EMERSON CENTER: HARDWARE

comp.chem.20

ssh –Y eclab@euch4e.chem.emory.edu
Passwd:

euch4e.chem.emory.edu
HOME=/home/chemistry/ch_res/eclab

cd spark

cd star

cd fire

$HOME/spark

mkdir USER
cd USER

Nodes = 36
Cores/node = 24
Speed = 2.6 GHz
Memory = 96 GB
Classes = spark24p
spark12p

spark (or spark.chem.emory.edu)

$HOME/star

mkdir USER
cd USER

Nodes = 36
Cores/node = 24, 16
Speed = 2.5 GHz
Memory = 80 GB
Classes = star24p
star16p
star8p
stars (1 core)

star (or star.chem.emory.edu)

$HOME/fire

mkdir USER
cd USER

Nodes = 16 + 1 GPU
Cores/node = 56 + 5000
Speed = 2.6 GHz
Memory = 196 GB
Classes = fire28p
fire-gpu

fire (or fire.chem.emory.edu)

Login the Emerson Center's Computers

From a Unix/MAC/iPad/iPhone terminal

ssh -Y eclab@euch4e.chem.emory.edu

From PC

1) Download and run PuTTY (www.putty.org)
2) Enable X-forwarding (Connection -> SSH -> Tunnels)
3) Under Session, choose SSH on port 22
4) Type **euch4e.chem.emory.edu** as host name
5) Click Open

A few UNIX commands and vi Editor

UNIX

Tree Structure: *Files and Directories*

cd - change directory: *cd directory_name*
rm - remove command: *rm file_name:* also: **rmdir, rm –I**
mv - move comman: *mv file_name*
mkdir - make directory: *mkdir directory_name*
cp - copy command: *cp file_name_1 file_name_2*
ls - list command

VI (View)

Command mode and **Insert mode**

vi *file_name*
Type **i** for insert command
Use backspace in order to correct mistake

:w **:w!** or **:wq** **:wq!** Write or write and quit
:q **:q!** quit
dd n delete
o Insert line

EMERSON CENTER:
Software (Selected List)

Electronic Structure

Gaussian-16, 09
Molpro-15.1
MOLCAS
GAMESS
TURBOMOLE
ORCA
VASP-5.2
DFTB+

MD Simulation & Modeling

GROMACS-19.1
NAMD-2.6
Rosetta
Amber-14

Graphics & Programming

MATLAB 2019
Mathematica 12.0
Gauss View 6

Command file (for LoadLeveler only):

```
#!/bin/ksh
#
###
# @ error = errcl.log
#
# @ initialdir = /star/chemistry/eclab/YOUR
# @ requirements = (Arch == "R6000") && (OpSys == "AIX53")
# @ notify_user = name@euch4e
# @ class = star16p
# @ group = ch_res
# @ queue
#
    INPF= test_inp
    OUTF= test_out

. /libs/scripts/g16/C01
chmod a+rw $OUTF
```

llsubmit xxxx.cmd

A Few LoadLeveler Commands

llq

```
Id                       Owner          Submitted   ST PRI Class        Running On
------------------------ ---------- ----------- -- --- ------------ -----------
euch4e.123949.0          nzhu        1/15 09:17   R  50  fire-gpu        euch7b
euch4e.123947.0          jamal       1/15 08:47   R  50  star24p         euch2c
euch4e.123944.0          zxk         1/14 11:48   R  50  spark24p        euch2d
euch4e.123950.0          jamal       1/15 11:17   R  50  spark24p        euch2d
euch4e.123929.0          zxk         1/13 09:49   R  50  spark24p        euch2d
euch4e.123926.0          zxk         1/13 09:46   R  50  spark24p        euch2d
euch4e.123928.0          zxk         1/13 09:48   R  50  spark24p        euch2d
euch4e.123927.0          zxk         1/13 09:46   R  50  spark24p        euch2d

8 job step(s) in queue, 0 waiting, 0 pending, 8 running, 0 held, 0 preempted
```

llcancel

EMORY Emerson Center for Scientific Computation

Setting up Input for GAUSSIAN

Resource Section: **%chk, %nproc=16, %mem=@**

The route section:
Which kind of job you want to run: methods and basis sets.
Starts with a # sign **Opt, freq, pop=full etc.**

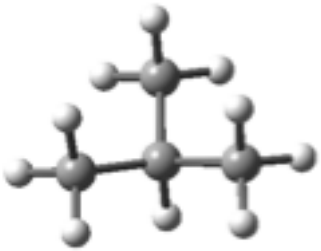
The title section: **ANY**

The Molecule specification section:
Charge on the molecule, Spin multiplicity**: 0 1 or -1 1 or 1 1, etc**
Molecular structure (x,y,z coordinates)

Basis sets (if necessary)

Other Specific Requirements

Input for GAUSSIAN: *t*Bu



%CHK=/starchk/chemistry/ch_res/eclab/**@YOUR**/h2o.chk
%nproc=16
%mem=2GB
B3LYP/**6-31G(d,p)** opt freq

tBu molecule

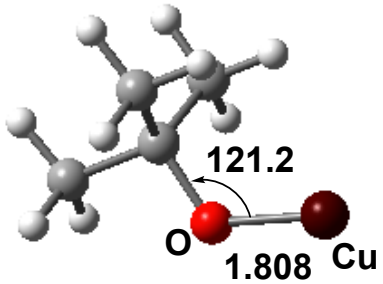
0 1

C	-1.49303751	0.44689800	0.00000000
C	0.02103049	0.44689800	0.00000000
H	0.37519549	0.98143900	-0.92732800
H	-1.88158751	1.49355300	0.00000000
H	-1.88160351	-0.07730300	-0.90591200
H	-1.88493351	-0.07546400	0.90578800
C	0.55417649	-0.96972900	-0.03454800
C	0.55380249	1.18729700	1.20842200
H	1.67031749	-0.96440100	-0.06053600
H	0.22450949	-1.53464200	0.87050700
H	0.17947749	-1.50407200	-0.94038700
H	0.22349649	0.68786100	2.15098600
H	1.66994849	1.20676800	1.19124900
H	0.17927949	2.23903500	1.21597100

Input for GAUSSIAN: Cu-O^{t}Bu

%chk=/starchk/chemistry/ch_res/eclab/jamal/CutBu.chk
%mem=2GB
%nproc=16
b3lyp/gen pseudo=read opt freq=noraman

Cu-tBu molecule



0 1

C	-1.49303751	0.44689800	0.00000000
C	0.02103049	0.44689800	0.00000000
O	0.44693349	1.08971312	-1.11516321
H	-1.88158751	1.49355300	0.00000000
H	-1.88160351	-0.07730300	-0.90591200
H	-1.88493351	-0.07546400	0.90578800
C	0.55417649	-0.96972900	-0.03454800
C	0.55380249	1.18729700	1.20842200
H	1.67031749	-0.96440100	-0.06053600
H	0.22450949	-1.53464200	0.87050700
H	0.17947749	-1.50407200	-0.94038700
H	0.22349649	0.68786100	2.15098600
H	1.66994849	1.20676800	1.19124900
H	0.17927949	2.23903500	1.21597100
Cu	1.04206053	1.98793796	-2.67341422

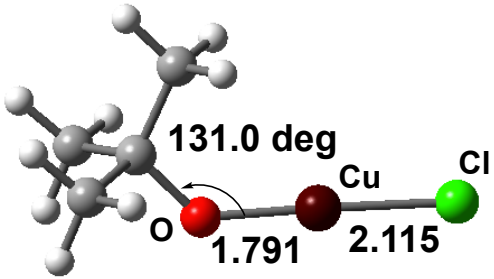
Cu 0
lanl2dz
****
H C O 0
6-31G(d,p)
****

Cu 0
lanl2dz

Input for GAUSSIAN: ClCu-O^{t}Bu

%chk=/starchk/chemistry/ch_res/eclab/jamal/CutBu.chk
%mem=2GB
%nproc=16
ub3lyp/gen pseudo=read opt freq=noraman

ClCu-tBu molecule



0 2

C	-2.46424600	1.34290700	-0.51202300
C	-1.99110800	0.00002500	-0.00005400
O	-0.64160700	-0.00002700	-0.00008600
H	-2.08852100	2.16285600	0.14569200
H	-2.08818300	1.51712900	-1.54850500
H	-3.57955700	1.38627600	-0.52877700
C	-2.46442200	-1.11494200	-0.90674600
C	-2.46418300	-0.22792600	1.41890900
H	-2.08838800	-2.09965200	-0.53927300
H	-3.57975300	-1.15095500	-0.93566900
H	-2.08888200	-0.95570000	-1.94583000
H	-3.57952600	-0.23472800	1.46487700
H	-2.08868500	-1.20757600	1.80017700
H	-2.08784800	0.58252200	2.08797000
Cu	1.16586400	-0.00001000	-0.00002900
Cl	2.11458960	-1.24988736	-0.93776982

Cu 0
lanl2dz
****
H C O Cl 0
6-31G(d,p)
****

Cu 0
lanl2dz

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OUTPUTS: tBu