Supplementary Information

Bettinger, H. F.; Sander, W.: **Dehydrophenylnitrenes: Quartet versus Doublet States**

1 4-Dehydrophenylnitrene (**3**)

1.1 $^4A_2$ State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.0358506806 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000023    RMS GRADIENT = 0.0000011
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.7861662512
 N           7.0  -0.0000000000   0.0000000000  -2.2844443589
 C           6.0  -0.0000000000   1.2319604655   1.1363708134
 C           6.0  -0.0000000000   1.2362102695  -0.2432042828
 C           6.0   0.0000000000   0.0000000000  -0.9643074285
 H           1.0  -0.0000000000   2.1548272864  -0.7962832210
 H           1.0  -0.0000000000   2.1494792499   1.6909726640
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.7861662512
 N           7.0  -0.0000000000   0.0000000000  -2.2844443589
 C           6.0  -0.0000000000  -1.2319604655   1.1363708134
 C           6.0  -0.0000000000   1.2319604655   1.1363708134
 C           6.0  -0.0000000000  -1.2362102695  -0.2432042828
 C           6.0  -0.0000000000   1.2362102695  -0.2432042828
 C           6.0   0.0000000000   0.0000000000  -0.9643074285
 H           1.0  -0.0000000000  -2.1548272864  -0.7962832210
 H           1.0  -0.0000000000   2.1548272864  -0.7962832210
 H           1.0  -0.0000000000  -2.1494792499   1.6909726640
 H           1.0  -0.0000000000   2.1494792499   1.6909726640

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

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

       FREQUENCY:        14.29       10.70        0.62        4.17       15.55
    IR INTENSITY:      0.01305     0.00338     0.00008     0.00126     0.00000

       FREQUENCY:        21.20      232.54      410.31      419.65      489.59
    IR INTENSITY:      0.01679     0.10213     0.00000     0.28752     0.20109

       FREQUENCY:       551.31      638.22      711.70      806.10      823.43
    IR INTENSITY:      0.01073     0.02444     0.06812     0.00000     1.71661

       FREQUENCY:       852.89      968.39      981.84      983.52     1057.87
    IR INTENSITY:      0.05291     0.00047     0.00000     0.05248     0.10293

       FREQUENCY:      1162.62     1202.08     1260.88     1360.88     1376.22
    IR INTENSITY:      0.08250     0.23515     0.05879     0.58727     0.05520

       FREQUENCY:      1467.86     1565.46     1601.95     1608.93     3330.56
    IR INTENSITY:      0.00843     0.00479     0.32442     0.06341     0.13279
```

```
       FREQUENCY:      3330.73     3347.85     3349.20
    IR INTENSITY:      0.00970     0.44645     0.00350

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    327.73327   578.37134   906.10461
 THE ROTATIONAL SYMMETRY NUMBER IS  2.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.50169     3.11753     1.98993
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
       0.081769 HARTREE/MOLECULE    17946.298524 CM**-1/MOLECULE
      51.311094 KCAL/MOL              214.685616 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                       1ST ORDER                       2ND ORDER
     1     E(MCSCF)=     -284.0358506808     E(MP2)=     -285.0343197556
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90511953

 Reference energy                   -283.94238843
 Nuclear energy                      241.98652229
 Kinetic energy                      284.51542671
 One electron energy                -862.22706399
 Two electron energy                 335.43828636
 Virial quotient                      -1.00100813
 Correlation energy                    -.85986692
 !CI(SD) STATE 1.4 ENERGY           -284.80225535
 Cluster corrected energies         -284.99197765 (Davidson)

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                       1ST ORDER                       2ND ORDER
     1     E(MCSCF)=     -283.9423884123     E(MP2)=     -285.0132055149
 ------------------------------------------------------------------------
```

1.2 $^2A_2$ State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.0257655142 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000091    RMS GRADIENT = 0.0000030
```

```
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.7822507611
 N           7.0   0.0000000000   0.0000000000  -2.3025411936
 C           6.0   0.0000000000   1.2269623241   1.1431658737
 C           6.0  -0.0000000000   1.2272145050  -0.2465027410
 C           6.0  -0.0000000000   0.0000000000  -0.9544289407
 H           1.0   0.0000000000   2.1467329070  -0.7983871680
 H           1.0  -0.0000000000   2.1455119102   1.6956469273
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.7822507611
 N           7.0   0.0000000000   0.0000000000  -2.3025411936
 C           6.0  -0.0000000000  -1.2269623241   1.1431658737
 C           6.0   0.0000000000   1.2269623241   1.1431658737
 C           6.0  -0.0000000000  -1.2272145050  -0.2465027410
 C           6.0  -0.0000000000   1.2272145050  -0.2465027410
 C           6.0  -0.0000000000   0.0000000000  -0.9544289407
 H           1.0  -0.0000000000  -2.1467329070  -0.7983871680
 H           1.0   0.0000000000   2.1467329070  -0.7983871680
 H           1.0  -0.0000000000  -2.1455119102   1.6956469273
 H           1.0  -0.0000000000   2.1455119102   1.6956469273

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:         4.99        2.13        0.31        3.20       16.07
    IR INTENSITY:      0.00921     0.00019     0.00000     0.00387     0.00000

       FREQUENCY:        19.17      238.29      409.83      416.59      468.67
    IR INTENSITY:      0.01885     0.10449     0.22331     0.00000     0.21740

       FREQUENCY:       547.38      642.82      678.50      819.05      829.47
    IR INTENSITY:      0.04732     0.01989     0.08149     1.63568     0.00000

       FREQUENCY:       861.36      958.74      967.46      979.12     1071.13
    IR INTENSITY:      0.00846     0.00003     0.32029     0.00000     0.18571

       FREQUENCY:      1099.55     1161.39     1220.49     1278.93     1386.69
    IR INTENSITY:      0.01018     0.53881     0.10882     0.30043     0.02660

       FREQUENCY:      1453.21     1568.04     1603.30     1638.15     3331.51
    IR INTENSITY:      0.01696     0.00752     0.31335     0.04449     0.10287

       FREQUENCY:      3332.14     3348.62     3349.84
    IR INTENSITY:      0.00005     0.38758     0.00680

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    324.40740   582.72326   907.13066
 THE ROTATIONAL SYMMETRY NUMBER IS  2.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.55810     3.09424     1.98768
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.081240 HARTREE/MOLECULE    17830.139894 CM**-1/MOLECULE
```

```
       50.978979 KCAL/MOL              213.296049 KJ/MOL

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -284.0257655143     E(MP2)=     -285.0258804624
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90566441

 Reference energy                    -283.94385509
 Nuclear energy                       241.97911277
 Kinetic energy                       284.52438284
 One electron energy                 -862.24003902
 Two electron energy                  335.45983138
 Virial quotient                       -1.00097254
 Correlation energy                     -.85723978
 !MRCI STATE 1.4 ENERGY              -284.80109486
 Cluster corrected energies          -284.98897834 (Davidson)

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -283.9438550755     E(MP2)=     -285.0065480529
 ------------------------------------------------------------------------
```

1.3 $^2B_2$ state

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -283.9997320251 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000033    RMS GRADIENT = 0.0000013
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.9189122074
 N           7.0  -0.0000000000   0.0000000000  -2.2643238858
 C           6.0   0.0000000000   1.2301111815   1.1112752095
 C           6.0   0.0000000000   1.2552329963  -0.2373964793
 C           6.0  -0.0000000000   0.0000000000  -0.9909429124
 H           1.0   0.0000000000   2.1714069329  -0.7962290385
 H           1.0  -0.0000000000   2.1610180346   1.6470908091
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.9189122074
 N           7.0  -0.0000000000   0.0000000000  -2.2643238858
 C           6.0  -0.0000000000  -1.2301111815   1.1112752095
 C           6.0   0.0000000000   1.2301111815   1.1112752095
```

```
 C           6.0  -0.0000000000  -1.2552329963  -0.2373964793
 C           6.0   0.0000000000   1.2552329963  -0.2373964793
 C           6.0  -0.0000000000   0.0000000000  -0.9909429124
 H           1.0  -0.0000000000  -2.1714069329  -0.7962290385
 H           1.0   0.0000000000   2.1714069329  -0.7962290385
 H           1.0  -0.0000000000  -2.1610180346   1.6470908091
 H           1.0  -0.0000000000   2.1610180346   1.6470908091


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -283.9997320252     E(MP2)=     -284.9794576452
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90465133

 Reference energy                    -283.90819803
 Nuclear energy                       239.88906684
 Kinetic energy                       284.46423307
 One electron energy                 -857.58716293
 Two electron energy                  332.93068000
 Virial quotient                       -1.00106580
 Correlation energy                     -.85921806
 !MRCI STATE 1.3 ENERGY              -284.76741609
 Cluster corrected energies          -284.95804049 (Davidson)
```

1.4 $^2A_1$ State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -283.9674518368 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000074    RMS GRADIENT = 0.0000024
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.7764231098
 N           7.0  -0.0000000000   0.0000000000  -2.3060493774
 C           6.0   0.0000000000   1.2298093593   1.1453246063
 C           6.0   0.0000000000   1.2217810945  -0.2437068731
 C           6.0  -0.0000000000   0.0000000000  -0.9531552815
 H           1.0  -0.0000000000   2.1346573438  -0.8058943210
 H           1.0   0.0000000000   2.1455501400   1.7022305678
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.7764231098
 N           7.0  -0.0000000000   0.0000000000  -2.3060493774
 C           6.0  -0.0000000000  -1.2298093593   1.1453246063
 C           6.0   0.0000000000   1.2298093593   1.1453246063
 C           6.0  -0.0000000000  -1.2217810945  -0.2437068731
 C           6.0   0.0000000000   1.2217810945  -0.2437068731
 C           6.0  -0.0000000000   0.0000000000  -0.9531552815
```

```
 H           1.0  -0.0000000000  -2.1346573438  -0.8058943210
 H           1.0  -0.0000000000   2.1346573438  -0.8058943210
 H           1.0  -0.0000000000  -2.1455501400   1.7022305678
 H           1.0   0.0000000000   2.1455501400   1.7022305678


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ---------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -283.9674518369     E(MP2)=     -284.9799789537
 ---------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90533010

 Reference energy                    -283.89285022
 Nuclear energy                       242.12261691
 Kinetic energy                       284.48946190
 One electron energy                 -862.44861975
 Two electron energy                  335.56982120
 Virial quotient                       -1.00093754
 Correlation energy                     -.86333142
 !MRCI STATE 1.1 ENERGY              -284.75618163
 Cluster corrected energies          -284.94616760 (Davidson)
```

1.5 $^2B_1$ State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -283.9291859284 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000087    RMS GRADIENT = 0.0000028
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.8152427498
 N           7.0   0.0000000000   0.0000000000  -2.3046460466
 C           6.0  -0.0000000000   1.2299034358   1.1700267469
 C           6.0   0.0000000000   1.2571314612  -0.2696277208
 C           6.0   0.0000000000   0.0000000000  -1.0334761961
 H           1.0  -0.0000000000   2.1841527136  -0.8035767737
 H           1.0  -0.0000000000   2.1482839945   1.7211806993
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   1.8152427498
 N           7.0   0.0000000000   0.0000000000  -2.3046460466
 C           6.0  -0.0000000000  -1.2299034358   1.1700267469
 C           6.0  -0.0000000000   1.2299034358   1.1700267469
 C           6.0  -0.0000000000  -1.2571314612  -0.2696277208
 C           6.0   0.0000000000   1.2571314612  -0.2696277208
 C           6.0   0.0000000000   0.0000000000  -1.0334761961
 H           1.0  -0.0000000000  -2.1841527136  -0.8035767737
 H           1.0  -0.0000000000   2.1841527136  -0.8035767737
 H           1.0  -0.0000000000  -2.1482839945   1.7211806993
```

```
 H           1.0  -0.0000000000   2.1482839945   1.7211806993


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -283.9291859284     E(MP2)=     -284.9354128150
 ------------------------------------------------------------------------
```

2 3-Dehydrophenylnitrene (**4**)

2.1 ^{4}A'' State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.0299086126 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000075    RMS GRADIENT = 0.0000032
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0042098147   1.0293092125   0.0000000000
 C           6.0  -1.2672644012   0.3735964814   0.0000000000
 C           6.0  -1.2587365780  -0.9949889304   0.0000000000
 C           6.0  -0.1222273632  -1.7896640861   0.0000000000
 C           6.0   1.1186770785  -1.1347324008   0.0000000000
 C           6.0   1.1833888175   0.2478299323   0.0000000000
 N           7.0   0.0708548284   2.3646185375   0.0000000000
 H           1.0  -2.1733994300   0.9461389271   0.0000000000
 H           1.0   2.1293690273   0.7524822901   0.0000000000
 H           1.0   2.0245608533  -1.7098344073   0.0000000000
 H           1.0  -0.1859400179  -2.8592275564   0.0000000000


MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:        36.41       10.20        4.72        1.32        8.38
    IR INTENSITY:      0.00293     0.01097     0.00227     0.00001     0.02581

       FREQUENCY:         9.60      223.65      412.07      419.83      517.37
    IR INTENSITY:      0.00951     0.03483     0.24869     0.06653     0.00006

       FREQUENCY:       544.98      645.20      668.62      788.82      860.64
    IR INTENSITY:      0.00027     0.00473     0.53034     1.18103     0.11894

       FREQUENCY:       872.05      900.12      997.47     1007.62     1076.14
    IR INTENSITY:      0.00158     0.17169     0.00005     0.25112     0.05994

       FREQUENCY:      1124.65     1176.54     1222.28     1302.74     1384.68
    IR INTENSITY:      0.20074     0.06066     0.65675     0.19943     0.01494

       FREQUENCY:      1466.21     1554.78     1616.29     1642.37     3320.65
    IR INTENSITY:      0.00285     0.02096     0.15922     0.13565     0.13617

       FREQUENCY:      3343.37     3345.09     3351.79
    IR INTENSITY:      0.18208     0.08432     0.27126

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

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    299.33808   613.34874   912.68682
 THE ROTATIONAL SYMMETRY NUMBER IS  1.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      6.02358     2.93974     1.97558
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
       0.081527 HARTREE/MOLECULE    17893.024186 CM**-1/MOLECULE
      51.158775 KCAL/MOL              214.048313 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -284.0299086129     E(MP2)=     -285.0298464175
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90545687

 Reference energy                   -283.94379954
 Nuclear energy                      241.86857219
 Kinetic energy                      284.52501035
 One electron energy                -861.99687459
 Two electron energy                 335.32629230
 Virial quotient                      -1.00097355
 Correlation energy                    -.85821057
 !CI(SD) STATE 1.2 ENERGY           -284.80201011
 Cluster corrected energies         -284.99058655 (Davidson)

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -283.9437995228     E(MP2)=     -285.0096222290
 ------------------------------------------------------------------------
```

2.2 ^{2}A'' State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.0373273274 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000095    RMS GRADIENT = 0.0000032
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0029950054   1.0381861805   0.0000000000
 C           6.0  -1.2748668214   0.3738283964   0.0000000000
```

```
 C           6.0  -1.2607917251  -0.9909995299   0.0000000000
 C           6.0  -0.1216788389  -1.7881903623   0.0000000000
 C           6.0   1.1212680726  -1.1330838134   0.0000000000
 C           6.0   1.1934736934   0.2458973836   0.0000000000
 N           7.0   0.0530468703   2.3510999676   0.0000000000
 H           1.0  -2.1768570451   0.9497953283   0.0000000000
 H           1.0   2.1406543096   0.7473458067   0.0000000000
 H           1.0   2.0251410508  -1.7109601540   0.0000000000
 H           1.0  -0.1873115716  -2.8573912034   0.0000000000


MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:        33.45       17.69       12.51        1.16        6.38
    IR INTENSITY:      0.00802     0.02550     0.01877     0.00003     0.00165

       FREQUENCY:         6.48      211.34      385.98      422.71      478.84
    IR INTENSITY:      0.00391     0.03000     0.00164     0.31912     0.03681

       FREQUENCY:       539.93      641.57      664.53      726.09      827.83
    IR INTENSITY:      0.00607     0.00780     0.64354     0.52568     0.64487

       FREQUENCY:       860.54      871.23      988.68      994.66     1069.05
    IR INTENSITY:      0.01862     0.17093     0.23639     0.00075     0.03608

       FREQUENCY:      1120.94     1190.42     1255.67     1333.14     1390.52
    IR INTENSITY:      0.21300     0.09423     0.27619     0.39147     0.05942

       FREQUENCY:      1438.59     1542.58     1595.38     1640.20     3323.43
    IR INTENSITY:      0.02398     0.02806     0.11191     0.12616     0.11565

       FREQUENCY:      3346.41     3353.80     3362.57
    IR INTENSITY:      0.19689     0.29106     0.01332

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    301.71463   610.22369   911.93832
 THE ROTATIONAL SYMMETRY NUMBER IS  1.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.97614     2.95480     1.97720
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.081050 HARTREE/MOLECULE    17788.322707 CM**-1/MOLECULE
       50.859418 KCAL/MOL              212.795804 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -284.0373273275     E(MP2)=     -285.0398683823
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)
```

```
Coefficient of reference function:   C(0) =  .90489747

 Reference energy                    -283.94257898
 Nuclear energy                       241.86495331
 Kinetic energy                       284.51831247
 One electron energy                 -861.96891412
 Two electron energy                  335.30052563
 Virial quotient                       -1.00100212
 Correlation energy                     -.86085618
 !MRCI STATE 1.2 ENERGY              -284.80343517
 Cluster corrected energies          -284.99377728 (Davidson)

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -283.9425789647     E(MP2)=     -285.0173024609
 ------------------------------------------------------------------------
```

2.3 ^{2}A' State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -283.9676005943 AFTER   3 ITERATIONS

          MAXIMUM GRADIENT =  0.0000037    RMS GRADIENT = 0.0000015
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0012686987   1.0235973062   0.0000000000
 C           6.0  -1.2608185395   0.3703900721   0.0000000000
 C           6.0  -1.2612799748  -1.0021397354   0.0000000000
 C           6.0  -0.1207525839  -1.7848157308   0.0000000000
 C           6.0   1.1195941166  -1.1397617575   0.0000000000
 C           6.0   1.1780723768   0.2465549454   0.0000000000
 N           7.0   0.0617911489   2.3711126757   0.0000000000
 H           1.0  -2.1582585612   0.9543851336   0.0000000000
 H           1.0   2.1190559745   0.7594526648   0.0000000000
 H           1.0   2.0231598073  -1.7179066745   0.0000000000
 H           1.0  -0.1842220659  -2.8553408994   0.0000000000


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -283.9676005945     E(MP2)=     -284.9827825781
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90517463

Reference energy                    -283.89070542
```

```
 Nuclear energy                        241.95187172
 Kinetic energy                        284.48779243
 One electron energy                  -862.10121720
 Two electron energy                   335.39475693
 Virial quotient                        -1.00093781
 Correlation energy                      -.86388313
 !MRCI STATE 1.1 ENERGY               -284.75458855
 Cluster corrected energies           -284.94498942 (Davidson)
```

3 2-Dehydrophenylnitrene (**5**)

3.1 ^{4}A'' State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.0348306263 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000060    RMS GRADIENT = 0.0000020
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0040471904   1.0995434936   0.0000000000
 C           6.0  -1.2143897051   0.3864239415   0.0000000000
 C           6.0  -1.3126783137  -0.9872296769   0.0000000000
 C           6.0  -0.1283685401  -1.7256588747   0.0000000000
 C           6.0   1.1188529725  -1.0654834140   0.0000000000
 C           6.0   1.2001441952   0.3078137225   0.0000000000
 N           7.0   0.0482318198   2.4197038208   0.0000000000
 H           1.0   2.1481107610   0.8090794852   0.0000000000
 H           1.0  -2.2686917443  -1.4726120895   0.0000000000
 H           1.0   2.0201131404  -1.6473687896   0.0000000000
 H           1.0  -0.1638717762  -2.7974836187   0.0000000000

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:        21.27        8.47        1.22       10.87       12.99
    IR INTENSITY:      0.03900     0.01414     0.00002     0.02242     0.01667

       FREQUENCY:        28.88      218.98      420.56      424.10      506.67
    IR INTENSITY:      0.00452     0.01458     0.18880     0.03898     0.01049

       FREQUENCY:       546.56      645.18      698.70      758.79      855.96
    IR INTENSITY:      0.01329     0.01952     0.08245     1.70506     0.02199

       FREQUENCY:       870.11      954.16      999.10     1005.38     1062.61
    IR INTENSITY:      0.03416     0.05768     0.00099     0.10738     0.04137

       FREQUENCY:      1154.40     1183.13     1267.78     1321.21     1351.09
    IR INTENSITY:      0.13255     0.11732     0.18020     0.03247     0.50094

       FREQUENCY:      1492.53     1528.60     1630.50     1647.94     3318.93
    IR INTENSITY:      0.00528     0.01641     0.09951     0.23451     0.02836

       FREQUENCY:      3331.11     3342.86     3350.00
    IR INTENSITY:      0.18745     0.42961     0.30994

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

```
 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    301.24803   622.00694   923.25497
 THE ROTATIONAL SYMMETRY NUMBER IS  1.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.98539     2.89882     1.95297
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.081757 HARTREE/MOLECULE    17943.481079 CM**-1/MOLECULE
       51.303038 KCAL/MOL              214.651912 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                       2ND ORDER
     1     E(MCSCF)=     -284.0348306264     E(MP2)=     -285.0332855395
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90515380

 Reference energy                   -283.94257990
 Nuclear energy                      241.16962664
 Kinetic energy                      284.51603781
 One electron energy                -860.58522086
 Two electron energy                 334.61363376
 Virial quotient                      -1.00100494
 Correlation energy                    -.85938056
 !CI(SD) STATE 1.2 ENERGY           -284.80196047
 Cluster corrected energies         -284.99149604 (Davidson)

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                       2ND ORDER
     1     E(MCSCF)=     -283.9425798839     E(MP2)=     -285.0121385779
 ------------------------------------------------------------------------
```

3.2 ^{2}A'' State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.0229441929 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000058    RMS GRADIENT = 0.0000019
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0064540388   1.0889172573   0.0000000000
 C           6.0  -1.2132876152   0.3779176700   0.0000000000
 C           6.0  -1.3143171994  -0.9790332571   0.0000000000
 C           6.0  -0.1150160792  -1.7287755266   0.0000000000
```

```
 C           6.0   1.1128244635  -1.0777026538   0.0000000000
 C           6.0   1.1870684191   0.3141593896   0.0000000000
 N           7.0   0.0593410878   2.4361532293   0.0000000000
 H           1.0   2.1359309291   0.8144608528   0.0000000000
 H           1.0  -2.2690015618  -1.4671829354   0.0000000000
 H           1.0   2.0189443932  -1.6517937176   0.0000000000
 H           1.0  -0.1574408760  -2.8003923085   0.0000000000


MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:        40.85       20.67       18.24        0.93        2.11
    IR INTENSITY:      0.02210     0.02410     0.03181     0.00004     0.00059

       FREQUENCY:        12.35      223.94      338.62      394.20      510.66
    IR INTENSITY:      0.00946     0.00329     0.16533     0.05424     0.00407

       FREQUENCY:       538.35      649.56      686.71      761.83      859.69
    IR INTENSITY:      0.03132     0.02241     0.06188     1.67233     0.04759

       FREQUENCY:       873.42      943.49      985.38     1001.34     1068.65
    IR INTENSITY:      0.00490     0.13020     0.34192     0.00348     0.05647

       FREQUENCY:      1146.25     1166.19     1192.10     1292.25     1346.95
    IR INTENSITY:      0.17491     0.48261     0.23043     0.10541     0.07871

       FREQUENCY:      1498.82     1541.57     1623.42     1672.91     3318.54
    IR INTENSITY:      0.01065     0.01331     0.16765     0.16321     0.01194

       FREQUENCY:      3330.28     3340.03     3348.84
    IR INTENSITY:      0.17048     0.40171     0.32998

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    299.11943   625.88625   925.00568
 THE ROTATIONAL SYMMETRY NUMBER IS  1.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      6.02799     2.88086     1.94927
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.081226 HARTREE/MOLECULE    17826.988101 CM**-1/MOLECULE
       50.969968 KCAL/MOL              213.258345 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ---------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -284.0229441930     E(MP2)=     -285.0217442855
 ---------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90563213
```

```
 Reference energy                   -283.94021910
 Nuclear energy                      241.07914056
 Kinetic energy                      284.52526190
 One electron energy                -860.43338616
 Two electron energy                 334.55721237
 Virial quotient                      -1.00095517
 Correlation energy                    -.85681413
 !MRCI STATE 1.2 ENERGY             -284.79703323
 Cluster corrected energies         -284.98489690 (Davidson)

SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -283.9402190772     E(MP2)=     -285.0021738129
 ------------------------------------------------------------------------
```

3.3 ^{2}A' State

(9,9)-CASSCF

```
FINAL MCSCF ENERGY IS     -283.9964220700 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000064    RMS GRADIENT = 0.0000030
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0020928469   1.0678339520   0.0000000000
 C           6.0  -1.3595431081   0.4700193261   0.0000000000
 C           6.0  -1.3064777804  -0.9812327187   0.0000000000
 C           6.0  -0.1484449772  -1.6897341345   0.0000000000
 C           6.0   1.1609715971  -1.0487233925   0.0000000000
 C           6.0   1.2476511507   0.2919348625   0.0000000000
 N           7.0   0.0485594572   2.3461643050   0.0000000000
 H           1.0   2.1860572528   0.8103747091   0.0000000000
 H           1.0  -2.2402059434  -1.5119240614   0.0000000000
 H           1.0   2.0392614160  -1.6639057838   0.0000000000
 H           1.0  -0.1784219112  -2.7640790653   0.0000000000


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -283.9964220702     E(MP2)=     -284.9786744040
 ------------------------------------------------------------------------
```

(3,3)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90448481

Reference energy                   -283.90585860
 Nuclear energy                     239.71619881
 Kinetic energy                     284.45388420
 One electron energy               -857.40474155
 Two electron energy                332.92243598
```

```
 Virial quotient                       -1.00109762
 Correlation energy                     -.86024816
 !MRCI STATE 1.1 ENERGY              -284.76610676
 Cluster corrected energies          -284.95733987 (Davidson)
```

4 Benzene (**6**), $^1A_{1g}$ State

(6,6)-CASSCF

```
FINAL MCSCF ENERGY IS     -230.8513201641 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000011    RMS GRADIENT = 0.0000005
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000313  -1.3920877312  -0.0000000000
 C           6.0   0.0000000293   1.3920877321  -0.0000000000
 C           6.0  -1.2055837850  -0.6960443237   0.0000000000
 C           6.0   1.2055838088  -0.6960443101  -0.0000000000
 C           6.0  -1.2055838043   0.6960443118   0.0000000000
 C           6.0   1.2055837894   0.6960443200   0.0000000000
 H           1.0   0.0000000016  -2.4654665048   0.0000000000
 H           1.0  -0.0000000005   2.4654665074   0.0000000000
 H           1.0  -2.1351565356  -1.2327335105  -0.0000000000
 H           1.0   2.1351564988  -1.2327335159  -0.0000000000
 H           1.0  -2.1351565030   1.2327335180  -0.0000000000
 H           1.0   2.1351565319   1.2327335070   0.0000000000


MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:        39.34       11.11        3.93        0.61        0.05
    IR INTENSITY:      0.00000     0.00000     0.00000     0.00000     0.00002

       FREQUENCY:        21.01      431.91      436.81      652.46      652.47
    IR INTENSITY:      0.00000     0.00000     0.00001     0.00000     0.00000

       FREQUENCY:       704.09      726.55      875.62      875.76     1000.76
    IR INTENSITY:      2.61037     0.00000     0.00000     0.00000     0.00000

       FREQUENCY:      1001.35     1030.98     1033.72     1098.66     1104.40
    IR INTENSITY:      0.00000     0.00000     0.00000     0.00000     0.05469

       FREQUENCY:      1104.57     1164.36     1264.39     1264.48     1325.79
    IR INTENSITY:      0.05407     0.00001     0.00000     0.00000     0.00004

       FREQUENCY:      1491.16     1615.64     1615.79     1722.21     1722.23
    IR INTENSITY:      0.00000     0.17170     0.16900     0.00000     0.00000

       FREQUENCY:      3301.00     3311.55     3311.63     3330.80     3330.89
    IR INTENSITY:      0.00001     0.00000     0.00000     1.45309     1.46851

       FREQUENCY:      3342.72
    IR INTENSITY:      0.00000

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

```
 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    314.76432   314.76438   629.52870
 THE ROTATIONAL SYMMETRY NUMBER IS  1.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.72838     5.72837     2.86419
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.104442 HARTREE/MOLECULE    22922.370954 CM**-1/MOLECULE
       65.538413 KCAL/MOL              274.212720 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -230.8513201642     E(MP2)=     -231.7376371988
 ------------------------------------------------------------------------
```

5 Phenyl radical (**7**), $^2A_1$ state

(7,7)-CASSCF

```
FINAL MCSCF ENERGY IS     -230.1995384641 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000057    RMS GRADIENT = 0.0000013
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000  -1.3211363869
 H           1.0   0.0000000000   0.0000000000  -2.3942727773
 C           6.0  -0.0000000000   0.0000000000   1.4052432769
 C           6.0  -0.0000000000   1.2110626999  -0.6310095624
 C           6.0   0.0000000000   1.2220627171   0.7648813831
 H           1.0   0.0000000000   2.1373395148  -1.1735682077
 H           1.0   0.0000000000   2.1432418048   1.3138573305
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000  -1.3211363869
 H           1.0   0.0000000000   0.0000000000  -2.3942727773
 C           6.0  -0.0000000000   0.0000000000   1.4052432769
 C           6.0  -0.0000000000  -1.2110626999  -0.6310095624
 C           6.0  -0.0000000000   1.2110626999  -0.6310095624
 C           6.0  -0.0000000000  -1.2220627171   0.7648813831
 C           6.0   0.0000000000   1.2220627171   0.7648813831
 H           1.0  -0.0000000000  -2.1373395148  -1.1735682077
 H           1.0   0.0000000000   2.1373395148  -1.1735682077
 H           1.0  -0.0000000000  -2.1432418048   1.3138573305
 H           1.0   0.0000000000   2.1432418048   1.3138573305

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:        36.26       20.52        7.03        0.64        1.89
    IR INTENSITY:      0.00000     0.00313     0.00206     0.00005     0.00001
```

```
       FREQUENCY:         6.84      424.86      441.98      641.59      648.95
    IR INTENSITY:      0.00350     0.00000     0.09109     0.00974     0.01452

       FREQUENCY:       693.45      739.08      846.04      913.05      991.76
    IR INTENSITY:      0.46528     1.78840     0.00000     0.01943     0.00000

       FREQUENCY:      1015.19     1037.82     1068.64     1095.12     1114.50
    IR INTENSITY:      0.00141     0.00329     0.04856     0.07130     0.04818

       FREQUENCY:      1181.73     1246.20     1312.78     1402.60     1559.61
    IR INTENSITY:      0.00045     0.00069     0.00065     0.01434     0.11808

       FREQUENCY:      1590.26     1679.92     1708.14     3306.79     3316.49
    IR INTENSITY:      0.18859     0.00065     0.02458     0.00309     0.19293

       FREQUENCY:      3330.38     3338.22     3343.63
    IR INTENSITY:      0.65772     0.86185     0.10531

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    286.45166   319.64395   606.09561
 THE ROTATIONAL SYMMETRY NUMBER IS  2.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      6.29456     5.64093     2.97492
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.091101 HARTREE/MOLECULE    19994.392429 CM**-1/MOLECULE
       57.166894 KCAL/MOL              239.186284 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -230.1995384642     E(MP2)=     -231.0560923555
 ------------------------------------------------------------------------
```

6 Phenylnitrene (**8**)

6.1 $^3A_2$ State

(8,8)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.6841630153 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000077    RMS GRADIENT = 0.0000027
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.8243728786
 N           7.0  -0.0000000000   0.0000000000  -2.3092748312
 C           6.0  -0.0000000000   1.2129601343   1.1251153728
 C           6.0  -0.0000000000   1.2254407937  -0.2561805481
```

```
C           6.0   0.0000000000   0.0000000000  -0.9765545046
H           1.0   0.0000000000   2.1480236980  -0.8025711649
H           1.0   0.0000000000   2.1397718746   1.6656342040
H           1.0   0.0000000000   0.0000000000   2.8967533917
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
C           6.0   0.0000000000   0.0000000000   1.8243728786
N           7.0  -0.0000000000   0.0000000000  -2.3092748312
C           6.0  -0.0000000000  -1.2129601343   1.1251153728
C           6.0  -0.0000000000   1.2129601343   1.1251153728
C           6.0  -0.0000000000  -1.2254407937  -0.2561805481
C           6.0  -0.0000000000   1.2254407937  -0.2561805481
C           6.0   0.0000000000   0.0000000000  -0.9765545046
H           1.0  -0.0000000000  -2.1480236980  -0.8025711649
H           1.0   0.0000000000   2.1480236980  -0.8025711649
H           1.0  -0.0000000000  -2.1397718746   1.6656342040
H           1.0   0.0000000000   2.1397718746   1.6656342040
H           1.0   0.0000000000   0.0000000000   2.8967533917

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

       FREQUENCY:         4.39        3.30        0.35        9.94       16.12
   IR INTENSITY:      0.00333     0.00086     0.00007     0.02161     0.03872

       FREQUENCY:        35.44      228.88      414.00      425.89      504.59
   IR INTENSITY:      0.00000     0.03110     0.24031     0.00000     0.06526

       FREQUENCY:       550.95      651.72      699.68      777.91      842.50
   IR INTENSITY:      0.00263     0.00229     0.69979     1.35177     0.00000

       FREQUENCY:       871.59      914.33      998.58     1009.89     1020.64
   IR INTENSITY:      0.01759     0.14901     0.00000     0.00109     0.14233

       FREQUENCY:      1069.60     1144.91     1171.49     1207.26     1311.46
   IR INTENSITY:      0.07238     0.10836     0.01892     0.38123     0.06606

       FREQUENCY:      1330.13     1417.06     1550.75     1579.70     1661.88
   IR INTENSITY:      0.41862     0.01160     0.00398     0.00034     0.25036

       FREQUENCY:      1663.17     3315.40     3323.22     3337.99     3344.83
   IR INTENSITY:      0.10727     0.00874     0.17615     0.42918     0.58756

       FREQUENCY:      3350.08
   IR INTENSITY:      0.20921

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    320.96934   618.64794   939.61727
 THE ROTATIONAL SYMMETRY NUMBER IS  2.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.61763     2.91456     1.91896
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.094977 HARTREE/MOLECULE    20845.047875 CM**-1/MOLECULE
       59.599042 KCAL/MOL              249.362393 KJ/MOL
```

```
SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ---------------------------------------------------------------------------
   STATE                        1ST ORDER                        2ND ORDER
     1     E(MCSCF)=     -284.6841630156     E(MP2)=     -285.7140391014
 ---------------------------------------------------------------------------
```

(2,2)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90452231

Reference energy                    -284.59883258
 Nuclear energy                       251.74694479
 Kinetic energy                       285.20120982
 One electron energy                 -882.59813489
 Two electron energy                  345.36949419
 Virial quotient                       -1.00098347
 Correlation energy                     -.88286333
 !CI(SD) STATE 1.4 ENERGY            -285.48169591
 Cluster corrected energies          -285.67791574 (Davidson)
```

6.2 $^1A_2$ State

(8,8)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.6568966472 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000073    RMS GRADIENT = 0.0000023
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.8259058554
 N           7.0  -0.0000000000   0.0000000000  -2.2809727830
 C           6.0   0.0000000000   1.2308321319   1.1138241913
 C           6.0  -0.0000000000   1.2565152248  -0.2477148884
 C           6.0   0.0000000000   0.0000000000  -1.0098113875
 H           1.0   0.0000000000   2.1769670164  -0.7957530280
 H           1.0  -0.0000000000   2.1526079331   1.6632634555
 H           1.0   0.0000000000   0.0000000000   2.8969315166
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.8259058554
 N           7.0  -0.0000000000   0.0000000000  -2.2809727830
 C           6.0  -0.0000000000  -1.2308321319   1.1138241913
 C           6.0   0.0000000000   1.2308321319   1.1138241913
 C           6.0  -0.0000000000  -1.2565152248  -0.2477148884
 C           6.0  -0.0000000000   1.2565152248  -0.2477148884
 C           6.0   0.0000000000   0.0000000000  -1.0098113875
 H           1.0  -0.0000000000  -2.1769670164  -0.7957530280
 H           1.0   0.0000000000   2.1769670164  -0.7957530280
 H           1.0  -0.0000000000  -2.1526079331   1.6632634555
 H           1.0  -0.0000000000   2.1526079331   1.6632634555
 H           1.0   0.0000000000   0.0000000000   2.8969315166

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.
```

```
      FREQUENCY:        17.30       12.73        5.94        0.48       11.18
   IR INTENSITY:      0.01638     0.00000     0.00815     0.00001     0.02784

      FREQUENCY:        24.55      156.59      378.54      426.88      446.47
   IR INTENSITY:      0.03956     0.07406     0.00000     0.36480     0.05756

      FREQUENCY:       539.06      620.55      633.05      731.15      765.21
   IR INTENSITY:      0.02900     0.00435     1.00931     0.50994     0.00000

      FREQUENCY:       816.40      823.34      981.37      983.38      999.56
   IR INTENSITY:      0.00187     0.61946     0.00000     0.04907     0.00906

      FREQUENCY:      1046.08     1111.12     1178.31     1245.81     1344.01
   IR INTENSITY:      0.00007     0.06372     0.07547     0.00330     0.16870

      FREQUENCY:      1388.31     1508.06     1534.10     1634.34     1635.69
   IR INTENSITY:      0.00800     0.00694     0.07502     0.04973     0.23746

      FREQUENCY:      1720.27     3318.26     3322.51     3348.38     3352.86
   IR INTENSITY:      0.01717     0.04748     0.30202     0.32562     0.40829

      FREQUENCY:      3358.13
   IR INTENSITY:      0.14804

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

 USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.
 P=  1.01325E+05 PASCAL.
 ALL FREQUENCIES ARE SCALED BY   1.00000
 THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)
    332.62027   612.56961   945.18988
 THE ROTATIONAL SYMMETRY NUMBER IS  2.0
 THE ROTATIONAL CONSTANTS ARE (IN GHZ)
      5.42086     2.94348     1.90765
 THE HARMONIC ZERO POINT ENERGY IS (SCALED BY   1.000)
        0.094197 HARTREE/MOLECULE    20673.877884 CM**-1/MOLECULE
       59.109642 KCAL/MOL              247.314744 KJ/MOL


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                      1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -284.6568966472     E(MP2)=     -285.6854041331
 ------------------------------------------------------------------------
```

(2,2)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90383759

Reference energy                   -284.56443863
 Nuclear energy                     250.85399998
 Kinetic energy                     285.12956975
 One electron energy               -880.66497165
 Two electron energy                344.35727286
 Virial quotient                     -1.00113678
 Correlation energy                   -.88926018
 !CI(SD) STATE 1.4 ENERGY          -285.45369881
```

```
 Cluster corrected energies          -285.65298780 (Davidson)
```

6.3 $^1A_1$ State

(8,8)-CASSCF

```
FINAL MCSCF ENERGY IS     -284.6191707181 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000035    RMS GRADIENT = 0.0000014
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.8207588578
 N           7.0  -0.0000000000   0.0000000000  -2.3248211270
 C           6.0  -0.0000000000   1.2121408695   1.1310550488
 C           6.0   0.0000000000   1.2152125692  -0.2552664646
 C           6.0  -0.0000000000   0.0000000000  -0.9687132510
 H           1.0   0.0000000000   2.1323478249  -0.8102650495
 H           1.0  -0.0000000000   2.1375827309   1.6735019897
 H           1.0   0.0000000000   0.0000000000   2.8940171334
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0   0.0000000000   0.0000000000   1.8207588578
 N           7.0  -0.0000000000   0.0000000000  -2.3248211270
 C           6.0  -0.0000000000  -1.2121408695   1.1310550488
 C           6.0  -0.0000000000   1.2121408695   1.1310550488
 C           6.0  -0.0000000000  -1.2152125692  -0.2552664646
 C           6.0   0.0000000000   1.2152125692  -0.2552664646
 C           6.0  -0.0000000000   0.0000000000  -0.9687132510
 H           1.0  -0.0000000000  -2.1323478249  -0.8102650495
 H           1.0   0.0000000000   2.1323478249  -0.8102650495
 H           1.0  -0.0000000000  -2.1375827309   1.6735019897
 H           1.0  -0.0000000000   2.1375827309   1.6735019897
 H           1.0   0.0000000000   0.0000000000   2.8940171334


SINGLE STATE MULTICONFIGURATIONAL PERTURBATION ENERGY

*** MC-QDPT2 ENERGIES ***
 ------------------------------------------------------------------------
   STATE                    1ST ORDER                      2ND ORDER
     1     E(MCSCF)=     -284.6191707181     E(MP2)=     -285.6611541618
 ------------------------------------------------------------------------
```

(2,2)-CASSCF

```
1PROGRAM * CI (Multireference internally contracted CI)

Coefficient of reference function:   C(0) =  .90447224

Reference energy                   -284.54671241
 Nuclear energy                      251.80429917
 Kinetic energy                      285.16408925
 One electron energy                -882.65313422
 Two electron energy                 345.41473412
 Virial quotient                      -1.00094686
 Correlation energy                    -.88738852
 !MRCI STATE 1.1 ENERGY             -285.43410093
 Cluster corrected energies         -285.63143909 (Davidson)
```

7 2-Iminyl-propa-1,3-diyl (**9**), $^3B_2$ State

(5,5)-CASSCF

```
FINAL MCSCF ENERGY IS     -170.3315441354 AFTER   2 ITERATIONS

          MAXIMUM GRADIENT =  0.0000060    RMS GRADIENT = 0.0000020
1     ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   0.1489270463
 N           7.0  -0.0000000000   0.0000000000   1.4164094754
 C           6.0   0.0000000000   1.2588214439  -0.6129852476
 H           1.0  -0.0000000000   2.1964280910  -0.0983958704
 H           1.0  -0.0000000000   1.2424659379  -1.6822351428
 COORDINATES OF ALL ATOMS ARE (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 C           6.0  -0.0000000000   0.0000000000   0.1489270463
 N           7.0  -0.0000000000   0.0000000000   1.4164094754
 C           6.0  -0.0000000000  -1.2588214439  -0.6129852476
 C           6.0   0.0000000000   1.2588214439  -0.6129852476
 H           1.0  -0.0000000000  -2.1964280910  -0.0983958704
 H           1.0  -0.0000000000   2.1964280910  -0.0983958704
 H           1.0  -0.0000000000  -1.2424659379  -1.6822351428
 H           1.0  -0.0000000000   1.2424659379  -1.6822351428
```