Computations using Gaussian programs via WebMO

The WebMO computational software facilitates computational chemistry via the WWW. WebMO permits the access of Gaussian software packages, which are installed on the Miami High Performance Computers (HPC), over the WWW using a web browser. Computational chemistry jobs can be created, queued, run, viewed, downloaded, and deleted all within the context of the WebMO interface. The following instructions allow you to perform calculations.

1. Use the URL link
http://miamioh.edu/webmo to navigate to the Web MO login page;
2. The first time you login, after entering your unique ID and password, you will be prompted to select a group. They should select chm255spring13 and enter the password chm255s13 when prompted;
3. From the Job Manager screen, using the pull-down menu
New Job --Create a New Job
to start a new window for building your molecule (Java must be enabled on your laptop)
4. In the Build Molecule screen, draw or use a template to place target molecule on the screen to be computed; Use the pull-down menu

clean-up --Add hydrogen

to correct carbon atoms' valences.
Use the pull-down menu
Clean-up--Mechanics--Optimize
to optimize your molecule before submission for Gaussian calculations.
5. Ignore the pop up warning about symmetry by click on OK;
6. Now your molecule is almost ready for calculations by the Gaussian program. Click the Job options button on the left panel;
Enter the following choices:
Job name: NHCAuCl (or any other names)
Calculation: Geometry Optimization
Theory: B3LYP
Basis Set: Other---then type gen in the pop up box
Charge: 0
Multiplicity: Singlet
In order to calculate heavy atom such as gold, additional steps must be added.
Click Advanced Tab, in the Additional Keywords box, type pseudo = read.
Then click the Preview Tab, click the button Generate. The input file will be generated and displayed in the text area. Scroll down to the last line, put one blank line and then the following basis sets information.

```
H C N O 0
6-31G(d)
```

```
****
Au 0
SDD
****
Au 0
SDD
```

One more cartridge return and submit job.

7. On the left panel, click Submit Job.
8. You will be directed back to the Job Manager screen, where you should be able to see the status of your Gaussian calculation. It takes from several seconds to a few hours to optimize the geometry of the molecule at the HF/6-31G(d) level of theory depending on the size of the molecule.
9. Once the status indicates complete, click on the right hand side button Actions--View to display the results of the calculations.
10. The displayed molecule is now geometry optimized. You can use this geometry to calculate a number of different properties of the molecule. What we need for the donor- acceptor experiment are the molecular orbital energies. At the bottom center of the screen, click the button New Job using this geometry.
11. On the next screen, click Job options. Change the Geometry optimization to Molecular orbitals. Then click Submit job. This should only take less than a minute.

12. Once the status turns to complete, click on the right hand side button of Actions--View to display the results of the calculations. Scroll down pass the graphical display, pass the other results including partial charges section. You should see a section labeled Molecular Orbitals. Find the HOMO and LUMO and copy the energies to your notebook. The occupied orbitals have occupancy of 2 and the unoccupied orbitals have occupancy of 0. The listed energies are in the unit of Hartrees. Convert them to kcal using the conversion factor 1 Hartree = 627.51 kcal. Negative values indicate lower energies.

Help is available

Miami Redhawk cluster computer help: anyone who has questions can contact rescomp@miamioh.edu. E-mail to this address will go to people involved in administrating the cluster compute