```
1          ****************************************************
           *            GAMESS VERSION =  6 MAY 1998            *
           *             FROM IOWA STATE UNIVERSITY             *
           * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
           *   M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,   *
           *          K.A.NGUYEN, S.J.SU, T.L.WINDUS,           *
           *       TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY       *
           *         J.COMPUT.CHEM.  14, 1347-1363(1993)        *
           ********** POWER MACINTOSH (MAC) VERSION ************

 EXECUTION OF GAMESS BEGUN 16:18:34 10-07-1999

            ECHO OF THE FIRST FEW INPUT CARDS -
 INPUT CARD> $CONTRL SCFTYP=RHF RUNTYP=HESSIAN $END
 INPUT CARD> $BASIS GBASIS=STO NGAUSS=3  $END
 INPUT CARD> $DATA
 INPUT CARD>    STO3G NH3
 INPUT CARD>    CNV  3
 INPUT CARD>
 INPUT CARD> N           7.0    .0000000000    .0000000000   -.0019717070
 INPUT CARD> H           1.0    .9405679704    .0000000000    .4239891888
 INPUT CARD>  $END
     750000 WORDS OF MEMORY AVAILABLE

     BASIS OPTIONS
     -------------
     GBASIS=STO          IGAUSS=       3      POLAR=NONE
     NDFUNC=       0     DIFFSP=       F
     NPFUNC=       0      DIFFS=       F


     RUN TITLE
     ---------
     STO3G NH3

 THE POINT GROUP OF THE MOLECULE IS CNV
 THE ORDER OF THE PRINCIPAL AXIS IS     3

 ATOM      ATOMIC                      COORDINATES (BOHR)
           CHARGE         X                  Y                  Z
 N           7.0      .0000000000         .0000000000        -.0037259860
 H           1.0     -.8887078684        1.5392871812         .8012233886
 H           1.0     -.8887078684       -1.5392871812         .8012233886
 H           1.0     1.7774157369         .0000000000         .8012233886

          INTERNUCLEAR DISTANCES (ANGS.)
          ------------------------------

                    N              H              H              H

  1  N               .0000000      1.0325264 *    1.0325264 *    1.0325264 *
  2  H              1.0325264 *     .0000000      1.6291115 *    1.6291115 *
  3  H              1.0325264 *    1.6291115 *     .0000000      1.6291115 *
  4  H              1.0325264 *    1.6291115 *    1.6291115 *     .0000000
```

```
 * ... LESS THAN  3.000


    ATOMIC BASIS SET
    ----------------
THE CONTRACTED PRIMITIVE FUNCTIONS HAVE BEEN UNNORMALIZED
THE CONTRACTED BASIS FUNCTIONS ARE NOW NORMALIZED TO UNITY

SHELL TYPE PRIM    EXPONENT          CONTRACTION COEFFICIENTS

N

  1   S    1      99.106169    3.454881 (   .154329)
  1   S    2      18.052312    3.341410 (   .535328)
  1   S    3       4.885660    1.041372 (   .444635)

  2   L    4       3.780456    -.193164 (  -.099967)     1.171553 (   .155916)
  2   L    5        .878497     .258372 (   .399513)      .736704 (   .607684)
  2   L    6        .285714     .194997 (   .700115)      .116706 (   .391957)

H

  5   S    7       3.425251     .276934 (   .154329)
  5   S    8        .623914     .267839 (   .535328)
  5   S    9        .168855     .083474 (   .444635)

TOTAL NUMBER OF SHELLS              =    5
TOTAL NUMBER OF BASIS FUNCTIONS     =    8
NUMBER OF ELECTRONS                 =   10
CHARGE OF MOLECULE                  =    0
STATE MULTIPLICITY                  =    1
NUMBER OF OCCUPIED ORBITALS (ALPHA) =    5
NUMBER OF OCCUPIED ORBITALS (BETA ) =    5
TOTAL NUMBER OF ATOMS               =    4
THE NUCLEAR REPULSION ENERGY IS       11.7371288162

    $CONTRL OPTIONS
    ---------------
    SCFTYP=RHF          RUNTYP=HESSIAN      EXETYP=RUN
    MPLEVL=       0     LOCAL =NONE         UNITS =ANGS
    MULT  =       1     ICHARG=       0     MAXIT =      30
    NPRINT=       7     IREST =       0     COORD =UNIQUE
    ECP   =NONE         NORMF =       0     NORMP =       0
    ITOL  =      20     ICUT  =       9     NZVAR =       0
    NOSYM =       0     INTTYP=POPLE        GEOM  =INPUT
    PLTORB=       F     MOLPLT=       F     RPAC  =       F
    AIMPAC=       F     FRIEND=             CITYP =NONE

    $SYSTEM OPTIONS
    ---------------
    KDIAG =       0     MEMORY=  750000     TIMLIM=    36000.0 SEC.
    COREFL=       F     PTIME =       F     XDR   =       F
    BALTYP=NXTVAL

         ----------------
```

```
          PROPERTIES INPUT
          ----------------

    MOMENTS            FIELD           POTENTIAL          DENSITY
IEMOM =       1   IEFLD =       0   IEPOT =       0   IEDEN =       0
WHERE =COMASS     WHERE =NUCLEI     WHERE =NUCLEI     WHERE =NUCLEI
OUTPUT=BOTH       OUTPUT=BOTH       OUTPUT=BOTH       OUTPUT=BOTH
IEMINT=       0   IEFINT=       0                     IEDINT=       0
                                                      MORB  =       0
          EXTRAPOLATION IN EFFECT

          ----------------------
          INTEGRAL INPUT OPTIONS
          ----------------------
NOPK  =       1 NORDER=       0 SCHWRZ=       F

    -------------------------------
    INTEGRAL TRANSFORMATION OPTIONS
    -------------------------------
    NWORD  =       0     CUTOFF = 1.0E-09
    MPTRAN =       0     DIRTRF =       F
    AOINTS =DUP

    -----------------------------------------
    THE POINT GROUP IS CNV, NAXIS= 3, ORDER= 6
    -----------------------------------------

    DIMENSIONS OF THE SYMMETRY SUBSPACES ARE
A1  =   4      A2  =   0      E   =   2

..... DONE SETTING UP THE RUN .....
STEP CPU TIME =      .28 TOTAL CPU TIME =         .2 (     .0 MIN)
TOTAL WALL CLOCK TIME=         .2 SECONDS, CPU UTILIZATION IS 100.00%

    --------------------------------
    HESSIAN MATRIX CONTROL PARAMETERS
    --------------------------------
    METHOD=ANALYTIC   NVIB  =       1   VIBSIZ=  .01000
    RDHESS=       F   PURIFY=       F   PRTIFC=       F
    VIBANL=       T   DECOMP=       F   PROJCT=       F
    SCLFAC= 1.00000   PRTSCN=       F   NPRT  =       0
    PULCOR=       F   NPUN  =       0   REDOVB=       T
    THERMOCHEMISTRY WILL BE PRINTED FOR    1 TEMPERATURES:
     298.15000

    -------------------------------
    CPHF RESPONSE SOLUTION OPTIONS
    -------------------------------
    POLAR  =       F     NWORD  =       0

          ********************
          1 ELECTRON INTEGRALS
          ********************
...... END OF ONE-ELECTRON INTEGRALS ......
STEP CPU TIME =      .02 TOTAL CPU TIME =         .2 (     .0 MIN)
```

```
TOTAL WALL CLOCK TIME=         .2 SECONDS, CPU UTILIZATION IS 100.00%

         GUESS OPTIONS
         -------------
         GUESS =HUCKEL
         NORB  =       0          NORDER=       0
         TOLZ  = 1.0E-08          TOLE  = 1.0E-05
         MIX   =       F          PRTMO =       F

INITIAL GUESS ORBITALS GENERATED BY HUCKEL   ROUTINE.
HUCKEL GUESS REQUIRES      3248 WORDS.

SYMMETRIES FOR INITIAL GUESS ORBITALS FOLLOW.   BOTH SET(S).
    5 ORBITALS ARE OCCUPIED (    1 CORE ORBITALS).
    2=A1       3=E        4=E        5=A1       6=E        7=E        8=A1
...... END OF INITIAL ORBITAL SELECTION ......
STEP CPU TIME =      .12 TOTAL CPU TIME =         .4 (     .0 MIN)
TOTAL WALL CLOCK TIME=         .4 SECONDS, CPU UTILIZATION IS 100.00%

         --------------------
         2 ELECTRON INTEGRALS
         --------------------

THE -PK- OPTION IS OFF, THE INTEGRALS ARE NOT IN SUPERMATRIX FORM.
STORING   15000 INTEGRALS/RECORD ON DISK, USING 12 BYTES/INTEGRAL.
TWO ELECTRON INTEGRAL EVALUATION REQUIRES   74416 WORDS OF MEMORY.
II,JST,KST,LST =  1  1  1  1 NREC =         1 INTLOC =    1
II,JST,KST,LST =  2  1  1  1 NREC =         1 INTLOC =    2
II,JST,KST,LST =  3  1  1  1 NREC =         1 INTLOC =   34
II,JST,KST,LST =  4  1  1  1 NREC =         1 INTLOC =   34
II,JST,KST,LST =  5  1  1  1 NREC =         1 INTLOC =   34
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS =                 164
         1 INTEGRAL RECORDS WERE STORED ON DISK FILE  8.
 ...... END OF TWO-ELECTRON INTEGRALS .....
STEP CPU TIME =      .08 TOTAL CPU TIME =         .5 (     .0 MIN)
TOTAL WALL CLOCK TIME=         .5 SECONDS, CPU UTILIZATION IS 100.00%

         -------------------
         RHF SCF CALCULATION
         -------------------

    NUCLEAR ENERGY =        11.7371288162
    MAXIT =   30     NPUNCH=    2
    EXTRAP=T  DAMP=F  SHIFT=F  RSTRCT=F  DIIS=F  DEM=F  SOSCF=F
    DENSITY CONV=  1.00E-05
    MEMORY REQUIRED FOR RHF STEP=     30560 WORDS.

ITER EX DEM  TOTAL ENERGY      E CHANGE  DENSITY CHANGE    DIIS ERROR
  1  0  0   -55.346372113   -55.346372113    .511470397    .000000000
  2  1  0   -55.447954090     -.101581977    .158614901    .000000000
  3  2  0   -55.454596941     -.006642851    .056548241    .000000000
  4  3  0   -55.455303843     -.000706902    .019809785    .000000000
  5  0  0   -55.455400963     -.000097120    .012289511    .000000000
  6  1  0   -55.455419563     -.000018600    .000422154    .000000000
  7  2  0   -55.455419770     -.000000207    .000172751    .000000000
```

```
  8  3  0   -55.455419793     -.000000023    .000069128    .000000000
  9  4  0   -55.455419796     -.000000003    .000029426    .000000000
 10  5  0   -55.455419797     -.000000001    .000013791    .000000000
 11  6  0   -55.455419797      .000000000    .000006155    .000000000

         -----------------
         DENSITY CONVERGED
         -----------------
    TIME TO FORM FOCK OPERATORS=        .2 SECONDS (        .0 SEC/ITER)
    TIME TO SOLVE SCF EQUATIONS=        .2 SECONDS (        .0 SEC/ITER)

FINAL ENERGY IS      -55.4554197971 AFTER  11 ITERATIONS

         ------------
         EIGENVECTORS
         ------------

                    1          2          3          4          5
                -15.3128    -1.0867     -.5615     -.5615     -.3585
                   A1         A1          E          E          A1
   1  N   1  S    .993452   -.218930    .000000    .000000    .095882
   2  N   1  S    .031334    .739763    .000000    .000000   -.481858
   3  N   1  X    .000000    .000000    .593384    .000000    .000000
   4  N   1  Y    .000000    .000000    .000000    .593384    .000000
   5  N   1  Z    .005194    .141219    .000000    .000000    .870687
   6  H   2  S   -.006465    .159051   -.250517    .433908    .138158
   7  H   3  S   -.006465    .159051   -.250517   -.433908    .138158
   8  H   4  S   -.006465    .159051    .501034    .000000    .138158

                    6          7          8
                  .6250      .7002      .7002
                   A1         E          E
   1  N   1  S   -.179971    .000000    .000000
   2  N   1  S   1.211420    .000000    .000000
   3  N   1  X    .000000   1.033441    .000000
   4  N   1  Y    .000000    .000000   1.033441
   5  N   1  Z    .612833    .000000    .000000
   6  H   2  S   -.701158    .487729   -.844772
   7  H   3  S   -.701158    .487729    .844772
   8  H   4  S   -.701158   -.975459    .000000
...... END OF RHF CALCULATION ......
STEP CPU TIME =      .60 TOTAL CPU TIME =        1.1 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.1 SECONDS, CPU UTILIZATION IS 100.00%

         -----------------
         ENERGY COMPONENTS
         -----------------

       WAVEFUNCTION NORMALIZATION =       1.0000000000

            ONE ELECTRON ENERGY =     -98.6230562919
            TWO ELECTRON ENERGY =      31.4305076785
         NUCLEAR REPULSION ENERGY =      11.7371288162
                                    ------------------
                     TOTAL ENERGY =     -55.4554197971
```

```
ELECTRON-ELECTRON POTENTIAL ENERGY =      31.4305076785
 NUCLEUS-ELECTRON POTENTIAL ENERGY =    -153.6981647772
  NUCLEUS-NUCLEUS POTENTIAL ENERGY =      11.7371288162
                                     ------------------
            TOTAL POTENTIAL ENERGY =    -110.5305282824
              TOTAL KINETIC ENERGY =      55.0751084853
                VIRIAL RATIO (V/T) =       2.0069053212

       ---------------------------------------
       MULLIKEN AND LOWDIN POPULATION ANALYSES
       ---------------------------------------

   MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL

                    1          2          3          4          5

                2.000000   2.000000   2.000000   2.000000   2.000000

  1             2.002409   1.430810   1.055655   1.055655   1.896133
  2             -.000803    .189730    .157391    .472172    .034622
  3             -.000803    .189730    .157391    .472172    .034622
  4             -.000803    .189730    .629563    .000000    .034622

            ----- POPULATIONS IN EACH AO -----
                          MULLIKEN      LOWDIN
           1  N   1  S     1.99557     1.99259
           2  N   1  S     1.62484     1.41343
           3  N   1  X     1.05566     1.08195
           4  N   1  Y     1.05566     1.08195
           5  N   1  Z     1.70894     1.71676
           6  H   2  S      .85311      .90444
           7  H   3  S      .85311      .90444
           8  H   4  S      .85311      .90444

       ----- MULLIKEN ATOMIC OVERLAP POPULATIONS -----
       (OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

          1          2          3          4

  1    6.4470902
  2     .3311907    .5909233
  3     .3311907   -.0345007    .5909233
  4     .3311907   -.0345007   -.0345007    .5909233

       TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
     ATOM         MULL.POP.    CHARGE          LOW.POP.     CHARGE
  1 N             7.440662   -.440662          7.286689   -.286689
  2 H              .853113    .146887           .904437    .095563
  3 H              .853113    .146887           .904437    .095563
  4 H              .853113    .146887           .904437    .095563

       -------------------------------
       BOND ORDER AND VALENCE ANALYSIS     BOND ORDER THRESHOLD= .050
       -------------------------------
```

```
                  BOND                          BOND                          BOND
 ATOM PAIR DIST  ORDER      ATOM PAIR DIST  ORDER      ATOM PAIR DIST  ORDER
   1   2  1.033   .962        1   3  1.033   .962        1   4  1.033   .962

                      TOTAL       BONDED        FREE
     ATOM            VALENCE     VALENCE     VALENCE
   1 N                 2.885       2.885        .000
   2 H                  .978        .978        .000
   3 H                  .978        .978        .000
   4 H                  .978        .978        .000

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

POINT   1           X           Y           Z (BOHR)    CHARGE
                .000000     .000000     .139212         .00 (A.U.)
        DX          DY          DZ         /D/  (DEBYE)
     .000000     .000000    1.875772    1.875772
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =      .28 TOTAL CPU TIME =        1.3 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.3 SECONDS, CPU UTILIZATION IS 100.00%

         --------------------
         2 ELECTRON INTEGRALS
         --------------------

THE -PK- OPTION IS OFF, THE INTEGRALS ARE NOT IN SUPERMATRIX FORM.
STORING   15000 INTEGRALS/RECORD ON DISK, USING 12 BYTES/INTEGRAL.
TWO ELECTRON INTEGRAL EVALUATION REQUIRES   74416 WORDS OF MEMORY.
II,JST,KST,LST =  1  1  1  1 NREC =         1 INTLOC =    1
II,JST,KST,LST =  2  1  1  1 NREC =         1 INTLOC =    2
II,JST,KST,LST =  3  1  1  1 NREC =         1 INTLOC =   34
II,JST,KST,LST =  4  1  1  1 NREC =         1 INTLOC =  145
II,JST,KST,LST =  5  1  1  1 NREC =         1 INTLOC =  316
TOTAL NUMBER OF NONZERO TWO-ELECTRON INTEGRALS =                538
         1 INTEGRAL RECORDS WERE STORED ON DISK FILE  8.
 ...... END OF TWO-ELECTRON INTEGRALS .....
STEP CPU TIME =      .08 TOTAL CPU TIME =        1.4 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.4 SECONDS, CPU UTILIZATION IS 100.00%

    -------------------------------
    PARTIAL INTEGRAL TRANSFORMATION
    -------------------------------

NUMBER OF CORE MOLECULAR ORBITALS     =    0
NUMBER OF OCCUPIED MOLECULAR ORBITALS =    5
TOTAL NUMBER OF MOLECULAR ORBITALS    =    8
TOTAL NUMBER OF ATOMIC ORBITALS       =    8
THRESHOLD FOR KEEPING TRANSFORMED 2E- INTEGRALS = 1.000E-09
AO INTEGRALS WILL BE READ IN FROM DISK...
# OF WORDS AVAILABLE =     750000
# OF WORDS NEEDED    =      61746 FOR IN MEMORY TRANSFORMATION
```

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CHOOSING IN MEMORY PARTIAL TRANSFORMATION...
TOTAL NUMBER OF TRANSFORMED 2E- INTEGRALS KEPT =       245
... END OF INTEGRAL TRANSFORMATION ...
STEP CPU TIME =      .20 TOTAL CPU TIME =        1.6 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.6 SECONDS, CPU UTILIZATION IS 100.00%

    ---------------------------------------------
    1ST AND 2ND INTEGRAL DERIVATIVE CONTRIBUTIONS
    ---------------------------------------------
...... END OF 1-ELECTRON GRAD+HESS+FOCKDER ......
STEP CPU TIME =      .18 TOTAL CPU TIME =        1.8 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.8 SECONDS, CPU UTILIZATION IS 100.00%

    ---------------------------------------------
    TWO ELECTRON INTEGRAL DERIVATIVE CONTRIBUTIONS
    ---------------------------------------------

     60769 WORDS REQUIRED,    750000 WORDS AVAILABLE
...... END OF 2-ELECTRON GRAD+HESS+FOCKDER ......
STEP CPU TIME =      .50 TOTAL CPU TIME =        2.3 (     .0 MIN)
TOTAL WALL CLOCK TIME=        2.3 SECONDS, CPU UTILIZATION IS 100.00%

    -----------------------------------------
    COUPLED-PERTURBED CLOSED SHELL HARTREE-FOCK
    -----------------------------------------
THE CPHF HAS      15 INDEPENDENT ORBITAL ROTATIONS.
CHOOSING IN MEMORY CPHF ALGORITHM
          -FA- WILL USE       828 WORDS,
          -TA- WILL USE      1640 WORDS,
         -FCK- WILL USE     31180 WORDS,
-WXY- AND -YA- WILL USE     30634 WORDS,
              THERE ARE    750000 WORDS AVAILABLE.
       TIME FOR -FA-   =         .117
       TIME FOR -TA-   =         .033
       TIME FOR -FCK-  =         .067
       TIME FOR -WXY-  =         .067
       TIME FOR -YA-   =         .000
...... DONE WITH CPHF CONTRIBUTIONS ......
STEP CPU TIME =      .53 TOTAL CPU TIME =        2.8 (     .0 MIN)
TOTAL WALL CLOCK TIME=        2.8 SECONDS, CPU UTILIZATION IS 100.00%

         ---------------
         ENERGY GRADIENT
         ---------------

     ATOM                E'X              E'Y              E'Z
   1 N                .000000000       .000000000      -.000002224
   2 H               -.000002645       .000004582       .000000741
   3 H               -.000002645      -.000004582       .000000741
   4 H                .000005290       .000000000       .000000741

         -------------------------------
         CARTESIAN FORCE CONSTANT MATRIX
         -------------------------------
```

			1			2		
			N			H		
			X	Y	Z	X	Y	Z
1	N	X	.840815	.000000	.000000	-.188524	.158911	.126928
		Y	.000000	.840815	.000000	.158911	-.372019	-.219846
		Z	.000000	.000000	.336186	.072490	-.125557	-.112062
2	H	X	-.188524	.158911	.072490	.191392	-.178131	-.094173
		Y	.158911	-.372019	-.125557	-.178131	.397080	.163112
		Z	.126928	-.219846	-.112062	-.094173	.163112	.114000
3	H	X	-.188524	-.158911	.072490	.015211	.029526	-.011072
		Y	-.158911	-.372019	.125557	-.029526	-.029175	.031430
		Z	.126928	.219846	-.112062	-.011072	-.031430	-.000969
4	H	X	-.463767	.000000	-.144981	-.018079	-.010306	-.021683
		Y	.000000	-.096776	.000000	.048746	.004114	.025304
		Z	-.253856	.000000	-.112062	.032755	-.006126	-.000969

			3			4		
			H			H		
			X	Y	Z	X	Y	Z
3	H	X	.191392	.178131	-.094173	-.018079	-.048746	.032755
		Y	.178131	.397080	-.163112	.010306	.004114	.006126
		Z	-.094173	-.163112	.114000	-.021683	-.025304	-.000969
4	H	X	-.018079	.010306	-.021683	.499924	.000000	.188346
		Y	-.048746	.004114	-.025304	.000000	.088548	.000000
		Z	.032755	.006126	-.000969	.188346	.000000	.114000

DIPOLE DERIVATIVE TENSOR

ATOM		UX	UY	UZ
N	D/DX	-.913621046	.000000000	.000000000
	D/DY	.000000000	-.913621046	.000000000
	D/DZ	.000000000	.000000000	-1.799881188
H	D/DX	.412017819	.186156440	.259172542
	D/DY	.186156440	.197062878	-.448900010
	D/DZ	.526843326	-.912519409	.599960396
H	D/DX	.412017819	-.186156440	.259172542
	D/DY	-.186156440	.197062878	.448900010
	D/DZ	.526843326	.912519409	.599960396
H	D/DX	.089585408	.000000000	-.518345083
	D/DY	.000000000	.519495290	.000000000
	D/DZ	-1.053686652	.000000000	.599960396

THE DIPOLE DERIVATIVE MATRIX IS IN DEBYE/ANGSTROM

NORMAL COORDINATE ANALYSIS IN THE HARMONIC APPROXIMATION

ATOMIC WEIGHTS (AMU)

1	N	14.00307
2	H	1.00782
3	H	1.00782
4	H	1.00782

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

FREQUENCIES IN CM**-1, IR INTENSITIES IN DEBYE**2/AMU-ANGSTROM**2

			1	2	3	4	5
	FREQUENCY:		.02	.02	.02	8.37	8.37
	INTENSITY:		.00000	.00000	.00000	1.96722	1.96722
1	N	X	.14070293	.19731820	-.00000485	.05347609	-.01841861
		Y	.19731820	-.14070293	.00000376	.01841861	.05347609
		Z	.00000025	-.00000613	-.24234649	.00000000	.00000000
2	H	X	.14070317	.19731853	-.00000485	-.24767109	.08530342
		Y	.19731853	-.14070317	.00000376	-.08530512	-.24766913
		Z	-.00000013	-.00000531	-.24234649	-.13413377	.69038584
3	H	X	.14070317	.19731853	-.00000485	-.24767036	.08530554
		Y	.19731853	-.14070317	.00000376	-.08530299	-.24766986
		Z	.00000115	-.00000622	-.24234649	-.53082479	-.46135617
4	H	X	.14070317	.19731853	-.00000485	-.24766888	.08530385
		Y	.19731853	-.14070317	.00000376	-.08530469	-.24767134
		Z	-.00000028	-.00000687	-.24234649	.66495856	-.22902966
TRANS. SAYVETZ		X	2.39568546	3.35964822	-.00008258	.00000503	-.00000173
		Y	3.35964822	-2.39568546	.00006409	.00000173	.00000503
		Z	.00000424	-.00010444	-4.12632342	.00000000	.00000000
		TOTAL	4.12632342	4.12632342	4.12632342	.00000532	.00000532
ROT. SAYVETZ		X	-.00000265	.00000189	.00000000	.82300853	2.38950079
		Y	.00000189	.00000265	.00000000	-2.38950079	.82300853
		Z	.00000000	.00000000	.00000000	.00000000	.00000000
		TOTAL	.00000326	.00000326	.00000000	2.52726276	2.52726276

			6	7	8	9	10
	FREQUENCY:		8.82	1411.64	**2076.31**	**2076.31**	3833.22
	INTENSITY:		.00000	1.91401	.03943	.03943	.18859
1	N	X	.00000000	.00000000	-.05150016	-.03264985	.00000000
		Y	.00000000	.00000000	.03264985	-.05150016	.00000000
		Z	.00000000	.10537393	.00000000	.00000000	.03971681
2	H	X	-.49805516	-.10141749	.21994958	.59921591	.26907398
		Y	-.28755228	.17566024	.29678367	.25709115	-.46604980
		Z	.00000000	-.48803398	-.22663801	.11861596	-.18394636
3	H	X	.49805516	-.10141749	.63578496	-.05670100	.26907398
		Y	-.28755228	-.17566024	-.35913324	-.15874423	.46604980
		Z	.00000000	-.48803398	.01059457	-.25558225	-.18394636
4	H	X	.00000000	.20283497	-.14017344	-.08886655	-.53814796
		Y	.57510456	.00000000	-.39129879	.61721417	.00000000
		Z	.00000000	-.48803398	.21604344	.13696629	-.18394636
TRANS. SAYVETZ		X	.00000000	.00000000	.00000000	.00000000	.00000000
		Y	.00000000	.00000000	.00000000	.00000000	.00000000
		Z	.00000000	.00000000	.00000000	.00000000	.00000000
		TOTAL	.00000000	.00000000	.00000000	.00000000	.00000000
ROT. SAYVETZ		X	.00000000	.00000000	-.00000515	.00000812	.00000000

```
                    Y   .00000000   .00000000  -.00000812  -.00000515   .00000000
                    Z  3.09059581   .00000000   .00000000   .00000000   .00000000
                TOTAL  3.09059581   .00000000   .00000961   .00000961   .00000000

                           11          12
      FREQUENCY:         4108.18     4108.18
      INTENSITY:          .11902      .11902

 1    N              X   .01775198  -.07381583
                     Y   .07381583   .01775198
                     Z   .00000000   .00000000
 2    H              X   .26312605   .23972493
                     Y  -.44402353  -.42756082
                     Z  -.23093421  -.21931915
 3    H              X  -.34335299   .09387269
                     Y  -.58987576   .17891822
                     Z   .30540306  -.09033532
 4    H              X  -.16642521   .69202506
                     Y   .00827661   .00199044
                     Z  -.07446885   .30965447

TRANS. SAYVETZ      X   .00000000   .00000000
                    Y   .00000000   .00000000
                    Z   .00000000   .00000000
                TOTAL   .00000000   .00000000

  ROT. SAYVETZ      X  -.00000278  -.00000067
                    Y   .00000067  -.00000278
                    Z   .00000000   .00000000
                TOTAL   .00000286   .00000286

REFERENCE ON SAYVETZ CONDITIONS - A. SAYVETZ, J.CHEM.PHYS., 7, 383-389(1939).

NOTE - THE MODES J,K ARE ORTHONORMALIZED ACCORDING TO
SUM ON I   M(I) * (X(I,J)*X(I,K) + Y(I,J)*Y(I,K) + Z(I,J)*Z(I,K)) = DELTA(J,K)

    ------------------------------
    THERMOCHEMISTRY AT T=  298.15 K
    ------------------------------

USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
P=  1.01325E+05 PASCAL.
ALL FREQUENCIES ARE SCALED BY   1.00000
THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
     6.38706     6.38706     9.55178
THE ROTATIONAL SYMMETRY NUMBER IS  3.0
THE ROTATIONAL CONSTANTS ARE (IN GHZ)
   282.30345   282.30345   188.76982
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        .040127 HARTREE/MOLECULE     8806.922200 CM**-1/MOLECULE
      25.180279 KCAL/MOL              105.354289 KJ/MOL

              Q              LN Q
ELEC.     1.00000E+00        .000000
TRANS.    2.76149E+06      14.831281
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ROT.      7.44840E+01       4.310585
VIB.      1.00119E+00        .001190
TOT.      2.05932E+08      19.143056

             E         H         G         CV        CP        S
          KJ/MOL    KJ/MOL    KJ/MOL   J/MOL-K   J/MOL-K   J/MOL-K
ELEC.       .000      .000      .000      .000      .000      .000
TRANS.     3.718     6.197   -36.766    12.472    20.786   144.099
ROT.       3.718     3.718   -10.686    12.472    12.472    48.312
VIB.     105.375   105.375   105.351      .500      .500      .080
TOTAL    112.812   115.291    57.900    25.443    33.757   192.491

             E         H         G         CV        CP        S
        KCAL/MOL  KCAL/MOL  KCAL/MOL CAL/MOL-K CAL/MOL-K CAL/MOL-K
ELEC.       .000      .000      .000      .000      .000      .000
TRANS.      .889     1.481    -8.787     2.981     4.968    34.441
ROT.        .889      .889    -2.554     2.981     2.981    11.547
VIB.      25.185    25.185    25.180      .119      .119      .019
TOTAL     26.963    27.555    13.838     6.081     8.068    46.006
......END OF NORMAL COORDINATE ANALYSIS......
STEP CPU TIME =      .15 TOTAL CPU TIME =        3.0 (     .0 MIN)
TOTAL WALL CLOCK TIME=        3.0 SECONDS, CPU UTILIZATION IS 100.00%
74416 WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY 16:18:37 10-07-1999
             AOINTS length        175 KB
             MOINTS length        176 KB
            DICTNRY length        415 KB
            FOCKDER length          3 KB
```