SHORT INTRODUCTION TO FIREFLY
WITH EXPERIENCE IN HPC2015 AND HTC

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OUTLINES

- Brief introduction to firefly(PCGAMESS).
- Firefly on windows and linux operating systems
- Performance on HPC2015 and HTC systems.
- Abilities and Limitations.
- GABEIT a graphical Interface to firefly.

GENERAL ATOMIC AND MOLECULAR ELECTRONIC STRUCTURE SYSTEM (GAMESS)

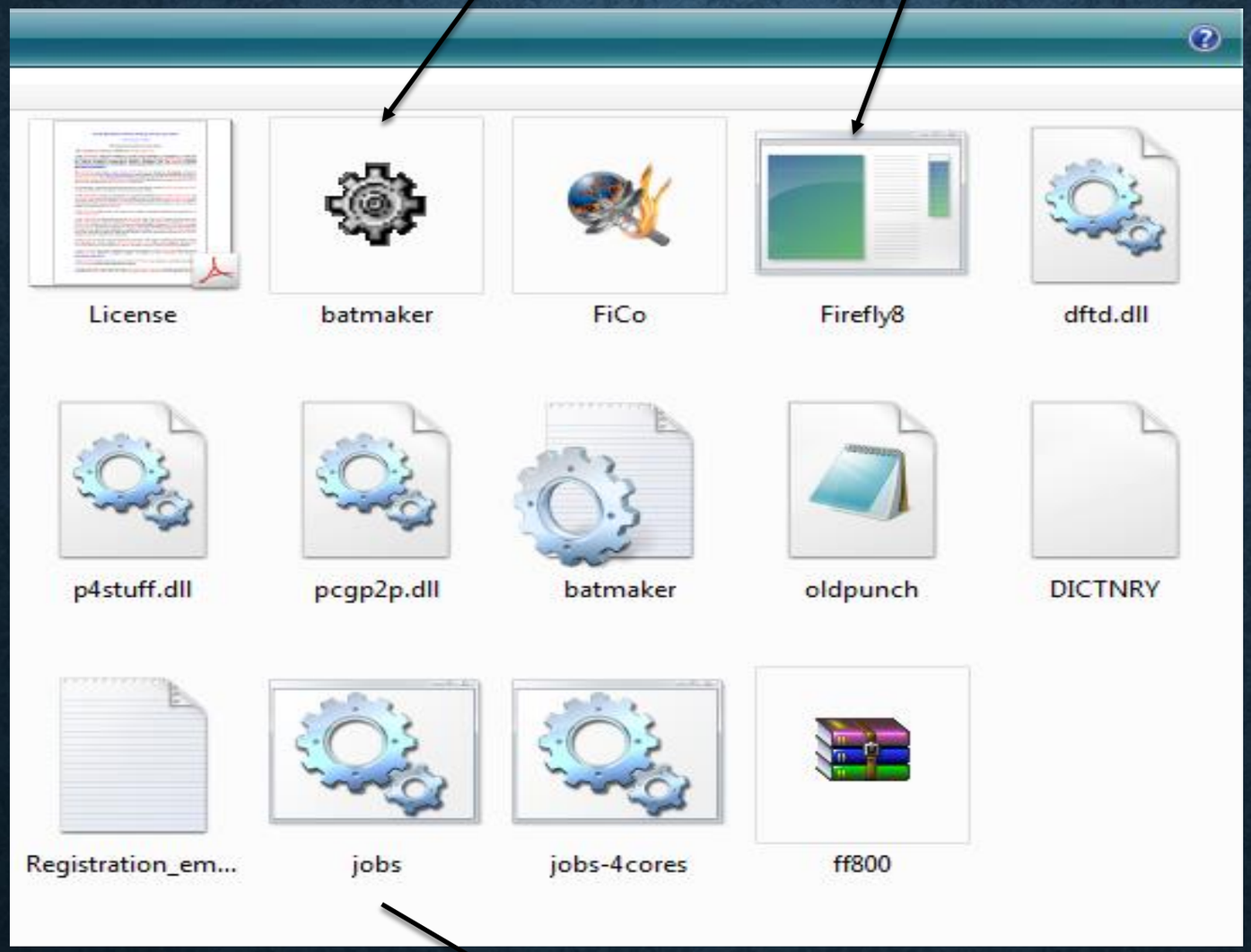
- PCGAMESS (Firefly)
- Last version is : 8.1.1
- Running on windows, linux and mac (32 and 64 bit mode)

- Ab initio and Density Functional Theory calculations as well as simulation methods
- Free of Charge and can be downloaded:
- http://classic.chem.msu.su/gran/gamess/index.html

FIREFLY ON WINDOWS OS

Batch maker

Firefly

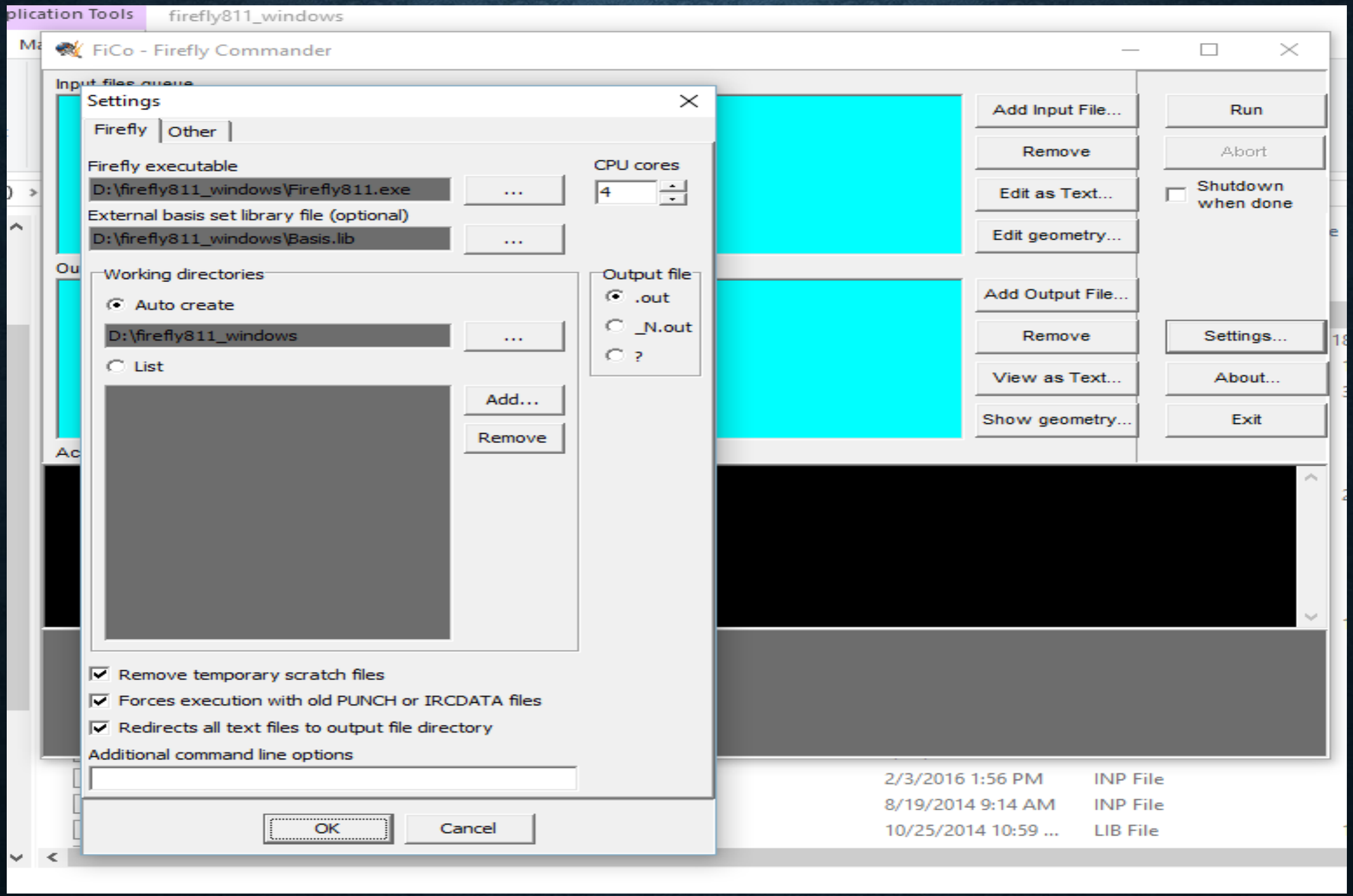


Executable

FIREFLY COMMAND LINES ON WINDOWS OS

- D:
- cd D:\firefly8_windows\
- del oldpunch.dat
- rename punch oldpunch.dat
- SET INPUT=D:\firefly8_windows\H2O-RHF.inp
- Firefly8.exe -f >D:\firefly8_windows\H2O-RHF.out

FIREFLY COMMANDER (FICO) ON WINDOWS



INPUT FILE FORMAT

The input file can be generated by any txt editors

```
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE $END
$SYSTEM TIMLIM=60000 MEMORY=90000000 $END
$BASIS  GBASIS=N311 NGAUSS=6 NDFUNC=1 NPFUNC=1 $END
$SCF    DIRSCF=.True. $END
$GUESS  GUESS=HUCKEL   $END
$DATA
H2O   Geometry optimization at RHF/6-311G(d,p)
C1
O  8.0    0.0    0.0    0.0
H  1.0    0.98   0.0    0.0
H  1.0    0.0    0.98   0.0
$END
```

TESTING THE SOFTWARE

Run all the test input files in the sample folder

! Bench 1

! This is a RHF/6-31G* run on silacyclopropane, with 61 AOs.

! It comes from a study of cycloalkanes and silacycloalkanes by

! J.A.Boatz, M.S.Gordon, and R.L.Hilderbrandt,

! J.Am.Chem.Soc., 1988, 110, 352-358.

!

! The FINAL energy is -368.0867960698 after 10 iterations,

! running the SCF in direct mode.

FIREFLY ON LINUX

- Statically linked version
- Dynamically linked version

[~@hpc2015-file firefly811_mpich-1_ssh]$

dftd.ex
fastdiag.ex
ffp2p.ex
firefly811
greetings.c
greetings-pgiompi
p4stuff.ex
pbs-ff-simple.cmd
pcgp2p.ex
procgrp

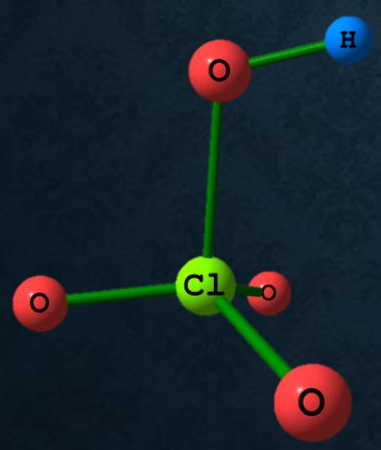
FIREFLY COMMANDER (PBS) ON LINUX

```
#!/bin/sh

####PBS -l nodes=2:ppn=2

###export IMPI_HOME=/home/ssadjadi/mpich-install
###export PATH=$IMPI_HOME/bin:$PATH
###export LD_LIBRARY_PATH=$IMPI_HOME/lib:$LD_LIBRARY_PATH
export FFHOME=/home/ssadjadi/firefly811_mpich-1_ssh
export WORK_DIR=/home/ssadjadi/work

###export I_MPI_DEVICE="rdssm:OpenIB-cma"
###export I_MPI_DEBUG=10

cd $WORK_DIR

time  $FFHOME/firefly811 -r -f -p -daf 2  -stdext  -ex $FFHOME -i
$FFHOME/Bench01.inp  -o $FFHOME/Bench01.out  -p4pg $FFHOME/procgrp
-b $FFHOME/Basis.lib
```

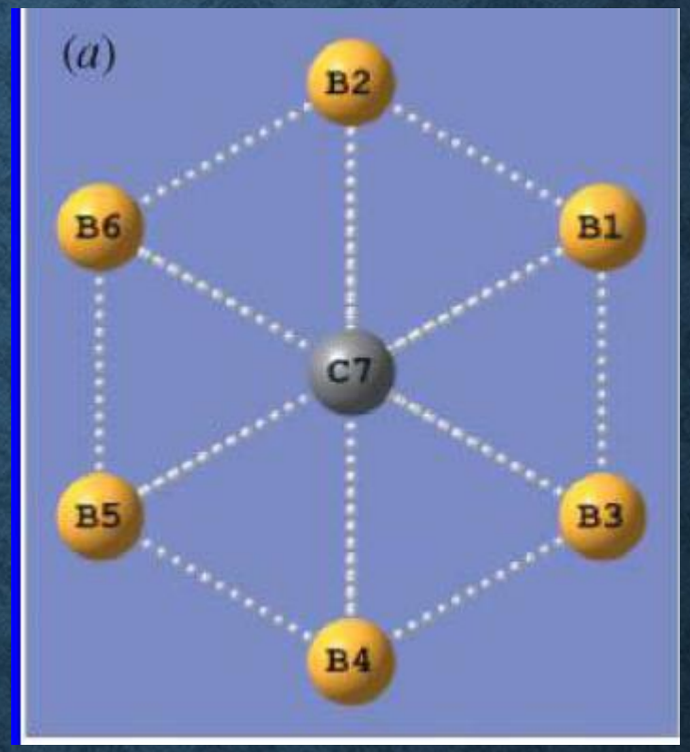
ABINITIO AND DFT CALCULATIONS

Geometry optimizations and Frequency calculations

RHF/6-311++G(d,p)



MP2(FC)/6-311++G(d,p)

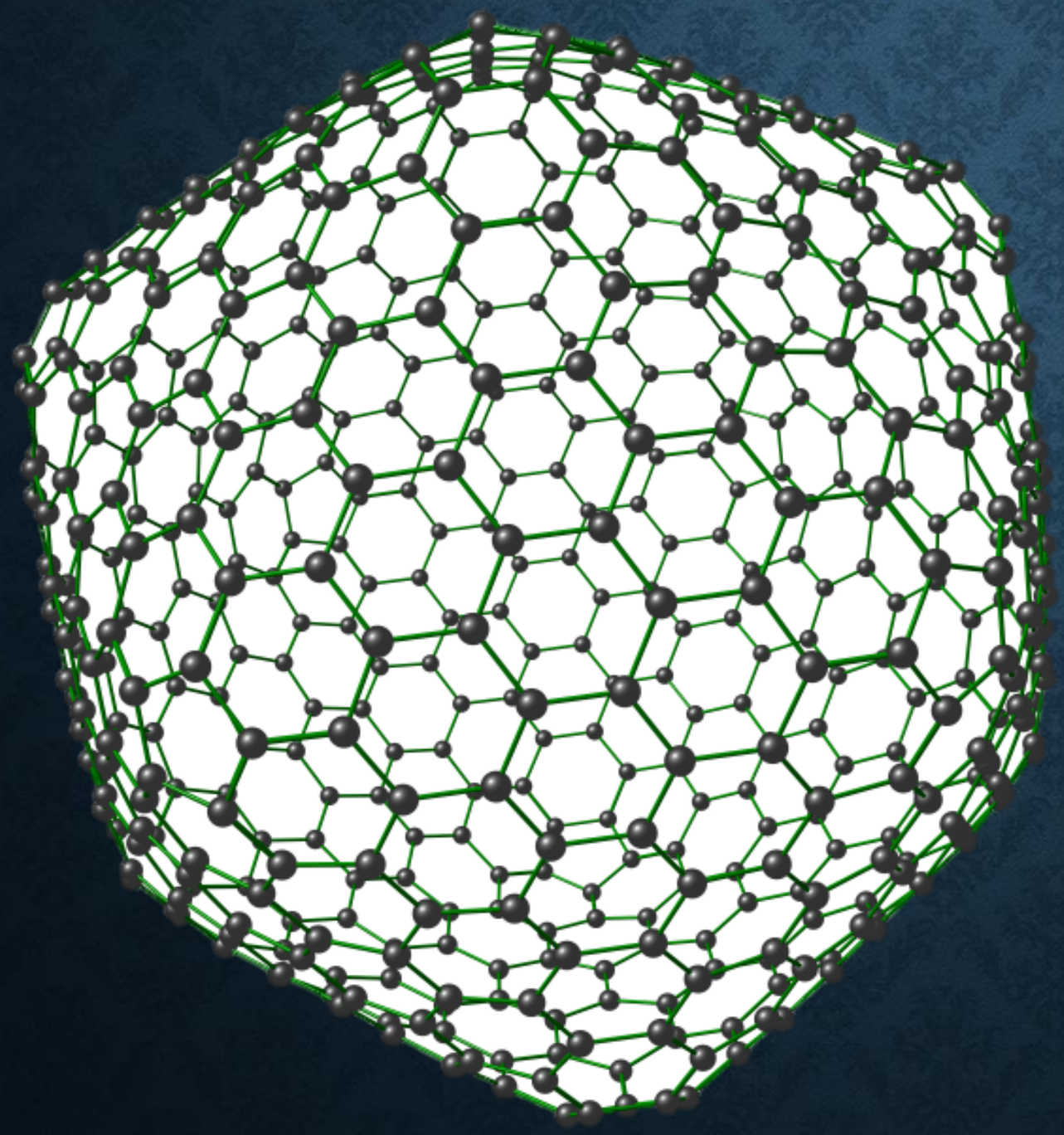


B6C(2-) at B3LYP/6-311+G*

Foroutan-Nejad, C., Shafiee, G. H., Sadjadi, A., Shahbazian, S. Canadian Journal of Chemistry, Vol 84 , Pages 771-781 (2006)

CALCULATIONS ON LARGE SYSTEMS

C540
A nano size molecule



Semi-empirical (AM1)
Geometry optimization
and
Frequency calculations

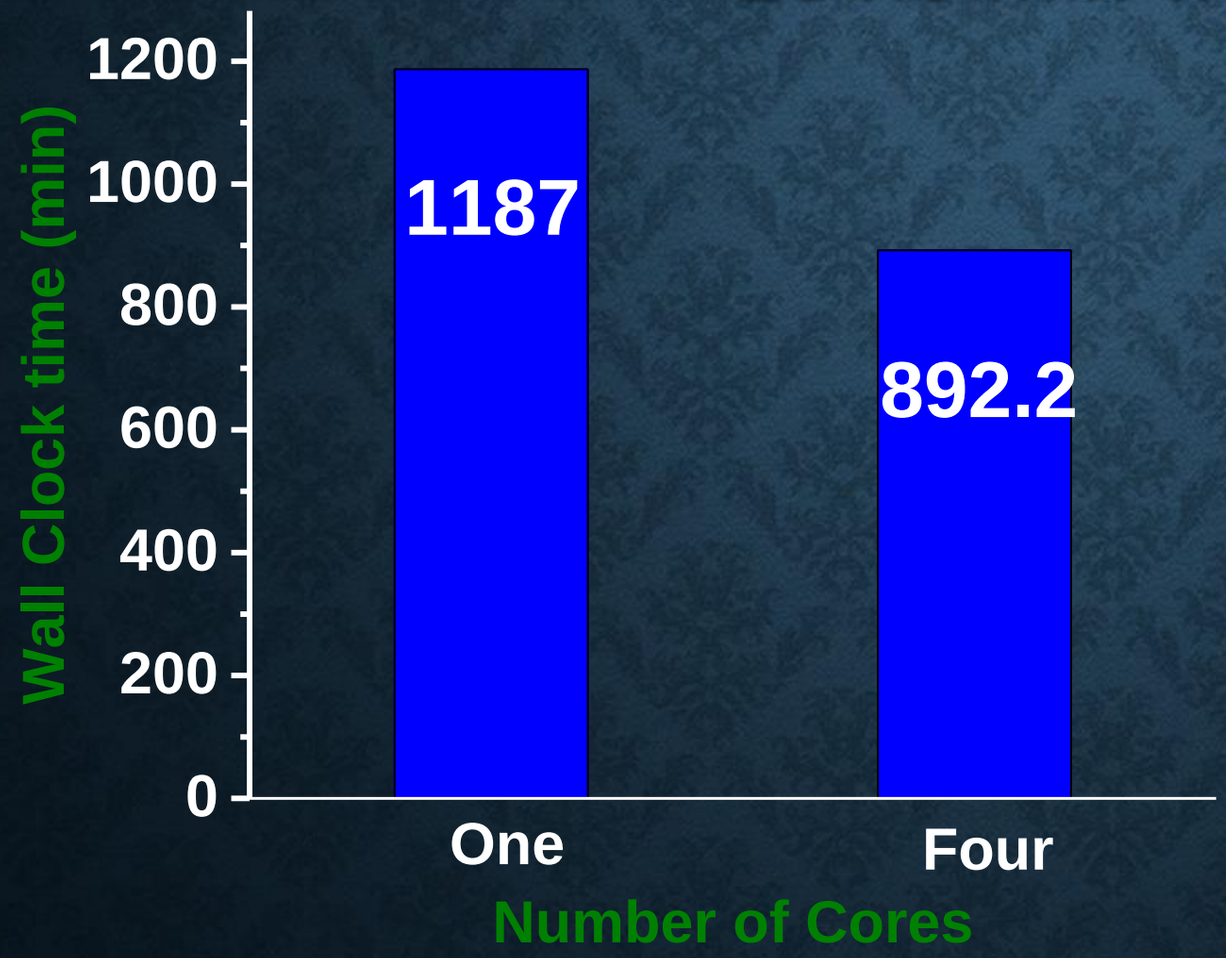
Within 359.8 min

On HTC platform

FIREFLY PERFORMANCE ON HTC PLATFORM

By using full CPU cores and threads

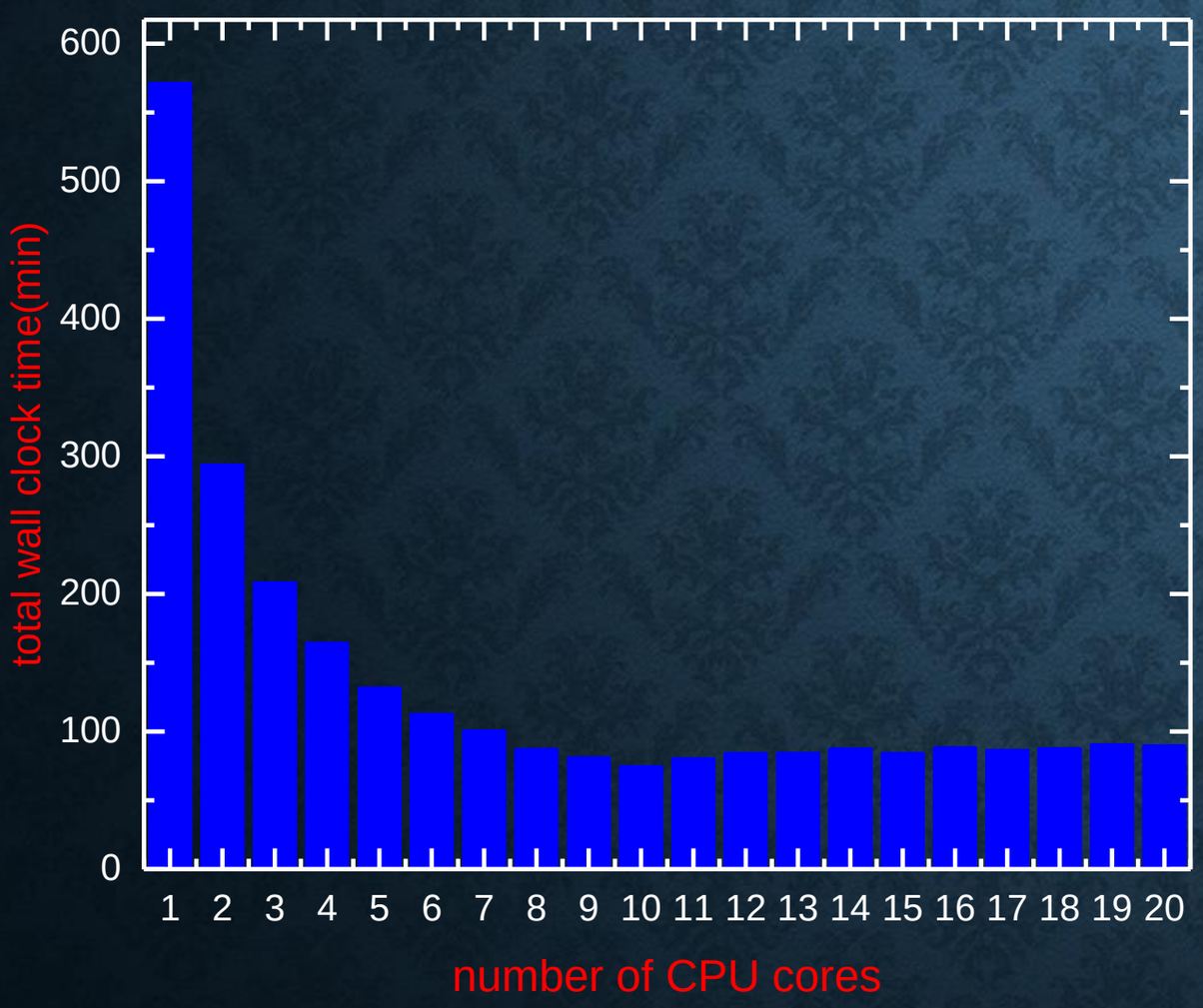
294.8 min was saved

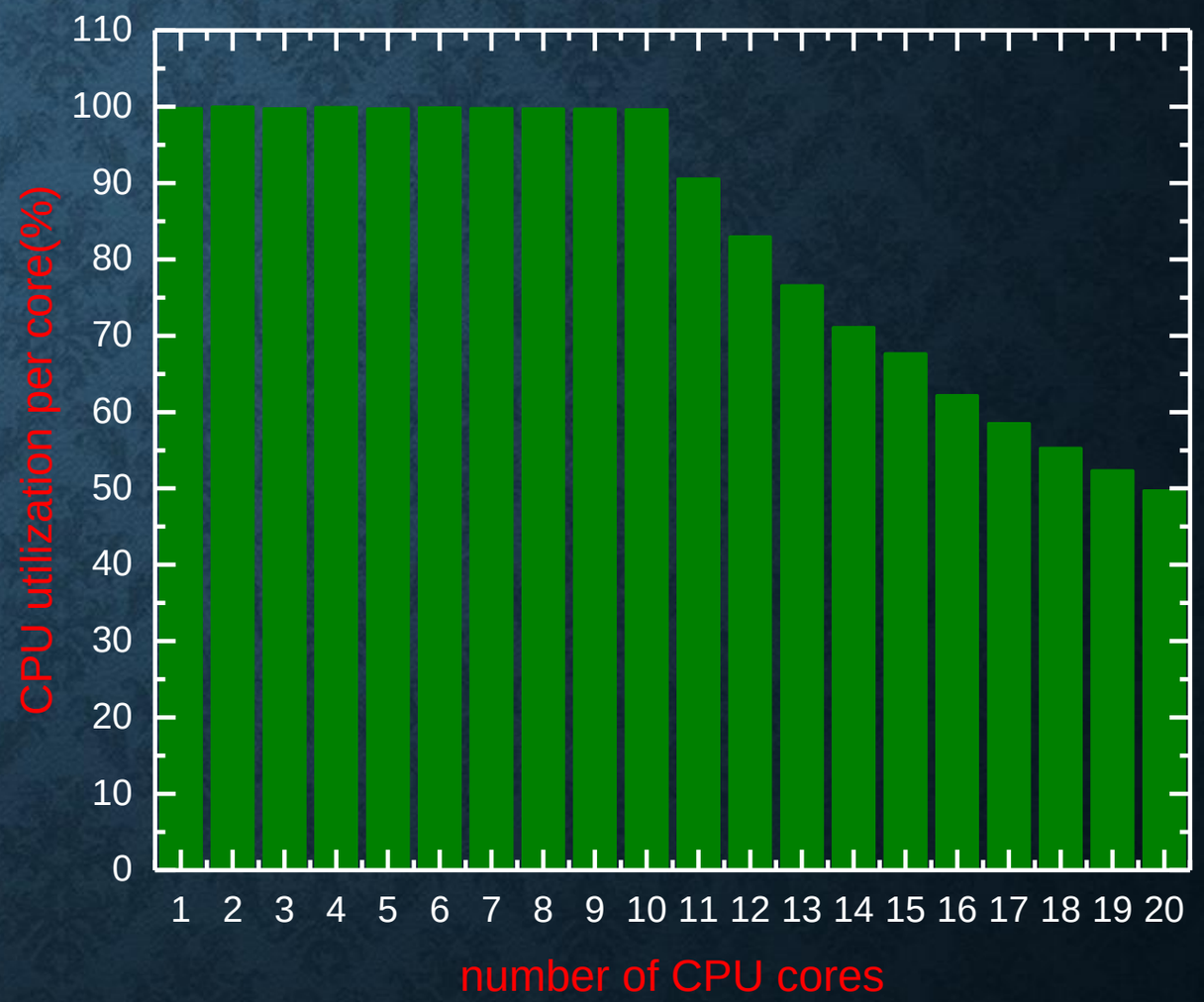


Si3C6H14
Optimization and Frequency calculations
RHF/6-311++G(d,p)

FIREFLY PERFORMANCE ON HPC2015 PLATFORM

Firefly810 (MPICH-1), Second order perturbation theory, geometry optimization and harmonic frequency calculations.
Cu2 , MP2(FC)/aug-cc-pVTZ , 238 basis functions. Core electrons: 36 , Correlated electrons: 22





PARALLEL VERSION (MPICH) RUNNING USING 3 PROCESSES (NODES)

SMT aware parts of program will use 2 threads.

SOME NOTES ABOUT FIREFLY

- Use exetyp=check in $CONTRL to set the correct memory request and check if the jobs can be done on the hardware platform. This save much of your time for figuring out the correct memory/disk configurations and provide the efficient usage of computing resources.
- Memory can not exceed 260MW on Windows 64 bit

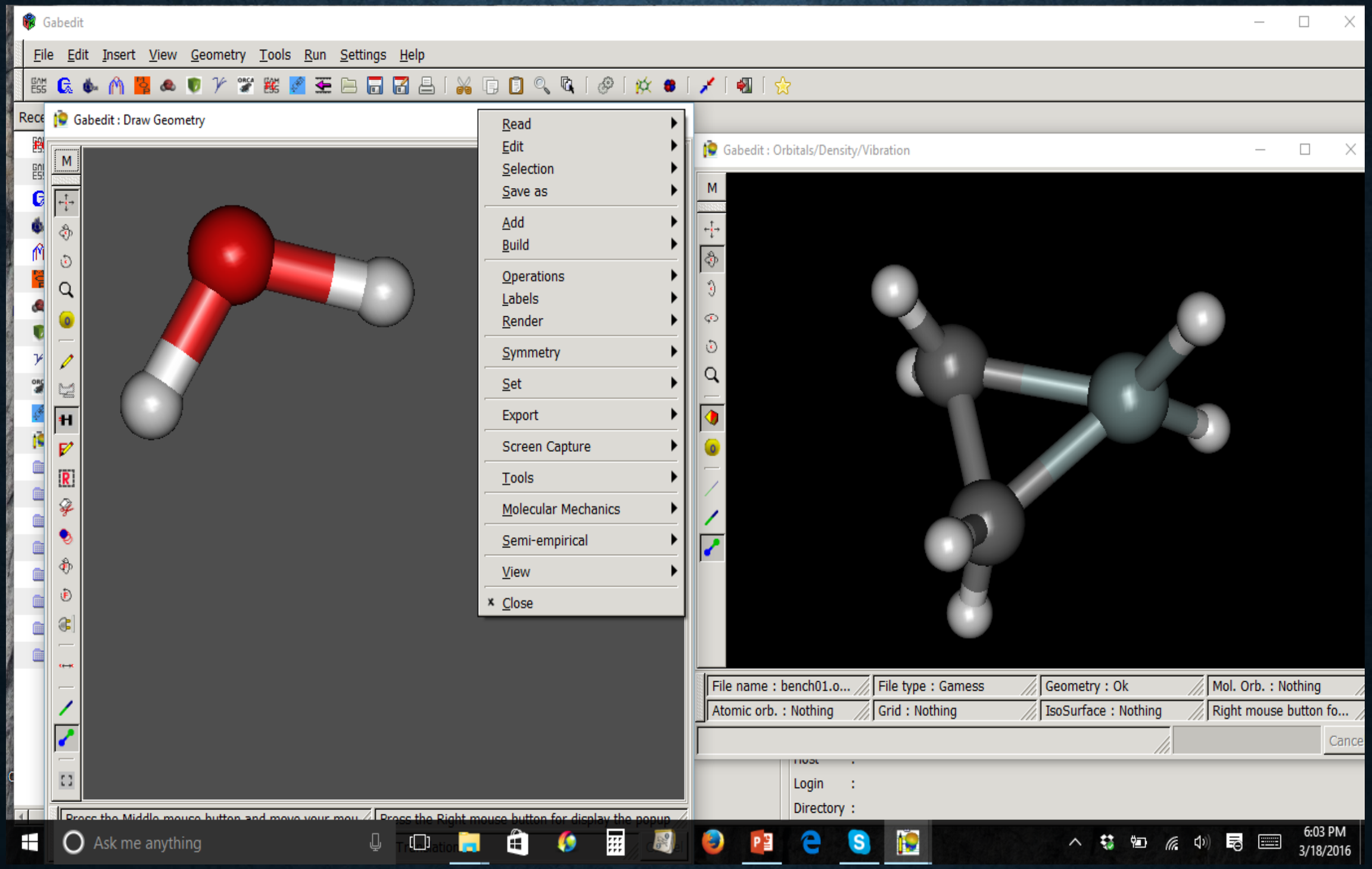
  $SYSTEM MWORDS=250 $END
- Semi-empirical calculations can not be done with more than 1012 atoms
- Coupled cluster (CC) calculations can be done by GAMESS(US). This version of GAMESS is available on HKU Gridpoint and it is very efficient coupled cluster code.

FIREFLY GRAPHICAL INTERFACE SOFTWARE

- Interface programs that help creating the input file and rendering/manupulating the information stored in the firefly output file
- Chemcraft
- Macmolplt
- Ghemical-GMS
- GABEDIT

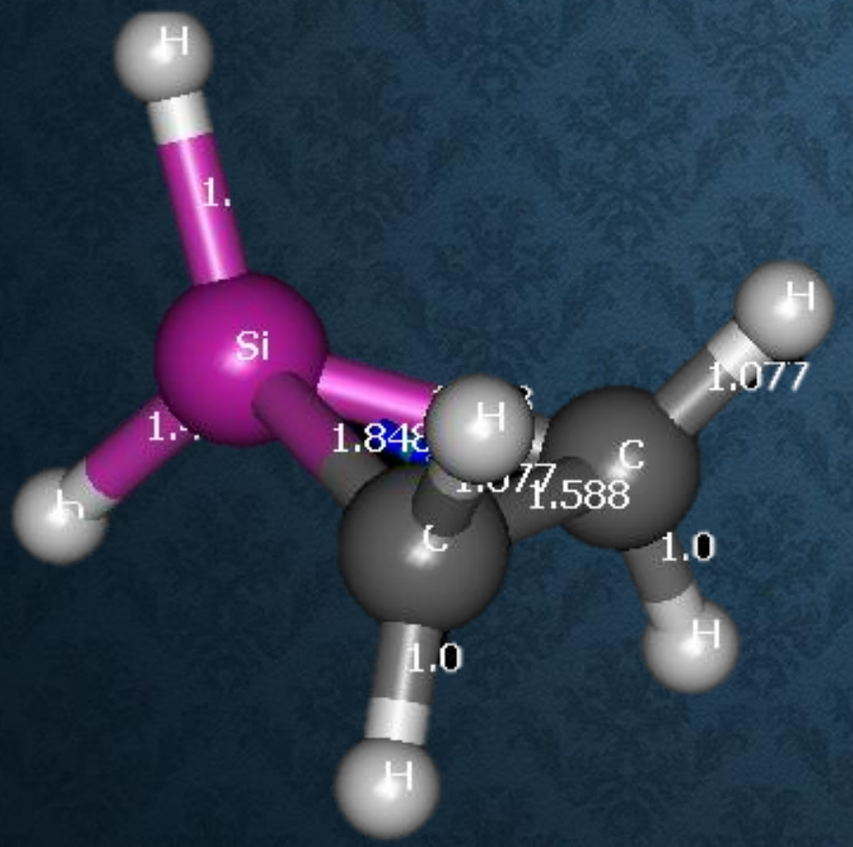
GABEDIT THE FIREFLY INTERFACE

WRITTEN BY: ABDUL-RAHMAN ALLOUCHE



BENCH 01

molecular structure

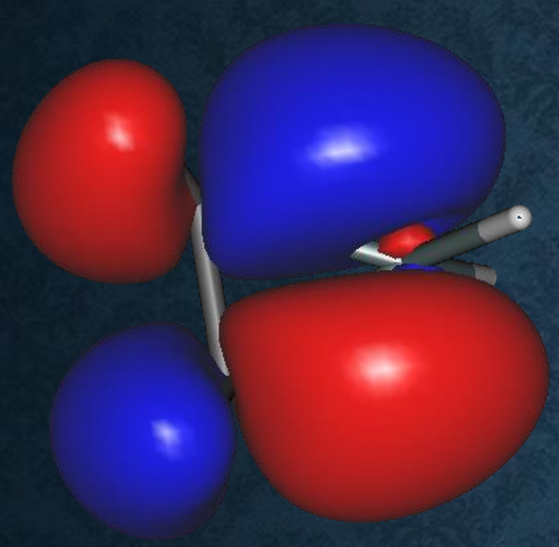


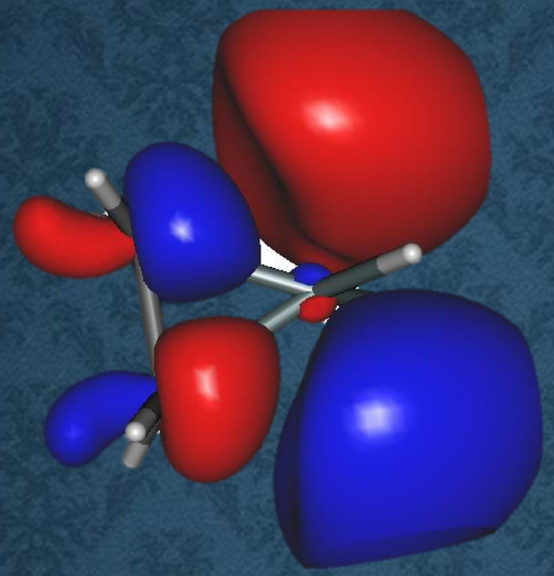
molecule formula: SiC2H6
charge:0 multiplicity:1
symmetry: C2v

TABLE OF BOND AND NON-BONDED DISTANCES

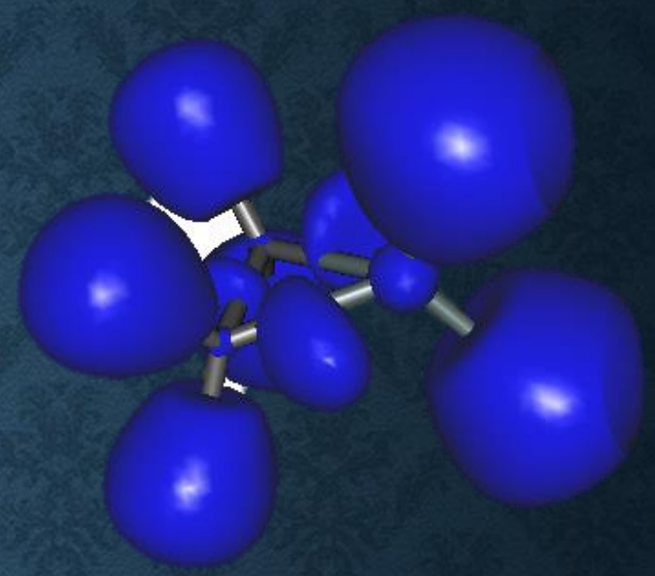
	distance	r(vdw)	r(covalent)	whether draw bond
r(Si-C)	1.8480995	3.19	1.88	yes
r(Si-H1)	1.4687996	2.79	1.43	no
r(Si-H2)	2.5643782	2.79	1.43	no
r(C-H1)	2.8745130	2.79	0.91	no
r(C-H2)	1.0767003	2.79	0.91	no
r(C-C)	1.5878680	3.4	1.36	no

FUNCTIONS PLOTTING IN GABEDIT

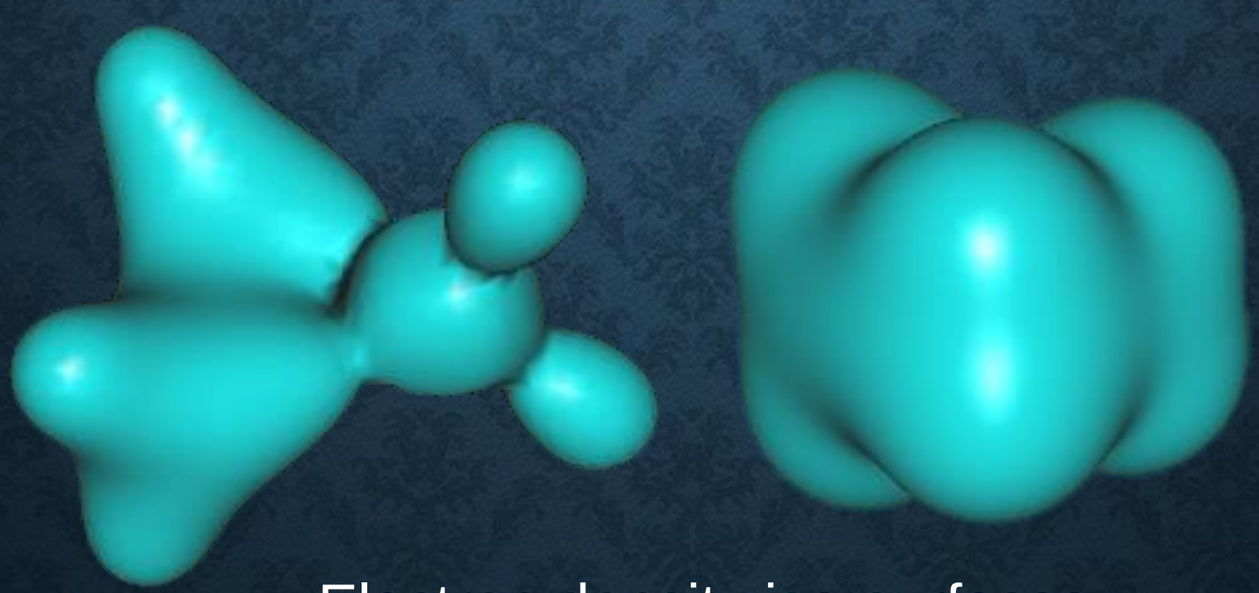




Molecular orbitals iso-surfaces

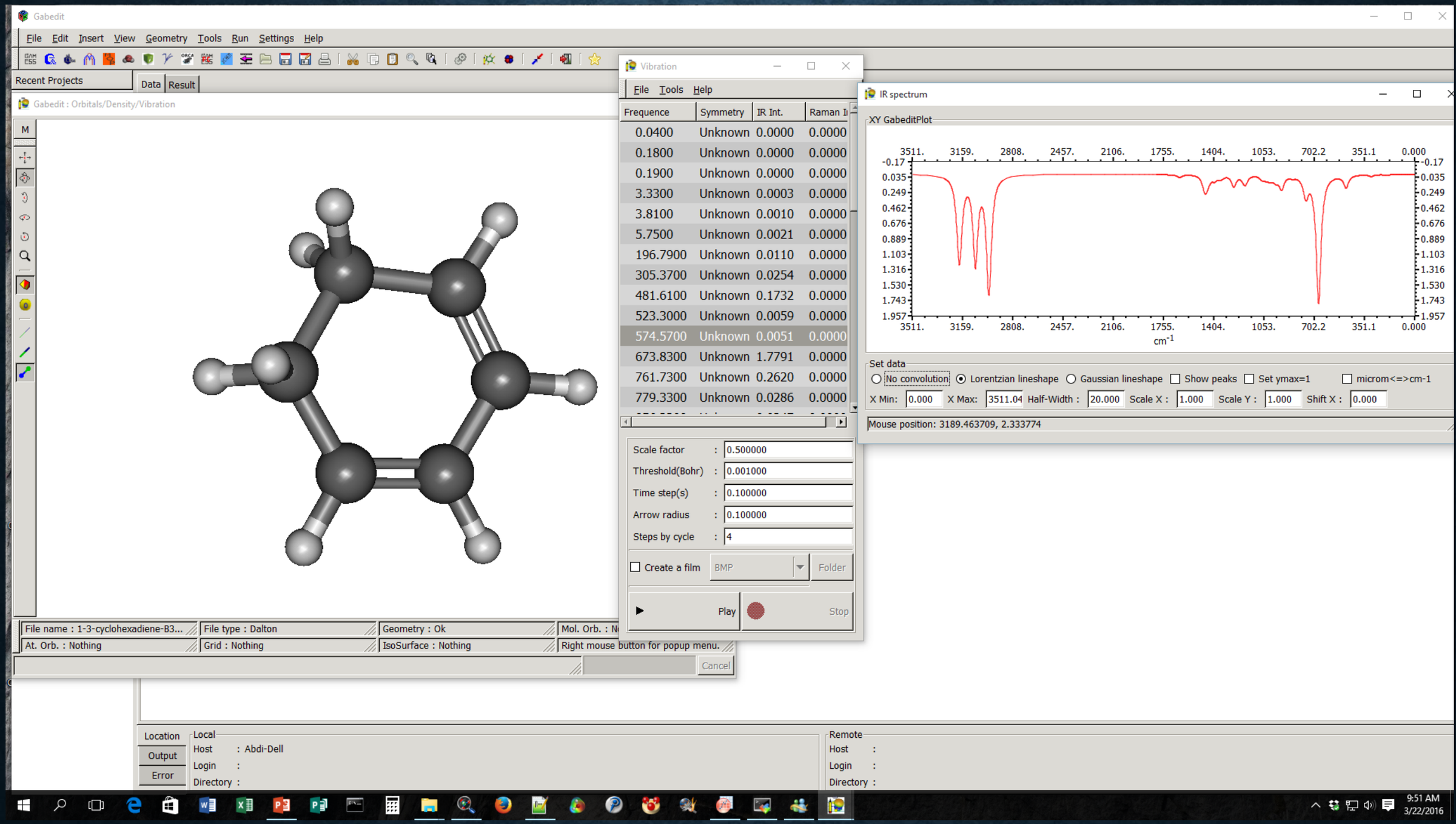


Electron location function (ELF)



Electron density iso-surfaces

ANIMATION OF VIBRATIONS IN GABEDIT



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JOB SUBMISSION AUTOMATION FOR FIREFLY ON HTC PLATFORM

Thank you Bill for helping us with this

```
ssadjadi@htclogin:~$ ls
7z.dll exe     firefly.bat     README  7z.exe    ff.7z     firefly.con   interlude.txt   7zip.dll  ff800.7z
gen_all.sh   job.bat        submit.condor
ff811.7z.zip     input
```

How to use

==========

- Put all your input files (*.inp) into the folder "input"
- Run chmod +x ./gen_all.sh
- Run ./gen_all.sh
- Run condor_submit submit.condor

CONCLUSIONS & REMARKS

- PCGAMESS over HTC and HPC2015 platfroms is reliable for Hartree-Fock, Post Hartree-Fock and Density Functional Theory calculations in combination with moderate and large size basis sets
- Moderate to large size molecules can be explored theoretically by present setup
- HTC is ready to cover the education and HPC 2015 for research purposes for broad range of users in different disciplines
- If a package of electron density analysis is installed on HTC and HPC2015 system, then the present computational chemistry services will reach to its ideal level.

We are grateful to our colleagues at ITS-High performance computing team:

Mr.Kwan, Miss Lillian Chan, Mr. Bill Yau and Dr. Mok Ngai Shing

Thank you for your attention