

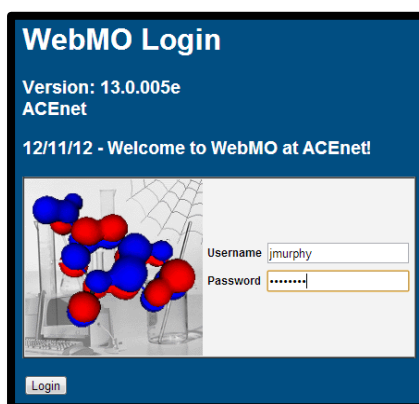
# CHEM 4305 Term Project:

## Simulating Molecular Liquids

### Part 1: Molecule Building and Charge Fitting

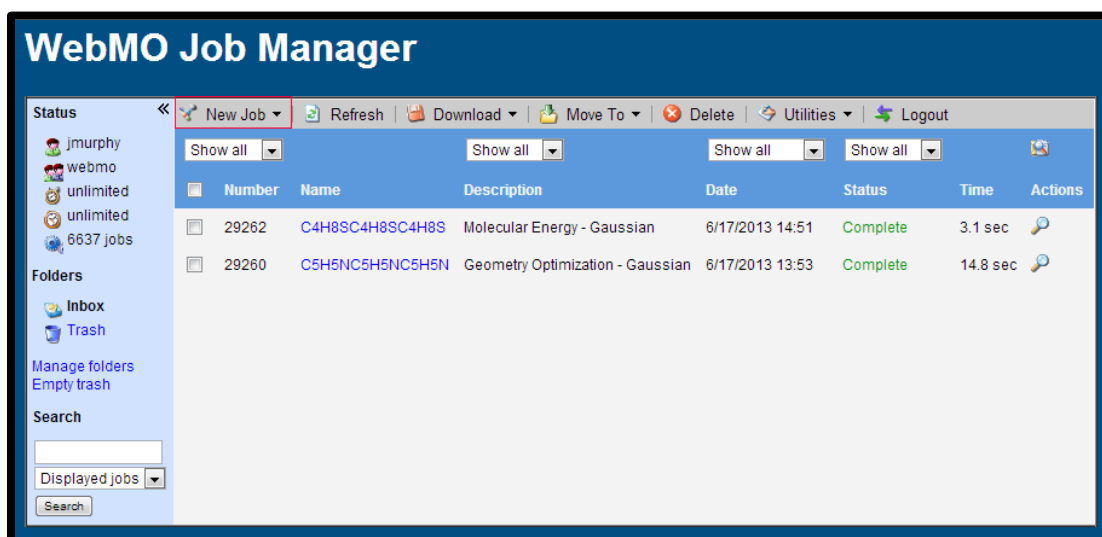
#### 1. Sign into WebMO.

Go to <https://webmo.ace-net.ca> and sign in using your ACEnet username and password.



The WebMO Login screen has a blue header with the title "WebMO Login". Below the header, it displays "Version: 13.0.005e" and "ACEnet". A welcome message reads "12/11/12 - Welcome to WebMO at ACEnet!". On the left, there is a 3D molecular model of a liquid. On the right, there are input fields for "Username" (containing "jmurphy") and "Password" (masked with dots). A "Login" button is located at the bottom left of the form area.

#### 2. Start a New Job

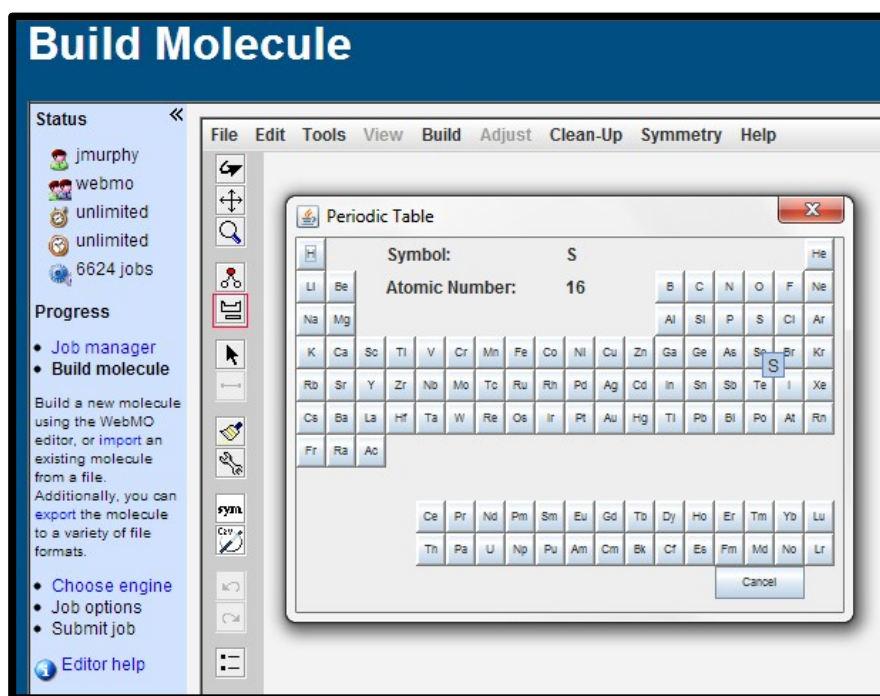


The WebMO Job Manager interface features a blue header with the title "WebMO Job Manager". Below the header is a toolbar with buttons for "New Job", "Refresh", "Download", "Move To", "Delete", "Utilities", and "Logout". The main area contains a table of jobs. On the left, there is a sidebar with "Status" information (jmurphy, webmo, unlimited, unlimited, 6637 jobs), "Folders" (Inbox, Trash), and a "Search" section. The table has columns for Number, Name, Description, Date, Status, Time, and Actions.

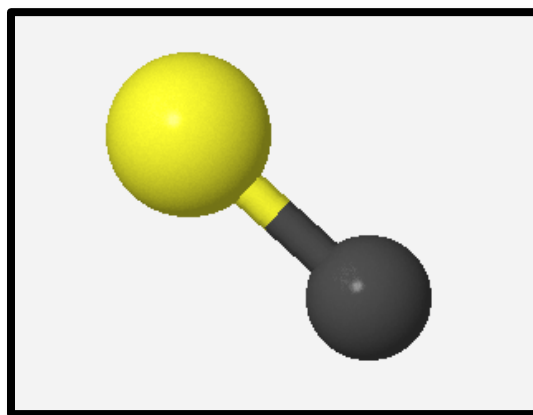
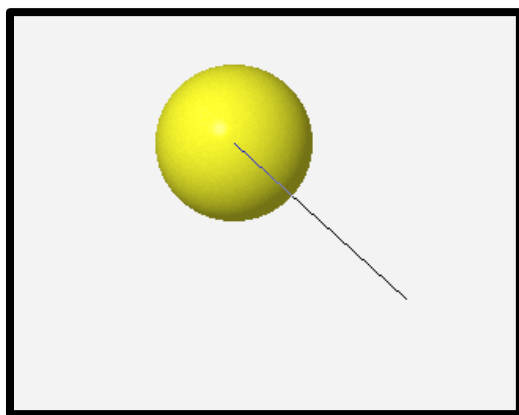
Number	Name	Description	Date	Status	Time	Actions
29262	C4H8SC4H8SC4H8S	Molecular Energy - Gaussian	6/17/2013 14:51	Complete	3.1 sec	
29260	C5H5NC5H5NC5H5N	Geometry Optimization - Gaussian	6/17/2013 13:53	Complete	14.8 sec	

### 3. Building a Molecule

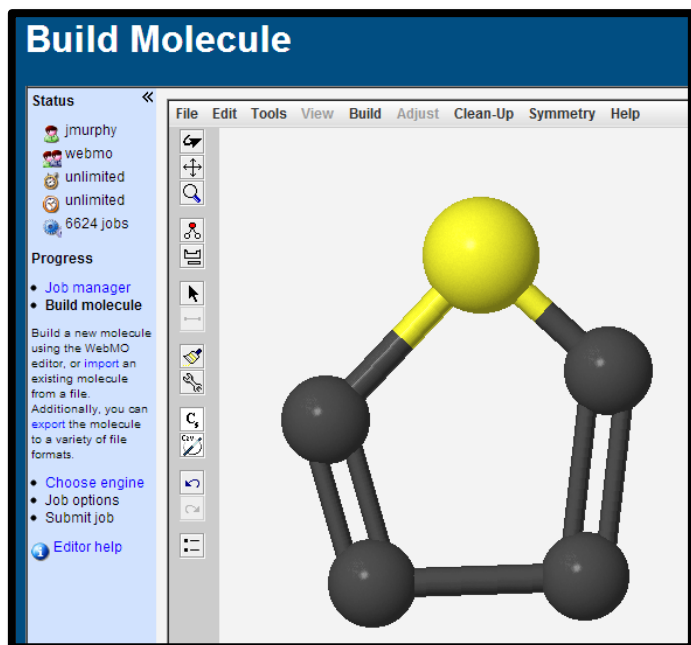
The molecule used in this example is thiophene. To begin, click on the **periodic table** and select the element you need. Sulfur is chosen in this example.



Click anywhere on the blank surface to add an atom. To add bonds, select the element required and **click and drag**.



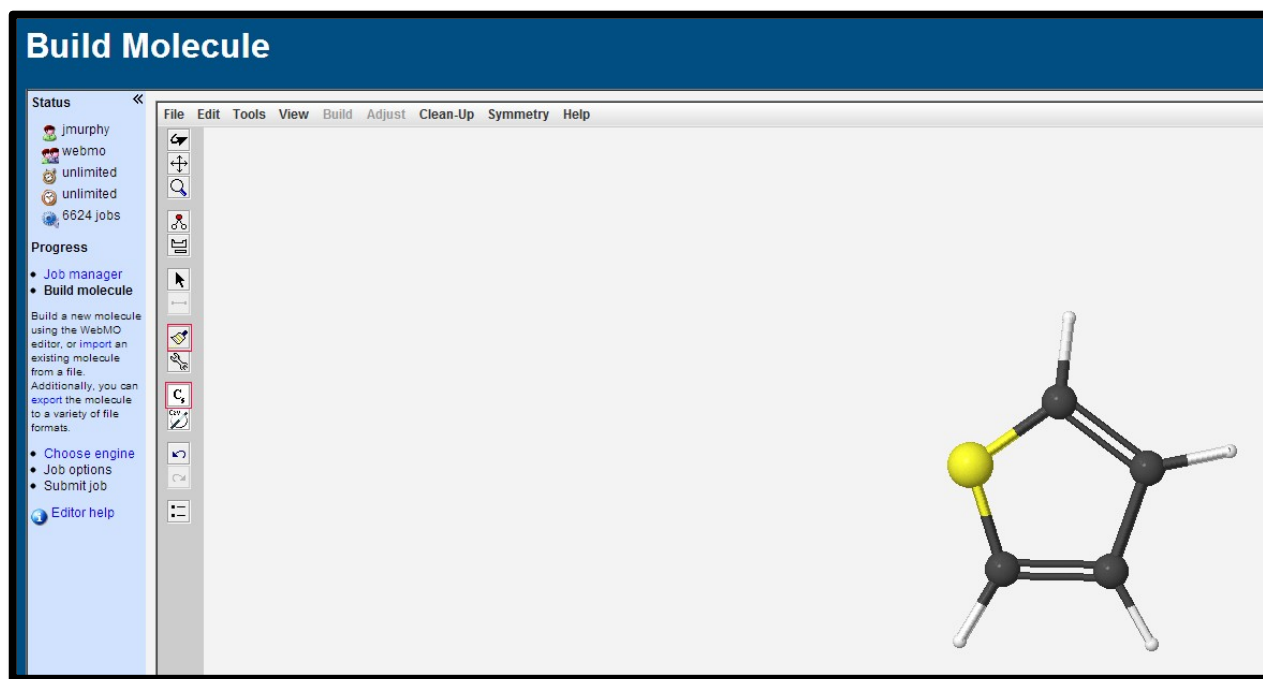
To make **double bonds**, draw a second bond between the atoms in the same way as you added the single bond.



#### 4. Clean Up Your Structure

Tidy up your bond angles and add hydrogen atoms by selecting the **broom** icon. Clicking the **symmetry** button adjusts the symmetry of your molecule so that it is in the highest point group available.

Save a screenshot of this page to submit for your term project.



To go to the next step, click the forward button at the bottom of the screen.

## 5. Choose a Computational Engine

Select the **Gaussian** computational engine and continue forward.

**Choose Computational Engine**

Engine	Description
<input type="radio"/> Gamess	Ab initio and semi-empirical calculations
<input checked="" type="radio"/> Gaussian	Ab initio and semi-empirical calculations
<input type="radio"/> QChem	Ab initio calculations

Select Queue:

Progress:

- Job manager
- Build molecule
- Choose engine

Choose the desired computational engine from those installed.

Job options

Submit job

Help

## 6. Geometry Optimization

Select '**Geometry Optimization**' under the calculation drop-down menu. Set the run time to **12** hours. Set the theory to **Hartree-Fock** and be sure that the basis set matches the one shown below.

**Configure Gaussian Job Options**

Status: jmurphy, webmo, unlimited, unlimited, 6616 jobs

Progress:

- Job manager
- Build molecule
- Choose engine
- Job options

Configure options for the selected job and computational engine.

Submit job

Help

Job Options

Job Name: C4H4S

Number of Processors: 1

Virtual Memory per Processor (h\_vmem): 2G

Job Time (h\_rt): 12 : 0 : 0

Calculation: Geometry Optimization

Theory: Hartree-Fock

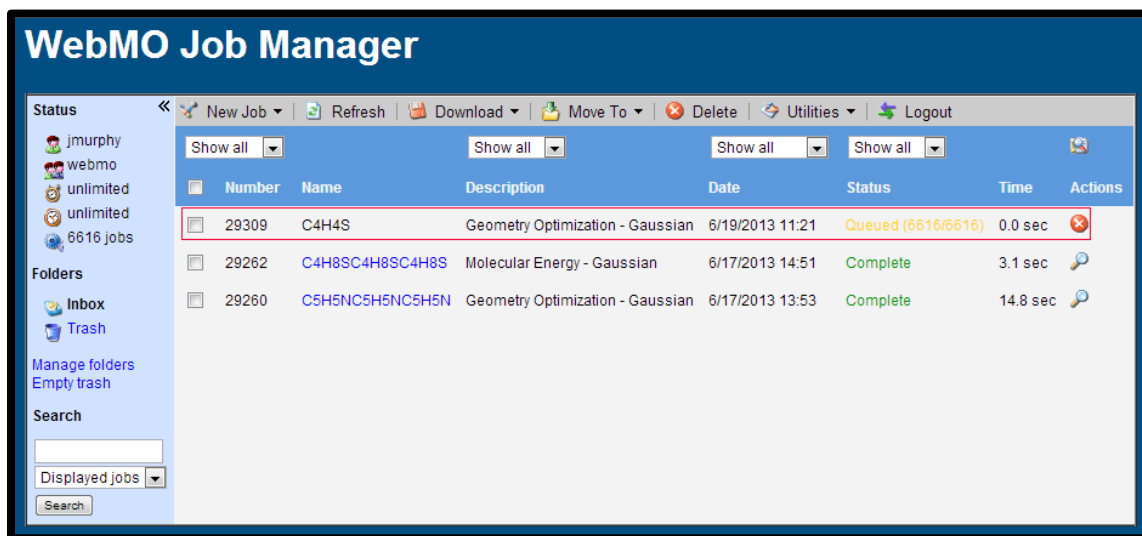
Basis Set: Routine: 6-31G(d)

Charge: 0

Multiplicity: Singlet

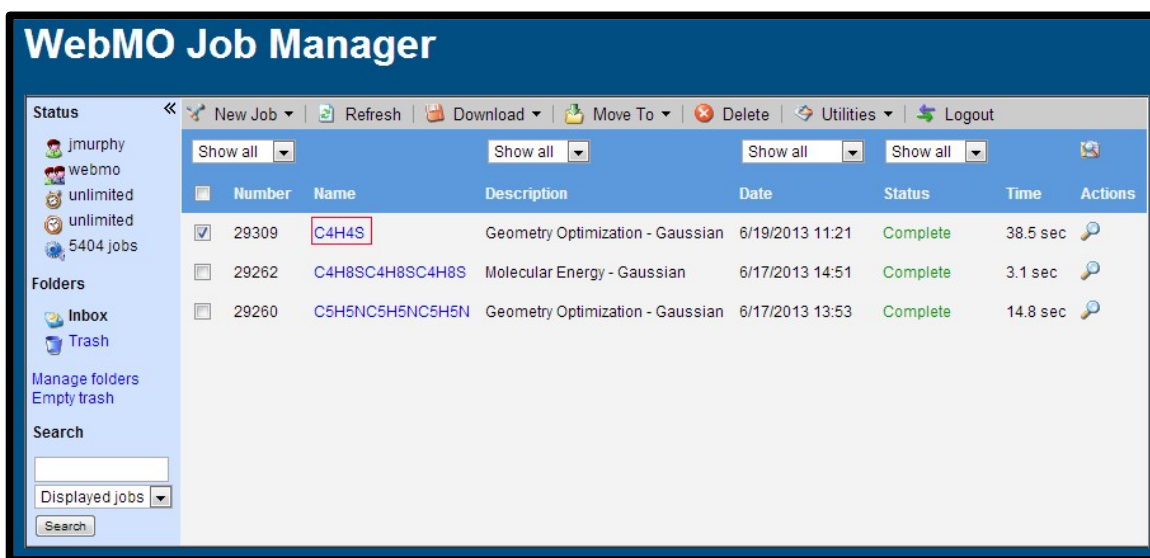
## 7. Wait for the Job to Complete

Your job will be placed in the ACEnet queue until a compute node is available. It will show “Queued” status until it is executed, when it will say “Running.” The job status will change to “Complete” when it is finished. Once your job is finished, click on the **chemical formula** corresponding to your molecule in the Job Manager screen.



The screenshot shows the WebMO Job Manager interface. On the left, a sidebar contains a 'Status' section with user information (jmurphy, webmo, unlimited, 6616 jobs), 'Folders' (Inbox, Trash), and a 'Search' section. The main area features a toolbar with 'New Job', 'Refresh', 'Download', 'Move To', 'Delete', 'Utilities', and 'Logout'. Below the toolbar is a table of jobs. The first job, with ID 29309 and name 'C4H4S', is in a 'Queued (6616/6616)' status. The other two jobs are 'Complete'.

Number	Name	Description	Date	Status	Time	Actions
29309	C4H4S	Geometry Optimization - Gaussian	6/19/2013 11:21	Queued (6616/6616)	0.0 sec	
29262	C4H8SC4H8SC4H8S	Molecular Energy - Gaussian	6/17/2013 14:51	Complete	3.1 sec	
29260	C5H5NC5H5NC5H5N	Geometry Optimization - Gaussian	6/17/2013 13:53	Complete	14.8 sec	

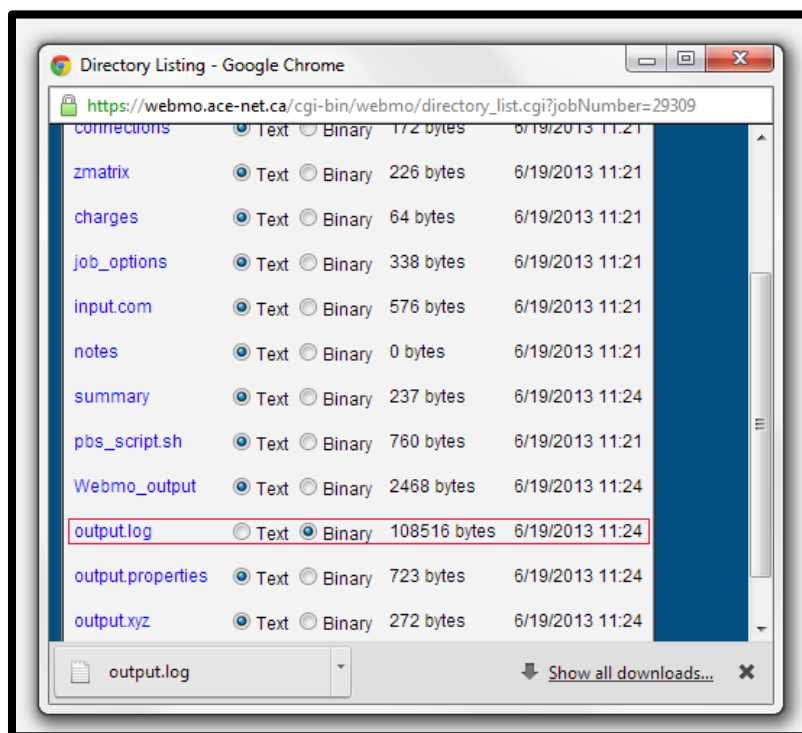


This screenshot shows the same WebMO Job Manager interface after the job has completed. The job with ID 29309 and name 'C4H4S' is now marked as 'Complete' and has a time of 38.5 sec. The 'C4H4S' text in the 'Name' column is highlighted with a red box. The 'Status' column now shows 'Complete' in green. The total number of jobs in the system is now 5404.

Number	Name	Description	Date	Status	Time	Actions
29309	C4H4S	Geometry Optimization - Gaussian	6/19/2013 11:21	Complete	38.5 sec	
29262	C4H8SC4H8SC4H8S	Molecular Energy - Gaussian	6/17/2013 14:51	Complete	3.1 sec	
29260	C5H5NC5H5NC5H5N	Geometry Optimization - Gaussian	6/17/2013 13:53	Complete	14.8 sec	

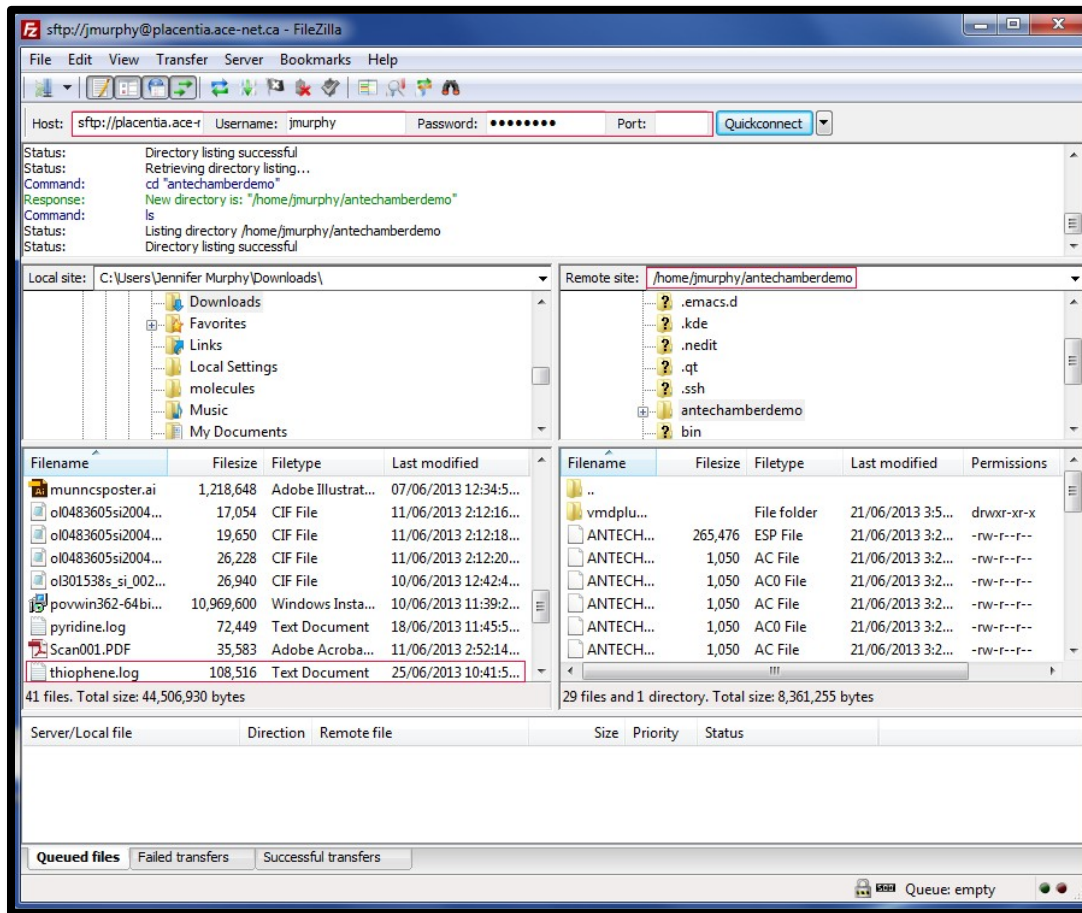
## 8. Downloading your .log File

Choose 'all files' on the left of the screen. Select the **binary** of output.log (you can rename it later) it will automatically download. This is the file that needs to be transferred to placentia using Filezilla or a SCP client like Filezilla.

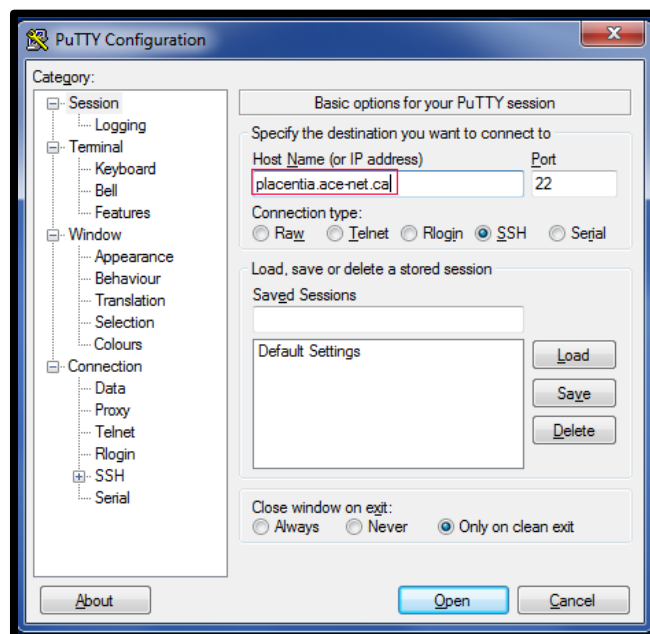


## 9. Transfer the output.log file to placentia using Filezilla

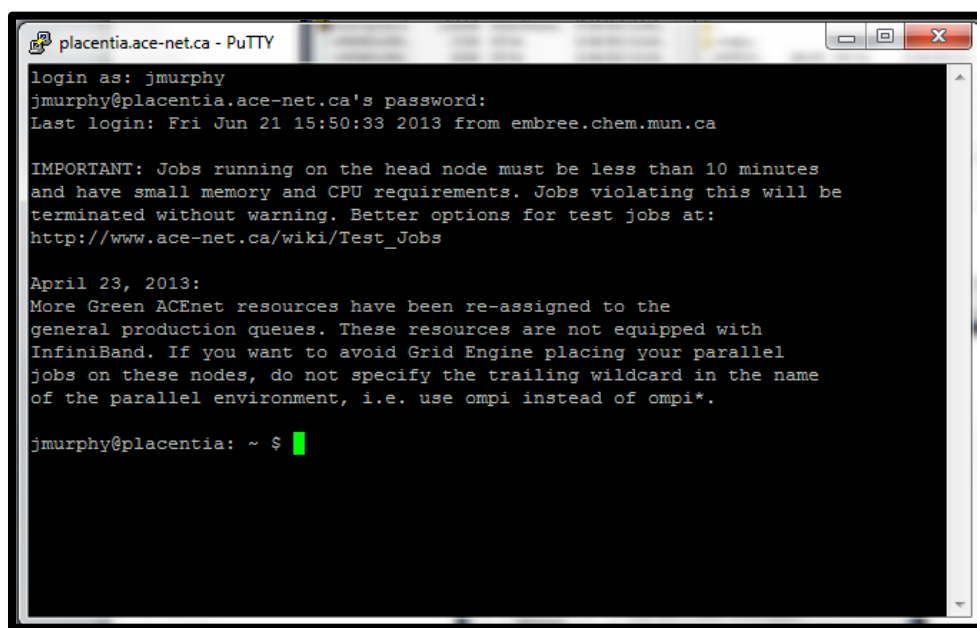
Open **Filezilla**, put in the host as **placentia.ace-net.ca** and enter your ACEnet **username** and **password**. The port is **22**. Once you have connected, get organized. Make a folder on placentia to put your .log file into. To do this, right click and make a new folder on the placentia side. Mine is called '**antechamber demo**'. Then, locate your output.log file in your downloads. I have renamed mine '**thiophene.log**', I suggest you rename yours appropriately. To transfer your file, click on the file and drag it into the new folder on placentia that you have made.



## 10. Open Putty and Log in to placentia.







```
placentia.ace-net.ca - PuTTY
login as: jmurphy
jmurphy@placentia.ace-net.ca's password:
Last login: Fri Jun 21 15:50:33 2013 from embree.chem.mun.ca

IMPORTANT: Jobs running on the head node must be less than 10 minutes
and have small memory and CPU requirements. Jobs violating this will be
terminated without warning. Better options for test jobs at:
http://www.ace-net.ca/wiki/Test_Jobs

April 23, 2013:
More Green ACEnet resources have been re-assigned to the
general production queues. These resources are not equipped with
InfiniBand. If you want to avoid Grid Engine placing your parallel
jobs on these nodes, do not specify the trailing wildcard in the name
of the parallel environment, i.e. use omp1 instead of omp1*.

jmurphy@placentia: ~ $
```

## 11. Change into the directory you put the output.log file in

Run the command 'ls' to check to make sure the antechamberdemo directory is present, then change into the antechamberdemo directory.

```
~ $ ls
    antechamberdemo  Bin                output_sulfur_molecules
    scratch          sulfur_molecules

~ $ cd antechamberdemo/
antechamberdemo $ ls
    pyridine.log  thiophene.log
```

## 12. Run Babel

Load the module for the openbabel program, then run the command **babel** to convert the Gaussian log file to a mol2 file. Use the command **less** to look at your mol2 file to confirm the conversion worked.

```
$ module load gcc openbabel
$ babel -i g09 thiophene.log -o mol2 thiophene.mol2
$ less thiophene.mol2
@<TRIPOS>MOLECULE
thiophene.log
  9 9 0 0 0
SMALL
USER_CHARGES
****
Gaussian 09 #N HF/6-31G(d) OPT Geom=Connectivity
@<TRIPOS>ATOM
      1 C      -1.2336   -0.0153   0.0000 C.ar      1  LIG1      -0.2774
      2 C      -0.7187   -1.2580   0.0000 C.ar      1  LIG1      -0.0932
      3 C       0.7185   -1.2582   0.0000 C.ar      1  LIG1      -0.0997
      4 C       1.2338   -0.0157   0.0000 C.ar      1  LIG1      -0.2726
      5 S       0.0000    1.1906   0.0000 S.2       1  LIG1       0.0224
      6 H       2.2668    0.2664   0.0000 H        1  LIG1       0.2255
      7 H       1.3156   -2.1501   0.0000 H        1  LIG1       0.1347
      8 H      -1.3155   -2.1501   0.0000 H        1  LIG1       0.1335
      9 H      -2.2666    0.2668   0.0000 H        1  LIG1       0.2268
```

**\*Press q to exit less**

### 13. Generate the Gaussian Input File Using Antechamber

Load the modules for antechamber program. Use the command **antechamber** to convert the mol2 file to a Gaussian input file, thiophene.gjf. Look at the file thiophene.gjf using less to make sure the conversion worked.

```
$ module load intel ambertools
$ export AMBERHOME=/usr/local/ambertools-13/
$ antechamber -fi mol2 -i thiophene.mol2 -fo gcrt -o thiophene.gjf
$ less thiophene.gjf
```

Your Gaussian input file should look like this:

```
--Link1--
%chk=molecule
#HF/6-31G* SCF=tight Test Pop=MK iop(6/33=2) iop(6/42=6) opt

remark line goes here

0 1
C 0.0000000000 0.7066000000 -1.2724000000
C 0.0000000000 1.2344000000 0.0014000000
S 0.0000000000 0.0000000000 1.1864000000
C 0.0000000000 -1.2344000000 0.0014000000
C 0.0000000000 -0.7066000000 -1.2724000000
H 0.0000000000 -1.3188000000 -2.1622000000
H 0.0000000000 -2.2708000000 0.2974000000
H 0.0000000000 2.2708000000 0.2974000000
H 0.0000000000 1.3188000000 -2.1622000000
```

## 14. Submit the Gaussian Calculation to the Queue

Running the Gaussian input file to calculate the electrostatic potential for charge fitting. This calculation will take longer, so it must be run through the queuing system. The program **nano** is an editor that will let you write a script to submit to the queuing system.

```
$ nano script-1.sh
```

Paste these lines into the editor:

```
#!/bin/sh
#$ -l h_rt=01:00:00
#$ -cwd

module load gaussian
g09 < thiophene.gjf 1>thiophene.out 2>thiophegjf.err
```

Save this script to disk by typing Ctrl-o and pressing Enter. Type Ctrl-x to exit back to the command line. Use the command **qsub** to submit this script to the queue. Check to see its status in the queue with the command **qstat**.

```
$ qsub script-1.sh
Your job 5693900 ("script-1.sh") has been submitted
$ qstat
```

job-ID	prior	name	user	state	submit/start at	queue
-----						
-----						
5693900	0.00000	script-3.s	jmurphy	qw	07/04/2013 15:01:58	1

You may have to wait up to a day for your job to be executed. The job will no longer be shown in the **qstat** output after it is complete. Once this has happened, you should be able to see a large output file (.out) in this directory list.

```
$ ls -l
```

-rw-r--r--	1	jmurphy	crowley	0	Jul	4	14:45	script-2.sh.o5693893
-rw-r--r--	1	jmurphy	crowley	1	Jul	4	14:56	script-2.sh.o5693899
-rw-r--r--	1	jmurphy	crowley	98	Jul	4	10:47	script-3.sh
-rw-r--r--	1	jmurphy	crowley	0	Jul	4	15:03	script-3.sh.e5693900
-rw-r--r--	1	jmurphy	crowley	0	Jul	4	15:03	script-3.sh.o5693900
-rw-r--r--	1	jmurphy	crowley	111	Jul	4	10:49	script-4.sh
-rw-r--r--	1	jmurphy	crowley	0	Jul	4	15:03	thiophegjf.err
-rw-r--r--	1	jmurphy	crowley	752	Jul	4	14:56	thiophene.gjf
-rw-r--r--	1	jmurphy	crowley	882193	Jul	4	10:06	thiophene.log
-rw-r--r--	1	jmurphy	crowley	1053	Jul	4	14:32	thiophene.mol2
-rw-r--r--	1	jmurphy	crowley	774402	Jul	4	15:18	thiophene.out

## 15. Use Antechamber to Generate Parameter and Topology Files

Run antechamber again on the Gaussian output file.

```
$ module load intel ambertools
$ export AMBERHOME=/usr/local/ambertools-13/
$ antechamber -fi gout -i thiophene.out -fo charmm -o thiophene -c resp

$ ls
ANTECHAMBER_AC.AC          babel.sh                   script-4.sh.e5693909
ANTECHAMBER_AC.AC0        Esout                     script-4.sh.o5693909
ANTECHAMBER_BOND_TYPE.AC  molecule.chk              thiophegjf.err
ANTECHAMBER_BOND_TYPE.AC0 Qout                      thiophene.gjf
ANTECHAMBER.ESP           AC0 QOUT                  thiophene.inp
ANTECHAMBER_PREP.AC       script-1.sh               thiophene.log
ANTECHAMBER_PREP.AC0      script-1.sh.e5693885      thiophene.mol2
ANTECHAMBER_RESP1.IN      script-1.sh.o5693885      thiophene.out
ANTECHAMBER_RESP1.OUT     script-2.sh               thiophene.prm
ANTECHAMBER_RESP2.IN      script-2.sh.e5693899      thiophene.rtf
ANTECHAMBER_RESP2.OUT     script-2.sh.o5693899
ANTECHAMBER_RESP.AC       script-3.sh
ATOMTYPE.INFO             script-3.sh.e5693900
```

## 16. Modify the CHARMM Input File

In order to create the .psf file, the CHARMM input file, thiophene.inp, must be edited using the 'nano' command. Add the following three lines to the end of the input file. To save the file: ctrl o, enter, ctrl x.

```
$ nano thiophene.inp
```

Add these lines to the bottom of the input file:

```
write psf card xplor name thiophene.psf
write coor card pdb name thiophene.pdb
stop
```

## 17. Execute CHARMM to Generate the PSF and PDB Files

Use the command **wget** to download the program charmm to your ACEnet account. Decompress this file using **tar**, then execute charm using the input file you've generated. There will be a series of files generated.

```
$ wget http://www.chem.mun.ca/homes/cnrhome/charmm.tgz
$ tar xzf charmm.tgz
$ ./charmm < thiophene.inp > thiophene.charmmout
$ ls
ANTECHAMBER_AC.AC          molecule.chk               script-5.sh.o5693912
ANTECHAMBER_AC.AC0        qout                     script-6.sh
ANTECHAMBER_BOND_TYPE.AC  AC0  QOUT                 script-6.sh.e5693920
ANTECHAMBER_BOND_TYPE.AC0 script-1.sh               script-6.sh.o5693920
ANTECHAMBER.ESP           script-1.sh.e5693885     thiophegjf.err
ANTECHAMBER_PREP.AC       script-1.sh.o5693885     thiophene.gjf
ANTECHAMBER_PREP.AC0      script-2.sh              thiophene.inp
ANTECHAMBER_RESP1.IN      script-2.sh.e5693899     thiophene.log
ANTECHAMBER_RESP1.OUT     script-2.sh.o5693899     thiophene.mol2
ANTECHAMBER_RESP2.IN      script-3.sh              thiophene.out
ANTECHAMBER_RESP2.OUT     script-3.sh.e5693900     thiophene.pdb
ANTECHAMBER_RESP.AC       script-4.sh.e5693909     thiophene.prm
ATOMTYPE.INF              script-4.sh.o5693909     thiophene.psf
babel.sh                  script-5.sh              thiophene.rtf
Esout                     script-5.sh.e5693912     tmp.out
```

## Stage 1 Complete

Download the psf and pdb files generated in the last step and submit them along with your WebMO screen shot.