

És el conjunt de funcions d'ona segons T.O.M. de la molècula AB₄:

$$\Psi = N \cdot \varphi_{A2s} + N' \cdot \varphi_{B2pz} + N'' \cdot \varphi_{B2pz} + N''' \cdot \varphi_{B2pz} + N^{IV} \cdot \varphi_{B2pz}$$

$$\Psi^* = N \cdot \varphi_{A2s} - N' \cdot \varphi_{B2pz} - N'' \cdot \varphi_{B2pz} - N''' \cdot \varphi_{B2pz} - N^{IV} \cdot \varphi_{B2pz}$$

$$\Psi' = N \cdot \varphi_{A2px} + N' \cdot \varphi_{B2pz} + N'' \cdot \varphi_{B2pz} + N''' \cdot \varphi_{B2pz} + N^{IV} \cdot \varphi_{B2pz}$$

$$\Psi'^* = N \cdot \varphi_{A2px} - N' \cdot \varphi_{B2px} - N'' \cdot \varphi_{B2py} - N''' \cdot \varphi_{B2px} - N^{IV} \cdot \varphi_{B2px}$$

$$\Psi_1 = N \cdot \varphi_{A2s} \pm N' \cdot \varphi_{B2py} \pm N'' \cdot \varphi_{B2py} \pm N''' \cdot \varphi_{B2py} \pm N^{IV} \cdot \varphi_{B2py}$$

$$\Psi_2 = N \cdot \varphi_{A2s} \pm N' \cdot \varphi_{B2px} \pm N'' \cdot \varphi_{B2px} \pm N''' \cdot \varphi_{B2px} \pm N^{IV} \cdot \varphi_{B2px}$$

$$\Psi_3 = N \cdot \varphi_{A2px} \pm N' \cdot \varphi_{B2py} \pm N'' \cdot \varphi_{B2py} \pm N''' \cdot \varphi_{B2py} \pm N^{IV} \cdot \varphi_{B2py}$$

$$\Psi_4 = N \cdot \varphi_{A2px} \pm N' \cdot \varphi_{B2px} \pm N'' \cdot \varphi_{B2px} \pm N''' \cdot \varphi_{B2px} \pm N^{IV} \cdot \varphi_{B2px}$$

$$\Psi_5 = N \cdot \varphi_{A2py} \pm N' \cdot \varphi_{B2py} \pm N'' \cdot \varphi_{B2py} \pm N''' \cdot \varphi_{B2py} \pm N^{IV} \cdot \varphi_{B2py}$$

$$\Psi_6 = N \cdot \varphi_{A2py} \pm N' \cdot \varphi_{B2px} \pm N'' \cdot \varphi_{B2px} \pm N''' \cdot \varphi_{B2px} \pm N^{IV} \cdot \varphi_{B2px}$$

$$\Psi_7 = N \cdot \varphi_{A2pz} \pm N' \cdot \varphi_{B2py} \pm N'' \cdot \varphi_{B2py} \pm N''' \cdot \varphi_{B2py} \pm N^{IV} \cdot \varphi_{B2py}$$

$$\Psi_8 = N \cdot \varphi_{A2pz} \pm N' \cdot \varphi_{B2px} \pm N'' \cdot \varphi_{B2px} \pm N''' \cdot \varphi_{B2px} \pm N^{IV} \cdot \varphi_{B2px}$$

$$\Psi'' = N \cdot \varphi_{A2py} + N' \cdot \varphi_{B2pz} + N'' \cdot \varphi_{B2pz} \pm N''' \cdot \varphi_{B2pz} \pm N^{IV} \cdot \varphi_{B2pz}$$

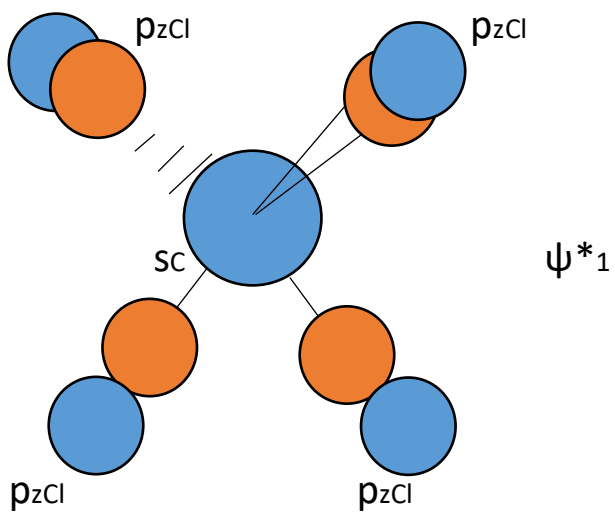
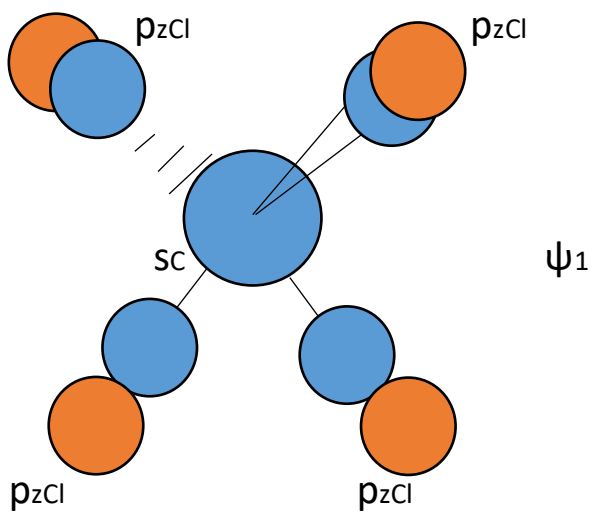
$$\Psi''' = N \cdot \varphi_{A2py} - N' \cdot \varphi_{B2pz} - N'' \cdot \varphi_{B2pz} \pm N''' \cdot \varphi_{B2pz} \pm N^{IV} \cdot \varphi_{B2pz}$$

$$\Psi'''' = N \cdot \varphi_{A2pz} \pm N' \cdot \varphi_{B2pz} \pm N'' \cdot \varphi_{B2pz} + N''' \cdot \varphi_{B2pz} + N^{IV} \cdot \varphi_{B2pz}$$

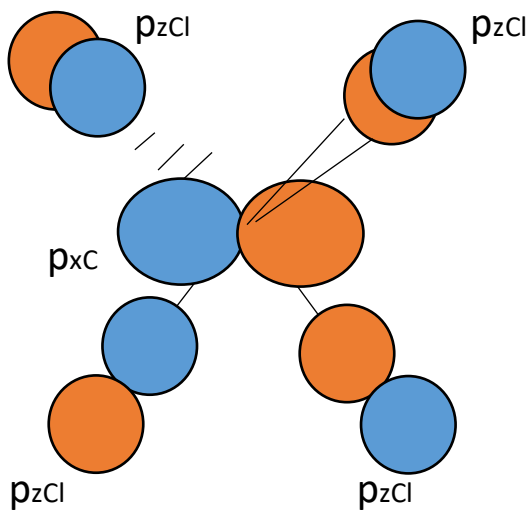
$$\Psi'''''' = N \cdot \varphi_{A2pz} \pm N' \cdot \varphi_{B2pz} \pm N'' \cdot \varphi_{B2pz} - N''' \cdot \varphi_{B2pz} - N^{IV} \cdot \varphi_{B2pz}$$

On de Ψ_1 a Ψ_8 són no enllaçants.

TOM CCl₄:



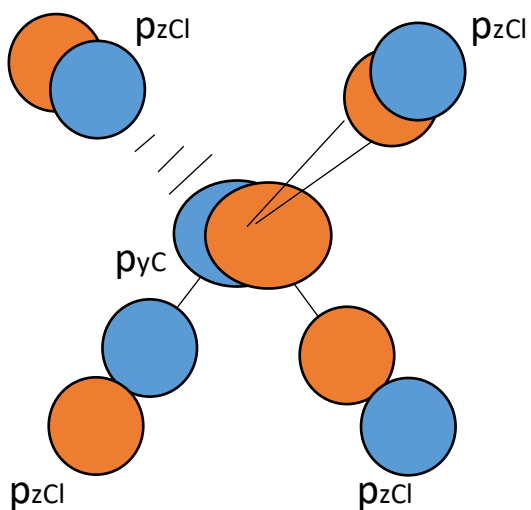
mentre que p_{xCl} i p_{yCl} no enllaçen



ψ_2

la ψ^*_2 és ràpid de deduir

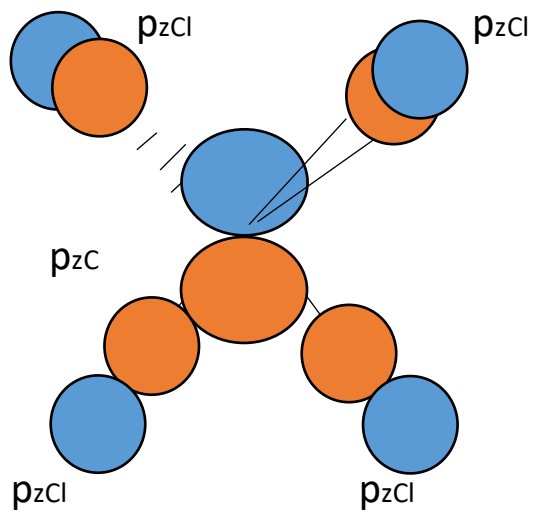
mentre que p_{xCl} i p_{yCl} continuen sense enllaçar



ψ_3

la ψ^*_3 és ràpid de deduir

p_{xCl} i p_{yCl} continuen sense enllaçar



ψ_4

la ψ^*_4 és ràpid de deduir

i p_{xCl} i p_{yCl} no enllaçen

per tant, tenim 16 Orbitals Atòmics que generen 16 Orbitals
Moleculars: $\psi_1, \psi^*_1 + p_{xCl} + p_{yCl}$

$\psi_2, \psi^*_2 + p_{xCl} + p_{yCl}$

$\psi_3, \psi^*_3 + p_{xCl} + p_{yCl}$

$\psi_4, \psi^*_4 + p_{xCl} + p_{yCl}$

16 O.M.