HNO MONOMER at MNDO

```
 ************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ************************************
 -------------------
 # mndo opt=z-matrix
 -------------------
 -----------
 HNO monomer
 -----------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 O     1     NO
 H     1     HN        2     HNO
       Variables:
  no                    1.4
  hn                    1.
  hno                 120.

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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 ---------------------------------------------------------------------
                         Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------
   1   1  N
   2   2  O     1   1.160986(  1)
   3   3  H     1   1.048315(  2)   2  113.755(  3)
 ---------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          8           0.000000    0.000000    1.160986
    3          1           0.959500    0.000000   -0.422285
 ---------------------------------------------------------
                   Distance matrix (angstroms):
              1          2          3
  1  N    0.000000
  2  O    1.160986   0.000000
  3  H    1.048315   1.851320   0.000000
                         Interatomic angles:
       O2-N1-H3=113.7547
 Stoichiometry    HNO
 Framework group  CS[SG(HNO)]
 Deg. of freedom    3
```

```
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          7           0.059969    0.554100    0.000000
   2          8           0.059969   -0.606886    0.000000
   3          1          -0.899531    0.976385    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    627.2740822     45.0698391     42.0486318
Isotopes: N-14,O-16,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of A'  symmetry.
There are     2 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
    9 basis functions       27 primitive gaussians
    6 alpha electrons        6 beta electrons
      nuclear repulsion energy        17.9129645158 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A") (A')
      Virtual   (A") (A') (A')
RHF-MNDO calculation of energy and first derivatives.
MO and density RWFs will be updated.
Closed-shell calculation:   6 occupied levels.
NNHCO=    0.
References:
 H: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
 N: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
 O: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.67D-01 DiagD=T ESCF=     30.565180 Diff=-1.28D+00 RMSDP= 5.44D-01.
It=  2 PL= 3.53D-02 DiagD=T ESCF=      2.979094 Diff=-2.76D+00 RMSDP= 1.28D-02.
It=  3 PL= 1.14D-02 DiagD=F ESCF=      1.761142 Diff=-1.22D-01 RMSDP= 6.23D-03.
It=  4 PL= 3.09D-03 DiagD=F ESCF=      1.585845 Diff=-1.75D-02 RMSDP= 9.61D-04.
It=  5 PL= 1.58D-03 DiagD=F ESCF=      1.637244 Diff= 5.14D-03 RMSDP= 4.90D-04.
It=  6 PL= 7.95D-04 DiagD=F ESCF=      1.636104 Diff=-1.14D-04 RMSDP= 5.46D-04.
It=  7 PL= 5.12D-05 DiagD=F ESCF=      1.635173 Diff=-9.31D-05 RMSDP= 2.48D-05.
It=  8 PL= 2.19D-05 DiagD=F ESCF=      1.635640 Diff= 4.67D-05 RMSDP= 1.28D-05.
It=  9 PL= 1.16D-05 DiagD=F ESCF=      1.635639 Diff=-9.31D-08 RMSDP= 1.48D-05.
Energy=    0.006010975861 NIter=  10.
Dipole moment= -0.413638  0.295425  0.000000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
   1          7           0.000006774    0.000000000    0.000007500
```

```
   2          8          -0.000003882    0.000000000   -0.000005398
   3          1          -0.000002893    0.000000000   -0.000002102
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000007500 RMS     0.000004205
-------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  O     1  -0.000005(   1)
  3  H     1  -0.000002(   2)  2   0.000006(   3)
-------------------------------------------------------------------
Internal  Forces:  Max     0.000006119 RMS     0.000004824

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  4  5  7
Trust test= 1.02D+00 RLast= 8.72D-04 DXMaxT set to 6.20D-01
The second derivative matrix:
                           no        hn        hno
          no           1.51995
          hn           0.10744   0.37560
          hno          0.11356   0.02131   0.33346
    Eigenvalues ---    0.32001   0.36808   1.54091
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.00148.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   no        2.19395  -0.00001   0.00000   0.00000   0.00000   2.19394
   hn        1.98103   0.00000   0.00000   0.00000   0.00000   1.98102
  hno        1.98539   0.00001   0.00000   0.00002   0.00002   1.98541
        Item               Value     Threshold  Converged?
Maximum Force            0.000006     0.000450     YES
RMS     Force            0.000005     0.000300     YES
Maximum Displacement     0.000020     0.001800     YES
RMS     Displacement     0.000012     0.001200     YES
Predicted change in Energy=-7.819020D-11
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       no          1.161    -DE/DX =    0.                            !
!       hn          1.0483   -DE/DX =    0.                            !
!       hno       113.7547   -DE/DX =    0.                            !
-------------------------------------------------------------------------
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```

```
**********************************************************************

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A') (A') (A') (A") (A') 
      Virtual   (A") (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --   -1.66816  -0.98716  -0.71423  -0.60560  -0.59122
Alpha  occ. eigenvalues --   -0.40340
Alpha virt. eigenvalues --   -0.00347   0.12438   0.26721
         Condensed to atoms (all electrons):
              1          2          3
 1  N    4.437333   0.273464   0.174920
 2  O    0.273464   5.910568  -0.015913
 3  H    0.174920  -0.015913   0.787158
Total atomic charges:
              1
 1  N    0.114283
 2  O   -0.168118
 3  H    0.053835
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  N    0.168118
 2  O   -0.168118
 3  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RMNDO\ZDO\H1N1O1\GLASER\07-Apr-1998\1\\# MNDO OPT=
Z-MATRIX\\HNO monomer\\0,1\N\O,1,no\H,1,hn,2,hno\\no=1.16098599\hn=1.0
4831502\hno=113.75473001\\Version=SGI-G94RevC.3\State=1-A'\HF=0.006011
\RMSD=0.000e+00\RMSF=4.205e-06\Dipole=0.4136383,0.,-0.295425\PG=CS [SG
(H1N1O1)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  6.9 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

HNO MONOMER at AM1

```
 ************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ************************************
 ------------------
 # AM1 opt=z-matrix
 ------------------
 ------------------
 HNO monomer at AM1
 ------------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 O     1     NO
 H     1     HN        2     HNO
       Variables:
  no                    1.4
  hn                    1.
  hno                 120.

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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 ---------------------------------------------------------------------
                         Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------
   1   1  N
   2   2  O     1   1.156829(  1)
   3   3  H     1   1.042419(  2)   2  115.420(  3)
 ---------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          8           0.000000    0.000000    1.156829
    3          1           0.941496    0.000000   -0.447463
 ---------------------------------------------------------
                   Distance matrix (angstroms):
              1          2          3
  1  N    0.000000
  2  O    1.156829   0.000000
  3  H    1.042419   1.860152   0.000000
                         Interatomic angles:
       O2-N1-H3=115.4202
 Stoichiometry    HNO
 Framework group  CS[SG(HNO)]
 Deg. of freedom    3
```

```
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          7           0.058843    0.550448    0.000000
   2          8           0.058843   -0.606381    0.000000
   3          1          -0.882652    0.997911    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    654.7600487     45.1679150     42.2531286
Isotopes: N-14,O-16,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of A'  symmetry.
There are     2 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
    9 basis functions       27 primitive gaussians
    6 alpha electrons        6 beta electrons
      nuclear repulsion energy        17.9682337562 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A") (A')
      Virtual   (A") (A') (A')
RHF-AM1 calculation of energy and first derivatives.
MO and density RWFs will be updated.
Closed-shell calculation:   6 occupied levels.
NNHCO=    0.
References:
 H: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
 N: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
 O: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.66D-01 DiagD=T ESCF=     30.370743 Diff=-1.30D+00 RMSDP= 5.44D-01.
It=  2 PL= 3.77D-02 DiagD=T ESCF=      2.374611 Diff=-2.80D+00 RMSDP= 1.32D-02.
It=  3 PL= 1.18D-02 DiagD=F ESCF=      1.070892 Diff=-1.30D-01 RMSDP= 6.39D-03.
It=  4 PL= 3.76D-03 DiagD=F ESCF=      0.882802 Diff=-1.88D-02 RMSDP= 1.10D-03.
It=  5 PL= 2.04D-03 DiagD=F ESCF=      0.934732 Diff= 5.19D-03 RMSDP= 5.96D-04.
It=  6 PL= 1.09D-03 DiagD=F ESCF=      0.933101 Diff=-1.63D-04 RMSDP= 7.47D-04.
It=  7 PL= 7.48D-05 DiagD=F ESCF=      0.931448 Diff=-1.65D-04 RMSDP= 3.54D-05.
It=  8 PL= 3.58D-05 DiagD=F ESCF=      0.932332 Diff= 8.84D-05 RMSDP= 1.92D-05.
It=  9 PL= 1.62D-05 DiagD=F ESCF=      0.932330 Diff=-2.05D-07 RMSDP= 2.38D-05.
It= 10 PL= 4.79D-06 DiagD=F ESCF=      0.932328 Diff=-2.00D-07 RMSDP= 1.50D-06.
It= 11 PL= 2.61D-06 DiagD=F ESCF=      0.932329 Diff= 1.05D-07 RMSDP= 8.10D-07.
Energy=    0.003426311836 NIter=  12.
Dipole moment= -0.482376  0.346253  0.000000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number             X             Y             Z
```

```
---------------------------------------------------------------------
   1          7          -0.000012320    0.000000000    0.000008058
   2          8          -0.000001486    0.000000000   -0.000000392
   3          1           0.000013806    0.000000000   -0.000007666
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000013806 RMS     0.000007215
---------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
---------------------------------------------------------------------------
  1  N
  2  O     1   0.000000(   1)
  3  H     1   0.000016(   2)  2   0.000002(   3)
---------------------------------------------------------------------------
Internal  Forces:  Max     0.000015760 RMS     0.000009172

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  4  5  7
Trust test= 1.02D+00 RLast= 5.81D-04 DXMaxT set to 6.25D-01
The second derivative matrix:
                           no        hn        hno
          no           1.38512
          hn           0.10576   0.39269
          hno          0.13376   0.04410   0.31134
    Eigenvalues ---    0.28506   0.39062   1.41347
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of  0.01277.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   no        2.18609   0.00000   0.00001  -0.00001   0.00000   2.18609
   hn        1.96989   0.00002   0.00000   0.00004   0.00004   1.96993
  hno        2.01446   0.00000   0.00000   0.00000   0.00000   2.01447
        Item               Value     Threshold  Converged?
Maximum Force            0.000016     0.000450     YES
RMS     Force            0.000009     0.000300     YES
Maximum Displacement     0.000042     0.001800     YES
RMS     Displacement     0.000024     0.001200     YES
Predicted change in Energy=-3.361919D-10
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
---------------------                           ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
---------------------------------------------------------------------------
!       no          1.1568   -DE/DX =    0.                             !
!       hn          1.0424   -DE/DX =    0.                             !
!       hno       115.4202   -DE/DX =    0.                             !
---------------------------------------------------------------------------
```

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

            Population analysis using the SCF density.

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

 Orbital Symmetries:
       Occupied  (A') (A') (A') (A') (A") (A')
       Virtual   (A") (A') (A')
  The electronic state is 1-A'.
 Alpha  occ. eigenvalues --   -1.55932  -1.01081  -0.71342  -0.60787  -0.60701
 Alpha  occ. eigenvalues --   -0.38887
 Alpha virt. eigenvalues --    0.00261   0.11820   0.23970
          Condensed to atoms (all electrons):
              1          2          3
  1  N    4.409043   0.322782   0.176827
  2  O    0.322782   5.891794  -0.022609
  3  H    0.176827  -0.022609   0.745164
 Total atomic charges:
              1
  1  N    0.091348
  2  O   -0.191967
  3  H    0.100619
 Sum of Mulliken charges=   0.00000
 Atomic charges with hydrogens summed into heavy atoms:
              1
  1  N    0.191967
  2  O   -0.191967
  3  H    0.000000
 Sum of Mulliken charges=   0.00000
 1\1\GINC-SHIVA\FOpt\RAM1\ZDO\H1N1O1\GLASER\07-Apr-1998\1\\# AM1 OPT=Z-
 MATRIX\\HNO monomer at AM1\\0,1\N\O,1,no\H,1,hn,2,hno\\no=1.15682908\h
 n=1.04241865\hno=115.42023475\\Version=SGI-G94RevC.3\State=1-A'\HF=0.0
 034263\RMSD=0.000e+00\RMSF=7.215e-06\Dipole=0.4823756,0.,-0.3462526\PG
 =CS [SG(H1N1O1)]\\@


 THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                     SHAKESPEARE
 Job cpu time:  0 days  0 hours  0 minutes  6.9 seconds.
 File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
 Normal termination of Gaussian 94
```

HNO MONOMER at PM3

```
 ***************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ***************************************
 ------------------
 # PM3 opt=z-matrix
 ------------------
 ------------------
 HNO monomer at PM3
 ------------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 O     1     NO
 H     1     HN        2     HNO
       Variables:
  no                    1.4
  hn                    1.
  hno                 120.

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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 ---------------------------------------------------------------------
                         Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------
   1   1  N
   2   2  O     1   1.175464(  1)
   3   3  H     1   0.997297(  2)   2  116.142(  3)
 ---------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          8           0.000000    0.000000    1.175464
    3          1           0.895280    0.000000   -0.439403
 ---------------------------------------------------------------
                   Distance matrix (angstroms):
              1          2          3
  1  N    0.000000
  2  O    1.175464   0.000000
  3  H    0.997297   1.846435   0.000000
                           Interatomic angles:
       O2-N1-H3=116.1418
 Stoichiometry    HNO
 Framework group  CS[SG(HNO)]
 Deg. of freedom    3
```

```
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          7           0.055955    0.560269    0.000000
   2          8           0.055955   -0.615195    0.000000
   3          1          -0.839325    0.999672    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    721.1793147     43.9245694     41.4028625
Isotopes: N-14,O-16,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of A'  symmetry.
There are     2 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
    9 basis functions       27 primitive gaussians
    6 alpha electrons        6 beta electrons
      nuclear repulsion energy        17.8781987690 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A')
RHF-PM3 calculation of energy and first derivatives.
MO and density RWFs will be updated.
Closed-shell calculation:   6 occupied levels.
NNHCO=    0.
References:
 H: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
 N: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
 O: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.74D-01 DiagD=T ESCF=     25.228706 Diff=-1.81D+00 RMSDP= 5.44D-01.
It=  2 PL= 4.42D-02 DiagD=T ESCF=      7.120529 Diff=-1.81D+00 RMSDP= 1.35D-02.
It=  3 PL= 1.64D-02 DiagD=F ESCF=      6.132417 Diff=-9.88D-02 RMSDP= 7.97D-03.
It=  4 PL= 1.32D-03 DiagD=F ESCF=      5.899459 Diff=-2.33D-02 RMSDP= 9.25D-04.
It=  5 PL= 8.68D-04 DiagD=F ESCF=      5.977396 Diff= 7.79D-03 RMSDP= 4.69D-04.
It=  6 PL= 4.96D-04 DiagD=F ESCF=      5.976277 Diff=-1.12D-04 RMSDP= 5.89D-04.
It=  7 PL= 6.54D-05 DiagD=F ESCF=      5.975208 Diff=-1.07D-04 RMSDP= 3.25D-05.
It=  8 PL= 2.56D-05 DiagD=F ESCF=      5.975832 Diff= 6.24D-05 RMSDP= 1.28D-05.
It=  9 PL= 1.33D-05 DiagD=F ESCF=      5.975831 Diff=-9.82D-08 RMSDP= 1.13D-05.
Energy=    0.021961200910 NIter=  10.
Dipole moment= -0.487074  0.427687  0.000000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
   1          7           0.000011753    0.000000000   -0.000000827
```

```
   2          8          -0.000000985    0.000000000   -0.000003708
   3          1          -0.000010769    0.000000000    0.000004535
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000011753 RMS     0.000005677
-------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  O     1  -0.000004(   1)
  3  H     1  -0.000012(   2)  2   0.000001(   3)
-------------------------------------------------------------------
Internal  Forces:  Max     0.000011665 RMS     0.000007105

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Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  4  5  7
Trust test= 1.01D+00 RLast= 8.31D-04 DXMaxT set to 2.51D-01
The second derivative matrix:
                           no        hn        hno
          no           1.22035
          hn           0.07924   0.47351
          hno          0.09582   0.05665   0.29033
    Eigenvalues ---    0.26873   0.47597   1.23949
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.00170.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   no        2.22130   0.00000   0.00000   0.00000   0.00000   2.22130
   hn        1.88462  -0.00001   0.00000  -0.00003  -0.00003   1.88459
  hno        2.02706   0.00000   0.00000   0.00001   0.00001   2.02707
        Item               Value     Threshold  Converged?
Maximum Force            0.000012     0.000450     YES
RMS     Force            0.000007     0.000300     YES
Maximum Displacement     0.000025     0.001800     YES
RMS     Displacement     0.000016     0.001200     YES
Predicted change in Energy=-1.586360D-10
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       no          1.1755   -DE/DX =    0.                            !
!       hn          0.9973   -DE/DX =    0.                            !
!       hno       116.1418   -DE/DX =    0.                            !
-------------------------------------------------------------------------
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```

```
 ****************************************************************

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --   -1.37603  -0.87030  -0.69001  -0.56533  -0.55918
Alpha  occ. eigenvalues --   -0.36168
Alpha virt. eigenvalues --    0.00262   0.11476   0.24537
         Condensed to atoms (all electrons):
             1          2          3
 1  N    4.235817   0.393155   0.125108
 2  O    0.393155   5.914538  -0.034476
 3  H    0.125108  -0.034476   0.882072
Total atomic charges:
             1
 1  N    0.245921
 2  O   -0.273216
 3  H    0.027296
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  N    0.273216
 2  O   -0.273216
 3  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RPM3\ZDO\H1N1O1\GLASER\07-Apr-1998\1\\# PM3 OPT=Z-
MATRIX\\HNO monomer at PM3\\0,1\N\O,1,no\H,1,hn,2,hno\\no=1.17546378\h
n=0.99729723\hno=116.14179222\\Version=SGI-G94RevC.3\State=1-A'\HF=0.0
219612\RMSD=0.000e+00\RMSF=5.677e-06\Dipole=0.4870738,0.,-0.4276872\PG
=CS [SG(H1N1O1)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  7.1 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

HNO MONOMER at CNDO

```
 ************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ************************************
 -------------------
 # CNDO opt=z-matrix
 -------------------
 -------------------
 HNO monomer at CNDO
 -------------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 O     1     NO
 H     1     HN        2     HNO
       Variables:
  no                    1.4
  hn                    1.
  hno                 120.

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 ---------------------------------------------------------------------
                         Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------
   1   1  N
   2   2  O     1   1.180269(  1)
   3   3  H     1   1.081578(  2)   2  111.405(  3)
 ---------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          8           0.000000    0.000000    1.180269
    3          1           1.006977    0.000000   -0.394725
 ---------------------------------------------------------
                   Distance matrix (angstroms):
              1          2          3
  1  N    0.000000
  2  O    1.180269   0.000000
  3  H    1.081578   1.869388   0.000000
                         Interatomic angles:
       O2-N1-H3=111.4047
 Stoichiometry    HNO
 Framework group  CS[SG(HNO)]
 Deg. of freedom    3
```

```
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          7           0.062936    0.565464    0.000000
   2          8           0.062936   -0.614805    0.000000
   3          1          -0.944041    0.960189    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    566.1128291     43.8715238     40.7161796
Isotopes: N-14,O-16,H-1
Standard basis: VSTO-3G* (5D, 7F)
There are     7 symmetry adapted basis functions of A'  symmetry.
There are     2 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
    9 basis functions       27 primitive gaussians
    6 alpha electrons        6 beta electrons
      nuclear repulsion energy        17.5953633673 Hartrees.
RHF-CNDO calculation of energy and first derivatives.
MO and density RWFs will be updated.
CNDO iteration  1 energy         -48.32587544 RMS DP=2.72D-01
CNDO iteration  2 energy         -48.33509736 RMS DP=1.02D-02
CNDO iteration  3 energy         -48.33674998 RMS DP=4.32D-03
CNDO iteration  4 energy         -48.33712312 RMS DP=2.16D-03
CNDO iteration  5 energy         -48.33721975 RMS DP=1.05D-03
CNDO iteration  6 energy         -48.33724760 RMS DP=6.23D-04
CNDO iteration  7 energy         -48.33725657 RMS DP=3.07D-04
CNDO iteration  8 energy         -48.33725972 RMS DP=2.05D-04
CNDO iteration  9 energy         -48.33726090 RMS DP=1.02D-04
CNDO iteration 10 energy         -48.33726138 RMS DP=7.49D-05
CNDO iteration 11 energy         -48.33726158 RMS DP=3.88D-05
CNDO iteration 12 energy         -48.33726167 RMS DP=2.99D-05
CNDO iteration 13 energy         -48.33726171 RMS DP=1.66D-05
CNDO iteration 14 4-point extrapolation.
CNDO iteration 15 energy         -48.33726175 RMS DP=1.80D-06
CNDO iteration 16 energy         -48.33726175 RMS DP=1.05D-06
CNDO iteration 17 energy         -48.33726175 RMS DP=6.55D-07
CNDO iteration 18 energy         -48.33726175 RMS DP=3.92D-07
CNDO iteration 19 energy         -48.33726175 RMS DP=2.58D-07
CNDO iteration 20 energy         -48.33726175 RMS DP=1.62D-07
CNDO iteration 21 energy         -48.33726175 RMS DP=1.11D-07
CNDO iteration 22 energy         -48.33726175 RMS DP=7.26D-08
Final CNDO energy   -30.74189838
Energy=  -30.741898380306 NIter=  22.
Dipole moment=  0.000000  0.000000  0.000000
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
```

```
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7           0.000018662    0.000000000   -0.000018334
   2          8          -0.000004773    0.000000000    0.000018527
   3          1          -0.000013890    0.000000000   -0.000000193
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000018662 RMS     0.000011754
-------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  O     1   0.000019(   1)
  3  H     1  -0.000013(   2)  2   0.000011(   3)
-------------------------------------------------------------------------
Internal  Forces:  Max     0.000018527 RMS     0.000014419

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   8 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  5  6  7  8
Trust test= 9.95D-01 RLast= 1.75D-03 DXMaxT set to 4.90D-01
The second derivative matrix:
                           no        hn        hno
          no           2.81776
          hn           0.16066   0.77089
          hno          0.05378   0.05221   0.31080
    Eigenvalues ---    0.30444   0.76340   2.83161
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.01318.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   no        2.23039   0.00002   0.00000   0.00001   0.00001   2.23039
   hn        2.04389  -0.00001   0.00001  -0.00003  -0.00002   2.04387
  hno        1.94438   0.00001   0.00002   0.00001   0.00004   1.94442
        Item               Value     Threshold  Converged?
Maximum Force            0.000019     0.000450     YES
RMS     Force            0.000014     0.000300     YES
Maximum Displacement     0.000037     0.001800     YES
RMS     Displacement     0.000025     0.001200     YES
Predicted change in Energy=-3.890273D-10
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
---------------------                            ---------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       no          1.1803   -DE/DX =    0.                           !
!       hn          1.0816   -DE/DX =    0.                           !
!       hno       111.4047   -DE/DX =    0.                           !
```

```
-------------------------------------------------------------------
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*********************************************************************

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A') (A') (A') (A') (A") (A')
      Virtual   (A") (A') (A')
 The electronic state is 1-A'.
Alpha  occ. eigenvalues --   -1.68639  -1.09644  -0.90416  -0.77084  -0.70841
Alpha  occ. eigenvalues --   -0.51593
Alpha virt. eigenvalues --    0.12226   0.26112   0.46216
         Condensed to atoms (all electrons):
             1          2          3
 1  N    4.364009   0.353131   0.225770
 2  O    0.353131   5.800504  -0.029075
 3  H    0.225770  -0.029075   0.735835
Total atomic charges:
             1
 1  N    0.057090
 2  O   -0.124560
 3  H    0.067470
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  N    0.124560
 2  O   -0.124560
 3  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RCNDO\ZDO\H1N1O1\GLASER\07-Apr-1998\1\\# CNDO OPT=
Z-MATRIX\\HNO monomer at CNDO\\0,1\N\O,1,no\H,1,hn,2,hno\\no=1.1802690
2\hn=1.08157821\hno=111.40468443\\Version=SGI-G94RevC.3\State=1-A'\HF=
-30.7418984\RMSD=0.000e+00\RMSF=1.175e-05\Dipole=0.,0.,0.\PG=CS [SG(H1
N1O1)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  5.5 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Cis HNO DIMER at MNDO

```
 ************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ************************************
 -------------------
 # mndo opt=z-matrix
 -------------------
 -------------
 cis HNO dimer
 -------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 N     1     NN
 O     2     NO        1     ONN
 O     1     NO        2     ONN       3     0.        0
 H     2     NH        1     HNN       3     180.      0
 H     1     NH        2     HNN       3     180.      0
       Variables:
  nn                    1.4
  no                    1.4
  nh                    1.
  onn                 120.
  hnn                 120.

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 ---------------------------------------------------------------------
                        Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------
   1   1  N
   2   2  N     1   1.322998(  1)
   3   3  O     2   1.219762(  2)   1  123.145(  6)
   4   4  O     1   1.219762(  3)   2  123.145(  7)   3    0.000( 10)   0
   5   5  H     2   1.038791(  4)   1  115.946(  8)   3  180.000( 11)   0
   6   6  H     1   1.038791(  5)   2  115.946(  9)   3  180.000( 12)   0
 ---------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          7           0.000000    0.000000    1.322998
    3          8           1.021290    0.000000    1.989921
    4          8           1.021290    0.000000   -0.666922
    5          1          -0.934085    0.000000    1.777501
    6          1          -0.934085    0.000000   -0.454502
```

```
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.322998   0.000000
 3  O    2.236698   1.219762   0.000000
 4  O    1.219762   2.236698   2.656843   0.000000
 5  H    2.007990   1.038791   1.966879   3.130287   0.000000
 6  H    1.038791   2.007990   3.130287   1.966879   2.232003
             6
 6  H    0.000000
                         Interatomic angles:
      N1-N2-O3=123.1453       N2-N1-O4=123.1453       N1-N2-H5=115.9464
      O3-N2-H5=120.9083       N2-N1-H6=115.9464       O4-N1-H6=120.9083
Stoichiometry    H2N2O2
Framework group  C2V[SGV(H2N2O2)]
Deg. of freedom    5
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          7           0.000000    0.661499    0.452265
   2          7           0.000000   -0.661499    0.452265
   3          8           0.000000   -1.328422   -0.569025
   4          8           0.000000    1.328422   -0.569025
   5          1           0.000000   -1.116002    1.386350
   6          1           0.000000    1.116002    1.386350
---------------------------------------------------------
Rotational constants (GHZ):     25.4737752      7.0962322      5.5501315
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of A1  symmetry.
There are     2 symmetry adapted basis functions of A2  symmetry.
There are     2 symmetry adapted basis functions of B1  symmetry.
There are     7 symmetry adapted basis functions of B2  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        70.6191401465 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (A1) (B1) (B2) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (B2) (A1) (B2)
RHF-MNDO calculation of energy and first derivatives.
MO and density RWFs will be updated.
Closed-shell calculation:  12 occupied levels.
```

```
NNHCO=    0.
References:
 H: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
 N: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
 O: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.46D-01 DiagD=T ESCF=     96.911551 Diff= 5.35D+00 RMSDP= 3.85D-01.
It=  2 PL= 5.53D-02 DiagD=T ESCF=     30.681818 Diff=-6.62D+00 RMSDP= 1.01D-02.
It=  3 PL= 1.64D-02 DiagD=F ESCF=     27.686187 Diff=-3.00D-01 RMSDP= 4.38D-03.
It=  4 PL= 3.98D-03 DiagD=F ESCF=     27.309994 Diff=-3.76D-02 RMSDP= 7.91D-04.
It=  5 PL= 1.96D-03 DiagD=F ESCF=     27.407736 Diff= 9.77D-03 RMSDP= 4.14D-04.
3-point extrapolation.
It=  6 PL= 1.10D-03 DiagD=F ESCF=     27.404753 Diff=-2.98D-04 RMSDP= 5.30D-04.
It=  7 PL= 6.32D-03 DiagD=F ESCF=     27.387311 Diff=-1.74D-03 RMSDP= 1.01D-03.
It=  8 PL= 2.75D-03 DiagD=F ESCF=     27.412546 Diff= 2.52D-03 RMSDP= 5.99D-04.
It=  9 PL= 1.56D-03 DiagD=F ESCF=     27.406358 Diff=-6.19D-04 RMSDP= 7.94D-04.
It= 10 PL= 1.14D-04 DiagD=F ESCF=     27.399419 Diff=-6.94D-04 RMSDP= 2.55D-05.
It= 11 PL= 7.35D-05 DiagD=F ESCF=     27.403364 Diff= 3.95D-04 RMSDP= 1.20D-05.
It= 12 PL= 4.03D-05 DiagD=F ESCF=     27.403361 Diff=-2.80D-07 RMSDP= 1.71D-05.
It= 13 PL= 3.34D-06 DiagD=F ESCF=     27.403358 Diff=-3.47D-07 RMSDP= 1.20D-06.
It= 14 PL= 1.93D-06 DiagD=F ESCF=     27.403360 Diff= 1.99D-07 RMSDP= 4.57D-07.
Energy=    0.100707451951 NIter=  15.
Dipole moment=  0.000000  0.000000  2.499590
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
   1          7          -0.000034401    0.000000000   -0.000026448
   2          7          -0.000034396    0.000000000    0.000026449
   3          8           0.000055217    0.000000000    0.000038579
   4          8           0.000055218    0.000000000   -0.000038580
   5          1          -0.000020820    0.000000000    0.000015403
   6          1          -0.000020817    0.000000000   -0.000015404
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000055218 RMS     0.000028069
---------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
---------------------------------------------------------------------------
  1  N
  2  N     1   0.000080(   1)
  3  O     2   0.000067(   2)  1   0.000005(   6)
  4  O     1   0.000067(   3)  2   0.000005(   7)  3   0.000000(  10)  0
  5  H     2   0.000025(   4)  1   0.000009(   8)  3   0.000000(  11)  0
  6  H     1   0.000025(   5)  2   0.000009(   9)  3   0.000000(  12)  0
---------------------------------------------------------------------------
Internal  Forces:  Max     0.000080432 RMS     0.000037696

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
```

```
Update second derivatives using information from points  2  3  4  5  7

Trust test= 9.79D-01 RLast= 1.24D-03 DXMaxT set to 4.24D-01
The second derivative matrix:
                           nn        no        nh        onn       hnn
          nn           0.68495
          no           0.17040   2.13310
          nh           0.05983   0.12562   0.82284
          onn          0.25741   0.09058  -0.04245   0.96992
          hnn          0.08194  -0.19945   0.02378   0.37643   0.64975
    Eigenvalues ---    0.35221   0.56597   0.82620   1.32370   2.19247
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.07061.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.50010   0.00008   0.00007   0.00002   0.00009   2.50020
   no        2.30502   0.00013   0.00005   0.00000   0.00005   2.30507
   nh        1.96303   0.00005   0.00000   0.00005   0.00005   1.96308
  onn        2.14929   0.00001   0.00002  -0.00005  -0.00003   2.14926
  hnn        2.02365   0.00002   0.00001   0.00003   0.00004   2.02368
        Item               Value     Threshold  Converged?
Maximum Force            0.000135     0.000450     YES
RMS     Force            0.000074     0.000300     YES
Maximum Displacement     0.000091     0.001800     YES
RMS     Displacement     0.000055     0.001200     YES
Predicted change in Energy=-7.529318D-09
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       nn          1.323    -DE/DX =    0.0001                         !
!       no          1.2198   -DE/DX =    0.0001                         !
!       nh          1.0388   -DE/DX =    0.0001                         !
!       onn       123.1453   -DE/DX =    0.                             !
!       hnn       115.9464   -DE/DX =    0.                             !
-------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (A1) (B1) (B2) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (B2) (A1) (B2)
 The electronic state is 1-A1.
```

```
Alpha  occ. eigenvalues --   -1.64115  -1.52340  -1.25308  -0.94113  -0.82962
Alpha  occ. eigenvalues --   -0.70303  -0.64877  -0.64740  -0.50951  -0.44262
Alpha  occ. eigenvalues --   -0.39864  -0.32119
Alpha virt. eigenvalues --   -0.02704  -0.01272   0.06780   0.18513   0.23987
Alpha virt. eigenvalues --    0.30199
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
 1  N    4.178431   0.270142  -0.009979   0.234763  -0.025831   0.273272
 2  N    0.270142   4.178431   0.234763  -0.009979   0.273272  -0.025831
 3  O   -0.009979   0.234763   6.141976   0.000464  -0.012542   0.000527
 4  O    0.234763  -0.009979   0.000464   6.141976   0.000527  -0.012542
 5  H   -0.025831   0.273272  -0.012542   0.000527   0.485665   0.002903
 6  H    0.273272  -0.025831   0.000527  -0.012542   0.002903   0.485665
Total atomic charges:
               1
 1  N    0.079203
 2  N    0.079203
 3  O   -0.355209
 4  O   -0.355209
 5  H    0.276006
 6  H    0.276006
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
               1
 1  N    0.355209
 2  N    0.355209
 3  O   -0.355209
 4  O   -0.355209
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RMNDO\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# MNDO OPT=
Z-MATRIX\\cis HNO dimer\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,onn,3,0.,0
\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,180.,0\\nn=1.32299835\no=1.21976
208\nh=1.03879084\onn=123.14531176\hnn=115.94640312\\Version=SGI-G94Re
vC.3\State=1-A1\HF=0.1007075\RMSD=0.000e+00\RMSF=2.807e-05\Dipole=-2.4
9959,0.,0.\PG=C02V [SGV(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  7.1 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Cis HNO DIMER at AM1

```
 ***************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ***************************************
 ------------------
 # am1 opt=z-matrix
 ------------------
---------------------
 cis HNO dimer at AM1
 ---------------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 N     1     NN
 O     2     NO        1     ONN
 O     1     NO        2     ONN       3     0.        0
 H     2     NH        1     HNN       3     180.      0
 H     1     NH        2     HNN       3     180.      0
       Variables:
  nn                    1.4
  no                    1.4
  nh                    1.
  onn                 120.
  hnn                 120.

 EDITED

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 ----------------------------------------------------------------------
                       Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ----------------------------------------------------------------------
   1   1  N
   2   2  N     1   1.309956(  1)
   3   3  O     2   1.217525(  2)   1  123.683(  6)
   4   4  O     1   1.217525(  3)   2  123.683(  7)   3    0.000( 10)   0
   5   5  H     2   1.026186(  4)   1  115.656(  8)   3  180.000( 11)   0
   6   6  H     1   1.026186(  5)   2  115.656(  9)   3  180.000( 12)   0
 ----------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          7           0.000000    0.000000    1.309956
    3          8           1.013129    0.000000    1.985186
    4          8           1.013129    0.000000   -0.675231
    5          1          -0.925012    0.000000    1.754264
```

```
   6          1          -0.925012    0.000000   -0.444308
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.309956   0.000000
 3  O    2.228765   1.217525   0.000000
 4  O    1.217525   2.228765   2.660417   0.000000
 5  H    1.983202   1.026186   1.951849   3.107866   0.000000
 6  H    1.026186   1.983202   3.107866   1.951849   2.198572
             6
 6  H    0.000000
                          Interatomic angles:
      N1-N2-O3=123.6827       N2-N1-O4=123.6827       N1-N2-H5=115.6562
      O3-N2-H5=120.6611       N2-N1-H6=115.6562       O4-N1-H6=120.6611
Stoichiometry    H2N2O2
Framework group  C2V[SGV(H2N2O2)]
Deg. of freedom    5
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          7           0.000000    0.654978    0.448751
   2          7           0.000000   -0.654978    0.448751
   3          8           0.000000   -1.330209   -0.564378
   4          8           0.000000    1.330209   -0.564378
   5          1           0.000000   -1.099286    1.373763
   6          1           0.000000    1.099286    1.373763
---------------------------------------------------------
Rotational constants (GHZ):     25.8980565      7.1125204      5.5800435
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of A1  symmetry.
There are     2 symmetry adapted basis functions of A2  symmetry.
There are     2 symmetry adapted basis functions of B1  symmetry.
There are     7 symmetry adapted basis functions of B2  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        70.9460455308 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (A1) (B1) (B2) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (B2) (A1) (B2)
RHF-AM1 calculation of energy and first derivatives.
MO and density RWFs will be updated.
```

```
Closed-shell calculation:  12 occupied levels.
NNHCO=    0.
References:
 H: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
 N: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
 O: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.57D-01 DiagD=T ESCF=    100.255866 Diff= 5.69D+00 RMSDP= 3.85D-01.
It=  2 PL= 6.02D-02 DiagD=T ESCF=     26.783201 Diff=-7.35D+00 RMSDP= 1.06D-02.
It=  3 PL= 1.73D-02 DiagD=F ESCF=     23.357334 Diff=-3.43D-01 RMSDP= 4.43D-03.
It=  4 PL= 3.40D-03 DiagD=F ESCF=     22.954350 Diff=-4.03D-02 RMSDP= 7.50D-04.
It=  5 PL= 1.62D-03 DiagD=F ESCF=     23.059046 Diff= 1.05D-02 RMSDP= 3.80D-04.
It=  6 PL= 8.89D-04 DiagD=F ESCF=     23.056539 Diff=-2.51D-04 RMSDP= 4.64D-04.
It=  7 PL= 8.64D-05 DiagD=F ESCF=     23.054135 Diff=-2.40D-04 RMSDP= 1.91D-05.
It=  8 PL= 4.66D-05 DiagD=F ESCF=     23.055452 Diff= 1.32D-04 RMSDP= 8.90D-06.
It=  9 PL= 2.64D-05 DiagD=F ESCF=     23.055451 Diff=-1.63D-07 RMSDP= 1.14D-05.
It= 10 PL= 3.22D-06 DiagD=F ESCF=     23.055449 Diff=-1.65D-07 RMSDP= 1.11D-06.
Energy=    0.084728866464 NIter=  11.
Dipole moment=  0.000000  0.000000  2.594422
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7           0.000113204    0.000000000    0.000004092
   2          7           0.000113199    0.000000000   -0.000004094
   3          8          -0.000127515    0.000000000   -0.000102936
   4          8          -0.000127519    0.000000000    0.000102939
   5          1           0.000014315    0.000000000   -0.000002516
   6          1           0.000014315    0.000000000    0.000002515
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000127519 RMS     0.000066583
-------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  N     1  -0.000110(   1)
  3  O     2  -0.000163(   2)  1  -0.000034(   6)
  4  O     1  -0.000163(   3)  2  -0.000034(   7)  3   0.000000(  10)  0
  5  H     2  -0.000014(   4)  1   0.000008(   8)  3   0.000000(  11)  0
  6  H     1  -0.000014(   5)  2   0.000008(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------
Internal  Forces:  Max     0.000163200 RMS     0.000075353

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  2  3  4  5  7

Trust test= 8.00D-01 RLast= 1.07D-03 DXMaxT set to 4.42D-01
The second derivative matrix:
```

```
                         nn        no        nh        onn       hnn
          nn           0.70481
          no           0.08390   1.76617
          nh           0.02489   0.02110   0.75784
          onn          0.12456  -0.10317  -0.12968   0.77086
          hnn          0.11934  -0.19216  -0.00793   0.39395   0.64578
    Eigenvalues ---    0.29143   0.59741   0.77716   1.14891   1.83055
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.20510.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.47546  -0.00011  -0.00011   0.00001  -0.00009   2.47537
   no        2.30079  -0.00033  -0.00011  -0.00003  -0.00014   2.30065
   nh        1.93921  -0.00003  -0.00010   0.00008  -0.00002   1.93919
  onn        2.15867  -0.00007  -0.00010  -0.00001  -0.00011   2.15856
  hnn        2.01858   0.00002   0.00007   0.00000   0.00007   2.01865
        Item               Value     Threshold  Converged?
Maximum Force            0.000326     0.000450     YES
RMS     Force            0.000158     0.000300     YES
Maximum Displacement     0.000140     0.001800     YES
RMS     Displacement     0.000095     0.001200     YES
Predicted change in Energy=-2.527156D-08
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       nn          1.31     -DE/DX =   -0.0001                         !
!       no          1.2175   -DE/DX =   -0.0003                         !
!       nh          1.0262   -DE/DX =    0.                            !
!       onn       123.6827   -DE/DX =   -0.0001                         !
!       hnn       115.6562   -DE/DX =    0.                            !
-------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

          Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (A1) (B1) (B2) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (B2) (A1) (B2)
 The electronic state is 1-A1.
Alpha  occ. eigenvalues --   -1.56033  -1.42535  -1.23572  -0.95554  -0.82554
Alpha  occ. eigenvalues --   -0.71905  -0.66345  -0.64040  -0.52066  -0.45065
Alpha  occ. eigenvalues --   -0.39879  -0.32434
Alpha virt. eigenvalues --   -0.01697  -0.00961   0.06815   0.18117   0.21725
```

```
Alpha virt. eigenvalues --    0.27909
         Condensed to atoms (all electrons):
             1          2          3          4          5          6
 1  N    4.152519   0.286288  -0.014461   0.281556  -0.035304   0.278833
 2  N    0.286288   4.152519   0.281556  -0.014461   0.278833  -0.035304
 3  O   -0.014461   0.281556   6.124714   0.000901  -0.018017   0.001086
 4  O    0.281556  -0.014461   0.000901   6.124714   0.001086  -0.018017
 5  H   -0.035304   0.278833  -0.018017   0.001086   0.443868   0.004327
 6  H    0.278833  -0.035304   0.001086  -0.018017   0.004327   0.443868
Total atomic charges:
             1
 1  N    0.050570
 2  N    0.050570
 3  O   -0.375778
 4  O   -0.375778
 5  H    0.325207
 6  H    0.325207
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  N    0.375778
 2  N    0.375778
 3  O   -0.375778
 4  O   -0.375778
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RAM1\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# AM1 OPT=Z-
MATRIX\\cis HNO dimer at AM1\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,onn,3
,0.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,180.,0\\nn=1.30995567\no=1.
21752455\nh=1.02618583\onn=123.68269248\hnn=115.656208\\Version=SGI-G9
4RevC.3\State=1-A1\HF=0.0847289\RMSD=0.000e+00\RMSF=6.658e-05\Dipole=-
2.5944224,0.,0.\PG=C02V [SGV(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  7.2 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Cis HNO DIMER at PM3

```
****************************************
Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
****************************************
------------------
# PM3 opt=z-matrix
------------------
--------------------
cis HNO dimer at PM3
--------------------
Symbolic Z-matrix:
   Charge = 0 Multiplicity = 1
N
N     1     NN
O     2     NO        1     ONN
O     1     NO        2     ONN       3     0.        0
H     2     NH        1     HNN       3     180.      0
H     1     NH        2     HNN       3     180.      0
      Variables:
 nn                    1.4
 no                    1.4
 nh                    1.
 onn                 120.
 hnn                 120.

EDITED

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

-----------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
-----------------------------------------------------------------------
  1   1  N
  2   2  N     1   1.318918(  1)
  3   3  O     2   1.248088(  2)   1  123.402(  6)
  4   4  O     1   1.248088(  3)   2  123.402(  7)   3    0.000( 10)   0
  5   5  H     2   0.994256(  4)   1  116.472(  8)   3  180.000( 11)   0
  6   6  H     1   0.994256(  5)   2  116.472(  9)   3  180.000( 12)   0
-----------------------------------------------------------------------
                Z-Matrix orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.000000    0.000000
   2          7           0.000000    0.000000    1.318918
   3          8           1.041943    0.000000    2.005997
   4          8           1.041943    0.000000   -0.687079
   5          1          -0.890008    0.000000    1.762124
```

```
   6          1          -0.890008    0.000000   -0.443206
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.318918   0.000000
 3  O    2.260458   1.248088   0.000000
 4  O    1.248088   2.260458   2.693076   0.000000
 5  H    1.974132   0.994256   1.947282   3.119460   0.000000
 6  H    0.994256   1.974132   3.119460   1.947282   2.205331
             6
 6  H    0.000000
                         Interatomic angles:
      N1-N2-O3=123.4017       N2-N1-O4=123.4017       N1-N2-H5=116.4724
      O3-N2-H5=120.1259       N2-N1-H6=116.4724       O4-N1-H6=120.1259
Stoichiometry    H2N2O2
Framework group  C2V[SGV(H2N2O2)]
Deg. of freedom    5
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          7           0.000000    0.659459    0.465346
   2          7           0.000000   -0.659459    0.465346
   3          8           0.000000   -1.346538   -0.576597
   4          8           0.000000    1.346538   -0.576597
   5          1           0.000000   -1.102665    1.355354
   6          1           0.000000    1.102665    1.355354
---------------------------------------------------------
Rotational constants (GHZ):     24.9115361      6.9579743      5.4388607
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of A1  symmetry.
There are     2 symmetry adapted basis functions of A2  symmetry.
There are     2 symmetry adapted basis functions of B1  symmetry.
There are     7 symmetry adapted basis functions of B2  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        70.1294110181 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (A1) (B2) (B1) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (B2) (A1) (B2)
RHF-PM3 calculation of energy and first derivatives.
MO and density RWFs will be updated.
```

```
Closed-shell calculation:  12 occupied levels.
NNHCO=    0.
References:
 H: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
 N: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
 O: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.61D-01 DiagD=T ESCF=     74.079460 Diff= 3.07D+00 RMSDP= 3.85D-01.
It=  2 PL= 5.12D-02 DiagD=T ESCF=     26.083498 Diff=-4.80D+00 RMSDP= 8.29D-03.
It=  3 PL= 1.26D-02 DiagD=F ESCF=     24.295058 Diff=-1.79D-01 RMSDP= 3.15D-03.
It=  4 PL= 2.11D-03 DiagD=F ESCF=     24.089016 Diff=-2.06D-02 RMSDP= 4.30D-04.
It=  5 PL= 8.73D-04 DiagD=F ESCF=     24.142213 Diff= 5.32D-03 RMSDP= 1.91D-04.
It=  6 PL= 3.89D-04 DiagD=F ESCF=     24.141390 Diff=-8.23D-05 RMSDP= 1.79D-04.
It=  7 PL= 2.35D-05 DiagD=F ESCF=     24.140915 Diff=-4.76D-05 RMSDP= 9.66D-06.
It=  8 PL= 1.63D-05 DiagD=F ESCF=     24.141140 Diff= 2.25D-05 RMSDP= 5.15D-06.
It=  9 PL= 9.19D-06 DiagD=F ESCF=     24.141139 Diff=-4.74D-08 RMSDP= 6.10D-06.
Energy=    0.088718777328 NIter=  10.
Dipole moment=  0.000000  0.000000  2.644962
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7           0.000006296    0.000000000   -0.000015216
   2          7           0.000006296    0.000000000    0.000015216
   3          8          -0.000005711    0.000000000   -0.000008849
   4          8          -0.000005708    0.000000000    0.000008849
   5          1          -0.000000587    0.000000000   -0.000004017
   6          1          -0.000000587    0.000000000    0.000004017
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000015216 RMS     0.000006655
-------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  N     1   0.000002(   1)
  3  O     2  -0.000010(   2)  1  -0.000010(   6)
  4  O     1  -0.000010(   3)  2  -0.000010(   7)  3   0.000000(  10)  0
  5  H     2  -0.000001(   4)  1  -0.000007(   8)  3   0.000000(  11)  0
  6  H     1  -0.000001(   5)  2  -0.000007(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------
Internal  Forces:  Max     0.000010011 RMS     0.000006455

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  2  3  4  5  7

Trust test= 1.00D+00 RLast= 1.31D-03 DXMaxT set to 4.24D-01
The second derivative matrix:
                       nn        no        nh        onn       hnn
```

```
          nn           0.56681
          no           0.13124   1.39865
          nh           0.01593   0.05332   0.94977
          onn          0.06078  -0.00423  -0.01170   0.85179
          hnn          0.02795  -0.11399   0.03062   0.36400   0.49990
    Eigenvalues ---    0.26171   0.53613   0.94496   1.08414   1.43998
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of  0.00876.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.49239   0.00000  -0.00001   0.00002   0.00001   2.49240
   no        2.35854  -0.00002  -0.00001  -0.00001  -0.00002   2.35853
   nh        1.87887   0.00000   0.00000   0.00000   0.00000   1.87887
  onn        2.15377  -0.00002  -0.00001  -0.00001  -0.00002   2.15375
  hnn        2.03283  -0.00001   0.00001  -0.00003  -0.00002   2.03281
        Item               Value     Threshold  Converged?
Maximum Force            0.000020     0.000450     YES
RMS     Force            0.000014     0.000300     YES
Maximum Displacement     0.000022     0.001800     YES
RMS     Displacement     0.000015     0.001200     YES
Predicted change in Energy=-4.783694D-10
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       nn          1.3189   -DE/DX =    0.                             !
!       no          1.2481   -DE/DX =    0.                             !
!       nh          0.9943   -DE/DX =    0.                             !
!       onn       123.4017   -DE/DX =    0.                             !
!       hnn       116.4724   -DE/DX =    0.                             !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (A1) (B2) (B1) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (B2) (A1) (B2)
 The electronic state is 1-A1.
Alpha  occ. eigenvalues --   -1.36462  -1.27148  -1.10641  -0.83588  -0.78250
Alpha  occ. eigenvalues --   -0.69810  -0.62635  -0.60402  -0.49358  -0.43396
Alpha  occ. eigenvalues --   -0.40602  -0.32817
Alpha virt. eigenvalues --   -0.02336   0.00098   0.05209   0.17006   0.20376
Alpha virt. eigenvalues --    0.25742
```

```
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
 1  N    3.597534   0.353181  -0.015499   0.341611  -0.060036   0.286962
 2  N    0.353181   3.597534   0.341611  -0.015499   0.286962  -0.060036
 3  O   -0.015499   0.341611   6.262073   0.000781  -0.030177   0.002460
 4  O    0.341611  -0.015499   0.000781   6.262073   0.002460  -0.030177
 5  H   -0.060036   0.286962  -0.030177   0.002460   0.740749  -0.004959
 6  H    0.286962  -0.060036   0.002460  -0.030177  -0.004959   0.740749
Total atomic charges:
              1
 1  N    0.496248
 2  N    0.496248
 3  O   -0.561249
 4  O   -0.561249
 5  H    0.065001
 6  H    0.065001
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  N    0.561249
 2  N    0.561249
 3  O   -0.561249
 4  O   -0.561249
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RPM3\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# PM3 OPT=Z-
MATRIX\\cis HNO dimer at PM3\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,onn,3
,0.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,180.,0\\nn=1.31891807\no=1.
2480878\nh=0.99425622\onn=123.40168106\hnn=116.47240531\\Version=SGI-G
94RevC.3\State=1-A1\HF=0.0887188\RMSD=0.000e+00\RMSF=6.655e-06\Dipole=
-2.6449618,0.,0.\PG=C02V [SGV(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  7.3 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Cis HNO DIMER at CNDO

```
****************************************
Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
****************************************
-------------------
# cndo opt=z-matrix
-------------------
----------------------
cis HNO dimer at CNDO
----------------------
Symbolic Z-matrix:
   Charge = 0 Multiplicity = 1
N
N     1     NN
O     2     NO        1     ONN
O     1     NO        2     ONN       3     0.        0
H     2     NH        1     HNN       3     180.      0
H     1     NH        2     HNN       3     180.      0
      Variables:
 nn                    1.4
 no                    1.4
 nh                    1.
 onn                 120.
 hnn                 120.

EDITED

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

-----------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
-----------------------------------------------------------------------
  1   1  N
  2   2  N     1   1.273507(  1)
  3   3  O     2   1.242241(  2)   1  124.591(  6)
  4   4  O     1   1.242241(  3)   2  124.591(  7)   3    0.000( 10)   0
  5   5  H     2   1.077969(  4)   1  115.789(  8)   3  180.000( 11)   0
  6   6  H     1   1.077969(  5)   2  115.789(  9)   3  180.000( 12)   0
-----------------------------------------------------------------------
                Z-Matrix orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.000000    0.000000
   2          7           0.000000    0.000000    1.273507
   3          8           1.022638    0.000000    1.978754
   4          8           1.022638    0.000000   -0.705246
   5          1          -0.970602    0.000000    1.742495
```

```
   6          1          -0.970602    0.000000   -0.468988
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.273507   0.000000
 3  O    2.227387   1.242241   0.000000
 4  O    1.242241   2.227387   2.684000   0.000000
 5  H    1.994582   1.077969   2.007193   3.156650   0.000000
 6  H    1.077969   1.994582   3.156650   2.007193   2.211482
             6
 6  H    0.000000
                         Interatomic angles:
      N1-N2-O3=124.5915       N2-N1-O4=124.5915       N1-N2-H5=115.7895
      O3-N2-H5=119.619        N2-N1-H6=115.7895       O4-N1-H6=119.619
Stoichiometry    H2N2O2
Framework group  C2V[SGV(H2N2O2)]
Deg. of freedom    5
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          7           0.000000    0.636754    0.450656
   2          7           0.000000   -0.636754    0.450656
   3          8           0.000000   -1.342000   -0.571982
   4          8           0.000000    1.342000   -0.571982
   5          1           0.000000   -1.105741    1.421258
   6          1           0.000000    1.105741    1.421258
---------------------------------------------------------
Rotational constants (GHZ):     25.1460244      7.0749448      5.5214582
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G* (5D, 7F)
There are     7 symmetry adapted basis functions of A1  symmetry.
There are     2 symmetry adapted basis functions of A2  symmetry.
There are     2 symmetry adapted basis functions of B1  symmetry.
There are     7 symmetry adapted basis functions of B2  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        70.2765010883 Hartrees.
RHF-CNDO calculation of energy and first derivatives.
MO and density RWFs will be updated.
CNDO iteration  1 energy        -131.66536194 RMS DP=1.92D-01
CNDO iteration  2 energy        -131.77557652 RMS DP=3.67D-02
CNDO iteration  3 energy        -131.86612135 RMS DP=2.75D-02
CNDO iteration  4 energy        -131.91329462 RMS DP=1.59D-02
CNDO iteration  5 energy        -131.92604169 RMS DP=8.95D-03
```

```
CNDO iteration  6 4-point extrapolation.
CNDO iteration  7 energy        -131.93176287 RMS DP=3.69D-04
CNDO iteration  8 energy        -131.93178256 RMS DP=2.94D-04
CNDO iteration  9 energy        -131.93178925 RMS DP=1.33D-04
CNDO iteration 10 energy        -131.93179185 RMS DP=9.58D-05
CNDO iteration 11 4-point extrapolation.
CNDO iteration 12 energy        -131.93179373 RMS DP=1.03D-05
CNDO iteration 13 energy        -131.93179374 RMS DP=7.75D-06
CNDO iteration 14 energy        -131.93179375 RMS DP=3.63D-06
CNDO iteration 15 energy        -131.93179375 RMS DP=2.39D-06
CNDO iteration 16 4-point extrapolation.
CNDO iteration 17 energy        -131.93179375 RMS DP=2.92D-07
CNDO iteration 18 energy        -131.93179375 RMS DP=1.04D-07
CNDO iteration 19 energy        -131.93179375 RMS DP=5.88D-08
Final CNDO energy   -61.65529266
Energy=  -61.655292662916 NIter=  19.
Dipole moment=  0.000000  0.000000  0.000000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7          -0.000156104    0.000000000    0.000096258
   2          7          -0.000156104    0.000000000   -0.000096258
   3          8           0.000162506    0.000000000    0.000093422
   4          8           0.000162507    0.000000000   -0.000093421
   5          1          -0.000006402    0.000000000    0.000012496
   6          1          -0.000006402    0.000000000   -0.000012496
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000162507 RMS     0.000087539
-------------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------------
  1  N
  2  N     1   0.000010(   1)
  3  O     2   0.000187(   2)  1  -0.000036(   6)
  4  O     1   0.000187(   3)  2  -0.000036(   7)  3   0.000000(  10)  0
  5  H     2   0.000011(   4)  1   0.000017(   8)  3   0.000000(  11)  0
  6  H     1   0.000011(   5)  2   0.000017(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------------
Internal  Forces:  Max     0.000186816 RMS     0.000078176

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   9 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  4  6  5  7  8
                                                         9
Trust test= 9.46D-01 RLast= 4.52D-03 DXMaxT set to 2.12D-01
The second derivative matrix:
                         nn        no        nh        onn       hnn
          nn           1.94462
```

```
          no           0.30999   3.76801
          nh           0.08599   0.09194   1.71897
          onn          0.15467   0.02292  -0.06207   0.71027
          hnn          0.15081  -0.11353   0.01109   0.37340   0.69207
    Eigenvalues ---    0.32281   1.01360   1.70546   1.96480   3.82727
RFO step:  Lambda=-3.39266697D-08.
Quartic linear search produced a step of -0.05100.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.40658   0.00001   0.00000  -0.00001  -0.00001   2.40657
   no        2.34749   0.00037   0.00002   0.00009   0.00010   2.34760
   nh        2.03707   0.00002   0.00006  -0.00006   0.00000   2.03706
  onn        2.17453  -0.00007  -0.00015  -0.00005  -0.00020   2.17434
  hnn        2.02091   0.00003   0.00017   0.00001   0.00018   2.02108
        Item               Value     Threshold  Converged?
Maximum Force            0.000374     0.000450     YES
RMS     Force            0.000171     0.000300     YES
Maximum Displacement     0.000196     0.001800     YES
RMS     Displacement     0.000127     0.001200     YES
Predicted change in Energy=-2.892109D-08
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       nn          1.2735   -DE/DX =    0.                            !
!       no          1.2422   -DE/DX =    0.0004                        !
!       nh          1.078    -DE/DX =    0.                            !
!       onn       124.5915   -DE/DX =   -0.0001                        !
!       hnn       115.7895   -DE/DX =    0.                            !
-------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

          Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (A1) (B2) (A1) (B2) (A1) (B1) (A1) (B2) (A2) (B2)
                (A1) (B1)
      Virtual   (A2) (B2) (A1) (A1) (B2) (B2)
 The electronic state is 1-A1.
Alpha  occ. eigenvalues --   -1.78698  -1.57901  -1.33376  -1.00021  -0.99587
Alpha  occ. eigenvalues --   -0.86666  -0.82824  -0.72837  -0.67077  -0.58992
Alpha  occ. eigenvalues --   -0.52997  -0.39799
Alpha virt. eigenvalues --    0.06983   0.21425   0.24563   0.40888   0.43921
Alpha virt. eigenvalues --    0.54164
         Condensed to atoms (all electrons):
```

```
             1          2          3          4          5          6
 1  N    3.968136   0.434955  -0.024452   0.218423  -0.041518   0.316949
 2  N    0.434955   3.968136   0.218423  -0.024452   0.316949  -0.041518
 3  O   -0.024452   0.218423   6.109109   0.000753  -0.023017   0.001167
 4  O    0.218423  -0.024452   0.000753   6.109109   0.001167  -0.023017
 5  H   -0.041518   0.316949  -0.023017   0.001167   0.600086  -0.008144
 6  H    0.316949  -0.041518   0.001167  -0.023017  -0.008144   0.600086
Total atomic charges:
             1
 1  N    0.127506
 2  N    0.127506
 3  O   -0.281984
 4  O   -0.281984
 5  H    0.154478
 6  H    0.154478
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  N    0.281984
 2  N    0.281984
 3  O   -0.281984
 4  O   -0.281984
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RCNDO\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# CNDO OPT=
Z-MATRIX\\cis HNO dimer at CNDO\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,on
n,3,0.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,180.,0\\nn=1.27350709\no
=1.2422405\nh=1.07796892\onn=124.59148144\hnn=115.78949167\\Version=SG
I-G94RevC.3\State=1-A1\HF=-61.6552927\RMSD=0.000e+00\RMSF=8.754e-05\Di
pole=0.,0.,0.\PG=C02V [SGV(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  6.3 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Trans HNO DIMER at MNDO

```
 ************************************
 Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
 ************************************
 -------------------
 # mndo opt=z-matrix
 -------------------
 ---------------
 trans HNO dimer
 ---------------
 Symbolic Z-matrix:
    Charge = 0 Multiplicity = 1
 N
 N     1     NN
 O     2     NO        1     ONN
 O     1     NO        2     ONN       3     180.      0
 H     2     NH        1     HNN       3     180.      0
 H     1     NH        2     HNN       3     0.        0
       Variables:
  nn                    1.4
  no                    1.4
  nh                    1.
  onn                 120.
  hnn                 120.

 EDITED

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 ----------------------------------------------------------------------
                        Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ----------------------------------------------------------------------
   1   1  N
   2   2  N     1   1.317043(  1)
   3   3  O     2   1.224592(  2)   1  119.959(  6)
   4   4  O     1   1.224592(  3)   2  119.959(  7)   3  180.000( 10)   0
   5   5  H     2   1.041254(  4)   1  118.264(  8)   3  180.000( 11)   0
   6   6  H     1   1.041254(  5)   2  118.264(  9)   3    0.000( 12)   0
 ----------------------------------------------------------------------
                 Z-Matrix orientation:
 ---------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------
    1          7           0.000000    0.000000    0.000000
    2          7           0.000000    0.000000    1.317043
    3          8           1.060964    0.000000    1.928583
    4          8          -1.060964    0.000000   -0.611540
    5          1          -0.917114    0.000000    1.810107
    6          1           0.917114    0.000000   -0.493064
```

```
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.317043   0.000000
 3  O    2.201154   1.224592   0.000000
 4  O    1.224592   2.201154   3.309805   0.000000
 5  H    2.029183   1.041254   1.981623   2.425916   0.000000
 6  H    1.041254   2.029183   2.425916   1.981623   2.944315
             6
 6  H    0.000000
                         Interatomic angles:
      N1-N2-O3=119.9592       N2-N1-O4=119.9592       N1-N2-H5=118.2636
      O3-N2-H5=121.7772       N2-N1-H6=118.2636       O4-N1-H6=121.7772
Stoichiometry    H2N2O2
Framework group  C2H[SGH(H2N2O2)]
Deg. of freedom    5
Full point group                 C2H     NOp   4
Largest Abelian subgroup         C2H     NOp   4
Largest concise Abelian subgroup C2      NOp   2
                  Standard orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.658521    0.000000
   2          7           0.000000   -0.658521    0.000000
   3          8           1.060964   -1.270062    0.000000
   4          8          -1.060964    1.270062    0.000000
   5          1          -0.917114   -1.151586    0.000000
   6          1           0.917114    1.151586    0.000000
---------------------------------------------------------
Rotational constants (GHZ):     58.4772243      5.2929486      4.8536318
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of AG  symmetry.
There are     2 symmetry adapted basis functions of BG  symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are     7 symmetry adapted basis functions of BU  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        69.8443990150 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AU) (AG) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (BU) (AG)
RHF-MNDO calculation of energy and first derivatives.
MO and density RWFs will be updated.
Closed-shell calculation:  12 occupied levels.
```

```
NNHCO=    0.
References:
 H: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
 N: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
 O: (MNDO):  M.J.S. DEWAR, W. THIEL, J. AM. CHEM. SOC., 99, 4907, (1977)
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.47D-01 DiagD=T ESCF=     93.812305 Diff= 5.04D+00 RMSDP= 3.85D-01.
It=  2 PL= 5.71D-02 DiagD=T ESCF=     27.373427 Diff=-6.64D+00 RMSDP= 9.70D-03.
It=  3 PL= 1.61D-02 DiagD=F ESCF=     24.422330 Diff=-2.95D-01 RMSDP= 4.64D-03.
It=  4 PL= 3.22D-03 DiagD=F ESCF=     24.016496 Diff=-4.06D-02 RMSDP= 7.29D-04.
It=  5 PL= 1.68D-03 DiagD=F ESCF=     24.136357 Diff= 1.20D-02 RMSDP= 3.79D-04.
It=  6 PL= 9.15D-04 DiagD=F ESCF=     24.133850 Diff=-2.51D-04 RMSDP= 4.65D-04.
It=  7 PL= 8.71D-05 DiagD=F ESCF=     24.131434 Diff=-2.42D-04 RMSDP= 2.13D-05.
It=  8 PL= 5.17D-05 DiagD=F ESCF=     24.132732 Diff= 1.30D-04 RMSDP= 9.90D-06.
It=  9 PL= 2.99D-05 DiagD=F ESCF=     24.132730 Diff=-1.93D-07 RMSDP= 1.36D-05.
It= 10 PL= 3.26D-06 DiagD=F ESCF=     24.132728 Diff=-2.25D-07 RMSDP= 8.74D-07.
It= 11 PL= 1.64D-06 DiagD=F ESCF=     24.132729 Diff= 1.25D-07 RMSDP= 3.64D-07.
Energy=    0.088687871100 NIter=  12.
Dipole moment=  0.000000  0.000000  0.000000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7           0.000044714    0.000000000   -0.000045614
   2          7          -0.000044809    0.000000000    0.000045611
   3          8           0.000054338    0.000000000    0.000035627
   4          8          -0.000054243    0.000000000   -0.000035625
   5          1          -0.000010506    0.000000000    0.000010663
   6          1           0.000010506    0.000000000   -0.000010663
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000054338 RMS     0.000030777
-------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  N     1   0.000092(   1)
  3  O     2   0.000065(   2)  1   0.000009(   6)
  4  O     1   0.000065(   3)  2   0.000009(   7)  3   0.000000(  10)  0
  5  H     2   0.000014(   4)  1   0.000009(   8)  3   0.000000(  11)  0
  6  H     1   0.000014(   5)  2   0.000009(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------
Internal  Forces:  Max     0.000091901 RMS     0.000038256

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  2  3  4  7
Trust test= 8.56D-01 RLast= 5.22D-04 DXMaxT set to 4.24D-01
The second derivative matrix:
                          nn        no        nh        onn       hnn
```

```
          nn           0.61417
          no           0.04847   1.93840
          nh           0.01742   0.07074   0.80765
          onn          0.18026   0.07167  -0.01126   0.95112
          hnn          0.07961  -0.16813  -0.01739   0.31723   0.70257
    Eigenvalues ---    0.45627   0.55683   0.80431   1.22873   1.96776
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.18035.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.48885   0.00009   0.00007   0.00003   0.00011   2.48896
   no        2.31414   0.00013   0.00004   0.00001   0.00005   2.31420
   nh        1.96768   0.00003   0.00000   0.00002   0.00003   1.96771
  onn        2.09368   0.00002   0.00004  -0.00006  -0.00002   2.09366
  hnn        2.06409   0.00002  -0.00002   0.00005   0.00003   2.06412
        Item               Value     Threshold  Converged?
Maximum Force            0.000130     0.000450     YES
RMS     Force            0.000073     0.000300     YES
Maximum Displacement     0.000107     0.001800     YES
RMS     Displacement     0.000056     0.001200     YES
Predicted change in Energy=-6.479147D-09
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       nn          1.317    -DE/DX =    0.0001                         !
!       no          1.2246   -DE/DX =    0.0001                         !
!       nh          1.0413   -DE/DX =    0.                             !
!       onn       119.9592   -DE/DX =    0.                             !
!       hnn       118.2636   -DE/DX =    0.                             !
-------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

          Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AU) (AG) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (BU) (AG)
 The electronic state is 1-AG.
Alpha  occ. eigenvalues --   -1.64606  -1.54620  -1.21961  -0.99195  -0.77982
Alpha  occ. eigenvalues --   -0.73629  -0.65255  -0.64852  -0.52021  -0.45508
Alpha  occ. eigenvalues --   -0.41317  -0.33236
Alpha virt. eigenvalues --   -0.03520  -0.00847   0.08550   0.16066   0.25648
Alpha virt. eigenvalues --    0.27821
```

```
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
 1  N    4.161297   0.276033  -0.012096   0.231129  -0.022337   0.269878
 2  N    0.276033   4.161297   0.231129  -0.012096   0.269878  -0.022337
 3  O   -0.012096   0.231129   6.203855   0.000050  -0.011107   0.002153
 4  O    0.231129  -0.012096   0.000050   6.203855   0.002153  -0.011107
 5  H   -0.022337   0.269878  -0.011107   0.002153   0.440941   0.002586
 6  H    0.269878  -0.022337   0.002153  -0.011107   0.002586   0.440941
Total atomic charges:
              1
 1  N    0.096097
 2  N    0.096097
 3  O   -0.413984
 4  O   -0.413984
 5  H    0.317886
 6  H    0.317886
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  N    0.413984
 2  N    0.413984
 3  O   -0.413984
 4  O   -0.413984
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RMNDO\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# MNDO OPT=
Z-MATRIX\\trans HNO dimer\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,onn,3,18
0.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,0.,0\\nn=1.31704299\no=1.224
59242\nh=1.041254\onn=119.95916533\hnn=118.26362597\\Version=SGI-G94Re
vC.3\State=1-AG\HF=0.0886879\RMSD=0.000e+00\RMSF=3.078e-05\Dipole=0.,0
.,0.\PG=C02H [SGH(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  7.3 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Trans HNO DIMER at AM1

```
****************************************
Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
****************************************
------------------
# am1 opt=z-matrix
------------------
----------------------
trans HNO dimer at AM1
----------------------
Symbolic Z-matrix:
   Charge = 0 Multiplicity = 1
N
N     1     NN
O     2     NO        1     ONN
O     1     NO        2     ONN       3     180.      0
H     2     NH        1     HNN       3     180.      0
H     1     NH        2     HNN       3     0.        0
      Variables:
 nn                    1.4
 no                    1.4
 nh                    1.
 onn                 120.
 hnn                 120.

EDITED

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

-----------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
-----------------------------------------------------------------------
  1   1  N
  2   2  N     1   1.301945(  1)
  3   3  O     2   1.222611(  2)   1  120.359(  6)
  4   4  O     1   1.222611(  3)   2  120.359(  7)   3  180.000( 10)   0
  5   5  H     2   1.027631(  4)   1  116.752(  8)   3  180.000( 11)   0
  6   6  H     1   1.027631(  5)   2  116.752(  9)   3    0.000( 12)   0
-----------------------------------------------------------------------
                Z-Matrix orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.000000    0.000000
   2          7           0.000000    0.000000    1.301945
   3          8           1.054961    0.000000    1.919873
   4          8          -1.054961    0.000000   -0.617928
   5          1          -0.917632    0.000000    1.764520
```

```
   6          1           0.917632    0.000000   -0.462575
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.301945   0.000000
 3  O    2.190629   1.222611   0.000000
 4  O    1.222611   2.190629   3.300334   0.000000
 5  H    1.988864   1.027631   1.978701   2.386403   0.000000
 6  H    1.027631   1.988864   2.386403   1.978701   2.885853
             6
 6  H    0.000000
                          Interatomic angles:
      N1-N2-O3=120.359        N2-N1-O4=120.359        N1-N2-H5=116.7525
      O3-N2-H5=122.8885       N2-N1-H6=116.7525       O4-N1-H6=122.8885
Stoichiometry    H2N2O2
Framework group  C2H[SGH(H2N2O2)]
Deg. of freedom    5
Full point group                 C2H     NOp   4
Largest Abelian subgroup         C2H     NOp   4
Largest concise Abelian subgroup C2      NOp   2
                  Standard orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.650972    0.000000
   2          7           0.000000   -0.650972    0.000000
   3          8           1.054961   -1.268900    0.000000
   4          8          -1.054961    1.268900    0.000000
   5          1          -0.917632   -1.113547    0.000000
   6          1           0.917632    1.113547    0.000000
---------------------------------------------------------
Rotational constants (GHZ):     60.2157171      5.3320260      4.8982887
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of AG  symmetry.
There are     2 symmetry adapted basis functions of BG  symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are     7 symmetry adapted basis functions of BU  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        70.2606811644 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AU) (AG) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (BU) (AG)
RHF-AM1 calculation of energy and first derivatives.
MO and density RWFs will be updated.
```

```
Closed-shell calculation:  12 occupied levels.
NNHCO=    0.
References:
 H: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
 N: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
 O: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.59D-01 DiagD=T ESCF=     96.249991 Diff= 5.29D+00 RMSDP= 3.85D-01.
It=  2 PL= 6.21D-02 DiagD=T ESCF=     21.963322 Diff=-7.43D+00 RMSDP= 1.03D-02.
It=  3 PL= 1.72D-02 DiagD=F ESCF=     18.511362 Diff=-3.45D-01 RMSDP= 4.77D-03.
It=  4 PL= 2.78D-03 DiagD=F ESCF=     18.056995 Diff=-4.54D-02 RMSDP= 7.19D-04.
It=  5 PL= 1.42D-03 DiagD=F ESCF=     18.189173 Diff= 1.32D-02 RMSDP= 3.63D-04.
It=  6 PL= 7.57D-04 DiagD=F ESCF=     18.186859 Diff=-2.31D-04 RMSDP= 4.34D-04.
It=  7 PL= 9.55D-05 DiagD=F ESCF=     18.184739 Diff=-2.12D-04 RMSDP= 2.06D-05.
It=  8 PL= 5.75D-05 DiagD=F ESCF=     18.185872 Diff= 1.13D-04 RMSDP= 1.02D-05.
It=  9 PL= 3.35D-05 DiagD=F ESCF=     18.185870 Diff=-2.18D-07 RMSDP= 1.36D-05.
It= 10 PL= 3.19D-06 DiagD=F ESCF=     18.185867 Diff=-2.42D-07 RMSDP= 9.52D-07.
It= 11 PL= 1.73D-06 DiagD=F ESCF=     18.185869 Diff= 1.33D-07 RMSDP= 4.20D-07.
Energy=    0.066833137284 NIter=  12.
Dipole moment=  0.000000  0.000000  0.000000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7          -0.000000225    0.000000000    0.000054972
   2          7           0.000000227    0.000000000   -0.000054970
   3          8          -0.000086526    0.000000000   -0.000085236
   4          8           0.000086524    0.000000000    0.000085234
   5          1           0.000011442    0.000000000    0.000007039
   6          1          -0.000011442    0.000000000   -0.000007039
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000086526 RMS     0.000044664
-------------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------------
  1  N
  2  N     1  -0.000133(   1)
  3  O     2  -0.000118(   2)  1  -0.000069(   6)
  4  O     1  -0.000118(   3)  2  -0.000069(   7)  3   0.000000(  10)  0
  5  H     2  -0.000007(   4)  1   0.000022(   8)  3   0.000000(  11)  0
  6  H     1  -0.000007(   5)  2   0.000022(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------------
Internal  Forces:  Max     0.000133167 RMS     0.000068334

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   7 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  2  3  4  5  7

Trust test= 6.48D-01 RLast= 8.23D-04 DXMaxT set to 4.42D-01
```

```
The second derivative matrix:
                           nn        no        nh        onn       hnn
          nn           0.69518
          no           0.09869   1.81969
          nh           0.03232   0.05629   0.78149
          onn          0.03939  -0.08804  -0.11511   0.78271
          hnn          0.14187  -0.14144   0.02353   0.30671   0.62473
    Eigenvalues ---    0.34314   0.63174   0.81702   1.05173   1.86017
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.28050.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.46032  -0.00013  -0.00011  -0.00003  -0.00013   2.46019
   no        2.31040  -0.00024  -0.00009   0.00000  -0.00008   2.31032
   nh        1.94194  -0.00001  -0.00010   0.00008  -0.00002   1.94192
  onn        2.10066  -0.00014  -0.00013  -0.00005  -0.00018   2.10048
  hnn        2.03772   0.00004   0.00009   0.00007   0.00016   2.03787
        Item               Value     Threshold  Converged?
Maximum Force            0.000235     0.000450     YES
RMS     Force            0.000137     0.000300     YES
Maximum Displacement     0.000183     0.001800     YES
RMS     Displacement     0.000129     0.001200     YES
Predicted change in Energy=-2.386176D-08
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
---------------------                           ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       nn           1.3019   -DE/DX =   -0.0001                        !
!       no           1.2226   -DE/DX =   -0.0002                        !
!       nh           1.0276   -DE/DX =    0.                           !
!       onn        120.359    -DE/DX =   -0.0001                        !
!       hnn        116.7525   -DE/DX =    0.                           !
-------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AU) (AG) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (BU) (AG)
 The electronic state is 1-AG.
Alpha  occ. eigenvalues --   -1.57183  -1.44537  -1.20524  -1.00306  -0.77351
Alpha  occ. eigenvalues --   -0.75876  -0.66864  -0.64300  -0.53304  -0.46551
Alpha  occ. eigenvalues --   -0.41635  -0.33766
```

```
Alpha virt. eigenvalues --   -0.02510  -0.00239   0.08534   0.15394   0.23564
Alpha virt. eigenvalues --    0.25645
         Condensed to atoms (all electrons):
              1         2         3         4         5         6
 1  N    4.140244   0.295509  -0.017548   0.276690  -0.031133   0.271443
 2  N    0.295509   4.140244   0.276690  -0.017548   0.271443  -0.031133
 3  O   -0.017548   0.276690   6.182015   0.000124  -0.015377   0.003979
 4  O    0.276690  -0.017548   0.000124   6.182015   0.003979  -0.015377
 5  H   -0.031133   0.271443  -0.015377   0.003979   0.400617   0.005386
 6  H    0.271443  -0.031133   0.003979  -0.015377   0.005386   0.400617
Total atomic charges:
              1
 1  N    0.064796
 2  N    0.064796
 3  O   -0.429883
 4  O   -0.429883
 5  H    0.365087
 6  H    0.365087
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  N    0.429883
 2  N    0.429883
 3  O   -0.429883
 4  O   -0.429883
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RAM1\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# AM1 OPT=Z-
MATRIX\\trans HNO dimer at AM1\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,onn
,3,180.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,0.,0\\nn=1.30194491\no=
1.22261094\nh=1.02763074\onn=120.35901752\hnn=116.75249663\\Version=SG
I-G94RevC.3\State=1-AG\HF=0.0668331\RMSD=0.000e+00\RMSF=4.466e-05\Dipo
le=0.,0.,0.\PG=C02H [SGH(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  7.3 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Trans HNO DIMER at PM3

```
****************************************
Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
****************************************
------------------
# pm3 opt=z-matrix
------------------
----------------------
trans HNO dimer at PM3
----------------------
Symbolic Z-matrix:
   Charge = 0 Multiplicity = 1
N
N     1     NN
O     2     NO        1     ONN
O     1     NO        2     ONN       3     180.      0
H     2     NH        1     HNN       3     180.      0
H     1     NH        2     HNN       3     0.        0
      Variables:
 nn                    1.4
 no                    1.4
 nh                    1.
 onn                 120.
 hnn                 120.

EDITED

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

-----------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
-----------------------------------------------------------------------
  1   1  N
  2   2  N     1   1.305405(  1)
  3   3  O     2   1.258280(  2)   1  117.325(  6)
  4   4  O     1   1.258280(  3)   2  117.325(  7)   3  180.000( 10)   0
  5   5  H     2   0.993536(  4)   1  120.757(  8)   3  180.000( 11)   0
  6   6  H     1   0.993536(  5)   2  120.757(  9)   3    0.000( 12)   0
-----------------------------------------------------------------------
               Z-Matrix orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.000000    0.000000
   2          7           0.000000    0.000000    1.305405
   3          8           1.117881    0.000000    1.882995
   4          8          -1.117881    0.000000   -0.577589
   5          1          -0.853792    0.000000    1.813492
   6          1           0.853792    0.000000   -0.508087
```

```
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.305405   0.000000
 3  O    2.189824   1.258280   0.000000
 4  O    1.258280   2.189824   3.324621   0.000000
 5  H    2.004424   0.993536   1.972898   2.405621   0.000000
 6  H    0.993536   2.004424   2.405621   1.972898   2.881939
             6
 6  H    0.000000
                         Interatomic angles:
      N1-N2-O3=117.3246       N2-N1-O4=117.3246       N1-N2-H5=120.7566
      O3-N2-H5=121.9188       N2-N1-H6=120.7566       O4-N1-H6=121.9188
Stoichiometry    H2N2O2
Framework group  C2H[SGH(H2N2O2)]
Deg. of freedom    5
Full point group                 C2H     NOp   4
Largest Abelian subgroup         C2H     NOp   4
Largest concise Abelian subgroup C2      NOp   2
                  Standard orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.652703    0.000000
   2          7           0.000000   -0.652703    0.000000
   3          8           1.117881   -1.230292    0.000000
   4          8          -1.117881    1.230292    0.000000
   5          1          -0.853792   -1.160790    0.000000
   6          1           0.853792    1.160790    0.000000
---------------------------------------------------------
Rotational constants (GHZ):     56.8550884      5.2850468      4.8355511
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G (5D, 7F)
There are     7 symmetry adapted basis functions of AG  symmetry.
There are     2 symmetry adapted basis functions of BG  symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are     7 symmetry adapted basis functions of BU  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        69.6052337251 Hartrees.
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AG) (AU) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (BU) (AG)
RHF-PM3 calculation of energy and first derivatives.
MO and density RWFs will be updated.
Closed-shell calculation:  12 occupied levels.
```

```
NNHCO=    0.
References:
 H: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
 N: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
 O: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).
Ext34=T Pulay=F Camp-King=F BShift= 0.00D+00
It=  1 PL= 9.64D-01 DiagD=T ESCF=     68.736571 Diff= 2.54D+00 RMSDP= 3.85D-01.
It=  2 PL= 5.49D-02 DiagD=T ESCF=     20.643220 Diff=-4.81D+00 RMSDP= 8.74D-03.
It=  3 PL= 1.52D-02 DiagD=F ESCF=     18.656137 Diff=-1.99D-01 RMSDP= 3.97D-03.
It=  4 PL= 2.40D-03 DiagD=F ESCF=     18.353221 Diff=-3.03D-02 RMSDP= 4.34D-04.
It=  5 PL= 1.11D-03 DiagD=F ESCF=     18.446499 Diff= 9.33D-03 RMSDP= 2.03D-04.
It=  6 PL= 5.43D-04 DiagD=F ESCF=     18.445615 Diff=-8.84D-05 RMSDP= 2.08D-04.
It=  7 PL= 5.50D-05 DiagD=F ESCF=     18.445024 Diff=-5.91D-05 RMSDP= 1.54D-05.
It=  8 PL= 3.51D-05 DiagD=F ESCF=     18.445307 Diff= 2.83D-05 RMSDP= 9.40D-06.
It=  9 PL= 2.17D-05 DiagD=F ESCF=     18.445306 Diff=-1.58D-07 RMSDP= 1.56D-05.
It= 10 PL= 3.19D-06 DiagD=F ESCF=     18.445303 Diff=-2.60D-07 RMSDP= 1.03D-06.
It= 11 PL= 1.28D-06 DiagD=F ESCF=     18.445305 Diff= 1.70D-07 RMSDP= 3.71D-07.
Energy=    0.067786565632 NIter=  12.
Dipole moment=  0.000000  0.000000  0.000000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7          -0.000201981    0.000000000    0.000135554
   2          7           0.000201978    0.000000000   -0.000135553
   3          8          -0.000152354    0.000000000   -0.000096392
   4          8           0.000152358    0.000000000    0.000096392
   5          1          -0.000028818    0.000000000   -0.000021840
   6          1           0.000028817    0.000000000    0.000021840
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000201981 RMS     0.000101643
-------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------
  1  N
  2  N     1  -0.000254(   1)
  3  O     2  -0.000180(   2)  1  -0.000037(   6)
  4  O     1  -0.000180(   3)  2  -0.000037(   7)  3   0.000000(  10)  0
  5  H     2   0.000014(   4)  1  -0.000063(   8)  3   0.000000(  11)  0
  6  H     1   0.000014(   5)  2  -0.000063(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------
Internal  Forces:  Max     0.000253786 RMS     0.000108010

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   5 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  1  2  3  4  5

Trust test= 8.48D-01 RLast= 1.76D-03 DXMaxT set to 4.24D-01
The second derivative matrix:
```

```
                          nn        no        nh        onn       hnn
          nn           0.47302
          no           0.00762   1.30149
          nh           0.01366   0.01961   0.94872
          onn          0.05688   0.07657  -0.00245   0.84310
          hnn         -0.02921  -0.10774   0.01932   0.33305   0.58251
    Eigenvalues ---    0.31682   0.49053   0.94812   1.07264   1.32072
RFO step:  Lambda=-2.12827305D-07.
Quartic linear search produced a step of -0.13491.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.46686  -0.00025  -0.00005  -0.00048  -0.00053   2.46633
   no        2.37780  -0.00036  -0.00011  -0.00018  -0.00029   2.37751
   nh        1.87751   0.00003  -0.00004   0.00008   0.00005   1.87756
  onn        2.04770  -0.00007  -0.00012   0.00022   0.00010   2.04780
  hnn        2.10760  -0.00013   0.00016  -0.00049  -0.00033   2.10727
        Item               Value     Threshold  Converged?
Maximum Force            0.000359     0.000450     YES
RMS     Force            0.000208     0.000300     YES
Maximum Displacement     0.000529     0.001800     YES
RMS     Displacement     0.000311     0.001200     YES
Predicted change in Energy=-1.267046D-07
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       nn          1.3054   -DE/DX =   -0.0003                         !
!       no          1.2583   -DE/DX =   -0.0004                         !
!       nh          0.9935   -DE/DX =    0.                            !
!       onn       117.3246   -DE/DX =   -0.0001                         !
!       hnn       120.7566   -DE/DX =   -0.0001                         !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

          Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AG) (AU) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (BU) (AG)
 The electronic state is 1-AG.
Alpha  occ. eigenvalues --   -1.37967  -1.28695  -1.07869  -0.87924  -0.73877
Alpha  occ. eigenvalues --   -0.73063  -0.62999  -0.60890  -0.50516  -0.44758
Alpha  occ. eigenvalues --   -0.42553  -0.34377
Alpha virt. eigenvalues --   -0.03012   0.00655   0.07215   0.14881   0.21201
```

```
Alpha virt. eigenvalues --    0.23444
         Condensed to atoms (all electrons):
             1          2          3          4          5          6
 1  N    3.591719   0.359028  -0.020728   0.330707  -0.052297   0.289930
 2  N    0.359028   3.591719   0.330707  -0.020728   0.289930  -0.052297
 3  O   -0.020728   0.330707   6.339926   0.000184  -0.024534   0.004611
 4  O    0.330707  -0.020728   0.000184   6.339926   0.004611  -0.024534
 5  H   -0.052297   0.289930  -0.024534   0.004611   0.639968   0.013797
 6  H    0.289930  -0.052297   0.004611  -0.024534   0.013797   0.639968
Total atomic charges:
             1
 1  N    0.501640
 2  N    0.501640
 3  O   -0.630166
 4  O   -0.630166
 5  H    0.128525
 6  H    0.128525
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  N    0.630166
 2  N    0.630166
 3  O   -0.630166
 4  O   -0.630166
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RPM3\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# PM3 OPT=Z-
MATRIX\\trans HNO dimer at PM3\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,onn
,3,180.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,0.,0\\nn=1.30540531\no=
1.2582796\nh=0.99353583\onn=117.32460191\hnn=120.75664093\\Version=SGI
-G94RevC.3\State=1-AG\HF=0.0677866\RMSD=0.000e+00\RMSF=1.016e-04\Dipol
e=0.,0.,0.\PG=C02H [SGH(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  6.1 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```

Trans HNO DIMER at CNDO

```
****************************************
Gaussian 94:  SGI-G94RevC.3 26-Sep-1995
               7-Apr-1998
****************************************
-------------------
# CNDO opt=z-matrix
-------------------
----------------------
trans HNO dimer at CNDO
----------------------
Symbolic Z-matrix:
   Charge = 0 Multiplicity = 1
N
N     1     NN
O     2     NO        1     ONN
O     1     NO        2     ONN       3     180.      0
H     2     NH        1     HNN       3     180.      0
H     1     NH        2     HNN       3     0.        0
      Variables:
 nn                    1.4
 no                    1.4
 nh                    1.
 onn                 120.
 hnn                 120.

EDITED

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

-----------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
-----------------------------------------------------------------------
  1   1  N
  2   2  N     1   1.271713(  1)
  3   3  O     2   1.243901(  2)   1  125.126(  6)
  4   4  O     1   1.243901(  3)   2  125.126(  7)   3  180.000( 10)   0
  5   5  H     2   1.079134(  4)   1  114.454(  8)   3  180.000( 11)   0
  6   6  H     1   1.079134(  5)   2  114.454(  9)   3    0.000( 12)   0
-----------------------------------------------------------------------
                Z-Matrix orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.000000    0.000000
   2          7           0.000000    0.000000    1.271713
   3          8           1.017378    0.000000    1.987418
   4          8          -1.017378    0.000000   -0.715704
   5          1          -0.982330    0.000000    1.718433
```

```
   6          1           0.982330    0.000000   -0.446720
---------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  N    0.000000
 2  N    1.271713   0.000000
 3  O    2.232686   1.243901   0.000000
 4  O    1.243901   2.232686   3.383357   0.000000
 5  H    1.979390   1.079134   2.017718   2.434390   0.000000
 6  H    1.079134   1.979390   2.434390   2.017718   2.923658
             6
 6  H    0.000000
                          Interatomic angles:
      N1-N2-O3=125.1256       N2-N1-O4=125.1256       N1-N2-H5=114.4539
      O3-N2-H5=120.4205       N2-N1-H6=114.4539       O4-N1-H6=120.4205
Stoichiometry    H2N2O2
Framework group  C2H[SGH(H2N2O2)]
Deg. of freedom    5
Full point group                 C2H     NOp   4
Largest Abelian subgroup         C2H     NOp   4
Largest concise Abelian subgroup C2      NOp   2
                  Standard orientation:
---------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------
   1          7           0.000000    0.635857    0.000000
   2          7           0.000000   -0.635857    0.000000
   3          8           1.017378   -1.351561    0.000000
   4          8          -1.017378    1.351561    0.000000
   5          1          -0.982330   -1.082576    0.000000
   6          1           0.982330    1.082576    0.000000
---------------------------------------------------------
Rotational constants (GHZ):     64.5877896      5.0866696      4.7153111
Isotopes: N-14,N-14,O-16,O-16,H-1,H-1
Standard basis: VSTO-3G* (5D, 7F)
There are     7 symmetry adapted basis functions of AG  symmetry.
There are     2 symmetry adapted basis functions of BG  symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are     7 symmetry adapted basis functions of BU  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   18 basis functions       54 primitive gaussians
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        69.2931649804 Hartrees.
RHF-CNDO calculation of energy and first derivatives.
MO and density RWFs will be updated.
CNDO iteration  1 energy        -130.71609655 RMS DP=1.92D-01
CNDO iteration  2 energy        -130.84766458 RMS DP=3.28D-02
CNDO iteration  3 energy        -130.91766532 RMS DP=2.22D-02
CNDO iteration  4 energy        -130.94582898 RMS DP=1.17D-02
CNDO iteration  5 energy        -130.95304183 RMS DP=6.42D-03
```

```
CNDO iteration  6 4-point extrapolation.
CNDO iteration  7 energy        -130.95589199 RMS DP=2.84D-04
CNDO iteration  8 energy        -130.95590299 RMS DP=2.15D-04
CNDO iteration  9 energy        -130.95590653 RMS DP=9.18D-05
CNDO iteration 10 energy        -130.95590787 RMS DP=6.62D-05
CNDO iteration 11 4-point extrapolation.
CNDO iteration 12 energy        -130.95590879 RMS DP=5.21D-06
CNDO iteration 13 energy        -130.95590879 RMS DP=3.55D-06
CNDO iteration 14 energy        -130.95590879 RMS DP=1.63D-06
CNDO iteration 15 energy        -130.95590879 RMS DP=1.04D-06
CNDO iteration 16 4-point extrapolation.
CNDO iteration 17 energy        -130.95590879 RMS DP=1.12D-07
CNDO iteration 18 energy        -130.95590879 RMS DP=4.57D-08
Final CNDO energy   -61.66274381
Energy=  -61.662743812893 NIter=  18.
Dipole moment=  0.000000  0.000000  0.000000
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          7           0.000090419    0.000000000   -0.000029678
   2          7          -0.000090421    0.000000000    0.000029676
   3          8           0.000050132    0.000000000    0.000023207
   4          8          -0.000050130    0.000000000   -0.000023205
   5          1          -0.000003040    0.000000000    0.000016719
   6          1           0.000003040    0.000000000   -0.000016719
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000090421 RMS     0.000037114
-------------------------------------------------------------------------------
          Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1     Length/X     N2     Alpha/Y      N3      Beta/Z       J
-------------------------------------------------------------------------------
  1  N
  2  N     1   0.000070(   1)
  3  O     2   0.000054(   2)  1  -0.000023(   6)
  4  O     1   0.000054(   3)  2  -0.000023(   7)  3   0.000000(  10)  0
  5  H     2   0.000010(   4)  1   0.000028(   8)  3   0.000000(  11)  0
  6  H     1   0.000010(   5)  2   0.000028(   9)  3   0.000000(  12)  0
-------------------------------------------------------------------------------
Internal  Forces:  Max     0.000069602 RMS     0.000033711

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Search for a local minimum.
Step number   9 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using information from points  3  5  6  7  8
                                                         9
Trust test= 1.01D+00 RLast= 3.67D-03 DXMaxT set to 2.12D-01
The second derivative matrix:
                          nn        no        nh        onn       hnn
          nn           1.80812
          no           0.21991   3.71478
```

```
          nh           0.19416   0.21155   1.60409
          onn          0.18143   0.05943  -0.07640   0.81335
          hnn          0.07827  -0.11216   0.06970   0.31243   0.68469
    Eigenvalues ---    0.41201   1.01490   1.51990   1.90909   3.76913
RFO step:  Lambda=-1.13609232D-08.
Quartic linear search produced a step of  0.02358.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   nn        2.40319   0.00007   0.00002   0.00002   0.00004   2.40323
   no        2.35063   0.00011   0.00002   0.00002   0.00003   2.35067
   nh        2.03927   0.00002   0.00005  -0.00006  -0.00001   2.03926
  onn        2.18385  -0.00005  -0.00004  -0.00008  -0.00012   2.18373
  hnn        1.99760   0.00006   0.00005   0.00009   0.00014   1.99774
        Item               Value     Threshold  Converged?
Maximum Force            0.000109     0.000450     YES
RMS     Force            0.000067     0.000300     YES
Maximum Displacement     0.000143     0.001800     YES
RMS     Displacement     0.000088     0.001200     YES
Predicted change in Energy=-1.015782D-08
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !   Optimized Parameters   !
                     ! (Angstroms and Degrees)  !
----------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       nn          1.2717   -DE/DX =    0.0001                         !
!       no          1.2439   -DE/DX =    0.0001                         !
!       nh          1.0791   -DE/DX =    0.                             !
!       onn       125.1256   -DE/DX =    0.                             !
!       hnn       114.4539   -DE/DX =    0.0001                         !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


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

           Population analysis using the SCF density.

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

Orbital Symmetries:
      Occupied  (AG) (BU) (AG) (BU) (AG) (BU) (AU) (AG) (BG) (BU)
                (AG) (AU)
      Virtual   (BG) (BU) (AG) (BU) (AG) (BU)
 The electronic state is 1-AG.
Alpha  occ. eigenvalues --   -1.77051  -1.59692  -1.26449  -1.09978  -0.87284
Alpha  occ. eigenvalues --   -0.86970  -0.85888  -0.68228  -0.65979  -0.60448
Alpha  occ. eigenvalues --   -0.51388  -0.37780
Alpha virt. eigenvalues --    0.07500   0.18863   0.25861   0.35892   0.49481
Alpha virt. eigenvalues --    0.52161
         Condensed to atoms (all electrons):
             1          2          3          4          5          6
```

```
 1  N    3.986265   0.434847  -0.025189   0.218235  -0.043793   0.312509
 2  N    0.434847   3.986265   0.218235  -0.025189   0.312509  -0.043793
 3  O   -0.025189   0.218235   6.141090   0.000226  -0.021223   0.000259
 4  O    0.218235  -0.025189   0.000226   6.141090   0.000259  -0.021223
 5  H   -0.043793   0.312509  -0.021223   0.000259   0.550359   0.005616
 6  H    0.312509  -0.043793   0.000259  -0.021223   0.005616   0.550359
Total atomic charges:
             1
 1  N    0.117126
 2  N    0.117126
 3  O   -0.313398
 4  O   -0.313398
 5  H    0.196272
 6  H    0.196272
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
 1  N    0.313398
 2  N    0.313398
 3  O   -0.313398
 4  O   -0.313398
 5  H    0.000000
 6  H    0.000000
Sum of Mulliken charges=   0.00000
1\1\GINC-SHIVA\FOpt\RCNDO\ZDO\H2N2O2\GLASER\07-Apr-1998\1\\# CNDO OPT=
Z-MATRIX\\trans HNO dimer at CNDO\\0,1\N\N,1,nn\O,2,no,1,onn\O,1,no,2,
onn,3,180.,0\H,2,nh,1,hnn,3,180.,0\H,1,nh,2,hnn,3,0.,0\\nn=1.27171348\
no=1.24390139\nh=1.07913442\onn=125.12559584\hnn=114.4539026\\Version=
SGI-G94RevC.3\State=1-AG\HF=-61.6627438\RMSD=0.000e+00\RMSF=3.711e-05\
Dipole=0.,0.,0.\PG=C02H [SGH(H2N2O2)]\\@


THERE'S SMALL CHOICE IN A BOWL OF ROTTEN APPLES.
                    SHAKESPEARE
Job cpu time:  0 days  0 hours  0 minutes  6.3 seconds.
File lengths (MBytes):  RWF=    5 Int=    0 D2E=    0 Chk=    2 Scr=    1
Normal termination of Gaussian 94
```