

# RUNNING GAUSSIAN 98 - A PRIMER

Version 1.1

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# 1 Overview

## 1.1 Objectives and Prerequisites

This tutorial serves as a quick guideline to the preparation and submission of computational chemistry jobs using Gaussian 98 (G98) at the Department of Chemistry, UW-Madison. The tutorial targets beginning users who have no previous experience with Gaussian. However, they should be rather familiar with the UNIX/Linux operating systems. Those who are not familiar with the UNIX/Linux systems should consult a Linux tutorial available at this web site or contact the Computational Chemistry Specialist for assistance.

The tutorial will present to the users a typical step-by-step procedure in order to prepare, submit, and process a Gaussian job. However, it is not meant to be comprehensive, nor is it a replacement of on-line manuals and help files provided from the software. The users are strongly recommended to finish the exercises presented herein.

## 1.2 Document Conventions

Several typefaces are used throughout the document, as shown below:

**Command** is printed in **boldface**

*User input* is printed in *italic*

# 2 Preparing Input Files

A G98 input file must be prepared before being submitted to run. To create your first (and simple) G98 input file, do the following:

- Create a directory called *myg98* (or anything you wish).
- Change the current directory to *myg98*.
- Use a text editor to create a file as shown below. Do not include the document start/end marks in your file. Note the mandatory extra blank line at the end of the file. (The number at the end of each line only shows the line number and must not be included in your actual input file.)

— Starts —

```
%chk=water.com.chk (1)
#T RHF/6-31G(d) Test (2)
(3)
Water HF Energy (4)
(5)
0 1 (6)
O -0.464 0.177 0.0 (7)
H -0.464 1.137 0.0 (8)
```

```
H 0.441 -0.143 0.0 (9)
(10)
— Ends —
```

**Note:** The file you created must be saved in ASCII (simple, DOS, text) format; otherwise, G98 will not run at all. If you are using a commercial word processing program (such as Microsoft Word or WordPerfect), you must save your file in text format. A popular text editor for Linux users is Vi.

## 2.1 Exercises

1. Create the file *water.com* as described in the text.
2. Open the file *water.com*, change the first line to `%chk=water.chk`. Save the new file as *water*.
3. Delete the first line in the file *water.com* above, then save it as *water\_nochk.txt*.

## 3 Submitting Gaussian Jobs

### 3.1 On GradLab

To submit your Gaussian jobs on a GradLab computer, use the following command:  
`$ g98 water.com`

### 3.2 On Bohr

```
$ qg 2 water.com
```

The number two is the number of microprocessors (2 microprocessors/node) of the cluster you request to run your job. Each user may have no more than 8 microprocessors (i.e. 4 nodes) running at any time. **Do not use the command 'g98' on the cluster Bohr, or your job will be terminated unceremoniously.**

### 3.3 Exercises

1. Submit and run *water.com* on both Bohr and GradLab. Write down the names of all the files containing the word *water* in them.
2. Do the same as in question 1, only this time use the file *water*.
3. Do the same as in question 1, only this time use the file *water\_nochk.txt*.
4. What observations have you made in terms of how G98 processes your submitted jobs?

## 4 Monitoring Gaussian Jobs

### 4.1 Watching it

Here are several ways to check the status of your jobs:

```
$ ps -u
```

 List currently run processes of the logged-in user.

**\$ tail -f *water.log*** This command allows you to watch the output file (in this case, *water.log*) while Gaussian continues to feed calculated results to the file. **Don't abuse this command, since it will take away computer resource from Gaussian, which makes the job even run more slowly.** (This is particularly true when you are running your jobs on a research cluster.)

## 4.2 Terminating Gaussian Jobs

For whatever the reason, if you need to remove a submitted job, use the commands described in the next sections.

### 4.2.1 On GradLab

**\$ jobs** To look for the job number (not the Process ID)

```
[1]-      Running          g98      10_01a.com &
[2]-      Running          g98      10_01b.com &
```

**\$ kill %1 %2** (Terminate jobs #1 and #2)

**\$ jobs** (Check again. *They are gone!*)

```
[1]-      Terminated     g98      10_01a.com &
[2]-      Terminated     g98      10_01b.com &
```

### 4.2.2 On Bohr

Use the following command to look up the PID and to remove a job from the queue.

**\$ qstat** shows the queue status

**\$ qstat -n** shows the nodes attached to a particular process

**\$ qdel PID** removes a job from the queue

## 4.3 Save Gaussian Output Files

### 4.3.1 On GradLab

The output of a Gaussian 98 job (i.e. the *filename.log* file) running on GradLab computers is in the same directory as the input file. Gradlab users need to save their files promptly to their Linux home account location if they wish to keep their files. Any files generated by GradLab users on local drive will be purged daily.

### 4.3.2 On Bohr

The output of a Gaussian 98 job (e.g. the *water.log* file) running on Bohr is in the user's home directory.

Contact your Computational Chemistry Specialist if you cannot find your output files.

## 4.4 Exercises

1. Locate your output file after the G98 run is completed.

# 5 Processing Gaussian Output Files

## 5.1 Using GaussView

GradLab users may look at their G98 results with GaussView using the following command:

GV (uppercase)

Then go to the directory that has the output file (*water.log*) to open it. A screen capture of *water.log* using GaussView is shown in Figure 1 (page 5).

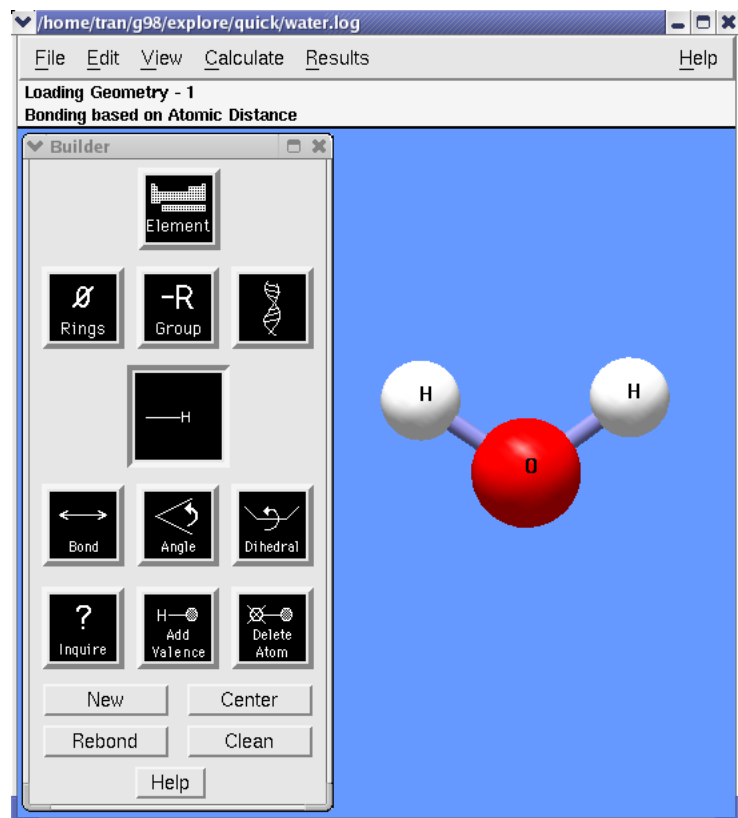


Figure 1: GaussView output of *water.log*

## 5.2 Using text editors

Gaussian output files are in text format and may be opened using any text editor. In addition, the following are a few commonly used command to investigate the contents of the output file.

`$ grep 'SCF Done: E(RHF)' water.log` Print out the RHF energy.

### 5.3 Exercises

1. Print out the line that shows you are the person who submitted the G98 job.

## 6 Getting Help

### 6.1 Geez... Help!!!

It's `ghelp`, that is! If you need general information about Gaussian, use the following command:  
`$ ghelp`

The program will print out a menu of options for you to choose from. More information can be found in the User's Reference available at the Chemistry Computer Center (Room 9311).

### 6.2 News from the Chemistry Computer Center

Please address your questions, report bugs, or simply share your success stories with Chemistry Computer Center. We'd like to hear from you.

## 7 Document History

### 7.1 Version History

**Version 1.1:** August 2004 - minor corrections

**Version 1.0:** February 2004

The on-line version can be found at <http://computing.chem.wisc.edu> (Go to: [Software](#) ⇒ [Chemistry](#) ⇒ [G](#) ⇒ [G98](#)).

### 7.2 Updates

Next scheduled update is August 2005.

## 8 Contact Information

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