Organisation de l'année — S. Humbel

Con.

TP 1 (2) (3) (4) 5 (6) (7) 8 (9) — (10)

10% + + + + — 50% — décembre

7 → MenS

20 + 5 pts. CR — QCM

Jours Examen

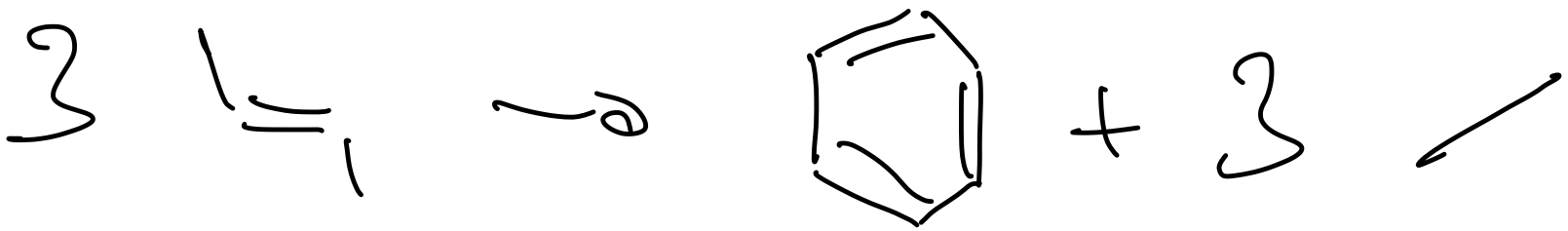
Note UE = 50% Examen

Équilibrer une réaction ; énergie d'une réaction

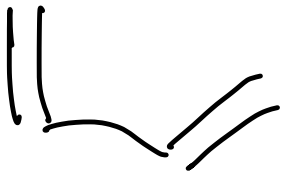
Expl. $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

$$\begin{cases} 4x = 6 + 2y \quad \times 3 \\ 8x = 6 + 6y \end{cases}$$

C:	4	6	2
H	8	6	6



Conjugaison
+ aromaticité



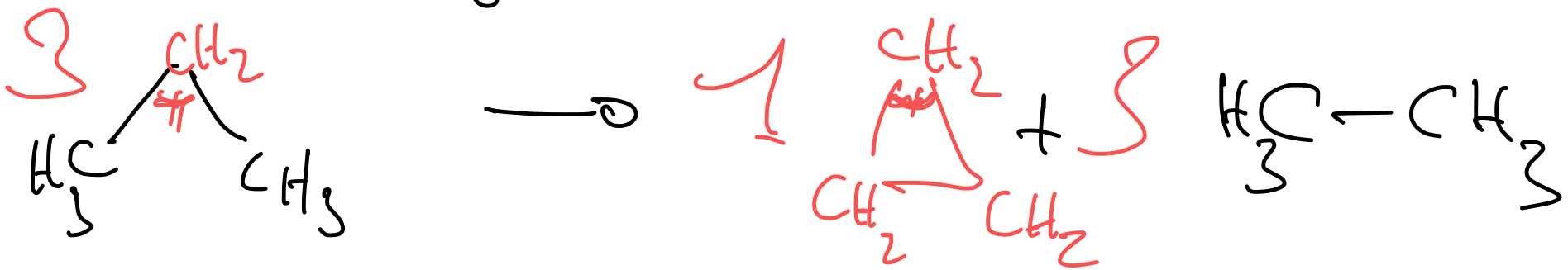
Réactions isodesmiques simple / double

Homodesmique

$\Delta p_3 - \Delta' p_3$
$\Delta p_2 - \Delta p_3$) $\neq$

Aromaticité + Conjugaison

Tension de cycle



Master 1 S1 : Laboratoire de Modélisation

Cours 1

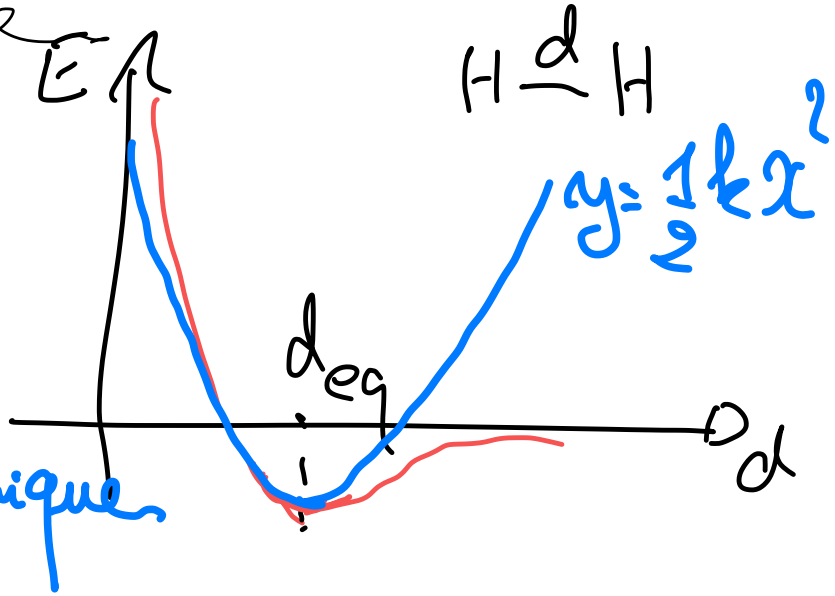
Chimie Théorique ; historique

Structure ⟷ Energie

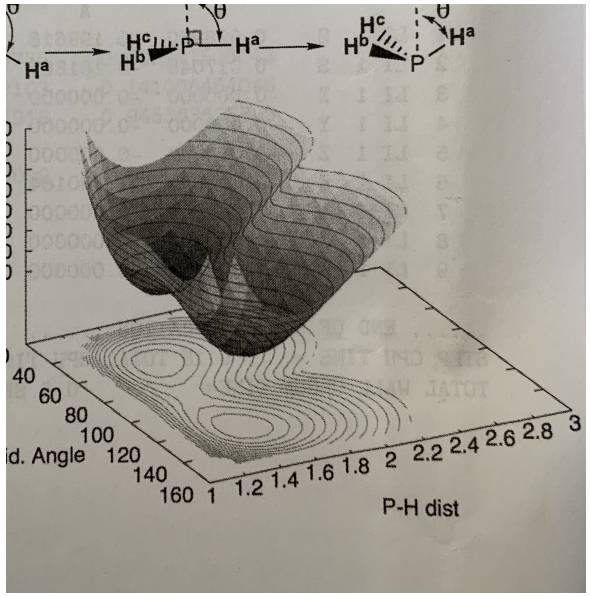
Harmonique

$x = d - d_{eq}$

$E_{MM} = f(x)$ dynamique



Coord_



Energie : $\hat{H}\,\Psi(M) = E\,\Psi(M)$

Schrödinger.

M : point autour de la molécule.

Hamiltonien : $\hat{T}$ cinétiq, V potentiel

H^{-1} -1 2^{-1} H

$+Z_A$ $+Z_B$

$$\hat{H} = \hat{T}_A + \hat{T}_B + \hat{T}_1 + \hat{T}_2$$

$$V_{A1} = \frac{Z_A(-1)}{r_{A1}} < 0$$

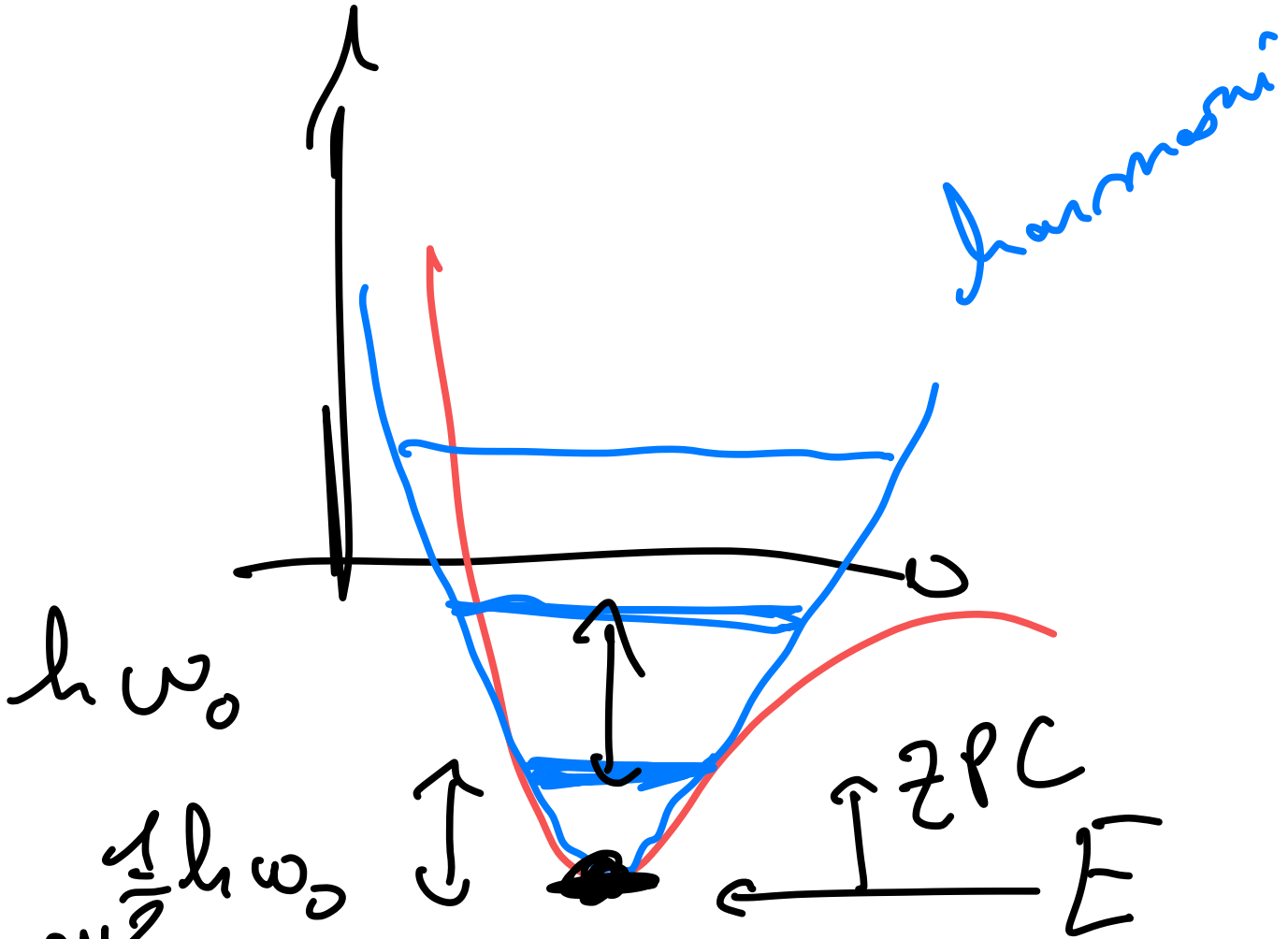
$$+V_{AB} + V_{A1} + V_{A2} + V_{B1} + V_{B2} + V_{12}$$

$+V_{AB} > 0$

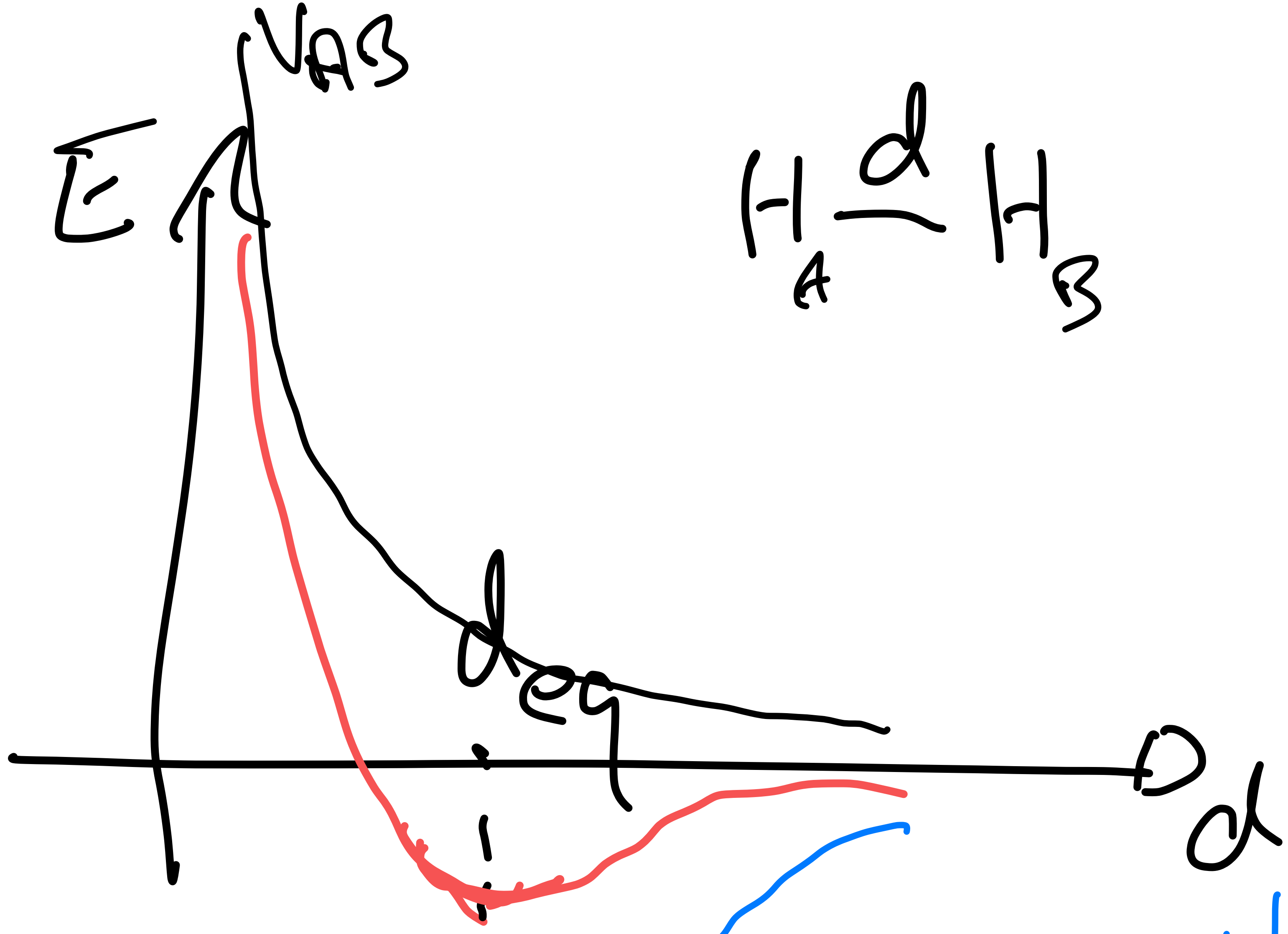
bielectronique > 0

Dans l'approximation Born-Oppenheimer

noyaux fixes $\vec{T}_A = \vec{T}_B = 0$



Zero Point Energy



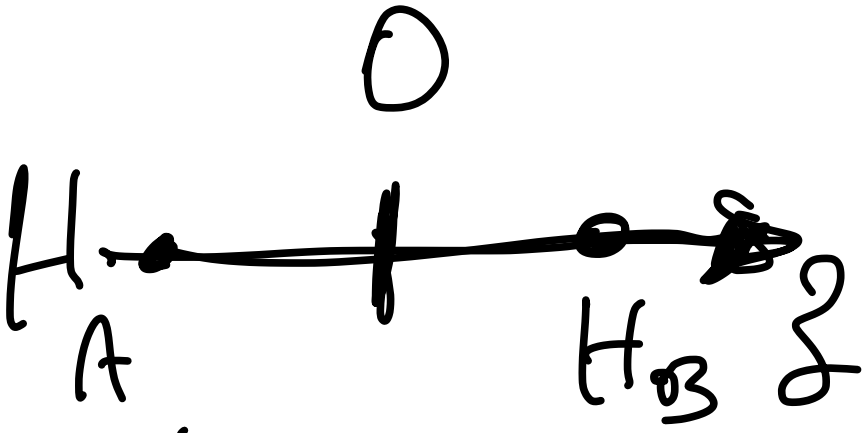
$H_A \overset{d}{—} H_B$

$$\hat{H} = V_{NN} + V_{Ne^-} (+ V_{e^-e^-}) \quad V_{Ne} = V_{A1} + V_{A2} + V_{B1} + V_{B2}$$

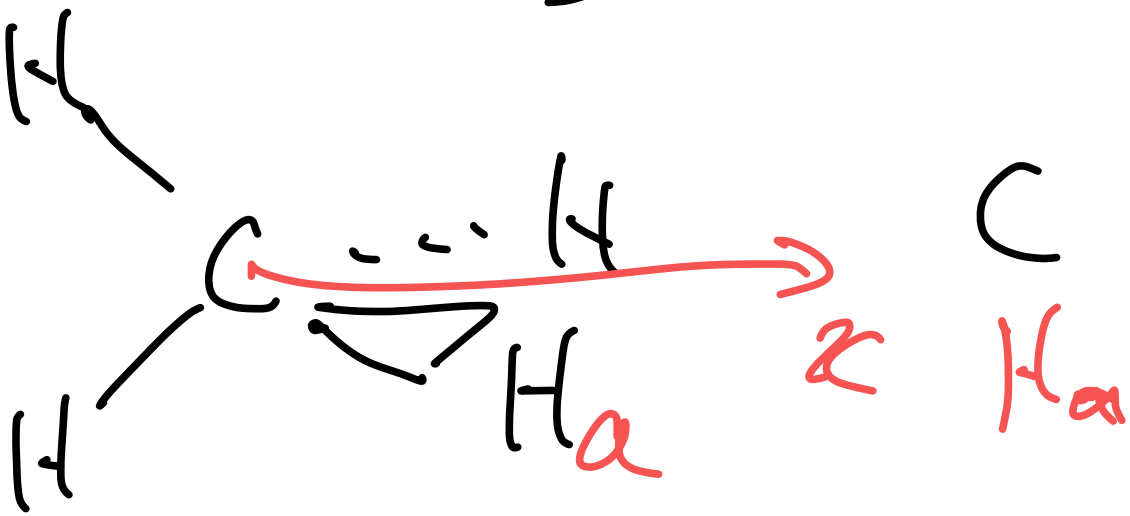
Geométrie :

coordonnées des atomes

- Cartésiennes

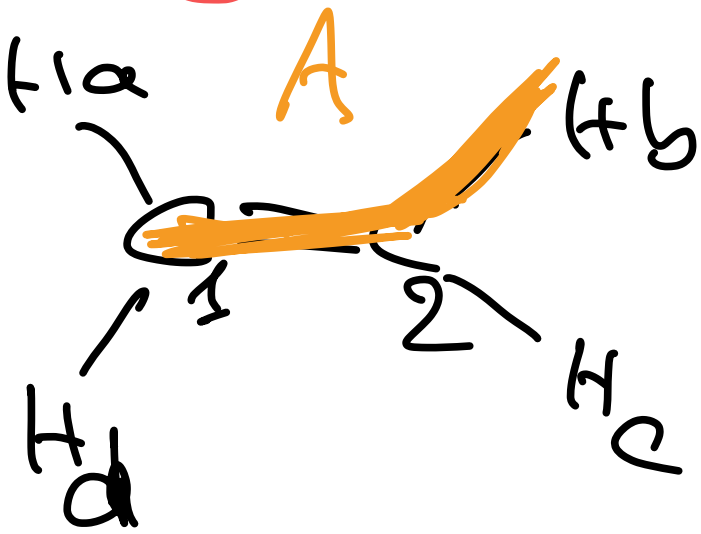


Sym	A	X	Y	Z
H		0.	0.	-0,37
H		0.	0.	+0,37



C	0.	0.	0.

Coordonnées internes - Z-matrix



R_{ab} distance

A_{abc} angle entre liaison

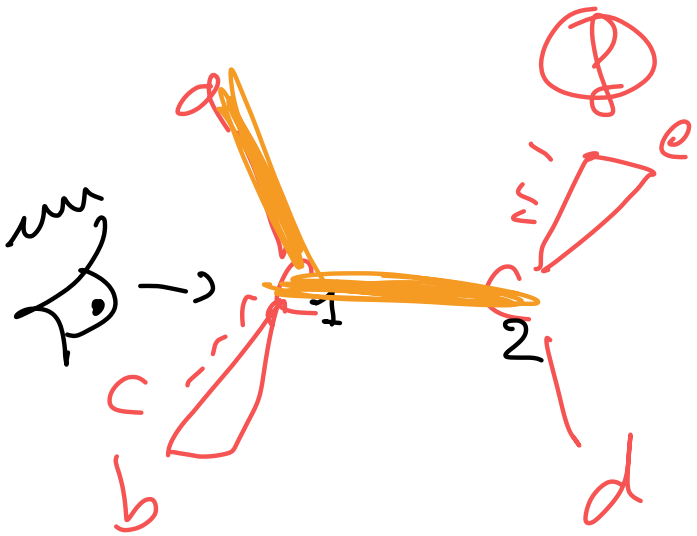
D_{abcd} angle dièdre entre plans

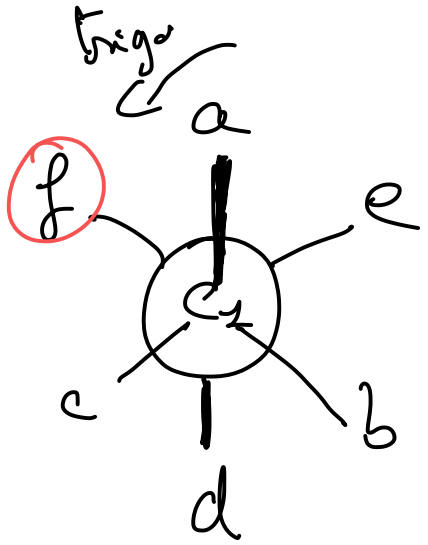
abc

bcd

a 1 2 b = 0°

d 1 2 b = 180°





a 1 2 d = 180°

a 1 2 b = -120

a 1 2 f = 60°

C_1

C_2 d_{CC} C_1

H_a d_{CH} C_1 A_{a12} C_2

H_b d_{CH} C_2 A_{b12} C_2 D_{b12a} a

↑

-120°