Working Session I : QTAIM / IQA/REG

https://moderm2023.sciencesconf.org/

Tuesday 5 sept. T. 42-43, basement	Wednesday 6 sept. T. 42-43, basement
QTAIM – IQA – REG	ELF, MESP & NCI
Lunch **Brasserie l'ardoise**	**Lunch** **Brasserie l'ardoise**
14h30-15h30 QTAIM – IQA - REG	Conceptual DFT
16h -17h30 ELF, MESP &NCI	

Working Session I

We provide all files needed for the working session:

✓A copy of useful articles and inputs for TopChem2 and ADF

✓For the first exercise of the session I, we have supplied all the requisite wfn/wfx files for TopChem2. Feel free to select the molecules from the provided list :

C_2H_6, C_2H_4, C_2H_2, C_6H_6, Cubane C_8H_8, H_2O, H_2CO, H_2O_2, CO, NO, CO_2, NH_3BH_3, B_2H_6, LiF, F_2, FH--CO, FH--OC, $ClF_3(C_{2v})$, FCl

The Working Session I

- **ADF**: https://www.scm.com/doc/ADF/.

Generalist quantum chemistry software that allows direct analyzes of molecular interactions, in particular those using the QTAIM/IQA approach and the descriptors of the conceptual DFT.

- **TopChem2**: https://www.lct.jussieu.fr/pagesperso/pilme/topchempage.html

It is a software for analyzing interactions using topological approaches and conceptual DFT. It is developed at the Laboratory of Theoretical Chemistry at Sorbonne University. It is free and the license allows free use for teaching or research activities.

Starting with Topchem2: Summary of main commands (page 32)

1. Open a linux terminal

2. Change the directory where the input files are located:

```
cd MoDerm/TP_Exercices/Inputs_MoDerm/SessionI
```

3. and start with the command-line,

```
topchem2 ….
```

Working Session I: QTAIM Analysis with Topchem2

QTAIM command-line,

- topchem2 **wfn**:c2h6.wfn **function**:rho **pop**:cov **cp**:y **refine**:f **proc**:4 **output**:c2h6.pop (optional: **atom_dist**:0.2) **vmd**

Working Session I: QTAIM Analysis with Topchem2

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Gaussian wfn file (or wfx)

Working Session I: QTAIM Analysis with Topchem2

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QTAIM analysis

Working Session I: QTAIM Analysis with Topchem2

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Compute population and the delocalization index

Working Session I: QTAIM Analysis with Topchem2

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Search the critical points

Working Session I: QTAIM Analysis with Topchem2

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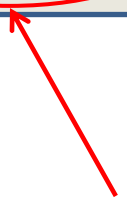


The file contains all your results

Working Session I: QTAIM Analysis with Topchem2

QTAIM command-line,

- topchem2 **wfn**:c2h6.wfn **function**:rho **pop**:cov **cp**:y **refine**:f **proc**:4 **output**:c2h6.pop (optional: **atom_dist**:0.2) **vmd**

Visualize Critical points with vmd

How to interpret your QTAIM results ?

Descriptors computed at the bond critical point bcp (3, -1)
→ bonding nature

Shared-shell (covalent):

- $\rho(\mathbf{r})$ high (> 0.15 e.bohr^{-3} in practical)

$$-\nabla^2\rho(x,y,z) = \frac{\partial^2\rho}{\partial x^2} + \frac{\partial^2\rho}{\partial y^2} + \frac{\partial^2\rho}{\partial z^2} < 0$$ (charge concentration)

- $|V|/G > 1$ and $H < 0$ (covalent or donor-acceptor)

$G(\mathbf{r})$: the positive kinetic energy density >0

$V(\mathbf{r})$: the potential energy density <0

$H(\mathbf{r}) = G(\mathbf{r}) + V(\mathbf{r})$, the total energy density <0

How to interpret your QTAIM results ?

- δ_{AB} is the delocalization index

It is connected to the *number of electron-pairs shared between two QTAIM basins A and B.* For closed-shell systems, the first-order matrix can be expanded in terms of overlap between molecular orbitals:

$$\delta(\Omega_A, \Omega_B) = 2 \sum_i \sum_j < \varphi_i | \varphi_j >_{\Omega_A} < \varphi_i | \varphi_j >_{\Omega_B}$$

It can be compared to other bond order indices.

Variance - Localization Index(LI)

basin	vol.	var.	fluct.	LI
1 C	103.041	1.946	0.325	4.049
2 C	103.041	1.892	0.316	4.103
3 H	679.264	0.513	0.512	0.489
4 H	657.407	0.561	0.560	0.441

Covariance Matrix

1 C	1.946	-0.475	-0.013	-0.479
2 C	-0.475	1.892	-0.446	-0.026
3 H	-0.013	-0.446	0.513	-0.009

Delocalization Index

1 C -	2 C	0.950
1 C -	3 H	0.025
1 C -	4 H	0.957

Search at the end of c2h6.pop, here δ_{CO} = 0.950

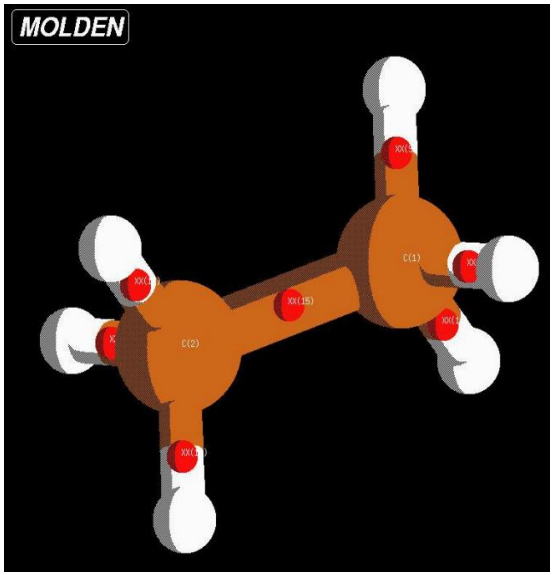
How to interpret your QTAIM results ?

	Scheme	ρ_{bcp}	$\nabla^2\rho_{bcp}$	$\lvert V_{bcp}\rvert/G_{bcp}$	H_{bcp}	δ
Closed-Shell	Van der Waals	Low	>0	≈1	>0	< 1
	ionic	Low	>0	≈1	>0	< 1
	donor-acceptor	Low	>0	≈1	<0	< 1
Shared -Shell	polar covalent	High	<0	>1	<0	> 1
	covalent	High	<0	>1	<0	> 1

How to visualize your QTAIM results ?

results : > vi your_file .pop

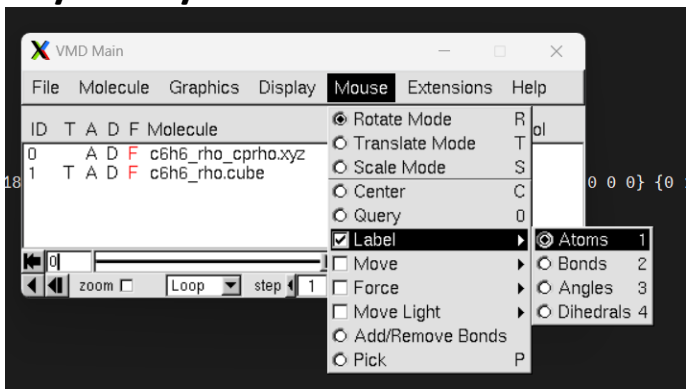
```
================================================
                POPULATION ANALYSIS SECTION
================================================

 Populations
 ================

 basin                vol.       pop.       q.

 1 C               103.041     5.9948     0.0052
 2 C               103.041     5.9948     0.0052
 3 H               679.264     1.0017    -0.0017
 4 H               657.407     1.0017    -0.0017
```

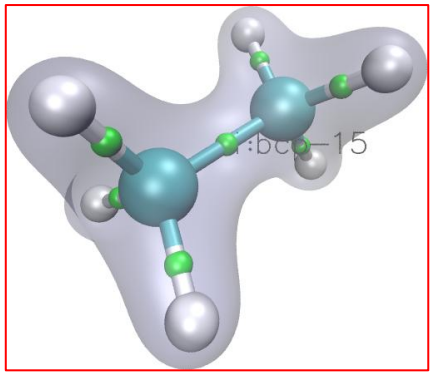


1. Visualize CP locations : > molden molecule _rho_cprho.xyz

2. Visualize CP locations : > vmd -e your_file_rho.vmd

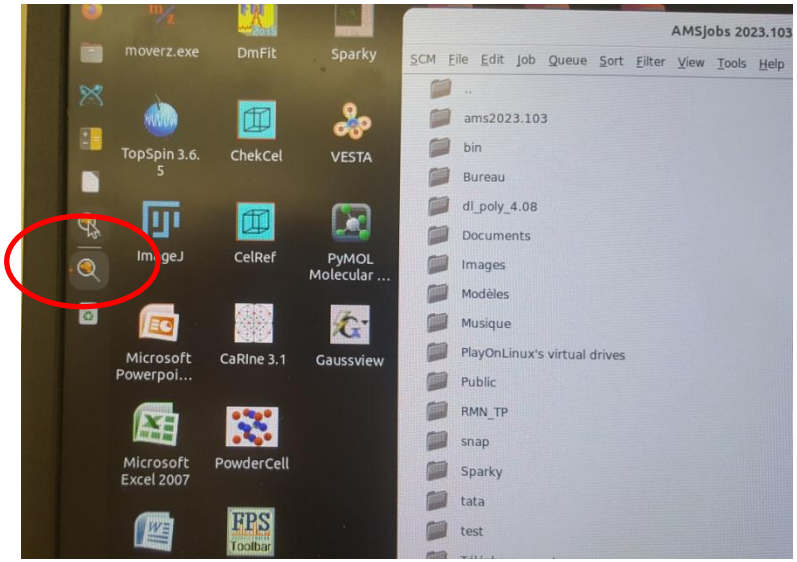
VMD Superpose CP + electron density : activate with **Mouse/Label/atoms** :





Working Session I : Source Function/IQA/REG Analysis with ADF

Run the AMS Graphical User Interface:



Please, read the document Practical Work with AMS 2023 (page 4) for an introduction to AMS Software Suite