```
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 16:14:46 10-07-1999

            ECHO OF THE FIRST FEW INPUT CARDS -
 INPUT CARD> $CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE $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   -.1592817187
 INPUT CARD> H           1.0    .7581807764    .0000000000    .4764258594
 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       -.3009988032
 H           1.0     -.7163769583       1.2408012891        .9003143277
 H           1.0     -.7163769583      -1.2408012891        .9003143277
 H           1.0     1.4327539166        .0000000000        .9003143277

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

                    N              H              H              H

  1  N               .0000000       .9894252 *     .9894252 *     .9894252 *
  2  H               .9894252 *     .0000000      1.3132076 *    1.3132076 *
  3  H               .9894252 *    1.3132076 *     .0000000      1.3132076 *
  4  H               .9894252 *    1.3132076 *    1.3132076 *     .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       12.4403893239

    $CONTRL OPTIONS
    ---------------
    SCFTYP=RHF          RUNTYP=OPTIMIZE     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%


         ----------------------------
         STATIONARY POINT LOCATION RUN
         ----------------------------

OBTAINING INITIAL HESSIAN, HESS=GUESS
DIAGONAL GUESS HESSIAN IN CARTESIAN COORDS IS H(I,I)=   .3333

         PARAMETERS CONTROLLING GEOMETRY SEARCH ARE
         METHOD =QA                  UPHESS =BFGS
         NNEG   =         0          NFRZ   =         0
         NSTEP  =        20          IFOLOW =         1
         HESS   =GUESS               RESTAR =         F
         IHREP  =         0          HSSEND =         F
         NPRT   =         0          NPUN   =         0
         OPTTOL = 1.000E-04          RMIN   = 1.500E-03
         RMAX   = 1.000E-01          RLIM   = 7.000E-02
         DXMAX  = 3.000E-01          PURIFY =         F
         MOVIE  =         F          TRUPD  =         T
         TRMAX  = 5.000E-01          TRMIN  = 5.000E-02
         ITBMAT =         5          STPT   =         F
```

```
          STSTEP = 1.000E-02          PROJCT=          T
1NSERCH=   0

 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.1592817187
 H           1.0    .7581807764    .0000000000    .4764258594
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.1592817187
 H           1.0   -.3790903882    .6566038130    .4764258594
 H           1.0   -.3790903882   -.6566038130    .4764258594
 H           1.0    .7581807764    .0000000000    .4764258594

          ********************
          1 ELECTRON INTEGRALS
          ********************
 ...... END OF ONE-ELECTRON INTEGRALS ......
 STEP CPU TIME =      .00 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 =      .18 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 =        12.4403893239
    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	-55.236796301	-55.236796301	.641250435	.000000000
2	1	0	-55.389542564	-.152746263	.199308844	.000000000
3	2	0	-55.397614739	-.008072175	.059028719	.000000000
4	3	0	-55.398242096	-.000627357	.018934149	.000000000
5	0	0	-55.398308575	-.000066478	.008890569	.000000000
6	1	0	-55.398319125	-.000010550	.000926130	.000000000
7	2	0	-55.398319570	-.000000445	.000413459	.000000000
8	3	0	-55.398319644	-.000000074	.000181179	.000000000
9	4	0	-55.398319657	-.000000013	.000077301	.000000000
10	5	0	-55.398319659	-.000000002	.000032538	.000000000
11	6	0	-55.398319659	.000000000	.000013599	.000000000
12	7	0	-55.398319660	.000000000	.000005662	.000000000

DENSITY CONVERGED

```
    TIME TO FORM FOCK OPERATORS=         .3 SECONDS (         .0 SEC/ITER)
    TIME TO SOLVE SCF EQUATIONS=         .2 SECONDS (         .0 SEC/ITER)

FINAL ENERGY IS      -55.3983196595 AFTER  12 ITERATIONS
```

EIGENVECTORS

				1	2	3	4	5
				-15.3397	-1.1745	**-.5510**	**-.5510**	-.4249
				A1	A1	E	E	A1
1	N	1	S	.993430	-.210674	.000000	.000000	.135631
2	N	1	S	.032053	.699044	.000000	.000000	-.677995
3	N	1	X	.000000	.000000	.627174	.000000	.000000
4	N	1	Y	.000000	.000000	.000000	.627174	.000000
5	N	1	Z	.008002	.216080	.000000	.000000	.737621
6	H	2	S	-.006646	.153182	-.260230	.450731	.174000
7	H	3	S	-.006646	.153182	-.260230	-.450731	.174000
8	H	4	S	-.006646	.153182	.520459	.000000	.174000

				6	7	8
				.6817	**.6817**	.6887
				E	E	A1
1	N	1	S	.000000	.000000	-.163556

```
   2  N   1  S    .000000    .000000   1.188896
   3  N   1  X   -.982777    .000000    .000000
   4  N   1  Y    .000000    .982777    .000000
   5  N   1  Z    .000000    .000000    .895741
   6  H   2  S   -.521487   -.903242   -.689269
   7  H   3  S   -.521487    .903242   -.689269
   8  H   4  S   1.042974    .000000   -.689269
...... END OF RHF CALCULATION ......
STEP CPU TIME =      .68 TOTAL CPU TIME =        1.2 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.2 SECONDS, CPU UTILIZATION IS 100.00%

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

       WAVEFUNCTION NORMALIZATION =       1.0000000000

            ONE ELECTRON ENERGY =     -99.5952450329
            TWO ELECTRON ENERGY =      31.7565360495
         NUCLEAR REPULSION ENERGY =      12.4403893239
                                    ------------------
                     TOTAL ENERGY =     -55.3983196595

ELECTRON-ELECTRON POTENTIAL ENERGY =      31.7565360495
 NUCLEUS-ELECTRON POTENTIAL ENERGY =    -154.9613183385
  NUCLEUS-NUCLEUS POTENTIAL ENERGY =      12.4403893239
                                    ------------------
           TOTAL POTENTIAL ENERGY =    -110.7643929651
             TOTAL KINETIC ENERGY =      55.3660733055
               VIRIAL RATIO (V/T) =       2.0005824208

         ---------------------------------------
         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             2.002742  1.393221  1.122364  1.122364  1.827597
   2             -.000914   .202260   .146273   .438818   .057468
   3             -.000914   .202260   .146273   .438818   .057468
   4             -.000914   .202260   .585090   .000000   .057468

              ----- POPULATIONS IN EACH AO -----
                            MULLIKEN      LOWDIN
             1  N   1  S     1.99623     1.99469
             2  N   1  S     1.76734     1.52992
             3  N   1  X     1.12236     1.16030
             4  N   1  Y     1.12236     1.16030
             5  N   1  Z     1.45999     1.47094
             6  H   2  S      .84390      .89462
             7  H   3  S      .84390      .89462
```

```
             8  H    4  S      .84390      .89462

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

                1          2          3          4

   1    6.5581892
   2     .3033664    .6493255
   3     .3033664   -.0543941    .6493255
   4     .3033664   -.0543941   -.0543941    .6493255

         TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
      ATOM         MULL.POP.    CHARGE          LOW.POP.     CHARGE
   1 N             7.468289    -.468289         7.316146    -.316146
   2 H              .843904     .156096          .894618     .105382
   3 H              .843904     .156096          .894618     .105382
   4 H              .843904     .156096          .894618     .105382

         -------------------------------
         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   .989   .973        1   3   .989   .973        1   4   .989   .973

                    TOTAL       BONDED        FREE
      ATOM         VALENCE     VALENCE     VALENCE
   1 N               2.920       2.920        .000
   2 H                .976        .976        .000
   3 H                .976        .976        .000
   4 H                .976        .976        .000

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

POINT   1           X           Y           Z (BOHR)    CHARGE
                .000000     .000000    -.087677         .00 (A.U.)
        DX          DY          DZ         /D/  (DEBYE)
     .000000     .000000    2.403172    2.403172
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =      .27 TOTAL CPU TIME =        1.5 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.5 SECONDS, CPU UTILIZATION IS 100.00%

BEGINNING ONE ELECTRON GRADIENT...
..... END OF 1-ELECTRON GRADIENT ......
STEP CPU TIME =      .02 TOTAL CPU TIME =        1.5 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.5 SECONDS, CPU UTILIZATION IS 100.00%

         ----------------------
         GRADIENT OF THE ENERGY
         ----------------------
SCHWARZ SCREENING SKIPPED          0 BLOCKS, COMPUTED         31 BLOCKS
```

```
...... END OF 2-ELECTRON GRADIENT ......
STEP CPU TIME =      .17 TOTAL CPU TIME =        1.6 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.6 SECONDS, CPU UTILIZATION IS 100.00%

         NSERCH=  0     ENERGY=     -55.3983197

                                 ----------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ----------------------
        ATOM     ZNUC        DE/DX         DE/DY         DE/DZ
 ------------------------------------------------------------------
  1  N            7.0       .0000000      .0000000     -.0093976
  2  H            1.0       .0549492     -.0951748      .0031325
  3  H            1.0       .0549492      .0951748      .0031325
  4  H            1.0     -.1098984       .0000000      .0031325

         MAXIMUM GRADIENT =   .1098984    RMS GRADIENT =  .0550384
         FORCE CONSTANT MATRIX NOT UPDATED --- TAKING FIRST STEP
         MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
              NR STEP HAS LENGTH         =    .571958
         TRIM/QA LAMBDA FOR NON-TS MODES =   -.30218515
         TRIM/QA STEP HAS LENGTH         =    .300000
         RADIUS OF STEP TAKEN=    .30000  CURRENT TRUST RADIUS=    .30000
1NSERCH=   1

 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.1514572584
 H           1.0    .8496884098    .0000000000    .4738177060
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.1514572584
 H           1.0   -.4248442049    .7358517482    .4738177060
 H           1.0   -.4248442049   -.7358517482    .4738177060
 H           1.0    .8496884098    .0000000000    .4738177060

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

                    N              H              H              H

  1  N               .0000000      1.0549593 *    1.0549593 *    1.0549593 *
  2  H              1.0549593 *     .0000000      1.4717035 *    1.4717035 *
  3  H              1.0549593 *    1.4717035 *     .0000000      1.4717035 *
  4  H              1.0549593 *    1.4717035 *    1.4717035 *     .0000000

  * ... LESS THAN  3.000

...... END OF ONE-ELECTRON INTEGRALS ......
STEP CPU TIME =      .03 TOTAL CPU TIME =        1.7 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.7 SECONDS, CPU UTILIZATION IS 100.00%
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 =      .25 TOTAL CPU TIME =        1.9 (     .0 MIN)
TOTAL WALL CLOCK TIME=        1.9 SECONDS, CPU UTILIZATION IS 100.00%

ITER EX DEM  TOTAL ENERGY      E CHANGE  DENSITY CHANGE    DIIS ERROR
  1  0  0   -55.432408323   -55.432408323    .028840249    .000000000
  2  1  0   -55.432896931     -.000488608    .006948927    .000000000
  3  2  0   -55.432923222     -.000026291    .002221418    .000000000
  4  3  0   -55.432925047     -.000001825    .000670694    .000000000
  5  0  0   -55.432925206     -.000000158    .000354489    .000000000
  6  1  0   -55.432925227     -.000000021    .000033875    .000000000
  7  2  0   -55.432925228     -.000000001    .000015040    .000000000

         -----------------
         DENSITY CONVERGED
         -----------------
    TIME TO FORM FOCK OPERATORS=        .2 SECONDS (        .0 SEC/ITER)
    TIME TO SOLVE SCF EQUATIONS=        .6 SECONDS (        .1 SEC/ITER)

FINAL ENERGY IS      -55.4329252278 AFTER   7 ITERATIONS
...... END OF RHF CALCULATION ......
STEP CPU TIME =      .95 TOTAL CPU TIME =        2.9 (     .0 MIN)
TOTAL WALL CLOCK TIME=        2.9 SECONDS, CPU UTILIZATION IS 100.00%
..... END OF 1-ELECTRON GRADIENT ......
STEP CPU TIME =      .05 TOTAL CPU TIME =        2.9 (     .0 MIN)
TOTAL WALL CLOCK TIME=        2.9 SECONDS, CPU UTILIZATION IS 100.00%

...... END OF 2-ELECTRON GRADIENT ......
STEP CPU TIME =      .15 TOTAL CPU TIME =        3.1 (     .1 MIN)
TOTAL WALL CLOCK TIME=        3.1 SECONDS, CPU UTILIZATION IS 100.00%

         NSERCH=  1     ENERGY=     -55.4329252

                              ----------------------
                              GRADIENT (HARTREE/BOHR)
                              ----------------------
       ATOM     ZNUC       DE/DX         DE/DY         DE/DZ
-------------------------------------------------------------------
 1  N            7.0      .0000000      .0000000     -.1006461
 2  H            1.0      .0115777     -.0200532      .0335487
 3  H            1.0      .0115777      .0200532      .0335487
 4  H            1.0     -.0231554      .0000000      .0335487

         MAXIMUM GRADIENT =   .1006461    RMS GRADIENT =  .0354903
         HESSIAN UPDATED USING THE BFGS FORMULA
            ACTUAL ENERGY CHANGE WAS   -.0346055682
         PREDICTED ENERGY CHANGE WAS   -.0421971198 RATIO=   .820
         MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
              NR STEP HAS LENGTH         =    .640438
         TRIM/QA LAMBDA FOR NON-TS MODES =   -.08755535
         TRIM/QA STEP HAS LENGTH         =    .424264
         RADIUS OF STEP TAKEN=    .42426  CURRENT TRUST RADIUS=    .42426
1NSERCH=   2
```

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COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
N           7.0    .0000000000    .0000000000   -.0019756812
H           1.0    .9325781996    .0000000000    .4239905136
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
N           7.0    .0000000000    .0000000000   -.0019756812
H           1.0   -.4662890998    .8076364119    .4239905136
H           1.0   -.4662890998   -.8076364119    .4239905136
H           1.0    .9325781996    .0000000000    .4239905136

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

                   N              H              H              H

 1  N               .0000000      1.0252557 *    1.0252557 *    1.0252557 *
 2  H              1.0252557 *     .0000000      1.6152728 *    1.6152728 *
 3  H              1.0252557 *    1.6152728 *     .0000000      1.6152728 *
 4  H              1.0252557 *    1.6152728 *    1.6152728 *     .0000000

 * ... LESS THAN  3.000

...... END OF ONE-ELECTRON INTEGRALS ......
STEP CPU TIME =      .10 TOTAL CPU TIME =        3.2 (     .1 MIN)
TOTAL WALL CLOCK TIME=        3.2 SECONDS, CPU UTILIZATION IS 100.00%
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 =      .23 TOTAL CPU TIME =        3.4 (     .1 MIN)
TOTAL WALL CLOCK TIME=        3.4 SECONDS, CPU UTILIZATION IS 100.00%

ITER EX DEM  TOTAL ENERGY      E CHANGE  DENSITY CHANGE    DIIS ERROR
  1  0  0   -55.443552497   -55.443552497    .176897960    .000000000
  2  1  0   -55.453208037     -.009655540    .075483513    .000000000
  3  2  0   -55.454886121     -.001678083    .028916443    .000000000
  4  3  0   -55.455182788     -.000296668    .012167765    .000000000
  5  0  0   -55.455235617     -.000052829    .008742275    .000000000
  6  1  0   -55.455247006     -.000011389    .000051746    .000000000
  7  2  0   -55.455247007     -.000000001    .000017485    .000000000
  8  3  0   -55.455247007      .000000000    .000006935    .000000000

         -----------------
         DENSITY CONVERGED
         -----------------
    TIME TO FORM FOCK OPERATORS=        .2 SECONDS (        .0 SEC/ITER)
    TIME TO SOLVE SCF EQUATIONS=        .6 SECONDS (        .1 SEC/ITER)

FINAL ENERGY IS      -55.4552470068 AFTER   8 ITERATIONS
...... END OF RHF CALCULATION ......
STEP CPU TIME =     1.08 TOTAL CPU TIME =        4.5 (     .1 MIN)
TOTAL WALL CLOCK TIME=        4.5 SECONDS, CPU UTILIZATION IS 100.00%
..... END OF 1-ELECTRON GRADIENT ......
```

```
 STEP CPU TIME =      .05 TOTAL CPU TIME =        4.5 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        4.5 SECONDS, CPU UTILIZATION IS 100.00%

 ...... END OF 2-ELECTRON GRADIENT ......
 STEP CPU TIME =      .15 TOTAL CPU TIME =        4.7 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        4.7 SECONDS, CPU UTILIZATION IS 100.00%

          NSERCH=  2     ENERGY=     -55.4552470

                                 ------------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ------------------------
        ATOM     ZNUC        DE/DX         DE/DY         DE/DZ
 ------------------------------------------------------------------
  1  N            7.0      .0000000      .0000000      .0067688
  2  H            1.0      .0038410     -.0066528     -.0022563
  3  H            1.0      .0038410      .0066528     -.0022563
  4  H            1.0     -.0076820      .0000000     -.0022563

          MAXIMUM GRADIENT =   .0076820    RMS GRADIENT =  .0044547
          HESSIAN UPDATED USING THE BFGS FORMULA
             ACTUAL ENERGY CHANGE WAS   -.0223217790
          PREDICTED ENERGY CHANGE WAS   -.0322741610 RATIO=   .692
          MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
               NR STEP HAS LENGTH         =    .027067
          RADIUS OF STEP TAKEN=    .02707  CURRENT TRUST RADIUS=    .42426
1NSERCH=   3

 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.0007237691
 H           1.0    .9408053620    .0000000000    .4235732095
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.0007237691
 H           1.0   -.4704026810    .8147613435    .4235732095
 H           1.0   -.4704026810   -.8147613435    .4235732095
 H           1.0    .9408053620    .0000000000    .4235732095

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

                     N              H              H              H

  1  N                .0000000      1.0320575 *    1.0320575 *    1.0320575 *
  2  H              1.0320575 *      .0000000      1.6295227 *    1.6295227 *
  3  H              1.0320575 *    1.6295227 *      .0000000      1.6295227 *
  4  H              1.0320575 *    1.6295227 *    1.6295227 *      .0000000

  * ... LESS THAN  3.000

 ...... END OF ONE-ELECTRON INTEGRALS ......
 STEP CPU TIME =      .08 TOTAL CPU TIME =        4.8 (     .1 MIN)
```

```
 TOTAL WALL CLOCK TIME=        4.8 SECONDS, CPU UTILIZATION IS 100.00%
 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 =      .23 TOTAL CPU TIME =        5.0 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        5.0 SECONDS, CPU UTILIZATION IS 100.00%

 ITER EX DEM  TOTAL ENERGY      E CHANGE  DENSITY CHANGE    DIIS ERROR
   1  0  0   -55.455413168   -55.455413168    .002117991    .000000000
   2  1  0   -55.455418469     -.000005301    .000353270    .000000000
   3  2  0   -55.455418594     -.000000125    .000079533    .000000000
   4  3  0   -55.455418597     -.000000004    .000015588    .000000000
   5  4  0   -55.455418597      .000000000    .000007875    .000000000
   6  5  0   -55.455418597      .000000000    .000002692    .000000000

          -----------------
          DENSITY CONVERGED
          -----------------
     TIME TO FORM FOCK OPERATORS=        .2 SECONDS (        .0 SEC/ITER)
     TIME TO SOLVE SCF EQUATIONS=        .7 SECONDS (        .1 SEC/ITER)

 FINAL ENERGY IS      -55.4554185975 AFTER   6 ITERATIONS
 ...... END OF RHF CALCULATION ......
 STEP CPU TIME =     1.05 TOTAL CPU TIME =        6.1 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        6.1 SECONDS, CPU UTILIZATION IS 100.00%
 ..... END OF 1-ELECTRON GRADIENT ......
 STEP CPU TIME =      .05 TOTAL CPU TIME =        6.1 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        6.1 SECONDS, CPU UTILIZATION IS 100.00%

 ...... END OF 2-ELECTRON GRADIENT ......
 STEP CPU TIME =      .15 TOTAL CPU TIME =        6.3 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        6.3 SECONDS, CPU UTILIZATION IS 100.00%

          NSERCH=  3     ENERGY=     -55.4554186

                                 ------------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ------------------------
        ATOM     ZNUC       DE/DX         DE/DY         DE/DZ
 ------------------------------------------------------------------
  1  N            7.0      .0000000      .0000000      .0008577
  2  H            1.0      .0001131     -.0001959     -.0002859
  3  H            1.0      .0001131      .0001959     -.0002859
  4  H            1.0     -.0002262      .0000000     -.0002859

          MAXIMUM GRADIENT =   .0008577    RMS GRADIENT =  .0003075
          HESSIAN UPDATED USING THE BFGS FORMULA
             ACTUAL ENERGY CHANGE WAS   -.0001715907
          PREDICTED ENERGY CHANGE WAS   -.0001684740 RATIO=  1.018
          MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
               NR STEP HAS LENGTH         =    .001716
          RADIUS OF STEP TAKEN=    .00172  CURRENT TRUST RADIUS=    .05413
1NSERCH=   4

 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
```

```
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
N           7.0    .0000000000    .0000000000   -.0014992957
H           1.0    .9407177355    .0000000000    .4238317184
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
N           7.0    .0000000000    .0000000000   -.0014992957
H           1.0   -.4703588678    .8146854568    .4238317184
H           1.0   -.4703588678   -.8146854568    .4238317184
H           1.0    .9407177355    .0000000000    .4238317184

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

                   N              H              H              H

 1  N                .0000000      1.0324032 *    1.0324032 *    1.0324032 *
 2  H               1.0324032 *     .0000000      1.6293709 *    1.6293709 *
 3  H               1.0324032 *    1.6293709 *     .0000000      1.6293709 *
 4  H               1.0324032 *    1.6293709 *    1.6293709 *     .0000000

 * ... LESS THAN  3.000

...... END OF ONE-ELECTRON INTEGRALS ......
STEP CPU TIME =      .10 TOTAL CPU TIME =        6.4 (     .1 MIN)
TOTAL WALL CLOCK TIME=        6.4 SECONDS, CPU UTILIZATION IS 100.00%
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 =      .25 TOTAL CPU TIME =        6.6 (     .1 MIN)
TOTAL WALL CLOCK TIME=        6.6 SECONDS, CPU UTILIZATION IS 100.00%

ITER EX DEM  TOTAL ENERGY      E CHANGE  DENSITY CHANGE    DIIS ERROR
  1  0  0   -55.455419241   -55.455419241    .000866684    .000000000
  2  1  0   -55.455419578     -.000000337    .000418036    .000000000
  3  2  0   -55.455419631     -.000000053    .000159294    .000000000
  4  3  0   -55.455419640     -.000000009    .000068050    .000000000
  5  4  0   -55.455419642     -.000000002    .000028163    .000000000
  6  5  0   -55.455419642      .000000000    .000011904    .000000000
  7  6  0   -55.455419642      .000000000    .000005016    .000000000

         -----------------
         DENSITY CONVERGED
         -----------------
    TIME TO FORM FOCK OPERATORS=        .2 SECONDS (        .0 SEC/ITER)
    TIME TO SOLVE SCF EQUATIONS=        .6 SECONDS (        .1 SEC/ITER)

FINAL ENERGY IS      -55.4554196422 AFTER   7 ITERATIONS
...... END OF RHF CALCULATION ......
STEP CPU TIME =      .95 TOTAL CPU TIME =        7.6 (     .1 MIN)
TOTAL WALL CLOCK TIME=        7.6 SECONDS, CPU UTILIZATION IS 100.00%
..... END OF 1-ELECTRON GRADIENT ......
STEP CPU TIME =      .03 TOTAL CPU TIME =        7.6 (     .1 MIN)
TOTAL WALL CLOCK TIME=        7.6 SECONDS, CPU UTILIZATION IS 100.00%
```

```
 ...... END OF 2-ELECTRON GRADIENT ......
 STEP CPU TIME =      .17 TOTAL CPU TIME =        7.8 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        7.8 SECONDS, CPU UTILIZATION IS 100.00%

          NSERCH=  4     ENERGY=     -55.4554196

                                  ----------------------
                                  GRADIENT (HARTREE/BOHR)
                                  ----------------------
         ATOM     ZNUC       DE/DX         DE/DY         DE/DZ
 ------------------------------------------------------------------
  1  N            7.0      .0000000      .0000000      .0002746
  2  H            1.0      .0000128     -.0000222     -.0000915
  3  H            1.0      .0000128      .0000222     -.0000915
  4  H            1.0     -.0000257      .0000000     -.0000915

          MAXIMUM GRADIENT =   .0002746    RMS GRADIENT =  .0000924
          HESSIAN UPDATED USING THE BFGS FORMULA
             ACTUAL ENERGY CHANGE WAS   -.0000010447
          PREDICTED ENERGY CHANGE WAS   -.0000007818 RATIO=  1.336
          MIN SEARCH, CORRECT HESSIAN, TRYING PURE NR STEP
               NR STEP HAS LENGTH         =    .001141
          RADIUS OF STEP TAKEN=    .00114  CURRENT TRUST RADIUS=    .05000
1NSERCH=   5

 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.0019717070
 H           1.0    .9405679704    .0000000000    .4239891888
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0    .0000000000    .0000000000   -.0019717070
 H           1.0   -.4702839852    .8145557563    .4239891888
 H           1.0   -.4702839852   -.8145557563    .4239891888
 H           1.0    .9405679704    .0000000000    .4239891888

          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

 ...... END OF ONE-ELECTRON INTEGRALS ......
 STEP CPU TIME =      .07 TOTAL CPU TIME =        7.8 (     .1 MIN)
 TOTAL WALL CLOCK TIME=        7.8 SECONDS, CPU UTILIZATION IS 100.00%
 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 =      .25 TOTAL CPU TIME =        8.1 (     .1 MIN)
TOTAL WALL CLOCK TIME=        8.1 SECONDS, CPU UTILIZATION IS 100.00%

ITER EX DEM  TOTAL ENERGY      E CHANGE  DENSITY CHANGE    DIIS ERROR
  1  0   0   -55.455419661   -55.455419661    .000534091    .000000000
  2  1   0   -55.455419774     -.000000114    .000246565    .000000000
  3  2   0   -55.455419793     -.000000019    .000095366    .000000000
  4  3   0   -55.455419796     -.000000003    .000040485    .000000000
  5  4   0   -55.455419797     -.000000001    .000016797    .000000000
  6  5   0   -55.455419797      .000000000    .000007093    .000000000

         -----------------
         DENSITY CONVERGED
         -----------------
    TIME TO FORM FOCK OPERATORS=        .2 SECONDS (        .0 SEC/ITER)
    TIME TO SOLVE SCF EQUATIONS=        .4 SECONDS (        .1 SEC/ITER)

FINAL ENERGY IS      -55.4554197971 AFTER   6 ITERATIONS
...... END OF RHF CALCULATION ......
STEP CPU TIME =      .80 TOTAL CPU TIME =        8.9 (     .1 MIN)
TOTAL WALL CLOCK TIME=        8.9 SECONDS, CPU UTILIZATION IS 100.00%
..... END OF 1-ELECTRON GRADIENT ......
STEP CPU TIME =      .03 TOTAL CPU TIME =        8.9 (     .1 MIN)
TOTAL WALL CLOCK TIME=        8.9 SECONDS, CPU UTILIZATION IS 100.00%

...... END OF 2-ELECTRON GRADIENT ......
STEP CPU TIME =      .17 TOTAL CPU TIME =        9.1 (     .2 MIN)
TOTAL WALL CLOCK TIME=        9.1 SECONDS, CPU UTILIZATION IS 100.00%

         NSERCH=  5     ENERGY=     -55.4554198

                                -----------------------
                                GRADIENT (HARTREE/BOHR)
                                -----------------------
       ATOM     ZNUC        DE/DX         DE/DY         DE/DZ
-------------------------------------------------------------
 1  N            7.0      .0000000      .0000000     -.0000023
 2  H            1.0     -.0000026      .0000046      .0000008
 3  H            1.0     -.0000026     -.0000046      .0000008
 4  H            1.0      .0000053      .0000000      .0000008

         MAXIMUM GRADIENT =   .0000053    RMS GRADIENT =  .0000028
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****

    STO3G NH3
COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
N           7.0    .0000000000    .0000000000   -.0019717070
H           1.0    .9405679704    .0000000000    .4239891888
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
```

```
N           7.0    .0000000000    .0000000000   -.0019717070
H           1.0   -.4702839852    .8145557563    .4239891888
H           1.0   -.4702839852   -.8145557563    .4239891888
H           1.0    .9405679704    .0000000000    .4239891888
```

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

NUCLEAR ENERGY = 11.7371288165
ELECTRONIC ENERGY = -67.1925486136
TOTAL ENERGY = -55.4554197971

MOLECULAR ORBITALS

				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	.739762	.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

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION = 1.0000000000

```
              ONE ELECTRON ENERGY =     -98.6230563272
              TWO ELECTRON ENERGY =      31.4305077135
         NUCLEAR REPULSION ENERGY =      11.7371288165
                                     ------------------
                     TOTAL ENERGY =     -55.4554197971

ELECTRON-ELECTRON POTENTIAL ENERGY =      31.4305077135
 NUCLEUS-ELECTRON POTENTIAL ENERGY =    -153.6981645646
  NUCLEUS-NUCLEUS POTENTIAL ENERGY =      11.7371288165
                                     ------------------
           TOTAL POTENTIAL ENERGY =    -110.5305280345
             TOTAL KINETIC ENERGY =      55.0751082374
               VIRIAL RATIO (V/T) =       2.0069053257

       ---------------------------------------
       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    6.4470900
  2     .3311908    .5909233
  3     .3311908   -.0345007    .5909233
  4     .3311908   -.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 =      .40 TOTAL CPU TIME =        9.5 (     .2 MIN)
 TOTAL WALL CLOCK TIME=        9.5 SECONDS, CPU UTILIZATION IS 100.00%
  $VIB
          IVIB=   0 IATOM=   0 ICOORD=   0 E=      -55.4554197971
  0.000000000E+00 0.000000000E+00-2.310490277E-06-2.648051331E-06 4.586559447E-
06
  7.701636593E-07-2.648051331E-06-4.586559447E-06 7.701636593E-07 5.296102663E-
06
  0.000000000E+00 7.701636593E-07
 -5.643854273E-15 1.235552199E-14 1.875771720E+00
 ......END OF GEOMETRY SEARCH......
 STEP CPU TIME =      .03 TOTAL CPU TIME =        9.5 (     .2 MIN)
 TOTAL WALL CLOCK TIME=        9.5 SECONDS, CPU UTILIZATION IS 100.00%
 74452 WORDS OF DYNAMIC MEMORY USED
 EXECUTION OF GAMESS TERMINATED NORMALLY 16:14:55 10-07-1999
              AOINTS length        175 KB
             DICTNRY length        343 KB
```