INCOOR = Coordinate file

INPUT_DMOL = DMol3 Program instructions

Job file = submit to the batch queue

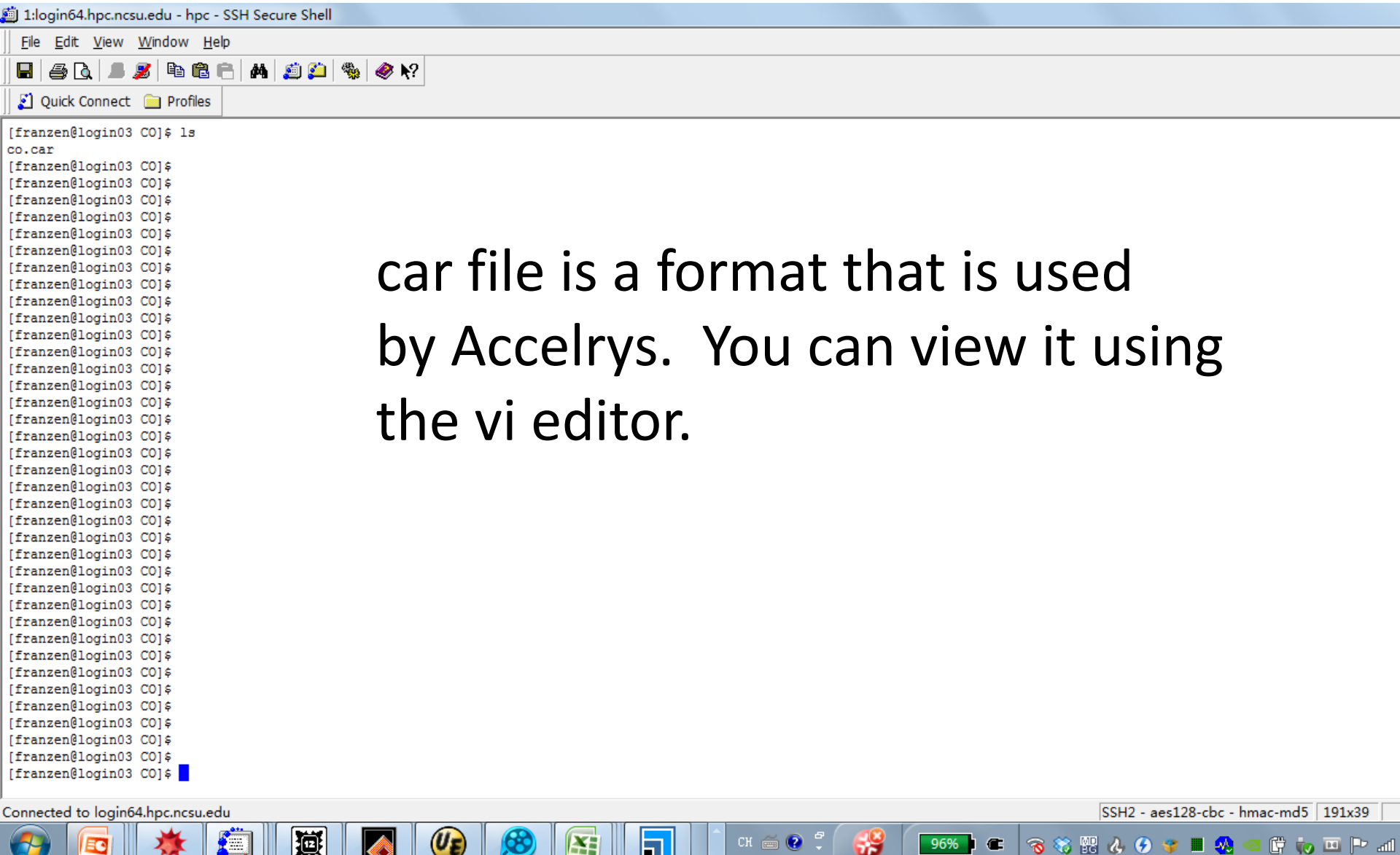
Running DMol3 Calculations

INCOOR

INPUT_DMOL

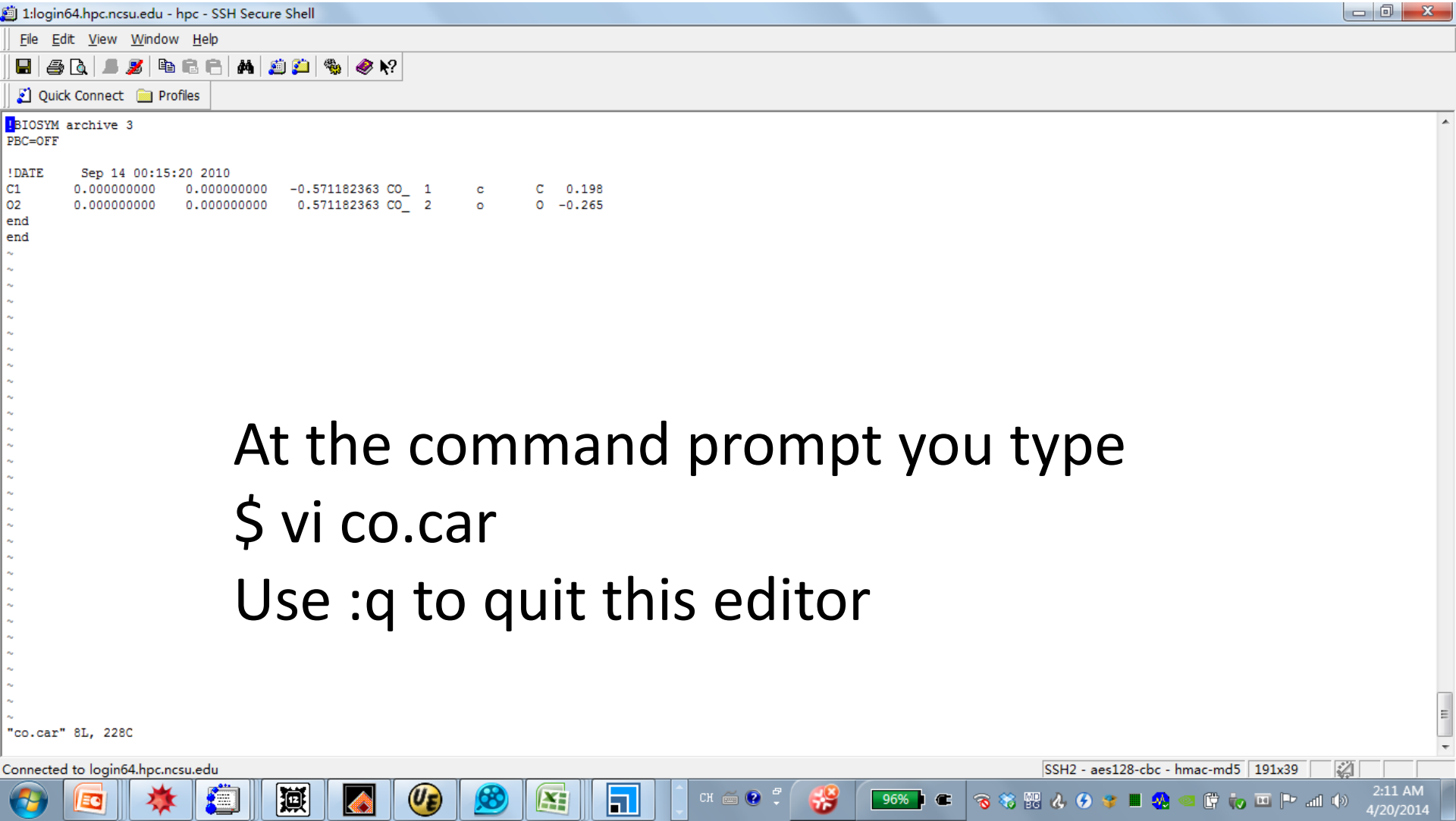
Job file

Start with a car file



car file is a format that is used by Accelrys. You can view it using the vi editor.

Viewing the file in vi editor

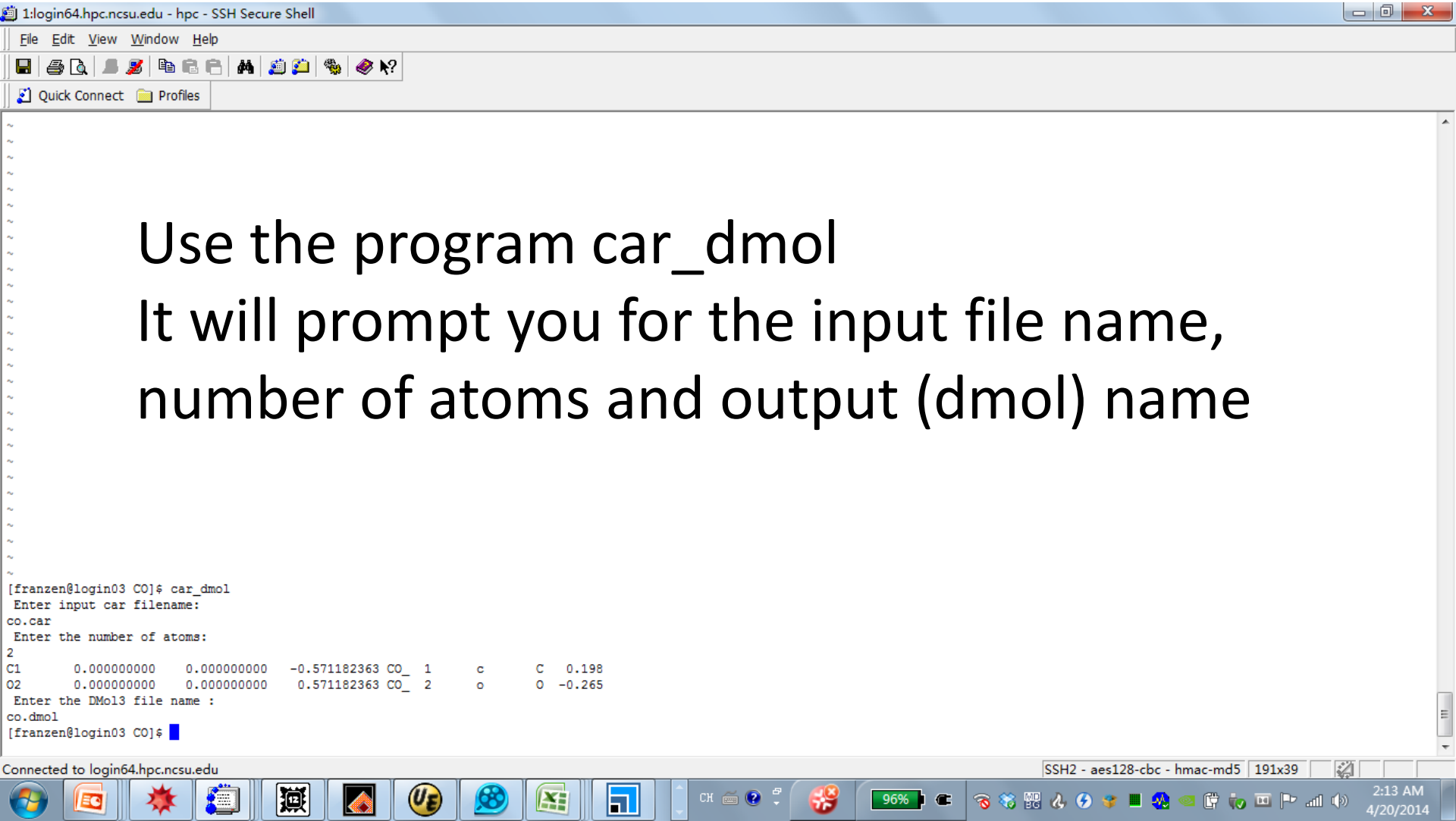


At the command prompt you type

$ vi co.car

Use :q to quit this editor

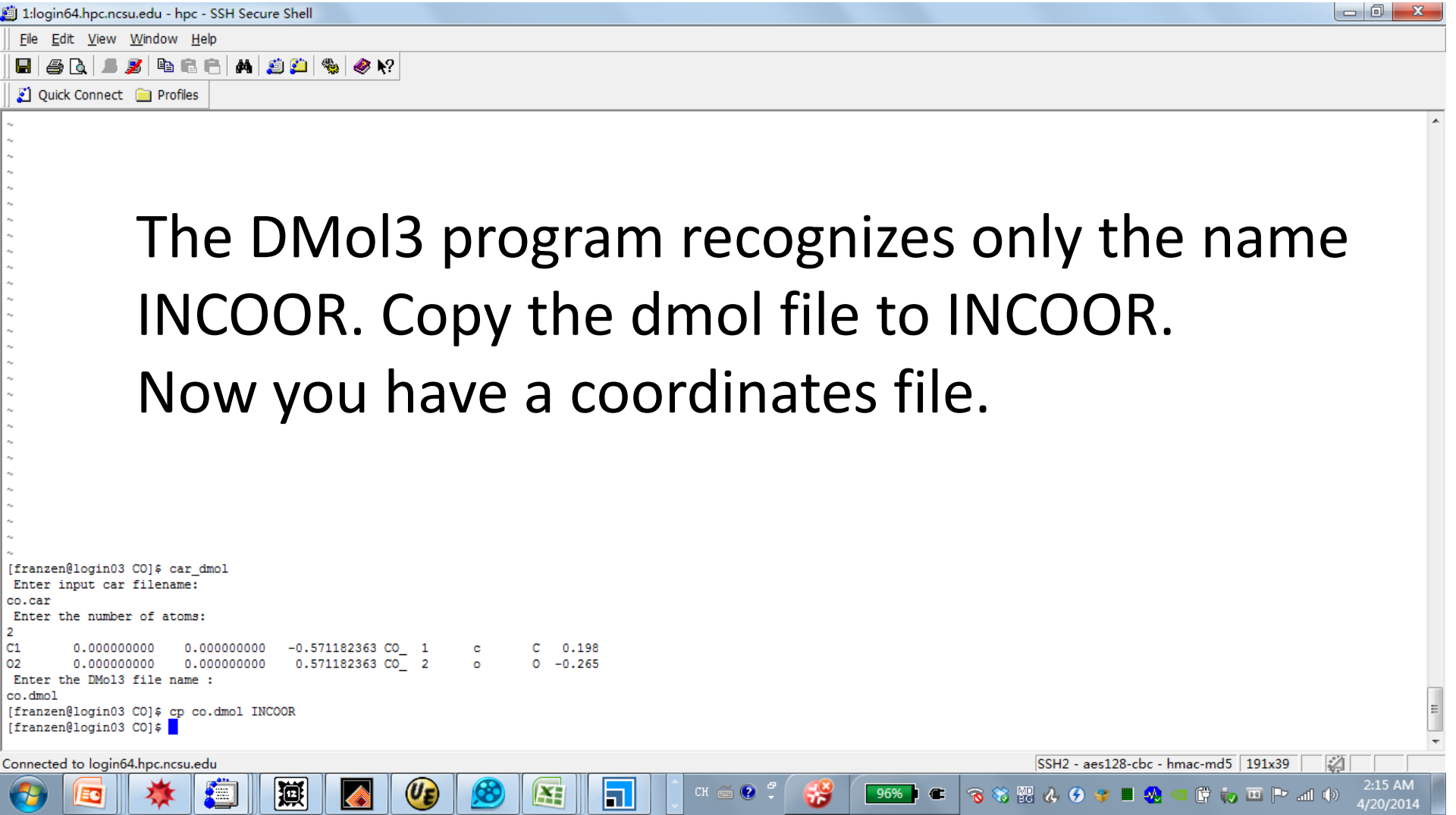
Convert the car file to dmol file format



Use the program car_dmol

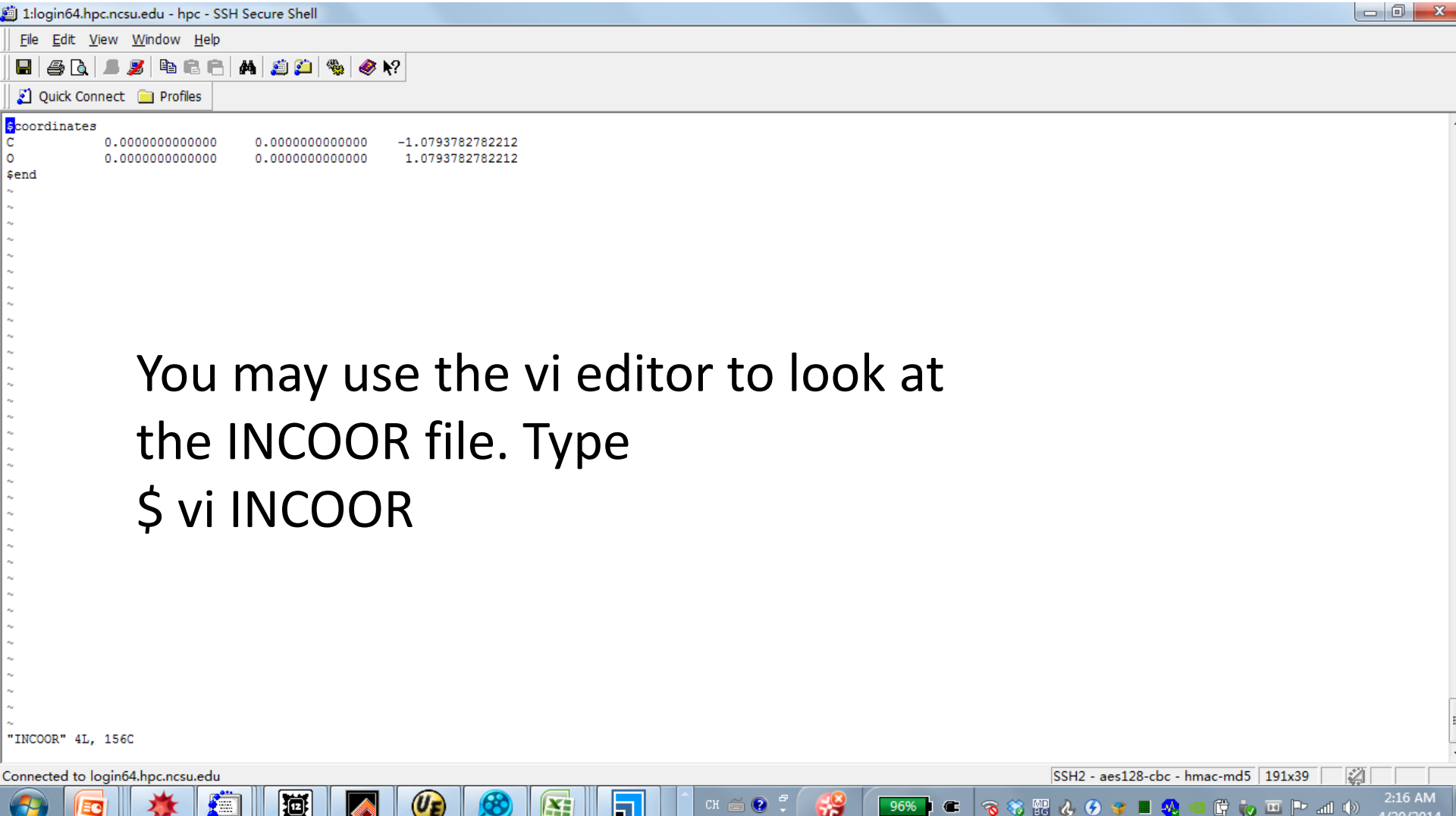
It will prompt you for the input file name, number of atoms and output (dmol) name

Making an INCOOR file



The DMol3 program recognizes only the name INCOOR. Copy the dmol file to INCOOR. Now you have a coordinates file.

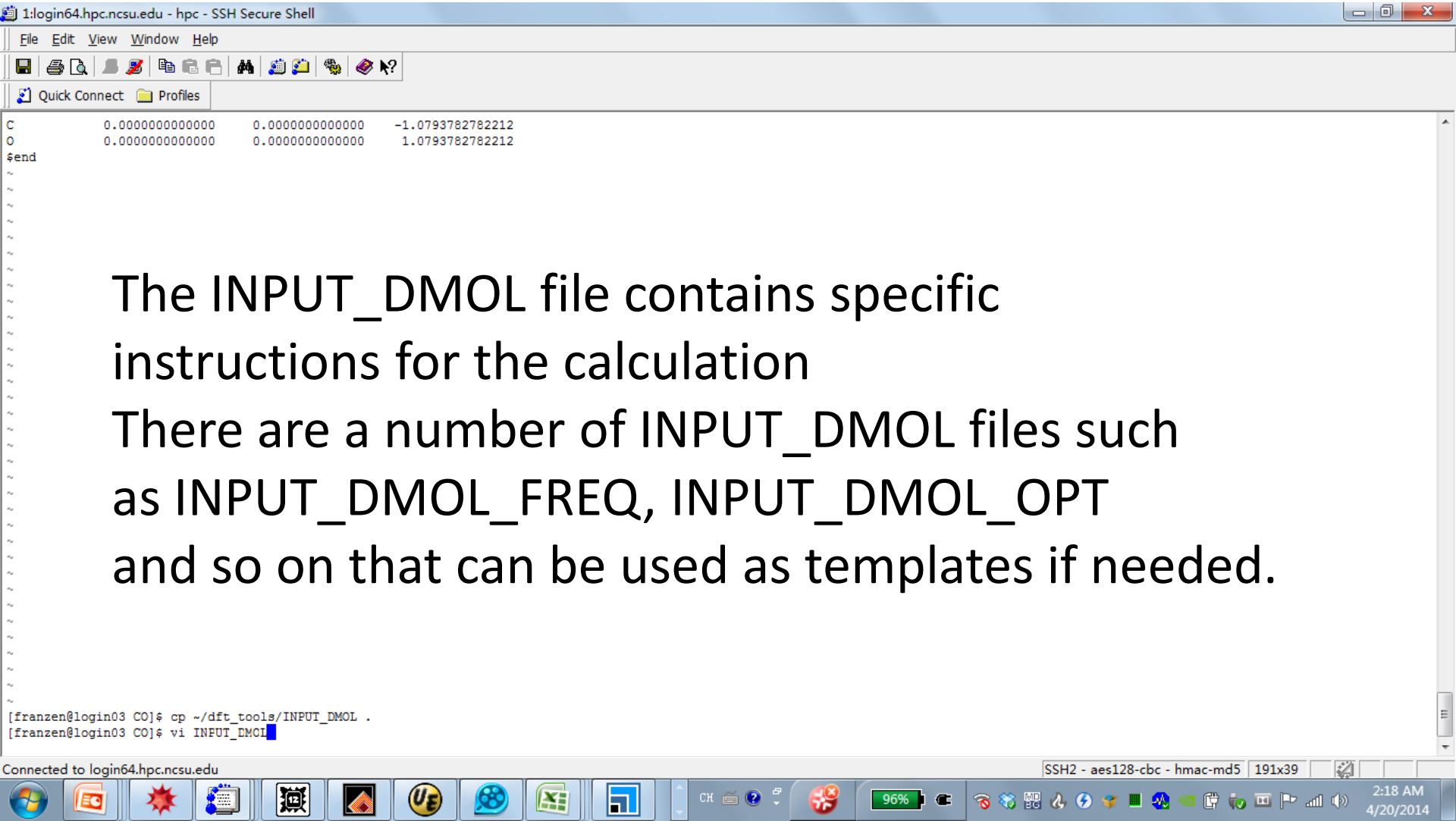
Examining the INCOOR file



You may use the vi editor to look at the INCOOR file. Type

$ vi INCOOR

Obtaining a INPUT_DMOL file



The INPUT_DMOL file contains specific instructions for the calculation

There are a number of INPUT_DMOL files such as INPUT_DMOL_FREQ, INPUT_DMOL_OPT and so on that can be used as templates if needed.

An INPUT_DMOL file for a single point calculation

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File Edit View Window Help

Quick Connect Profiles

```
# -----  Type of Calculation:

Calculate               energy

Functional              pbe

Basis                   dnp

Spin                    0.000

Charge                  0.000

# -----   Properties Keywords


#  -----   SCF keywords:

# -----  Optimization keywords:


~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
"INPUT_DMOL" 23L, 279C
```

The “energy” keyword refers to a single calculation

You may need to change the Charge and Spin keywords for your molecule.

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An INPUT_DMOL file for a geometry optimization and frequency calculation

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File Edit View Window Help

Quick Connect Profiles

```
# -----  Type of Calculation:
Calculate               optimize_frequency
Functional              pbe
Basis                   dnp
Charge                  0.000
Spin                    0.000

# -----   Properties Keywords
#Vibration_restart       on
#  -----   SCF keywords:
Occupation  Thermal 0.005
# -----  Optimization keywords:
OPT_Coordinate_System   Cartesian
Print   Eigval_Last_It
~
~
~
~
~
~
~
~
~
~
```

The # means that a line is commented out

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The text of the cbrc script is given below.
The paths need to be modified to have your name.

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File Edit View Window Help

Quick Connect Profiles

```
echo '#!/bin/tcsh -f'
echo '#BSUB -o "$1".error -e "$1".error"
echo '#BSUB -W 1440 '
echo '#BSUB -n 8 '
echo '#BSUB -J '$1
echo '#BSUB -q brc'
echo '  '
echo '# Set some environmental variables '
echo 'setenv DMOL_DATA /home/franzen/dmol_data '
echo '  '
echo '# move to requested directory'
echo '  '
echo 'cd /share2/franzen/dft/'$2
echo 'cp "$1".dmol INCOOR"
echo '  '
echo '#'
echo '# Call DMol executable'
echo '  '
echo '# Run DMol:'
echo '  '
echo '/home/franzen/bin/Dmol39m10m > "$1".outmol"
echo '  '
echo '  '
echo '  exit'
```

Modify the path for the DMOL_DATA
/home/YOUR_DIRECTORY/dmol_data

Modify the path for working directory
/share2/YOUR_DIRECTORY/$1

Modify the path for bin directory
/home/YOUR_DIRECTORY/bin/Dmol3 etc.

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The job file submits the job to the queue.
The submitter on the HPC is the bsub command.
You can generate a job file using a script.
Please use cbrc (for the brc queue) or
ccos (for the cos queue).

To run the script you need to provide the
file name (root name without extension) and
directory name. The format is

$ cbrc FILE_NAME DIR_NAME > FILE_NAME.job

When you have INCOOR, INPUT_DMOL and Job file you may run the job.

$ bsub < FILE_NAME.job

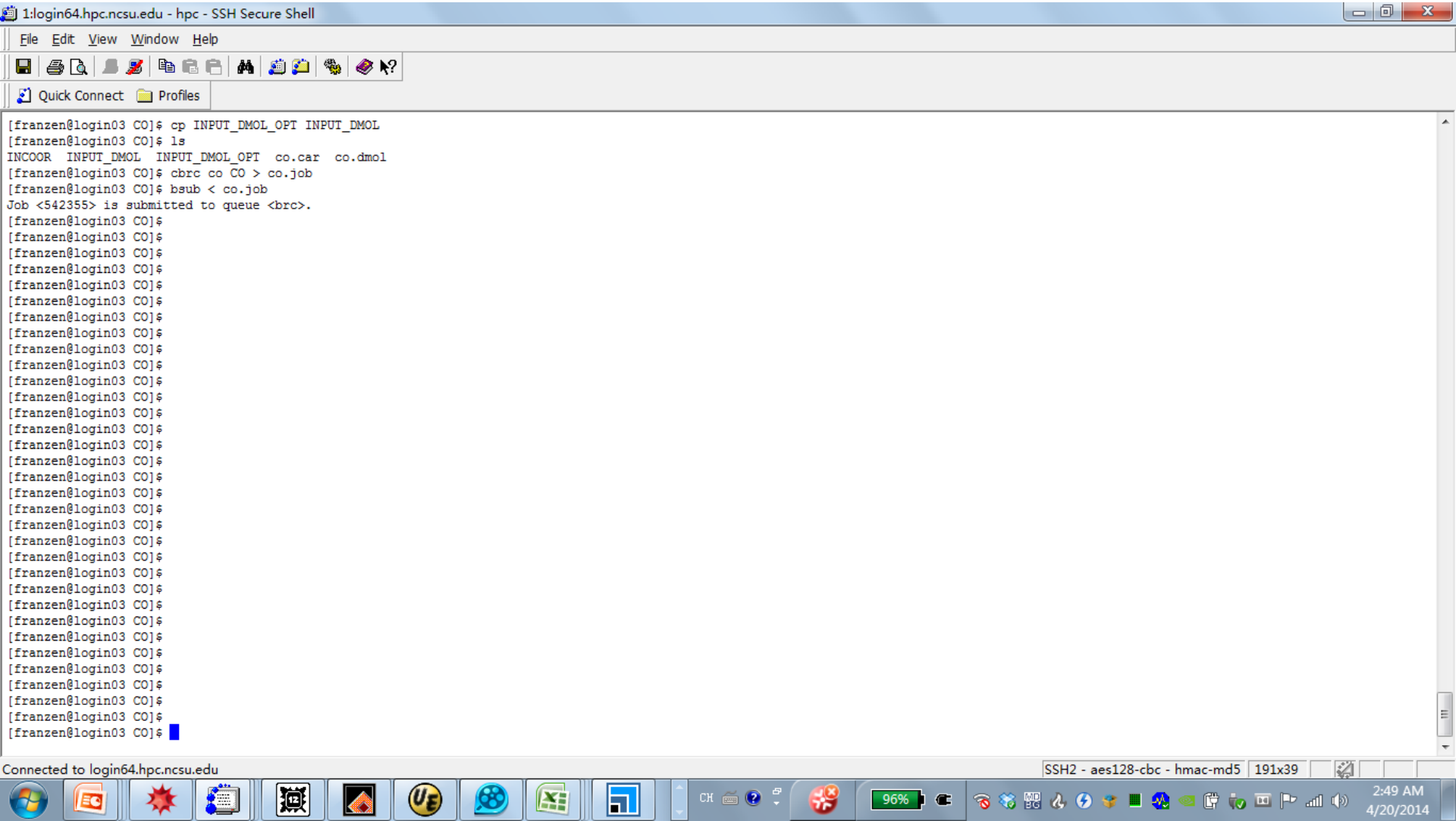
To check that the job is running use

$ bjobs

To kill the job use

$ bkill PROCESS_ID

For example, for CO you would use
$ cbrc co CO > co.job



Check the output in the co.outmol file

$ vi co.outmol

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File Edit View Window Help

Quick Connect Profiles

```
   z      0.0000      0.0000      0.0000      0.0000     -0.6548     -0.7558
O  x      0.0000      0.0000      0.0000      1.0000      0.0000      0.0000
   y      0.0000      0.0000      1.0000      0.0000      0.0000      0.0000
   z      0.0000      0.0000      0.0000      0.0000     -0.7558      0.6548


 Zero point vibrational energy:      0.207 au_amu


Standard thermodynamic quantities at   298.15 K  and    1.00 atm

   Zero point vibrational energy:        3.042 kcal/mol

   H,Trans:                0.889 kcal/mol
   H,Rot  :                0.592 kcal/mol
   H,pV   :                0.592 kcal/mol
   H,Vib - ZPVE:           0.000 kcal/mol
   S,Trans:               35.925  cal/mol.K
   S,Rot  :               11.344  cal/mol.K
   S,Vib  :                0.001  cal/mol.K
   C,Trans:                4.968  cal/mol.K
   C,Rot  :                1.987  cal/mol.K
   C,Vib  :                0.007  cal/mol.K
   ========================================
   H,Total - ZPVE:         2.074 kcal/mol
   S,Total:               47.270  cal/mol.K
   C,Total (p):            6.962  cal/mol.K
   G,Total:              -12.020 kcal/mol

Symmetry analysis for vibrations:c4v symdec file generated by DMol
      freq       a1    e
      cm-1       %
    2127.9     100.   0.

Wall_clock_time calculate diag       0.0 m        0.9 s
Wall_clock_time calc not diag        0.1 m        3.7 s
Wall_clock_time total,  1 proc       0.1 m        4.6 s
 time all done       0.31m       18.87s
[franzen@login03 CO]$ vi co.outmol
```

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The bottom of the co.outmol should have the appearance on the left.

Compile the program mpnm_diatomic
Use the f77 fortran compiler

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File Edit View Window Help

Quick Connect Profiles

```
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$
[franzen@login03 CO]$ f77 mpnm_diatomic.f -o mpnm_diatomic
[franzen@login03 CO]$ mpnm_diatomic
 Enter outmol filename:
co.outmol
 Enter 1 for linear, Enter 0 for non-linear:
1
 Enter number of atoms:
2
 Enter maximum displacement(e.g. 1.0) :
2.0
 Enter number of steps (e.g. 21):
21
 ibeg =  0
 ifreq =  1
     C   0.000000000    0.000000000   -1.079378278
     O   0.000000000    0.000000000    1.079378278
    1    0.000000         0.0        0.00
 Enter car filename:
co.car
C1        0.000000000    0.000000000   -0.571182363 CO_  1      c
O2        0.000000000    0.000000000    0.571182363 CO_  2      o
 Enter rootname:
co__
 PROGRAM COMPLETE
 DMOL INPUT FILES HAVE BEEN GENERATED
[franzen@login03 CO]$
```

The command for compilation is:
$ f77 mpnm_diatomic.f –o mpnm
The –o flag tells the final name of the compiled program. You may call it anything you want.

Here you see the instructions to run the program and generate output files (normal mode projections)

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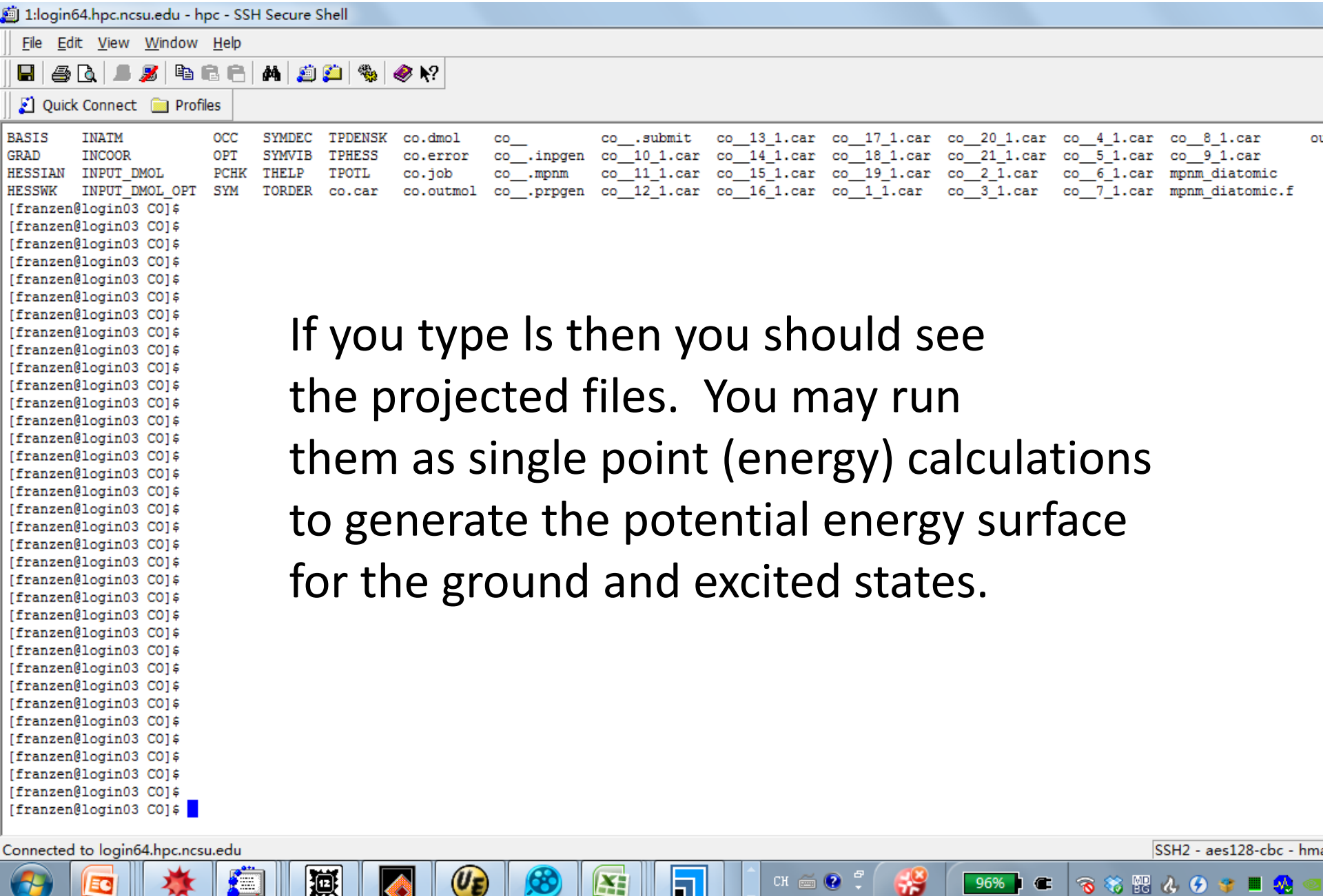
96% 2:53 AM 4/20/2014


1:login64.hpc.ncsu.edu - hpc - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
BASIS INATM OCC SYMDEC TPDENSK co.dmol co__ co__.submit co__13_1.car co__17_1.car co__20_1.car co__4_1.car co__8_1.car
GRAD INCOOR OPT SYMVIB TPHESS co.error co__.inpgen co__10_1.car co__14_1.car co__18_1.car co__21_1.car co__5_1.car co__9_1.car
HESSIAN INPUT_DMOL PCHK THELP TPOTL co.job co__.mpnm co__11_1.car co__15_1.car co__19_1.car co__2_1.car co__6_1.car mpnm_diatomic
HESSWK INPUT_DMOL_OPT SYM TORDER co.car co.outmol co__.prpgen co__12_1.car co__16_1.car co__1_1.car co__3_1.car co__7_1.car mpnm_diatomic.f
[franzen@login03 CO]$
If you type ls then you should see the projected files. You may run them as single point (energy) calculations to generate the potential energy surface for the ground and excited states.
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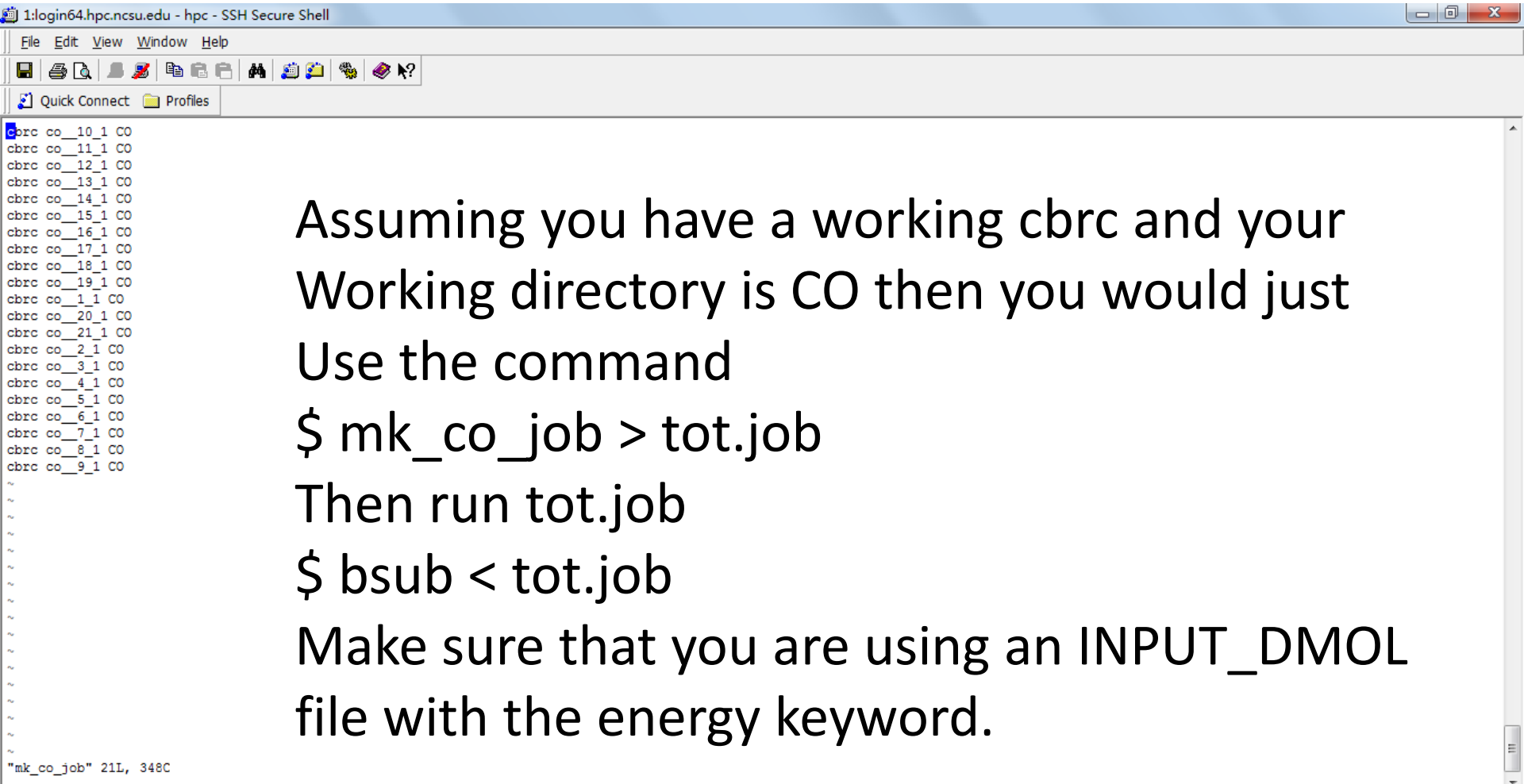
SSH2 - aes128-cbc - hma
96%

To run multiple files you may wish to create
a script that creates a job file to run multiple files.
an example is the script mk_co_job



Assuming you have a working cbrc and your
Working directory is CO then you would just
Use the command

$ mk_co_job > tot.job

Then run tot.job

$ bsub < tot.job

Make sure that you are using an INPUT_DMOL
file with the energy keyword.

To efficiently extract information for the outmol files use the “grep” command.
For example
$ grep energy *.outmol

You will see a list of the energies. If you want to save them to a file, use the redirect (>) like this.
$ grep energy *.outmol > co_energy

LINUX has a somewhat different order for the files so you many need to change the order, but energies will be in this file.
.

To extract the energies of the LUMO you will need to figure out which line in each output file contains the LUMO. Then use the appropriate grep command to extract those energies.