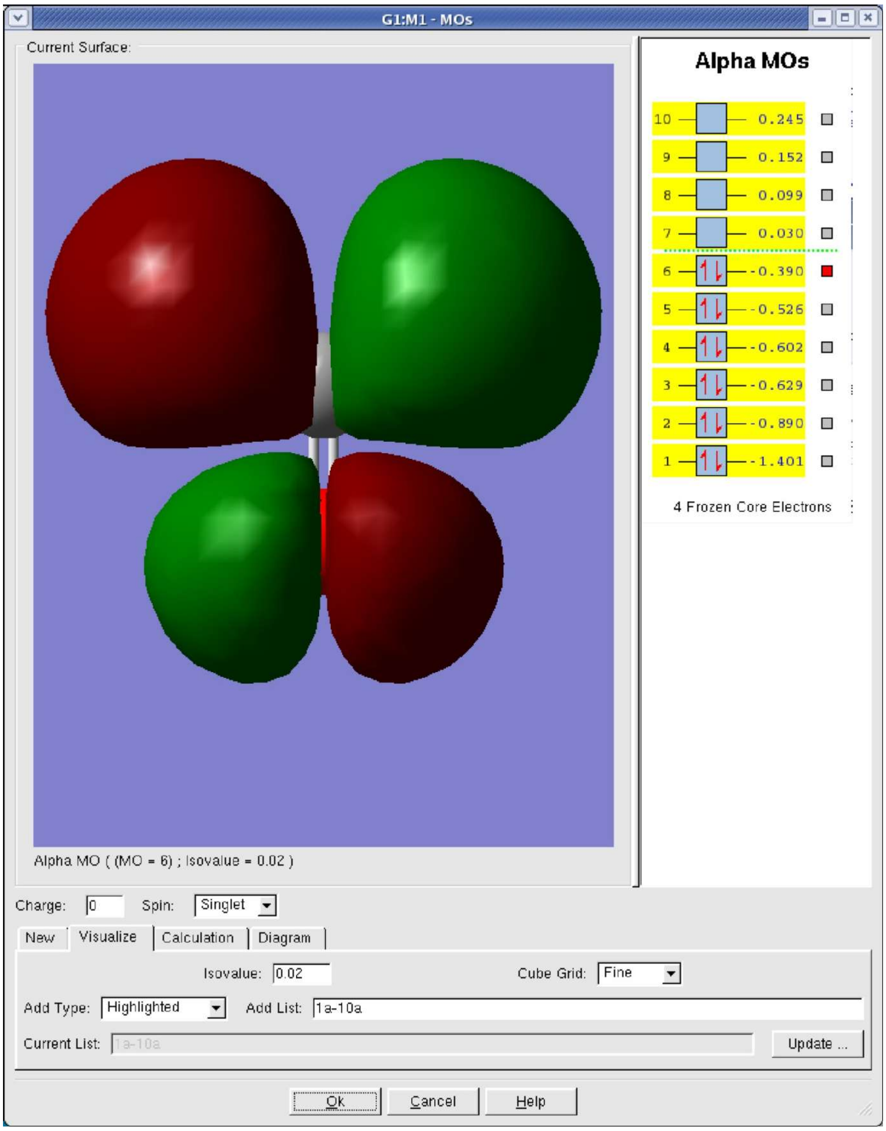
Quantum Chemical Calculations

Part II – GaussView and Gaussian



10 0.245
9 0.152
8 0.099
7 0.030
6 -0.390
5 -0.526
4 -0.602
3 -0.629
2 -0.890
1 -1.401

4 Frozen Core Electrons

Alpha MO ((MO = 6) ; Isovalue = 0.02)

Charge: 0
Spin: Singlet
Isovalue: 0.02
Cube Grid: Fine
Add Type: Highlighted
Add List: 1a-10a
Current List: 1a-10a

Brought to You
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1. How to login and print your files

1.1 How to login

You will get your username and password from the assistants.

After logging in open a terminal window and start GaussView by giving the command: **GView**

Note: Due to quota restrictions (you have a limit on how much disk space you can have), it might be better to do:

```
cd /tmp
mkdir $LOGNAME             or: mkdir <your username>
cd $LOGNAME                or: cd <your username>
GView
```

1.2 How to print the output files

You can print your output (**.log**) files either by opening them in GaussView (**Open** under the **File** menu), choose **View File...** under the **Results** menu and then choose **Print**, or by printing the file directly in a terminal window: **lp -d** <*name of printer*> **filename.log**

2. How to use the Mouse

The three buttons on the mouse has the following functions:

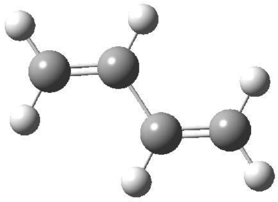
left:	Choose in menus To select items Click and hold to rotate the molecule To add atoms/groups/fragments
middle	Translations
right	Zoom

3. To build/edit a molecule

1. Select **New : Create MolGroup** from the **File** menu or, if you want to change your existing molecule, choose the window with your molecule in.

2. Select an atom from the **Element Fragment** window (accessed by clicking on the **^{6}C** – button and choose want kind of bond/hybridization you want and click with the left button in the **Molecule** window. Be careful of where the **Hot** label is, in the main **Gauss View** window. If it's not on the center atom then you might end up with unexpected results.
   To connect an atom to another, click with left button on the hydrogen (yellow) and the selected atom will be bonded.

Example: How to build 1-3-butadiene.



1. Select a carbon with four bonds from the panel.
2. Click with the left button on the builder area (a carbon with four bonds appears in the middle of the builder area
3. Click with the left button on one of the hydrogens.
4. Repeat this two more times and, hopefully, you will have butane on the screen. In order to create the double bonds, select the **Modify Bond** button.
5. Click (left button) on one of the carbons at the end, then on the carbon next to it. In the window that opens, choose the double bond (two lines) and click **OK**. A double bond will appear!
6. Repeat for the other end carbon.
7. Then select the **Delete Atom** button. Click on one hydrogen on each carbon to reduce the number of hydrogens to the correct number.

Another way to do the same thing is to choose the carbon with two single and one double bond, place it on the builder area, click on the double bond (and you will join a similar atom to the double bond). Then click on one of the hydrogens to create a single bonded atom. Finally click on the free double bond and voilá 1-3-butadiene.

3. In order to get a better geometry, choose **Clean** in the **Edit** menu.

4. To save your work, choose **Save** in the **File** menu. This is not necessary if you are going to perform a calculation on your molecule, just follow the steps in **4.1**.

To build more complicated molecules it might help to look for rings, fragments or other parts by using the **Ring Fragment**, **R-Group Fragment** or **Biological Fragment** buttons.

4. Performing calculations

4.1 Setting up a PM3 geometry optimization calculation

Select **Gaussian** in the **Calculate** menu.

1. In the **Job Type** tab choose which kind of calculation you want to perform. Usually in the *Quantum Chemical Calculation* exercise you should choose: **Optimization** or **Opt+Freq** in order to do a geometry optimization with or without a frequency calculation. A **Geometry Optimization** will tell the program to try to find the best (lowest energy and energy gradient) geometry for the selected molecule. This is achieved by doing an energy calculation of the initial geometry and then calculate the energy gradient. Gaussian will then move each atom in the molecule according to the gradient in order to minimize both the energy and the gradient. Then the program will recalculate the energy and the gradient and continue moving the atoms until all convergence criteria are met. These criteria are usually that the energy difference between two consecutive calculations are smaller than a certain value ε or the energy gradient is sufficient small (see theory part, section 1).
   You should choose: **Optimization**
   Optimize to a **Minimum**
   Calculate Force Constants **Never**
   and for **Opt+Freq**: Compute Raman **Default**

2. In the **Method** tab you specify a lot of things. Most of the time you should choose: **Ground State Semi-empirical..**.
   Default Spin
   PM3
   And the correct **Charge** and **Spin** for your molecule. Always check that you have the correct values.
3. In the **Title** tab enter title for your job.
4. The rest of the tabs are not necessary to use in the exercises.
5. Then, when you are satisfied with your input, you must select **Submit...** button(under **Gaussian** in the **Calculate** menu). You must then save your input specifications and then click on **OK** when the program asks you if you want to run Gaussian.

4.2 Investigating and changing distances, angles and dihedral angles

If you want to examine or change a bond or distance then click on the **Modify Bond** button and choose two atoms, in the new window that appears the bond length (or distance if two non-bonding atoms are chosen) in Ångströms.
The same can be done for angles (choose three atoms) and dihedral angles (choose four atoms). Gaussian reports angles in degrees.

4.3 Calculating Properties

In some cases you might want Gaussian to print the molecular orbitals (the coefficients of the LCAO, c_i in the first exercise). Due to a bug in Gaussian this is a bit complicated for semi empirical calculations. Do the following:

1. Create your molecule and run a geometry optimization as stated in **3** and **4.1**.
2. Submit.
3. Open your results (**.chk** file)
4. Create a new input from your old results, i.e. choose **Gaussian...** under the **Calculate** menu.
5. Under the **Job Type** tab choose **Energy**.
6. In the **Additional Keywords:** field (in the bottom part of the window) add: **geom=check guess=read pop=full**
7. Click on **Submit**, when **GaussView** prompts you to save your file do so under a new name.
8. Click on **OK** to start the calculation when asked if you want to submit the file to Gaussian.
9. Gaussian might warn you that there were errors but it doesn't matter, Gaussian has printed the information we wanted before the error. Click on **Yes** in the window that asks if you want to view your results and opend the .log file.
10. GaussView opens a window with your molecule in, you have to choose: **View File ...** under the **Results** menu to view the text in your log file.

4.4 Viewing Molecular Orbitals

If you want to visualize the orbitals you must first have performed a calculation, either a single point (choose **Energy** under the **Job Type** tab) or a Geometry Optimization (**Optimization** under the **Job Type** tab). When the calculation is finished open the **.chk** file. Now you can very easy visualize the molecular orbitals:

1. Choose **MOs** under the **Edit** menu.
2. A new window will open, where you have your molecule on the left and a graph of your occupied and unoccupied molecular orbitals on the right. Choose all the orbitals you are interested in by clicking on the number or the energy value in the graph on the left, they will be marked in yellow. Continue marking orbitals until you have marked all that you are interested in. Don't click on the arrows representing the electrons, unless you want to rearrange the electrons.
3. Choose the **Visualize** tab and click on the **Update ...** button. Wait a few seconds (the bigger the molecule and the higher number of orbitals the longer) and then you will see the molecular orbital in superimposed on your molecule in the left part of the window.
4. Click on the box to the right of the orbital in the graph on the right to change orbital displayed on the left.
5. Click on **OK** when you have finished viewing the orbitals.

4.5 Finding Transition States

To find a transition state the following procedure must be undertaken (see theory part, section 5.1).

1. Create the reactant and run a geometry optimization (as described in **3** and **4.1**). Make sure that you open the **.chk** file when the calculation is finished.
2. Create the product and run a geometry optimization.
3. Open a new molecule window (**New: Create MolGroup** under the **File** menu).
4. Copy (Ctrl+C) and paste (Ctrl+V) the reactant molecule (from the **.chk** file) into the new window.
5. Choose **New: Add to MolGroup** under the **File** menu.
6. Copy and paste the product molecule into the new window.
7. In this window click on the top, rightmost button, to make GaussView display both the reactant and the product in the same window.
8. Choose the **Connection Editor ...** under the **Edit** menu.
9. On the reactant molecule, number the atoms by clicking on them with the middle mouse button, from 1 until the last atom. Try to do this in a logical way, i.e. First number the carbon atoms, then the other heavy atoms and last the hydrogens.
10. Choose the product molecule in the other part of this window.
11. Repeat point 9 for this molecule. Number the atoms in the exact same order as for the product, even the hydrogens must be numbered in the same way for both reactant and product. This is very important!
12. Close the Connection Editor window by clicking on **OK**.
13. Choose **Gaussian** under the **Calculate** menu.
14. In the **Job Type** tab, choose:
    Opt+Freq
    Optimize to a TS (QST2)
    Keep the other options unchanged.
15. In the **Method** tab, choose (as before):
    Ground State
    Semi-empirical...
    Default Spin
    PM3
    Set the **Charge** and **Spin** to the correct values.
16. Click on the **Submit...** button and save under a new name, and click on **OK** to start the calculation.

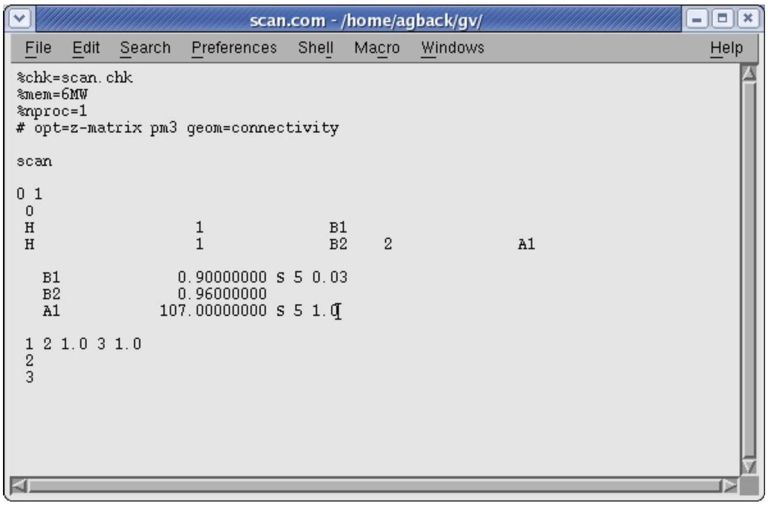
4.6 Scanning the potential energy surface

To scan a part of the potential surface you can follow this steps:

1. Build your molecule (see **3**). If you want you can first run a geometry optimization (see 4.1).
2. Open the **Gaussian...** window under the **Calculate** menu.
3. Under the **Job Type** tab, choose:
   Scan
   Relaxed (Z-Matrix)
4. Under the Method tab choose (as usual):
   Method: Ground State
   Semi-empirical...
   Default Spin
   PM3
   and the correct **Charge** and **Spin**
5. Click on the **Edit...** button, save your file.
6. In the input file, find the variable(s) you want to scan and add on the same line:
   S [no. steps] [step size]
   Example:
   Change:
   B1 0.90000000
   To:
   B1 0.90000000 S 10 0.05
   To make a scan of the B1 distance in 11 steps increasing the distance with 0.05 Å every step.
7. Save and click on the **Submit** button.

8. When the calculation is finished choose the **.log** file and check the **Read Intermediate Geometries (Optimizations Only)** box. Click on the **Open** button.

It is possible to scan several variable at the same time, just remember that the number of steps can increase fast.



```
%chk=scan.chk
%mem=6MW
%nproc=1
# opt=z-matrix pm3 geom=connectivity

scan

0 1
 O
 H                  1              B1
 H                  1              B2    2              A1

   B1             0.90000000 S 5 0.03
   B2             0.96000000
   A1           107.00000000 S 5 1.0

 1 2 1.0 3 1.0
 2
 3
```

Fig 2. *Example of potential energy surface scan.*

5. The Results menu

5.1 Summary

When you choose **Summary...** under the **Results** menu you get a summary of your calculation. You can use this in order to find the **Total Energy** in an easy way.

5.2 Charges

In order to examine the atomic charges, choose **Charges...** under the **Results** menu.

5.3 Surfaces

It's only possible to choose **Surfaces...** under the **Results** menu if you have opened a **.chk** or **.cube** file.
If you have an **.chk** file, you must choose **New Cube** in the **Cube Actions...** drop down menu. In the new window you can specify what kind of surface you want (usually **Molecular Orbital** and then you have to specify which orbitals, you can choose **All**). Click on **OK** to generate the surfaces specified.

After you have generated some surfaces you can choose which you want to display. In the second from the top drop down menu, choose which surface or orbital you want to display and in the next menu (**Surface Actions...**) choose **New Surface** in order to view it.
In the fourth menu you can see all the surfaces you have displayed or are displaying. Remember to look only at one molecular orbital at a time, overlaying two orbitals is not good.

5.4 Vibrations

If you have performed a frequency calculation you can investigate your results by opening your **.log** file (**Open** under the **File** menu) not the **.chk** file (this is a bug for Gaussian on SUN).
After opening the file you can choose **Vibrations...** under the **Results** menu,. In the new window that opens you can choose which vibrational mode you want to display. Click on the one you want and then click on the **Start** button. In some cases it might help to check the **Show Displacement Vectors** box. This will show arrows indicating the atom displacement, the longer the arrow the larger the displacement.
To view another vibrational mode click on another frequency in the list.
When you are finished looking at the vibrations, click on the **Stop** button.

5.5 Scan

If you have performed a potential energy surface scan or a geometry optimization you can investigate your results by opening your **.log** file (**Open** under the **File** menu) and marking the **Read Intermediate Geometries (Optimizations Only)** box.
After opening the file you can choose **Scan...** under the **Results** menu, whereafter a new window opens. In this window you get information about your calculation, two plots, one energy plot and one gradiant plot.

5.6 The .log file

The **.log** file contains a lot of information. To view it choose **View File ...** under the **Results** menu. This will open a new window displaying the file. It is also possible to print it (see **1.2**). If you are interested in the MO-LCAO coefficients you should use some caution when reading the results. It's easy to misinterpret the table.

Example:

```
     Molecular Orbital Coefficients
                           1         2         3         4         5
                        (SG)--O   (SG)--O   (PI)--O   (PI)--O   (SG)--O
     EIGENVALUES --    -1.47103  -0.76015  -0.59361  -0.59361  -0.47877
   1 1   C  1S          0.40616  -0.56411   0.00000   0.00000   0.66059
   2        1PX         0.00000   0.00000   0.28733   0.42838   0.00000
   3        1PY         0.00000   0.00000   0.42838  -0.28733   0.00000
   4        1PZ         0.33883  -0.07727   0.00000   0.00000  -0.58791
   5 2   O  1S          0.82117   0.48423   0.00000   0.00000   0.03727
   6        1PX         0.00000   0.00000   0.47721   0.71148   0.00000
   7        1PY         0.00000   0.00000   0.71148  -0.47721   0.00000
   8        1PZ        -0.21426   0.66433   0.00000   0.00000   0.46539
                           6         7         8
                        (PI)--V   (PI)--V   (SG)--V
     EIGENVALUES --     0.03674   0.03674   0.22350
   1 1   C  1S          0.00000   0.00000   0.28360
   2        1PX         0.80898  -0.28193   0.00000
   3        1PY         0.28193   0.80898   0.00000
   4        1PZ         0.00000   0.00000   0.73047
   5 2   O  1S          0.00000   0.00000  -0.29968
   6        1PX        -0.48709   0.16975   0.00000
   7        1PY        -0.16975  -0.48709   0.00000
   8        1PZ         0.00000   0.00000   0.54422
```

Eigenvalues: This row shows the energy for the molecular orbitals,in atomic units (convert to eV by multiplying by **27.212**).

Atomic Orbitals: This column specifies which atomic orbital the coefficients relates to. NOTE: By some reason Gaussian writes a number in front of the atomic orbital. This number is not connected to the letter that follows. This example should be interpreted as (since it is from a semi-empirical calculation on carbonmonoxide, CO):

`S` = 2S from carbon
`PX` = 2PX from carbon
`PY` = 2PY from carbon
`PZ` = 2PZ from carbon
`S` = 2S from oxygen
`PX` = 2PX from oxygen
`PY` = 2PY from oxygen
`PZ` = 2PZ from oxygen

Molecular orbital 1: This column tells you everything about the first molecular orbital. It gives the energy, symmetry and how the molecular orbital is formed from the atomic orbitals (MO-LCAO). The rows should be interpreted as:

`1` = Molecular orbital 1
`(SG)--O` = The symmetry of the orbital, Sigma .
`-1.47103` = The energy, 40.03 eV.
`0.40616` = How much the C_{2S} AO is contributing to the MO.
`0.00000` = No contribution from C_{2Px}
`0.00000` = No contribution from C_{2Py}
`0.33883` = The contribution from C_{2Pz}
`0.82117` = The contribution from O_{2S} to the MO.
...

6. About different file types in GaussView and Gaussian.

There are some different file types used in Gaussian. They are specified by their file extension.

- **.com** This is the input file. All your specifications on what molecule and what to calculate is stored in text format in this file. The file is created by **GaussView** when you click on **Save**.
- **.log** This is an output file that is created by Gaussian when you click on the Submit button. It contains all information in text format about your calculation.
- **.chk** This file is also created by Gaussian when you submit your job. It is not a text file. From this file you can create surfaces.
- **.fchk** This file is usually not needed. It's a readable version of the .chk file.
- **.cube** This file is for displaying surfaces. It is created by Gaussian whenever you want to display a surface. It's not in a readable format.