaison)

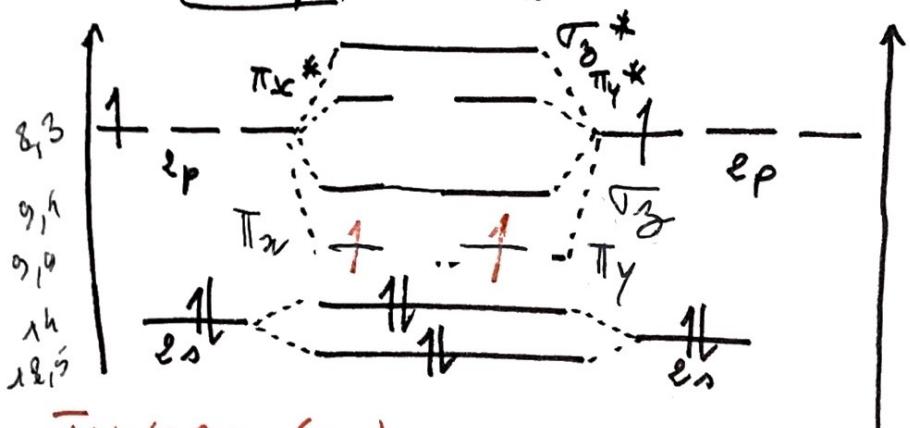
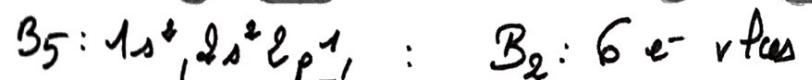


σ_z



σ_z^*
2 plans modaux

TD-8-

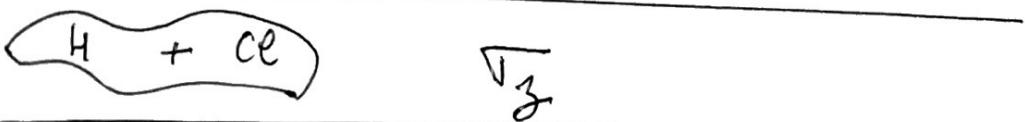


INVERSION(π_3) de (π_x)(π_y) jusqu'à N.

$$OL: \frac{1}{2} [\text{nbr } e^- \text{ liant} - \text{nbr } e^- \text{ anti-liant}] = \frac{1}{2} [4 - 2] = 1 \text{ liaison}$$

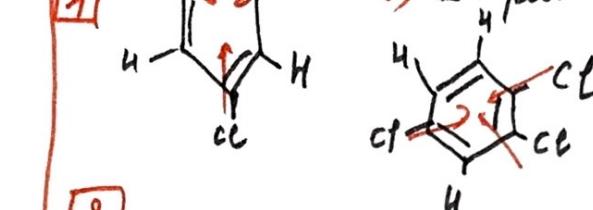
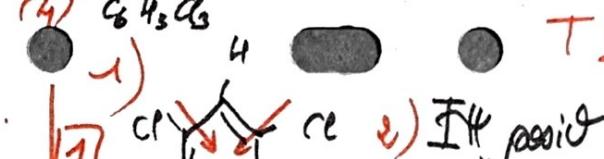
→ λ E photon $> 9,4 \text{ eV} \Rightarrow$ ionisat molécule: $B_2 + h\nu = B_2^+ + e^-$
 → $\lambda = 8,48 \mu\text{m} \Leftrightarrow 0,5 \text{ eV}$ ou $-9,7 + 9,9 = +0,2 \text{ eV} \Rightarrow B_2^*$ excita.

+ OL \rightarrow + LL \downarrow (longueur liaison)

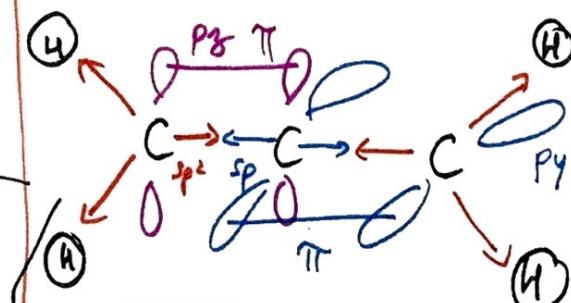
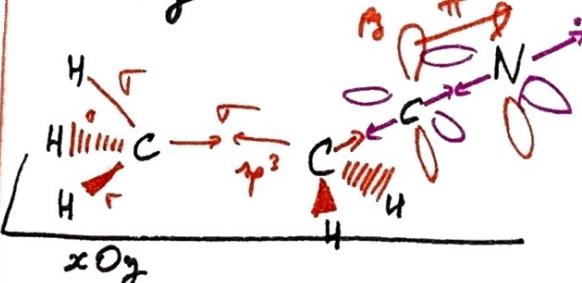
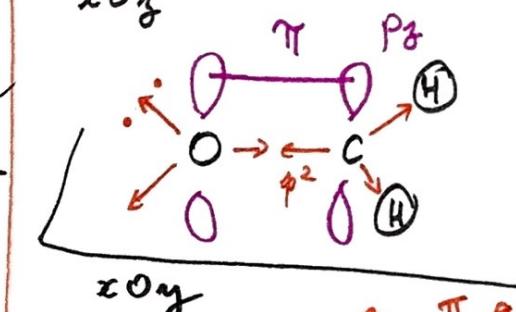
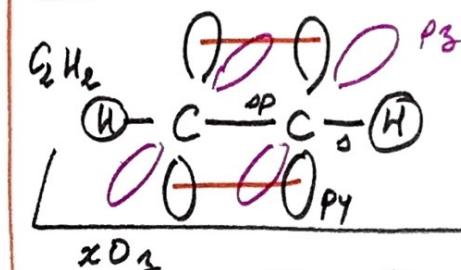


Paramagn.

TD-9



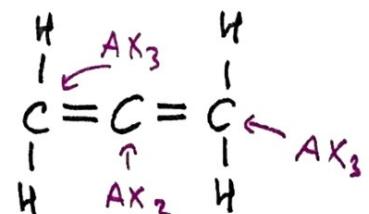
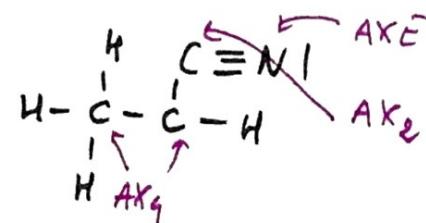
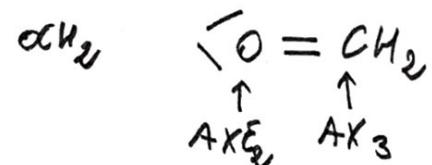
3)

3) $\chi(C) > \chi(H)$ \hookrightarrow polarisat liaison $\hookrightarrow \mu_{tot} + élévé$

$$\vec{\mu}_t = 1.6 + 2.1,6 \cos\left(\frac{180^\circ}{2}\right)$$

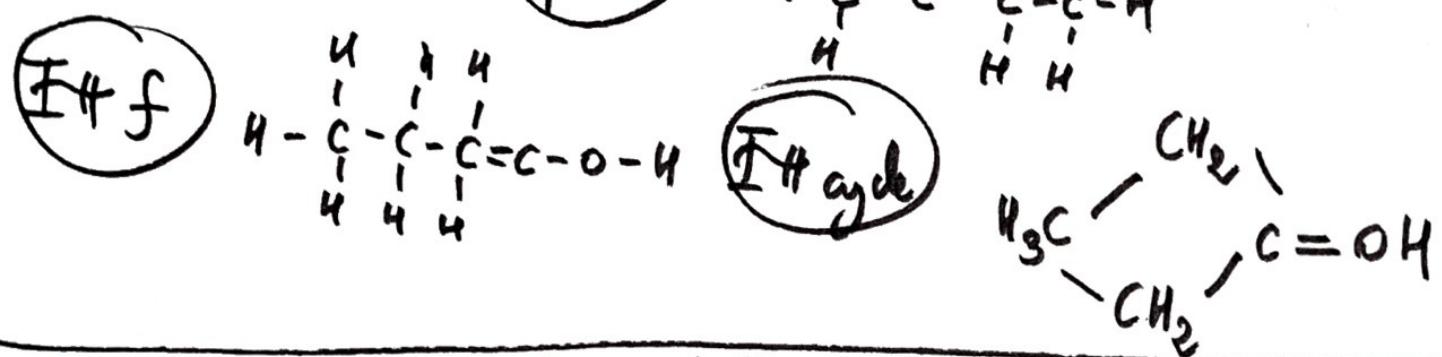
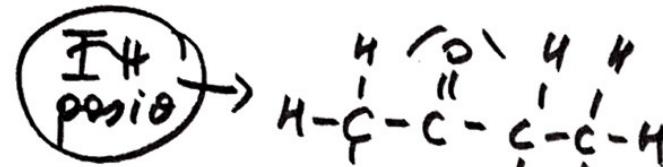
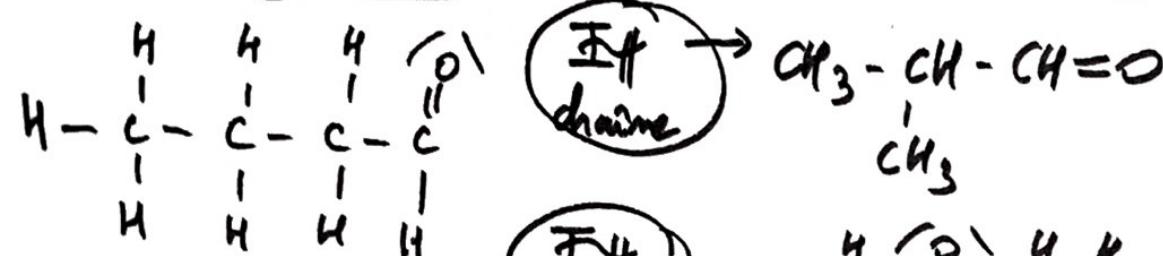
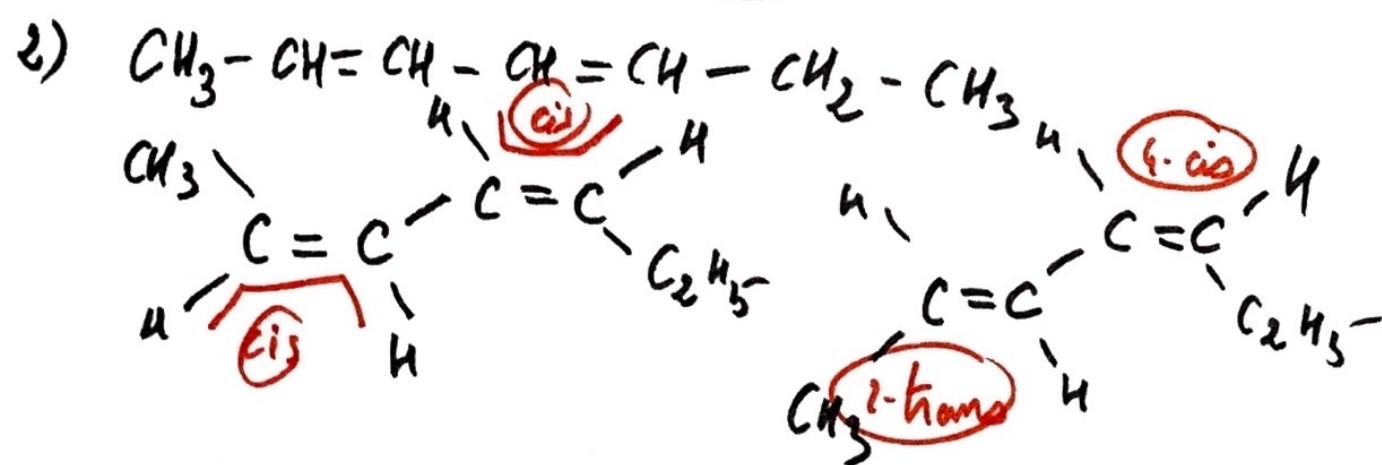
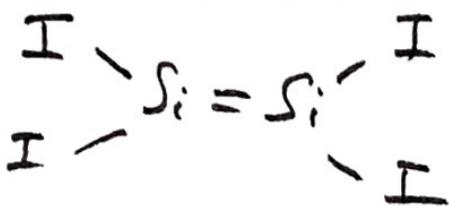
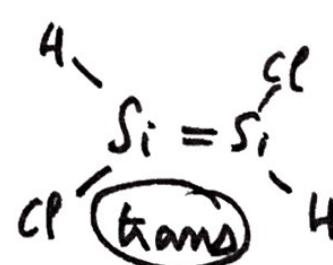
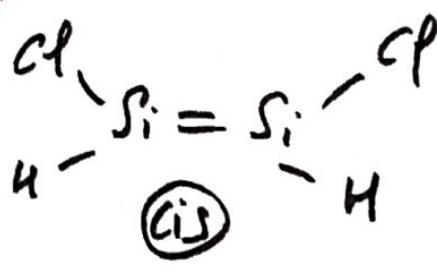
ERR

AX ₂ en AXE	2	sp lin
AX ₃	3	sp ² tri
AX ₄	4	sp ³ tétra
AX ₅	5	sp ³ d B3
AX ₆	6	sp ³ d ² B3'



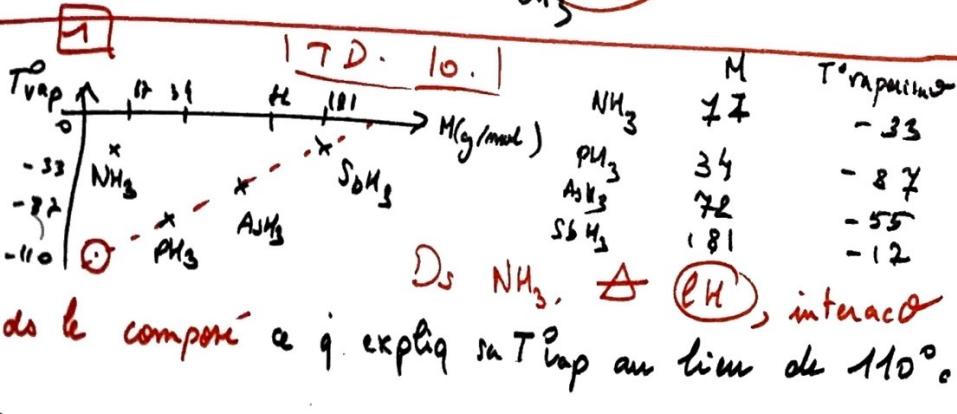
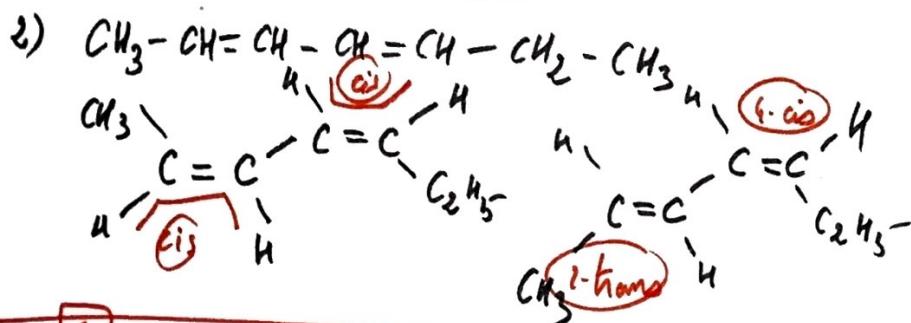
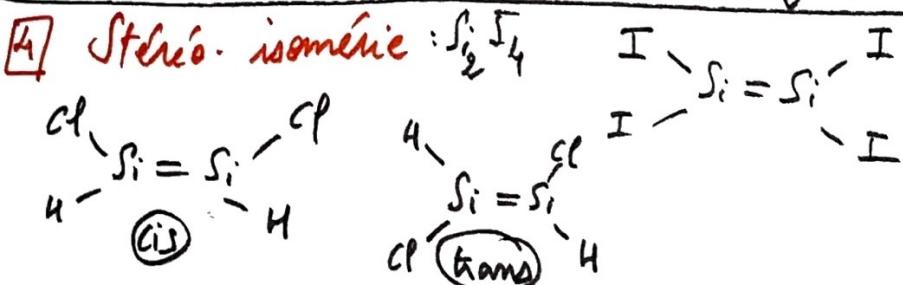
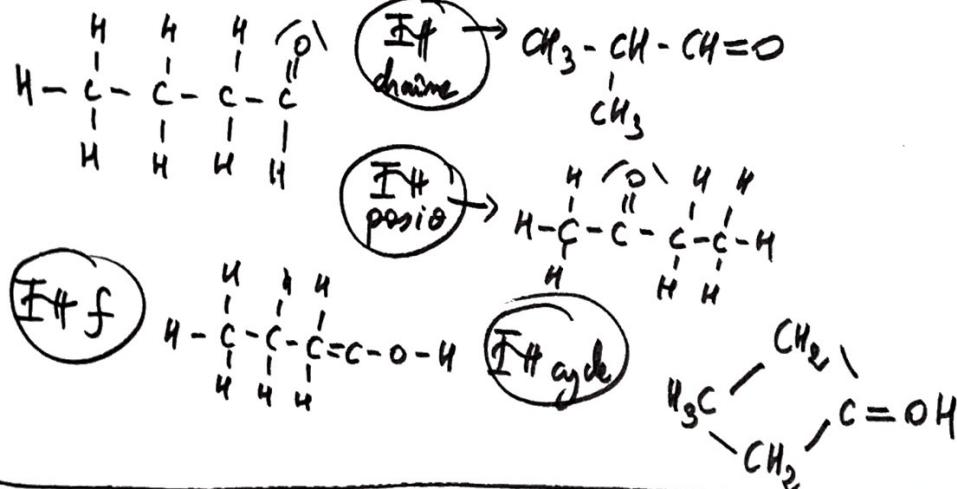
3

ETH Constitution

4 Stereo-isomeric: Si_2I_4 I - $\text{Si}=\text{Si}-\text{I}$ 

3

Etat constitutif



7

8

M	T_{fusion}	$T_{\text{ébull}}$	T_{ambiante}
F_2	-220	-188	gazeux
Cl_2	-100	-34	gazeux
Br_2	-7	+59	liquide
I_2	114	184	solide

- $\rightarrow T_{\text{fusion}} \& T_{\text{ébull}} \uparrow$ \rightarrow masse mol.
- \rightarrow Composé dihalog \Rightarrow composé apolaire $\Rightarrow \cancel{\mu}$
- \rightarrow Δ forces London (propt μ & M)
- \rightarrow forces Keesom \downarrow

3) Liaison ionique : si $\Delta X \geq 1.5$. simm Covalente

4) $\text{CH}_3-\text{CH}_2-\bar{\text{O}}-\text{CH}_2-\text{CH}_3$ & $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}_2-\bar{\text{O}}-\text{H}$

\rightarrow Keesom, Debye, London

\rightarrow no Keesom, Debye, London, LH

(LH : + énergétiques mais \ominus énergétiques que liaisons covalentes).

