Starting up instructions

All the files are in deuterium (rfct_tp@lct.jussieu.fr), at the directory TP_topologie

Important files:

- **Linux reminder: linux.pdf**
- **Instructions on how to use the program: software.pdf**
- **These exercises: exercices.pdf**
- **Theory overview: theory.pdf**
- **Cube files: http://www.lct.jussieu.fr/pagesperso/contrera/nci-exercises.html**

Getting started (see linux reminder above if necessary)

1. **Remember to create a working directory (e.g. with your name(s))**
2. **Copy the files to it**
3. **Start going! ELF exercises take much longer, bare it in mind for distributing your time**
4. **Remember to write a Compte Rendu. You will have to hand it at the end of the session.**

ELF

1. BONDS: analyzing bond order in ethane vs ethylene

a) Perform ELF analysis and obtain the ELF for ethane and ethylene (ethene) [Follow instructions in software.pdf].

b) Check that the integration of electrons (total number of electrons) corresponds to the expected number. This should be done each time to check the accuracy of the integration.

c) Draw the Lewis structure of both compounds and identify all the pairs predicted by Lewis theory. Remember to include core electrons, since they will also appear in the ELF results.

d) Look at the output from bas09:

   i. Identify the attractors with your Lewis picture and explain the ELF notation for each of them. Find the bonding attractor(s). What is the ELF notation for them?

ii. Look at the bonding attractors: How many are there in each case? Why? Where and why are they located? (check xyz position and angles)

iii. Look at the H-C-H and H-C-C angles and check how they deform from the ideal value according (or not) to VSEPR.

e) Look at the output from pop09:

i. What is the charge for the single and for the double bond according to the output? Does it agree with what you expected? Comment on the differences.

ii. Look at the volumes. Do they agree with VSEPR? (exclude hydrogenated bonds, i.e. comment on cores, non-hydrogenated bonds and lone pairs)

f) Download the cube files http://www.lct.jussieu.fr/pagesperso/contrera/nci-exercises.html and visualize them using VMD [Follow instructions in software.pdf] How do both bonds look like?

2. LONE PAIRS: analyzing VSEPR in ethanol vs chloroethane

a) Perform ELF analysis and obtain the ELF for ethanol and chloroetane [Follow instructions in software.pdf].

b) Check that the integration of electrons (total number of electrons) corresponds to the expected number. This should be done each time to check the accuracy of the integration.

c) Draw the Lewis structure of both compounds and identify all the pairs predicted by Lewis theory. Remember to include core electrons, since they will also appear in the ELF results.

d) Look at the output from bas09:

i. Identify the attractors with your Lewis picture and explain the ELF notation for each of them. Find the lone pair attractor(s). What is the ELF notation for them?

ii. Look at the lone pair attractors: How many are there in each case? Why? (check xyz position and angles). Compare the distance from the lone pair and the C-O bond to the oxygen. Why are they different?

You will see that one of the lone pairs of C2H5Cl appears as shared, you can ignore it in your analysis and take it as a mere lone pair since the distances are very different to C and to Cl (the program uses the gradient to find the connections).

iii. Look at the angles around the oxygen and check how they deform from the ideal value according (or not) to VSEPR.

e) Look at the output from pop09:

i. Hydrogens were all equivalent in ethane and ethylene, but not in these molecules. Why?
ii. Look at the charge of the C-O and C-Cl bonds. How is it? Why?
iii. Calculate the total charge in the O and Cl lone pairs. How is it with respect to your prediction from the Lewis structure?
iv. Look at the volumes of the lone pairs. Are they bigger or smaller than non-hydrogenated bonds? Does this agree with VSEPR?
v. Why is oxygen core smaller than the carbon one?
vi. Is the charge in the chlorine core correct?

f) Download the cube files http://www.lct.jussieu.fr/pagesperso/contrera/nci-exercises.html and visualize them using VMD [Follow instructions in software.pdf]
i. How do the lone pairs look like?
ii. Check in internet what halogen bonds are. How does this bond relate to what you see in chloroethane?

NCI

1. Looking at non covalent interactions

Run promolecular NCI analysis for a peptide (`peptide.xyz`) and identify the different types of bonds.

2. Analysing intermolecular interactions (*ideal for ligand-protein interactions*)

Analyze the interactions in the inclusion complex between the 7-cucurbit and a bicycle derivative (files: `cb7.xyz` and `bcb.xyz`). This complex has a binding energy of the order of protein-ligand interactions. What interactions are responsible for the stabilization? Use the `intermolecular` keyword and compare the result with the one from a normal run.

EXTENSION (OPTIONAL)

1. Solvation

Check the interactions responsible for the solvation of the cation K^+ in water (`khoh6.wfn`). What do you observe? What parameters did you need to adjust?

2. Big systems

If you are interested in big systems, you can have a look at the interactions determining the stabilization of β-sheets (`sheet.xyz`). Which are the main interactions? Which atoms are involved?

Now have a look at the interactions in the base pairs: You can repeat the exercise for the adenyn-thymine complex (`AT.xyz, A.xyz, T.xyz` files). Remember that you may want to look only at intermolecular interactions.