SUPPLEMENTARY INFORMATION: "Noncovalent Interaction": A Chemical Misnomer that Inhibits Proper Understanding of Hydrogen Bonding, Rotation Barriers, and Other Topics

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INTRODUCTION

This SI file consists of ready-to-run *Gaussian 16* input files, each containing optimized geometrical coordinates as well as extended "title" sections summarizing vibrational frequencies, thermochemical values, and other calculated properties, followed by $NBO...$END keylist input with selected analysis keywords. Following the plan of the paper, the SI file is divided into separate "**HYDROGEN BONDING**," "**ROTATION BARRIER**," and "**STERIC REPULSION**" sections. Each section includes the input files for ordinary optimizations ("`pop=nbo7read`") followed by those for $DEL-deletion optimizations ("`pop=nbo7del`"). These files serve to re-generate all numerical values and graphical PLOT files (as displayed in the orbital images generated by the *NBOPro7@jmol* program) of the main paper.

HYDROGEN BONDING

```
%mem=2gb
%nprocshared=8
%chk=fh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
FH, E=-100.482383390  (dE= )
nu: 4098
 Vibrational temperatures:   5895.45
         (Kelvin)
 Zero-point correction=                     0.009335 (Hartree/Particle)
 Thermal correction to Energy=              0.011695
 Thermal correction to Enthalpy=            0.012640
 Thermal correction to Gibbs Free Energy=  -0.007072
 Sum of electronic and zero-point Energies=       -100.473048
 Sum of electronic and thermal Energies=          -100.470688
 Sum of electronic and thermal Enthalpies=        -100.469744
 Sum of electronic and thermal Free Energies=     -100.489455
Total dipole moment   0.00  0.00 -1.98  1.98    0.00  0.00 -1.98  1.98
0 1
F
H    1   0.9222
$nbo file=fh dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=clh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
ClH, E=-460.834022055  (dE= )
nu: 2934
 Vibrational temperatures:   4222.04
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```
           (Kelvin)
 Zero-point correction=                              0.006685 (Hartree/Particle)
 Thermal correction to Energy=                       0.009046
 Thermal correction to Enthalpy=                     0.009990
 Thermal correction to Gibbs Free Energy=           -0.011204
 Sum of electronic and zero-point Energies=              -460.827337
 Sum of electronic and thermal Energies=                 -460.824976
 Sum of electronic and thermal Enthalpies=               -460.824032
 Sum of electronic and thermal Free Energies=            -460.845226
Total dipole moment    0.00  0.00 -1.40  1.40     0.00  0.00 -1.40  1.40
0 1
Cl
H    1   1.2869
$nbo file=clh dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=brh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
BrH, E=-2574.75317353  (dE= )
nu: 2605
 Vibrational temperatures:   3747.31
          (Kelvin)
 Zero-point correction=                              0.005934 (Hartree/Particle)
 Thermal correction to Energy=                       0.008294
 Thermal correction to Enthalpy=                     0.009238
 Thermal correction to Gibbs Free Energy=           -0.013296
 Sum of electronic and zero-point Energies=             -2574.747240
 Sum of electronic and thermal Energies=                -2574.744880
 Sum of electronic and thermal Enthalpies=              -2574.743935
 Sum of electronic and thermal Free Energies=           -2574.766470
Total dipole moment    0.00  0.00 -1.08  1.08     0.00  0.00 -1.08  1.08
0 1
Br
H    1   1.4273
$nbo file=brh dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=hh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
HH, E=-1.17957156591  (dE= )
nu: 4418
 Vibrational temperatures:   6356.61
          (Kelvin)
 Zero-point correction=                              0.010065 (Hartree/Particle)
 Thermal correction to Energy=                       0.012426
 Thermal correction to Enthalpy=                     0.013370
 Thermal correction to Gibbs Free Energy=           -0.001426
 Sum of electronic and zero-point Energies=                -1.169506
 Sum of electronic and thermal Energies=                   -1.167146
 Sum of electronic and thermal Enthalpies=                 -1.166202
 Sum of electronic and thermal Free Energies=              -1.180997
Total dipole moment    0.00  0.00  0.00  0.00     0.00  0.00  0.00  0.00
0 1
H
H    1   0.7442
$nbo file=hh dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=hh_brh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
HH...BrH, E=-2575.93273798  (dE=+0.0048)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 27,31,111
 Vibrational temperatures:      39.44    44.05   159.13   185.11  3748.13
          (Kelvin)                6350.97
```

```
 Zero-point correction=                          0.016668 (Hartree/Particle)
 Thermal correction to Energy=                    0.022656
 Thermal correction to Enthalpy=                  0.023600
 Thermal correction to Gibbs Free Energy=        -0.012760
 Sum of electronic and zero-point Energies=          -2575.916070
 Sum of electronic and thermal Energies=             -2575.910082
 Sum of electronic and thermal Enthalpies=           -2575.909138
 Sum of electronic and thermal Free Energies=        -2575.945498
    1. HBr                       1.09 -0.01  0.00  1.09    1.21 -0.04  0.00  1.21
                                                    deloc: -0.12  0.03  0.00  0.12
    2. H2                        0.00  0.02  0.00  0.02    0.00  0.02  0.00  0.02
0 1
              35              0.000000   0.217550   0.000000
               1              1.426926   0.186963   0.000000
               1             -0.750089  -4.270970   0.000000
               1             -0.676837  -3.530234   0.000000
$nbo file=hh_brh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=hh_clh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
HH...ClH, E=-462.013704938  (dE=-0.07)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 40,64,146,...
 Vibrational temperatures:     57.31    91.51   210.01   234.60   4220.29
         (Kelvin)           6348.10
 Zero-point correction=                          0.017674 (Hartree/Particle)
 Thermal correction to Energy=                    0.023441
 Thermal correction to Enthalpy=                  0.024385
 Thermal correction to Gibbs Free Energy=        -0.009072
 Sum of electronic and zero-point Energies=          -461.996031
 Sum of electronic and thermal Energies=             -461.990264
 Sum of electronic and thermal Enthalpies=           -461.989320
 Sum of electronic and thermal Free Energies=        -462.022777
    1. HCl                       1.41 -0.12  0.00  1.41    1.57 -0.18  0.00  1.58
                                                    deloc: -0.17  0.06  0.00  0.18
    2. H2                        0.00  0.03  0.00  0.03    0.00  0.03  0.00  0.03
0 1
              17              0.000000   0.380003  -0.000000
               1              1.280477   0.250120  -0.000000
               1             -0.658932  -3.726854   0.000000
               1             -0.621544  -2.983324   0.000000
$nbo file=hh_clh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=hh_fh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
HH...FH, E=-101.662377949  (dE=-0.27)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 79,116,227,...
 Vibrational temperatures:    114.15   167.55   326.67   340.04   5890.74
         (Kelvin)           6338.88
 Zero-point correction=                          0.020866 (Hartree/Particle)
 Thermal correction to Energy=                    0.026203
 Thermal correction to Enthalpy=                  0.027147
 Thermal correction to Gibbs Free Energy=        -0.002526
 Sum of electronic and zero-point Energies=          -101.641512
 Sum of electronic and thermal Energies=             -101.636175
 Sum of electronic and thermal Enthalpies=           -101.635231
 Sum of electronic and thermal Free Energies=        -101.664904
    1. HF                        1.61  1.18  0.00  1.99    1.79  1.30  0.00  2.21
                                                    deloc: -0.18 -0.12  0.00  0.22
    2. H2                        0.00  0.08  0.00  0.08    0.01  0.08  0.00  0.09
```

```
0 1
              9                    0.000000   0.451609   0.000000
              1                    0.746640   0.993348   0.000000
              1                   -0.399769  -2.900430  -0.000000
              1                   -0.346871  -2.157402  -0.000000
$nbo file=hh_fh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=brh_brh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
BrH...BrH, E= -5149.50797736  (dE=-1.02)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 37,96,173,...
 Vibrational temperatures:     53.85   138.23   248.35   372.90  3659.65
         (Kelvin)           3741.29
 Zero-point correction=                            0.013007 (Hartree/Particle)
 Thermal correction to Energy=                     0.018521
 Thermal correction to Enthalpy=                   0.019466
 Thermal correction to Gibbs Free Energy=         -0.018302
 Sum of electronic and zero-point Energies=        -5149.494971
 Sum of electronic and thermal Energies=           -5149.489456
 Sum of electronic and thermal Enthalpies=         -5149.488512
 Sum of electronic and thermal Free Energies=      -5149.526279
   1. HBr                  -1.13 -0.40  0.00  1.20    -1.24  0.00  0.00  1.24
                                                 deloc:  0.11 -0.40  0.00  0.42
   2. HBr                   0.13 -1.20  0.00  1.20     0.13 -1.34  0.00  1.35
0 1
             35                    0.018027  -2.102222   0.000000
              1                   -1.408607  -2.168100   0.000000
             35                    0.018027   2.143678   0.000000
              1                    0.146735   0.717134   0.000000
$nbo file=brh_brh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=brh_clh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
BrH...ClH, E=-3035.58908266  (dE=-1.18)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 48,105,167...
 Vibrational temperatures:     68.96   150.84   239.97   391.88  3685.98
         (Kelvin)           4209.92
 Zero-point correction=                            0.013851 (Hartree/Particle)
 Thermal correction to Energy=                     0.019319
 Thermal correction to Enthalpy=                   0.020263
 Thermal correction to Gibbs Free Energy=         -0.016123
 Sum of electronic and zero-point Energies=        -3035.575232
 Sum of electronic and thermal Energies=           -3035.569764
 Sum of electronic and thermal Enthalpies=         -3035.568820
 Sum of electronic and thermal Free Energies=      -3035.605205
   1. HCl                  -1.44  0.40  0.00  1.50    -1.60  0.13  0.00  1.61
                                                 deloc:  0.16  0.27  0.00  0.31
   2. HBr                   0.17  1.19  0.00  1.20     0.18  1.34  0.00  1.35
                                                 deloc: -0.01 -0.16  0.00  0.16
0 1
             17                    0.020399   2.724414  -0.000000
              1                   -1.259279   2.870995   0.000000
             35                    0.020399  -1.405720   0.000000
              1                    0.198506   0.014166  -0.000000
$nbo file=brh_clh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=brh_fh
```

```
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
BrH...FH, E=-2675.23940475  (dE=-2.41)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 87,135,235,...
 Vibrational temperatures:    125.01   194.36   338.82   441.36  3701.25
          (Kelvin)           5860.50
 Zero-point correction=                           0.016881 (Hartree/Particle)
 Thermal correction to Energy=                     0.022062
 Thermal correction to Enthalpy=                   0.023007
 Thermal correction to Gibbs Free Energy=         -0.010771
 Sum of electronic and zero-point Energies=          -2675.222524
 Sum of electronic and thermal Energies=             -2675.217342
 Sum of electronic and thermal Enthalpies=           -2675.216398
 Sum of electronic and thermal Free Energies=        -2675.250175
   1. HF                    -1.64  1.34  0.00  2.12    -1.81  1.30  0.00  2.23
                                               deloc:  0.17  0.04  0.00  0.17
   2. HBr                    0.13  1.34  0.00  1.34     0.14  1.50  0.00  1.51
                                               deloc:  0.00 -0.16  0.00  0.16
0 1
                9               0.013843   2.729208   -0.000000
                1              -0.732269   3.274315    0.000000
               35               0.013843  -0.812897   -0.000000
                1               0.123170   0.614227   -0.000000
$nbo file=brh_fh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=clh_brh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
ClH...BrH, E=-3035.58948228  (dE=-1.44)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 55,108,207,...
 Vibrational temperatures:     79.77   154.75   297.36   425.11  3739.48
          (Kelvin)           4097.27
 Vibrational temperatures:     79.77   154.75   297.36   425.11  3739.48
          (Kelvin)           4097.27
 Zero-point correction=                           0.013924 (Hartree/Particle)
 Thermal correction to Energy=                     0.019277
 Thermal correction to Enthalpy=                   0.020221
 Thermal correction to Gibbs Free Energy=         -0.015784
 Sum of electronic and zero-point Energies=          -3035.575558
 Sum of electronic and thermal Energies=             -3035.570206
 Sum of electronic and thermal Enthalpies=           -3035.569261
 Sum of electronic and thermal Free Energies=        -3035.605266
   1. HBr                    0.47  1.14  0.00  1.24     0.04  1.25  0.00  1.25
                                               deloc:  0.43 -0.11  0.00  0.45
   2. HCl                    1.50 -0.16  0.00  1.51     1.71 -0.17  0.00  1.71
                                               deloc: -0.20  0.01  0.00  0.20
0 1
               35              -1.309859  -0.039403    0.000002
                1              -1.396827   1.386314   -0.000016
               17               2.696059   0.006404    0.000008
                1               1.408902  -0.116073   -0.000211
$nbo file=clh_brh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=clh_clh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
ClH...ClH, E=-921.670558460  (dE=-1.58)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 65,113,199,...
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```
     Vibrational temperatures:     93.22    163.27    286.10    445.42    4129.22
            (Kelvin)           4208.27
 Zero-point correction=                             0.014766 (Hartree/Particle)
 Thermal correction to Energy=                      0.020083
 Thermal correction to Enthalpy=                    0.021027
 Thermal correction to Gibbs Free Energy=          -0.013646
 Sum of electronic and zero-point Energies=            -921.655792
 Sum of electronic and thermal Energies=               -921.650476
 Sum of electronic and thermal Enthalpies=             -921.649531
 Sum of electronic and thermal Free Energies=          -921.684204
   1. HCl                      -0.45  1.45  0.00  1.52    -0.15  1.61  0.00  1.62
                                                  deloc: -0.30 -0.16  0.00  0.34
   2. HCl                      -1.49 -0.26  0.00  1.51    -1.70 -0.28  0.00  1.72
                                                  deloc:  0.21  0.02  0.00  0.21
0 1
            17                   -1.904641   -0.070217   -0.000015
             1                   -2.057085    1.208964    0.000074
            17                    1.983989    0.010337   -0.000021
             1                    0.708167   -0.190990    0.000546
$nbo file=clh_clh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=clh_fh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
ClH...FH, E=-561.321312583  (dE=-3.08)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 112,161,292,....
 Vibrational temperatures:    160.70    232.10    419.69    523.81    4141.07
            (Kelvin)           5854.40
 Zero-point correction=                             0.017943 (Hartree/Particle)
 Thermal correction to Energy=                      0.022888
 Thermal correction to Enthalpy=                    0.023833
 Thermal correction to Gibbs Free Energy=          -0.008107
 Sum of electronic and zero-point Energies=            -561.303370
 Sum of electronic and thermal Energies=               -561.298424
 Sum of electronic and thermal Enthalpies=             -561.297480
 Sum of electronic and thermal Free Energies=          -561.329420
   1. HF                       -1.69  1.30  0.00  2.14    -1.86  1.23  0.00  2.23
                                                  deloc:  0.17  0.07  0.00  0.18
   2. HCl                       0.17  1.63  0.00  1.64     0.18  1.85  0.00  1.85
                                                  deloc: -0.02 -0.22  0.00  0.22
0 1
             9                    0.023339    2.067101   -0.000000
             1                   -0.742198    2.585194   -0.000000
            17                    0.023339   -1.248692    0.000000
             1                    0.135379    0.038657   -0.000000
$nbo file=clh_fh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=fh_brh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
FH...BrH, E=-2675.23977260  (dE=-2.65)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 96,145,337,...
 Vibrational temperatures:    138.07    209.26    485.16    642.11    3734.92
            (Kelvin)           5663.42
 Zero-point correction=                             0.017216 (Hartree/Particle)
 Thermal correction to Energy=                      0.022085
 Thermal correction to Enthalpy=                    0.023029
 Thermal correction to Gibbs Free Energy=          -0.010544
 Sum of electronic and zero-point Energies=           -2675.222556
 Sum of electronic and thermal Energies=              -2675.217687
 Sum of electronic and thermal Enthalpies=            -2675.216743
```

```
   Sum of electronic and thermal Free Energies=        -2675.250317
     1. HBr                     -0.61  1.18  0.00  1.33    -0.09  1.28  0.00  1.29
                                             deloc: -0.52 -0.10  0.00  0.53
     2. HF                      -2.06 -0.26  0.00  2.08    -2.29 -0.28  0.00  2.31
                                             deloc:  0.23  0.02  0.00  0.23
 0 1
              35              -0.718359   -0.039414   -0.000002
               1              -0.763678    1.388916    0.000015
               9               2.682823    0.010399   -0.000017
               1               1.760836   -0.103009    0.000212
$nbo file=fh_brh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=fh_clh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
FH...ClH, E=-561.320823712  (dE=-2.77)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 104,155,344...
 Vibrational temperatures:   150.11   223.64   494.92   670.92  4199.60
         (Kelvin)           5695.20
 Zero-point correction=                          0.018105 (Hartree/Particle)
 Thermal correction to Energy=                   0.022916
 Thermal correction to Enthalpy=                 0.023861
 Thermal correction to Gibbs Free Energy=       -0.008327
 Sum of electronic and zero-point Energies=      -561.302718
 Sum of electronic and thermal Energies=         -561.297907
 Sum of electronic and thermal Enthalpies=       -561.296963
 Sum of electronic and thermal Free Energies=    -561.329151
     1. HCl                     -0.55  1.49  0.00  1.59    -0.14  1.65  0.00  1.65
                                             deloc: -0.41 -0.15  0.00  0.43
     2. HF                      -2.04 -0.38  0.00  2.08    -2.27 -0.41  0.00  2.31
                                             deloc:  0.23  0.04  0.00  0.23
 0 1
              17              -1.128882   -0.071457   -0.000003
               1              -1.248200    1.212058    0.000013
               9               2.135246    0.016820   -0.000009
               1               1.221986   -0.148675    0.000114
$nbo file=fh_clh archive nrt plot dipole $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=fh_fh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
FH...FH, E=-200.972811239  (dE=-5.05)
FH, E=-100.482383390  (dE= )
ClH, E=-460.834022055  (dE= )
BrH, E=-2574.75317353  (dE= )
HH, E=-1.17957156591  (dE= )
nu: 161,220,456...
 Vibrational temperatures:   232.18   317.65   655.94   829.39  5695.68
         (Kelvin)           5838.65
 Zero-point correction=                          0.021486 (Hartree/Particle)
 Thermal correction to Energy=                   0.025903
 Thermal correction to Enthalpy=                 0.026848
 Thermal correction to Gibbs Free Energy=       -0.002861
 Sum of electronic and zero-point Energies=      -200.951325
 Sum of electronic and thermal Energies=         -200.946908
 Sum of electronic and thermal Enthalpies=       -200.945964
 Sum of electronic and thermal Free Energies=    -200.975672
     1. HF                      -1.86 -1.13  0.00  2.18    -2.04 -0.96  0.00  2.25
                                             deloc:  0.18 -0.17  0.00  0.25
     2. HF                       0.31 -2.13  0.00  2.15     0.34 -2.38  0.00  2.40
                                             deloc: -0.03  0.25  0.00  0.25
 0 1
               9               0.034957   -1.306771   -0.000000
               1              -0.793920   -1.718253   -0.000000
               9               0.034957    1.439904    0.000000
```

```
              1                     0.164698    0.520062    0.000000
$nbo file=fh_fh archive nrt plot dipole $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** opt=calcall polar pop=nbo7read
XH...YH, E=  (dE= )
0 1
Y
H    1   1.
X    1   3.    2   110.
H    3   1.    2    30.    1    0.
$nbo file=xh_yh archive nrt plot dipole $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
HH...BrH, E($DEL)=-2575.932652176 (dE=0.06)
0 1
 Br
 H   1    r1
 x   1    1.      2     90.
 H   1    r2      2     a1       3    10.
 x   4    1.      1     90.      3    180.
 H   4    r3      5     a2       1    tw
r1   1.4270
r2   4.3650
r3   0.7443
a1   186.13
a2   -45.89
tw   -101.31
$nbo print=0 $end
$del
  delete 2 orbitals 20 21
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
FH...FH, E($DEL)=  (dE= )
0 1
 F
 H   1    r1
 x   1    1.      2     90.
 F   1    r2      2     a1       3    10.
 x   4    1.      1     90.      3    180.
 H   4    r3      5     a2       1    tw
r1   1.
r2   3.
r3   1.
a1   120.
a2   90.
tw   20.
$nbo print=0 $end
$del
  delete 2 orbitals 11 12
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
FH...FH, E($DEL)=-200.969569707  (dE=-3.01)
0 1
```

```
 F
 H    1    r1
 x    1    1.     2     90.
 F    1    r2     2     a1      3      10.
 x    4    1.     1     90.     3      180.
 H    4    r3     5     a2      1      tw
r1   0.9239
r2   3.1797
r3   0.9227
a1   129.70
a2   76.36
tw   -3.84
$nbo print=0 $end
$del
  delete 2 orbitals 11 12
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
FH...ClH, E($DEL)=-561.319081897  (dE=)
             17          0      0.000000    0.000000    0.000000
              1          0      0.000000    0.000000    1.286382
              9          0      1.950572   -0.343938    2.935405
              1          0      2.791390   -0.334628    2.553954
0 1
 Cl
 H    1    r1
 x    1    1.     2     90.
 F    1    r2     2     a1      3      10.
 x    4    1.     1     90.     3      180.
 H    4    r3     5     a2      1      tw
r1   1.2864
r2   3.5411
r3   0.9233
a1   34.01
a2   189.36
tw   13.53
$nbo print=0 $end
$del
  delete 2 orbitals 15 16
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
FH...BrH, E($DEL)=-2675.237584089  (dE=-1.27)
             35                 0.000000    0.000000    0.000000
              1                 0.000000    0.000000    1.426300
              9                 2.444453   -0.431023    2.691414
              1                 2.990902   -0.343013    1.952644
0 1
 Br
 H    1    r1
 x    1    1.     2     90.
 F    1    r2     2     a1      3      10.
 x    4    1.     1     90.     3      180.
 H    4    r3     5     a2      1      tw
r1   1.4263
r2   3.316613
r3   0.9231
a1   42.68
a2   168.06
tw   -9.01
$nbo print=0 $end
$del
  delete 2 orbitals 24 25
```

```
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
ClH...FH, E($DEL)=-561.319088228  (dE=-1.68 )
0 1
 F
 H   1    r1
 x   1    1.      2      90.
 Cl  1    r2      2      a1       3      10.
 x   4    1.      1      90.      3      180.
 H   4    r3      5      a2       1      tw
r1   0.9232
r2   3.6872
r3   1.2861
a1   116.69
a2   67.54
tw   -9.16
$nbo print=0 $end
$del
  delete 2 orbitals 15 16
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
ClH...ClH, E($DEL)=-921.669650599  (dE=-1.01)
0 1
 Cl
 H   1    r1
 x   1    1.      2      90.
 Cl  1    r2      2      a1       3      10.
 x   4    1.      1      90.      3      180.
 H   4    r3      5      a2       1      tw
r1   1.2874
r2   4.0333
r3   1.2871
a1   54.84
a2   143.60
tw   -15.53
$nbo print=0 $end
$del
  delete 2 orbitals 19 20
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
ClH...BrH, E($DEL)=-3035.587950624  (dE=-0.47)
0 1
 Br
 H   1    r1
 x   1    1.      2      90.
 Cl  1    r2      2      a1       3      10.
 x   4    1.      1      90.      3      180.
 H   4    r3      5      a2       1      tw
r1   1.4272
r2   5.0997
r3   1.2870
a1   101.36
a2   82.63
tw   0.01
$nbo print=0 $end
$del
```

```
   delete 2 orbitals 28 29
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
BrH...FH, E($DEL)=-2675.237558498  (dE=-1.26)
0 1
 F
 H   1     r1
 x   1     1.      2     90.
 Br  1     r2      2     a1       3     10.
 x   4     1.      1     90.      3     180.
 H   4     r3      5     a2       1     tw
r1   0.9230
r2   3.9294
r3   1.4261
a1   117.52
a2   67.26
tw   -9.03
$nbo print=0 $end
$del
   delete 2 orbitals 24 25
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
BrH...ClH, E($DEL)=-3035.588046795 (dE=-0.53)
0 1
 Cl
 H   1     r1
 x   1     1.      2     90.
 Br  1     r2      2     a1       3     10.
 x   4     1.      1     90.      3     180.
 H   4     r3      5     a2       1     tw
r1   1.2870
r2   4.8190
r3   1.4265
a1   96.41
a2   77.05
tw   -13.65
$nbo print=0 $end
$del
   delete 2 orbitals 28 29
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
BrH...BrH, E($DEL)=-5149.506516181* (dE=-0.11)
0 1
 Br
 H   1     r1
 x   1     1.      2     90.
 Br  1     r2      2     a1       3     10.
 x   4     1.      1     90.      3     180.
 H   4     r3      5     a2       1     tw
r1   1.4261
r2   4.6019
r3   1.4292
a1   221.98
a2   42.66
tw   2.67
$nbo print=0 $end
```

```
$del
  delete 2 orbitals 37 38
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
HH...FH, E($DEL)=-101.662438626 (dE=-0.30)
0 1
 F
 H    1    r1
 x    1    1.      2     90.
 H    1    r2      2     a1       3     10.
 x    4    1.      1     90.      3     180.
 H    4    r3      5     a2       1     tw
r1   0.9222
r2   3.4401
r3   0.7451
a1   5.65
a2   352.25
tw   -213.18
$nbo print=0 $end
$del
  delete 2 orbitals 7 8
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=xh_yh
#b3lyp/6-311++g** nosymm opt=(maxcycles=100) pop=nbo7del
HH...ClH, E($DEL)=-462.013682447 (dE=-0.06)
0 1
 Cl
 H    1    r1
 x    1    1.      2     90.
 H    1    r2      2     a1       3     10.
 x    4    1.      1     90.      3     180.
 H    4    r3      5     a2       1     tw
r1   1.2876
r2   5.3140
r3   0.7429
a1   12.66
a2   42.14
tw   103.34
$nbo print=0 $end
$del
  delete 2 orbitals 11 12
$end
--Link1--
--Link1—
```

ROTATION BARRIERS

```
----
HOOH
----
full: -151.6021697 @ 121.12
 DEL: -151.5777827 @ 130.44
%-Del-E = 0.016%
------
CH3CH3
------
full: -79.8565753 @ 60.12
 DEL: -79.8179280 @ 63.26
%-Del-E = 0.048%
------
CH3NH2
------
```

```
full: -95.8938910
 DEL: -95.8466542
%-Del-E = 0.049%
------
HCONH2
------
full: -169.954848506
 DEL: -169.769538009
%-Del-E = 0.684%
------------------------------------------------------------------------
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=0), E(DEL)=-169.767055457 (1.56)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0500
r3   1.2982
a3   116.52
r4   1.5477
a4   130.02
d4   178.47
r5   1.0094
a5   105.48
r6   1.0096
a6   107.92
d6   246.08
tau  0.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=10), E(DEL)=-169.767655109 (1.18)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0496
r3   1.2994
a3   116.64
r4   1.5469
a4   129.72
d4   177.93
r5   1.0105
a5   105.37
r6   1.0108
a6   107.67
d6   256.39
tau  10.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
```

```
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=20), E(DEL)=-169.768249692 (0.81)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0490
r3   1.3007
a3   116.96
r4   1.5452
a4   129.18
d4   177.62
r5   1.0112
a5   105.37
r6   1.0116
a6   107.42
d6   266.61
tau  20.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=30), E(DEL)= -169.768798741 (0.46)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0486
r3   1.3019
a3   117.17
r4   1.5437
a4   128.80
d4   177.72
r5   1.0122
a5   105.40
r6   1.0126
a6   107.02
d6   277.02
tau  30.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=40), E(DEL)=-169.769234708 (0.19)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0482
r3   1.3029
a3   117.34
r4   1.5421
```

```
a4   128.50
d4   178.25
r5   1.0129
a5   105.58
r6   1.0131
a6   106.65
d6   287.20
tau  40.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=50), E(DEL)=-169.769489864 (0.03)
0 1
H
C    1   r2
O    2   r3    1    a3
N    2   r4    1    a4    3   d4
H    4   r5    2    a5    3   tau
H    4   r6    2    a6    3   d6
r2   1.0479
r3   1.3036
a3   117.49
r4   1.5415
a4   128.38
d4   179.32
r5   1.0130
a5   105.84
r6   1.0131
a6   106.28
d6   297.14
tau  50.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=60), E(DEL)=-169.769525017 (0.01)
0 1
H
C    1   r2
O    2   r3    1    a3
N    2   r4    1    a4    3   d4
H    4   r5    2    a5    3   tau
H    4   r6    2    a6    3   d6
r2   1.0479
r3   1.3037
a3   117.53
r4   1.5403
a4   128.22
d4   180.46
r5   1.0130
a5   106.32
r6   1.0130
a6   106.08
d6   306.78
tau  60.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
```

```
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=70), E(DEL)=-169.768978994 (0.35)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0484
r3   1.3022
a3   117.29
r4   1.5419
a4   128.54
d4   182.22
r5   1.0117
a5   107.32
r6   1.0115
a6   105.88
d6   325.47
tau  70.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=80), E(DEL)=-169.768978994 (0.35)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0484
r3   1.3022
a3   117.29
r4   1.5419
a4   128.54
d4   182.22
r5   1.0117
a5   107.32
r6   1.0115
a6   105.88
d6   325.47
tau  80.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=90), E(DEL)=-169.768490053 (0.66)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0488
```

```
r3   1.3011
a3   117.08
r4   1.5431
a4   128.86
d4   182.46
r5   1.0106
a5   107.80
r6   1.0104
a6   105.91
d6   334.74
tau  90.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=100), E(DEL)=-169.767931662 (1.01)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0493
r3   1.2998
a3   116.88
r4   1.5445
a4   129.24
d4   182.44
r5   1.0097
a5   108.14
r6   1.0096
a6   105.94
d6   344.33
tau  100.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=110), E(DEL)=-169.767349406 (1.37)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0498
r3   1.2986
a3   116.69
r4   1.5453
a4   129.68
d4   182.03
r5   1.0085
a5   108.48
r6   1.0085
a6   106.04
d6   353.82
tau  110.
$nbo print=0 $end
$DEL
```

```
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=120), E(DEL)=-169.766761745 (1.74)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0503
r3   1.2975
a3   116.50
r4   1.5461
a4   130.16
d4   181.34
r5   1.0076
a5   108.65
r6   1.0078
a6   106.04
d6   363.70
tau  120.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=130), E(DEL)=-169.761210536 (5.22)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  tau
H   4  r6   2   a6   3  d6
r2   1.0481
r3   1.3020
a3   117.19
r4   1.5345
a4   125.52
d4   181.91
r5   1.0080
a5   109.77
r6   1.0081
a6   109.40
d6   250.60
tau  130.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=140), E(DEL)=-169.761016586 (5.35)
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
```

```
H    4   r5   2   a5   3   tau
H    4   r6   2   a6   3   d6
r2   1.0484
r3   1.3015
a3   117.09
r4   1.5358
a4   125.77
d4   183.53
r5   1.0079
a5   109.80
r6   1.0080
a6   109.14
d6   260.26
tau  140.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=150), E(DEL)=-169.760840721 (5.46)
0 1
H
C    1   r2
O    2   r3   1   a3
N    2   r4   1   a4   3   d4
H    4   r5   2   a5   3   tau
H    4   r6   2   a6   3   d6
r2   1.0488
r3   1.3008
a3   116.92
r4   1.5374
a4   126.26
d4   184.33
r5   1.0074
a5   109.86
r6   1.0075
a6   109.00
d6   270.28
tau  150.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=160), E(DEL)=-169.760844945 (5.46)
0 1
H
C    1   r2
O    2   r3   1   a3
N    2   r4   1   a4   3   d4
H    4   r5   2   a5   3   tau
H    4   r6   2   a6   3   d6
r2   1.0493
r3   1.3000
a3   116.61
r4   1.5385
a4   127.02
d4   184.87
r5   1.0067
a5   109.94
r6   1.0067
a6   108.88
d6   280.53
```

```
tau  160.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=170), E(DEL)=-169.761156673 (5.26)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0498
r3   1.2988
a3   116.50
r4   1.5394
a4   127.77
d4   184.84
r5   1.0057
a5   110.03
r6   1.0057
a6   108.73
d6   290.88
tau  170.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HCONH2 (tau=180), E(DEL)=-169.761773208 (4.87)
0 1
H
C   1   r2
O   2   r3   1   a3
N   2   r4   1   a4   3   d4
H   4   r5   2   a5   3   tau
H   4   r6   2   a6   3   d6
r2   1.0505
r3   1.2969
a3   116.42
r4   1.5400
a4   128.50
d4   184.19
r5   1.0048
a5   109.84
r6   1.0056
a6   108.56
d6   300.53
tau  180.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=z-matrix freq
cis-CHFCHF, E(full)=-277.142846266
nu:237,510,771,...
```

```
 Vibrational temperatures:    340.39   733.61  1108.85  1116.07  1251.17
         (Kelvin)            1452.66  1617.65  1842.14  1988.01  2526.05
                             4625.18  4658.01
 Zero-point correction=                           0.036830 (Hartree/Particle)
 Thermal correction to Energy=                    0.040698
 Thermal correction to Enthalpy=                  0.041642
 Thermal correction to Gibbs Free Energy=         0.010510
 Sum of electronic and zero-point Energies=          -277.106017
 Sum of electronic and thermal Energies=             -277.102148
 Sum of electronic and thermal Enthalpies=           -277.101204
 Sum of electronic and thermal Free Energies=        -277.132336
0 1
H
C    1    r2
C    2    r3   1   a3
F    2    r4   3   a4   1   d4
H    3    r5   2   a5   1   d5
F    3    r6   2   a6   4   d6
r2   1.0811
r3   1.3238
a3   122.98
r4   1.3432
a4   122.59
d4   180.00
r5   1.0811
a5   122.99
d5   0.00
r6   1.3432
a6   122.59
d6   0.
$nbo file=cis_chfchf $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix freq
cis-CHFCHF, E(DEL)=-276.972503939
nu:317,334,551,...
 Vibrational temperatures:    456.74   480.82   793.04  1186.31  1301.63
         (Kelvin)            1628.46  1652.72  1851.36  1874.84  2505.74
                             4634.46  4644.87
 Zero-point correction=                           0.036436 (Hartree/Particle)
 Thermal correction to Energy=                    0.040427
 Thermal correction to Enthalpy=                  0.041371
 Thermal correction to Gibbs Free Energy=         0.010285
 Sum of electronic and zero-point Energies=          -277.105129
 Sum of electronic and thermal Energies=             -277.101138
 Sum of electronic and thermal Enthalpies=           -277.100193
 Sum of electronic and thermal Free Energies=        -277.131279
0 1
H
C    1    r2
C    2    r3   1   a3
F    2    r4   3   a4   1   d4
H    3    r5   2   a5   1   d5
F    3    r6   2   a6   4   d6
r2   1.0601
r3   1.3520
a3   133.70
r4   1.4945
a4   115.34
d4   179.97
r5   1.0601
a5   133.70
d5   0.01
r6   1.4946
a6   115.35
d6   -0.02
$nbo print=0 $end
$del
```

```
    lewis
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=z-matrix freq
trans-CHFCHF, E(full)=-277.141564470
nu:317,334,551,...
 Vibrational temperatures:     456.74   480.82   793.04  1186.31  1301.63
         (Kelvin)             1628.46  1652.72  1851.36  1874.84  2505.74
                             4634.46  4644.87
 Zero-point correction=                           0.036436 (Hartree/Particle)
 Thermal correction to Energy=                    0.040427
 Thermal correction to Enthalpy=                  0.041371
 Thermal correction to Gibbs Free Energy=         0.010285
 Sum of electronic and zero-point Energies=          -277.105129
 Sum of electronic and thermal Energies=             -277.101138
 Sum of electronic and thermal Enthalpies=           -277.100193
 Sum of electronic and thermal Free Energies=        -277.131279
0 1
H
C    1    r2
C    2    r3   1   a3
F    2    r4   3   a4   1   d4
H    3    r5   2   a5   1   d5
F    3    r6   2   a6   4   d6
r2   1.0814
r3   1.3222
a3   125.71
r4   1.3500
a4   120.03
d4   180.00
r5   1.0814
a5   125.71
d5   180.00
r6   1.3500
a6   120.03
d6   180.00
$nbo file=cis_chfchf $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm freq
trans-CHFCHF, E(DEL)=-276.979176905
nu: 298,332,478,...
 Vibrational temperatures:     429.09   477.08   688.24  1257.74  1268.76
         (Kelvin)             1506.44  1527.42  1714.19  1776.49  2831.66
                             5012.92  5106.04
 Zero-point correction=                           0.037362 (Hartree/Particle)
 Thermal correction to Energy=                    0.041449
 Thermal correction to Enthalpy=                  0.042394
 Thermal correction to Gibbs Free Energy=         0.010983
 Sum of electronic and zero-point Energies=          -276.941815
 Sum of electronic and thermal Energies=             -276.937727
 Sum of electronic and thermal Enthalpies=           -276.936783
 Sum of electronic and thermal Free Energies=        -276.968194
0 1
H
C    1    r2
C    2    r3   1   a3
F    2    r4   3   a4   1   d4
H    3    r5   2   a5   1   d5
F    3    r6   2   a6   4   d6
r2   1.0621
r3   1.3493
a3   133.44
r4   1.4935
```

```
a4  114.04
d4  179.96
r5  1.0621
a5  133.44
d5  180.06
r6  1.4935
a6  114.01
d6  180.01
$nbo print=0 $end
$del
  lewis
$end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=z-matrix freq
HOOH, E(full)=-151.602169726
nu:365,934,1296,...
 Vibrational temperatures:    525.24  1344.14  1865.30  2090.70  5434.06
         (Kelvin)            5435.42
 Zero-point correction=                           0.026435 (Hartree/Particle)
 Thermal correction to Energy=                    0.029677
 Thermal correction to Enthalpy=                  0.030621
 Thermal correction to Gibbs Free Energy=         0.004121
 Sum of electronic and zero-point Energies=          -151.575735
 Sum of electronic and thermal Energies=             -151.572493
 Sum of electronic and thermal Enthalpies=           -151.571549
 Sum of electronic and thermal Free Energies=        -151.598049
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9672
r3   1.4540
a3   100.47
r4   0.9672
a4   100.47
tw   121.12
$nbo file=HOOH $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm freq
HOOH, E(DEL)=-151.577782680
nu: 196,930,1461,...
 Vibrational temperatures:    281.53  1337.88  2101.83  2326.79  5368.40
         (Kelvin)            5422.73
 Zero-point correction=                           0.026663 (Hartree/Particle)
 Thermal correction to Energy=                    0.030120
 Thermal correction to Enthalpy=                  0.031064
 Thermal correction to Gibbs Free Energy=         0.004630
 Sum of electronic and zero-point Energies=          -151.551119
 Sum of electronic and thermal Energies=             -151.547662
 Sum of electronic and thermal Enthalpies=           -151.546718
 Sum of electronic and thermal Free Energies=        -151.573153
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9720
r3   1.5196
a3   95.41
r4   0.9720
a4   95.41
tw   130.44
```

```
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=modredundant
HOOH rotation barrier
 Summary of Optimized Potential Surface Scan (add -151.0 to energies):
                                  1               2               3               4
5
     Eigenvalues --        -0.588669 (8.47)  -0.588981 (8.28)  -0.589869 (7.72)  -0.591216
(6.87)  -0.592872 (5.83)
          R1                 0.967354        0.967452        0.967627        0.967904
0.968229
          R2                 1.462041        1.462287        1.460884        1.458740
1.456203
          R3                 0.967353        0.967452        0.967627        0.967904
0.968230
          A1               105.323500      105.216869      104.988747      104.649150
104.236775
          A2               105.323472      105.216774      104.989227      104.648880
104.237009
          D1                 0.000000       10.000000       20.000000       30.000000
40.000000
                                  6               7               8               9
10
     Eigenvalues --        -0.594679 (4.70)  -0.596480 (3.57)  -0.598145 (2.53)  -0.599577
(1.63)  -0.600718 (0.91)
          R1                 0.968535        0.968753        0.968830        0.968739
0.968481
          R2                 1.453641        1.451409        1.449799        1.449008
1.449113
          R3                 0.968535        0.968752        0.968830        0.968738
0.968481
          A1               103.785411      103.318931      102.848653      102.373679
101.889558
          A2               103.785464      103.318761      102.848824      102.373432
101.889686
          D1                50.000000       60.000000       70.000000       80.000000
90.000000
                                 11              12              13              14
15
     Eigenvalues --        -0.601531 (0.40)  -0.602005 (0.10)  -0.602168 (0.00)  -0.602089
(0.05)  -0.601855 (0.20)
          R1                 0.968097        0.967661        0.967240        0.966879
0.966598
          R2                 1.450065        1.451713        1.453826        1.456149
1.458426
          R3                 0.968097        0.967661        0.967240        0.966879
0.966598
          A1               101.406120      100.941009      100.509068      100.119859
99.783429
          A2               101.406047      100.941142      100.509274      100.119977
99.783802
          D1               100.000000      110.000000      120.000000      130.000000
140.000000
                                 16              17              18              19
     Eigenvalues --        -0.601555 (0.39)  -0.601268 (0.57)  -0.601063 (0.69)  -0.600988
(0.74)
          R1                 0.966402        0.966281        0.966221        0.966223
          R2                 1.460439        1.462008        1.463008        1.463002
          R3                 0.966402        0.966281        0.966221        0.966223
          A1                99.510911       99.311488       99.191589       99.192705
          A2                99.510817       99.311853       99.191450       99.192640
          D1               150.000000      160.000000      170.000000      180.000000
0 1
H
```

```
O    1    r2
O    2    r3    1    a3
H    3    r4    2    a4    1    tw
r2    0.9720
r3    1.5196
a3    95.41
r4    0.9720
a4    95.41
tw    0.
1 2 3 4 S 18 10.
$nbo print=0 $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=0)=-151.561164017(NNYY) (10.43)
0 1
H
O    1    r2
O    2    r3    1    a3
H    3    r4    2    a4    1    tw
r2    0.9749
r3    1.5312
a3    99.94
r4    0.9749
a4    99.94
tw    0.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=10)=-151.561484852(YYYY) (10.23)
0 1
H
O    1    r2
O    2    r3    1    a3
H    3    r4    2    a4    1    tw
r2    0.9762
r3    1.5294
a3    99.85
r4    0.9762
a4    99.85
tw    10.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=20)=-151.562428514(NNYY) (9.63)
0 1
H
O    1    r2
O    2    r3    1    a3
H    3    r4    2    a4    1    tw
r2    0.9767
r3    1.5269
a3    99.79
r4    0.9767
a4    99.82
tw    20.
```

```
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=30)=-151.563970462(YYYY) (8.67)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9739
r3   1.5272
a3   98.91
r4   0.9739
a4   98.91
tw   30.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=40)=-151.565871693(YYYY) (7.47)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9739
r3   1.5254
a3   98.31
r4   0.9739
a4   98.31
tw   40.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=50)=-151.567965276 (6.16)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9739
r3   1.5236
a3   97.69
r4   0.9739
a4   97.69
tw   50.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
```

```
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=60)=-151.570068697 (4.84)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9741
r3   1.5229
a3   97.08
r4   0.9741
a4   97.08
tw   60.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=70)=-151.572041240 (3.60)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9740
r3   1.5212
a3   96.60
r4   0.9740
a4   96.60
tw   70.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=80)=-151.573787126 (2.51)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9739
r3   1.5200
a3   96.21
r4   0.9739
a4   96.21
tw   80.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=90)=-151.575261231 (1.58)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9736
```

```
r3   1.5192
a3   95.92
r4   0.9736
a4   95.92
tw   90.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=100)= -151.576397011 (0.87)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9733
r3   1.5195
a3   95.69
r4   0.9733
a4   95.69
tw   100.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=110)=-151.577189565 (0.37)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9728
r3   1.5190
a3   95.52
r4   0.9728
a4   95.52
tw   110.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=120)=-151.577639459 (0.09)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9720
r3   1.5196
a3   95.41
r4   0.9720
a4   95.41
tw   120.
$nbo print=0 $end
$DEL
 Lewis
```

```
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=130)=-151.577782480 (0.00)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9720
r3   1.5196
a3   95.41
r4   0.9720
a4   95.41
tw   130.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=140)=-151.577686248 (0.06)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9720
r3   1.5196
a3   95.41
r4   0.9720
a4   95.41
tw   140.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=150)=-151.577450750 (0.21)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9714
r3   1.5212
a3   95.54
r4   0.9714
a4   95.54
tw   150.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=160)=-151.577183862 (0.38)
0 1
```

```
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9712
r3   1.5214
a3   95.58
r4   0.9712
a4   95.58
tw   160.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=170)=-151.576981609 (0.50)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9711
r3   1.5219
a3   95.64
r4   0.9711
a4   95.64
tw   170.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
HOOH, E(DEL; tau=180)=-151.576907220 (0.55)
0 1
H
O   1   r2
O   2   r3   1   a3
H   3   r4   2   a4   1   tw
r2   0.9711
r3   1.5222
a3   95.66
r4   0.9711
a4   95.66
tw   180.
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=z-matrix freq
CH3CH3, E(full)=-79.8565752846
nu: 307,827(2),...
 Vibrational temperatures:     442.41  1189.83  1189.97  1432.90  1751.90
         (Kelvin)             1751.96  2026.18  2047.75  2162.85  2162.97
                              2165.96  2166.09  4350.46  4350.69  4416.15
                              4416.26  4452.09  4452.20
 Zero-point correction=                        0.074307 (Hartree/Particle)
 Thermal correction to Energy=                 0.077794
 Thermal correction to Enthalpy=               0.078738
```

```
 Thermal correction to Gibbs Free Energy=          0.051189
 Sum of electronic and zero-point Energies=          -79.782268
 Sum of electronic and thermal Energies=            -79.778781
 Sum of electronic and thermal Enthalpies=          -79.777837
 Sum of electronic and thermal Free Energies=       -79.805386
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.5309
r3  1.0937
a3  111.36
r4  1.0937
a4  111.35
d4  119.98
r5  1.0937
a5  111.36
d5  120.01
r6  1.0937
a6  111.36
tw  60.12
r7  1.0937
a7  111.35
d7  119.98
r8  1.0937
a8  111.36
d8  120.01
$nbo file=ch3ch3 $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** nosymm opt=(ts,z-matrix,calcfc) freq
CH3CH3 (eclipsed t.s.), -79.8522677640
nu: -299,896(2),991,...
 Vibrational temperatures:   1288.47  1288.52  1426.25  1683.22  1683.24
          (Kelvin)          2023.87  2069.64  2160.67  2160.73  2173.64
                            2173.69  4361.51  4371.92  4429.42  4429.46
                            4462.17  4462.21
 Zero-point correction=                      0.073864 (Hartree/Particle)
 Thermal correction to Energy=               0.076915
 Thermal correction to Enthalpy=             0.077859
 Thermal correction to Gibbs Free Energy=    0.050985
 Sum of electronic and zero-point Energies=          -79.778404
 Sum of electronic and thermal Energies=            -79.775353
 Sum of electronic and thermal Enthalpies=          -79.774409
 Sum of electronic and thermal Free Energies=       -79.801283
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.5447
r3  1.0925
a3  111.79
r4  1.0925
a4  111.79
d4  120.00
r5  1.0925
a5  111.79
d5  120.00
```

```
r6   1.0925
a6   111.79
r7   1.0925
a7   111.79
d7   120.00
r8   1.0925
a8   111.79
d8   120.00
tw   0.
$nbo file=ch3ch3_ecl archive nrt plot steric $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm freq
CH3CH3, E(DEL)=-79.817928022 (YYYY) (0.00)
nu: 29,918(2),938,1219(2),1475,1518,1599(2),1602(2),3130(2),3144(2),3253,3284
 Vibrational temperatures:     41.86  1320.25  1320.34  1350.26  1753.47
         (Kelvin)            1753.50  2122.29  2184.01  2299.29  2299.97
                             2305.30  2305.98  4503.55  4503.77  4523.09
                             4523.32  4681.05  4725.22
 Zero-point correction=                           0.076821 (Hartree/Particle)
 Thermal correction to Energy=                    0.080735
 Thermal correction to Enthalpy=                  0.081679
 Thermal correction to Gibbs Free Energy=         0.051902
 Sum of electronic and zero-point Energies=          -79.741107
 Sum of electronic and thermal Energies=             -79.737193
 Sum of electronic and thermal Enthalpies=           -79.736249
 Sum of electronic and thermal Free Energies=        -79.766026
0 1
C
C   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
H   2   r8   1  a8   7  d8
r2  1.6826
r3  1.0928
a3  109.74
r4  1.0928
a4  109.74
d4  120.00
r5  1.0928
a5  109.74
d5  120.00
r6  1.0928
a6  109.74
tw  63.26
r7  1.0928
a7  109.74
d7  119.99
r8  1.0928
a8  109.74
d8  120.00

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** nosymm opt=modredundant
CH3CH3 barrier, E(full)
 Summary of Optimized Potential Surface Scan (add -79.0 to energies):
```

	1	2	3	4	5
Eigenvalues --	-0.852268 (2.70)	-0.852584 (2.50)	-0.853423 (1.98)	-0.854520 (1.29)	-0.855569 (0.63)
R1	1.544148	1.543269	1.540409	1.536779	1.533572
R2	1.092586	1.092665	1.092813	1.093072	1.093356
R3	1.092587	1.092230	1.092139	1.092399	1.092801
R4	1.092586	1.093070	1.093659	1.094069	1.094188
R5	1.092586	1.092665	1.092813	1.093072	1.093356
R6	1.092587	1.092230	1.092139	1.092399	1.092801
R7	1.092586	1.093070	1.093659	1.094069	1.094188
A1	111.806253	111.758520	111.649178	111.518526	111.407470
A2	111.805871	112.046617	112.131997	112.068873	111.876239
A3	111.805901	111.496508	111.229159	111.085747	111.073808
A4	107.038763	107.717215	108.234283	108.460842	108.374103
A5	107.038943	106.435767	106.097952	106.126374	106.445440
A6	107.038906	107.080920	107.201209	107.304672	107.419792
A7	111.806253	111.758520	111.649177	111.518522	111.407466
A8	111.805860	112.046619	112.132005	112.068874	111.876241
A9	111.805911	111.496505	111.229154	111.085751	111.073806
A10	107.038789	107.717212	108.234259	108.460847	108.374101
A11	107.038916	106.435769	106.097975	106.126368	106.445443
A12	107.038906	107.080921	107.201207	107.304671	107.419794
D1	-0.000009	10.000183	20.000306	30.000412	40.000308
D2	119.999953	131.007720	141.659087	151.813138	161.484589
D3	-120.000171	-108.987028	-98.308963	-88.165206	-78.485998
D4	119.999927	131.007722	141.659112	151.813133	161.484593
D5	-120.000110	-107.984742	-96.682107	-86.374142	-77.031126
D6	-0.000234	12.020510	23.349843	33.647515	42.998287
D7	-120.000197	-108.987027	-98.308937	-88.165213	-78.485997
D8	-0.000234	12.020510	23.349844	33.647512	42.998284
D9	119.999641	132.025762	143.381794	153.669169	163.027697

	6	7	8	9	10
Eigenvalues --	-0.856309 (0.17)	-0.856575 (0.00)	-0.856309 (0.17)	-0.855567 (0.63)	-0.854517 (1.29)
R1	1.531433	1.530681	1.531412	1.533534	1.536717
R2	1.093561	1.093681	1.093639	1.093497	1.093221
R3	1.093275	1.093706	1.094028	1.094122	1.093982

R4	1.094047	1.093690	1.093236	1.092755	1.092377
R5	1.093561	1.093681	1.093639	1.093497	1.093221
R6	1.093275	1.093706	1.094028	1.094122	1.093982
R7	1.094047	1.093690	1.093236	1.092755	1.092377
A1	111.338211	111.355649	111.424669	111.547763	111.644941
A2	111.624781	111.345250	111.127259	110.991706	111.028661
A3	111.176512	111.361326	111.589961	111.826185	112.013305
A4	108.033110	107.523392	106.958091	106.455977	106.146932
A5	106.955006	107.512501	108.015078	108.327345	108.398476
A6	107.497109	107.537608	107.509527	107.447485	107.332900
A7	111.338208	111.355645	111.424672	111.547763	111.644952
A8	111.624783	111.345248	111.127260	110.991693	111.028662
A9	111.176517	111.361323	111.589972	111.826176	112.013318
A10	108.033122	107.523391	106.958102	106.455973	106.146932
A11	106.954991	107.512507	108.015058	108.327362	108.398460
A12	107.497106	107.537613	107.509520	107.447495	107.332889
D1	50.000251	60.000347	70.000368	80.000106	90.000279
D2	170.822613	179.994025	-170.821384	-161.462896	-151.763633
D3	-69.149591	-59.990399	-50.834872	-41.488333	-31.783080
D4	170.822598	179.994031	-170.821400	-161.462883	-151.763641
D5	-68.355040	-60.012291	-51.643152	-42.925885	-33.527553
D6	51.672756	60.003285	68.343359	77.048679	86.452999
D7	-69.149608	-59.990396	-50.834888	-41.488317	-31.783084
D8	51.672753	60.003282	68.343360	77.048681	86.453003
D9	171.700550	-179.981142	-171.670128	-162.976755	-153.566444

	11	12	13	14	15
Eigenvalues --	-0.853420 (1.98)	-0.852582 (2.51)	-0.852268 (2.70)	-0.852583 (2.51)	-0.853422 (1.98)
R1	1.540314	1.543267	1.544452	1.543318	1.540365
R2	1.092941	1.092670	1.092556	1.092600	1.092818
R3	1.093556	1.093023	1.092515	1.092256	1.092266
R4	1.092170	1.092224	1.092539	1.093037	1.093550
R5	1.092941	1.092670	1.092556	1.092600	1.092818
R6	1.093556	1.093023	1.092515	1.092256	1.092266
R7	1.092169	1.092224	1.092539	1.093037	1.093550
A1	111.725507	111.757957	111.766122	111.743338	111.679394

A2	111.200553	111.499814	111.810451	112.056826
112.169238
A3	112.107349	112.042053	111.820366	111.487735
111.167237
A4	106.132485	106.456783	107.040433	107.694986
108.201317
A5	108.151903	107.658630	107.024061	106.467789
106.157335
A6	107.225764	107.121207	107.074902	107.086248
107.168341
A7	111.725503	111.757959	111.766112	111.743338
111.679392
A8	111.200544	111.499831	111.810463	112.056851
112.169253
A9	112.107335	112.042058	111.820349	111.487724
111.167217
A10	106.132474	106.456763	107.040410	107.694963
108.201309
A11	108.151932	107.658634	107.024093	106.467803
106.157350
A12	107.225774	107.121198	107.074910	107.086241
107.168341
D1	100.000227	110.000265	120.000334	130.000335
140.000309
D2	-141.615909	-130.984015	-120.022244	-109.024410
-98.335043
D3	-21.589281	-10.928034	0.036961	10.988593
21.637372
D4	-141.615888	-130.984002	-120.022215	-109.024398
-98.335042
D5	-23.232024	-11.968283	-0.044793	11.950856
23.329607
D6	96.794604	108.087699	120.014412	131.963859
143.302021
D7	-21.589257	-10.928024	0.036984	10.988604
21.637376
D8	96.794607	108.087696	120.014406	131.963859
143.302024
D9	-143.178765	-131.856323	-119.926389	-108.023138
-96.725561

	16	17	18	19
Eigenvalues --	-0.854521 (1.29)	-0.855570 (0.63)	-0.856310 (0.17)	-0.856575 (0.00)
R1	1.536752	1.533546	1.531410	1.530662
R2	1.093112	1.093402	1.093598	1.093664
R3	1.092516	1.092892	1.093330	1.093740
R4	1.093919	1.094055	1.093960	1.093687
R5	1.093112	1.093402	1.093598	1.093664
R6	1.092516	1.092892	1.093331	1.093741
R7	1.093919	1.094055	1.093960	1.093686
A1	111.577630	111.463295	111.371380	111.328778
A2	112.133656	111.953155	111.678903	111.373092
A3	110.964690	110.944481	111.096256	111.373554
A4	108.423435	108.342536	108.011031	107.518058
A5	106.176184	106.480607	106.969426	107.513786
A6	107.286887	107.410030	107.496347	107.527564
A7	111.577633	111.463293	111.371387	111.328785
A8	112.133678	111.953178	111.678903	111.373140
A9	110.964673	110.944455	111.096220	111.373495
A10	108.423432	108.342543	108.011038	107.518073
A11	106.176182	106.480604	106.969411	107.513774
A12	107.286882	107.410031	107.496340	107.527565
D1	150.000230	160.000329	170.000247	-179.999769
D2	-88.146321	-78.461885	-69.145089	-60.012148
D3	31.812980	41.518322	50.863561	60.017826
D4	-88.146336	-78.461910	-69.145132	-60.012204
D5	33.707113	43.075875	51.709531	59.975417
D6	153.666414	163.056083	171.718182	-179.994609
D7	31.812968	41.518300	50.863523	60.017776
D8	153.666417	163.056085	171.718186	-179.994603
D9	-86.374282	-76.963708	-68.273163	-59.964629

```
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6826
r3  1.0928
a3  109.74
r4  1.0928
a4  109.74
d4  120.00
r5  1.0928
a5  109.74
d5  120.00
r6  1.0928
a6  109.74
r7  1.0928
a7  109.74
d7  119.99
r8  1.0928
a8  109.74
d8  120.00
tw  0.

3 1 2 6 S 18 10.
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=0,-79.817850906 (0.05)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6775
r3  1.0929
a3  109.67
r4  1.0929
a4  109.67
d4  120.00
r5  1.0929
a5  109.67
d5  120.00
r6  1.0929
a6  109.67
r7  1.0929
a7  109.67
d7  120.00
r8  1.0929
a8  109.67
d8  120.00
tw  0.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
```

```
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=10,-79.817857087 (0.04)
0 1
C
C   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
H   2   r8   1  a8   7  d8
r2  1.6778
r3  1.0929
a3  109.67
r4  1.0929
a4  109.68
d4  120.01
r5  1.0929
a5  109.67
d5  120.00
r6  1.0929
a6  109.67
r7  1.0929
a7  109.68
d7  120.01
r8  1.0929
a8  109.67
d8  120.00
tw  10.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=20,-79.817873243 (0.03)
0 1
C
C   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
H   2   r8   1  a8   7  d8
r2  1.6788
r3  1.0929
a3  109.68
r4  1.0928
a4  109.69
d4  120.02
r5  1.0929
a5  109.68
d5  120.00
r6  1.0929
a6  109.68
r7  1.0928
a7  109.69
d7  120.02
r8  1.0929
a8  109.68
d8  120.00
tw  20.

$nbo print=0 $end
$DEL
  Lewis
```

```
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=30,-79.817892776 (0.02)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6798
r3  1.0928
a3  109.66
r4  1.0928
a4  109.66
d4  120.03
r5  1.0928
a5  109.66
d5  120.01
r6  1.0928
a6  109.66
r7  1.0928
a7  109.65
d7  120.03
r8  1.0928
a8  109.66
d8  120.02
tw  30.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=40,-79.817850906 (0.05)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6775
r3  1.0929
a3  109.67
r4  1.0929
a4  109.67
d4  120.00
r5  1.0929
a5  109.67
d5  120.00
r6  1.0929
a6  109.67
r7  1.0929
a7  109.67
d7  120.00
r8  1.0929
a8  109.67
d8  120.00
```

```
tw  40.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=50,-79.817924097 (0.00)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6826
r3  1.0928
a3  109.74
r4  1.0928
a4  109.74
d4  120.00
r5  1.0928
a5  109.74
d5  120.00
r6  1.0928
a6  109.74
r7  1.0928
a7  109.74
d7  119.99
r8  1.0928
a8  109.74
d8  120.00
tw  50.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=60,-79.817928455 (0.00)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6826
r3  1.0928
a3  109.74
r4  1.0928
a4  109.74
d4  120.00
r5  1.0928
a5  109.74
d5  120.00
r6  1.0928
a6  109.74
r7  1.0928
```

```
a7  109.74
d7  119.99
r8  1.0928
a8  109.74
d8  120.00
tw  60.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=70,-79.817924132 (0.00)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6826
r3  1.0928
a3  109.74
r4  1.0928
a4  109.74
d4  120.00
r5  1.0928
a5  109.74
d5  120.00
r6  1.0928
a6  109.74
r7  1.0928
a7  109.74
d7  119.99
r8  1.0928
a8  109.74
d8  120.00
tw  70.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=80,-79.817911711 (0.01)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6812
r3  1.0928
a3  109.70
r4  1.0928
a4  109.70
d4  119.98
r5  1.0928
```

```
a5  109.70
d5  119.99
r6  1.0928
a6  109.70
r7  1.0928
a7  109.70
d7  119.98
r8  1.0928
a8  109.70
d8  120.00
tw  80.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=90, -79.817892715 (0.02)
0 1
C
C    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
H    2    r8    1    a8    7    d8
r2  1.6798
r3  1.0928
a3  109.66
r4  1.0928
a4  109.66
d4  119.97
r5  1.0928
a5  109.66
d5  119.99
r6  1.0928
a6  109.66
r7  1.0928
a7  109.65
d7  119.97
r8  1.0928
a8  109.66
d8  119.99
tw  90.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=100,-79.817873261 (0.03)
0 1
C
C    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
H    2    r8    1    a8    7    d8
r2  1.6788
r3  1.0929
```

```
a3  109.70
r4  1.0929
a4  109.68
d4  119.98
r5  1.0928
a5  109.69
d5  120.00
r6  1.0929
a6  109.69
r7  1.0929
a7  109.68
d7  119.98
r8  1.0928
a8  109.69
d8  120.00
tw  100.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=110,-79.817857100 (0.04)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6778
r3  1.0929
a3  109.68
r4  1.0929
a4  109.67
d4  119.99
r5  1.0929
a5  109.68
d5  120.00
r6  1.0929
a6  109.68
r7  1.0929
a7  109.67
d7  119.99
r8  1.0929
a8  109.68
d8  120.00
tw  110.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=120,-79.817850906 (0.05)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
```

```
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6775
r3  1.0929
a3  109.67
r4  1.0929
a4  109.67
d4  120.00
r5  1.0929
a5  109.67
d5  120.00
r6  1.0929
a6  109.67
r7  1.0929
a7  109.67
d7  120.00
r8  1.0929
a8  109.67
d8  120.00
tw  120.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=130,-79.817857086 (0.04)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6778
r3  1.0929
a3  109.67
r4  1.0929
a4  109.68
d4  120.01
r5  1.0929
a5  109.67
d5  120.00
r6  1.0929
a6  109.67
r7  1.0929
a7  109.68
d7  120.01
r8  1.0929
a8  109.67
d8  120.00
tw  130.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=140,-79.817873244 (0.03)
0 1
```

```
C
C    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
H    2    r8    1    a8    7    d8
r2   1.6788
r3   1.0929
a3   109.68
r4   1.0928
a4   109.69
d4   120.02
r5   1.0929
a5   109.68
d5   120.00
r6   1.0929
a6   109.68
r7   1.0928
a7   109.69
d7   120.02
r8   1.0928
a8   109.68
d8   120.00
tw   140.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=150,-79.817892775 (0.02)
0 1
C
C    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
H    2    r8    1    a8    7    d8
r2   1.6798
r3   1.0928
a3   109.66
r4   1.0928
a4   109.66
d4   120.02
r5   1.0928
a5   109.66
d5   120.01
r6   1.0928
a6   109.66
r7   1.0928
a7   109.65
d7   120.03
r8   1.0928
a8   109.66
d8   120.02
tw   150.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
```

```
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=160,-79.817911752 (0.01)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6812
r3  1.0928
a3  109.70
r4  1.0928
a4  109.70
d4  120.02
r5  1.0928
a5  109.70
d5  120.01
r6  1.0928
a6  109.70
r7  1.0928
a7  109.69
d7  120.02
r8  1.0928
a8  109.70
d8  120.01
tw  160.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=170,-79.817924097 (0.002)
0 1
C
C   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
H   2   r8   1   a8   7   d8
r2  1.6826
r3  1.0928
a3  109.74
r4  1.0928
a4  109.74
d4  120.00
r5  1.0928
a5  109.74
d5  120.00
r6  1.0928
a6  109.74
r7  1.0928
a7  109.74
d7  119.99
r8  1.0928
a8  109.74
d8  120.00
tw 170.

$nbo print=0 $end
```

```
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3CH3 barrier, E(DEL), tau=180,-79.817928455 (0.00)
0 1
C
C    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
H    2    r8    1    a8    7    d8
r2   1.6826
r3   1.0928
a3   109.74
r4   1.0928
a4   109.74
d4   120.00
r5   1.0928
a5   109.74
d5   120.00
r6   1.0928
a6   109.74
r7   1.0928
a7   109.74
d7   119.99
r8   1.0928
a8   109.74
d8   120.00
tw   180.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=z-matrix freq
CH3NH2, E(FULL)=-95.8938909670 (0.00)
nu: 304,821,973,...
 Vibrational temperatures:      437.08   1180.77   1400.08   1518.14   1673.21
           (Kelvin)            1930.46   2100.26   2154.21   2182.47   2398.47
                               4261.82   4397.11   4448.64   5046.96   5158.75
 Zero-point correction=                            0.063793 (Hartree/Particle)
 Thermal correction to Energy=                     0.067231
 Thermal correction to Enthalpy=                   0.068175
 Thermal correction to Gibbs Free Energy=          0.040861
 Sum of electronic and zero-point Energies=            -95.830098
 Sum of electronic and thermal Energies=               -95.826660
 Sum of electronic and thermal Enthalpies=             -95.825716
 Sum of electronic and thermal Free Energies=          -95.853030
0 1
C
N    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
r2   1.4656
r3   1.0927
a3   109.18
```

```
r4  1.0928
a4  109.17
d4  116.82
r5  1.1003
a5  115.17
d5  121.58
r6  1.0141
a6  111.18
tw  61.90
r7  1.0141
a7  111.18
d7  119.37

$nbo file=ch3nh2 $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm freq
CH3NH2, E(DEL)=-95.846654215 (0.00)
nu: 36,898,969,...
 Vibrational temperatures:       51.71  1292.39  1394.50  1517.79  1627.43
         (Kelvin)              1928.36  2094.39  2265.24  2275.13  2521.01
                               4585.94  4612.08  4793.03  5158.17  5251.56
 Zero-point correction=                            0.065503 (Hartree/Particle)
 Thermal correction to Energy=                     0.069373
 Thermal correction to Enthalpy=                   0.070317
 Thermal correction to Gibbs Free Energy=          0.040963
 Sum of electronic and zero-point Energies=            -95.781151
 Sum of electronic and thermal Energies=               -95.777282
 Sum of electronic and thermal Enthalpies=             -95.776337
 Sum of electronic and thermal Free Energies=          -95.805691
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6042
r3  1.0849
a3  107.90
r4  1.0857
a4  105.73
d4  119.78
r5  1.0848
a5  107.92
d5  119.80
r6  1.0111
a6  107.13
tw  2.16
r7  1.0111
a7  107.14
d7  115.17

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g**  nosymm opt=modredundant
CH3NH2 rot. barrier
 Summary of Optimized Potential Surface Scan (add -95.0 to energies):
                                  1              2              3              4
5
```

```
     Eigenvalues --            -0.890808 (1.93)  -0.891004 (1.81)  -0.891594 (1.44)  -0.892394
(0.94)  -0.893166 (0.45)
          R1                   1.471384          1.472949          1.472153          1.470745
1.468483
          R2                   1.093994          1.095362          1.096928          1.098369
1.099367
          R3                   1.094804          1.094692          1.094726          1.094316
1.093885
          R4                   1.094226          1.092759          1.091888          1.091465
1.091762
          R5                   1.011117          1.012136          1.013169          1.014000
1.014499
          R6                   1.011128          1.011990          1.013031          1.013936
1.014471
          A1                 111.770082        112.802905        113.730522        114.415772
114.857730
          A2                 110.683928        110.341061        110.004530        109.641919
109.418698
          A3                 111.901829        111.073137        110.344165        109.741145
109.386027
          A4                 107.581067        107.341744        107.148686        107.148760
107.351859
          A5                 107.105543        107.642559        108.118827        108.415452
108.403118
          A6                 107.574278        107.408973        107.240830        107.209553
107.137481
          A7                 112.223747        111.824287        111.466379        111.154770
111.033789
          A8                 112.226026        111.541097        110.964480        110.558014
110.546470
          A9                 107.828645        106.991515        106.351471        106.074983
106.197257
          D1                  -0.000157         -9.999916        -20.000124        -30.000380
-40.000506
          D2                 121.616998        109.769330         98.334943         87.530401
77.599131
          D3                 119.896748        110.046890        100.185842         90.386599
80.785680
          D4                -118.486096       -130.183865       -141.479092       -152.082620
-161.614684
          D5                -120.127145       -130.953111       -141.689417       -152.107252
-162.132411
          D6                   1.490010        -11.183865        -23.354351        -34.576471
-44.532774
          D7                   0.000157          9.999916         20.000124         30.000380
40.000506
                                      6                 7                 8                 9
10
     Eigenvalues --            -0.893707 (0.12)  -0.893891 (0.00)  -0.893687 (0.13)  -0.893151
(0.46)  -0.892414 (0.93)
          R1                   1.466938          1.465428          1.465078          1.464883
1.465910
          R2                   1.100122          1.100448          1.100293          1.099784
1.098703
          R3                   1.093306          1.092687          1.092143          1.091694
1.091615
          R4                   1.092096          1.092816          1.093424          1.094239
1.094764
          R5                   1.014466          1.014152          1.013326          1.012434
1.011462
          R6                   1.014459          1.014124          1.013383          1.012601
1.011780
          A1                 115.086098        115.187005        115.104682        114.882380
114.423369
          A2                 109.241572        109.177960        109.181162        109.349236
109.663360
          A3                 109.195400        109.198352        109.329546        109.590565
109.902642
          A4                 107.626276        107.944509        108.184914        108.305443
108.235916
```

A5	108.238009	107.907335	107.614940	107.312040	107.205221
A6	107.163512	107.127799	107.130735	107.109761	107.134695
A7	111.056677	111.203613	111.494522	111.827766	112.179201
A8	110.773057	111.191224	111.726613	112.260882	112.671957
A9	106.656234	107.192131	107.865212	108.362961	108.737306
D1	-50.000469	-60.000414	-70.000411	-80.000456	-90.000259
D2	68.328456	59.369083	50.786500	42.048798	33.109549
D3	71.166356	61.603206	51.862407	41.992800	31.818620
D4	-170.504720	-179.027297	172.649319	164.042053	154.928428
D5	-171.930647	178.428927	168.767856	159.119011	149.341801
D6	-53.601722	-62.201576	-70.445232	-78.831735	-87.548391
D7	50.000469	60.000414	70.000411	80.000456	90.000259

	11	12	13	14	15
Eigenvalues --	-0.891651 (1.41)	-0.891058 (1.78)	-0.890809 (1.93)	-0.890991 (1.82)	-0.891554 (1.47)
R1	1.467316	1.469268	1.471137	1.472217	1.471927
R2	1.097395	1.095611	1.094225	1.093069	1.092387
R3	1.091880	1.092646	1.093969	1.095639	1.097300
R4	1.095178	1.095252	1.094923	1.094382	1.093820
R5	1.010818	1.010533	1.011132	1.011984	1.013000
R6	1.011152	1.010734	1.011091	1.011821	1.012749
A1	113.767152	112.896786	111.943240	110.978041	110.145428
A2	110.194075	110.845511	111.766455	112.664644	113.449929
A3	110.255494	110.562561	110.690924	110.674527	110.532932
A4	107.984083	107.613388	107.136963	106.812104	106.659918
A5	107.168283	107.330711	107.528999	107.775940	107.957117
A6	107.213787	107.355478	107.546353	107.713017	107.874768
A7	112.413868	112.477432	112.217803	111.905849	111.568312
A8	112.857756	112.759728	112.228022	111.632971	111.041247
A9	108.777589	108.556867	107.810113	107.097111	106.503481
D1	-100.000291	-110.000399	-120.000353	-130.000123	-140.000167
D2	23.486398	13.166224	1.589743	-9.976460	-21.357322
D3	21.428133	10.816797	0.193225	-10.277524	-20.528492
D4	144.914823	133.983419	121.783322	109.746139	98.114353
D5	139.581885	129.747518	120.048527	110.385334	100.785836
D6	-96.931425	-107.085859	-118.361376	-129.591003	-140.571319

```
          D7                   100.000291        110.000399        120.000353        130.000123
140.000167
                                      16                17                18                19
     Eigenvalues --           -0.892328 (0.98)  -0.893093 (0.50)  -0.893655 (0.15)  -0.893888
(0.00)
          R1                     1.470670          1.468758          1.467005          1.465628
          R2                     1.092068          1.092131          1.092334          1.092726
          R3                     1.098731          1.099778          1.100299          1.100466
          R4                     1.093350          1.093000          1.092860          1.092687
          R5                     1.013886          1.014403          1.014507          1.014184
          R6                     1.013659          1.014241          1.014417          1.014158
          A1                   109.472309        109.146024        109.020077        109.167405
          A2                   114.107708        114.603689        114.942778        115.176129
          A3                   110.303716        109.942527        109.586372        109.190574
          A4                   106.739914        107.007084        107.439268        107.853002
          A5                   107.999883        107.852374        107.573512        107.193403
          A6                   107.993519        108.053913        108.022671        107.968801
          A7                   111.260340        111.085889        111.081993        111.156425
          A8                   110.609077        110.543151        110.701854        111.111314
          A9                   106.177119        106.250643        106.607582        107.127364
          D1                  -150.000410       -160.000388       -170.000418        179.999643
          D2                   -32.244099        -42.304072        -51.761676        -60.796479
          D3                   -30.468216        -40.032653        -49.340826        -58.531913
          D4                    87.288095         77.663663         68.897917         60.671966
          D5                    91.295003         81.888304         72.506846         63.105533
          D6                  -150.948687       -160.415380       -169.254412       -177.690588
          D7                   150.000410        160.000388        170.000418       -179.999643
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.4656
r3  1.0927
a3  109.18
r4  1.0928
a4  109.17
d4  116.82
r5  1.1003
a5  115.17
d5  121.58
r6  1.0141
a6  111.18
r7  1.0141
a7  111.18
d7  119.37
tw  0.
3 2 1 6 S 18 10.
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=0), E(DEL)= -95.846651723 (0.002)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6043
r3  1.0846
a3  108.01
r4  1.0857
a4  105.77
```

```
d4  119.77
r5  1.0851
a5  107.78
d5  119.80
r6  1.0111
a6  107.16
r7  1.0110
a7  107.14
d7  115.16
tw  0.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=10), E(DEL)=-95.846644356 (0.01)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6042
r3  1.0843
a3  108.15
r4  1.0855
a4  106.04
d4  120.01
r5  1.0857
a5  107.44
d5  119.71
r6  1.0109
a6  107.28
r7  1.0108
a7  107.16
d7  115.34
tw  10.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=20), E(DEL)= -95.846636374 (0.01)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6048
r3  1.0842
a3  108.16
r4  1.0853
a4  106.41
d4  120.16
r5  1.0862
a5  107.15
```

```
d5  119.73
r6  1.0106
a6  107.40
r7  1.0105
a7  107.25
d7  115.54
tw  20.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=30), E(DEL)=-95.846632640 (0.01)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6050
r3  1.0842
a3  108.07
r4  1.0849
a4  106.85
d4  120.30
r5  1.0867
a5  106.90
d5  119.76
r6  1.0102
a6  107.51
r7  1.0101
a7  107.36
d7  115.75
tw  30.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=40), E(DEL)=-95.84663238 (0.01)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6051
r3  1.0843
a3  107.89
r4  1.0846
a4  107.27
d4  120.40
r5  1.0871
a5  106.74
d5  119.80
r6  1.0099
a6  107.57
```

```
r7  1.0099
a7  107.46
d7  115.89
tw  40.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=50), E(DEL)= -95.846632763 (0.01)
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6051
r3  1.0844
a3  107.63
r4  1.0844
a4  107.64
d4  120.45
r5  1.0872
a5  106.68
d5  119.85
r6  1.0098
a6  107.56
r7  1.0098
a7  107.54
d7  115.94
tw  50.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=60), E(DEL)=-95.846632611 (0.01)
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6052
r3  1.0847
a3  107.30
r4  1.0842
a4  107.92
d4  120.44
r5  1.0872
a5  106.72
d5  119.91
r6  1.0098
a6  107.50
r7  1.0099
a7  107.56
d7  115.89
```

```
tw  60.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=70), E(DEL)=-95.846632500 (0.01)
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6052
r3  1.0849
a3  106.92
r4  1.0841
a4  108.10
d4  120.38
r5  1.0869
a5  106.84
d5  119.98
r6  1.0101
a6  107.40
r7  1.0102
a7  107.51
d7  115.74
tw  70.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=80), E(DEL)=-95.846634570 (0.01)
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6050
r3  1.0852
a3  106.53
r4  1.0841
a4  108.19
d4  120.28
r5  1.0865
a5  107.04
d5  120.07
r6  1.0104
a6  107.29
r7  1.0105
a7  107.41
d7  115.55
tw  80.

$nbo print=0 $end
```

```
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=90), E(DEL)=-95.846640184 (0.01)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6048
r3  1.0854
a3  106.18
r4  1.0842
a4  108.20
d4  120.17
r5  1.0860
a5  107.29
d5  120.17
r6  1.0107
a6  107.19
r7  1.0108
a7  107.29
d7  115.37
tw  90.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=100), E(DEL)=-95.846640184 (0.01)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6048
r3  1.0854
a3  106.18
r4  1.0842
a4  108.20
d4  120.17
r5  1.0860
a5  107.29
d5  120.17
r6  1.0107
a6  107.19
r7  1.0108
a7  107.29
d7  115.37
tw  100.

$nbo print=0 $end
$DEL
  Lewis
$END
```

```
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=110), E(DEL)=-95.846648413 (0.00)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6045
r3  1.0855
a3  105.91
r4  1.0844
a4  108.14
d4  120.06
r5  1.0855
a5  107.96
d5  120.25
r6  1.0110
a6  107.13
r7  1.0111
a7  107.19
d7  115.21
tw  110.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=120), E(DEL)=-95.846653476 (0.00)
0 1
C
N   1   r2
H   1   r3   2   a3
H   1   r4   2   a4   3   d4
H   1   r5   2   a5   4   d5
H   2   r6   1   a6   3   tw
H   2   r7   1   a7   6   d7
r2  1.6043
r3  1.0856
a3  105.77
r4  1.0848
a4  107.98
d4  119.96
r5  1.0851
a5  107.80
d5  120.28
r6  1.0111
a6  107.12
r7  1.0111
a7  107.12
d7  115.14
tw  120.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
```

```
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=130), E(DEL)=-95.846651417 (0.00)
0 1
C
N    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
r2   1.6043
r3   1.0856
a3   105.82
r4   1.0852
a4   107.75
d4   119.88
r5   1.0847
a5   107.99
d5   120.25
r6   1.0111
a6   107.17
r7   1.0111
a7   107.11
d7   115.17
tw   130.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=150), E(DEL)=-95.846636303 (0.01)
0 1
C
N    1    r2
H    1    r3    2    a3
H    1    r4    2    a4    3    d4
H    1    r5    2    a5    4    d5
H    2    r6    1    a6    3    tw
H    2    r7    1    a7    6    d7
r2   1.6047
r3   1.0852
a3   106.38
r4   1.0863
a4   107.18
d4   119.78
r5   1.0842
a5   108.14
d5   120.04
r6   1.0106
a6   107.39
r7   1.0105
a7   107.24
d7   115.51
tw   150.

$nbo print=0 $end
$DEL
   Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=160), E(DEL)=-95.846632843 (0.01)
```

```
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6049
r3  1.0849
a3  106.78
r4  1.0868
a4  106.94
d4  119.74
r5  1.0841
a5  108.09
d5  119.92
r6  1.0103
a6  107.50
r7  1.0102
a7  107.35
d7  115.73
tw  160.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=170), E(DEL)=-95.846632652 (0.01)
0 1
C
N   1   r2
H   1   r3   2  a3
H   1   r4   2  a4   3  d4
H   1   r5   2  a5   4  d5
H   2   r6   1  a6   3  tw
H   2   r7   1  a7   6  d7
r2  1.6049
r3  1.0847
a3  107.19
r4  1.0872
a4  106.77
d4  119.72
r5  1.0842
a5  107.94
d5  119.83
r6  1.0100
a6  107.58
r7  1.099
a7  107.47
d7  115.91
tw  170.

$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm opt=z-matrix
CH3NH2 (tau=180), E(DEL)=-95.846633379 (0.01)
0 1
C
N   1   r2
```

```
H    1   r3   2   a3
H    1   r4   2   a4   3   d4
H    1   r5   2   a5   4   d5
H    2   r6   1   a6   3   tw
H    2   r7   1   a7   6   d7
r2   1.6047
r3   1.0844
a3   107.58
r4   1.0873
a4   106.68
d4   119.71
r5   1.0843
a5   107.73
d5   119.75
r6   1.0097
a6   107.61
r7   1.0097
a7   107.59
d7   116.08
tw   180.


$nbo print=0 $end
$DEL
  Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7read nosymm opt=z-matrix freq
HCONH2, E(full)=-169.954848506
nu:233,568,635,...
 Vibrational temperatures:     335.43   817.38   913.54   1492.61   1515.05
          (Kelvin)            1815.98  2038.15  2328.27   2577.26   4238.56
                              5148.90  5345.83
 Zero-point correction=                         0.045233 (Hartree/Particle)
 Thermal correction to Energy=                  0.048983
 Thermal correction to Enthalpy=                0.049927
 Thermal correction to Gibbs Free Energy=       0.020701
 Sum of electronic and zero-point Energies=        -169.909615
 Sum of electronic and thermal Energies=           -169.905866
 Sum of electronic and thermal Enthalpies=         -169.904922
 Sum of electronic and thermal Free Energies=      -169.934148
0 1
H
C    1   r2
O    2   r3   1   a3
N    2   r4   1   a4   3   d4
H    4   r5   2   a5   3   d5
H    4   r6   2   a6   3   d6
r2   1.1059
r3   1.2115
a3   122.69
r4   1.3610
a4   112.38
d4   180.00
r5   1.0093
a5   119.42
d5   0.00
r6   1.0067
a6   121.42
d6   180.00
$nbo file=hconh2 $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** pop=nbo7del nosymm freq
HCONH2, E(DEL)=-169.769538009
```

```
nu: 197,500,835,...
 Vibrational temperatures:     282.81    719.63   1200.96   1427.56   1672.33
         (Kelvin)             1862.03   2054.75   2545.64   2635.60   5228.67
                              5239.23   5281.13
 Zero-point correction=                           0.047740 (Hartree/Particle)
 Thermal correction to Energy=                     0.051510
 Thermal correction to Enthalpy=                   0.052454
 Thermal correction to Gibbs Free Energy=          0.022881
 Sum of electronic and zero-point Energies=            -169.721798
 Sum of electronic and thermal Energies=               -169.718028
 Sum of electronic and thermal Enthalpies=             -169.717084
 Sum of electronic and thermal Free Energies=          -169.746657
0 1
H
C    1   r2
O    2   r3    1   a3
N    2   r4    1   a4    3   d4
H    4   r5    2   a5    3   d5
H    4   r6    2   a6    3   d6
r2   1.0478
r3   1.3037
a3   117.59
r4   1.5411
a4   128.20
d4   179.82
r5   1.0131
a5   106.08
d5   56.12
r6   1.0131
a6   106.16
d6   303.08
$nbo print=0 $end
$DEL
 Lewis
$END
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=rot_barr
#b3lyp/6-311++g** nosymm pop=nbo7read opt=modredundant
HCONH2, E(full)=-169.954848506
 Summary of Optimized Potential Surface Scan (add -169.0 to energies):
                                   1              2              3              4
5
      Eigenvalues --        -0.954849 (0.00)  -0.954688 (0.10)  -0.954021 (0.52)  -0.952580
(1.42)  -0.950276 (2.87)
          R1             1.105900        1.106040        1.106197        1.106500
1.106946
          R2             1.211500        1.211373        1.210798        1.209402
1.208164
          R3             1.361000        1.362785        1.367284        1.373444
1.379757
          R4             1.009300        1.009728        1.010965        1.012046
1.013033
          R5             1.006700        1.007359        1.008922        1.010554
1.012133
          A1           122.690000      122.649436      122.490422      122.369331
122.130860
          A2           112.380000      112.385256      112.519924      112.556113
112.669768
          A3           124.930000      124.941054      124.884813      124.840177
124.806521
          A4           119.420000      118.847886      117.638714      116.737063
116.064576
          A5           121.420000      120.529627      118.792788      116.812490
114.925973
          A6           119.160000      118.346865      116.511102      114.333219
112.149333
          D1           180.000000     -171.757085     -163.656455     -155.469287
-147.090356
```

```
         D2          0.000000       -9.168882      -14.030585      -14.975499
-13.449826
         D3          0.000000        9.999944       20.000035       29.999896
39.999919
         D4        180.000000      172.588147      169.625905      170.493683
173.640449
                         6               7               8               9
10
    Eigenvalues --     -0.947171 (4.82)  -0.943417 (7.17)  -0.939236 (9.80)  -0.934900
(12.52)  -0.930735 (15.13)
         R1          1.107214        1.107922        1.108087        1.108673
1.109073
         R2          1.207001        1.205406        1.203846        1.202066
1.200156
         R3          1.386917        1.394380        1.403201        1.411856
1.420985
         R4          1.014063        1.014985        1.016149        1.017341
1.018596
         R5          1.013638        1.015001        1.016562        1.017957
1.019410
         A1        121.822284      121.516813      121.245516      120.984666
120.831305
         A2        112.939107      113.237124      113.710003      114.287128
114.936617
         A3        124.693460      124.580711      124.332968      124.051463
123.685324
         A4        115.483566      115.035854      114.323541      113.469388
112.341871
         A5        113.261434      111.692866      110.293645      109.135268
108.151445
         A6        110.105639      108.195738      106.495485      105.068955
103.993102
         D1       -138.367738     -129.262461     -119.594959     -109.376377
-98.439646
         D2        -10.096850       -5.433397        0.363257        7.409102
15.756387
         D3         49.999892       59.999949       69.999924       79.999925
89.999946
         D4        178.270780     -176.170987     -170.041860     -163.214596
-155.804021
                        11              12              13              14
15
    Eigenvalues --     -0.927102 (17.41)  -0.924386 (19.12)  -0.923009 (19.98)  -0.948861
(3.76)   -0.951390 (2.17)
         R1          1.109845        1.110187        1.110557        1.104925
1.105380
         R2          1.198088        1.196485        1.195526        1.208549
1.209314
         R3          1.429746        1.436280        1.439509        1.384760
1.377989
         R4          1.019984        1.020775        1.020187        1.013360
1.011768
         R5          1.020623        1.021369        1.020325        1.016016
1.014340
         A1        120.739184      120.688562      120.626715      122.403678
122.503250
         A2        115.585880      116.148056      116.471529      112.656334
112.551720
         A3        123.324611      123.017909      122.893466      124.932969
124.944971
         A4        110.934833      109.691033      109.052342      115.429402
116.666999
         A5        107.526080      107.424846      108.500318      111.624592
113.475380
         A6        103.403576      103.489385      105.016659      110.724868
112.812846
         D1        -86.764170      -74.363629      -61.042867      -49.052516
-39.913640
         D2         25.636826       37.474820       52.823699     -176.641794
-173.634263
```

	16	17	18	19

```
          D3                   99.999946        109.999913        119.999960        130.000032
139.999997
          D4                  -147.599058       -138.161638       -126.133473          2.410754
6.279374
                                   16                17                18                19
      Eigenvalues --           -0.953181 (1.05)  -0.954249 (0.38)  -0.954731 (0.07)  -0.954848
(0.00)
          R1                    1.105565          1.105835          1.106021          1.105965
          R2                    1.210302          1.210839          1.211562          1.211742
          R3                    1.371835          1.366665          1.362379          1.360805
          R4                    1.010004          1.008486          1.007103          1.006616
          R5                    1.012584          1.010993          1.009622          1.009141
          A1                  122.599110        122.637282        122.658345        122.683609
          A2                  112.547029        112.473229        112.409514        112.381861
          A3                  124.850497        124.881378        124.926642        124.934530
          A4                  118.071492        119.474162        120.746255        121.384993
          A5                  115.291711        117.247329        118.767243        119.475501
          A6                  114.985604        116.944192        118.569032        119.139360
          D1                  -30.654510        -21.016047        -10.836557          0.004907
          D2                 -172.048659       -172.238940       -174.854819       -179.854523
          D3                  150.000061        160.000065        170.000061       -179.999974
          D4                    8.605911          8.777172          5.981799          0.140596
0 1
H
C   1  r2
O   2  r3   1   a3
N   2  r4   1   a4   3  d4
H   4  r5   2   a5   3  d5
H   4  r6   2   a6   3  d6
r2  1.1059
r3  1.2115
a3  122.69
r4  1.3610
a4  112.38
d4  180.00
r5  1.0093
a5  119.42
d5  0.00
r6  1.0067
a6  121.42
d6  180.00
3 2 4 5 S 18 10.
$nbo file=hconh2 archive $end
--Link1--
--Link1—
```

STERIC REPULSIONS

```
%mem=2gb
%nprocshared=8
%chk=he_he
#b3lyp/6-311++g** pop=nbo7read
He...He (R=5), -5.82708671068 (dE=0.00)
0 1
He
He   1   5.
$nbo file=he_he_5 archive steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=he_he
#b3lyp/6-311++g** pop=nbo7read
He...He (R=4), -5.82707721566 (dE=0.007)
0 1
He
He   1   4.
$nbo file=he_he_4 archive steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=he_he
```

```
#b3lyp/6-311++g** pop=nbo7read
He...He (R=3), -5.82701220107 (dE=0.05)
0 1
He
He   1   3.
$nbo file=he_he_3 archive steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=he_he
#b3lyp/6-311++g** pop=nbo7read
He...He (R=2), -5.82522970796 (dE=1.17)
0 1
He
He   1   2.
$nbo file=he_he_2 archive steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=he_he
#b3lyp/6-311++g** pop=nbo7read
He...He (R=1), -5.68164563835 (dE=91.27)
0 1
He
He   1   1.
$nbo file=he_he_1 archive steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=chfchf_cis
#b3lyp/6-311++g** pop=nbo7read opt freq
cis-CHF=CHF (C2v), -277.142846492 (dE=0.00 kcal/mol)
nu: 236,510,771,...
 Vibrational temperatures:    340.26   733.63  1108.84  1115.38  1250.73
         (Kelvin)            1452.32  1617.68  1842.23  1987.87  2526.19
                             4626.36  4659.17
 Zero-point correction=                           0.036831 (Hartree/Particle)
 Thermal correction to Energy=                    0.040700
 Thermal correction to Enthalpy=                  0.041644
 Thermal correction to Gibbs Free Energy=         0.011166
 Sum of electronic and zero-point Energies=          -277.106015
 Sum of electronic and thermal Energies=             -277.102147
 Sum of electronic and thermal Enthalpies=           -277.101202
 Sum of electronic and thermal Free Energies=        -277.131681
0 1
C
C   1   1.3238
H   1   1.0810    2   122.96
F   1   1.3432    2   122.62  3   180.
H   2   1.0810    1   122.96  3     0.
F   2   1.3432    1   122.62  3   180.
$nbo file=chfchf_cis archive nrt plot steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=chfchf_trans
#b3lyp/6-311++g** pop=nbo7read opt freq
trans-CHF=CHF (C2h), -277.141563885 (dE=0.80 kcal/mol)
nu: 317,334,551,...
 Vibrational temperatures:    456.51   480.63   793.18  1185.63  1300.77
         (Kelvin)            1628.85  1653.17  1851.01  1874.46  2504.93
                             4635.61  4646.00
 Zero-point correction=                           0.036435 (Hartree/Particle)
 Thermal correction to Energy=                    0.040427
 Thermal correction to Enthalpy=                  0.041371
 Thermal correction to Gibbs Free Energy=         0.010939
 Sum of electronic and zero-point Energies=          -277.105129
 Sum of electronic and thermal Energies=             -277.101137
 Sum of electronic and thermal Enthalpies=           -277.100193
 Sum of electronic and thermal Free Energies=        -277.130625
0 1
```

```
C
C    1   1.3234
H    1   1.0813    2   125.70
F    1   1.3499    2   120.01   3   180.
H    2   1.0813    1   125.70   3   180.
F    2   1.3499    1   120.01   3    0.
$nbo file=chfchf_trans archive nrt plot steric $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=0)=-157.272643068 (dE=0.00)
Total steric exchange energy:   135.22 kcal/mol
dE(SXE)=2.01
dE(SXE;i,j)=2.06
0 1
                6        0.000000    1.590550   -0.521941
                6        0.000000    0.667983    0.663470
                6       -0.000000   -0.667983    0.663470
                1        0.000000    1.060210   -1.475268
                1       -0.878256    2.245715   -0.502836
                1        0.878256    2.245715   -0.502836
                1        0.000000    1.165182    1.631762
                1       -0.000000   -1.165182    1.631762
                6       -0.000000   -1.590550   -0.521941
                1       -0.000000   -1.060210   -1.475268
                1        0.878256   -2.245715   -0.502836
                1       -0.878256   -2.245715   -0.502836
$nbo file=cis_2_butene_0 archive steric nrt plot $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=10)=-157.272543650 (dE=0.06)
Total steric exchange energy:   135.13 kcal/mol
dE(SXE)=1.92
dE(SXE;i,j)=2.01
0 1
                6        1.589478   -0.522182    0.000621
                6        0.667862    0.664514   -0.004684
                6       -0.668169    0.664048    0.000502
                1        1.068902   -1.466558   -0.164703
                1        2.350729   -0.422014   -0.780286
                1        2.126825   -0.595161    0.953478
                1        1.164573    1.632781    0.005117
                1       -1.165879    1.631916    0.005330
                6       -1.589091   -0.522555   -0.000207
                1       -1.057295   -1.474767   -0.020574
                1       -2.228099   -0.516279    0.890149
                1       -2.260238   -0.492870   -0.865899
$nbo file=cis_2_butene_10 archive steric nrt plot $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=20)=-157.272268007 (dE=0.24)
Total steric exchange energy:   134.81 kcal/mol
dE(SXE)=1.60
dE(SXE;i,j)=1.87
0 1
                6        1.585613   -0.523088    0.001047
                6        0.667337    0.667895   -0.008226
                6       -0.668600    0.666167    0.000871
                1        1.093857   -1.440283   -0.327651
                1        2.440885   -0.354096   -0.660499
                1        1.993525   -0.698865    1.003585
                1        1.163762    1.635958    0.009250
                1       -1.168780    1.632661    0.009746
```

```
                6          -1.584069   -0.524527   -0.000485
                1          -1.046981   -1.473282   -0.039480
                1          -2.208401   -0.532613    0.900336
                1          -2.269550   -0.488162   -0.854525
$nbo file=cis_2_butene_20 archive steric nrt plot $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=30)=-157.271883143 (dE=0.48)
Total steric exchange energy:   134.31 kcal/mol
dE(SXE)=1.10
dE(SXE;i,j)=1.65
0 1
                6           1.579485   -0.524684    0.001142
                6           0.666776    0.673153   -0.009334
                6          -0.669044    0.669391    0.000872
                1           1.136176   -1.395288   -0.486859
                1           2.513951   -0.300051   -0.520365
                1           1.848378   -0.813352    1.024027
                1           1.162982    1.640758    0.012225
                1          -1.173127    1.633808    0.010987
                6          -1.576331   -0.527371   -0.000709
                1          -1.031286   -1.471305   -0.049761
                1          -2.192169   -0.546216    0.905921
                1          -2.270223   -0.491288   -0.847994
$nbo file=cis_2_butene_30 archive steric nrt plot $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=40)=-157.271489489 (dE=0.72)
Total steric exchange energy:   133.77 kcal/mol
dE(SXE)=0.56
dE(SXE;i,j)=1.32
0 1
                6           1.571893   -0.526597    0.000890
                6           0.665924    0.679087   -0.007938
                6          -0.669708    0.673593    0.000686
                1           1.199497   -1.332706   -0.636439
                1           2.568619   -0.262233   -0.360336
                1           1.694462   -0.931719    1.012000
                1           1.162707    1.646138    0.010767
                1          -1.178162    1.635501    0.010241
                6          -1.566859   -0.530810   -0.000814
                1          -1.011167   -1.468625   -0.050413
                1          -2.182764   -0.556492    0.905582
                1          -2.260693   -0.501505   -0.848344
$nbo file=cis_2_butene_40 archive steric nrt plot $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=50)=-157.271200474 (dE=0.91)
Total steric exchange energy:   133.38 kcal/mol
dE(SXE)=0.17
dE(SXE;i,j)=0.94
0 1
                6           1.565698   -0.527991    0.000352
                6           0.665181    0.684119   -0.004359
                6          -0.670213    0.676916    0.000082
                1           1.286529   -1.252591   -0.770293
                1           2.602853   -0.241236   -0.184857
                1           1.541353   -1.049099    0.963838
                1           1.162322    1.650678    0.007353
                1          -1.182891    1.636592    0.005691
                6          -1.558634   -0.533606   -0.000513
                1          -0.994296   -1.467204   -0.033383
```

```
              1           -2.187877   -0.554624    0.896841
              1           -2.240189   -0.519146   -0.858559
$nbo file=cis_2_butene_50 archive steric nrt plot $end
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** pop=nbo7read
cis_2_butene methyl rotation, E(tau=60)=-157.271092891 (dE=0.97)
Total steric exchange energy:   133.21 kcal/mol
dE(SXE)=0.00
dE(SXE;i,j)=0.56
0 1
              6            1.563242   -0.528484    0.000012
              6            0.664998    0.686084   -0.000089
              6           -0.670311    0.678434    0.000055
              1            1.398197   -1.159612   -0.879432
              1            2.614775   -0.235447   -0.002794
              1            1.402029   -1.156412    0.882483
              1            1.162543    1.652444   -0.000050
              1           -1.184448    1.637244    0.000183
              6           -1.555282   -0.534665   -0.000023
              1           -0.987068   -1.466519   -0.001014
              1           -2.210301   -0.540559    0.878703
              1           -2.211608   -0.539351   -0.877812
$nbo file=cis_2_butene_60 archive steric nrt plot $end
--Link1--
--Link1--
%mem=2gb
%nprocshared=8
%chk=cis_2_butene_rb
#b3lyp/6-311++G** opt=modredundant
cis_2_butene methyl rotation, E(tau)
0 1
C
C   1   r2
C   2   r3   1   a3
H   1   r4   2   a4   3   tau
H   1   r5   2   a5   4   tw5
H   1   r6   2   a6   4   tw6
H   2   r7   1   a7   3   d7
H   3   r8   2   a8   7   d8
C   3   r9   2   a9   7   d9
H   9   r10  3   a10  2   d10
H   9   r11  3   a11  10  d11
H   9   r12  3   a12  10  d12
r2  1.5
r3  1.3
a3  120.
r4  1.
a4  110.
tau 0.
r5  1.
a5  110.
tw5 120.
r6  1.
a6  110.
tw6 -120.
r7  1.
a7  120.
d7  180.
r8  1.
a8  120.
d8  0.
r9  1.5
a9  120.
d9  180.
r10 1.
a10 110.
d10 0.
r11 1.
```

```
a11 110.
d11 120.
r12 1.
a12 110.
d12 -120.
3 2 1 4  S  6  10.
$nbo file-propene steric nrt $end
--Link1--
--Link1--
```