CM2 – Description quantique de la liaison métal-ligand

1. Structure électronique des complexes

1.1. Ligands σ-donneurs

1.2. Effets π

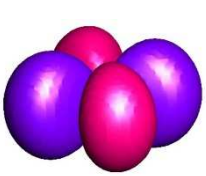
1.3. Un peu de spectroscopie

2. Activation des ligands

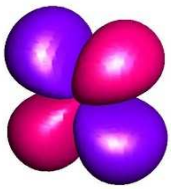
2.1. Alcènes

2.2. Carbonyle

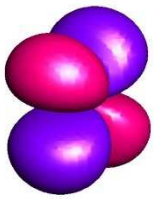
2.3. Dihydrogène



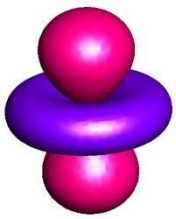
orbitale $3d_{xy}$



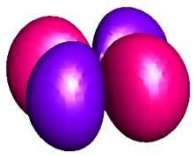
orbitale $3d_{yz}$



orbitale $3d_{xz}$



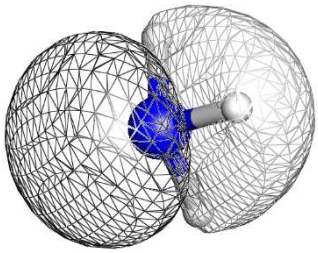
orbitale $3d_{z^2}$



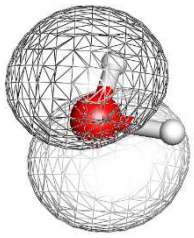
orbitale $3d_{x^2-y^2}$

Orbitales moléculaires de quelques ligands et complexes (calculs Jimp2) :

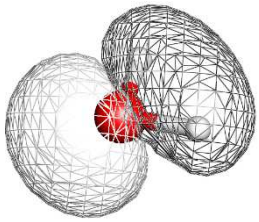
HOMO de NH_3 (E = −13,48 eV ; calculs Jimp2) :



H_2O :

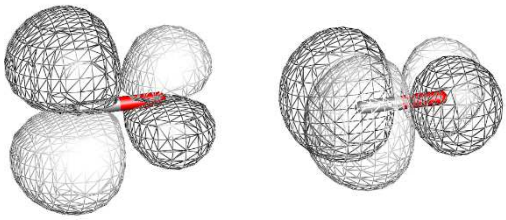


HOMO (−14,23 eV)

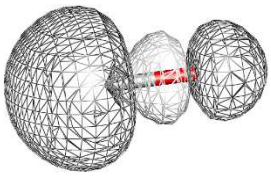


HOMO−1 (−17,14 eV)

CO :

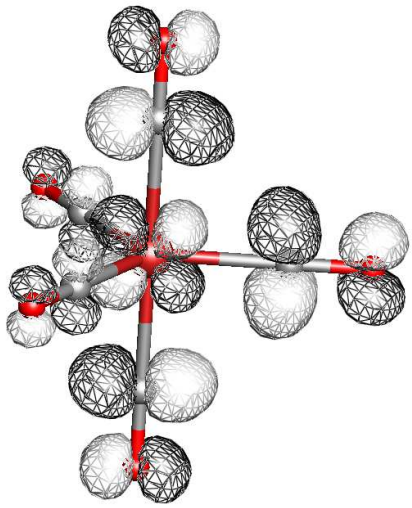


LUMO (0,48 eV, 2 OM dégénérées)

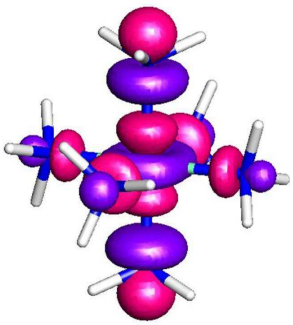


HOMO (−12,76 eV)

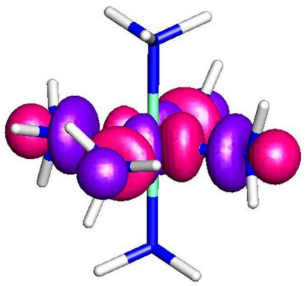
LUMO de $Fe(CO)_5$:



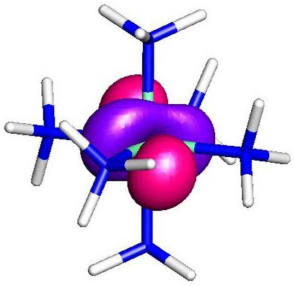
Orbitales frontalières (bloc d) du complexe $Ni(NH_3)_6^{2+}$ (calcul Jimp2) :



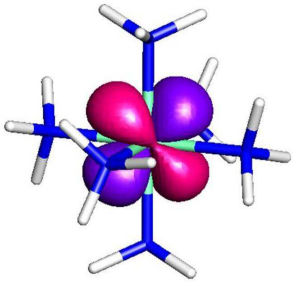
ψ_4



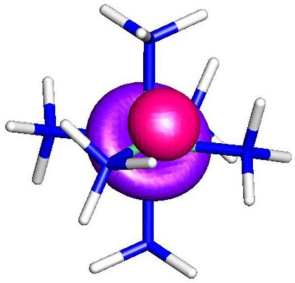
ψ_5



ψ_1



ψ_2



ψ_3