Practical Class
Introduction to numerical quantum chemistry

This pratical work comes from David Lauvergnat, Orsay 2013, from a master1 program.

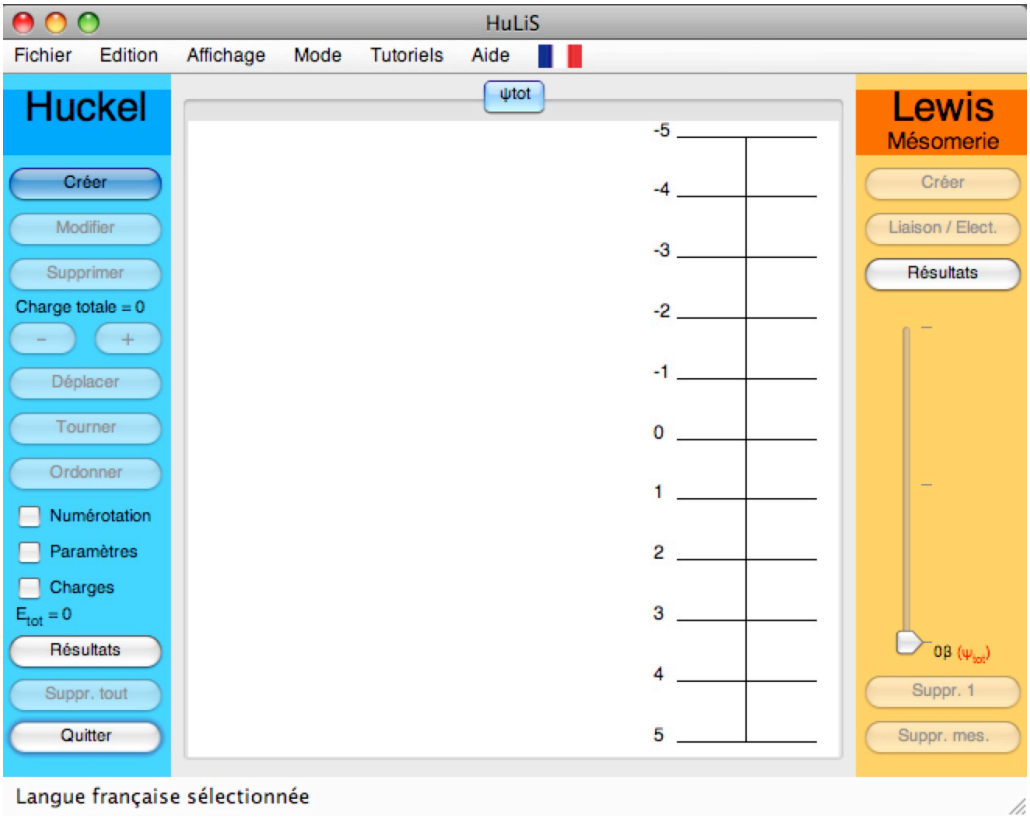
MO diagrams with Hückel model

The Hückel model is used to describe the π-electron system. In 1930, E. Hückel has rationalized some reactivity's of cyclic conjugated molecular systems and he has defined the so-called "Hückel rule" for aromatic compounds.

We are going to use another software, named "***HuLis***", made especially for Hückel molecular orbital calculations.

1) The ethylene ($H_2C=CH_2$), methylene-imine ($H_2C=NH$) and methanal ($H_2C=0$) molecules

To Launch the "***Hulis***" program, click on "". The following window appears:



The English language can be selected using the flag button.
Then, to learn rapidly how to use "***HuLis***", you should run the tutorial (click on "***Tutorials***", and select "***Tutorial 0 : Build***").

a. Build the ethylene molecule.
   Report and draw the doubly-occupied and the unoccupied orbitals *(obtained by clicking the "**Results**" button)*.

Q1: Using the coefficients of molecular orbitals, check that each MO is an eigenvector of the Hückel Hamiltonian.

Q2: Calculate the π-electronic density on each carbon. What are the atomic charges?

b. Build the methylene-imine ($H_2C=NH$) and then the methanal ($H_2C=O$) molecules.
For each molecule, report and draw the doubly-occupied orbital and the unoccupied one *(obtained by clicking the "**Results**" button).*

Q3: Calculate the π-electronic density and the charge on the atoms (C, N, O). What are their atomic charges? Comment the evolution of the charge in this series (ethylene, methylene-imine, methanal).

2) Benzene and cyclo-butadiene molecules

a. Build the benzene molecule.
Report and draw the doubly-occupied and the unoccupied orbitals *(obtained by clicking the "**Results**" button).*

*Q1: Using the coefficients of molecular orbitals (obtained by clicking the "**Results**" button), check that each MO is an eigenvector of the Hückel Hamiltonian.*

Q2: Calculate the π-electronic density on each carbon. What are the atomic charges?

Q3: Calculate the total electronic energy.

b. Build one Kekulé structure of benzene.
Report and draw the doubly-occupied and the unoccupied orbitals *(obtained by clicking the "**Results**" button).*

To set-up a Kekulé structure, you have to remove three β-interactions between three C-C bonds. To remove one β-interaction, proceed as follow: (i) Click on the "***change***" button. (ii) Click on one benzene bond. (iii) Change the value of "***Hxy***" to zero.

Q4: Calculate the total electronic energy and compare its energy to the energy of three ethylenes.
Compare the Kekulé energy and the benzene one.

c. Build the cyclo-butadiene molecule.

Q5: Calculate its total electronic energy. Compare this energy to the energy of two ethylenes.

Q6: Following Hückel rule, a planar ring molecule is said aromatic when its π-electron number is equal to 4n+2 (n is an integer). Check that benzene is aromatic and cyclo-butadiene is antiaromatic.