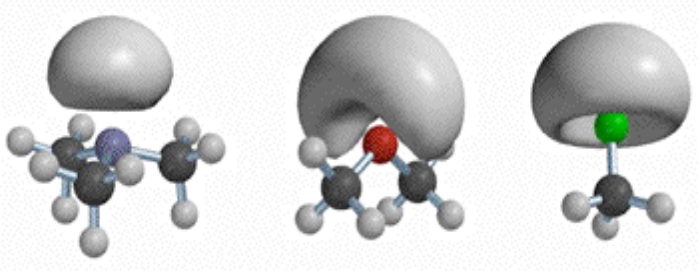
NCSSM Chemistry
The North Carolina School of Science and Mathematics

Troubleshooting Difficult Jobs



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General Comments

- Jobs done in "Intro" level classes always work
  - Instructor has tested multiple times
- Jobs at the research level will fail more often than not
- ENTIRE PAPERS are written on getting a job to run

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        ELECTROSTATIC MOMENTS
        --------------------

POINT   1          X           Y           Z (BOHR)    CHARGE
             0.000000    0.000000    0.000000        0.00 (A.U.)
       DX          DY          DZ        /D/  (DEBYE)
-3273.979737 -443.217695   90.957048 3305.095827
 ..... END OF PROPERTY EVALUATION .....
STEP CPU TIME =     0.59 TOTAL CPU TIME =      132.6 (    2.2 MIN)
TOTAL WALL CLOCK TIME=      133.8 SECONDS, CPU UTILIZATION IS  99.16%

ENERGY DID NOT CONVERGE...ABORTING HESSIAN

EXECUTION OF GAMESS TERMINATED -ABNORMALLY- AT Wed Jul 12 06:47:00 2006
695053 WORDS OF DYNAMIC MEMORY USED
STEP CPU TIME =     0.00 TOTAL CPU TIME =      132.6 (    2.2 MIN)
TOTAL WALL CLOCK TIME=      133.8 SECONDS, CPU UTILIZATION IS  99.16%
A fatal error occurr on DDI Process 0.
ddikick.x: application process 0 quit unexpectedly.
ddikick.x: Fatal error detected.
The error is most likely to be in the application, so check for
input errors, disk space, memory needs, application bugs, etc.
ddikick.x will now clean up all processes, and exit...
ddikick.x: Sending kill signal to DDI processes.
ddikick.x: Execution terminated due to error(s).
```

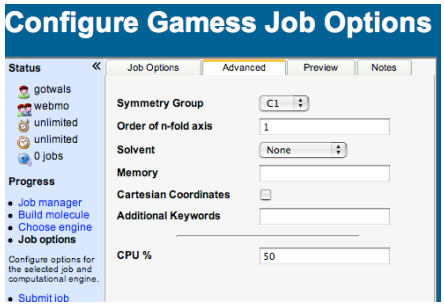
Types of Failures

Streptomycin	Molecular Energy - Gamess	7/12/2006 8:48	Complete	8:37
streptomycin	Geometry Optimization - Gamess	7/12/2006 7:18	Failed	2:13
Streptomycin	Vibrational Frequencies - Gamess	7/12/2006 6:44	Failed	2:12

- True "failed" failures
  - Examples
    - Geometry optimizations
    - Linear molecules
    - Amino groups
    - Convergence errors
- Successful jobs with bogus results
- Where to find errors?
  - In log file

Keywords

- All codes have rich list of keywords
  - WebMO
    - Use "Advanced" tab
    - Must have EXACTLY correct syntax
  - Links on Moodle

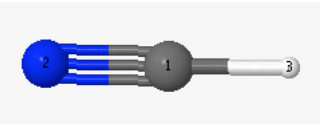


Geometry Optimizations

- All molecules should be optimized prior to performing meaningful calculations
  - Caveat: sometimes optimization IS the meaningful calculation!
- "Washing" your molecule
  - Comprehensive cleanup: performs a molecular mechanics/dynamics (MM/MD) optimization
  - Run a PM3/AM1 semi-empirical optimization
  - Run your final *ab initio* optimization

Linear Molecules

- Bond angles of 180 degrees
- Classic example: HCN
- Often fail, especially in GAMESS
- Options
  - Dummy atoms
  - Run with cartesian coordinate geometries
  - Under "Advanced" menu

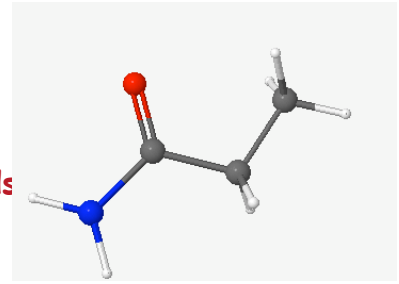



```
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE
     ICHARG=0 MULT=1 COORD=ZMTMPC $END
$BASIS GBASIS=N21 NGAUSS=3 $END
 $DATA
CHN
C1 1
C 0.0000000 0 0.0000000 0 0.0000000 0 0 0 0
N 1.1371365 1 0.0000000 0 0.0000000 0 1 0 0
H 1.0502355 1 180.00000 1 0.0000000 0 1 2 0
 $END
```

```
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE
     ICHARG=0 MULT=1 COORD=CART $END
$BASIS GBASIS=N21 NGAUSS=3 $END
 $DATA
CHN
C1 1
C 6 0.00000000 0.00000000 0.00000000
N 7 0.00000000 0.00000000 1.13713650
H 1 0.00000000 0.00000000 -1.05023553
 $END
```

Amino Groups

- H-N-C=O groups
- Will often fail, especially in MOPAC
- Use NOMM or MMOK keywords
  - "No" molecular mechanics corrections
  - "Molecular mechanics OK"

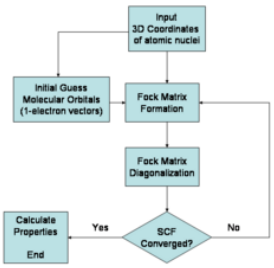


```
   MOLECULAR POINT GROUP    :   CS
H: (PM3): J. J. P. STEWART, J. COMP. CHEM.      10, 209 (1989).
C: (PM3): J. J. P. STEWART, J. COMP. CHEM.      10, 209 (1989).
N: (PM3): J. J. P. STEWART, J. COMP. CHEM.      10, 209 (1989).
O: (PM3): J. J. P. STEWART, J. COMP. CHEM.      10, 209 (1989).

         RHF CALCULATION, NO. OF DOUBLY OCCUPIED LEVELS = 15
THIS SYSTEM CONTAINS -HNCO- GROUPS.
YOU MUST SPECIFY "NOMM" OR "MMOK" REGARDING MOLECULAR MECHANICS CORRECTION
```


Convergence Errors

- SCF: self-consistent field theory
- Calculations run until one of two things happens:
  - Calculation converges
  - Job runs out of cycles (set at 250)
- Changing # of cycles
  - Gaussian: opt=(maxcycles=n)
  - GAMESS: maxit=
  - MOPAC: ITRY=




```
>>>>>>>>>> Convergence criterion not met.
 SCF Done:  E(RHF) =  -112.176862421     A.U. after  129 cycles
            Convg  =    0.5429D-05             -V/T =  2.0034
            S**2   =   0.0000
 Convergence failure -- run terminated.
 Error termination via Lnk1e in /usr/local/g03/l502.exe at Fri Jul  7 11:47:27 2006.
 Job cpu time:  0 days  0 hours  0 minutes  9.4 seconds.
 File lengths (MBytes):  RWF=     11 Int=      0 D2E=      0 Chk=      1 Scr=      1
```

http://en.wikipedia.org/wiki/Hartree-Fock

Gaussian Checkpoint files

- Use of "checkpoint" files
  - Consider ALWAYS saving a checkpoint file
  - On restart: use checkpoint file (by job number)
  - Various keyword options available