

m#+LATEX\HHEAD: enumerate

Computational Chemistry Laboratory II (CBE 60547)

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09-20-2019

1 Electronic Structure Calculations using GAMESS and Avogadro

In this lab session we will learn how to run and visualize the results of electronic structure calculations utilizing the GAMESS and Avogadro software on the CRC machines.

1.1 Logging In With FastX

Go to <https://crcfe01.crc.nd.edu> and log in using your ND credentials. Then choose a single xterm session to get started. Alternatively, download [fastX](#) software.

1.2 Loading the required modules

- The shell command `module avail` shows a list of software installed on the CRC machines which you can load and use

```
1 module avail
```

- The modules we will need to load are `avogadro`, `gamess`, and `openbabel`.

```
1 module load avogadro
2 module load gamess
3 module load openbabel
```

1.3 Avogadro

- To launch avogadro type

```
1 avogadro &
```

- We are going to set up and run a calculation for N_2
- In the draw settings section select nitrogen from the element drop down menu
- Uncheck adjust hydrogens (this will put hydrogens on your atom and construct NH_3)
- Clicking in the view window will create a nitrogen atom
- Place two nitrogen atoms next to each other to make a N_2 molecule
- Hovering over any of the icons in the top bar will display a description of that option.

- The click to measure tool will allow you to measure distances (select two atoms) and angles (select 3 atoms). Select both nitrogens, #1 and #2 will appear on them and the distance will be displayed below
- Click on the manipulation tool (the hand with a finger pointing)
- Click and drag one of the nitrogens until the bond length is 1.1 Å\ (later we will learn methods for optimizing geometry, but for right now we will set it based on the experimental distance <http://cccbdb.nist.gov/exp2.asp?casno=7727379>)

1.4 GAMESS

1.4.1 Creating Input files

- We are ready to generate our input file now. From the extensions menu select **GAMESS** and click on **Input Generator**
- A window will pop-up. The setup for this calculation right now is a single point energy calculation, the method is restricted Hartree-Fock, with the STO-3G basis. In the lower right click generate
- Name your input file and save it in a new folder
- Alternately, you could also have typed in the input file by hand

1.4.2 Running calculations

- Go back to the terminal cd into the directory where you saved the input file
- The command below will run games on your input file and generate an output file called N2.log

```
1  rungms N2.inp > N2.log
```

To queue a job, create and save gamess.sh:

```
#!/bin/bash
#$ -pe smp 4
#$ -q debug
#$ -N gamess
module load gamess

cat <<EOF > ~/.gmsrc
set SCR=/scratch365/$USER
set USERSCR=$PWD
EOF

rungms $1.inp > $1.out
```

```
1  qsub gamess.sh N2
```

1.4.3 Analyzing the output

- Open the output file in a text editor, either gedit or emacs.

```
1 emacs N2.log &
```

- The structure of the output file is
 - summary of the input
 - initialization messages
 - store 1 and 2 electron integrals
 - SCF calculation details
 - final orbital populations and energies
- Now go back to Avogadro and open the log file
- From here you can view the orbitals and their energies
- You can also measure any angles and bond lengths in the same manner as we did when setting up the input calculation

1.4.4 Run a series of jobs

```
1  #!/bin/bash
2  #$ -pe smp 4
3  #$ -q debug
4  #$ -N gamess
5  module load gamess
6
7  cat <<EOF > ~/.gmsrc
8  set SCR=/scratch365/$USER
9  set USERSCR=$PWD
10 EOF
11
12 rm -f dist template summary.dat
13
14 cat <<EOF > dist
15 0.5
16 0.6
17 0.7
18 0.8
19 0.9
20 1.0
21 1.1
22 1.2
23 1.3
24 1.4
25 1.5
26 1.6
27 1.7
28 1.8
29 1.9
30 2.0
31 2.1
32 2.2
33 2.3
34 2.4
35 2.5
36 2.6
```

```

37  2.7
38  2.8
39  2.9
40  3.0
41  EOF
42
43  cat <<'EOF' > template
44    $BASIS GBASIS=STO NGAUSS=3 $END
45    $CONTRL SCFTYP=RHF RUNTYP=ENERGY ICHARG=1 MULT=1 $END
46    $DATA
47    Title
48    C1
49    H      1.0      0.      0.      0.
50    He     2.0      0.      0.    XXX
51    $END
52    EOF
53
54  for i in $(cat dist); do
55    echo $i
56    sed s/XXX/$i/ < template > $i.inp
57    echo $i.inp
58    runrms $i.inp > $i.out
59    ENERGY=$(grep '^ FINAL RHF' $i.out | gawk '{print $5}')
60    echo "$i $ENERGY" >> summary.dat
61  done

```

1.4.5 Plot output