

Problemas T4

4.1 [Ne] 3s<sup>1</sup> 3d<sup>1</sup>

$$\begin{array}{l}
 s^1 \rightarrow \begin{cases} l=0 \\ s=1/2 \end{cases} \left\{ \begin{array}{l} 2S \\ 2D \end{array} \right. \\
 d^1 \rightarrow \begin{cases} l=2 \\ s=1/2 \end{cases}
 \end{array}
 \left\{ \begin{array}{l} L_T = 2 \\ S_T = 1, 0 \end{array} \right\}
 \left\{ \begin{array}{l} 1D \\ 3D \end{array} \right.$$

habría de ser el de E pero no lo es !!

4.2 [1s<sup>2</sup> 2s<sup>2</sup>] p<sup>2</sup> 3s<sup>1</sup> de N

$$\begin{array}{l}
 p^2: 3P, 1D, 1S \\
 s^1: 2S
 \end{array}
 \left\{ \begin{array}{l} 3P \\ 2S \end{array} \right.
 \left\{ \begin{array}{l} L_T = 0+1=1 \\ S_T = \frac{1}{2} + 1, \frac{1}{2} \end{array} \right\}
 \left\{ \begin{array}{l} 4P \\ 2P \end{array} \right.$$

+ estable (-E) ↑S

$$\begin{array}{l}
 1D \\
 2S
 \end{array}
 \left\{ \begin{array}{l} L_T = 2 \\ S_T = \frac{1}{2} \end{array} \right\}
 2D$$

$$\begin{array}{l}
 1S \\
 2S
 \end{array}
 \left\{ \begin{array}{l} L_T = 0 \\ S_T = 1/2 \end{array} \right\}
 2S$$

4.3 [1s<sup>2</sup> 2s<sup>2</sup>] 2p<sup>5</sup> 3s<sup>1</sup> 3d<sup>1</sup>

$$p^5 = p^1 \rightarrow \begin{cases} l=1 \\ s=1/2 \end{cases} \left\{ \begin{array}{l} 2P \\ 2S \end{array} \right.
 \left\{ \begin{array}{l} L_T = 1 \\ S_T = 1, 0 \end{array} \right\}
 \left\{ \begin{array}{l} 1P \\ 3P \end{array} \right.$$

$$s^1 \Rightarrow \begin{cases} l=0 \\ s=1/2 \end{cases} \left\{ \begin{array}{l} 2S \\ 2D \end{array} \right.$$

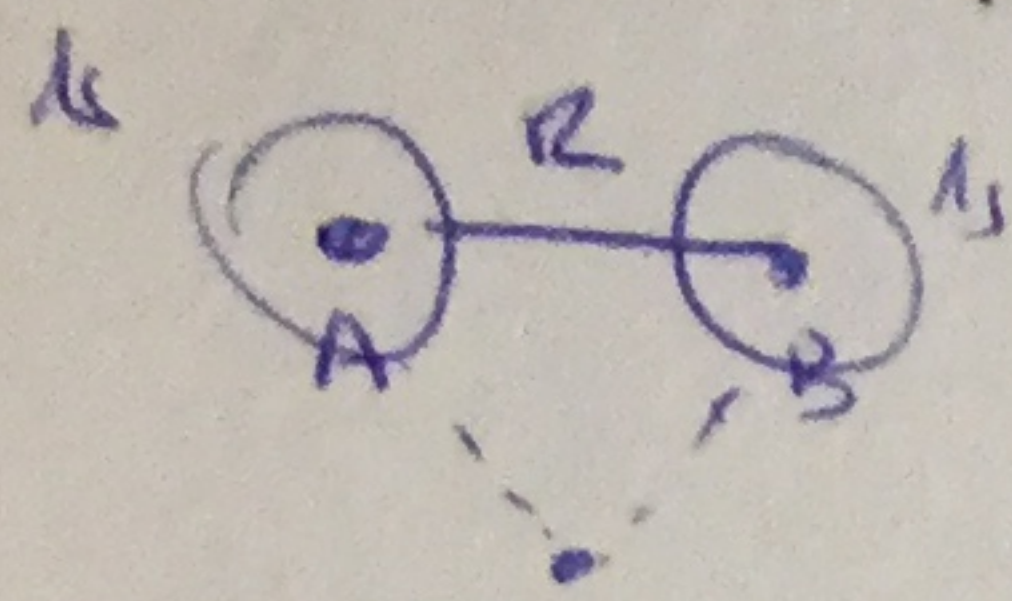
$$d^1 \rightarrow \begin{cases} l=2 \\ s=1/2 \end{cases} \left\{ \begin{array}{l} 2D \\ 3P \end{array} \right.
 \left\{ \begin{array}{l} L_T = 3, 2, 1 \\ S_T = 3/2, 1/2 \end{array} \right\}
 \left\{ \begin{array}{l} 4F \\ 2F \end{array} \right.
 \left\{ \begin{array}{l} 4D \\ 2D \end{array} \right.
 \left\{ \begin{array}{l} 4P \\ 2P \end{array} \right.$$

$$\begin{array}{l}
 2P \\
 2D
 \end{array}
 \left\{ \begin{array}{l} L_T = 3, 2, 1 \\ S_T = 0 + 1/2 \end{array} \right\}
 \left\{ \begin{array}{l} 2F \\ 2D \\ 2P \end{array} \right.$$

↗ ≠ ✓

4.4.  $H_2^+$

Met variational linear.



$$\Phi_1 = \frac{1}{\sqrt{2+2S_{AB}}} (\chi_A + \chi_B)$$

$$\Phi_2 = \frac{1}{\sqrt{2-2S_{AB}}} (\chi_A - \chi_B)$$

HFLCAO com linear de orb. atômicos normalizados

$$H = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{AB} & H_{BB} \end{pmatrix} = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{AB} & H_{BB} \end{pmatrix}$$

$$S = \begin{pmatrix} 1 & S_{AB} \\ S_{AB} & 1 \end{pmatrix}$$

$$(H_{AA} - W)^2 - (H_{AB} - WS_{AB})^2 = 0$$

$$H_{AA} - W = \pm (H_{AB} - WS_{AB}) \rightarrow H_{AA} = +W \pm (H_{AB} - WS_{AB})$$

$$\oplus \quad \boxed{W_+ = \frac{H_{AA} - H_{AB}}{1 - S_{AB}}}$$

$$\ominus \quad \boxed{W_- = \frac{H_{AA} + H_{AB}}{1 + S_{AB}}}$$

$$(H_{AA} - W_-)C_{A-} + (H_{AB} - W_-S_{AB})C_{B-}$$