Problemes T4

4.1 [Ne] $3s^1$ $3d^1$

$s^1 \to l=0, s=1/2 \} \ {}^2S$

$d^1 \to l=2, s=1/2 \} \ {}^2D$

$\} \ L_T = 2, \ S_T = 1, 0 \} \ {}^1D, \ {}^3D$ (circled) havia de ser el de − E però no ho és !!

4.2 [$1s^2$ $2s^2$] $2p^2$ $3s^1$ de (N)

p^2: ${}^3P$, ${}^1D$, ${}^1S$

s^1: ${}^2S$

${}^3P$, ${}^2S \} \ L_T = 0 + 1 = 1, \ S_T = \frac{1}{2} + 1, \frac{1}{2} \} \ {}^4P$ (circled), ${}^2P$

+ estable (− E) (↑S)

${}^1D$, ${}^2S \} \ L_T = 2, \ S_T = \frac{1}{2} \} \ {}^2D$

${}^1S$, ${}^2S \} \ L_T = 0, \ S_T = 1/2 \} \ {}^2S$

4.3 [$1s^2$ $2s^2$] $2p^5$ $3s^1$ $3d^1$

$p^5 = p^1 \to l = 1, s = 1/2 \} \ {}^2P$

$s^1 \Rightarrow l = 0, s = 1/2 \} \ {}^2S$

$\} \ L_T = 1, \ S_T = 1, 0 \} \ {}^1P, \ {}^3P$

$d^1 \to l = 2, s = 1/2 \} \ {}^2D$

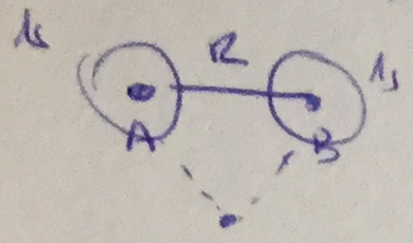
${}^3P$, ${}^2D \} \ L_T = 3, 2, 1, \ S_T = 3/2, 1/2 \} \ {}^4F \ {}^4D \ {}^4P$, ${}^2F \ {}^2D \ {}^2P$

↗↙ ≠

${}^1P$, ${}^2D \} \ L_T = 3, 2, 1, \ S_T = 0 + 1/2 \} \ {}^2F \ {}^2D \ {}^2P$ ✓

4.4. H_2^+

Met variacional lineal.



$$\Phi_1 = \frac{1}{\sqrt{2+2S_{AB}}}\chi_A + \chi_B \qquad \Phi_2 = \frac{1}{\sqrt{2-2S_{AB}}}(\chi_A - \chi_B)$$

HFLCAO combs lineal de orb. atómicos normalizados

$$HO = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{AB} & H_{BB} \end{pmatrix} = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{AB} & H_{BB} \end{pmatrix} \qquad S = \begin{pmatrix} 1 & S_{AB} \\ S_{AB} & 1 \end{pmatrix}$$

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

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

(+) ~~ANO~~ $$W_+ = \frac{H_{AA} - H_{AB}}{1 - S_{AB}}$$

(−) $$W_- = \frac{H_{AA} + H_{AB}}{1 + S_{AB}}$$

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