Entering Gaussian System, Link 0=g98
Initial command:
/ual/usr/local/g98/l1.exe /ual/airk/lab/h2o/Gau-12349.inp -
scdir=/ual/airk/lab/h2o/
Entering Link 1 = /ual/usr/local/g98/l1.exe PID= 12352.

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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
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R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov, G. Liu,
A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin,
D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara,
C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen,
M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon,
E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA.1998,

-18 Feb-2004
*****************************************************************************
# p RHF/STO-3G SCF=Tight freq

H2O
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
O
H        1 R
H        1 R      2 A
Variables:
R 1.09894
A 100.0284
Leaves Link 1 at Wed Feb 18 15:57:59 2004, MaxMem=          0 cpu:       0.2
Enter /ua1/usr/local/g98/l101.exe(---

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

---

Initial Parameters!

---

!) Name          Value Derivative information (Atomic Units! { (Angstroms and Degrees! ( !

---

! R 0.9994 calculate D2E/DX2 analytically!

! A 100.0284 calculate D2E/DX2 analytically!

---

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

---

Leave Link 103 at Wed Feb 18 15:58:00 2004, MaxMem= 6291456 cpu: 0.1

) Enter /ua1/usr/local/g98/l301.exe

---

Z-MATRIX (ANGSTROMS AND DEGREES)

---

CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J

---

1 1 O 2 2 H 1 0.989400(1)

3 3 H 1 0.989400(2) 2 100.028(3)

---

Z-Matrix orientation :

---

Center Atomic Atomic Coordinates (Angstroms( Number Number Type X Y Z

---

0.000000 0.000000 0.000000 0 8 1

0.989400 0.000000 0.000000 0 1 2

0.172290- 0.000000 0.974284 0 1 3

---

Distance matrix (angstroms):

---

3 2 1

1 0 0.000000

2 H 0.989400 0.000000

3 H 0.989400 1.516164 0.000000

Interatomic angles:

H2-O1-H3=100.0284

Stoichiometry H2O

Framework group C2V(C2(O),SGV(H2){

Deg. of freedom 2

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2 NOp 2

Standard orientation :

---

Center Atomic Atomic Coordinates (Angstroms( Number Number Type X Y Z

---

0.127157 0.000000 0.000000 0 8 1

0.508629- 0.758082 0.000000 0 1 2

0.508629- 0.758082- 0.000000 0 1 3

---

Rotational constants (GHz): 698.4339218 436.2844998 268.5387744

Isotopes: O-16,H-1,H-1

Leave Link 202 at Wed Feb 18 15:58:00 2004, MaxMem= 6291456 cpu: 0.2

) Enter /ua1/usr/local/g98/1301.exe

Standard basis: STO-3G (5D, 7F)

There are 4 symmetry adapted basis functions of A1 symmetry.
There are 0 symmetry adapted basis functions of A2 symmetry.
There are 1 symmetry adapted basis functions of B1 symmetry.
There are 2 symmetry adapted basis functions of B2 symmetry.
Crude estimate of integral set expansion from redundant integrals=1.296.
Integral buffers will be 131072 words long.
Two-electron integral symmetry is turned on.
7 basis functions 21 primitive gaussians
5 alpha electrons 5 beta electrons
nuclear repulsion energy 8.9065697394 Hartrees.
Leave Link 301 at Wed Feb 18 15:58:00 2004, MaxMem= 6291456 cpu: 0.2
) Enter /ual/usr/local/g98/l302.exe
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
NBasis= 7 RedAO= T NBF= 4 0 1 2
NbsUse= 7 1.00D-04 NBFU= 4 0 1 2
Leave Link 302 at Wed Feb 18 15:58:01 2004, MaxMem= 6291456 cpu: 0.5
) Enter /ual/usr/local/g98/l303.exe
DipDrv: MaxL=1.
Leave Link 303 at Wed Feb 18 15:58:01 2004, MaxMem= 6291456 cpu: 0.2
) Enter /ual/usr/local/g98/l401.exe
Projected INDO Guess.
Initial guess orbital symmetries:
Virtual  (A1) (B2)
Leave Link 401 at Wed Feb 18 15:58:02 2004, MaxMem= 6291456 cpu: 0.4
) Enter /ual/usr/local/g98/l502.exe
IExCor=   0 DFT=F Ex=HF Corr=None ScaHFX= 1.0000
ScaDFX=  0.0000  0.0000  0.0000  0.0000
IRadAn=      0 IRanWt=     -1 IRanGd=            0 ICorTp=0
Using DIIS extrapolation.
Closed shell SCF:
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral symmetry usage will be decided dynamically.
Keep RI integrals in memory in canonical form, NReq= 806476.
IEnd=  6056 IEndB=  6056 NGot=  6291456 MDV=  6289667
LenX=  6289667
Symmetry not used in FoFDir.
MinBra= 0 MaxBra= 1 Meth= 1.
IRaf=       0 NMat=   1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.
Cycle  1 Pass 1 IDiag 1:
E=-0.838073586097085D+02
DIIS: error= 3.56D-01 at cycle  1.
T= 1000. NK=0 NO(<0.9)= 0 NV(>0.1)= 0 5.00e < EF 0.00e >EF Err=0.0D+00
RMSDP=1.76D-02 MaxDP=3.69D-02
Cycle  2 Pass 1 IDiag 1:
E=-0.838720725422508D+02 Delta-E= -0.064713932542
DIIS: error= 1.23D-02 at cycle  2.
T=  927. NK=0 NO(<0.9)= 0 NV(>0.1)= 0 5.00e < EF 0.00e >EF Err=0.0D+00
RMSDP=3.63D-03 MaxDP=1.25D-02
Cycle  3 Pass 1 IDiag 1:
E=-0.838724369328D+02 Delta-E= -0.00354992387
DIIS: error= 1.40D-03 at cycle  3.
Coeff: 0.8760-01-0.108D+01
T=  800. NK=0 NO(<0.9)= 0 NV(>0.1)= 0 5.00e < EF 0.00e >EF Err=0.0D+00
RMSDP=1.27D-03 MaxDP=4.64D-03
Cycle 4 Pass 1 IDiag 1:

E=-0.838724649658831D+02 Delta-E= -0.000037431245
DIIS: error= 5.20D-04 at cycle 4.
Coeff: -0.197D-01 0.472D+00-0.145D+01
RMSDP=6.37D-04 MaxDP=2.01D-03

Cycle 5 Pass 1 IDiag 1:

E=-0.838724707818147D+02 Delta-E= -0.000005815932
DIIS: error= 9.11D-05 at cycle 5.
Coeff: -0.191D-03-0.219D-01 0.373D-01 0.161D+00-0.118D+01
RMSDP=1.05D-04 MaxDP=3.09D-04

Cycle 6 Pass 1 IDiag 1:

E=-0.838724709538061D+02 Delta-E= -0.000000171991
DIIS: error= 1.16D-05 at cycle 6.
Coeff: 0.833D-03-0.212D-01 0.373D-01 0.161D+00-0.118D+01
RMSDP=9.84D-06 MaxDP=3.16D-05

Cycle 7 Pass 1 IDiag 1:

E=-0.838724709562590D+02 Delta-E= -0.000000002453
DIIS: error= 3.37D-08 at cycle 7.
Coeff: -0.115D-06 0.489D-05-0.124D-03 0.917D-03-0.274D-02-0.998D+00
RMSDP=1.58D-08 MaxDP=3.16D-05

Cycle 8 Pass 1 IDiag 1:

E=-0.838724709562590D+02 Delta-E= -0.000000000000
DIIS: error= 3.37D-11 at cycle 8.
Coeff: -0.100D+01
RMSDP=1.84D-11 MaxDP=5.75D-11

SCF Done: E(RHF) = -74.9659012168 A.U. after 8 cycles
Convg = 0.1836D-10 -V/T = 2.0060
S**2 = 0.0000

KE= 7.451862833339D+01 PE= 1.963529057548D+02 EE= 3.796180646517D+01
Leave Link 502 at Wed Feb 18 15:58:02 2004, MaxMem=6291456 cpu: 0.2
)
Enter /ual/usr/local/g98/l801.exe(

Range of M.O.s used for correlation: 1 7
NBasis= 7 NAE= 5 NBE= 5 NFC= 0 NFV= 0
NRorb= 7 NOA= 5 NOB= 5 NVA= 2 NVB= 2
Leave Link 801 at Wed Feb 18 15:58:02 2004, MaxMem=6291456 cpu: 0.0
)
Enter /ual/usr/local/g98/l1002.exe(

Minotr: Closed-shell wavefunction.
Direct CPHF calculation.
Solving linear equations simultaneously.
Using symmetry in CPHF.
Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.
Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.
Differentiating once with respect to electric field.
with respect to dipole field.
NewPWx=F KeepS1=T KeepFl=T KeepIn=T MapXYZ=F.
MDV= 6291456
Using IRadAn= 2.
Store integrals in memory, NReq= 820522.
Symmetry not used in FoFDir.
MinBr= 0 MaxBr= 1 Meth= 1.
IRaf= 0 NMat= 1 IRCut= 1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E= 0.
There are 3 degrees of freedom in the 1st order CPHF.
3 vectors were produced by pass 0.
AX will form 3 AO Fock derivatives at one time.
2 vectors were produced by pass 1.
vectors were produced by pass 2.
vectors were produced by pass 3.
Inv2: IOpt= 1 Iter= 1 AM= 3.21D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 9 with in-core refinement.
Leave Link 1002 at Wed Feb 18 15:58:02 2004, MaxMem= 6291456 cpu: 0.1
) Enter /ual/usr/local/g98/l1101.exe(
Using compressed storage.
Will process 3 atoms per pass.
Leave Link 1101 at Wed Feb 18 15:58:03 2004, MaxMem= 6291456 cpu: 0.5
) Enter /ual/usr/local/g98/l1102.exe(
Use density number 0.
Leave Link 1102 at Wed Feb 18 15:58:03 2004, MaxMem= 6291456 cpu: 0.2
) Enter /ual/usr/local/g98/l1110.exe(
Forming Gx(P) for the SCF density.
Integral derivatives from FoFDir, PRISM(SPDF).
Do as many integral derivatives as possible in FoFDir.
G2DrvN: MDV= 6291456.
G2DrvN: will do 3 atoms at a time, making 1 passes doing MaxLOS=1.
Petite list used in FoFDir.
MinBra= 0 MaxBra= 1 Meth= 1.
IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1 JSym2E=1.
FoFDir used for L=0 through L=1.
Leave Link 1110 at Wed Feb 18 15:58:03 2004, MaxMem= 6291456 cpu: 0.2
) Enter /ual/usr/local/g98/l1102.exe(
Minotr: Closed-shell wavefunction.
Direct CPHF calculation.
Solving linear equations simultaneously.
Using symmetry in CPHF.
Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.
Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.
Differentiating once with respect to electric field.
with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
NewPWx=T KeepS1=F KeepF1=F KeepIn=F MapXYZ=F.
MDV= 6291456
Using IRadAn= 2.
Store integrals in memory, NReq= 820579.
Symmetry not used in FoFDir.
MinBra= 0 MaxBra= 1 Meth= 1.
IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.
There are 9 degrees of freedom in the 1st order CPHF.
8 vectors were produced by pass 0.
AX will form 8 AO Fock derivatives at one time.
2 vectors were produced by pass 1.
Inv2: IOpt= 1 Iter= 1 AM= 1.87D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 10 with in-core refinement.
Leave Link 1002 at Wed Feb 18 15:58:04 2004, MaxMem= 6291456 cpu: 0.3
) Enter /ual/usr/local/g98/1601.exe(
Copying SCF densities to generalized density rwf, ISCF=0 IROHF=0.

********************************************************************************
Population analysis using the SCF density.

********************************************************************************

Orbital Symmetries:
Virtual (A1) (B2)
The electronic state is 1-A1.
Alpha occ. eigenvalues -- -20.25157 -1.25755 -0.59386 -0.45973 -0.39262
Alpha virt. eigenvalues --   0.58180   0.69269
Condensed to atoms (all electrons):

\[
\begin{align*}
3 & \quad 2 \quad 1 \\
1 & \quad 0 \quad 7.822771 \quad 0.253884 \quad 0.253884 \\
2 & \quad H \quad 0.253884 \quad 0.626246 \quad -0.045400 \\
3 & \quad H \quad 0.253884 \quad -0.045400 \quad 0.626246 \\
\end{align*}
\]

Total atomic charges:

\[
\begin{align*}
1 & \quad 0 \quad -0.330540 \\
2 & \quad H \quad 0.165270 \\
3 & \quad H \quad 0.165270 \\
\end{align*}
\]

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

\[
\begin{align*}
1 & \quad 0 \quad 0.000000 \\
2 & \quad H \quad 0.000000 \\
3 & \quad H \quad 0.000000 \\
\end{align*}
\]

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au):  \(<R^2>= 18.2684\)

Charge= 0.0000 electrons

Dipole moment (Debye):

\[
X = 0.0000 \\
Y = 0.0000 \\
Z = -1.7092 \\
\text{Tot}= 1.7092
\]

Quadrupole moment (Debye-Ang):

\[
\begin{align*}
XX &= -6.1257 \\
YY &= -4.4856 \\
ZZ &= -5.3333 \\
XY &= 0.0000 \\
XZ &= 0.0000 \\
YZ &= 0.0000
\end{align*}
\]

Octapole moment (Debye-Ang**2):

\[
\begin{align*}
XXX &= 0.0000 \\
YYY &= 0.0000 \\
ZZZ &= 0.0000 \\
XYZ &= 0.0000 \\
XXZ &= 0.0000 \\
YZZ &= 0.0000 \\
XYZ &= 0.0000
\end{align*}
\]

Hexadecapole moment (Debye-Ang**3):

\[
\begin{align*}
XXXX &= -3.2653 \\
YYYY &= -6.7334 \\
ZZZZ &= -5.2196 \\
XXXXY &= 0.0000 \\
XXXY &= 0.0000 \\
XXZZ &= 0.0000 \\
YYZZ &= 0.0000 \\
XYZ &= 0.0000
\end{align*}
\]

N-N= 8.906569739431D+00  E-N=-1.963529057543D+02  KE= 7.451862833339D+01

Symmetry A1 KE= 6.651704420488D+01
Symmetry A2 KE= 0.000000000000D+00
Symmetry B1 KE= 5057462452019.D+00
Symmetry B2 KE= 2.944121676499D+00

Exact polarizability:  0.040   0.000   5.508   0.000   0.000   2.566
Approx polarizability:  0.040   0.000   5.508   0.000   0.000   2.606

Leave Link  601 at Wed Feb 18 15:58:04 2004, MaxMem= 6291456 cpu: 0.3

Enter /ua1/usr/local/g98/l701.exe

Compute integral second derivatives.

... and contract with generalized density number  0.

Leave Link  701 at Wed Feb 18 15:58:05 2004, MaxMem= 6291456 cpu: 0.6

Enter /ua1/usr/local/g98/l702.exe

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link  702 at Wed Feb 18 15:58:05 2004, MaxMem= 6291456 cpu: 0.0

Enter /ua1/usr/local/g98/l703.exe

Integral derivatives from FoFDir, PRISM(SPD) Scalar Rys(F).

Petite list used in FoFDir.

MinBra= 0 MaxBra= 2 Meth= 1.
IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1 JSym2E=1.

Leave Link  703 at Wed Feb 18 15:58:06 2004, MaxMem= 6291456 cpu: 1.1

Enter /ua1/usr/local/g98/l716.exe

Dipole =-3.44485441D-17 0.00000000D+00-6.72455877D-01
Polarizability= 4.00614661D-02 3.18275704D-16 5.50797998D+00
1.58798725 D-16-2.22044605D-16 2.56576708D+00
HyperPolar =-3.59205161D-17 8.82132963D-17-2.96841989D-16
H₂O is a linear molecule with 3 atoms; we have 3 normal modes. There are five normal modes with a minus sign (here the sign jumped to the end of the number due to WORD) representing kinetic and rotation modes.

**Thermochemistry**

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 8 and mass 15.99491
Atom 2 has atomic number 1 and mass 1.00783
Atom 3 has atomic number 1 and mass 1.00783
Molecular mass: 18.01056 amu.

Principal axes and moments of inertia in atomic units:

<table>
<thead>
<tr>
<th>EIGENVALUES</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.58398</td>
<td>4.13662</td>
<td>6.72060</td>
<td></td>
</tr>
</tbody>
</table>

This molecule is an asymmetric top.

Rotational Symmetry Number 2.

Rotational Temperatures (Kelvin): 33.51935 20.93823 12.88775
Rotational Constants (GHz): 698.43392 436.28450 268.53877

Zero-point vibrational energy: 64008.0 Joules/Mol

Vibrational Temperatures: 3122.15 5956.64 6317.89 K

Zero-point correction = 0.024379 (Hartree/Particle)
Thermal correction to Energy = 0.027212
Thermal correction to Enthalpy = 0.028156
Thermal correction to Gibbs Free Energy = 0.006642

Sum of electronic and zero-point Energies = -74.941522
Sum of electronic and thermal Energies = -74.938689
Sum of electronic and thermal Enthalpies = -74.937745
Sum of electronic and thermal Free Energies = -74.959260

<table>
<thead>
<tr>
<th>E (Thermal)</th>
<th>CV</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>kcal/mol</td>
<td>cal/mol-Kelvin</td>
<td>cal/mol-Kelvin</td>
</tr>
<tr>
<td>TOTAL</td>
<td>17.076</td>
<td>5.968</td>
</tr>
<tr>
<td>ELECTRONIC</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>TRANSLATIONAL</td>
<td>0.889</td>
<td>2.981</td>
</tr>
<tr>
<td>ROTATIONAL</td>
<td>0.889</td>
<td>2.981</td>
</tr>
<tr>
<td>VIBRATIONAL</td>
<td>15.298</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Note: there are other properties like Raman freq, IR intensity, Thermochemistry, etc.
<table>
<thead>
<tr>
<th></th>
<th>Q</th>
<th>LOG10(Q)</th>
<th>LN(Q)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL BOT</td>
<td>0.881269D-03</td>
<td>-3.054892</td>
<td>-7.034148</td>
</tr>
<tr>
<td>TOTAL V=0</td>
<td>0.144130D+09</td>
<td>8.158754</td>
<td>18.785226</td>
</tr>
<tr>
<td>VIB (BOT)</td>
<td>0.611457D-11</td>
<td>-11.213634</td>
<td>-25.820346</td>
</tr>
<tr>
<td>VIB (V=0)</td>
<td>0.100003D+01</td>
<td>0.000012</td>
<td>0.000028</td>
</tr>
<tr>
<td>ELECTRONIC</td>
<td>0.100000D+01</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>TRANSLATIONAL</td>
<td>0.300436D+07</td>
<td>6.477751</td>
<td>14.915574</td>
</tr>
<tr>
<td>ROTATIONAL</td>
<td>0.479723D+02</td>
<td>1.680991</td>
<td>3.870624</td>
</tr>
</tbody>
</table>

Illustration of the IR spectrum, frequencies and intensities.
Cartesian Forces: Max 0.00014019 RMS 0.00007901

Internal Coordinate Forces (Hartree/Bohr or radian):

<table>
<thead>
<tr>
<th>Cent</th>
<th>Atom</th>
<th>N1</th>
<th>Length/X</th>
<th>N2</th>
<th>Alpha/Y</th>
<th>N3</th>
<th>Beta/Z</th>
<th>J</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O</td>
<td>1</td>
<td>0.000010(1)</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>H</td>
<td>1</td>
<td>0.000010(2)</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Internal Forces: Max 0.00010065 RMS 0.00009044

Force constants in Cartesian coordinates:

<table>
<thead>
<tr>
<th>5</th>
<th>4</th>
<th>3</th>
<th>2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.704733</td>
<td>1</td>
<td>D+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.000000</td>
<td>2</td>
<td>D+00</td>
<td>-0152289, D-04</td>
<td></td>
</tr>
<tr>
<td>0.832544</td>
<td>3</td>
<td>D-01</td>
<td>0.000000D+00</td>
<td>0.734178D+00</td>
</tr>
<tr>
<td>0.798532</td>
<td>4</td>
<td>D-01</td>
<td>0.000000D+00</td>
<td>-0.669774D-01</td>
</tr>
<tr>
<td>0.000000</td>
<td>5</td>
<td>D+00</td>
<td>0.761447D-05</td>
<td>0.000000D+00</td>
</tr>
<tr>
<td>0.538504</td>
<td>6</td>
<td>D-01</td>
<td>0.000000D+00</td>
<td>-0.639602D+00</td>
</tr>
<tr>
<td>0.624880</td>
<td>7</td>
<td>D+00</td>
<td>0.000000D+00</td>
<td>0.150232D+00</td>
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<tr>
<td>0.000000</td>
<td>8</td>
<td>D+00</td>
<td>0.761447D-05</td>
<td>0.000000D+00</td>
</tr>
<tr>
<td>0.294040</td>
<td>9</td>
<td>D-01</td>
<td>0.000000D+00</td>
<td>-0.945757D-01</td>
</tr>
</tbody>
</table>

Force constants in internal coordinates:

<table>
<thead>
<tr>
<th>3</th>
<th>2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.654122</td>
<td>6</td>
<td>D+00</td>
</tr>
<tr>
<td>0.336883</td>
<td>7</td>
<td>D-01</td>
</tr>
<tr>
<td>0.000000</td>
<td>8</td>
<td>D+00</td>
</tr>
<tr>
<td>0.145195</td>
<td>9</td>
<td>D-01</td>
</tr>
</tbody>
</table>

Search for a local minimum.
Step number 1 out of a maximum of 20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
The second derivative matrix:

R A
R 1.24695
A 0.07540 0.29688

Eigenvalues --- 0.29093 1.25290

Angle between quadratic step and forces = 38.23 degrees.
Linear search not attempted -- first point.

Variable Old X -DE/DX Delta X Delta X Delta X New X
<table>
<thead>
<tr>
<th>Linear</th>
<th>(Quad)</th>
<th>(Total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>1.86969</td>
<td>0.00002</td>
</tr>
<tr>
<td>A</td>
<td>1.74582</td>
<td>-0.00001</td>
</tr>
</tbody>
</table>

Item Value Threshold Converged?
| Maximum Force | 0.000020 | 0.000450 | YES |
| RMS Force | 0.000015 | 0.000300 | YES |
| Maximum Displacement | 0.000027 | 0.001800 | YES |
| RMS Displacement | 0.000023 | 0.001200 | YES |

Predicted change in Energy = -2.654501D-10
Optimization completed.
Stationary point found.

Optimized Parameters!

Angstroms and Degrees!

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Derivative information (Atomic Units!)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>0.9894</td>
<td>-DE/DX = 0!</td>
</tr>
<tr>
<td>A</td>
<td>100.028</td>
<td>-DE/DX = 0!</td>
</tr>
</tbody>
</table>

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Feb 18 15:58:08 2004, MaxMem= 6291456 cpu: 0.2

Enter /u/b/local/g98/19999.exe

\1\ GINC-ATTO\Freq\RHF\STO-3G\H2O\ARIK\18-Feb-2004\1\#/P RHF/STO-3G S
CF=TIGHT FREQ\H2O\0,1\O\H,1,R\H,1,R,2,A\R=0.9894\A=100.0284\Versio
n=DEC-AXP-OSF/1-G98RevA.4\State=1-A1\HF=-74.9659012\RMSD=1.836e-11\RMS
F=7.901e-06\Dipole=0.5152382,0.,0.4321186\DipoleDeriv=0.036166,0.,0.05
.0.0934912,0.,0.0161967,0.1683745,0.,0.056462,0.,0.5596981,0.,-0.6462,0
0.27,0.0370292,0.,0.2045404,0.,-0.1945558,0.,0.0289163,0.,-0.2798491,0
0.1783591,0.0275457,0.,-0.98491,0 Polar=3.7807005,0.,0.0406156,-1.44863
4.2930466,02,0 PolarDeriv=-4.991107,0.,0.0139236,-0.3327678,0.,-1.145
0.9281,-0.0116774,0.5154286,0.,-1.3508651,0.,-1.16107089,0.,-0.9654,0
0.,0.5198693,0.,0.0270535,1.8029034,0.,-0.440508,0.,-4.6315952,0.,-691,0
5.7879,0.884405,0.,0.0181178,0.3496552,0.,-2.1376814,0.,0.421006,0
0.,0.2.0317095,0.,0.6260691,0.,1.4701356,0.,-0.0131299,78,5.431615,0
1.1563828,-0.0297952,1.8125741,0.,-0.1657734,0.,7868163,0. HyperPolar
9.02,0.0489901,0.0186431,0.,1.8779942,0.,-0.0584135,0.,-8.5063201,0=
7688 PG=C02V [C2 (01), SGV (H2)] \Nimag=0\0.0.70473285,0.,-0.00001523,-0.08
0.000007,-0.06697742,0.08492041,0.,-0.07985315,0.,-0.73417797,0.325445,0
0.654121,0.02016213,0.63960226,0.,0.00000571,0.05385040,0.,-0.61,0
0.03368827,0.62994696,0.,-0.00506726,0.,-0.15023186,0.62487970,0.,-74
0.094575,-0.00000571,0.02940405,0.,-0.00000190,0.,-0.00000761,0
0.00001402,0\0.10909519,0.11654359,0.,-0.01451948,0.,-0.08713955,0
0\0.00000169,0.00001052,0.,-0.0001007,0.,0.00000350,0.,-0.0001176

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CHARLES DARWIN

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Normal termination of Gaussian 98.