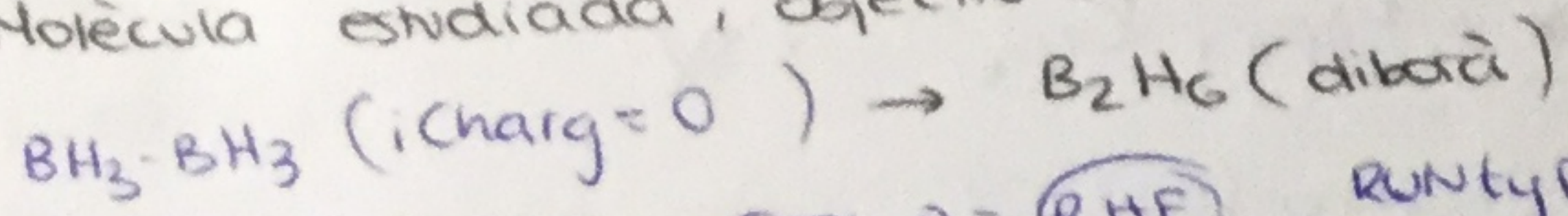


GEN 2016 : Problemes

PC5

1. Molècula estudiada, objectiu del càlcul (mètode unitat):



Del INPUT: \$CONTROL SCFTYP = **RHF** RUNTYP = Optimize

Objectiu: optimitzar la geometria d'equilibri i càlcul MMW

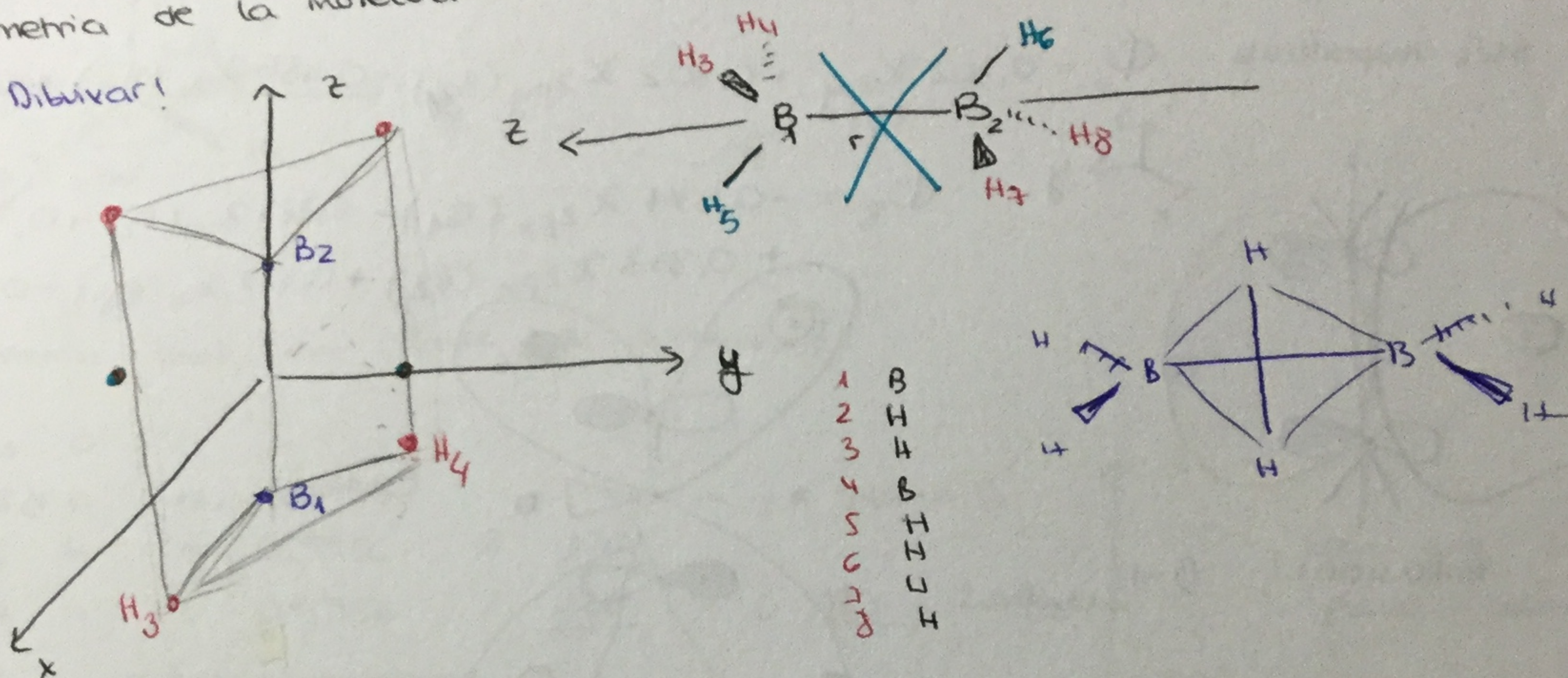
Mètode: Restricted Hartree Fock (RHF) amb una base mínima STO-3G

Gauss = STO  $\rightarrow$  ~~base~~ orbitals de Slater

nGauss = 3 **STO-3G** amb a base mínima

b) Geometria de la molècula en forma Z matrix: una vegada optimitzat!!

1) Dibujar!



Atom	d	$\alpha$ (ABC)	d(ABCD)
1 B			
2 B	1	r <sub>BB</sub>	
3 H	1	r <sub>HB1</sub>	
4 H	1	r <sub>HB1</sub>	2 118,8
5 H	1	r <sub>HB2</sub>	
6 H	2	r <sub>HB1</sub>	
7 H	2	r <sub>HB1</sub>	
8 H	2	r <sub>HB2</sub>	

Coordenates angulars

$r_{BB} = 1,80457$

$r_{HB1} = 1,1540$

$r_{HB2} = 1,3264$

$\alpha$

ZMatrix

Atom	d	$\alpha$ (Bend) ABC	$\alpha$ (Torsion) ABCD
1 B			
2 B	1	1,154	
3 H	1	1,154	2 122,54
4 B	1	1,805	2 118,80
5 H	4	1,154	1 118,80
6 H	4	1,154	2 118,84
7 H	1	1,326	4 47,13
8 H	1	1,326	4 47,13

d en Å ;  $\alpha$  en degrees (°) (angles)

6)

$^1H : \chi_{1s} \times 6$

$5B : [1s^2 2s^2] \underline{2p^1} \rightarrow \chi_{1s}, \chi_{2s}, \chi_{2p_x}, \chi_{2p_y}, \chi_{2p_z} \times 5$

$\boxed{10 + 6 = 16}$   $e^-$  totals:  $10 + 6 = 16 / 2 \rightarrow 8$  OMs ocupats  
lincials

$16$  OAs  $\rightarrow 16$  OMs =  $8$  OMs ocupats +  $8$  OMs virtuals de valència

Dels orbitals ( $6 - 10$ )  $\rightarrow$  Tots són de valència. No són  $n=1$

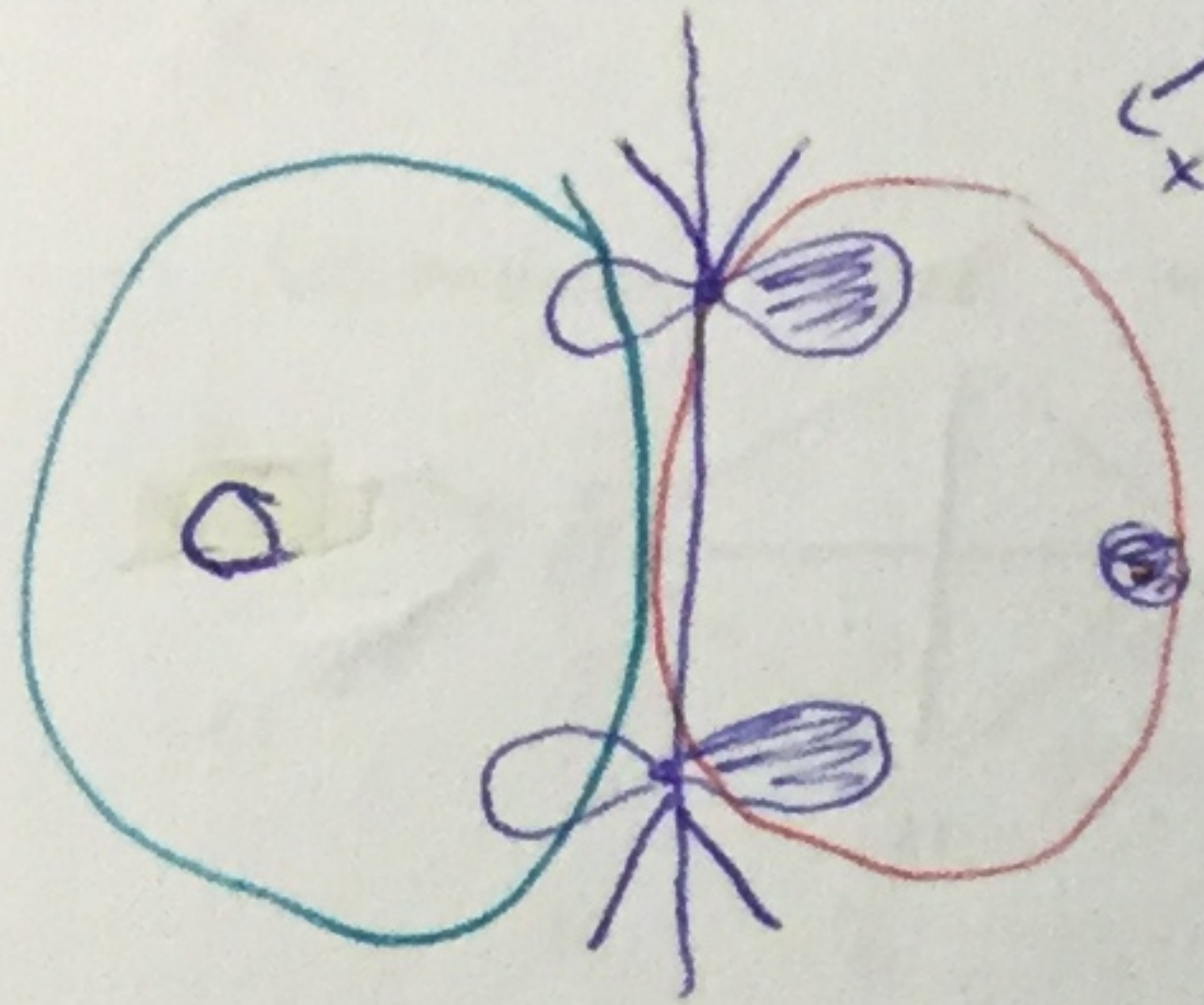
d) Representació contribució  $\Phi_6$  i  $\Phi_8$

$E_6 < 0$  ocupat

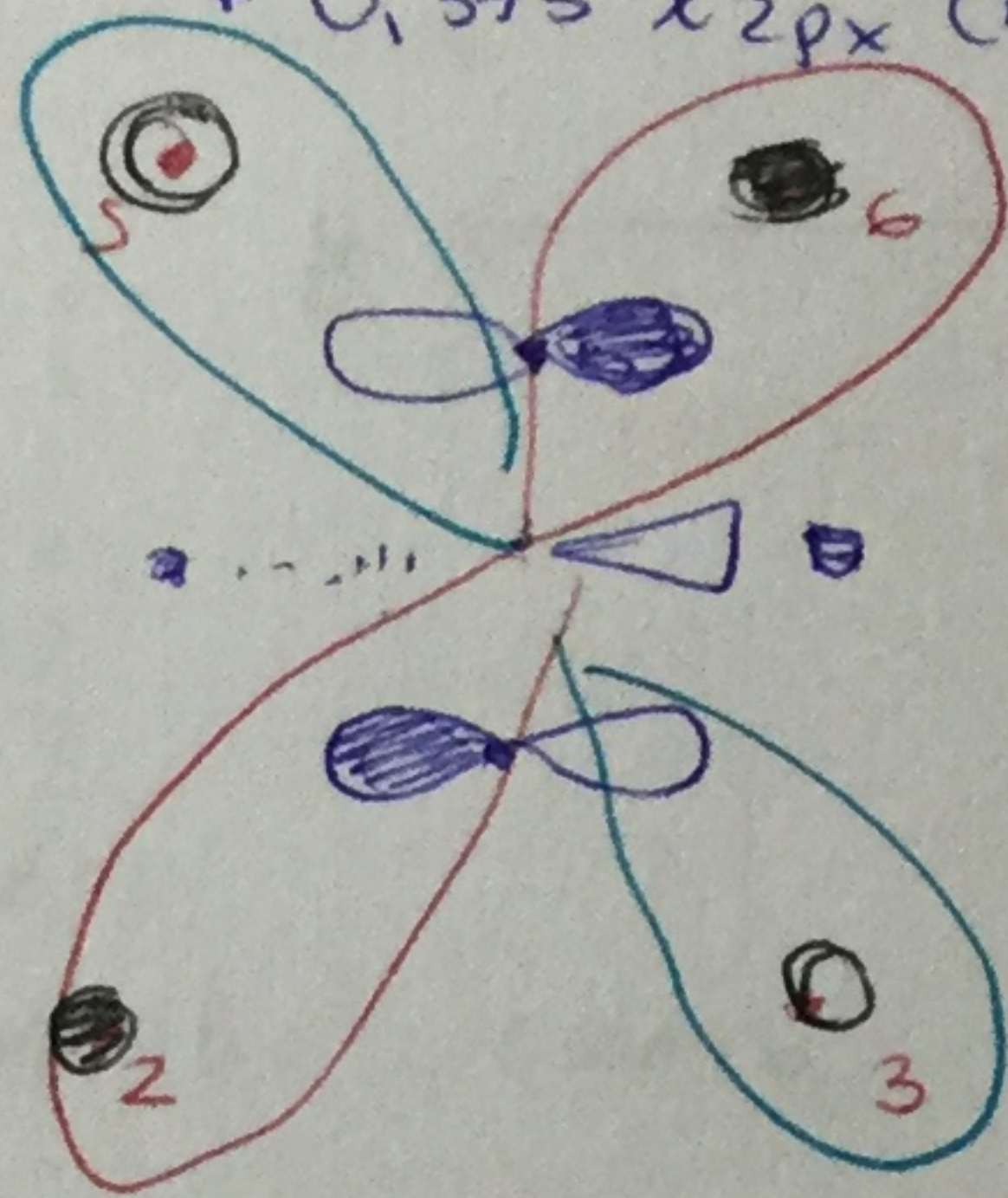
Més important

$\Phi_6 = 0,302 \chi_{2p_y}(B) + 0,302 \chi_{2p_y}(B2) - 0,486 \chi_{1s}(H7) + 0,486 \chi_{1s}(H8)$

$\Phi_8 = -0,574 \chi_{2p_x}(B1) - 0,327 \chi_{1s}(H2) + 0,327 \chi_{1s}(H3) + 0,327 \chi_{2p_x}(B2) + 0,327 \chi_{1s}(H5) - 0,327 \chi_{1s}(H6)$



enllaçant! B-H central.



Enllaçant B-H terminal

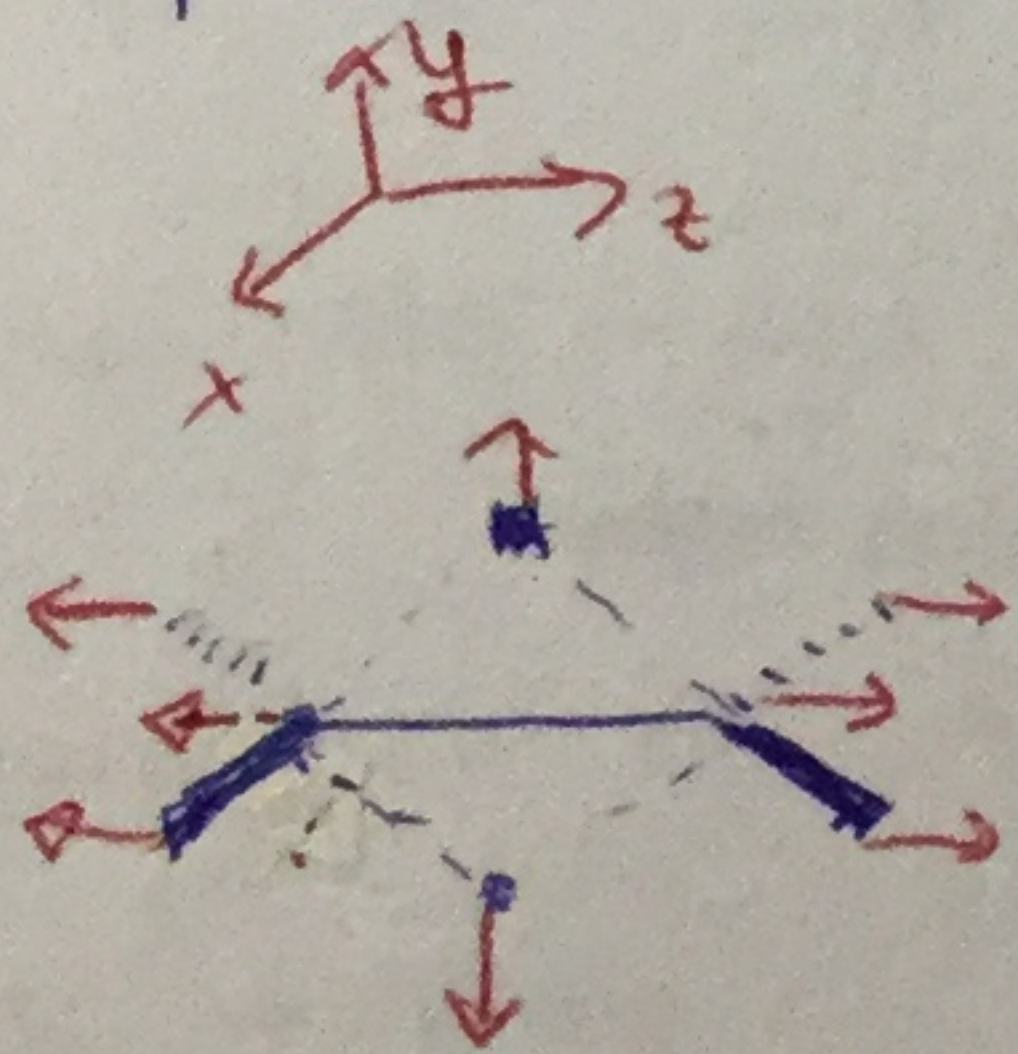
NSERCH: (9) 9 punts.

$V_{rep\ e-l} > < \neq V_{rep\ nuc}$

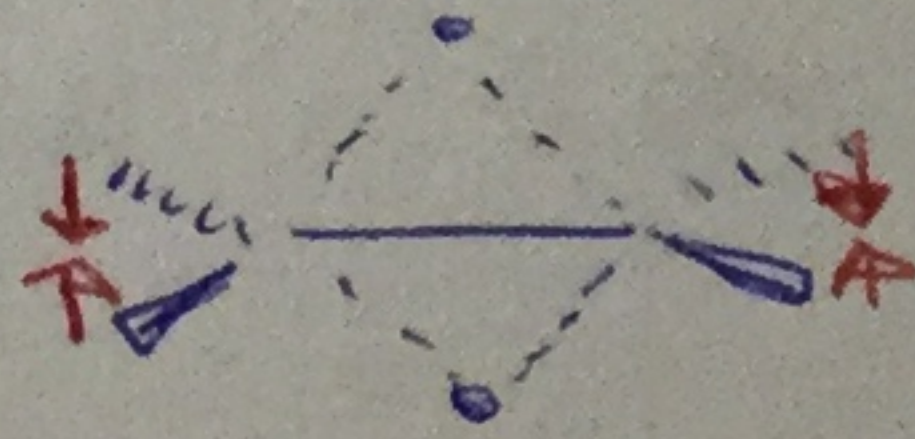
$V_{rep\ e-l-e} = 47,59$  hartree

$V_{ec} > V_{nn}$

$V_{rep\ n-n} = 32,15$  hartree



Stanul:leu  
 $\vec{d} = 0$   
 No active IR

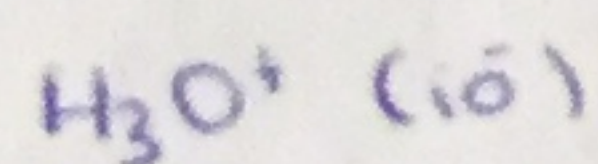


Stanul:leu  
 No active IR

$\left(\frac{\partial d}{\partial Q}\right)_e = 0$

JUNY 2015. Pràctiques QF III

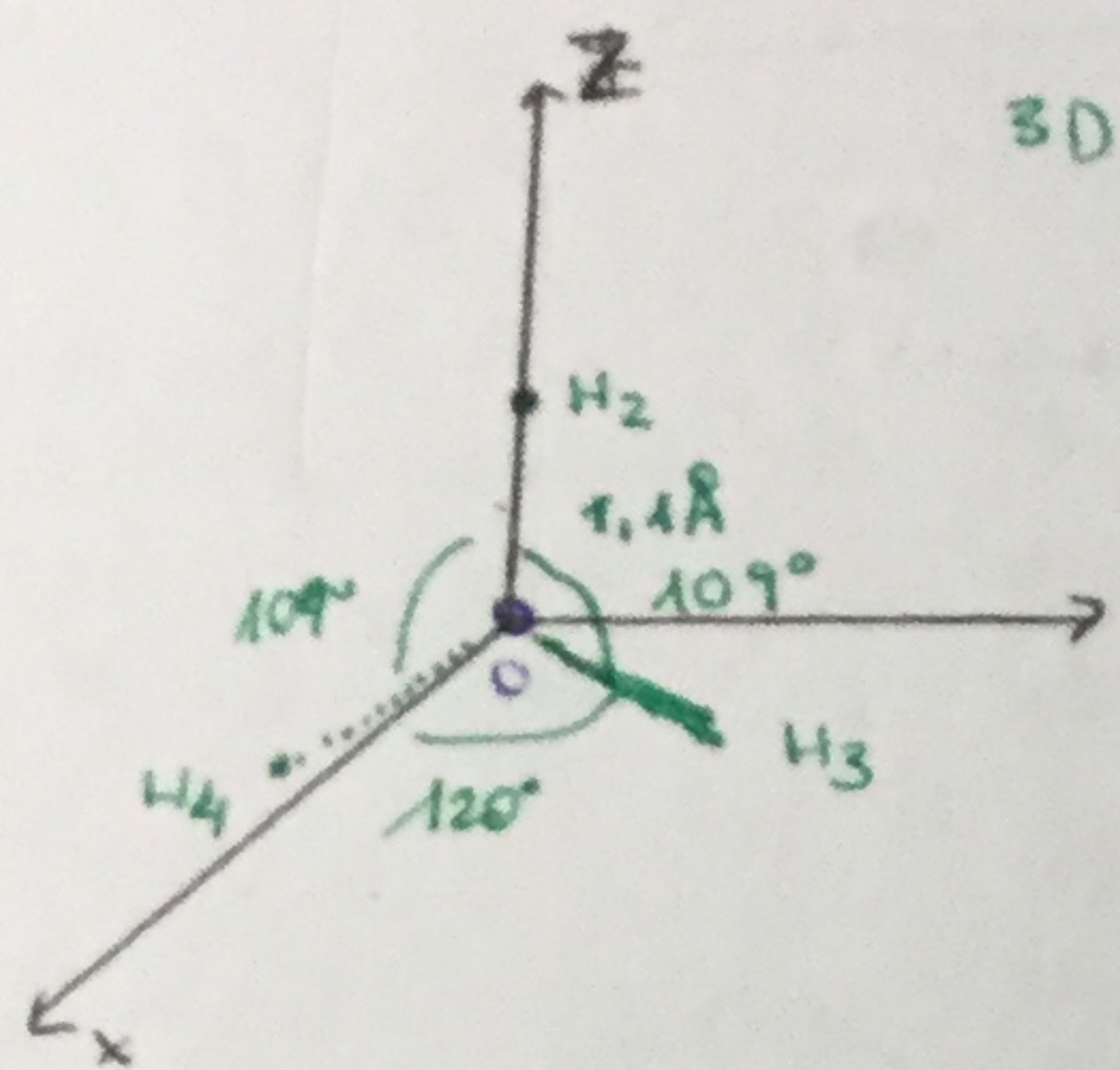
a) Mòdul, objectiu, mètode:



Trobar el solitari point ET (puntu de nitat) Estret estacionari

Mètode RHF STO-3G MPEVL=2.

b) Geometria inicial? Mitjançant el input



no plane.

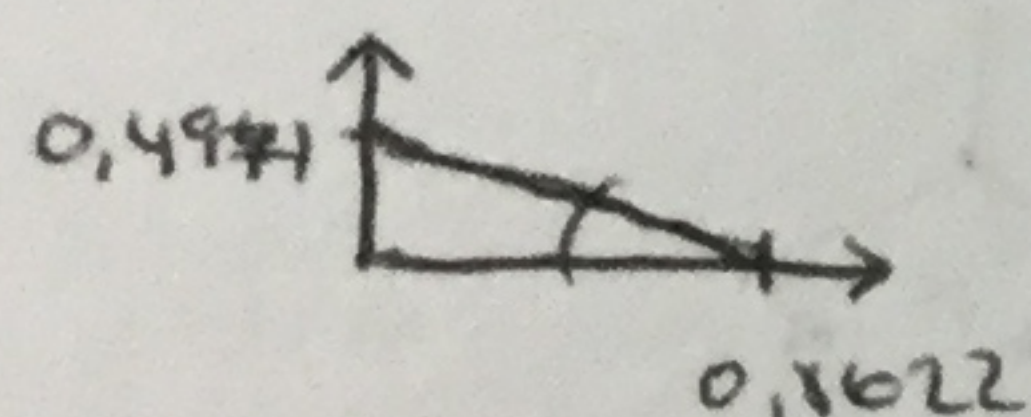
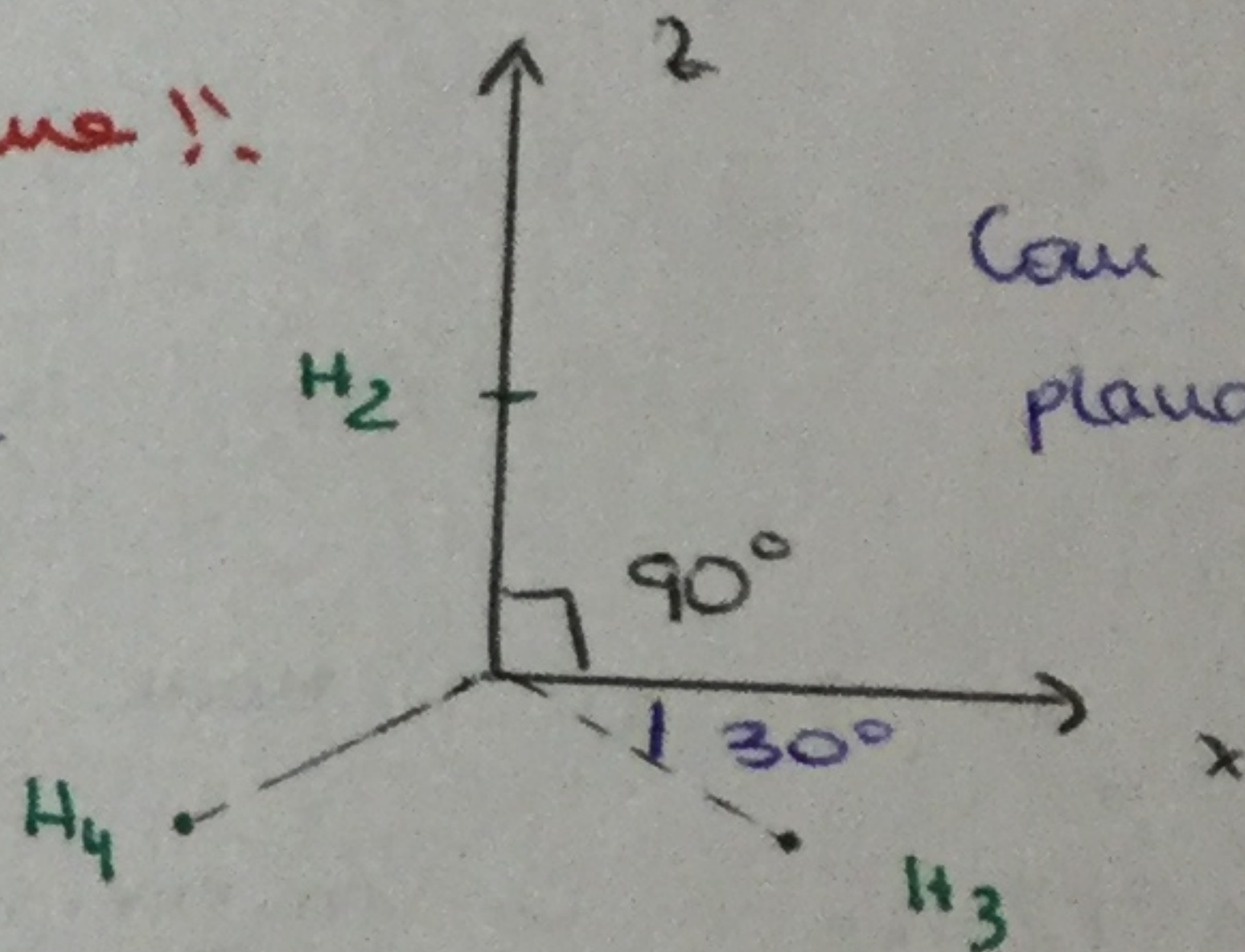
c) Geometria final en base de Z-Matrix:

1	O					
2	H	1	0,9956			
3	H	1	0,9956	2	120	
4	H	1	0,9956	2	120	3 120

$$d(OH_2) = \sqrt{(0,862)^2 + (0,4978)^2} = 0,9956$$

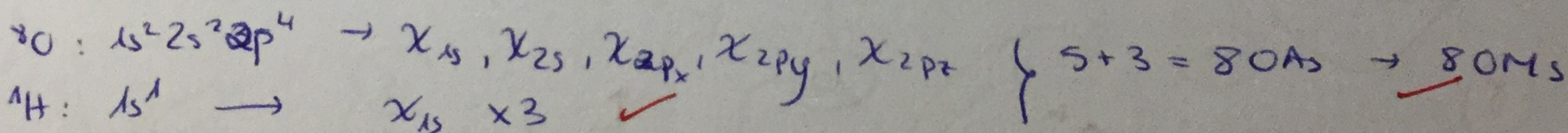
Plane !!

Com que és plana  $360^\circ - 240^\circ = 120$



$$\tan \alpha = \frac{0,4978}{0,8622}$$

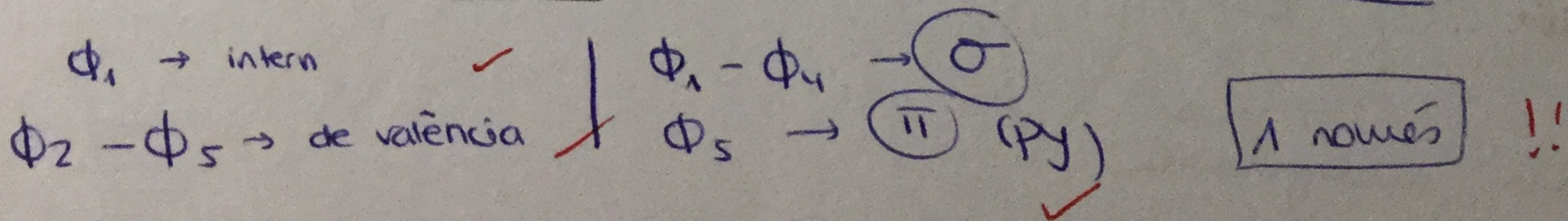
d) Funcions utilitzades de base. Ocupats virtuals? Intens, valència?  $\sigma$ ;  $\pi$ ?  $\pi$ ?



Tenim  $Me^- - Ae^- = 10e^- \rightarrow 5 OMs \text{ ocupats i } 3 OMs \text{ virtuals.} \checkmark$

capítol càtio  $\checkmark$

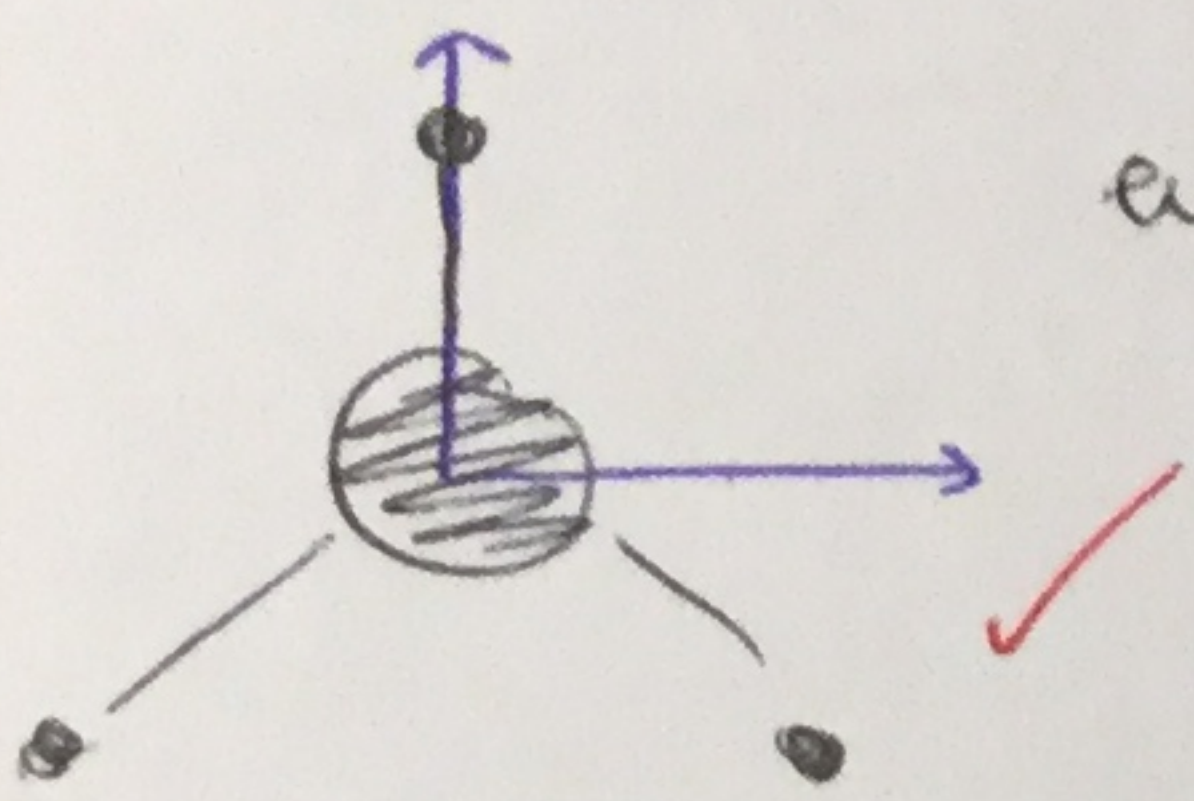
Classifiqueu els mostrats  $\rightarrow$  Tots estan ocupats !!  $E < 0$



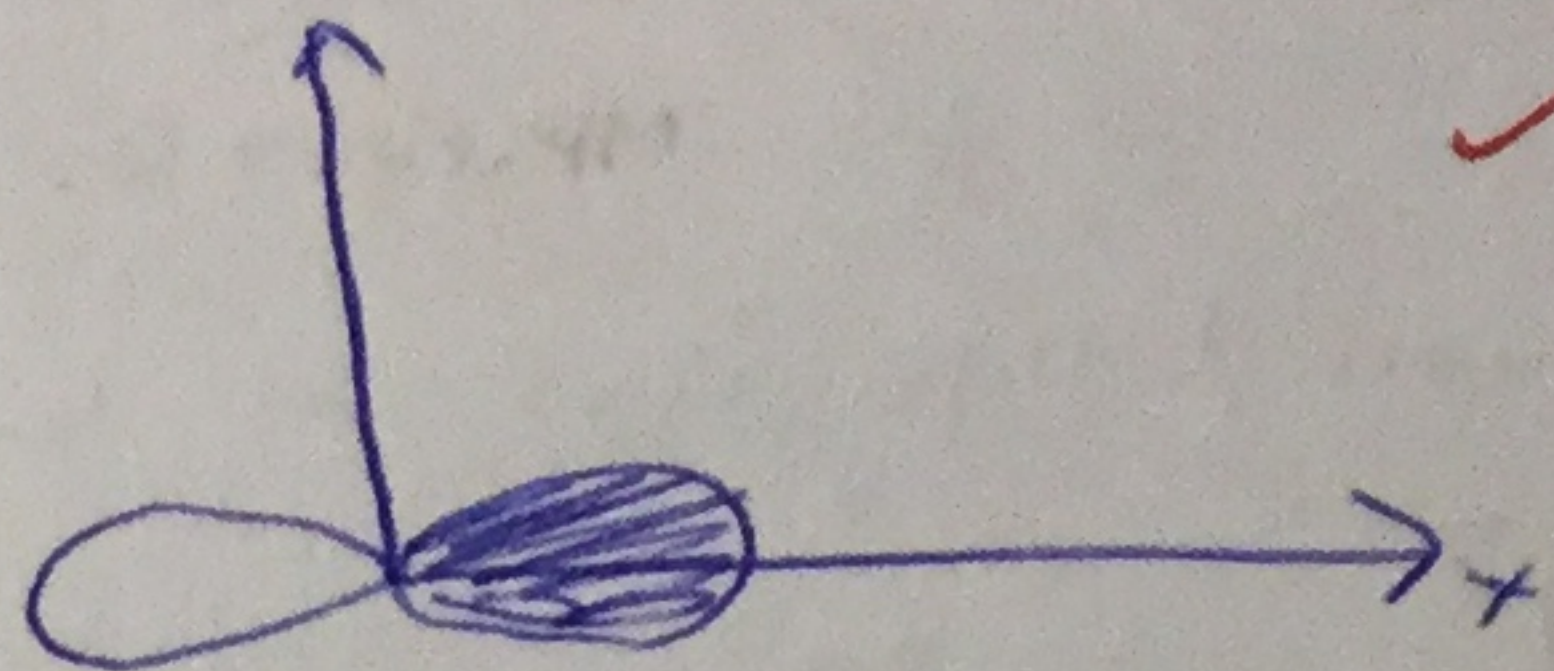
e)  $\Phi_2, \Phi_4, \Phi_5$  ? representar!!

$$\Phi_2 = 0,24 \chi_{1s} - 0,876 \chi_{2s} - 0,101 \chi_{1s}(H) \times 3$$

$$\Phi_4 = -0,69978 \chi_{2p_x} - 0,344 \chi_{1s}(H_2) + 0,344 \chi_{1s}(H_3)$$

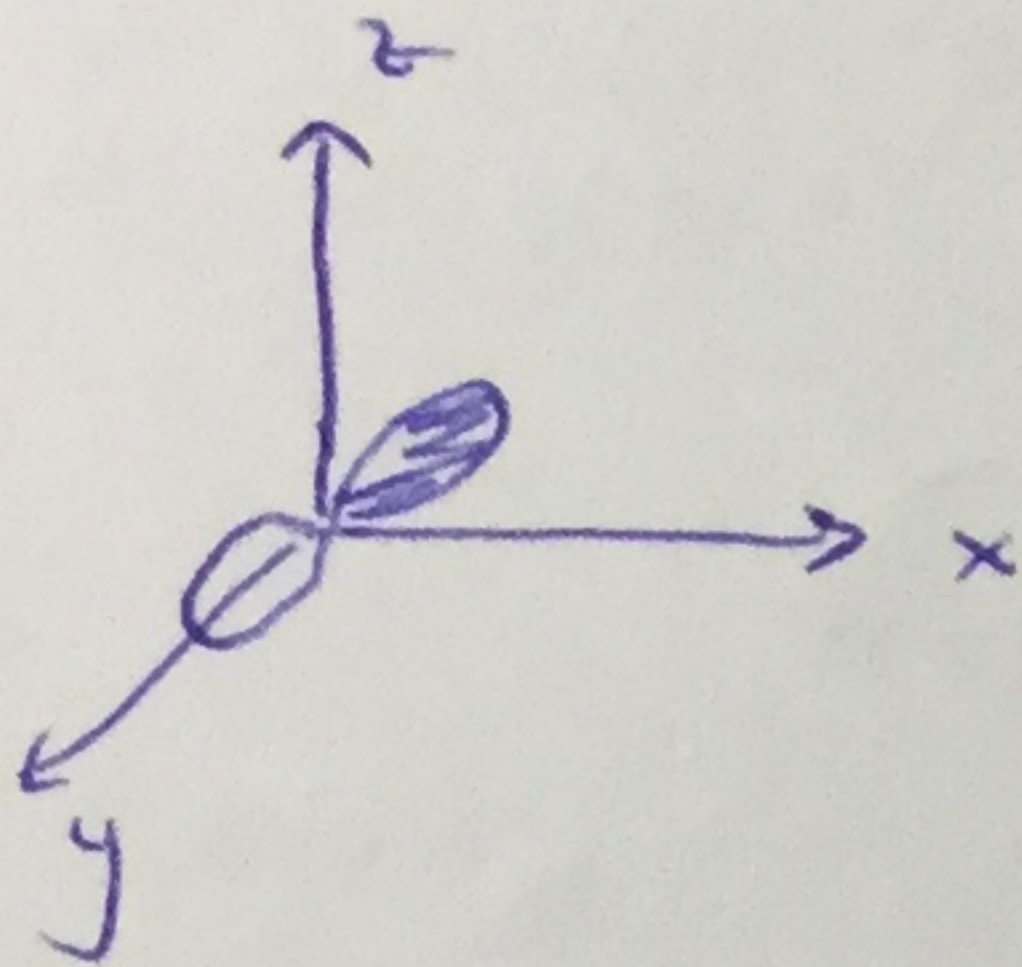


entlastet



entlastet!

$$\Phi_5 = 1 \chi_{2p_y} (0)$$



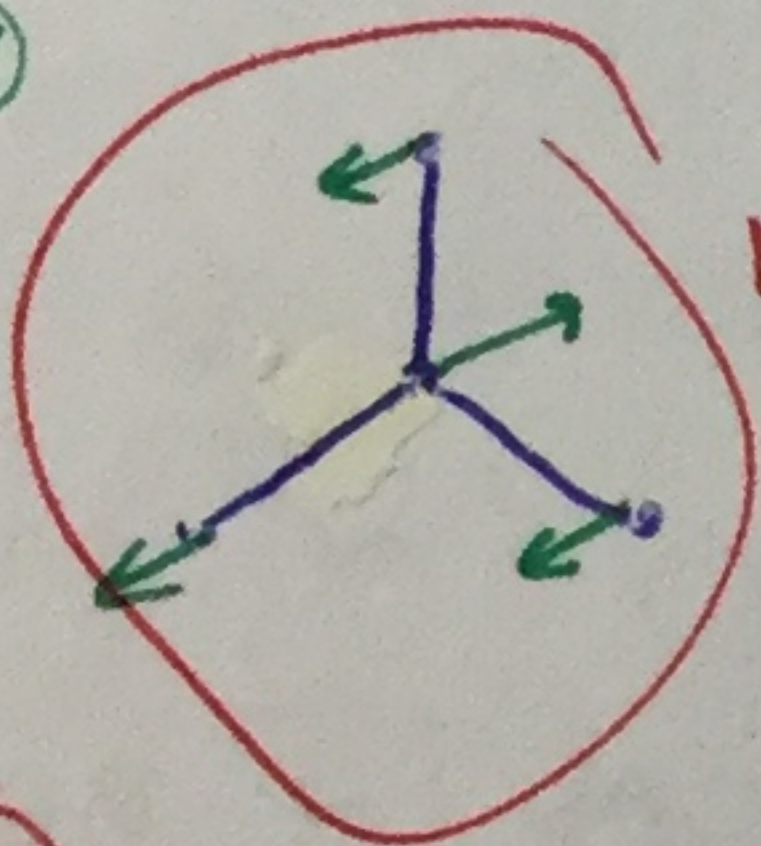
No entlastet

f.)  $|D| = 0$  debe ~~ser~~ si que cambia porque hay carga neta +1.

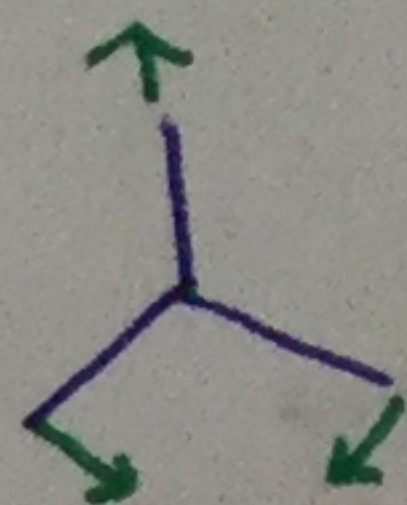
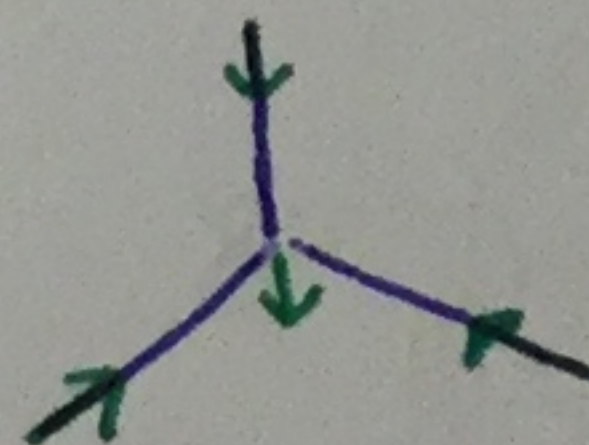
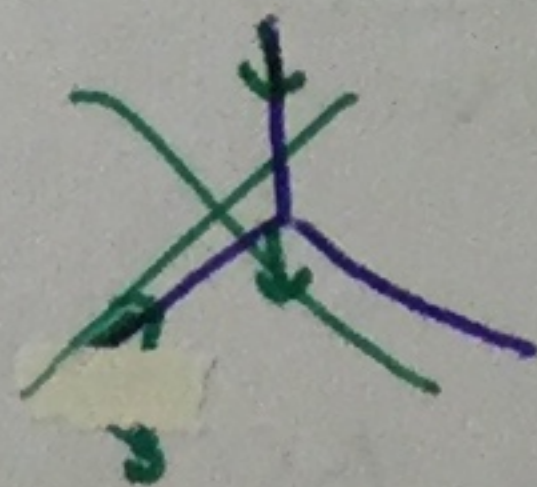
g) m.n.v. 1, 8, 10 Mode 1? Actos 8 : 10 112?

$$3N - 6 = 12 - 6 = 6 \text{ m.n.v.}$$

(1)

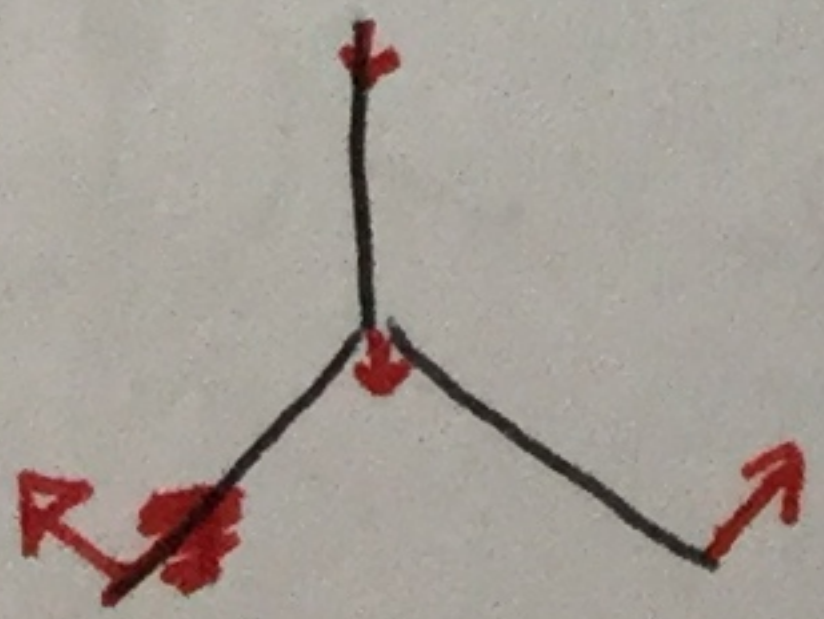


Imaginario!!



~~flexión~~

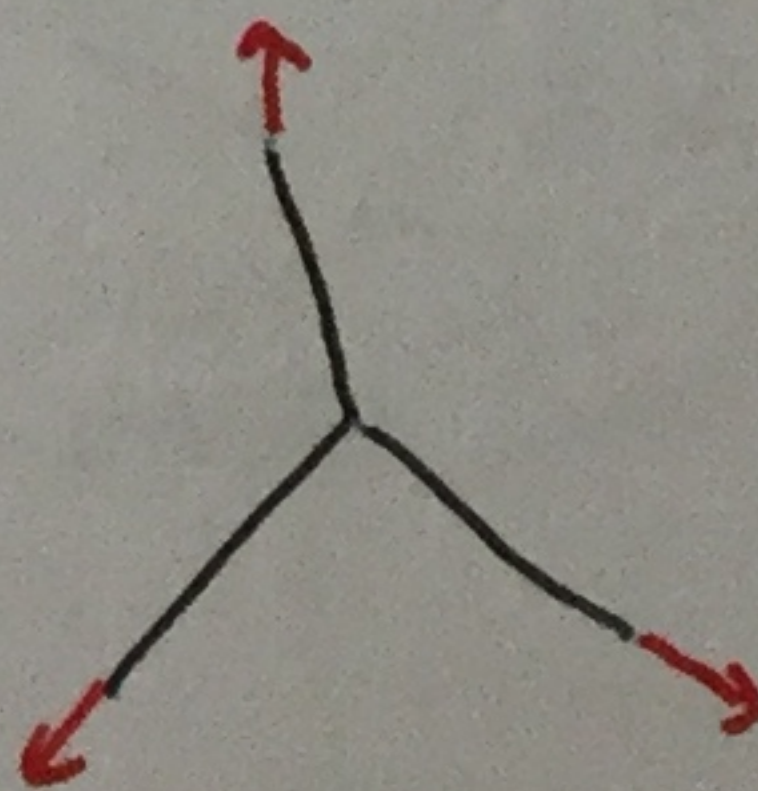
(8)



flexión ?

$\uparrow^+$   
x

(10)



tenión simétrica activa 12.  
stretching

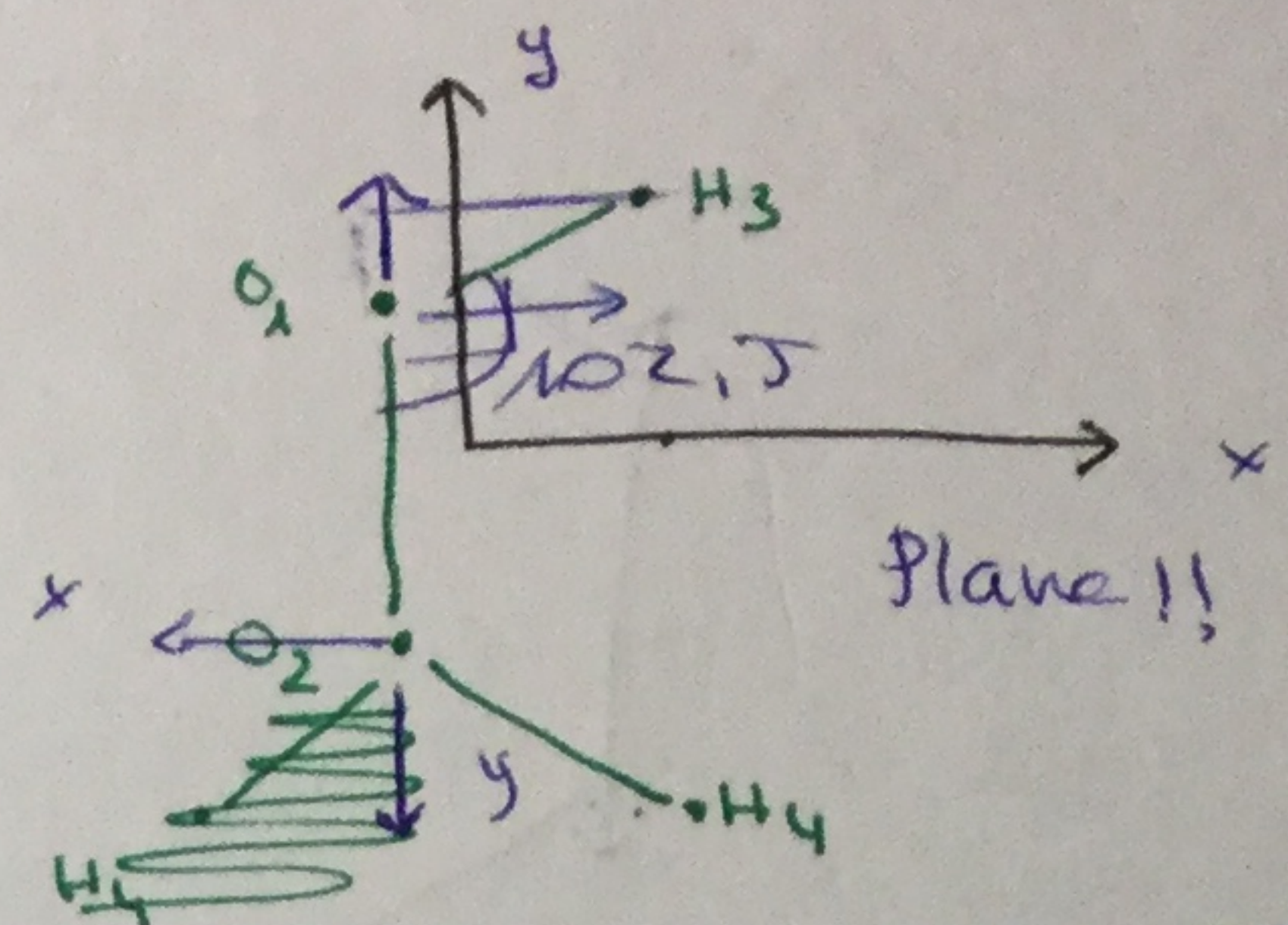
(1) Activación imaginaria

GEN 2015

1. H<sub>2</sub>O<sub>2</sub> obiectiv puncte de alta ET  
RHF, MP2, STO-3G.

no vcm

2.  
1 0  
2 0 1 1,4568  
3 H 1  
4 H 2



1	0						
2	0	1	1,4568	3	3		
3	H	1	1,027	2	102,5		
4	H	2	1,027	1	102,5	3	180

$$d_{OH} = \sqrt{(0,2214645)^2 + \dots} = 1,027$$

e  $\alpha = \cos^{-1}(\dots) = 77,55 \rightarrow 102,5$

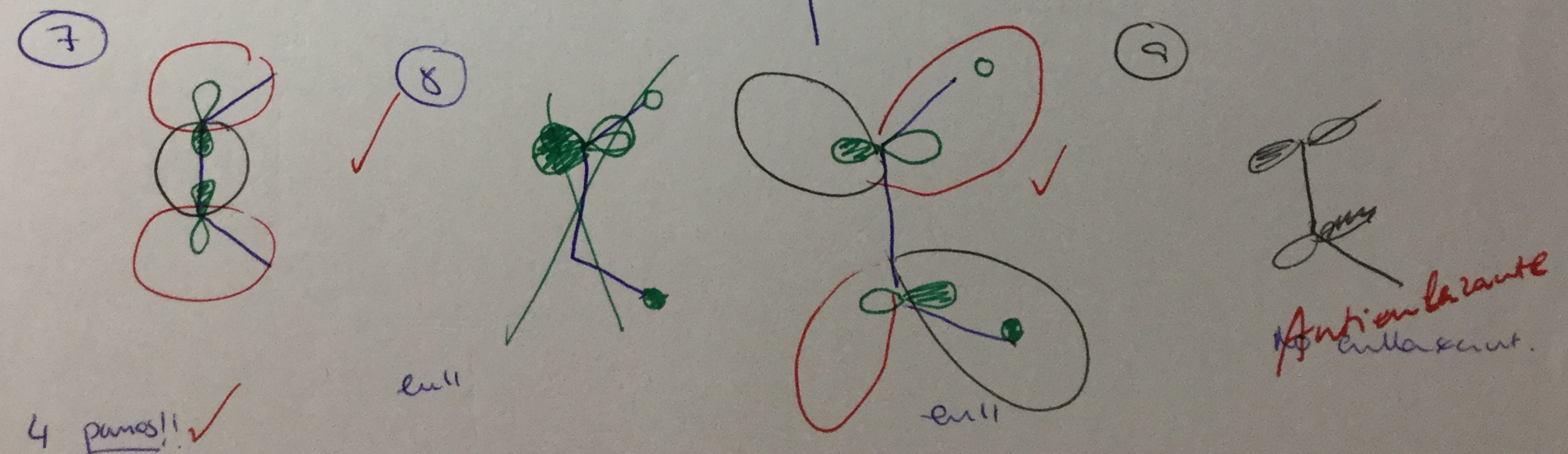
1,00305

8 O: 1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>4</sup> → x<sub>1s</sub>, x<sub>2s</sub>, x<sub>2p<sub>x</sub></sub>, x<sub>2p<sub>y</sub></sub>, x<sub>2p<sub>z</sub></sub> → 5 × 2 = 10 OA  
 1 H: 1s<sup>1</sup> → x<sub>1s</sub> × 2 → 120 OA → 120 OM ✓

8+8+2 = 18e<sup>-</sup> / 2 → 9 OM<sub>s</sub> ocupats ✓  
 3 OM<sub>s</sub> urmas ✓

Φ<sub>6</sub> - Φ<sub>9</sub> ocupats | Toti sau de valenta! ✓  
 Φ<sub>10</sub> vacant

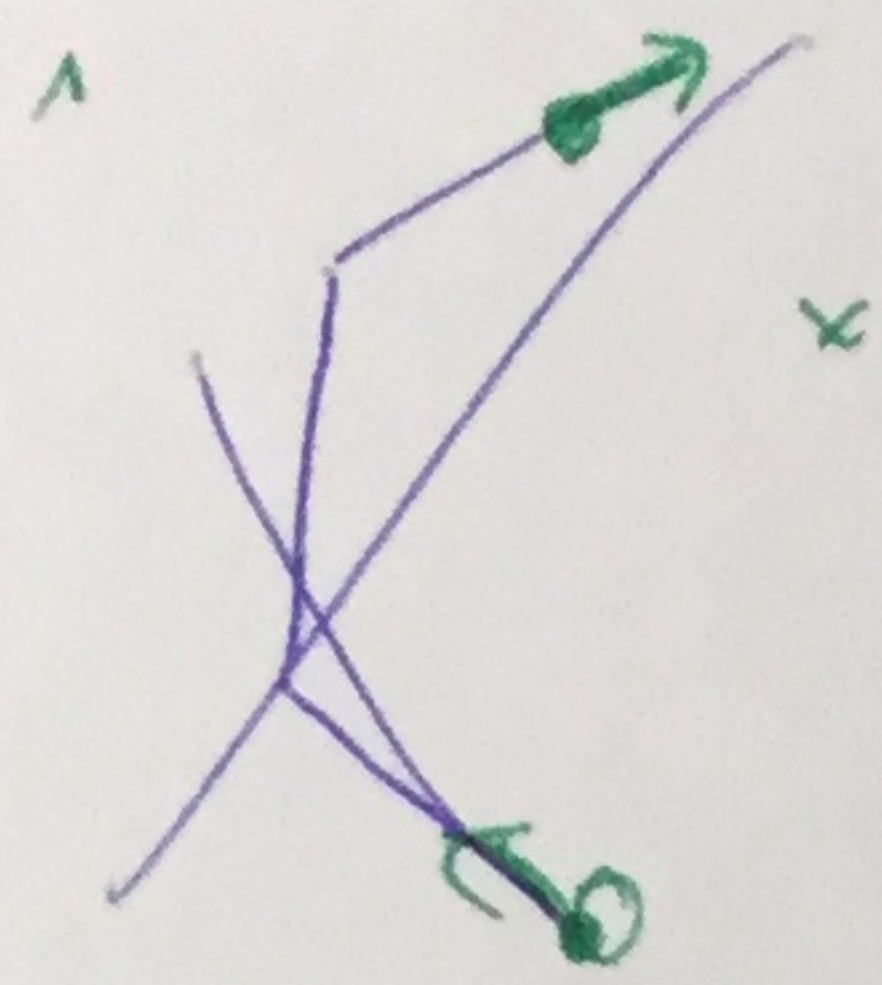
Φ<sub>6</sub> : π | Φ<sub>7</sub> ; Φ<sub>10</sub> → Φ<sub>8</sub> → σ  
 Φ<sub>9</sub> : π ✓



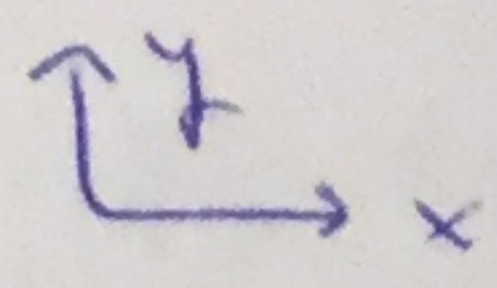
4 pures!! ✓

1e<sup>-</sup> E  
 2e<sup>-</sup> E

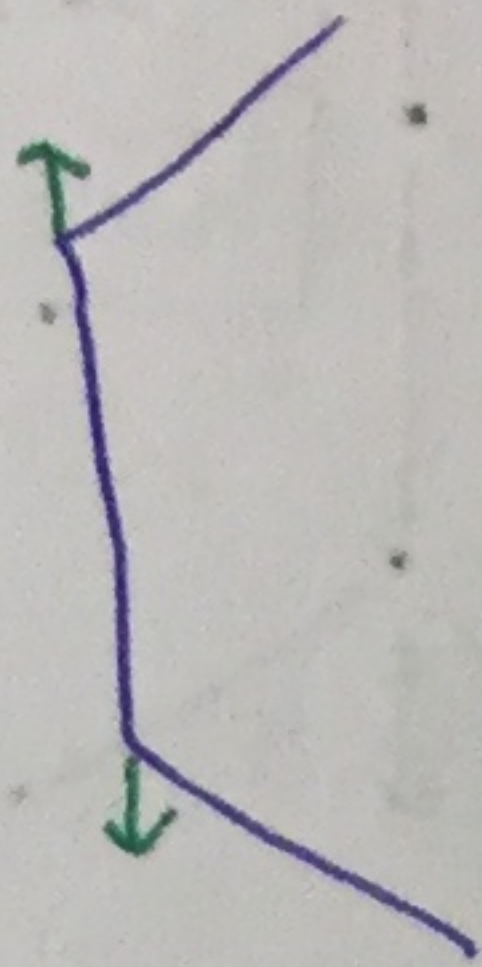
MNU. 1, 8, 9



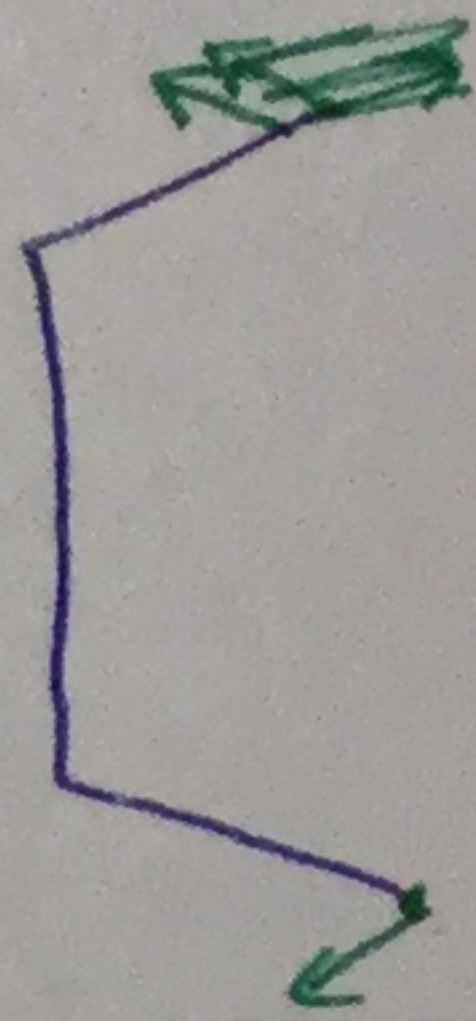
(wajinai!!)



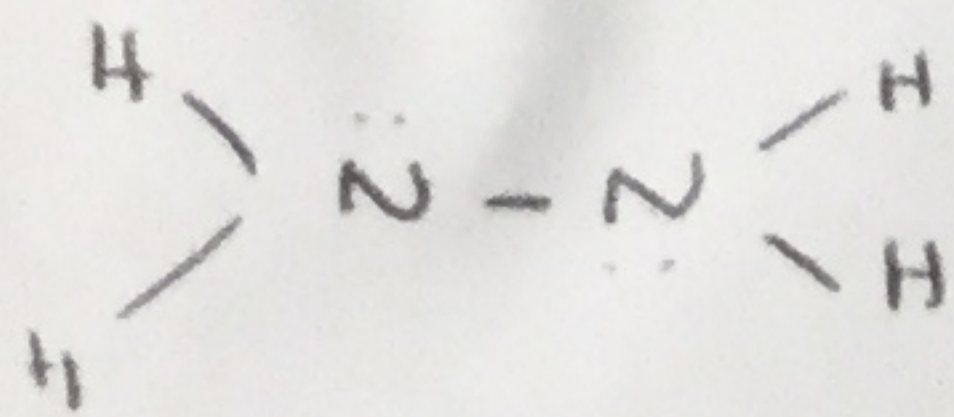
8



9



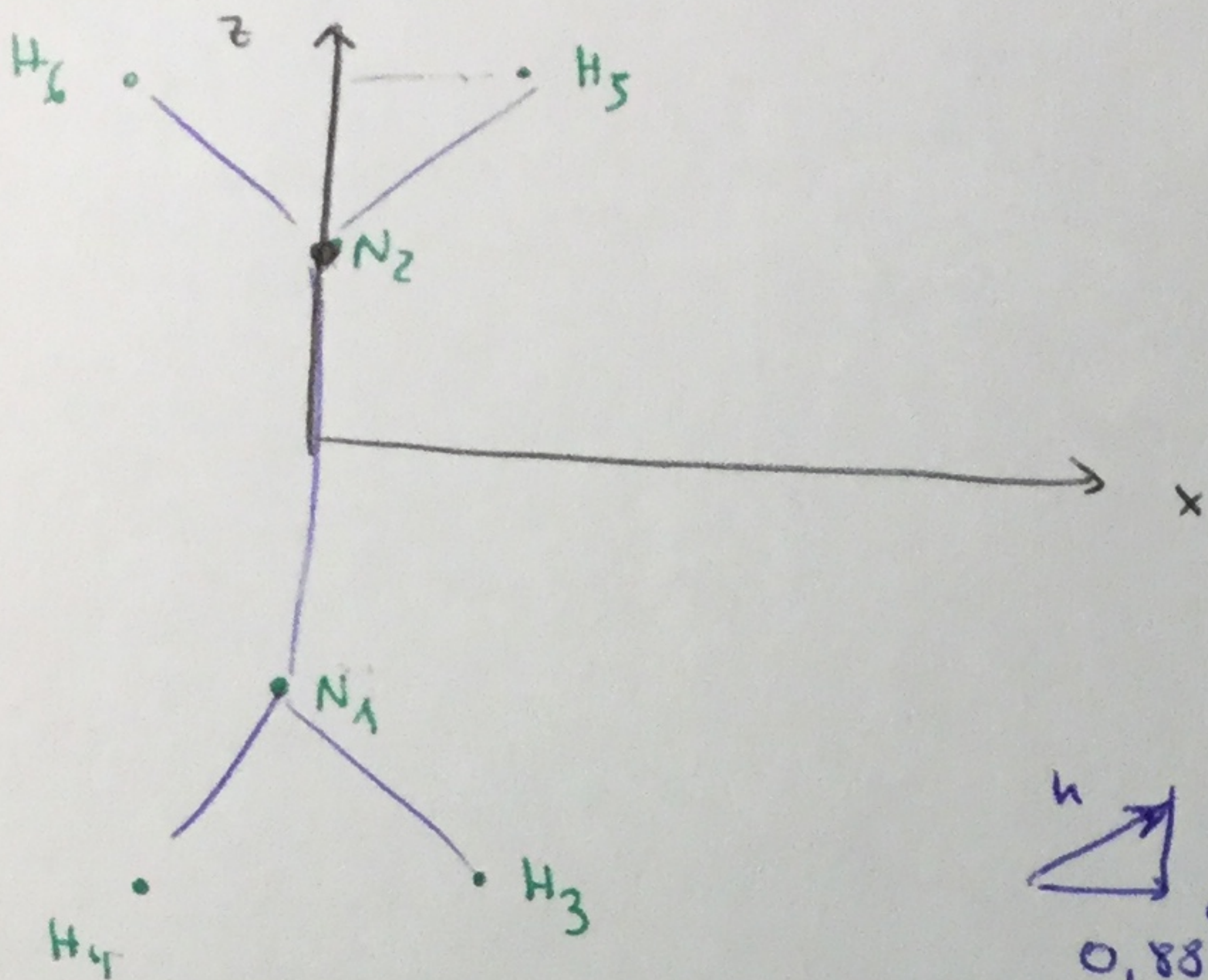
JUNY 2014



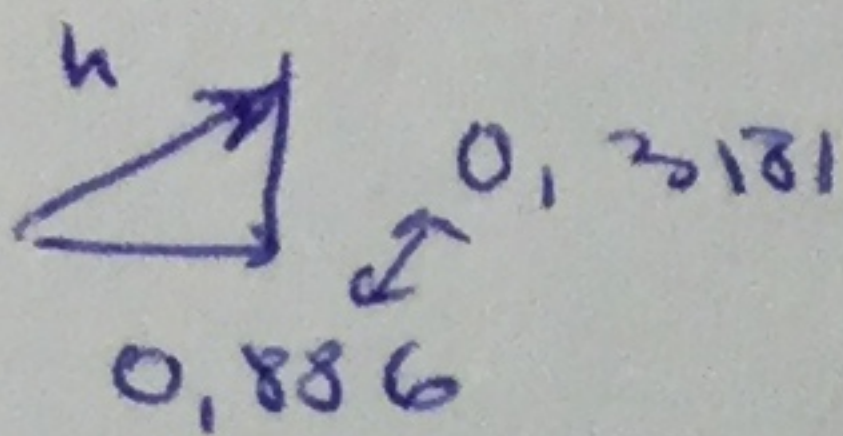
NH<sub>2</sub>

Optimize → Buscar secuencia d'equilibrio  
RHF STO-3G

Plane

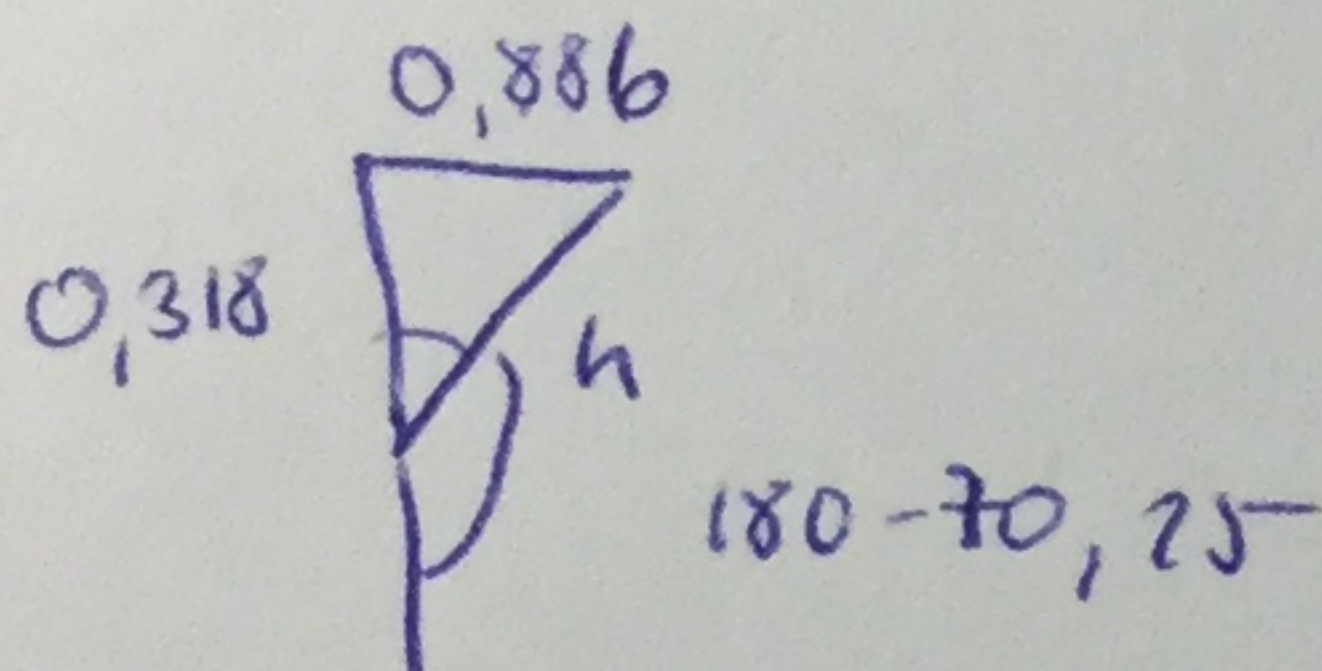


1	N						
2	N	1	1,4				
3	H	1	0,941	2	109,75		
4	H	1	0,941	2	109,75	6	180
5	H	2	0,941	1	109,75	8	<u>diatere not 0</u>
6	H	2	0,941	1	109,75	4	180



$h = 0,941$

$\alpha = \arctan \frac{0,3181}{0,886} = 70,25^\circ$



140ms 9 or + swirl.

N: ~~2s~~ 1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>6</sup> 3s<sup>2</sup> 3p<sup>6</sup> 3d<sup>10</sup>  
 ↑ ↑ ↑ ↑ ↑ ↑  
 1 1 3 1 3 6 → 15 × 2 = 30 DM<sub>J</sub>

H: 1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>6</sup> → 1+1+3 = 5 × 4 = 20 → 500ms.

ET