

Basics of Running G03 on a PC
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The objective of using Gaussian in this course is to understand better chemical reactions and transition state theory, in addition to the computations of thermochemistry. With this in mind, our objective is to give you simple, illustrative calculations, and to sacrifice accuracy for speed and simplicity. Additional information can be found at the web site below:

General Gaussian site:

<http://www.gaussian.com/>

At this site, you can download the Gaussian03 manual or access the Gaussian03 manual on-line. The syntax should not be too much different for Gaussian98 and Gaussian03.

Also note that Gaussian's units of energy is the Hartree,
1 Hartree = 27.21 eV = 627.46 kcal/mol

1. Run G03W from GaussView

Start GaussView from the Start menu.

Either open a previously saved file (.gif or .log) or construct a new molecule structure. Under the *Calculate* menu, choose *Gaussian*

You now must choose a job type, typically Optimization or Opt+Freq.

Optimization: geometry optimization of the molecule

Opt+Freq: geometry optimization and then frequency calculation, including thermodynamic properties

Next, you must choose a *Method*, including *Basis Set*. The *Method* is the type of quantum calculation and determines the accuracy of the calculation.

The *Basis Set* is the mathematical description of the wavefunction that you will calculate. In general, the bigger the *Basis Set* is, the better.

Each homework set will tell you which *Method* and which *Basis Set* to use.

Note that for methods that are not on the pulldown menu, you can either edit the .gif file (see two lines down) directly, or you can choose "Hartree-Fock" and then type in directly the method that you wish to use in the line after "Additional Keywords:".

After setting the jobs, choose *Submit*

Save the .gif file first (You do not need to add the .gif extension, since that is done automatically.), then the job will automatically run.

The output file will have the same name as the input file, but with a .log extension.

The other important file will be in the Scratch directory. It will have a .chk extension, and will contain all important information.

2. How to visualize frequencies and non-0 K properties

- 1) You need to have performed an Opt+Freq calculation first.
- 2) In GaussViewW, go to *File-Open* and open the .log file. Next go to *Results-Vibrations*.

3. How to compute thermodynamic properties of molecules at conditions other than 1 atm and 298.15 K

- 1) You need to have performed an Opt+Freq calculation first.
- 2) Move the .chk file into the main G03W directory. (It is likely in the Scratch directory.)
- 3) You will now use the freqchk.exe utility.
- 4) To do so, you need to first create an input file, called for example in.txt with the following contents:

```
<filename>.chk  
n  
Temperature in K  
Pressure in atm  
1  
Y
```

- 5) Open a DOS prompt and cd to the G03W directory
- 6) Use the following command to compute the new thermodynamic data and output it to the file out.txt:

```
freqchk.exe < in.txt > out.txt
```

4. Performing a transition state calculation

As discussed in class, finding a transition state is equivalent to finding a saddle point. A saddle point is a point on the energy hypersurface in which all first derivatives are zero and all second derivative but one are positive. The other derivative is negative (single negative eigenvalue).

WARNING: Gaussian will find the closest saddle point, in other words, the closest point with one negative frequency (second derivative). It may not be the correct transition state. You must visualize the frequency, as demonstrated in class, to determine whether this is correct or not. If it is not, you will have to adjust the input reactant and product structures to be closer to the transition state structure that you are trying to find.

- 1) Draw the product structure and choose Method and Basis set.
- 2) Choose the “Opt+Freq” option for Job Type. Also, choose Optimize to a “TS” and Calculate Force constants “always” which means to calculate force constants, at every point. The “Calculate force constants” will make the calculation much more expensive, but will give you a much greater chance of finding the saddle point. This option makes the program calculate the force constants (second derivatives) analytically, as opposed to estimating them. Why does this make such a difference? (Try without this option.) You might also need to add “noeigentest” in the keywords for opt to prevent it to stop whenever it finds a negative eigenvalue even it has more than one negative eigenvalues.

A sample file, for the H-HBr reaction is below: (See also the next to the last example at the end of these notes.)

```
%mem=6MW  
%nproc=1  
%chk=HHBrReact.chk  
# opt=(CalcAll,ts) freq=noraman ublyp/3-21g
```

Title Card Required

```
0 2
Br      0      0.000000      0.000000      0.000000
H       0      0.000000      0.000000      Z1
H       0      X1      0.000000      Z2

Z1      1.410000
Z2      1.550000
X1      0.000000
```

(Don't forget always to leave one blank space at the end.)

5. Restart a Gaussian job from the checkpoint file.

(Not necessary for SMA 5413, but OK to do.)

In order to save computer time, restarting job from a previous run is possible. For instance, we want to use more accurate methods or larger basis sets to calculate the energy or analyze the frequency from an optimized geometry of a previous run. Say, we have a checkpoint file zh1.chk which is the result of a zeolite cluster optimization. If we want to use BLYP method and a larger basis set 6-31G* to calculate a more accurate energy of the cluster, a simple restarting input file can be generated like this:

(single-point calculation, at a fixed geometry)

```
%Chk=zh1
#BLYP/6-31G(d) Guess=Read Geom=Checkpoint
```

zeolite energy calculation

```
0 1
```

Save the file with whatever name you want, i.e. zh1_1.gif, and put the file at the same place as the zh1.chk file. Don't forget to leave a blank space after **0 1** in zh1_1.gif. Since the checkpoint file will be modified after the energy is calculated and the optimization is the most time-consuming part, ALWAYS REMEMBER TO KEEP A COPY OF CHECKPOINT FILE AFTER THE OPTIMIZATION IS FINISHED so that you won't have to rerun it if the checkpoint file is altered.

(Geometry optimization)

```
%Chk=zh1
#BLYP/6-31G(d) Opt Guess=Read Geom=Checkpoint
```

zeolite energy calculation

```
0 1
```

(Frequency and thermodynamic properties calculation)

If you want to do a frequency analysis of the optimized geometry, just add one more keyword to zh1_1.gif as below:

```
%Chk=zh1
#BLYP/6-31G(d) Guess=Read Geom=Checkpoint Freq
```

zeolite energy calculation

0 1

(Geometry optimization and frequency calculation w/thermodynamic properties)

```
%Chk=zh1
#BLYP/6-31G(d) Opt Guess=Read Geom=Checkpoint Freq
```

zeolite energy calculation

0 1

(Transition state calculation)

```
%Chk=zh1
#BLYP/6-31G(d) Opt=(CalcFC,TS,NoEigentest,MaxCycle=300) Guess=Read
Geom=Checkpoint Freq
```

zeolite transition state calculation

0 1

6. Meaning of sample input file

```
%Chk=zh1
#P BLYP/6-31G(d) Opt Guess=Read Geom=Checkpoint Freq
```

zeolite energy calc

0 1

%Chk=zh1	This sets the name of the checkpoint file to be zh1.chk
#	Starts the command line
P	Detailed output (blank for no detailed output)
BLYP BPW91, SPL, etc.	Choice of method. Other possible methods are RHF, MP2, B3LYP,
6-31G(d) etc.	Choice of basis set. Other possible choices are 3-21G, 6-31G*, D95,
Opt	Optimize geometry (This is different for a transition state calculation. See above)
Guess=Read	Choose initial guess for the wavefunction from the checkpoint file
Geom=Checkpoint	Choose initial geometry from the checkpoint file
Freq	Perform a frequency calculation
Zeolite energy calc	Label with no meaning, except it must be there
0 1	0=Charge, 1=Spin multiplicity
	Blank space must be left here
...	Geometry of structure follows