Example of IR frequency calculations of the H_2O molecule.

```
 Entering Gaussian System, Link 0=g98
 Initial command:
/ ua1/usr/local/g98/l1.exe /ua1/arik/lab/h2o/Gau-12349.inp -
scrdir=/ua1/arik/lab/h2o/
 Entering Link 1 = /ua1/usr/local/g98/l1.exe PID=     12352.

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 Gaussian 98, Revision A.4,
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**********************************************
 Gaussian 98:  DEC-AXP-OSF/1-G98RevA.4 11-Sep-1998
-18                     Feb-2004
**********************************************
------------------------------
# p RHF/STO-3G SCF=Tight freq
------------------------------
;1/1,3=1,38=4,30=1/10
;5/2=6,18=2/17
;1/1,2,3=1,30=1,25=3/11
;1/1=4/7
;4/2=2,38=2,32=5/5
;11/1=4,11=8/6
;10/2=10/13
;11/1,2,10=111,16=11,15=1,9=2,8=11/6
;1/2=10/6
;1/1=1,28=2,18=2,10=2,9=2,8=6/7
;1/1,2,3,16=1,25=1,10=7/8
;1/3=4,30=1/10
;99//99
 Leave Link    1 at Wed Feb 18 15:57:59 2004, MaxMem=          0 cpu:       0.2
) Enter /ua1/usr/local/g98/l101.exe(
---
 H2O
---
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 O
 H                    1    R
 H                    1    R        2    A
      Variables:
  R                     0.9894
  A                   100.0284
 Leave Link  101 at Wed Feb 18 15:57:59 2004, MaxMem=    6291456 cpu:       0.2
) Enter /ua1/usr/local/g98/l103.exe(

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
```
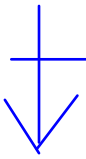

the keywork for calculating IR frequencies.

```
 Initialization pass.
----------------------------
    !                       Initial Parameters!
) !                      Angstroms and Degrees!  (
----------------------                                ----------------------
      ! Name          Value   Derivative information (Atomic Units!     (
-------------------------------------------------------------------------
        ! R          0.9894   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.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Wed Feb 18 15:58:00 2004, MaxMem=    6291456 cpu:       0.1
) Enter /ua1/usr/local/g98/l202.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     O    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/l301.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.
 Raffenetti 1 integral format.
 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 /ua1/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 /ua1/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 /ua1/usr/local/g98/l401.exe(
 Projected INDO Guess.
 Initial guess orbital symmetries:
       Occupied  (A1) (A1) (B2) (A1) (B1(
       Virtual   (A1) (B2(
 Leave Link  401 at Wed Feb 18 15:58:02 2004, MaxMem=    6291456 cpu:       0.4
) Enter /ua1/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 R1 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=-0.838724275346382D+02 Delta-E=       -0.000354992387
 DIIS: error= 1.40D-03 at cycle   3.
 Coeff: 0.786D-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
```



begining of the SCF iterative process

```
 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:-0.191D0.218-03-D-01 0.229D+00-0.121D+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=6.18D-08

 Cycle   8  Pass 1  IDiag 1:
 E=-0.838724709562590D+02 Delta-E=        0.000000000000
 DIIS: error= 3.37D-11 at cycle   8.
 Coeff: 0.685D-11 0.201D-08-0.324D-07 0.155D-06-0.449D-06 0.897D-03
 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 /ua1/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 /ua1/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 KeepF1=T KeepIn=T MapXYZ=F.
          MDV=  6291456
          Using IRadAn=       2.
          Store integrals in memory, NReq=      820522.
 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   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.
```

end of the process

```
 2   vectors were produced by pass  2.
 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 /ua1/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 /ua1/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 /ua1/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 /ua1/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.
          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:       03.
) Enter /ua1/usr/local/g98/l601.exe(
 Copying SCF densities to generalized density rwf, ISCF=0 IROHF=0.

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

            Population analysis using the SCF density.

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

 Orbital Symmetries:
       Occupied  (A1) (A1) (B2) (A1) (B1(
       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:(
3          2          1
  1  O    7.822771   0.253884   0.253884
  2  H    0.253884   0.626246  -0.045400
  3  H    0.253884  -0.045400   0.626246
 Total atomic charges:
1
  1  O   -0.330540
  2  H    0.165270
  3  H    0.165270
 Sum of Mulliken charges=   0.00000
 Atomic charges with hydrogens summed into heavy atoms:
1
  1  O    0.000000
  2  H    0.000000
  3  H    0.000000
 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  Tot=     1.7092
 Quadrupole moment (Debye-Ang:(
   XX=    -6.1257   YY=    -4.4856   ZZ=    -5.3333
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Octapole moment (Debye-Ang**2:(
  XXX=     0.0000  YYY=     0.0000  ZZZ=    -0.1745  XYY=     0.0000
  XXY=     0.0000  XXZ=     0.0192  XZZ=     0.0000  YZZ0.0000     =
  YYZ=    -0.5314  XYZ=     0.0000
 Hexadecapole moment (Debye-Ang**3:(
 XXXX=    -3.2653 YYYY=    -6.7334 ZZZZ=    -5.2196 XXXY=     0.0000
 XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
 ZZZY=     0.0000 XXYY=    -1.8084 XXZZ=    -1.4597 YYZZ=    -1.7391
 XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
 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:   0.020   0.000   3.938   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(
 Compute integral second derivatives.
 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
```

begining of the freq calc,

H2O is a linear molecule with 3 atoms we have 3*3-5 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.

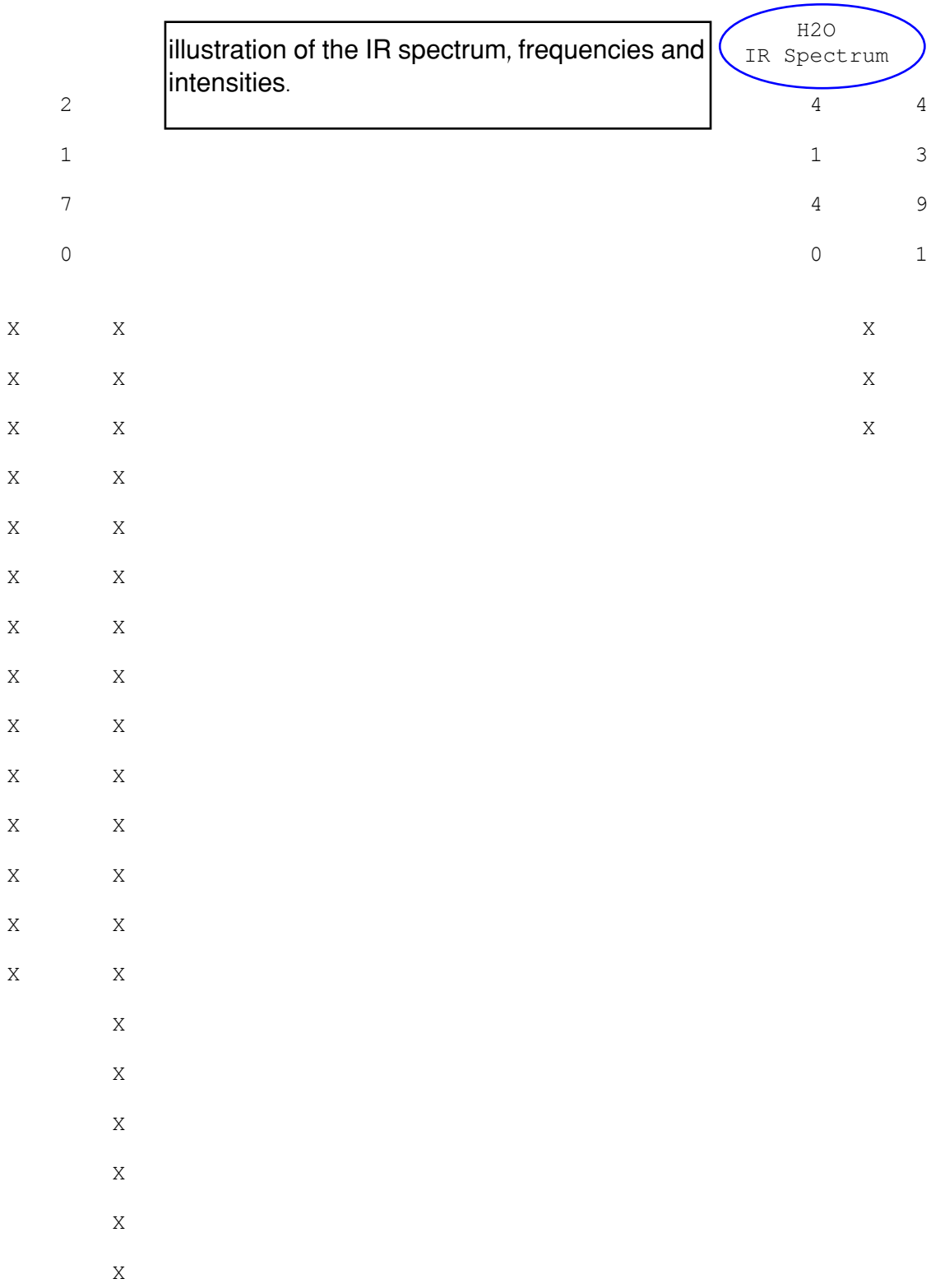
```
6.67386607                D-15 7.62375429D-02-3.00222083D-16
7.01220372-               D+00-1.56018150D-16-5.26407256D-16
4.11403190-               D+00
 Full mass-weighted force constant matrix:
 Low frequencies ---  -14.9935 0.0014    0.0007-   0.0012-   9.9999-   12.1649-
 Low frequencies --- 2170.0154 4140.0992 4391.1813
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),(
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
3                      2                      1
                      A1                     A1                     B2
 Frequencies --  2170.0154              4140.0992              4391.1813
 Red. masses --     1.0785                 1.0491                 1.0774
 Frc consts  --     2.9922                10.5946                12.2398
 IR Inten    --     7.2388                44.2856                29.9692
 Raman Activ --     9.2666                47.8189                21.5537
 Depolar     --     0.7246                 0.1791                 0.7500
 Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
0.00   0.07   0.00     0.05   0.00   0.00     0.07   0.00   0.00     8    1
0.45   0.54-  0.00     0.42-  0.57   0.00     0.54-  0.45-  0.00     1    2
0.45-  0.54-  0.00     0.42-  0.57-  0.00     0.54-  0.45   0.00     1    3

 -------------------
 - 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:
3         2         1
     EIGENVALUES --     2.58398   4.13662   6.72060
           X            0.00000   0.00000   1.00000
           Y            1.00000   0.00000   0.00000
           Z            0.00000   1.00000   0.00000
 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(
) 15.29827                                   Kcal/Mol(
 VIBRATIONAL TEMPERATURES:   3122.15  5956.64  6317.89
)          KELVIN(

 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

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  17.076             5.968            45.282
 ELECTRONIC              0.000             0.000             0.000
 TRANSLATIONAL           0.889             2.981            34.609
 ROTATIONAL              0.889             2.981            10.673
 VIBRATIONAL            15.298             0.006             0.001
```

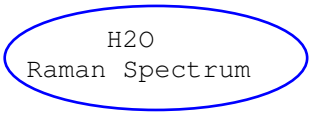
the 3*3-5 freq.

Note: there are other properties like Raman freq, IR intensity, Thermo-chemistry, etc.

	Q	LOG10(Q)	LN(Q(
TOTAL BOT	0.881269D-03	-3.054892	-7.034148
TOTAL V=0	0.144130D+09	8.158754	18.786226
VIB (BOT)	0.611457D-11	-11.213634	-25.820346
VIB (V=0)	0.100003D+01	0.000012	0.000028
ELECTRONIC	0.100000D+01	0.0000000.000000	
TRANSLATIONAL	0.300436D+07	6.477751	14.915574
ROTATIONAL	0.479723D+02	1.680991	3.870624

illustration of the IR spectrum, frequencies and intensities.





2 4 4

1 1 3

7 4 9

0 0 1

X X X

X X X

X X X

X X X

X X

X X

X X

X X

X X

X X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

***** Axes restored to original set*****

Center Number	Atomic Number	Forces (Hartrees/Bohr(X	Y	Z
0.000011758-	0.000000000	0.000014019-	8	1

```
0.000010065    0.000000000    0.000003499           1          2
0.000001693    0.000000000    0.000010521           1          3
--------------------------------------------------------------------
 Cartesian Forces:  Max     0.000014019 RMS     0.000007901
--------------------------------------------------------------------
           Internal Coordinate Forces (Hartree/Bohr or radian(
 Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
--------------------------------------------------------------------
  1   O
  2   H     1   0.000010(   1(
  3   H     1   0.000010(   2)  2  -0.000007(   3(
--------------------------------------------------------------------
 Internal  Forces:  Max     0.000010065 RMS     0.000009044
 Force constants in Cartesian coordinates :
5             4             3             2             1
0.704733  1   D+00
0.000000  2   D+00 -0152289.D-04
0.832544- 3   D-01  0.000000D+00  0.734178D+00
0.798532- 4   D-01  0.000000D+00 -0.669774D-01  0.849204D-01
0.000000  5   D+00  0.761447D-05  0.000000D+00  0.000000D+00 -0.571417D-05
0.538504  6   D-01  0.000000D+00 -0.639602D+00 -0.201621D-01  0.000000D+00
0.624880- 7   D+00  0.000000D+00  0.150232D+00 -0.506726D-02  0.000000D+00
0.000000  8   D+00  0.761447D-05  0.000000D+00  0.000000D+00 -0.190030D-05
0.294040  9   D-01  0.000000D+00 -0.945757D-01  0.871395D-01  0.000000D+00
9             8             7             6
0.654122  6   D+00
0.336883- 7   D-01  0.629947D+00
0.000000  8   D+00  0.000000D+00 -0.571417D-05
0.145195- 9   D-01 -0.116544D+00  0.000000D+00  0.109095D+00
 Force constants in internal coordinates :
3             2             1
0.654122  1   D+00
0.306452- 2   D-01  0.654122D+00
0.377005  3   D-01  0.377005D-01  0.296880D+00
 Leave Link  716 at Wed Feb 18 15:58:06 2004, MaxMem=    6291456 cpu:       0.1
) Enter /ua1/usr/local/g98/l103.exe(

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 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
)                                 Linear)    (Quad)   (Total(
    R         1.86969   0.00002   0.00000   0.00002   0.00002   1.86971
    A         1.74582  -0.00001   0.00000  -0.00003  -0.00003   1.74580
         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.
```

Frequency calculations are very sensitive to the geometry of the molecule, thus we must check if the geometry we are using is optimized.

This is an optimized geometry!

```
 --    Stationary point found.
----------------------------
   !                        Optimized Parameters!
) !                         Angstroms and Degrees!   (
----------------------                                ----------------------
      ! Name          Value   Derivative information (Atomic Units!     (
-------------------------------------------------------------------------
        ! R          0.9894   -DE/DX =    0!                            .
        ! A        100.0284   -DE/DX =    0!                            .
-------------------------------------------------------------------------
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link  103 at Wed Feb 18 15:58:08 2004, MaxMem=    6291456 cpu:       0.2
) Enter /ua1/usr/local/g98/l9999.exe(
\1\1 GINC-ATTO\Freq\RHF\STO-3G\H2O1\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-,.6462,0
0.27,.0.0370292,0,.0.2045404,0-,0.1945558-,.0.0289163,0-,.0.2798491,0,
\0.1783591,.0.0275457,0-,.98491,0 Polar=3.7807005,0.,0.0400615,-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-,.0,.1.6107089,0-,.9654,0
0-,.0.5198963,0,.0.0270535,1.8029034,0-,.0.440508,0-,4.6315952-,.691,0
5.7879,.0.884405,0-,0.0181178,.0.3496552,0,.2.1376814,0,.0,.4210006,0.
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(O1),SGV(H2)]\NImag=0\\0.70473285,0.,-0.00001523,-0.08
0.000007,.0.06697742,0.08492041,0-,.0.07985315,0-,0.73417797,.325445,0
0.654121,.0.02016213,0-,0.63960226-,.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,.0.00000190,0-,.0,.0.00000761,0
,.0.00001402,0\\0.10909519,.0.11654359,0-,0.01451948-,.71,0.08713955,0
@\\\0.00000169-,.0.00001052,0-,0.00001007-,.0.00000350,0-,0.00001176


 NATURE WILL TELL YOU A DIRECT LIE IF SHE CAN.

 --                                  CHARLES DARWIN
 Job cpu time:  0 days  0 hours  0 minutes  7.8 seconds.
 File lengths (MBytes):  RWF=    11 Int=     0 D2E=     0 Chk=     8 Scr=     1
 Normal termination of Gaussian 98.
```