Computational Chemistry With HTC System

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Outlines

- Software
- Testing the Software
- Performance
- Abilities and Limitations

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Software

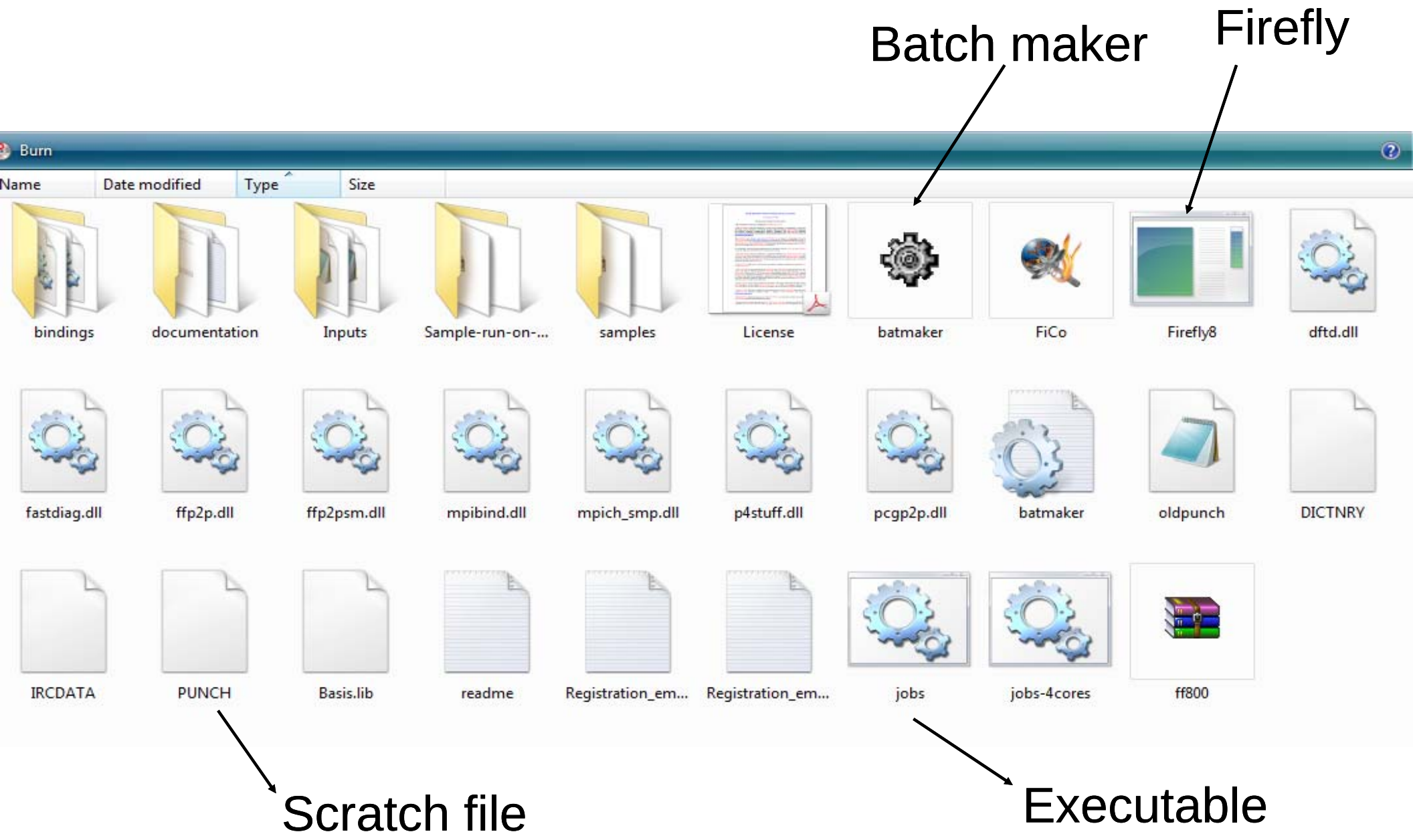
- PCGAMESS (Firefly)

- Last version is : 8.0.0
- Running on :

- Free of Charge and can be downloaded:

http://classic.chem.msu.su/gran/gamess/index.html

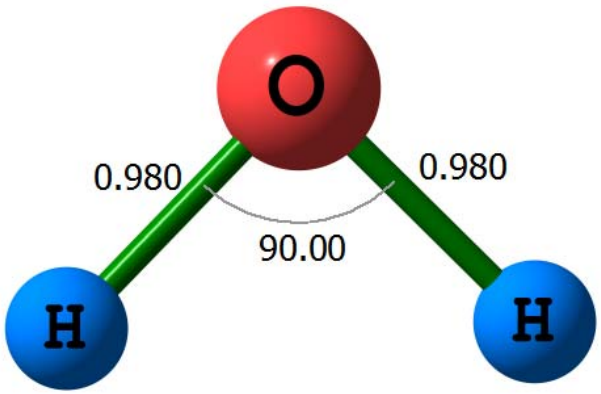
Software


Batch maker
Firefly
Burn
Name
Date modified
Type
Size
bindings
documentation
Inputs
Sample-run-on-...
samples
License
batmaker
FiCo
Firefly8
dftd.dll
fastdiag.dll
ffp2p.dll
ffp2psm.dll
mpibind.dll
mpich_smp.dll
p4stuff.dll
pcgp2p.dll
batmaker
oldpunch
DICTNRY
IRCDATA
PUNCH
Basis.lib
readme
Registration_em...
Registration_em...
jobs
jobs-4cores
ff800
Scratch file
Executable

Software

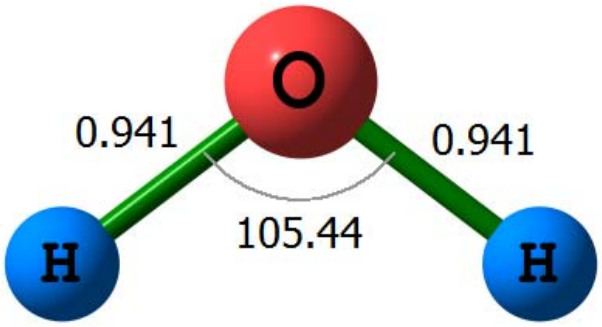
The input file can be generated by any txt editors

```
$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
```



Software

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



Software

- Interface programs that help for creating the input file and rendering the information stored in the pcgamess output file
- Chemcraft 
- Macmolplt 
- Ghemical-GMS 

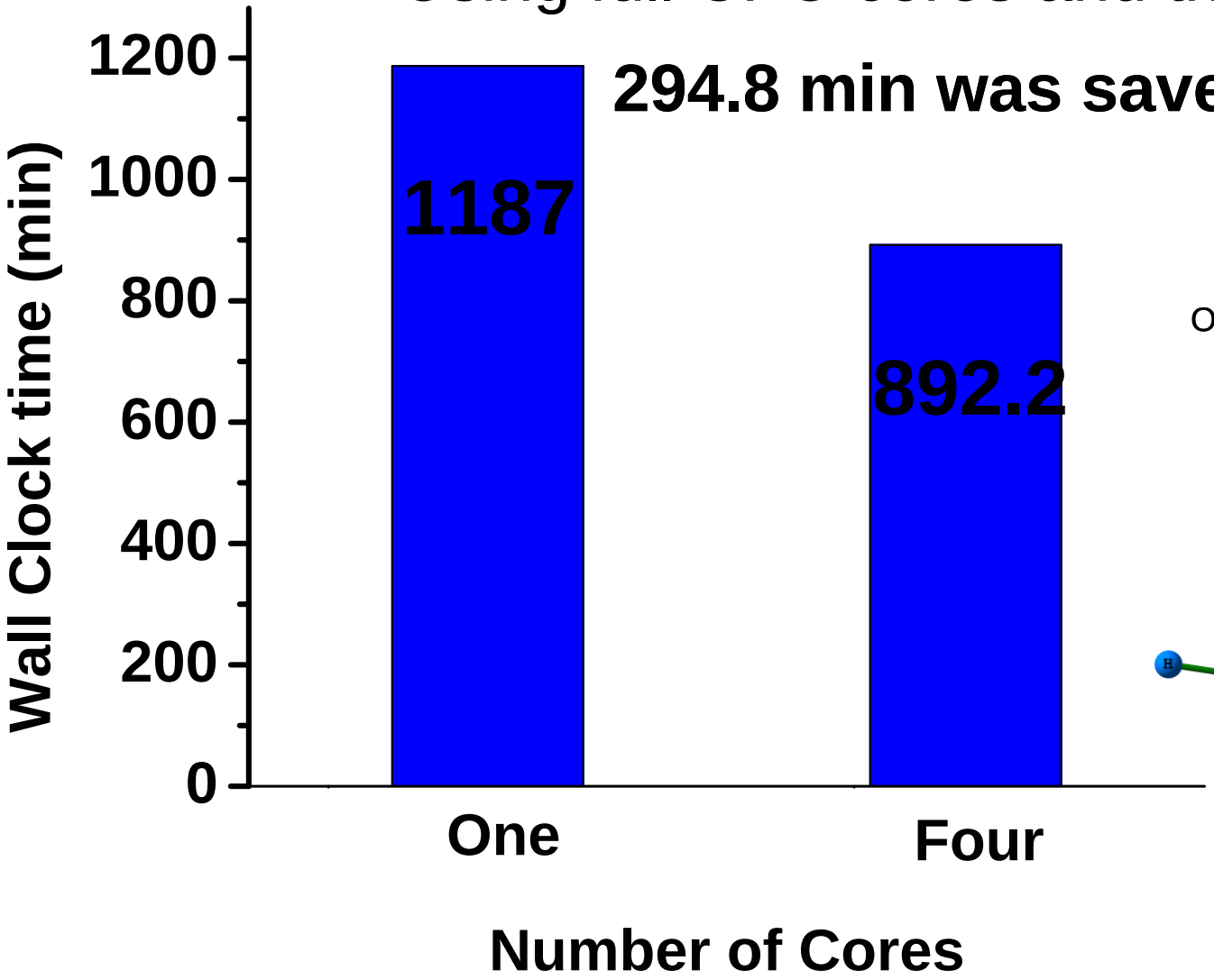
Testing the Software

Properties	Standard	HTC	Delta
Energy(hartree)	-368.0867960698	-368.0867960555	1.430004203939E-8
Energy	-290.0124281332	-290.0124281400	6.800007668062E-9
Energy	-580.1097061958	-580.1097061806	1.519993020338E-8
Energy	-407.1472108663	-407.1472108451	2.119998043781E-8
Energy	-115.7534036796	-115.7534036778	1.800003701646E-9
Energy	-231.8224047596	-231.8224047290	3.060000608457E-8
Energy	-6642.1898266163	-6642.1898264568	1.594999048393E-7
Gradient RMS	0.0013151940	0.0013151650	2.899999999991E-8
Gradient RMS	0.0196184750	0.0196184750	0.0000000000
S-Squared	2.013	2.013	0.0000000000
Dipole moment(Debye)	0.0250990000	0.0250990000	0.0000000000

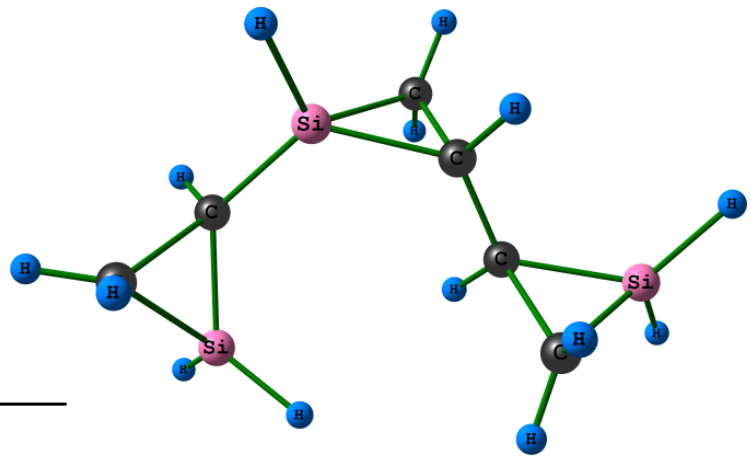
Errors in energy are well below 10^{-6} hartree

Performance

Using full CPU cores and threads

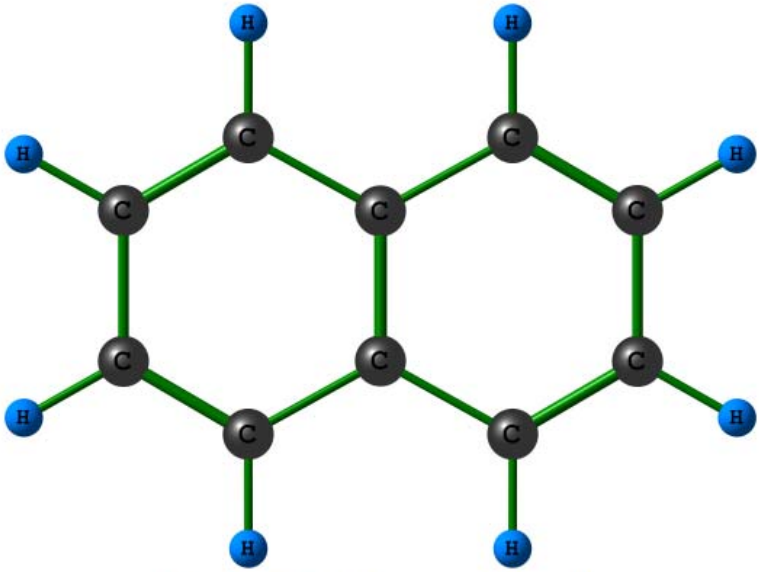


Si3C6H14
Optimization and Frequency calculations
RHF/6-311++G(d,p)

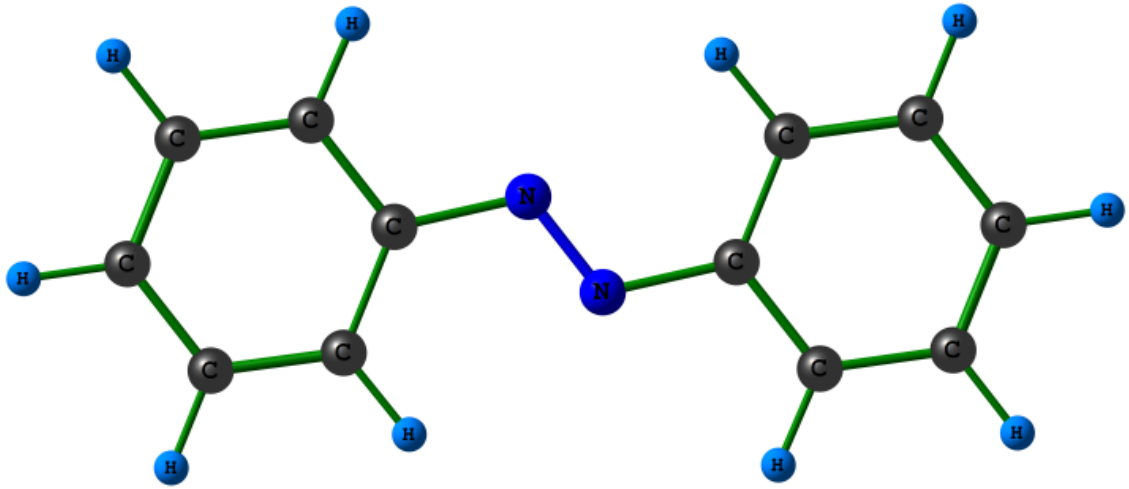


Abilities

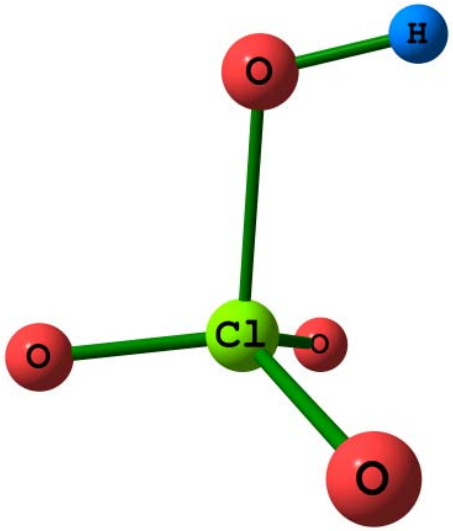
Geometry optimizations and Frequency calculations



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

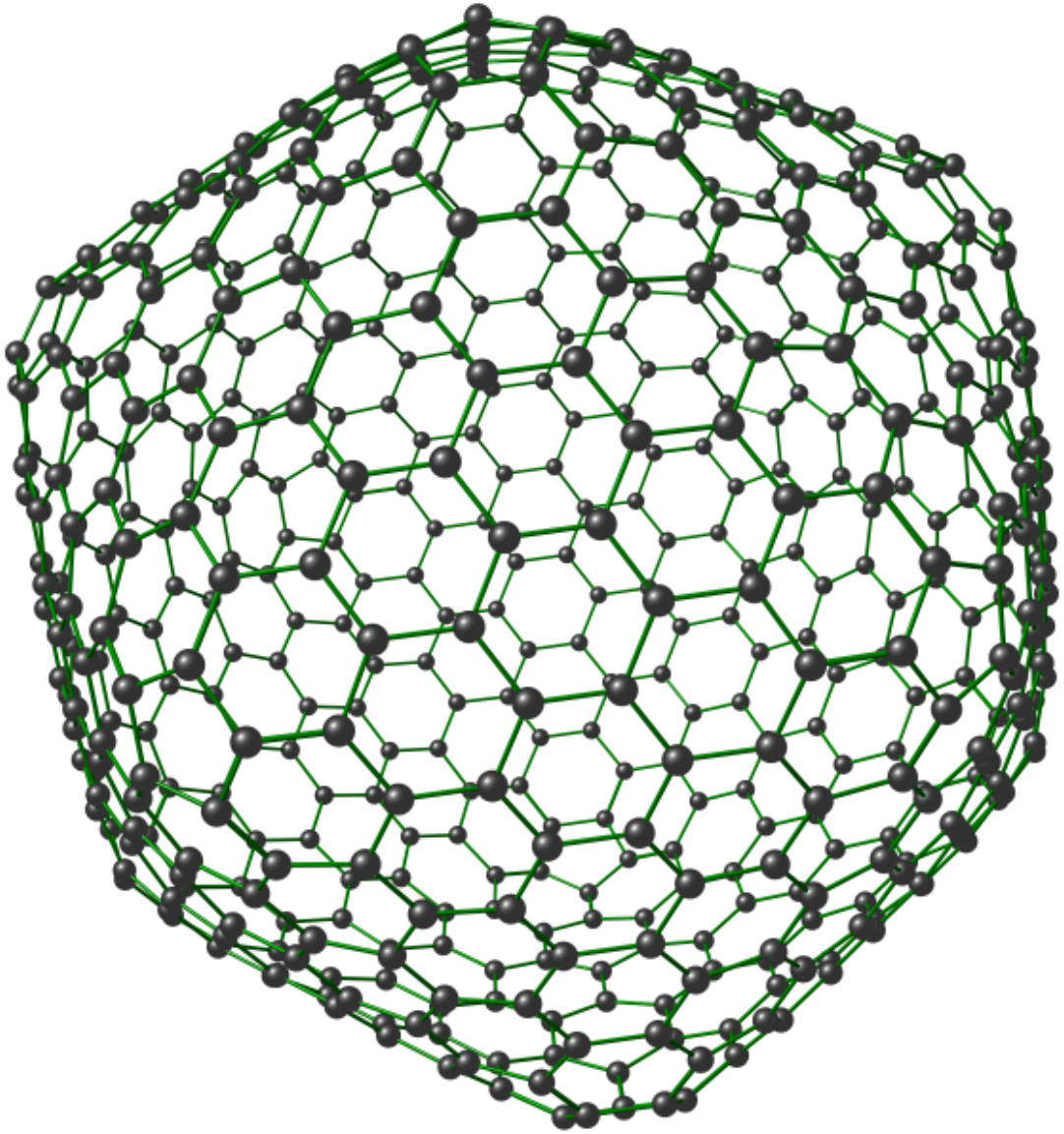


B3LYP/6-311++G(d,p)



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

Abilities



C540
A nano size molecule

Semi-empirical (AM1)
Geometry optimization and
Frequency calculations

Within 359.8 min

Limitations

1- Memory can not exceed 260MW on Windows 64 bit

$SYSTEM MWORDS=250 $END

2- Semi-empirical calculations can not be done with more than 1012 atoms

Conclusions & Remarks

1- PCGAMESS over HTC is reliable

2- Hartree-Fock, Post Hartree-Fock and Density Functional Theory methods can be applied in combination with moderate size basis sets

3- Moderate to large size molecules can be explored theoretically by present setup

4- HTC is ready to cover both the education and research ereas for broad range of users in different disciplines

5- If a package of electron density analysis is installed on HTC system, then the present computational chemistry service will reach to its ideal level.

I am grateful to my colleagues at ITS-High performance computing team:

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

That gave me this opportunity to collaborate with them in HTC project.

Thank you All for your attention