Chemistry 438/550: Computational Chemistry, Spring 2022

Homework #3, due Feb. 16

1. First, build the formaldehyde molecule. There are lots of ways to do this, but here is a simple approach you can do in a browser window:

   (a) In your browser, visit https://www.webmo.net/demo/index.html

   (b) Follow steps 1-3 in the tutorial there. (You can go further if you want, but on the first time, just stop after step 3.)

   (c) Now choose File → Export Molecule → XYZ format. Save the file when requested: default name will be *molecule.xyz*

2. Next, edit the *molecule.xyz* file with a text editor. The format is very simple: the first line gives the number of atoms; the second line is blank; remaining lines have the element name, followed by *xyz* coordinates. This format is very similar to what Gaussian wants. To carry out the conversion from .xyz to Gaussian .com format, do this:

   (a) Change the first two lines to the following five lines:

   ```
   # HF/6-31G* opt
   <blank line>
   my first trial run on formaldehyde
   <blank line>
   0  1
   ```

   Note the blank line before and after the "title line". The coordinate lines should follow right after the "0 1" line. Finally, add a blank line at the bottom of the file. Name the file *formaldehyde.com*

3. Next, you need to transfer (copy) this file from your laptop to amarel. If you are in a Mac/Linux terminal, you can just do this:

   ```
   rsync -av formaldehyde.com netid@amarel.rutgers.edu:
   ```

   Change *netid* your your netid. Note the ":" at the end of the command: that tells the rsync program that *amarel.rutgers.edu* is a machine name, not a file name. If you are using putty as your terminal, see chapter 5 in the Putty user manual; your command will look very much like the one above:

   ```
   pscp formaldehyde.com netid@amarel.rutgers.edu:
   ```

   If you are using some other terminal program, check its instructions about how to transfer files to and from a remote server.

4. Now login to amarel; you should find the *formaldehyde.com* file in your home directory. You might want to create a new working directory, and move it there. Next, in that working directory, do this:

   ```
   cp /projects/community/classes/ccb550/g16.pbs.template formaldehyde.pbs
   ```

   Note that you will now edit a copy of the template file, called `formaldehyde.pbs`. Instructions for editing are in the file itself: you will change STARTDIR to your working directory (something like `/home/netid/homework3`); change NETID to your netid; change JOB to formaldehyde. Finally, run the job this way:

```
sbatch formaldehyde.pbs
```

5. You can monitor the progress of your job by typing '`squeue | grep netid`'; once your job is completed, you should see a `formaldehyde.log` file in your working directory. Take a deep breath, and examine that file to see how much of it you can understand. It is good to see the final line say "`Normal termination of Gaussian 16`". If you don't see this, try to figure out what went wrong. Send me email giving details if you can't figure it out – you are jumping in with both feet to Gaussian, so glitches are to be expected.

6. "Hand in" your homework this way, changing *lastname* to your lastname:

```
cp formaldehyde.log \
      /projects/community/classes/ccb550/homework3/lastname.log
```

   (Above command should all be on one line.)