Chemistry 416, Dr. Glaser
Applications of IR/Raman Spectra: Water and Ammonia

Attached you will find the printouts of *ab initio* calculations of H_20 and NH_3. The calculations were carried out at the RHF/3-21G level, but we need not be concerned with the computational details. What is of interest here, are the vibrational frequencies computed, the associated normal modes, and their IR and Raman intensities. All the important sections in each printout are highlighted in bold face for your convenience.

(a) Make a drawing of the molecule using the Cartesian coordinates found in the section "Standard Orientation".

(b) Find the highlighted section that contains the frequencies and associated information.

(c) Draw the normal mode representations. Here is how you do this: For every atom in the molecule (denoted by their atomic number and sequence number) you will find the x, y, and z components of the vector that shows the displacement of that atom for each particular frequency. Draw these vectors for all the atoms for each vibration. This displacement information is given with respect to the coordinate system shown in the "standard orientation".

(d) Considering your drawings of the normal modes, name these vibrations as "stretching" and "bending" modes and so on and state whether they are "symmetric" or "asymmetric".

(e) Below the frequencies, you will find the intensities computed for the IR and Raman spectra. As you can see, the relative intensities for the various frequencies are quite different in the two cases. Explain why that is so in light of your drawings of the vibrational modes.

(f) Now let's consider the number of frequencies in each case. Calculate the number of vibrations using 3N-6. How many frequencies are we observing for water and for ammonia? Explain the discrepancy (if any).

(g) Look up the actual experimental spectra for water and ammonia (in the gas phase) and comment on the accuracy of the calculations.

(2 attachments, freq. calc. of H_20 and NH_3 at RHF/3-21G).

```
****************************************
Gaussian 88:  VAX-VMS-G88RevC  19-Aug-1988
    VAX-3100  VMS-5.2  Sun 26-SEP-1993
****************************************
Default route: RHF/6-31G* Name=GLASER 6D 10F
----------------------------------------
# RHF/3-21G guess=read geom=checkpoint freq
----------------------------------------
1/10=4,29=10002,30=1/1,3;
2/10=1,12=2/2;
3/5=5,11=1,25=14,30=1/1,2,3,11,14;
4/5=1,7=1/1;
5//1;
8/6=4,11=10/1;
10/8=1,13=10/2;
11/6=2,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,8=1,9=1/2;
7/8=1,10=1,25=1/7,2,3,16;
1/10=4,30=1/3;
6/7=2,8=2,9=2,10=2,18=1/1;
99//99;
----------
water freq
----------
   Charge = 0 Multiplicity = 1
Z-Matrix taken from the checkpoint file:
DKB0:[GROUP.GLASER]WATER.CHK;1
O
H,1,ho
H,1,ho,2,hoh
     Variables:
ho=0.96666468
hoh=107.68075609
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                      ----------------------------
                      !   Initial Parameters    !
                      ! (Angstroms and Degrees) !
----------------------                          ------------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       ho          0.9667   calculate D2E/DX2 analytically            !
!       hoh       107.6808   calculate D2E/DX2 analytically            !
--------------------------------------------------------------------------------
Initial trust radius is 3.000D-01.
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
--------------------------------------------------------------------------------
                         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   0.966665(  1)
  3   3  H     1   0.966665(  2)   2  107.681(  3)
--------------------------------------------------------------------------------
                 Z-Matrix orientation:
---------------------------------------------------------------------
```

```
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------
   1          8           0.000000    0.000000    0.000000
   2          1           0.000000    0.000000    0.966665
   3          1           0.921003    0.000000   -0.293589
---------------------------------------------------------------
                   Distance matrix (angstroms):
             1          2          3
 1  O    0.000000
 2  H    0.966665   0.000000
 3  H    0.966665   1.560924   0.000000
                         Interatomic angles:
      H2-O1-H3=107.6808
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              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------
   1          8           0.000000    0.000000    0.114074
   2          1           0.000000    0.780462   -0.456294
   3          1           0.000000   -0.780462   -0.456294
---------------------------------------------------------------
Rotational constants (GHZ):    867.8358164    411.6218181    279.1965493
Isotopes: O-16,H-1,H-1
Radii and axes of the molecular ellipsoid:
                         1         2         3
    EIGENVALUES --     1.83986   1.07042   0.69800
        1              0.00000   0.00000   1.00000
        2             -1.00000   0.00000   0.00000
        3              0.00000   1.00000   0.00000
Standard basis: 3-21G     (S, S=P, 6D, 7F)
THERE ARE   7 SYMMETRY ADAPTED BASIS FUNCTIONS OF A1  SYMMETRY.
THERE ARE   0 SYMMETRY ADAPTED BASIS FUNCTIONS OF A2  SYMMETRY.
THERE ARE   2 SYMMETRY ADAPTED BASIS FUNCTIONS OF B1  SYMMETRY.
THERE ARE   4 SYMMETRY ADAPTED BASIS FUNCTIONS OF B2  SYMMETRY.
Crude estimate of integral set expansion from redundant integrals=1.247.
Integral buffers will be     16256 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
 13 basis functions      21 primitive gaussians
  5 alpha electrons        5 beta electrons
    nuclear repulsion energy    9.0978291294 Hartrees.
ONE-ELECTRON INTEGRAL SYMMETRY USED IN STVINT.
RysSet:  KIntrp=       98   KCalc=        0   KAssym=       73
The smallest eigenvalue of the overlap matrix is  1.106D-01
DipDrv:  will hold 34 matrices at once.
Out2E:  integral cutoff =  1.00D-10
Standard cutoffs selected in Shell.
    1314 INTEGRALS PRODUCED FOR A TOTAL OF      1314
SHELL:  FMTGEN WAS CALLED       97 TIMES.
Phoenix requires      17280 words of memory.
```

```
Out2E:  integral cutoff =  1.00D-10
Phenix exits -- no d or f functions.
       0 INTEGRALS PRODUCED FOR A TOTAL OF      1314
PHOENIX SHELL PASSES=       0  NUMBER PROCESSED=       0
         FAST PASSES=       0
RysSet:  KIntrp=        0   KCalc=        0   KAssym=        0
Initial guess read from the checkpoint file:
DKB0:[GROUP.GLASER]WATER.CHK;1
Guess basis functions will be translated to current atomic coordinates.
INITIAL GUESS ORBITAL SYMMETRIES.
      OCCUPIED  (A1) (A1) (B2) (A1) (B1)
      VIRTUAL   (A1) (B2) (B2) (A1) (B1) (A1) (B2) (A1)
Alpha deviation from unit magnitude is 4.16D-17 for orbital    1.
Alpha deviation from orthogonality  is 4.86D-17 for orbitals  13   2.
Using DIIS extrapolation.
RHF CLOSED SHELL SCF.
REQUESTED CONVERGENCE ON DENSITY MATRIX  0.1000D-08 WITHIN  64 CYCLES.
RHFClo:  Unsorted integral processing.
RHFCLO:  NGOT=   620032
Two-electron integrals will be kept in memory.
Orbital symmetries in FixScr:
  1=1   2=1   3=4   4=1   5=3   6=1   7=4   8=4   9=1  10=3
 11=1  12=4  13=1

                    -75.5859597587
                    -75.5859597587
                    -75.5859597587
                    -75.5859597587
SCF DONE:  E(RHF) =  -75.5859597587     A.U. AFTER    3 CYCLES
           CONVG  =    0.8498E-12             -V/T =  2.0021
KE= 7.542491888244D+01 PE=-1.979109210540D+02 EE= 3.780221328343D+01
RANGE OF M.O.'S USED FOR CORRELATION:   1  13
Minotr:  Closed-shell wavefunction.
         Using unsorted AO integrals in the linear equations.
         Solving linear equations separately.
         Using symmetry in CPHF.
         Requested convergence is 1.0D-09 RMS, and 1.0D-08 maximum.
         Differentiating once with respect to electric field.
               with respect to dipole field.
         MDV=   620032
         There are   3 degrees of freedom in the 1st order CPHF.
AX will form   3 AO Fock derivatives at one time.
Linear equations solution converged to 1.000D-09 1.000D-08 after  9
iterations.
Grad1E:  Ngot =   620032
Grad1E:  In-core method used.
RysSet:  KIntrp=      156   KCalc=        0   KAssym=       96
Grad2E:  fast logic used.
Standard cutoffs used.
PQCut1= 1.00D-20 PQCut2= 1.00D-20 PQCut3= 1.00D+02
PQCut4= 1.00D-20 PQCut6= 1.00D-20
Grad2E:  Fast passes=     226
RysSet:  KIntrp=     1903   KCalc=        0   KAssym=       46
Minotr:  Closed-shell wavefunction.
         Using unsorted AO integrals in the linear equations.
         Solving linear equations separately.
         Using symmetry in CPHF.
         Requested convergence is 1.0D-09 RMS, and 1.0D-08 maximum.
```

```
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         MDV=   620032
         There are   9 degrees of freedom in the 1st order CPHF.
Recover   3 previous solutions.
AX will form   6 AO Fock derivatives at one time.
Linear equations solution converged to 1.000D-09 1.000D-08 after  9
iterations.
RysSet:  KIntrp=      162   KCalc=        0   KAssym=       90
TWLHES:  FMTGEN WAS CALLED        73 TIMES.
Compute integral second derivatives.
DF integral derivatives using scalar Rys method.
Standard cutoffs used.
PQCut1= 1.00D-20 PQCut2= 1.00D-20 PQCut3= 1.00D+02 PQCut4= 1.00D-20
DDPhnx exits -- no d or f functions.
RysSet:  KIntrp=        0   KCalc=        0   KAssym=        0
Full mass-weighted force constant matrix:
Low frequencies ---   -0.0023   -0.0011   -0.0005    5.6420    7.1377
9.5472
Low frequencies --- 1799.3079 3812.3289 3945.7746
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:
                          1         2         3
                         A1        A1        B2
      Frequencies ---  1799.3079 3812.3289 3945.7746
   Reduced masses ---     1.0898    1.0386    1.0850
  Force constants ---     2.0788    8.8935    9.9528
   IR Intensities ---    79.9505    0.0486    9.1665
 Raman Activities ---    11.4941   95.6646   44.0833
  Depolarizations ---     0.4298    0.2180    0.7500
Coord Atom Element:
  4     1     8          0.00000   0.00000   0.00000
  4     1     8          0.00000   0.00000  -0.07176
  4     1     8         -0.07397   0.04530   0.00000
  4     2     1          0.00000   0.00000   0.00000
  4     2     1          0.39078   0.60805   0.56943
  4     2     1          0.58699  -0.35950  -0.41614
  4     3     1          0.00000   0.00000   0.00000
  4     3     1         -0.39078  -0.60805   0.56943
  4     3     1          0.58699  -0.35950   0.41614
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:
                     1                     2                     3
                    A1                    A1                    B2
Frequencies --  1799.3079             3812.3289             3945.7746
Red. masses --     1.0898                1.0386                1.0850
Frc consts  --     2.0788                8.8935                9.9528
IR Inten    --    79.9505                0.0486                9.1665
Raman Activ --    11.4941               95.6646               44.0833
Depolar     --     0.4298                0.2180                0.7500
Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
  1   8     0.00   0.00  -0.07     0.00   0.00   0.05     0.00  -0.07   0.00
  2   1     0.00   0.39   0.59     0.00   0.61  -0.36     0.00   0.57  -0.42
  3   1     0.00  -0.39   0.59     0.00  -0.61  -0.36     0.00   0.57   0.42
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- 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.
Principle axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --     2.07959   4.38446   6.46405
          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)     41.64931    19.75462    13.39924
ROTATIONAL CONSTANTS (GHZ)          867.83582   411.62182   279.19655
ZERO-POINT VIBRATIONAL ENERGY      57166.0 (JOULES/MOL)
                                  13.66301 (KCAL/MOL)
                                 0.0217734 (HARTREE/PARTICLE)
VIBRATIONAL TEMPERATURES:   2588.79  5485.06  5677.06
         (KELVIN)
SUM OF THERMAL ENERGIES:    0.0246073 (HARTREE/PARTICLE)
SUM OF HARTREE-FOCK AND THERMAL ENERGIES:  -75.5613524 (HARTREE/PARTICLE)
                       E                 CV                S
                   JOULES/MOL     JOULES/MOL-KELVIN   JOULES/MOL-KELVIN
TOTAL               64606.586             25.050            188.647
ELECTRONIC              0.000              0.000              0.000
TRANSLATIONAL        3718.457             12.472            144.802
ROTATIONAL           3718.457             12.472             43.831
VIBRATIONAL         57169.672              0.106              0.014
                       E                 CV                S
                   KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                 15.441              5.987             45.088
ELECTRONIC             0.000              0.000              0.000
TRANSLATIONAL          0.889              2.981             34.609
ROTATIONAL             0.889              2.981             10.476
VIBRATIONAL           13.664              0.025              0.003
                     Q            LOG10(Q)             LN(Q)
TOTAL BOT       0.126139E-01         -1.899152         -4.373127
TOTAL V=0       0.130570E+09          8.115844         18.687251
VIB (BOT)       0.966225E-10        -10.014922        -23.060209
VIB (V=0)       0.100017E+01          0.000074          0.000169
ELECTRONIC      0.100000E+01          0.000000          0.000000
TRANSLATIONAL   0.300436E+07          6.477751         14.915574
ROTATIONAL      0.434529E+02          1.638019          3.771678
***** AXES RESTORED TO ORIGINAL SET *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          8           0.000005375    0.000000000    0.000003928
   2          1          -0.000001631    0.000000000   -0.000003409
   3          1          -0.000003744    0.000000000   -0.000000518
-------------------------------------------------------------------
          MAX     0.000005375     RMS     0.000002846
-------------------------------------------------------------------
```

```
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
--------------------------------------------------------------------------
 1   O
 2   H     1  -0.000003 (  1)
 3   H     1  -0.000003 (  2)  2   0.000003 (  3)
--------------------------------------------------------------------------
                 MAX     0.000003409     RMS     0.000003272
FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).
           1             2             3             4             5
  1  0.532909D+00
  2 -0.172694D-16  0.617591D-05
  3 -0.133354D+00 -0.246251D-16  0.617928D+00
  4 -0.548533D-01  0.444216D-17 -0.400849D-01  0.591985D-01
  5  0.548981D-18 -0.308760D-05  0.275736D-16 -0.149156D-17  0.215066D-05
  6  0.385344D-01  0.240516D-16 -0.520565D+00 -0.234317D-01 -0.257076D-16
  7 -0.478056D+00  0.128272D-16  0.173439D+00 -0.434519D-02  0.942574D-18
  8  0.167204D-16 -0.308760D-05 -0.294854D-17 -0.295060D-17  0.936588D-06
  9  0.948196D-01  0.573449D-18 -0.973626D-01  0.635166D-01 -0.186597D-17
           6             7             8             9
  6  0.540343D+00
  7 -0.151027D-01  0.482401D+00
  8  0.165602D-17 -0.137698D-16  0.215066D-05
  9 -0.197781D-01 -0.158336D+00  0.129252D-17  0.117141D+00
FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).
           1             2             3
  1  0.540343D+00
  2 -0.838245D-02  0.540343D+00
  3  0.428017D-01  0.428017D-01  0.197536D+00
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:
                         ho        hoh
          ho           1.06392
          hoh          0.08560   0.19754
    Eigenvalues ---    0.18916   1.07230
Angle between quadratic step and forces=  43.29 degrees.
Linear search not attempted -- first point.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)

   ho        1.82673  -0.00001   0.00000  -0.00001  -0.00001   1.82672
  hoh        1.87938   0.00000   0.00000   0.00002   0.00002   1.87940
        Item               Value     Threshold  Converged?
Maximum Force            0.000007     0.000450     YES
RMS     Force            0.000005     0.000300     YES
Maximum Displacement     0.000019     0.001800     YES
RMS     Displacement     0.000014     0.001200     YES
Predicted change in energy=-5.449593D-11
Optimization completed.
   -- Stationary point found.
                       ----------------------------
                       !  Optimized Parameters   !
                       ! (Angstroms and Degrees) !
```

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!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       ho          0.9667   -DE/DX =   -0.000007                      !
!       hoh       107.6808   -DE/DX =    0.000003                      !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Copying SCF densities to generalized density rwf.

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

          Population analysis using the SCF density.

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

ORBITAL SYMMETRIES.
      OCCUPIED  (A1) (A1) (B2) (A1) (B1)
      VIRTUAL   (A1) (B2) (B2) (A1) (B1) (A1) (B2) (A1)
 THE ELECTRONIC STATE IS 1-A1.
Alpha eigenvalues --  -20.42722  -1.32097  -0.68554  -0.52983  -0.47723
Alpha eigenvalues --    0.26107   0.36033   1.20665   1.27667   1.78397
Alpha eigenvalues --    1.86334   2.02480   3.10330
         Condensed to atoms (all electrons):
             1          2          3
 1  O    8.204676   0.264079   0.264079
 2  H    0.264079   0.407946  -0.038443
 3  H    0.264079  -0.038443   0.407946
Total atomic charges:
             1
 1  O   -0.732834
 2  H    0.366417
 3  H    0.366417
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
Charge= 0.0000 esu
Dipole moment (Debye):
   X=     0.0000    Y=     0.0000    Z=    -2.3874  Tot=     2.3874
Quadrupole moment (Debye-Ang):
  XX=    -6.8381   YY=    -3.9719   ZZ=    -5.8823
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -1.1881  XYY=     0.0000
 XXY=     0.0000  XXZ=    -0.3033  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.2229  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=    -4.2011 YYYY=    -5.4004 ZZZZ=    -5.2845 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -1.8619 XXZZ=    -1.6231 YYZZ=    -1.4986
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 9.097829129430D+00 E-N=-1.979109210540D+02  KE= 7.542491888244D+01
 Exact polarizability:   0.783   0.000   6.802   0.000   0.000   3.627
Approx polarizability:   0.581   0.000   4.867   0.000   0.000   2.824
Unable to assign archive entry number now.
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```
1\1\UMC-RGPSI\FREQ\RHF\3-21G\H2O1\GLASER\26-SEP-1993\1\\# RHF/3-21G GU
ESS=READ GEOM=CHECKPOINT FREQ\\water freq\\0,1\O\H,1,ho\H,1,ho,2,hoh\\
ho=0.966665\hoh=107.680756\\Version=VAX-VMS-G88RevC\State=1-A1\HF=-75.
5859598\RMSD=0.850D-12\RMSF=0.285D-05\Dipole=0.7583463,0.,0.5542053\Di
poleDeriv=-0.349642,0.,0.0274502,0.,-0.8714406,0.,0.0274502,0.,-0.3671
427,0.3085573,0.,-0.0929317,0.,0.4357203,0.,-0.019781,0.,0.049835,0.04
10847,0.,0.0654814,0.,0.4357203,0.,-0.0076693,0.,0.3173076\Polar=4.732
1877,0.,0.7834907,-1.5125139,0.,5.6964779\PolarDeriv=-7.6779752,0.,0.3
877201,0.7365787,0.,-2.2599733,0.,-2.1298598,0.,0.,-1.5565179,0.,-0.00
16315,0.,0.2833489,-1.2498441,0.,-7.2610977,0.2605339,0.,-0.0190259,1.
7595556,0.,0.9629948,0.,-0.1389286,0.,0.,2.4255575,0.,0.3545643,0.,-0.
3809086,-0.8385932,0.,8.4018771,7.4174413,0.,-0.3686942,-2.4961343,0.,
1.2969785,0.,2.2687884,0.,0.,-0.8690396,0.,-0.3529328,0.,0.0975597,2.0
884373,0.,-1.1407795\HyperPolar=23.3536856,0.,0.5868588,0.,-7.4414723,
0.,0.4288809,2.3743139,0.,26.2436922\PG=C02V [C2(O1),SGV(H2)]\NIMAG=0\
\0.53290903,0.0,0.00000618,-0.13335399,0.0,0.61792772,-0.05485326,0.0,
-0.04008492,0.05919845,0.0,-0.00000309,0.0,0.0,0.00000215,0.03853437,0
.0,-0.52056512,-0.02343165,0.0,0.54034323,-0.47805578,0.0,0.17343892,-
0.00434519,0.0,-0.01510272,0.48240097,0.0,-0.00000309,0.0,0.0,0.000000
94,0.0,0.0,0.00000215,0.09481963,0.0,-0.09736260,0.06351657,0.0,-0.019
77811,-0.15833620,0.0,0.11714071\\-0.00000537,0.0,-0.00000393,0.000001
63,0.0,0.00000341,0.00000374,0.0,0.00000052\\@


WE LOSE BECAUSE WE WIN

GAMBLERS,

RECOLLECTING WHICH,

TOSS THEIR DICE AGAIN....


                        EMILY DICKINSON  BOLTS OF MELODY NO. 533

Final File Lengths (Blocks):
GAUSS_RWF       6408 -- deleted
GAUSS_INT       2541 -- deleted
GAUSS_CHK        948

Time used:
 IO time  0 days  0 hours  5 minutes 48.7 seconds.
CPU time  0 days  0 hours  3 minutes 57.8 seconds.
TOT time  0 days  0 hours  9 minutes 46.5 seconds.
  RAINER       job terminated at 26-SEP-1993 16:17:06.67

  Accounting information:
  Buffered I/O count:         2187      Peak working set size: 10200
  Direct I/O count:          17436      Peak page file size:   25266
  Page faults:               48381      Mounted volumes:           0
  Charged CPU time:     0 00:03:58.71   Elapsed time:     0 00:13:28.31
```

```
****************************************
Gaussian 88:  VAX-VMS-G88RevC  19-Aug-1988
    VAX-3100  VMS-5.2  Sun 26-SEP-1993
****************************************
Default route: RHF/6-31G* Name=GLASER 6D 10F
-----------------------------------------
# RHF/3-21G guess=read geom=checkpoint freq
-----------------------------------------
1/10=4,29=10002,30=1/1,3;
2/10=1,12=2/2;
3/5=5,11=1,25=14,30=1/1,2,3,11,14;
4/5=1,7=1/1;
5//1;
8/6=4,11=10/1;
10/8=1,13=10/2;
11/6=2,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,8=1,9=1/2;
7/8=1,10=1,25=1/7,2,3,16;
1/10=4,30=1/3;
6/7=2,8=2,9=2,10=2,18=1/1;
99//99;
------------
ammonia freq
------------
   Charge = 0 Multiplicity = 1
Z-Matrix taken from the checkpoint file:
DKB0:[GROUP.GLASER]AMMONIA.CHK;1
N
X,1,1.
H,1,hn,2,hnx
H,1,hn,2,hnx,3,120.,0
H,1,hn,2,hnx,3,-120.,0
     Variables:
hn=1.00259511
hnx=106.38373576
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                      ----------------------------
                      !   Initial Parameters    !
                      ! (Angstroms and Degrees) !
---------------------                            ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       hn          1.0026   calculate D2E/DX2 analytically            !
!       hnx       106.3837   calculate D2E/DX2 analytically            !
--------------------------------------------------------------------------------
Initial trust radius is 3.000D-01.
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
--------------------------------------------------------------------------------
                        Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------------
  1   1  N
  2      X     1   1.000000(  1)
  3   2  H     1   1.002595(  2)   2  106.384(  5)
  4   3  H     1   1.002595(  3)   2  106.384(  6)   3  120.000(  8)   0
```

```
  5   4  H     1   1.002595(  4)   2  106.384(  7)   3 -120.000(  9)   0
--------------------------------------------------------------------------
                Z-Matrix orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          7           0.000000    0.000000    0.000000
   2         -1           0.000000    0.000000    1.000000
   3          1           0.961884    0.000000   -0.282801
   4          1          -0.480942   -0.833016   -0.282801
   5          1          -0.480942    0.833016   -0.282801
---------------------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  X    1.000000   0.000000
 3  H    1.002595   1.603371   0.000000
 4  H    1.002595   1.603371   1.666032   0.000000
 5  H    1.002595   1.603371   1.666032   1.666032   0.000000
                        Interatomic angles:
      X2-N1-H3=106.3837       X2-N1-H4=106.3837       H3-N1-H4=112.3743
      X2-N1-H5=106.3837       H3-N1-H5=112.3743       H4-N1-H5=112.3743
STOICHIOMETRY    H3N
FRAMEWORK GROUP  C3V[C3(N),3SGV(H)]
DEG. OF FREEDOM    2
FULL POINT GROUP                 C3V     NOP  6
LARGEST ABELIAN SUBGROUP         CS      NOP  2
LARGEST CONCISE ABELIAN SUBGROUP CS      NOP  2
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          7           0.000000    0.000000    0.084840
   2          1           0.000000    0.961884   -0.197961
   3          1           0.833016   -0.480942   -0.197961
   4          1          -0.833016   -0.480942   -0.197961
---------------------------------------------------------------------
Rotational constants (GHZ):    316.3445851    316.3445851    180.6615026
Isotopes: N-14,H-1,H-1,H-1
Radii and axes of the molecular ellipsoid:
                         1         2         3
    EIGENVALUES --     1.93917   1.72827   0.80296
        1              0.50000  -0.86603   0.00000
        2             -0.86603  -0.50000   0.00000
        3              0.00000   0.00000   1.00000
Standard basis: 3-21G     (S, S=P, 6D, 7F)
THERE ARE  11 SYMMETRY ADAPTED BASIS FUNCTIONS OF A'  SYMMETRY.
THERE ARE   4 SYMMETRY ADAPTED BASIS FUNCTIONS OF A"  SYMMETRY.
Crude estimate of integral set expansion from redundant integrals=1.305.
Integral buffers will be     16256 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
 15 basis functions      24 primitive gaussians
  5 alpha electrons        5 beta electrons
    nuclear repulsion energy   12.0368402125 Hartrees.
ONE-ELECTRON INTEGRAL SYMMETRY USED IN STVINT.
```

```
RysSet:  KIntrp=      197   KCalc=        0   KAssym=      167
The smallest eigenvalue of the overlap matrix is  7.101D-02
DipDrv:  will hold 34 matrices at once.
Out2E:  integral cutoff =  1.00D-10
Standard cutoffs selected in Shell.
    3638 INTEGRALS PRODUCED FOR A TOTAL OF      3638
SHELL:  FMTGEN WAS CALLED      402 TIMES.
Phoenix requires      17280 words of memory.
Out2E:  integral cutoff =  1.00D-10
Phenix exits -- no d or f functions.
       0 INTEGRALS PRODUCED FOR A TOTAL OF      3638
PHOENIX SHELL PASSES=       0  NUMBER PROCESSED=       0
         FAST PASSES=       0
RysSet:  KIntrp=        0   KCalc=        0   KAssym=        0
Initial guess read from the checkpoint file:
DKB0:[GROUP.GLASER]AMMONIA.CHK;1
Guess basis functions will be translated to current atomic coordinates.
INITIAL GUESS ORBITAL SYMMETRIES.
      OCCUPIED  (A1) (A1) (E) (E) (A1)
      VIRTUAL   (A1) (E) (E) (E) (E) (A1) (A1) (E) (E) (A1)
Alpha deviation from unit magnitude is 8.33D-17 for orbital   15.
Alpha deviation from orthogonality  is 1.04D-16 for orbitals  15   2.
Using DIIS extrapolation.
RHF CLOSED SHELL SCF.
REQUESTED CONVERGENCE ON DENSITY MATRIX  0.1000D-08 WITHIN  64 CYCLES.
RHFClo:  Unsorted integral processing.
RHFCLO:  NGOT=   620032
Two-electron integrals will be kept in memory.
Orbital symmetries in FixScr:
  1=1   2=1   3=2   4=1   5=1   6=1   7=1   8=2   9=2  10=1
 11=1  12=1  13=2  14=1  15=1

                    -55.8722034683
                    -55.8722034683
                    -55.8722034683
                    -55.8722034683
SCF DONE:  E(RHF) =  -55.8722034683     A.U. AFTER    3 CYCLES
           CONVG  =    0.7100E-12             -V/T =  2.0020
KE= 5.575882517059D+01 PE=-1.552144339754D+02 EE= 3.154656512398D+01
RANGE OF M.O.'S USED FOR CORRELATION:   1  15
Minotr:  Closed-shell wavefunction.
         Using unsorted AO integrals in the linear equations.
         Solving linear equations separately.
         Using symmetry in CPHF.
         Requested convergence is 1.0D-09 RMS, and 1.0D-08 maximum.
         Differentiating once with respect to electric field.
               with respect to dipole field.
         MDV=   620032
         There are   3 degrees of freedom in the 1st order CPHF.
AX will form   3 AO Fock derivatives at one time.
Linear equations solution converged to 1.000D-09 1.000D-08 after  8
iterations.
Grad1E:  Ngot =   620032
Grad1E:  In-core method used.
RysSet:  KIntrp=      295   KCalc=        0   KAssym=      213
Grad2E:  fast logic used.
Standard cutoffs used.
PQCut1= 1.00D-20 PQCut2= 1.00D-20 PQCut3= 1.00D+02
```

```
PQCut4= 1.00D-20 PQCut6= 1.00D-20
Grad2E:  Fast passes=     610
RysSet:  KIntrp=     4636   KCalc=        0   KAssym=      215
Minotr:  Closed-shell wavefunction.
         Using unsorted AO integrals in the linear equations.
         Solving linear equations separately.
         Using symmetry in CPHF.
         Requested convergence is 1.0D-09 RMS, and 1.0D-08 maximum.
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         MDV=   620032
         There are  12 degrees of freedom in the 1st order CPHF.
Recover   3 previous solutions.
AX will form   9 AO Fock derivatives at one time.
Linear equations solution converged to 1.000D-09 1.000D-08 after  9
iterations.
RysSet:  KIntrp=      322   KCalc=        0   KAssym=      186
TWLHES:  FMTGEN WAS CALLED       318 TIMES.
Compute integral second derivatives.
DF integral derivatives using scalar Rys method.
Standard cutoffs used.
PQCut1= 1.00D-20 PQCut2= 1.00D-20 PQCut3= 1.00D+02 PQCut4= 1.00D-20
DDPhnx exits -- no d or f functions.
RysSet:  KIntrp=        0   KCalc=        0   KAssym=        0
Full mass-weighted force constant matrix:
Low frequencies ---  -23.8996  -20.3446  -20.3443    0.0006    0.0007
0.0009
Low frequencies ---  856.1289 1858.0312 1858.0312
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:
                          1         2         3         4         5
                         A1         E         E        A1         E
      Frequencies ---   856.1289 1858.0312 1858.0312 3644.6745 3800.8265
   Reduced masses ---     1.1947    1.0787    1.0787    1.0163    1.0938
  Force constants ---     0.5159    2.1941    2.1941    7.9543    9.3099
   IR Intensities ---   380.7176   22.7108   22.7108    0.2738    0.9365
 Raman Activities ---     8.8333   10.4123   10.4123  108.6895   47.2013
  Depolarizations ---     0.0562    0.7500    0.7500    0.1210    0.7500
Coord Atom Element:
  6     1     7          0.00000   0.00000  -0.07384   0.00000   0.00000
  6     1     7          0.00000  -0.07384   0.00000   0.00000   0.08134
  6     1     7         -0.11992   0.00000   0.00000   0.02557   0.00000
  6     2     1          0.00000   0.00000   0.78283   0.00000   0.00000
  6     2     1          0.14159  -0.09888   0.00000   0.56488  -0.78252
  6     2     1          0.55542  -0.20109   0.00000  -0.11843   0.22151
  6     3     1          0.12262   0.38179   0.12155   0.48920   0.35145
  6     3     1         -0.07079   0.56240   0.38179  -0.28244  -0.17379
  6     3     1          0.55542   0.10054  -0.17414  -0.11843  -0.11075
  6     4     1         -0.12262  -0.38179   0.12155  -0.48920  -0.35145
  6     4     1         -0.07079   0.56240  -0.38179  -0.28244  -0.17379
  6     4     1          0.55542   0.10054   0.17414  -0.11843  -0.11075
                           6
                           E
      Frequencies ---  3800.8265
   Reduced masses ---     1.0938
  Force constants ---     9.3099
```

```
   IR Intensities ---     0.9365
 Raman Activities ---    47.2013
  Depolarizations ---     0.7500
Coord Atom Element:
  7     1     7         -0.08134
  7     1     7          0.00000
  7     1     7          0.00000
  7     2     1         -0.02912
  7     2     1          0.00000
  7     2     1          0.00000
  7     3     1          0.57961
  7     3     1         -0.35145
  7     3     1         -0.19183
  7     4     1          0.57961
  7     4     1          0.35145
  7     4     1          0.19183
```

Harmonic frequencies (cm-1), IR intensities (KM/Mole),**
Raman scattering activities (A4/AMU), Raman depolarization ratios,**
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1			2			3	
	A1			E			E	
Frequencies --	**856.1289**			**1858.0312**			**1858.0312**	
Red. masses --	**1.1947**			**1.0787**			**1.0787**	
Frc consts --	**0.5159**			**2.1941**			**2.1941**	
IR Inten --	**380.7176**			**22.7108**			**22.7108**	
Raman Activ --	**8.8333**			**10.4123**			**10.4123**	
Depolar --	**0.0562**			**0.7500**			**0.7500**	
Atom AN	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
1 7	**0.00**	**0.00**	**-0.12**	**0.00**	**-0.07**	**0.00**	**-0.07**	**0.00**	**0.00**
2 1	**0.00**	**0.14**	**0.56**	**0.00**	**-0.10**	**-0.20**	**0.78**	**0.00**	**0.00**
3 1	**0.12**	**-0.07**	**0.56**	**0.38**	**0.56**	**0.10**	**0.12**	**0.38**	**-0.17**
4 1	**-0.12**	**-0.07**	**0.56**	**-0.38**	**0.56**	**0.10**	**0.12**	**-0.38**	**0.17**

	4			5			6	
	A1			E			E	
Frequencies --	**3644.6745**			**3800.8265**			**3800.8265**	
Red. masses --	**1.0163**			**1.0938**			**1.0938**	
Frc consts --	**7.9543**			**9.3099**			**9.3099**	
IR Inten --	**0.2738**			**0.9365**			**0.9365**	
Raman Activ --	**108.6895**			**47.2013**			**47.2013**	
Depolar --	**0.1210**			**0.7500**			**0.7500**	
Atom AN	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
1 7	**0.00**	**0.00**	**0.03**	**0.00**	**0.08**	**0.00**	**-0.08**	**0.00**	**0.00**
2 1	**0.00**	**0.56**	**-0.12**	**0.00**	**-0.78**	**0.22**	**-0.03**	**0.00**	**0.00**
3 1	**0.49**	**-0.28**	**-0.12**	**0.35**	**-0.17**	**-0.11**	**0.58**	**-0.35**	**-0.19**
4 1	**-0.49**	**-0.28**	**-0.12**	**-0.35**	**-0.17**	**-0.11**	**0.58**	**0.35**	**0.19**

```
-------------------
- THERMOCHEMISTRY -
-------------------
TEMPERATURE   298.150 KELVIN.
PRESSURE      1.00000 ATM.
ATOM  1 HAS ATOMIC NUMBER  7 AND MASS  14.00307
ATOM  2 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM  3 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM  4 HAS ATOMIC NUMBER  1 AND MASS   1.00783
Molecular mass:    17.02655 amu.
Principle axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --     5.70499   5.70499   9.98963
```

```
          X            1.00000   0.00000   0.00000
          Y            0.00000  -1.00000   0.00000
          Z            0.00000   0.00000   1.00000
THIS MOLECULE IS AN OBLATE SYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  3.
ROTATIONAL TEMPERATURES (KELVIN)     15.18206    15.18206     8.67034
ROTATIONAL CONSTANTS (GHZ)          316.34459   316.34459   180.66150
ZERO-POINT VIBRATIONAL ENERGY      94615.8 (JOULES/MOL)
                                  22.61371 (KCAL/MOL)
                                 0.0360372 (HARTREE/PARTICLE)
VIBRATIONAL TEMPERATURES:   1231.77  2673.28  2673.28  5243.84  5468.51
         (KELVIN)           5468.51
SUM OF THERMAL ENERGIES:    0.0389356 (HARTREE/PARTICLE)
SUM OF HARTREE-FOCK AND THERMAL ENERGIES:  -55.8332678 (HARTREE/PARTICLE)
                      E                  CV                  S
                 JOULES/MOL     JOULES/MOL-KELVIN   JOULES/MOL-KELVIN
TOTAL            102225.529             27.469             192.377
ELECTRONIC            0.000              0.000               0.000
TRANSLATIONAL      3718.457             12.472             144.101
ROTATIONAL         3718.457             12.472              47.560
VIBRATIONAL       94788.615              2.525               0.716
                      E                  CV                  S
                  KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL               24.432              6.565              45.979
ELECTRONIC           0.000              0.000               0.000
TRANSLATIONAL        0.889              2.981              34.441
ROTATIONAL           0.889              2.981              11.367
VIBRATIONAL         22.655              0.604               0.171
                     Q            LOG10(Q)             LN(Q)
TOTAL BOT      0.507203E-08         -8.294818        -19.115970
TOTAL V=0      0.191007E+09          8.281050         19.051377
VIB (BOT)      0.269944E-16        -16.568726        -38.150901
VIB (V=0)      0.101658E+01          0.007143          0.016446
ELECTRONIC     0.100000E+01          0.000000          0.000000
TRANSLATIONAL  0.276153E+07          6.441150         14.831297
ROTATIONAL     0.680389E+02          1.832757          4.220080
***** AXES RESTORED TO ORIGINAL SET *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7           0.000000000    0.000000000   -0.000034817
   2          1           0.000039596    0.000000000    0.000011606
   3          1          -0.000019798   -0.000034291    0.000011606
   4          1          -0.000019798    0.000034291    0.000011606
-------------------------------------------------------------------
          MAX     0.000039596     RMS     0.000022949
-------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
 1   N
     X     1   0.000000 (  1)
 2   H     1   0.000035 (  2)  2  -0.000042 (  5)
 3   H     1   0.000035 (  3)  2  -0.000042 (  6)  3   0.000000 (  8)  0
 4   H     1   0.000035 (  4)  2  -0.000042 (  7)  3   0.000000 (  9)  0
-------------------------------------------------------------------------
                MAX     0.000042256     RMS     0.000031574
```

```
FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).
           1             2             3             4             5
  1  0.777871D+00
  2 -0.146422D-15  0.777871D+00
  3  0.616979D-16 -0.119642D-15  0.128889D+00
  4 -0.436479D+00  0.634258D-17  0.952643D-01  0.472857D+00
  5 -0.173472D-17 -0.821017D-01 -0.384892D-17  0.867362D-18  0.758148D-01
  6  0.152454D+00  0.705070D-17 -0.429629D-01 -0.117303D+00  0.203288D-18
  7 -0.170696D+00 -0.153450D+00 -0.476322D-01 -0.181889D-01 -0.419694D-01
  8 -0.153450D+00 -0.347885D+00 -0.825013D-01  0.502082D-02  0.314343D-02
  9 -0.762269D-01 -0.132029D+00 -0.429629D-01  0.110191D-01  0.139327D-01
 10 -0.170696D+00  0.153450D+00 -0.476322D-01 -0.181889D-01  0.419694D-01
 11  0.153450D+00 -0.347885D+00  0.825013D-01 -0.502082D-02  0.314343D-02
 12 -0.762269D-01  0.132029D+00 -0.429629D-01  0.110191D-01 -0.139327D-01
           6             7             8             9            10
  6  0.441882D-01
  7 -0.175756D-01  0.175075D+00
  8 -0.257651D-02  0.171924D+00  0.373596D+00
  9 -0.612621D-03  0.586513D-01  0.101587D+00  0.441882D-01
 10 -0.175756D-01  0.138096D-01 -0.234951D-01  0.655650D-02  0.175075D+00
 11  0.257651D-02  0.234951D-01 -0.288550D-01  0.165092D-01 -0.171924D+00
 12 -0.612621D-03  0.655650D-02 -0.165092D-01 -0.612621D-03  0.586513D-01
          11            12
 11  0.373596D+00
 12 -0.101587D+00  0.441882D-01
FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).
           1             2             3             4             5
  1  0.000000D+00
  2  0.000000D+00  0.502238D+00
  3  0.000000D+00 -0.164400D-02  0.502238D+00
  4  0.000000D+00 -0.164400D-02 -0.164400D-02  0.502238D+00
  5  0.000000D+00 -0.328829D-01 -0.203027D-01 -0.203027D-01  0.532157D-01
  6  0.000000D+00 -0.203027D-01 -0.328829D-01 -0.203027D-01  0.207396D-01
  7  0.000000D+00 -0.203027D-01 -0.203027D-01 -0.328829D-01  0.207396D-01
  8  0.000000D+00  0.247041D-01  0.591257D-09 -0.247041D-01 -0.637742D-01
  9  0.000000D+00 -0.247041D-01  0.247041D-01 -0.591257D-09  0.637742D-01
           6             7             8             9
  6  0.532157D-01
  7  0.207396D-01  0.532157D-01
  8  0.117538D-08  0.637742D-01  0.250566D+00
  9 -0.637742D-01 -0.117538D-08 -0.125283D+00  0.250566D+00
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
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:
                         hn        hnx
          hn           1.49685
          hnx         -0.22046   0.28408
    Eigenvalues ---    0.24525   1.53568
Angle between quadratic step and forces=  38.84 degrees.
Linear search not attempted -- first point.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)

   hn        1.89463   0.00010   0.00000   0.00000   0.00000   1.89463
```

```
  hnx        1.85675  -0.00013   0.00000  -0.00044  -0.00044   1.85630
        Item               Value     Threshold  Converged?
Maximum Force            0.000127     0.000450     YES
RMS     Force            0.000116     0.000300     YES
Maximum Displacement     0.000443     0.001800     YES
RMS     Displacement     0.000313     0.001200     YES
Predicted change in energy=-2.829714D-08
Optimization completed.
   -- Stationary point found.
                       ---------------------------
                       !  Optimized Parameters   !
                       ! (Angstroms and Degrees) !
---------------------                            ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------
!       hn          1.0026   -DE/DX =    0.000104                      !
!       hnx       106.3837   -DE/DX =   -0.000127                      !
--------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Copying SCF densities to generalized density rwf.

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

           Population analysis using the SCF density.

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

ORBITAL SYMMETRIES.
      OCCUPIED  (A1) (A1) (E) (E) (A1)
      VIRTUAL   (A1) (E) (E) (E) (E) (A1) (A1) (E) (E) (A1)
 THE ELECTRONIC STATE IS 1-A1.
Alpha eigenvalues --  -15.43154  -1.12009  -0.62031  -0.62031  -0.38898
Alpha eigenvalues --    0.27526   0.37736   0.37736   1.18644   1.18644
Alpha eigenvalues --    1.28990   1.41270   1.59869   1.59869   2.57458
         Condensed to atoms (all electrons):
              1          2          3          4
 1  N    6.867170   0.336328   0.336328   0.336328
 2  H    0.336328   0.436193  -0.032286  -0.032286
 3  H    0.336328  -0.032286   0.436193  -0.032286
 4  H    0.336328  -0.032286  -0.032286   0.436193
Total atomic charges:
              1
 1  N   -0.876155
 2  H    0.292052
 3  H    0.292052
 4  H    0.292052
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  N    0.000000
 2  H    0.000000
 3  H    0.000000
 4  H    0.000000
Sum of Mulliken charges=   0.00000
Charge= 0.0000 esu
Dipole moment (Debye):
   X=     0.0000    Y=     0.0000    Z=    -1.7534  Tot=     1.7534
Quadrupole moment (Debye-Ang):
```

```
  XX=    -5.7305   YY=    -5.7305   ZZ=    -8.6919
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     0.0000  YYY=     0.9183  ZZZ=    -1.2946  XYY=     0.0000
 XXY=    -0.9183  XXZ=    -0.7238  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -0.7238  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=    -8.4230 YYYY=    -8.4230 ZZZZ=    -7.7585 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=    -0.2480 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8077 XXZZ=    -2.8578 YYZZ=    -2.8578
XXYZ=     0.2480 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 1.203684021246D+01 E-N=-1.552144339754D+02  KE= 5.575882517059D+01
 Exact polarizability:   7.936   0.000   7.936   0.000   0.000   2.409
Approx polarizability:   5.906   0.000   5.906   0.000   0.000   1.882
Unable to assign archive entry number now.
1\1\UMC-RGPSI\FREQ\RHF\3-21G\H3N1\GLASER\26-SEP-1993\1\\# RHF/3-21G GU
ESS=READ GEOM=CHECKPOINT FREQ\\ammonia freq\\0,1\N\X,1,1.\H,1,hn,2,hnx
\H,1,hn,2,hnx,3,120.,0\H,1,hn,2,hnx,3,-120.,0\\hn=1.002595\hnx=106.383
736\\Version=VAX-VMS-G88RevC\State=1-A1\HF=-55.8722035\RMSD=0.710D-12\
RMSF=0.229D-04\Dipole=0.,0.,-0.6898411\DipoleDeriv=-0.3463854,0.,0.,0.
,-0.3463854,0.,0.,0.,-0.9660575,0.0622884,0.,0.0721185,0.,0.1686352,0.
,0.1851159,0.,0.3220191,0.1420485,-0.0460495,-0.0360593,-0.0460495,0.0
888751,-0.0624565,-0.092558,-0.1603151,0.3220191,0.1420485,0.0460495,-
0.0360593,0.0460495,0.0888751,0.0624565,-0.092558,0.1603151,0.3220191\
Polar=7.9360047,0.,7.9360047,0.,0.,2.4086503\PolarDeriv=-3.5413823,0.,
3.5413823,2.9737636,0.,0.,0.,3.5413823,0.,0.,2.9737636,0.,4.0924344,0.
,4.0924344,0.,0.,3.7551364,7.7351846,0.,0.0814574,-1.1039184,0.,-0.264
0793,0.,1.4659421,0.,0.,-0.8785907,0.,-2.0582736,0.,-0.6700161,2.61011
,0.,-1.2517121,-2.0969012,-2.2918521,-1.8114198,-0.9349226,-0.0975698,
0.1320397,-1.0928532,-2.5036622,-5.6765574,-0.0975698,-1.0475865,0.228
6994,-1.0170804,-0.6011332,-1.7112092,-1.305055,-2.2604216,-1.2517121,
-2.0969012,2.2918521,-1.8114198,-0.9349226,0.0975698,0.1320397,1.09285
32,-2.5036622,5.6765574,0.0975698,-1.0475865,-0.2286994,-1.0170804,0.6
011332,-1.7112092,-1.305055,2.2604216,-1.2517121\HyperPolar=20.9409941
,0.,-20.9409941,0.,-10.3415882,0.,-10.3415882,0.,0.,-2.4506764\PG=C03V
 [C3(N1),3SGV(H1)]\NIMAG=0\\0.77787084,0.0,0.77787084,0.0,0.0,0.128888
83,-0.43647890,0.0,0.09526431,0.47285661,0.0,-0.08210167,0.0,0.0,0.075
81481,0.15245385,0.0,-0.04296294,-0.11730258,0.0,0.04418818,-0.1706959
8,-0.15344984,-0.04763216,-0.01818885,-0.04196942,-0.01757563,0.175075
26,-0.15344984,-0.34788459,-0.08250131,0.00502082,0.00314343,-0.002576
51,0.17192414,0.37359616,-0.07622692,-0.13202890,-0.04296294,0.0110191
4,0.01393269,-0.00061262,0.05865129,0.10158702,0.04418818,-0.17069598,
0.15344984,-0.04763216,-0.01818885,0.04196942,-0.01757563,0.01380957,-
0.02349512,0.00655650,0.17507526,0.15344984,-0.34788459,0.08250131,-0.
00502082,0.00314343,0.00257651,0.02349512,-0.02885499,0.01650920,-0.17
192414,0.37359616,-0.07622692,0.13202890,-0.04296294,0.01101914,-0.013
93269,-0.00061262,0.00655650,-0.01650920,-0.00061262,0.05865129,-0.101
58702,0.04418818\\0.0,0.0,0.00003482,-0.00003960,0.0,-0.00001161,0.000
01980,0.00003429,-0.00001161,0.00001980,-0.00003429,-0.00001161\\@


ONE OF THE BENEFITS OF A COLLEGE EDUCATION
IS TO SHOW THE BOY ITS LITTLE AVAIL
                                    EMERSON IN 'CULTURE'

Final File Lengths (Blocks):
GAUSS_RWF       6408 -- deleted
GAUSS_INT       2541 -- deleted
```

```
GAUSS_CHK        951

Time used:
 IO time  0 days  0 hours  6 minutes 45.8 seconds.
CPU time  0 days  0 hours  5 minutes  3.1 seconds.
TOT time  0 days  0 hours 11 minutes 48.9 seconds.
  RAINER       job terminated at 26-SEP-1993 16:44:20.68

  Accounting information:
  Buffered I/O count:         2196      Peak working set size: 10200
  Direct I/O count:          20290      Peak page file size:   25266
  Page faults:               50058      Mounted volumes:           0
  Charged CPU time:     0 00:05:04.07   Elapsed time:     0 00:27:13.03
```