Molecular Dynamics

Molecular Dynamics Simulation

For electrons we have to solve the quantum Schroedinger Equation
For nuclei we only consider that they move classically

$$\vec{F} = m\vec{a} = m\frac{d^2\vec{x}}{dt^2} = m\ddot{\vec{x}} = -\frac{dV}{d\vec{x}}$$

Force on nuclei can be obtained from potential derivative

$$\vec{x}(t+\Delta t) \approx \vec{x}(t) + \dot{\vec{x}}(t)\Delta t$$

$$\dot{\vec{x}}(t+\Delta t) \approx \dot{\vec{x}}(t) + \ddot{\vec{x}}(t)\Delta t$$

$$\ddot{\vec{x}}(t) = -\frac{1}{m}\frac{dV}{d\vec{x}}\bigg|_{\vec{x}(t)}$$

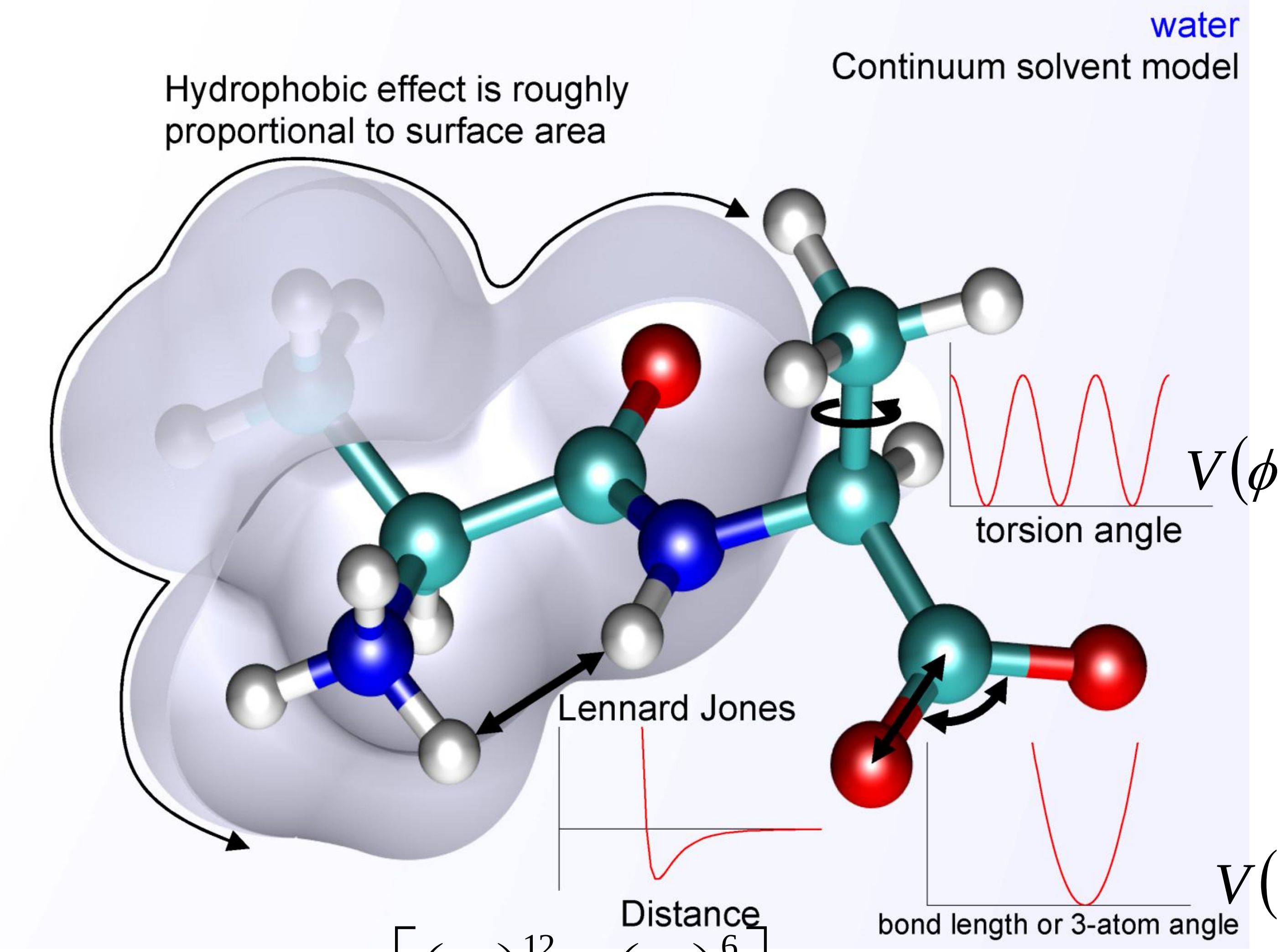
Initial Condition: You give starting geometry and velocity then you calculate the force from your potential energy surface. Using the force you calculate the velocity and position change, then continue on.

For example for harmonic oscillator

$$V(x) = \frac{1}{2}k\left(x - x_{eq}\right)^2$$

$$-\frac{dV}{dx} = -k\left(x - x_{eq}\right)$$

Types of Force Fields used in Molecular Mechanics



$$V(\phi) = V_0 \cos(a\phi)$$

$$V(x) = \frac{1}{2} k \left(x - x_{eq}\right)^2$$

$$V(x) = 4\varepsilon\left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6}\right]$$

Wikipedia “Molecular Mechanics”

On the fly simulation

At every time step solve the electronic Schrodinger equation

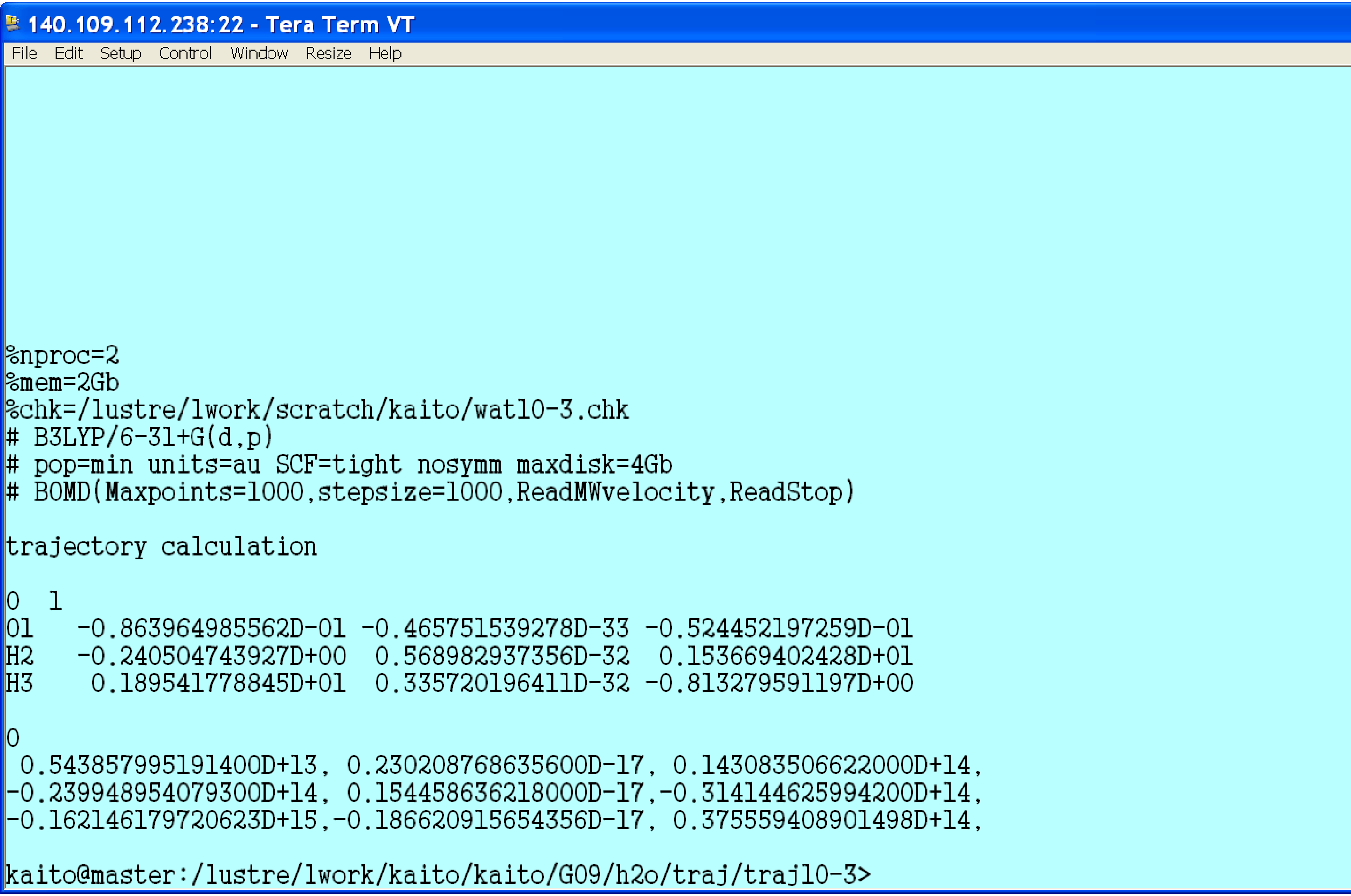
Good Points

1. Accurate
2. Can describe reaction
3. Do not have to worry about fitting problems

Bad Points

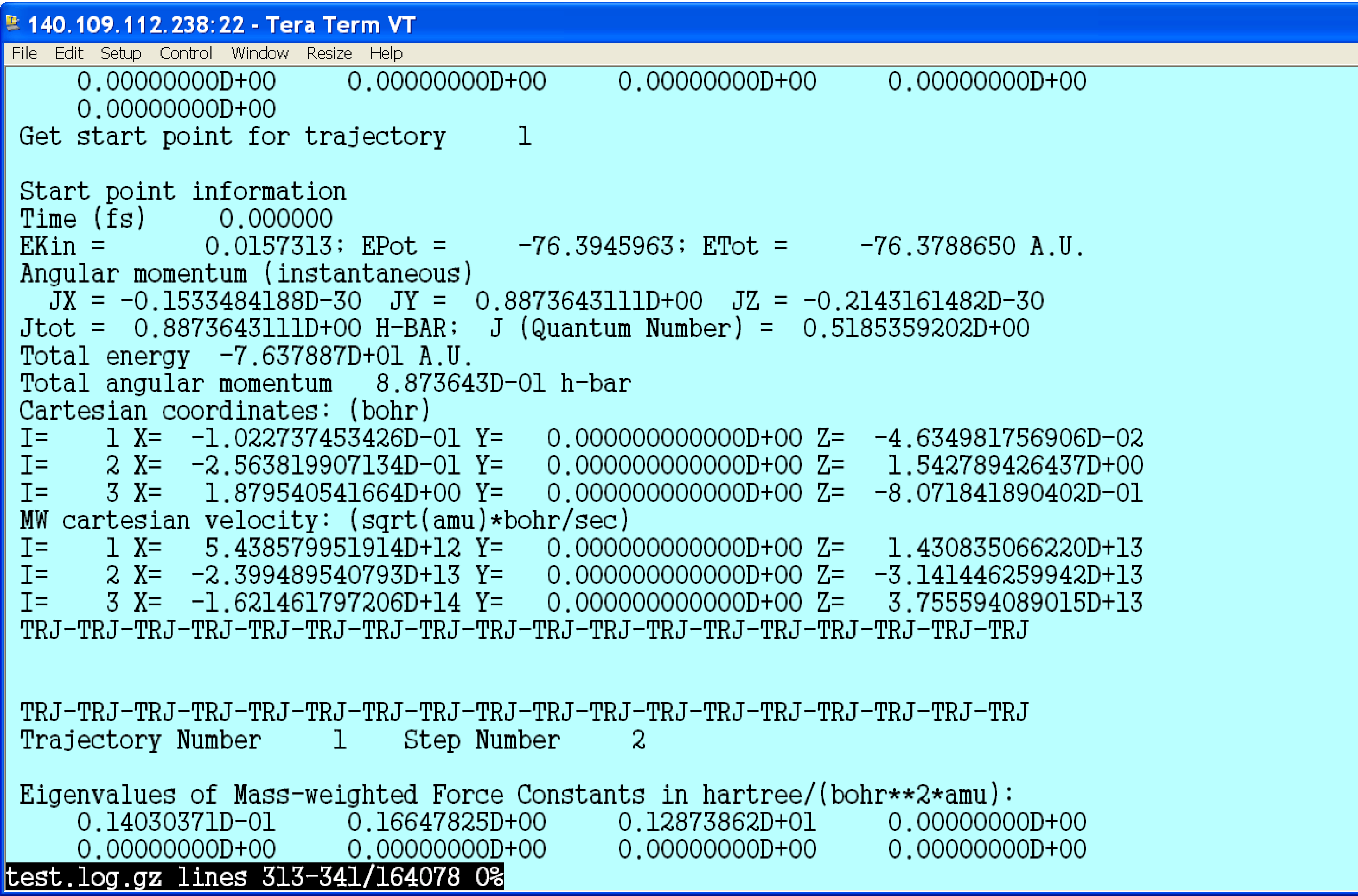
1. Computational time is great so can only be used for short time propagation
2. Can not perform detailed analysis

Gaussian 09 BOMD input



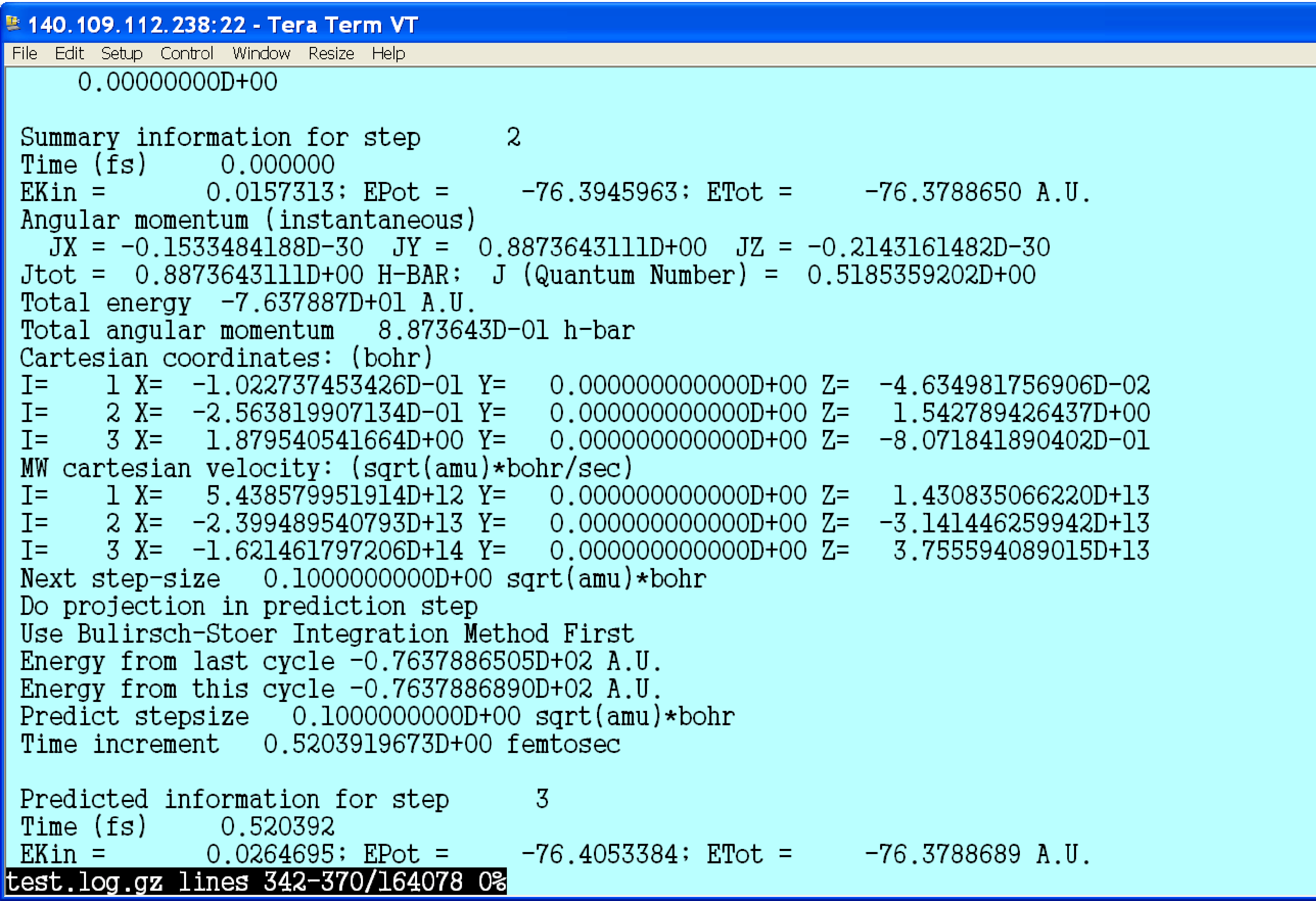
```
%nproc=2
%mem=2Gb
%chk=/lustre/lwork/scratch/kaito/wat10-3.chk
# B3LYP/6-31+G(d,p)
# pop=min units=au SCF=tight nosymm maxdisk=4Gb
# BOMD(Maxpoints=1000,stepsize=1000,ReadMWvelocity,ReadStop)

trajectory calculation

0  1
O1   -0.863964985562D-01 -0.465751539278D-33 -0.524452197259D-01
H2   -0.240504743927D+00  0.568982937356D-32  0.153669402428D+01
H3    0.189541778845D+01  0.335720196411D-32 -0.813279591197D+00

0
 0.543857995191400D+13, 0.230208768635600D-17, 0.143083506622000D+14,
-0.239948954079300D+14, 0.154458636218000D-17,-0.314144625994200D+14,
-0.162146179720623D+15,-0.186620915654356D-17, 0.375559408901498D+14,

kaito@master:/lustre/lwork/kaito/kaito/G09/h2o/traj/traj10-3>
```

G09 BOMD output 1



```
     0.00000000D+00     0.00000000D+00     0.00000000D+00     0.00000000D+00
     0.00000000D+00
 Get start point for trajectory     1

 Start point information
 Time (fs)    0.000000
 EKin =       0.0157313; EPot =     -76.3945963; ETot =    -76.3788650 A.U.
 Angular momentum (instantaneous)
   JX = -0.1533484188D-30  JY =  0.8873643111D+00  JZ = -0.2143161482D-30
 Jtot =  0.8873643111D+00 H-BAR:  J (Quantum Number) =  0.5185359202D+00
 Total energy  -7.637887D+01 A.U.
 Total angular momentum   8.873643D-01 h-bar
 Cartesian coordinates: (bohr)
 I=     1 X=  -1.022737453426D-01 Y=   0.000000000000D+00 Z=  -4.634981756906D-02
 I=     2 X=  -2.563819907134D-01 Y=   0.000000000000D+00 Z=   1.542789426437D+00
 I=     3 X=   1.879540541664D+00 Y=   0.000000000000D+00 Z=  -8.071841890402D-01
 MW cartesian velocity: (sqrt(amu)*bohr/sec)
 I=     1 X=   5.438579951914D+12 Y=   0.000000000000D+00 Z=   1.430835066220D+13
 I=     2 X=  -2.399489540793D+13 Y=   0.000000000000D+00 Z=  -3.141446259942D+13
 I=     3 X=  -1.621461797206D+14 Y=   0.000000000000D+00 Z=   3.755594089015D+13
 TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ


 TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ
 Trajectory Number      1     Step Number      2

 Eigenvalues of Mass-weighted Force Constants in hartree/(bohr**2*amu):
     0.14030371D-01     0.16647825D+00     0.12873862D+01     0.00000000D+00
     0.00000000D+00     0.00000000D+00     0.00000000D+00     0.00000000D+00
test.log.gz lines 313-341/164078 0%
```

G09 BOMD output 2



```
     0.00000000D+00


 Summary information for step      2
 Time (fs)     0.000000
 EKin =        0.0157313; EPot =      -76.3945963; ETot =      -76.3788650 A.U.
 Angular momentum (instantaneous)
   JX = -0.1533484188D-30  JY =  0.8873643111D+00  JZ = -0.2143161482D-30
 Jtot =  0.8873643111D+00 H-BAR;  J (Quantum Number) =  0.5185359202D+00
 Total energy  -7.637887D+01 A.U.
 Total angular momentum   8.873643D-01 h-bar
 Cartesian coordinates: (bohr)
 I=     1 X=  -1.022737453426D-01 Y=   0.000000000000D+00 Z=  -4.634981756906D-02
 I=     2 X=  -2.563819907134D-01 Y=   0.000000000000D+00 Z=   1.542789426437D+00
 I=     3 X=   1.879540541664D+00 Y=   0.000000000000D+00 Z=  -8.071841890402D-01
 MW cartesian velocity: (sqrt(amu)*bohr/sec)
 I=     1 X=   5.438579951914D+12 Y=   0.000000000000D+00 Z=   1.430835066220D+13
 I=     2 X=  -2.399489540793D+13 Y=   0.000000000000D+00 Z=  -3.141446259942D+13
 I=     3 X=  -1.621461797206D+14 Y=   0.000000000000D+00 Z=   3.755594089015D+13
 Next step-size   0.1000000000D+00 sqrt(amu)*bohr
 Do projection in prediction step
 Use Bulirsch-Stoer Integration Method First
 Energy from last cycle -0.7637886505D+02 A.U.
 Energy from this cycle -0.7637886890D+02 A.U.
 Predict stepsize   0.1000000000D+00 sqrt(amu)*bohr
 Time increment   0.5203919673D+00 femtosec

 Predicted information for step      3
 Time (fs)     0.520392
 EKin =        0.0264695; EPot =      -76.4053384; ETot =      -76.3788689 A.U.
test.log.gz lines 342-370/164078 0%
```

Method of Propagation1

Goal:

$$\frac{dx}{dt} = f(x,t); \qquad x(t_0) = x_0 \rightarrow x(t_{final}) \ \text{ in time step } \ \Delta t$$

- Euler method (first order method take gradient)

$$x_{n+1} = x_n + f(x_n, t_n)\Delta t$$

- 4th order Runge-Kutta propagation : add up contribution along the way

$$x_{n+1} = x_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\Delta t$$

$$k_1 = f(x_{n,} t_n); \qquad k_2 = f(x_n + 0.5k_1\Delta t, t_n + 0.5\Delta t)$$

$$k_3 = f(x_n + 0.5k_2\Delta t, t_n + 0.5\Delta t); \ k_4 = f(x_n + k_3\Delta t, t_n + \Delta t)$$

Method of Propagation 2

- Predictor Corrector : repeated Euler

$$x_{n+1}^{1} = x_n + f\left(x_n, t_n\right)\Delta t$$

$$x_{n+1}^{2} = x_n + \frac{1}{2}\left(f\left(x_n, t_n\right) + f\left(x_{n+1}^{1}, t_{n+1}\right)\right)\Delta t$$

$$x_{n+1}^{3} = x_n + \frac{1}{2}\left(f\left(x_n, t_n\right) + f\left(x_{n+1}^{2}, t_{n+1}\right)\right)\Delta t$$

$$\ldots$$

$$x_{n+1}^{m} = x_n + \frac{1}{2}\left(f\left(x_n, t_n\right) + f\left(x_{n+1}^{m-1}, t_{n+1}\right)\right)\Delta t$$

$$\text{stop if } \left|x_{n+1}^{m} - x_{n+1}^{m-1}\right| < \text{threshold}$$

Method of Propagation 3

- Symplectic Integrator: special integrator for classical mechanics made to satisfy Hamilton's Equation $$\frac{dp}{dt} = -\frac{\partial H}{\partial q}; \qquad \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

Second order Symplectic assume H=T(p)+V(q)

$$p_{n+0.5} = p_n + 0.5\dot{p}_n \Delta t = p_n + 0.5\left(-\frac{\partial V(q_n)}{\partial q}\right)\Delta t$$

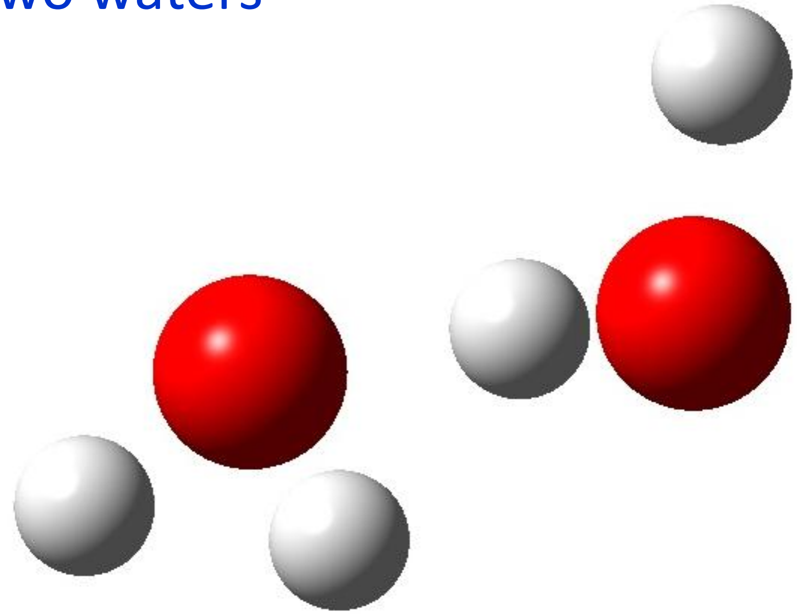
$$q_{n+1} = q_n + \frac{\partial T(p_{n+0.5})}{\partial p}\Delta t$$

$$p_{n+1} = p_{n+0.5} + 0.5\left(-\frac{\partial V(q_{n+1})}{\partial q}\right)\Delta t$$

Intermolecular Interaction: Super Molecule Approximation

Super Molecule Approximation

To obtain the interaction between two waters perform calculation of two waters

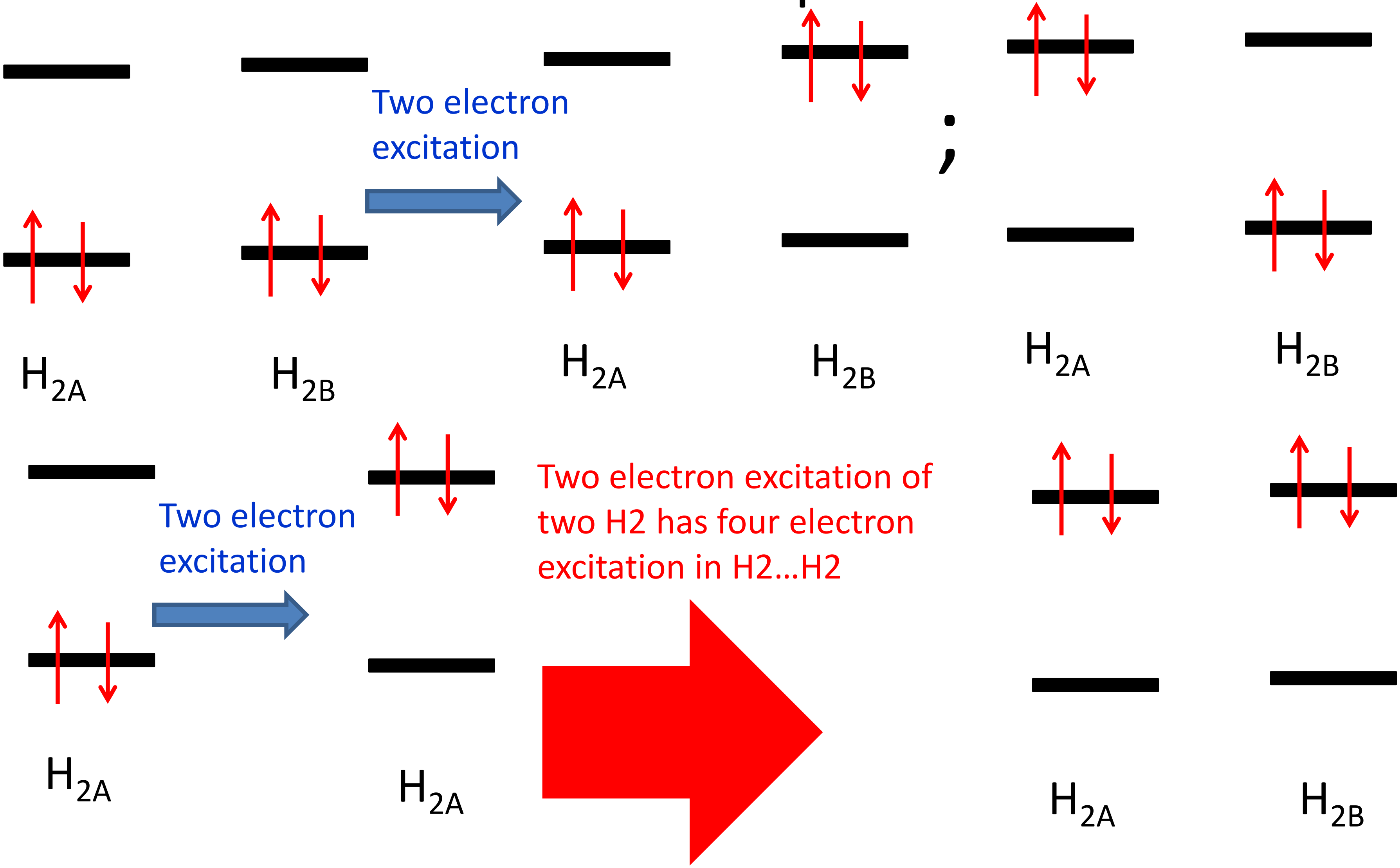


Two things to be careful

- Size Consistency
- Basis set super position erro

Size Consistancy

- Consider H2…H2 with CISD infinite far away result for H2…H2 is not equal to 2 H2!!



Two electron excitation of two H2 has four electron excitation in H2…H2

Size Consistent Methods

- MP2
- CCSD

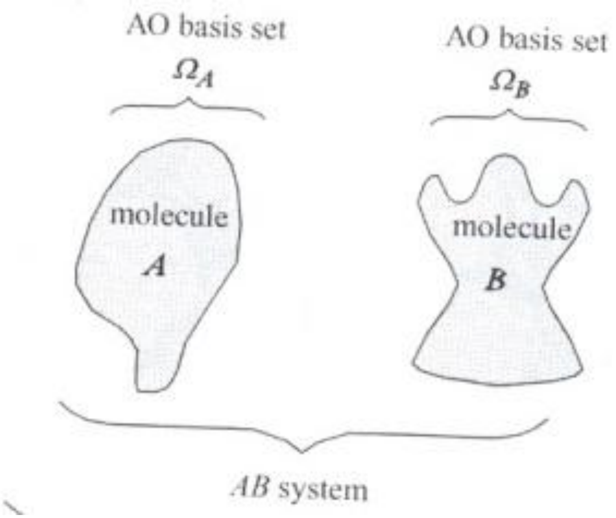
$$CCSD = \exp^{T_1+T_2} D_0$$

$$= T_1 D_0 + T_2 D_0 + \frac{1}{2}\left[T_1 T_1 D_0 + T_2 T_2 D_0 + T_1 T_2 D_0\right]$$

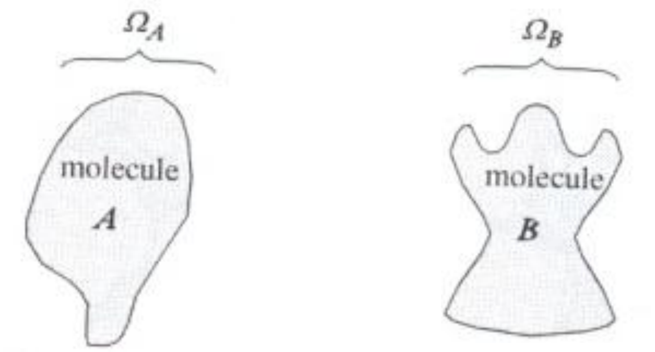
Pople et al. have defined an empirical estimation of the four electron excitation contribution MRSDCI had defined +Q so for bond dissociation and potential energy surface calculation people use MRSDCI+Q to approximately take care of the size consistancy problem

Basis Set Super Position Error

- When calculating the energy of a supermolecule we use the basis set of Molecule A and Molecule B together, when we calculate the separated products we calculate molecule A with basis of A, molecule B with basis of B

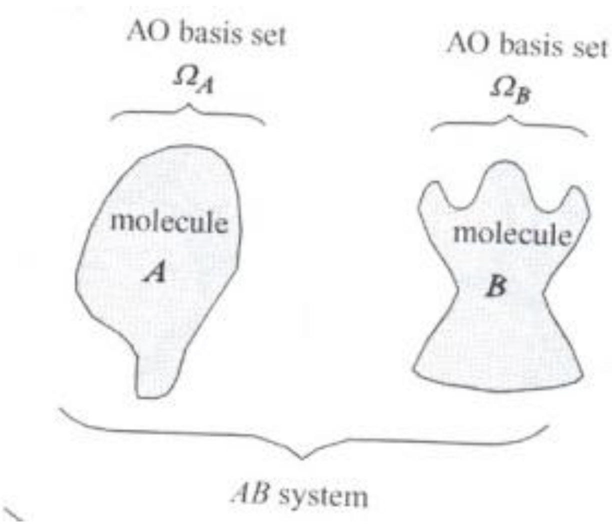


VS

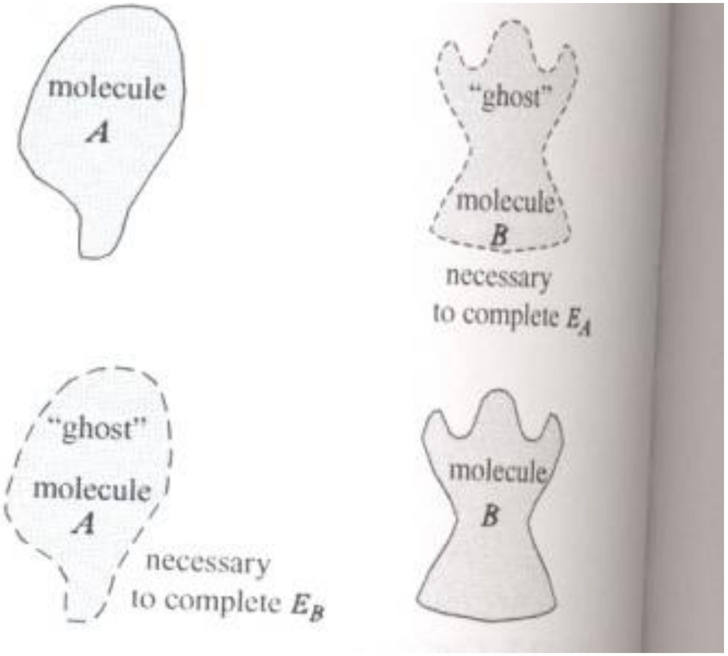


Counter Poise Correction

- Boys Lanbardi method: use ghost atoms (no charge just position to put basis)and put the basis for the respective partner in the energy calculation for molecule A and B

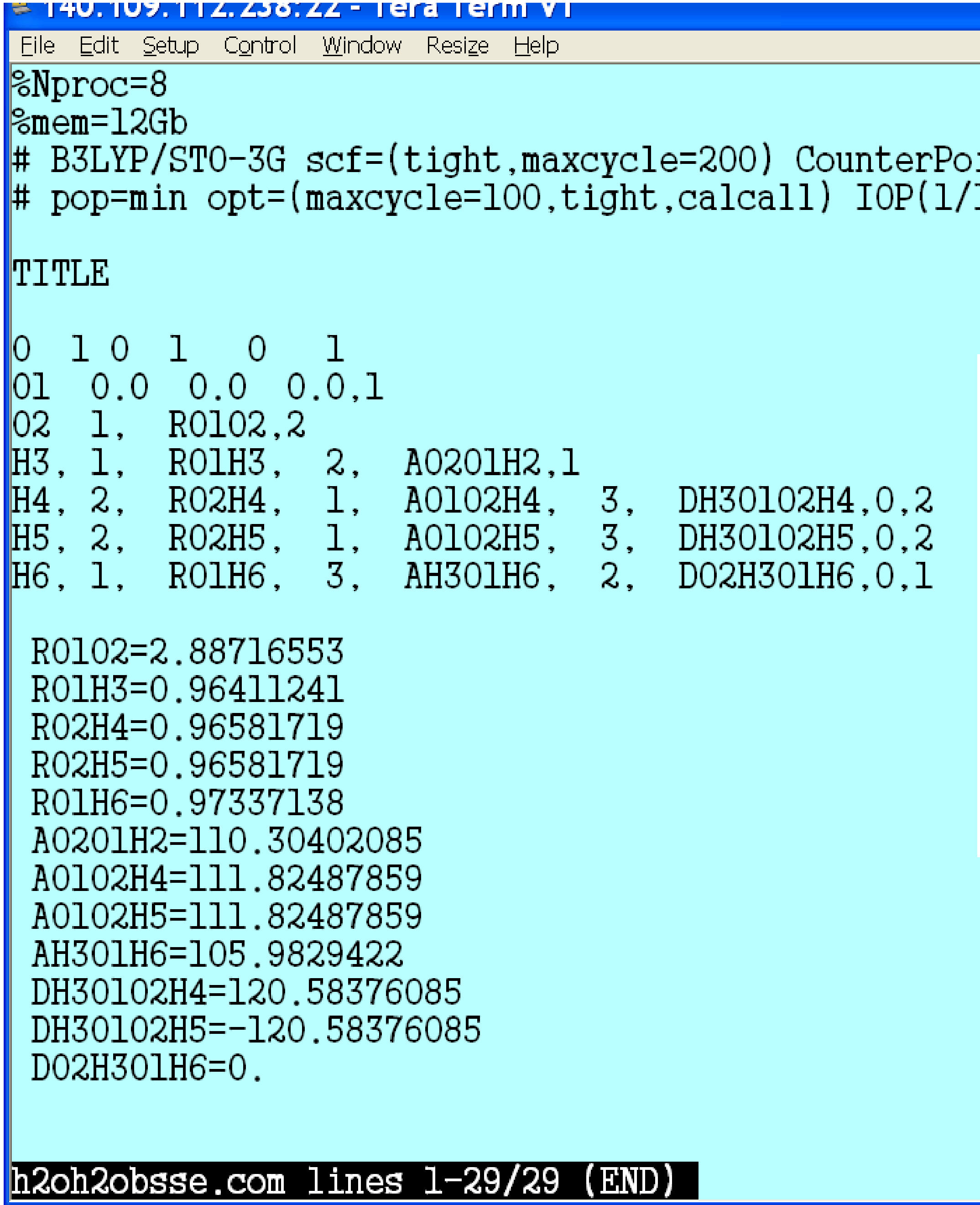


VS

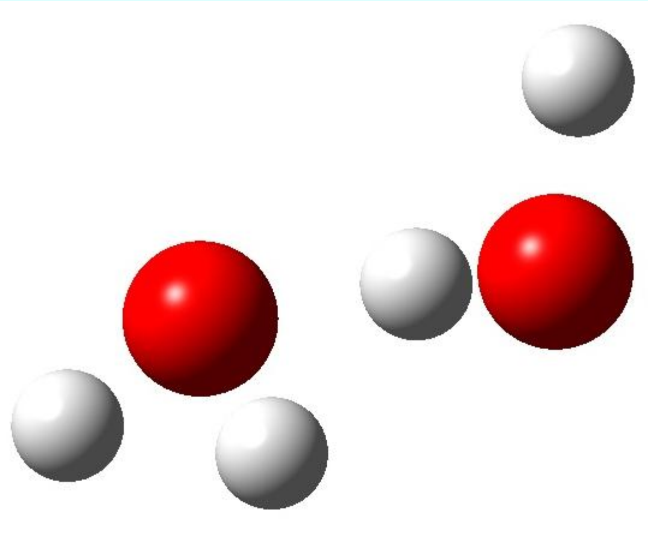


BSSE big for small basis sets

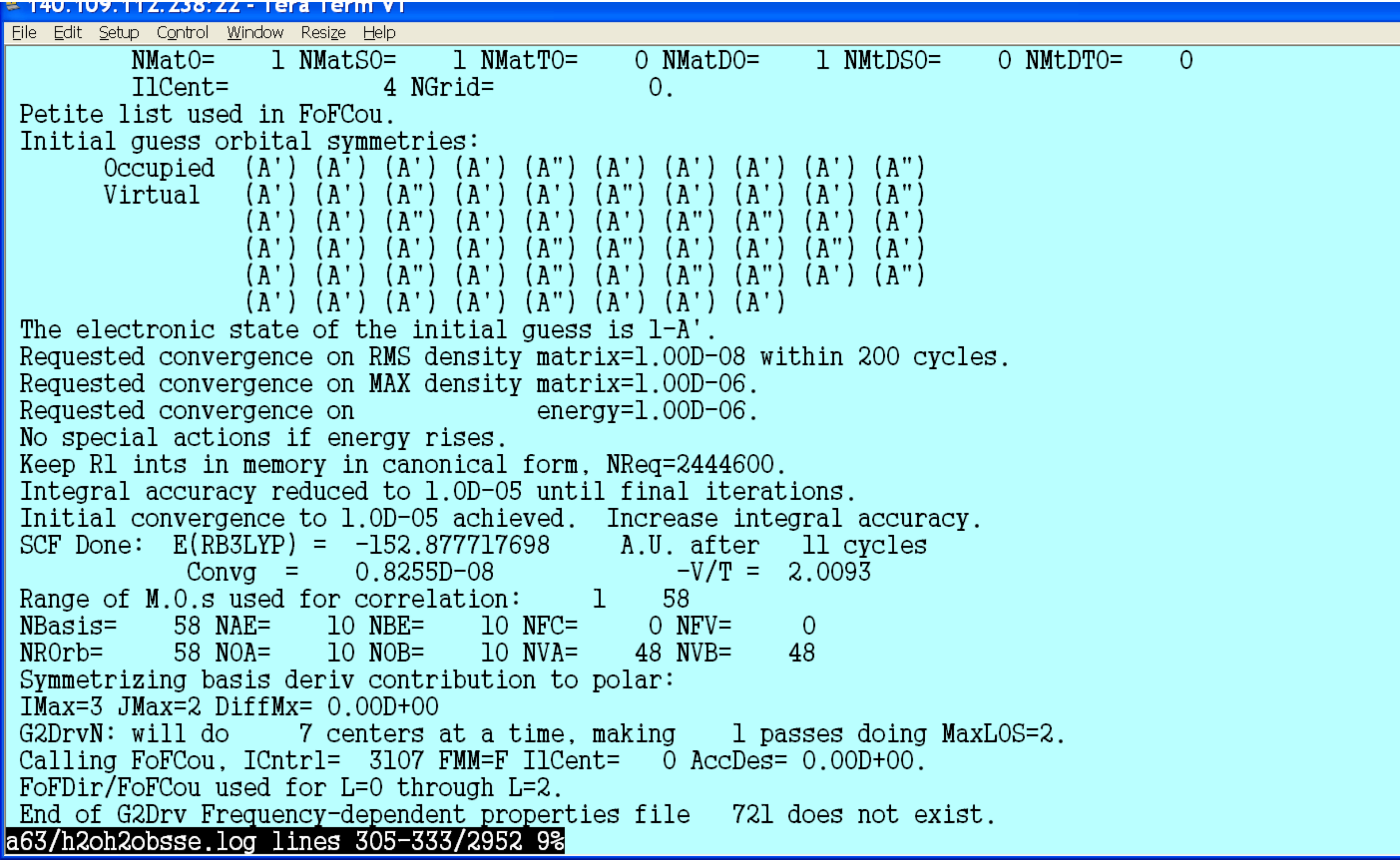
Gaussian CP Input



```
%Nproc=8
%mem=12Gb
# B3LYP/STO-3G scf=(tight,maxcycle=200) CounterPoise=2
# pop=min opt=(maxcycle=100,tight,calcall) IOP(1/11=1,99/14=1)

TITLE

0  1 0  1   0   1
O1  0.0  0.0  0.0,1
O2  1,   RO1O2,2
H3, 1,   RO1H3,  2,  AO2O1H2,1
H4, 2,   RO2H4,  1,  AO1O2H4,  3,  DH3O1O2H4,0,2
H5, 2,   RO2H5,  1,  AO1O2H5,  3,  DH3O1O2H5,0,2
H6, 1,   RO1H6,  3,  AH3O1H6,  2,  DO2H3O1H6,0,1

 RO1O2=2.88716553
 RO1H3=0.96411241
 RO2H4=0.96581719
 RO2H5=0.96581719
 RO1H6=0.97337138
 AO2O1H2=110.30402085
 AO1O2H4=111.82487859
 AO1O2H5=111.82487859
 AH3O1H6=105.9829422
 DH3O1O2H4=120.58376085
 DH3O1O2H5=-120.58376085
 DO2H3O1H6=0.

h2oh2obsse.com lines 1-29/29 (END)
```

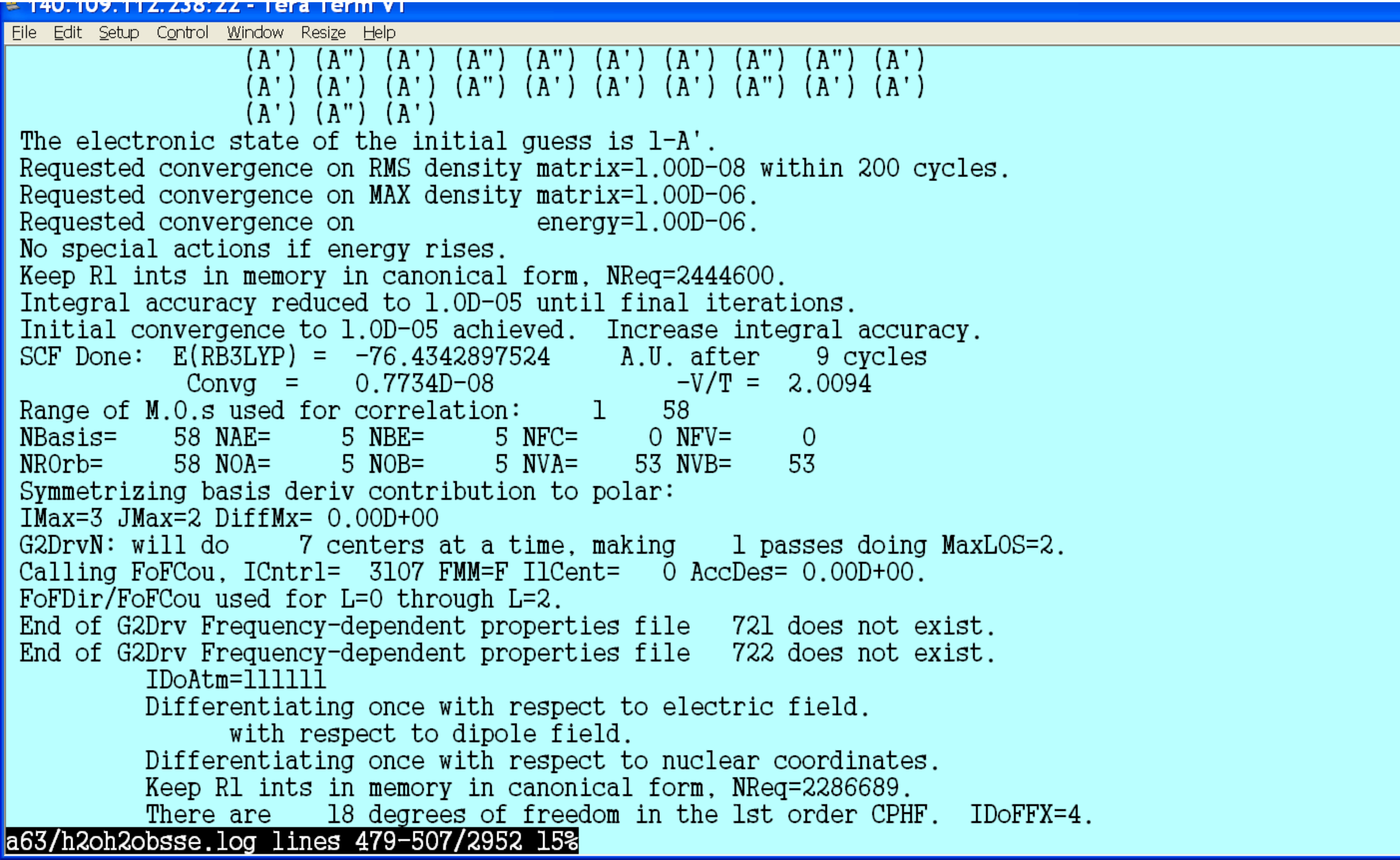


G09 CP output 1



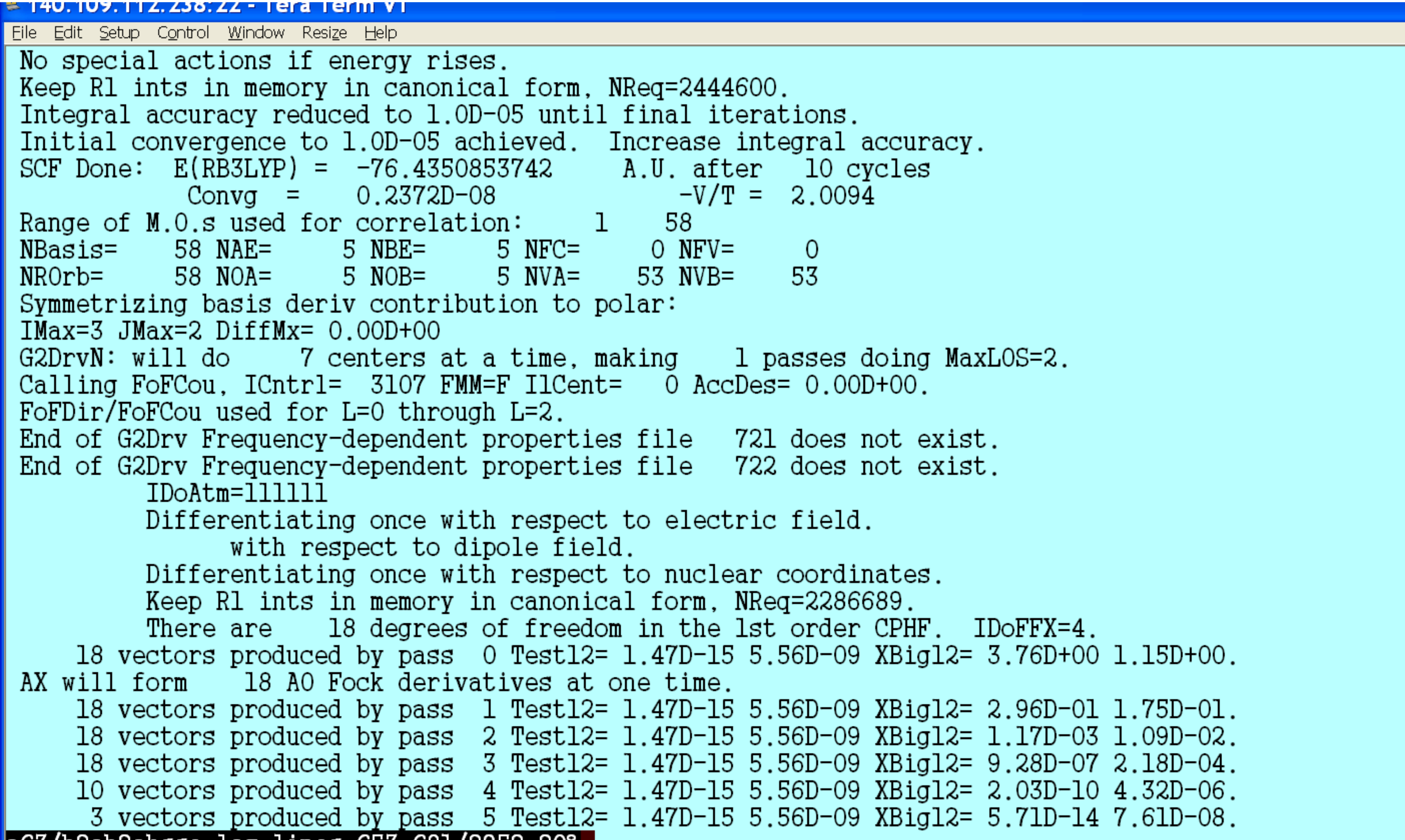
```
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=          4 NGrid=          0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A') (A') (A') (A') (A") (A') (A') (A') (A') (A")
       Virtual   (A') (A') (A") (A') (A') (A") (A') (A') (A') (A")
                 (A') (A') (A") (A') (A') (A') (A") (A") (A') (A')
                 (A') (A') (A') (A') (A") (A") (A') (A') (A") (A')
                 (A') (A') (A") (A') (A") (A') (A") (A") (A') (A")
                 (A') (A') (A') (A') (A") (A') (A') (A')
 The electronic state of the initial guess is 1-A'.
 Requested convergence on RMS density matrix=1.00D-08 within 200 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=2444600.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB3LYP) =  -152.877717698     A.U. after   11 cycles
             Convg  =    0.8255D-08             -V/T =  2.0093
 Range of M.O.s used for correlation:     1    58
 NBasis=    58 NAE=    10 NBE=    10 NFC=     0 NFV=     0
 NROrb=     58 NOA=    10 NOB=    10 NVA=    48 NVB=    48
 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do     7 centers at a time, making    1 passes doing MaxLOS=2.
 Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
 FoFDir/FoFCou used for L=0 through L=2.
 End of G2Drv Frequency-dependent properties file   721 does not exist.
a63/h2oh2obsse.log lines 305-333/2952 9%
```

G09 CP output2



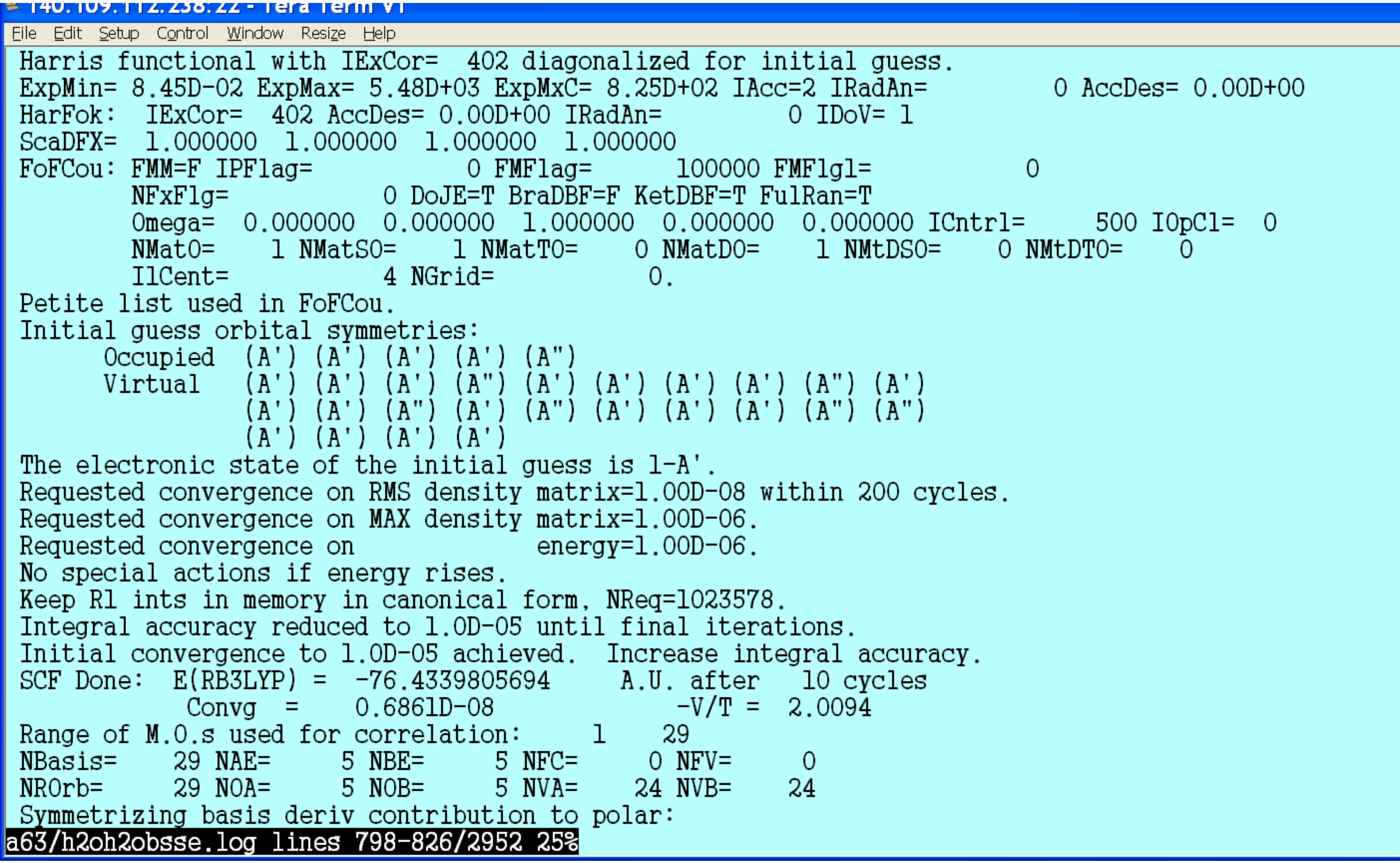
```
                 (A') (A") (A') (A") (A") (A') (A') (A") (A") (A')
                 (A') (A') (A') (A") (A') (A') (A') (A") (A') (A')
                 (A') (A") (A')
 The electronic state of the initial guess is 1-A'.
 Requested convergence on RMS density matrix=1.00D-08 within 200 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=2444600.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB3LYP) =  -76.4342897524     A.U. after    9 cycles
             Convg  =    0.7734D-08             -V/T =  2.0094
 Range of M.O.s used for correlation:     1    58
 NBasis=    58 NAE=     5 NBE=     5 NFC=     0 NFV=     0
 NROrb=     58 NOA=     5 NOB=     5 NVA=    53 NVB=    53
 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do     7 centers at a time, making    1 passes doing MaxLOS=2.
 Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
 FoFDir/FoFCou used for L=0 through L=2.
 End of G2Drv Frequency-dependent properties file   721 does not exist.
 End of G2Drv Frequency-dependent properties file   722 does not exist.
          IDoAtm=111111
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
          Keep R1 ints in memory in canonical form, NReq=2286689.
          There are    18 degrees of freedom in the 1st order CPHF.  IDoFFX=4.
a63/h2oh2obsse.log lines 479-507/2952 15%
```

G09 CP output3



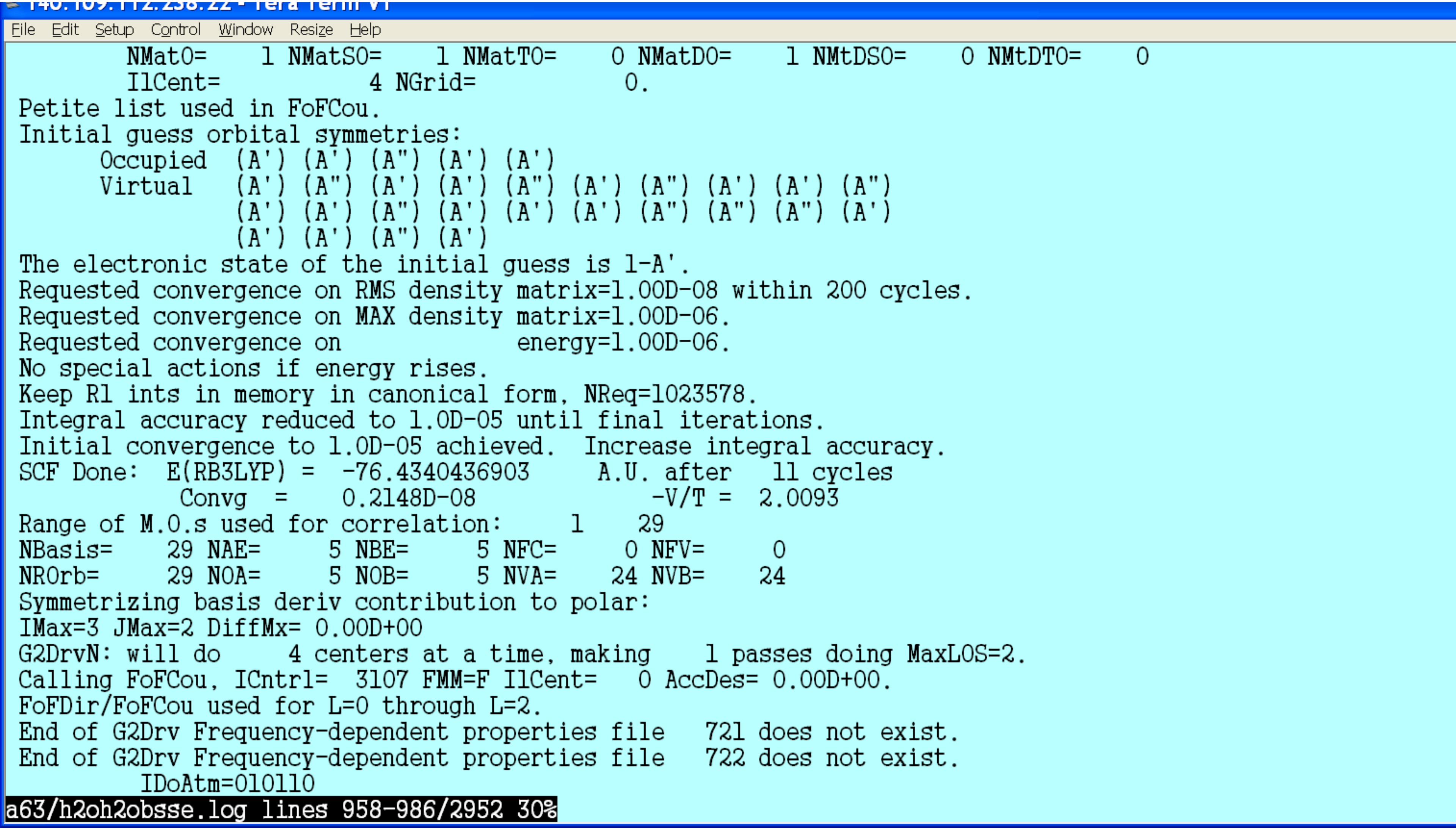
```
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=2444600.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RB3LYP) =  -76.4350853742     A.U. after   10 cycles
           Convg  =    0.2372D-08             -V/T =  2.0094
Range of M.O.s used for correlation:     1    58
NBasis=    58 NAE=     5 NBE=     5 NFC=     0 NFV=     0
NROrb=     58 NOA=     5 NOB=     5 NVA=    53 NVB=    53
Symmetrizing basis deriv contribution to polar:
IMax=3 JMax=2 DiffMx= 0.00D+00
G2DrvN: will do     7 centers at a time, making    1 passes doing MaxLOS=2.
Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
FoFDir/FoFCou used for L=0 through L=2.
End of G2Drv Frequency-dependent properties file   721 does not exist.
End of G2Drv Frequency-dependent properties file   722 does not exist.
         IDoAtm=111111
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Keep R1 ints in memory in canonical form, NReq=2286689.
         There are    18 degrees of freedom in the 1st order CPHF.  IDoFFX=4.
    18 vectors produced by pass  0 Test12= 1.47D-15 5.56D-09 XBig12= 3.76D+00 1.15D+00.
AX will form    18 AO Fock derivatives at one time.
    18 vectors produced by pass  1 Test12= 1.47D-15 5.56D-09 XBig12= 2.96D-01 1.75D-01.
    18 vectors produced by pass  2 Test12= 1.47D-15 5.56D-09 XBig12= 1.17D-03 1.09D-02.
    18 vectors produced by pass  3 Test12= 1.47D-15 5.56D-09 XBig12= 9.28D-07 2.18D-04.
    10 vectors produced by pass  4 Test12= 1.47D-15 5.56D-09 XBig12= 2.03D-10 4.32D-06.
     3 vectors produced by pass  5 Test12= 1.47D-15 5.56D-09 XBig12= 5.71D-14 7.61D-08.
```

G09 CP output4



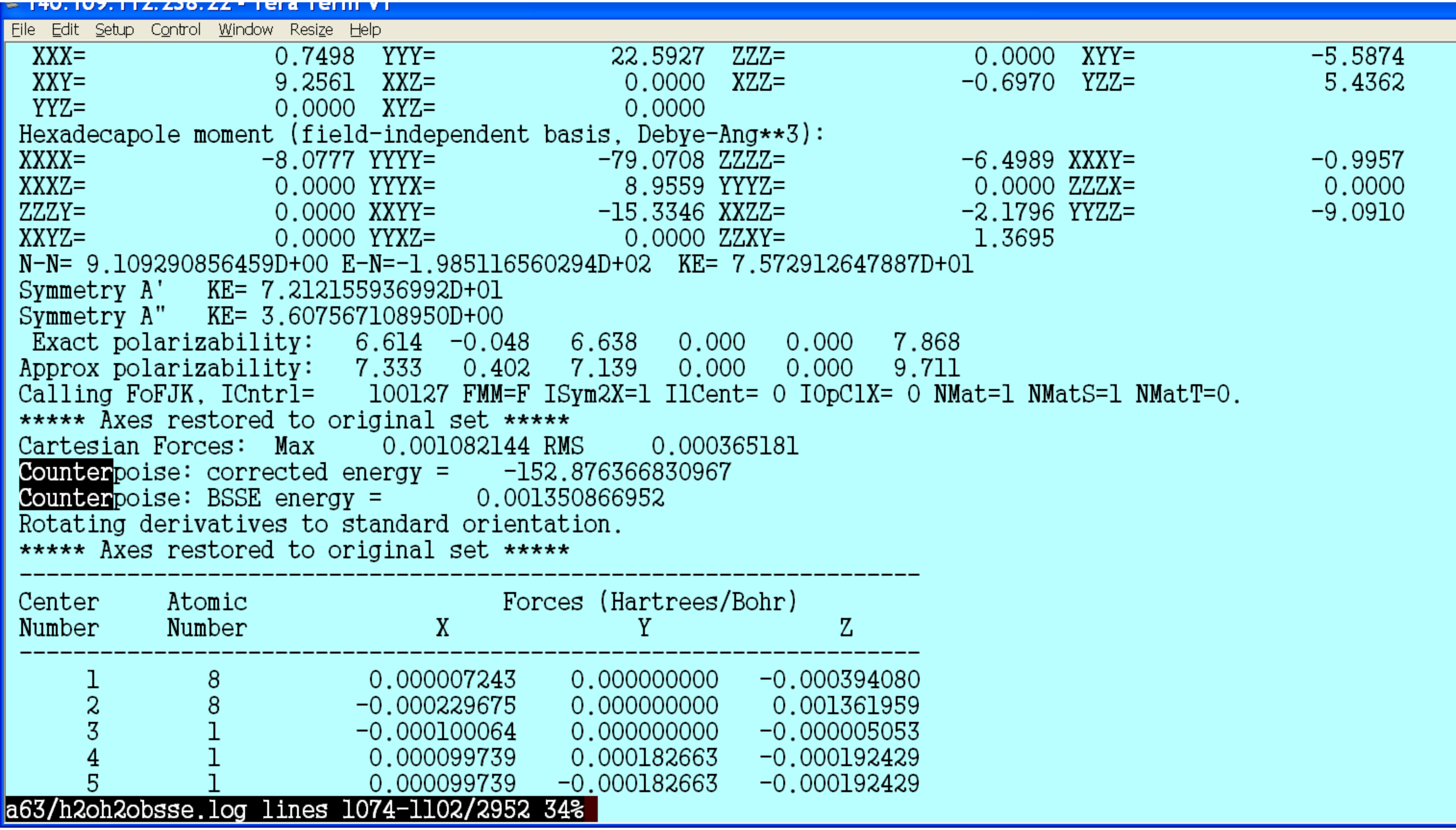
```
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 8.45D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=         0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A') (A') (A') (A') (A")
       Virtual   (A') (A') (A') (A") (A') (A') (A') (A') (A") (A')
                 (A') (A') (A") (A') (A") (A') (A') (A') (A") (A")
                 (A') (A') (A') (A')
 The electronic state of the initial guess is 1-A'.
 Requested convergence on RMS density matrix=1.00D-08 within 200 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=1023578.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB3LYP) =  -76.4339805694     A.U. after   10 cycles
             Convg  =    0.6861D-08             -V/T =  2.0094
 Range of M.O.s used for correlation:     1    29
 NBasis=    29 NAE=     5 NBE=     5 NFC=     0 NFV=     0
 NROrb=     29 NOA=     5 NOB=     5 NVA=    24 NVB=    24
 Symmetrizing basis deriv contribution to polar:
a63/h2oh2obsse.log lines 798-826/2952 25%
```

G09 CP Output 5



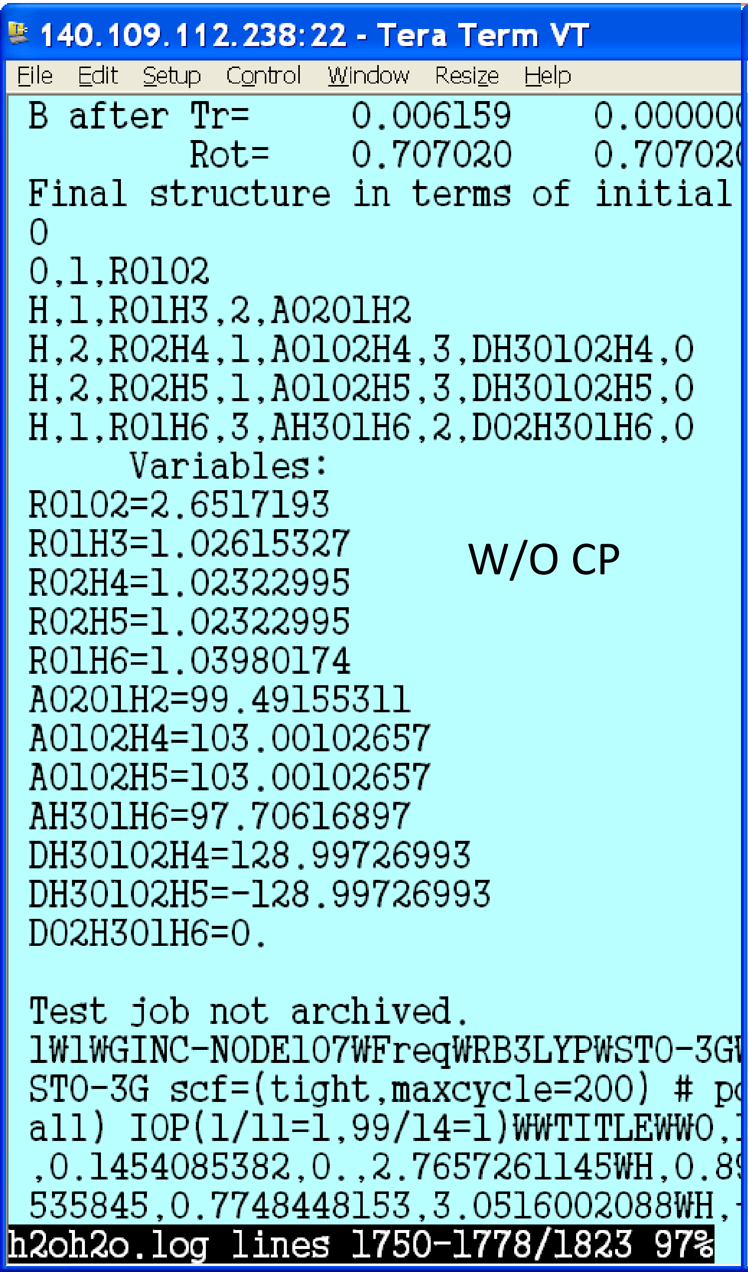
```
         NMatO=     1 NMatSO=     1 NMatTO=     0 NMatDO=     1 NMtDSO=     0 NMtDTO=     0
         IlCent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A') (A') (A") (A') (A')
       Virtual   (A') (A") (A') (A') (A") (A') (A") (A') (A') (A")
                 (A') (A') (A") (A') (A') (A') (A") (A") (A") (A')
                 (A') (A') (A") (A')
 The electronic state of the initial guess is 1-A'.
 Requested convergence on RMS density matrix=1.00D-08 within 200 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=1023578.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB3LYP) =  -76.4340436903     A.U. after   11 cycles
             Convg  =    0.2148D-08             -V/T =  2.0093
 Range of M.O.s used for correlation:     1    29
 NBasis=    29 NAE=     5 NBE=     5 NFC=     0 NFV=     0
 NROrb=     29 NOA=     5 NOB=     5 NVA=    24 NVB=    24
 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do    4 centers at a time, making    1 passes doing MaxLOS=2.
 Calling FoFCou, ICntrl=  3107 FMM=F IlCent=   0 AccDes= 0.00D+00.
 FoFDir/FoFCou used for L=0 through L=2.
 End of G2Drv Frequency-dependent properties file   721 does not exist.
 End of G2Drv Frequency-dependent properties file   722 does not exist.
          IDoAtm=010110
a63/h2oh2obsse.log lines 958-986/2952 30%
```

G09 CP output 6



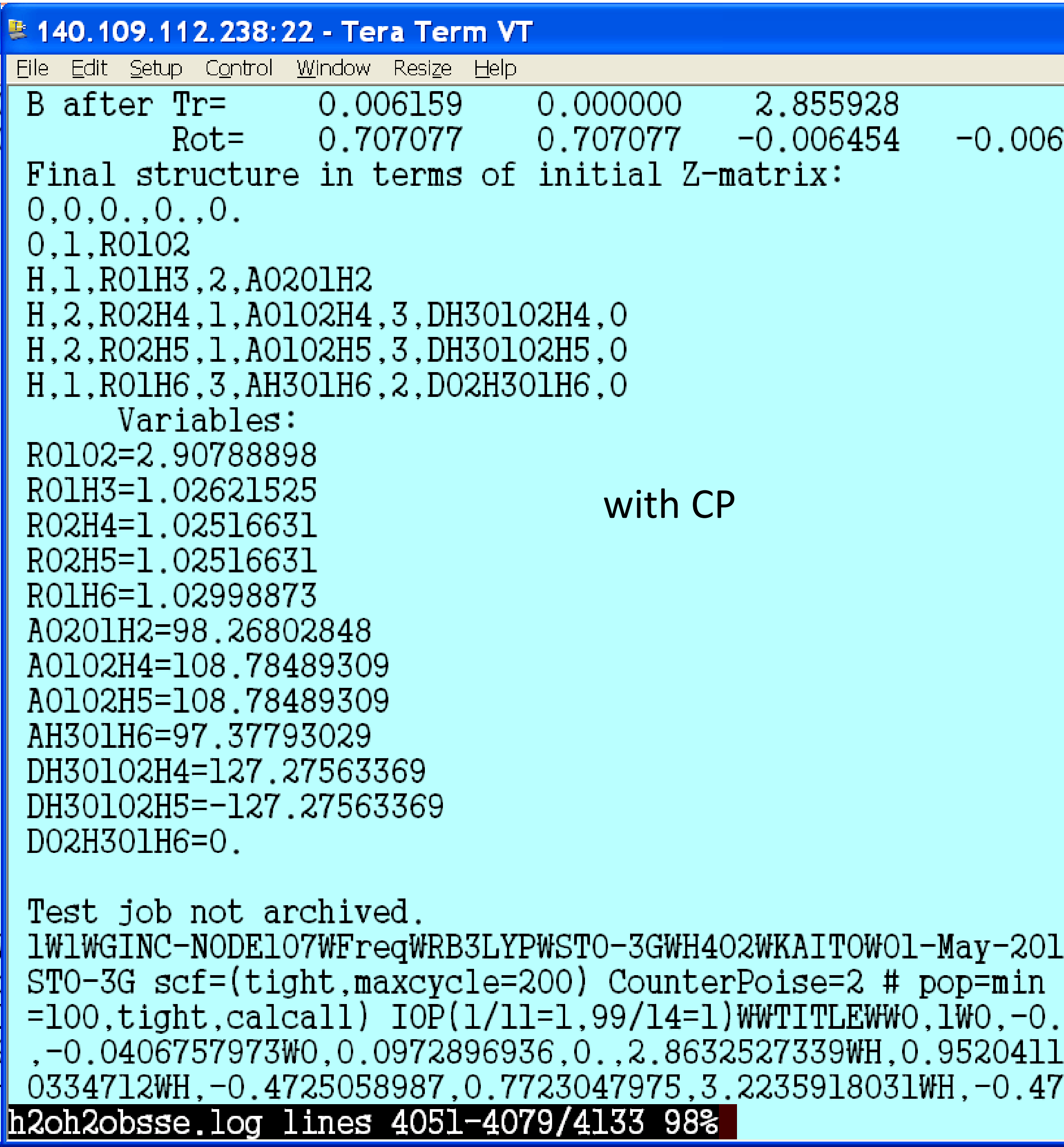
```
 XXX=              0.7498  YYY=             22.5927  ZZZ=              0.0000  XYY=             -5.5874
 XXY=              9.2561  XXZ=              0.0000  XZZ=             -0.6970  YZZ=              5.4362
 YYZ=              0.0000  XYZ=              0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=             -8.0777 YYYY=            -79.0708 ZZZZ=             -6.4989 XXXY=             -0.9957
XXXZ=              0.0000 YYYX=              8.9559 YYYZ=              0.0000 ZZZX=              0.0000
ZZZY=              0.0000 XXYY=            -15.3346 XXZZ=             -2.1796 YYZZ=             -9.0910
XXYZ=              0.0000 YYXZ=              0.0000 ZZXY=              1.3695
N-N= 9.109290856459D+00 E-N=-1.985116560294D+02  KE= 7.572912647887D+01
Symmetry A'   KE= 7.212155936992D+01
Symmetry A"   KE= 3.607567108950D+00
 Exact polarizability:   6.614  -0.048   6.638   0.000   0.000   7.868
Approx polarizability:   7.333   0.402   7.139   0.000   0.000   9.711
Calling FoFJK, ICntrl=    100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces:  Max      0.001082144 RMS      0.000365181
Counterpoise: corrected energy =    -152.876366830967
Counterpoise: BSSE energy =       0.001350866952
Rotating derivatives to standard orientation.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1          8          0.000007243    0.000000000   -0.000394080
     2          8         -0.000229675    0.000000000    0.001361959
     3          1         -0.000100064    0.000000000   -0.000005053
     4          1          0.000099739    0.000182663   -0.000192429
     5          1          0.000099739   -0.000182663   -0.000192429
a63/h2oh2obsse.log lines 1074-1102/2952 34%
```

Optimized Geometry CP



```
B after Tr=      0.006159      0.00000
        Rot=     0.707020      0.70702
Final structure in terms of initial
O
O,1,RO1O2
H,1,RO1H3,2,AO2O1H2
H,2,RO2H4,1,AO1O2H4,3,DH3O1O2H4,0
H,2,RO2H5,1,AO1O2H5,3,DH3O1O2H5,0
H,1,RO1H6,3,AH3O1H6,2,DO2H3O1H6,0
     Variables:
RO1O2=2.6517193
RO1H3=1.02615327
RO2H4=1.02322995
RO2H5=1.02322995
RO1H6=1.03980174
AO2O1H2=99.49155311
AO1O2H4=103.00102657
AO1O2H5=103.00102657
AH3O1H6=97.70616897
DH3O1O2H4=128.99726993
DH3O1O2H5=-128.99726993
DO2H3O1H6=0.

Test job not archived.
1W1WGINC-NODE107WFreqWRB3LYPWSTO-3GW
STO-3G scf=(tight,maxcycle=200) # po
all) IOP(1/11=1,99/14=1)WWTITLEWWO,1
,0.1454085382,0.,2.7657261145WH,0.89
535845,0.7748448153,3.0516002088WH,-
h2oh2o.log lines 1750-1778/1823 97%
```

W/O CP



```
B after Tr=      0.006159      0.000000      2.855928
        Rot=     0.707077      0.707077     -0.006454     -0.006
Final structure in terms of initial Z-matrix:
O,0,0.,0.,0.
O,1,RO1O2
H,1,RO1H3,2,AO2O1H2
H,2,RO2H4,1,AO1O2H4,3,DH3O1O2H4,0
H,2,RO2H5,1,AO1O2H5,3,DH3O1O2H5,0
H,1,RO1H6,3,AH3O1H6,2,DO2H3O1H6,0
     Variables:
RO1O2=2.90788898
RO1H3=1.02621525
RO2H4=1.02516631
RO2H5=1.02516631
RO1H6=1.02998873
AO2O1H2=98.26802848
AO1O2H4=108.78489309
AO1O2H5=108.78489309
AH3O1H6=97.37793029
DH3O1O2H4=127.27563369
DH3O1O2H5=-127.27563369
DO2H3O1H6=0.

Test job not archived.
1W1WGINC-NODE107WFreqWRB3LYPWSTO-3GWH4O2WKAITOW01-May-201
STO-3G scf=(tight,maxcycle=200) CounterPoise=2 # pop=min
=100,tight,calcall) IOP(1/11=1,99/14=1)WWTITLEWWO,1WO,-0.
,-0.0406757973WO,0.0972896936,0.,2.8632527339WH,0.952041l
0334712WH,-0.4725058987,0.7723047975,3.2235918031WH,-0.47
h2oh2obsse.log lines 4051-4079/4133 98%
```

with CP

Excited Electronic States Calculation

Method for Excited States

- Use more than one slater determinant
    - CISD: Configuration Interaction Singles and Doubles
    - CCSD: Coupled Cluster Singles and Doubles
    - MCSCF: Multiconfigurational Self Consistent Field
    - MR-CISD: Multireference CISD
- CAS MP2
    - MP2,3,4: Mollar Plesset perturbation theory
- Equation of Motion CCSD
- Time Dependent DFT