Supporting Material
for

Q-band EPR Spectroscopy of Photogenerated Quartet State Organic Nitreno-radicals

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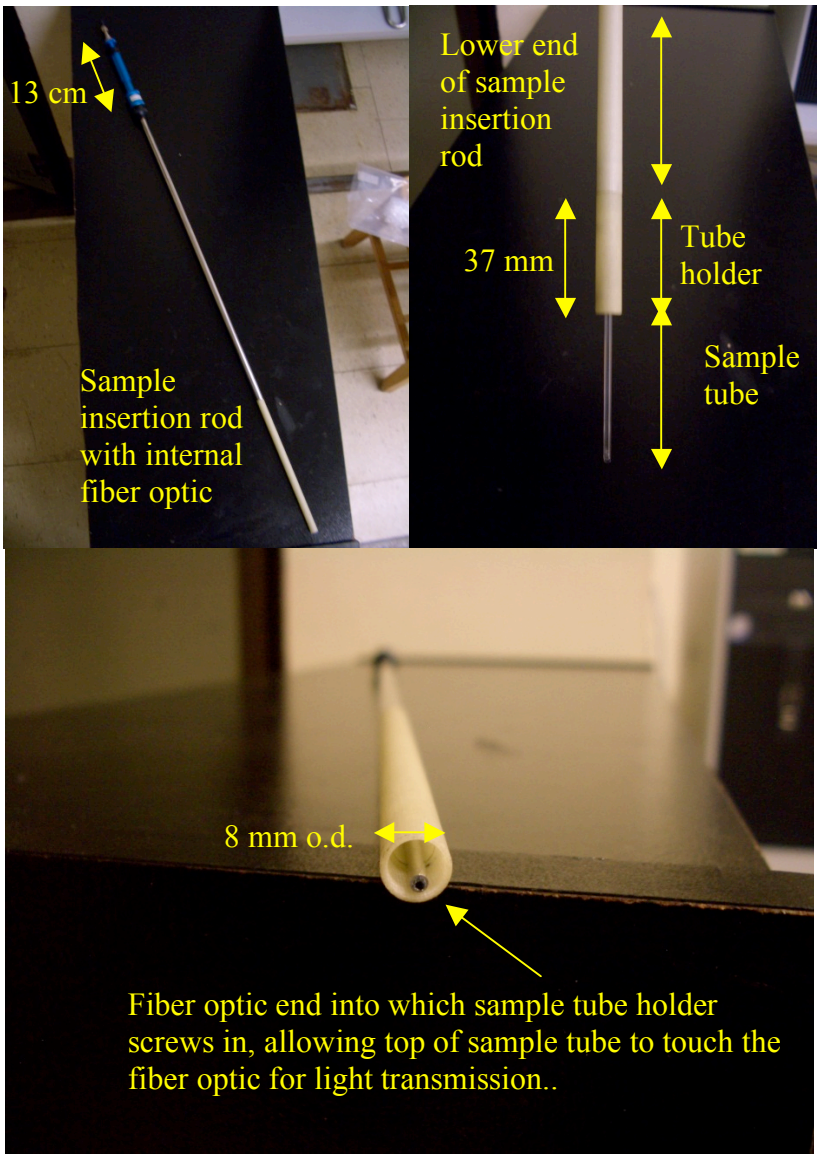
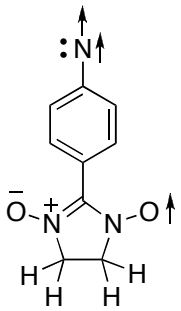
Figure 1S. Modified Bruker E600-1021RL Q-band sample insertion rod for in-resonator photolysis.



Assembly of sample insertion rod plus screw-in sample tube holder plus sample tube, ready to insert into resonator.

Archive summaries for computations in Table 2, coordinates and energies

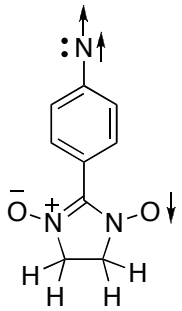
Planar quartet of NPhNN model system, UB3LYP/6-31G*



$^4A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C9H8N3O2(4)\LAHTI\13-Jan-2011\0\\#
 P UB3LYP/6-31G* GFINPUT IOP(6/7=3) TEST OPT\\Burak quartet p-nitrenoph
 enyl-NN\\0,4\O,0.,2.339552,-1.453353\O,0.,-2.339552,-1.453353\C,0.,0.7
 63607,-3.229762\C,0.,-0.763607,-3.229762\N,0.,1.11244,-1.789063\N,0.,-
 1.11244,-1.789063\C,0.,0.,0.460396\C,0.,0.,-0.978738\C,0.,0.,3.316108\
 C,0.,1.226514,1.192811\C,0.,-1.226514,1.192811\C,0.,1.232087,2.564584\
 C,0.,-1.232087,2.564584\N,0.,0.,4.627562\H,0.,2.159348,0.646424\H,0.,-
 2.159348,0.646424\H,0.,2.167421,3.114563\H,0.,-2.167421,3.114563\H,0.8
 88415,1.210526,-3.683141\H,0.888415,-1.210526,-3.683141\H,-0.888415,1.
 210526,-3.683141\H,-0.888415,-1.210526,-3.683141\\Version=SGI64-G03Rev
 B.03\State=4-A1\HF=-662.259356\S2=3.875509\S2-1=0.\S2A=3.754887\RMSD=4
 .740e-09\RMSF=4.955e-05\Dipole=0.,0.,-2.2463026\PG=C02V [C2(C1C1C1N1),
 SGV(C6H4N2O2),X(H4)]\\@
```

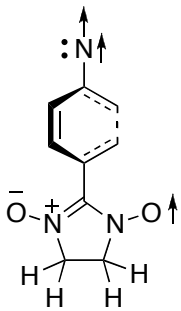
Planar doublet of NPhNN model system, UB3LYP/6-31G*



$^2A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C9H8N3O2(2)\LAHTI\25-Jan-2011\0\\#
 P UB3LYP/6-31G* GFINPUT IOP(6/7=3) TEST OPT GUESS=READ\\Burak doublet
 p-nitrenophenyl-NN\\0,2\O,0.,2.3367790394,-1.453743368\O,0.,-2.3367790
 394,-1.453743368\C,0.,0.76344395,-3.2343590241\C,0.,-0.76344395,-3.234
 3590241\N,0.,1.1092761668,-1.7912735284\N,0.,-1.1092761668,-1.79127352
 84\C,0.,0.,0.4700279722\C,0.,0.,-0.9968109925\C,0.,0.,3.3126722967\C,0
 .,1.22031053,1.1909458407\C,0.,-1.22031053,1.1909458407\C,0.,1.2256770
 023,2.5718333196\C,0.,-1.2256770023,2.5718333196\N,0.,0.,4.6417798737\
 H,0.,2.1534177718,0.6450492174\H,0.,-2.1534177718,0.6450492174\H,0.,2.
 1623285735,3.1195506489\H,0.,-2.1623285735,3.1195506489\H,0.8884484221
 ,1.2127837393,-3.6850782141\H,0.8884484221,-1.2127837393,-3.6850782141
 \H,-0.8884484221,1.2127837393,-3.6850782141\H,-0.8884484221,-1.2127837
 393,-3.6850782141\\Version=SGI64-G03RevB.03\State=2-A1\HF=-662.2508591
 \S2=1.820785\S2-1=0.\S2A=0.999409\RMSD=9.890e-09\RMSF=5.349e-05\Dipole
 =0.,0.,-2.0998888\PG=C02V [C2(C1C1C1N1),SGV(C6H4N2O2),X(H4)]\\@
```

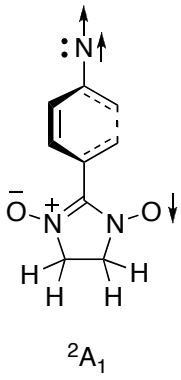
Twisted quartet of NPhNN model system, UB3LYP/6-31G*



$^4A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C9H8N3O2(4)\LAHTI\10-Jan-2011\0\\#
 P UB3LYP/6-31G* GFINPUT IOP(6/7=3) TEST OPT\\Burak quartet p-nitrenoph
 enyl-NN, bisected\\0,4\O,2.3240192116,0.,-1.3915748006\O,-2.3240192116
 ,0.,-1.3915748006\C,0.7676567334,0.,-3.2289908575\C,-0.7676567334,0.,-
 3.2289908575\N,1.1164168617,0.,-1.7802973025\N,-1.1164168617,0.,-1.780
 2973025\C,0.,0.,0.4595835707\C,0.,0.,-1.0131645233\C,0.,0.,3.283590396
 5\C,0.,1.2181151257,1.1668490684\C,0.,-1.2181151257,1.1668490684\C,0.,
 1.2321403511,2.5478363945\C,0.,-1.2321403511,2.5478363945\N,0.,0.,4.61
 00701672\H,0.,2.1542965362,0.616873832\H,0.,-2.1542965362,0.616873832\
 H,0.,2.1652605861,3.1009258678\H,0.,-2.1652605861,3.1009258678\H,1.214
 5853053,0.8885193393,-3.6812808633\H,-1.2145853053,0.8885193393,-3.681
 2808633\H,1.2145853053,-0.8885193393,-3.6812808633\H,-1.2145853053,-0.
 8885193393,-3.6812808633\\Version=SGI64-G03RevB.03\State=4-A1\HF=-662.
 2412453\S2=3.856827\S2-1=0.\S2A=3.754522\RMSD=3.620e-09\RMSF=1.720e-04
 \Dipole=0.,0.,-1.8812144\PG=C02V [C2(C1C1C1N1),SGV(C4H4),SGV'(C2N2O2),
 X(H4)]\\@
```

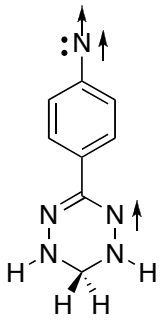
Twisted doublet of NPhNN model system, UB3LYP/6-31G*



$^2A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C9H8N3O2(2)\LAHTI\10-Jan-2011\0\\#
 P UB3LYP/6-31G* GFINPUT IOP(6/7=3) TEST OPT\\Burak doublet p-nitrenoph
 enyl-NN, bisected\\0,2\O,2.3239312813,0.,-1.3915275907\O,-2.3239312813
 ,0.,-1.3915275907\C,0.7678294714,0.,-3.228643754\C,-0.7678294714,0.,-3
 .228643754\N,1.1163174993,0.,-1.7806497352\N,-1.1163174993,0.,-1.78064
 97352\C,0.,0.,0.4597417183\C,0.,0.,-1.0135587009\C,0.,0.,3.2834002698\
 C,0.,1.2179568244,1.1667071397\C,0.,-1.2179568244,1.1667071397\C,0.,1.
 2319020332,2.5480066212\C,0.,-1.2319020332,2.5480066212\N,0.,0.,4.6108
 625813\H,0.,2.1542448518,0.616847823\H,0.,-2.1542448518,0.616847823\H,
 0.,2.1652573622,3.1008401663\H,0.,-2.1652573622,3.1008401663\H,1.21441
 33753,0.8883691497,-3.6820540271\H,-1.2144133753,0.8883691497,-3.68205
 40271\H,1.2144133753,-0.8883691497,-3.6820540271\H,-1.2144133753,-0.88
 83691497,-3.6820540271\\Version=SGI64-G03RevB.03\State=2-A1\HF=-662.24
 09868\S2=1.852982\S2-1=0.\S2A=1.119894\RMSD=4.922e-09\RMSF=4.644e-05\D
 ipole=0.,0.,-1.8795217\PG=C02V [C2(C1C1C1N1),SGV(C4H4),SGV'(C2N2O2),X(
 H4)]\\@
```

Planar quartet of NPhVerd model system, UB3LYP/6-31G*



$^4A_1$

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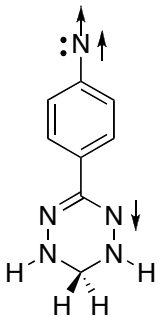
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C8H8N5(4)\LAHTI\19-Mar-2004\0\\# T
 EST OPT B3LYP DIRECT 6-31G(D)\\Nitrenophenyl verdazyl model (no phenyl
  groups\\0,4\N,0.,0.,-4.6410806496\C,0.,0.,-3.3266029553\C,0.,0.,-0.47
 42292532\C,-1.231645084,0.,-2.5745701019\C,1.231645084,0.,-2.574570101
 9\C,1.218530947,0.,-1.2002282964\C,-1.218530947,0.,-1.2002282964\H,-2.
 1668876572,0.,-3.1252686751\H,2.1668876572,0.,-3.1252686751\H,2.151787
 2624,0.,-0.6479709213\H,-2.1517872624,0.,-0.6479709213\C,0.,0.,0.98744
 78578\C,0.,0.,3.7999082652\N,1.1960979729,0.,1.6066736182\N,-1.1960979
 729,0.,1.6066736182\N,-1.1750222141,0.,2.9471824566\N,1.1750222141,0.,
 2.9471824566\H,0.,-0.8904488579,4.4519271183\H,2.0864177765,0.,3.37732
 0874\H,-2.0864177765,0.,3.377320874\H,0.,0.8904488579,4.4519271183\\Ve
 rsion=SGI64-G03RevB.03\State=4-A1\HF=-583.2401014\S2=3.845\S2-1=0.\S2A
 =3.753185\RMSD=8.580e-09\RMSF=5.317e-05\Dipole=0.,0.,3.4558084\PG=C02V
  [C2(C1C1C1C1N1),SGV(C4H6N4),SGV'(H2)]\\@
```

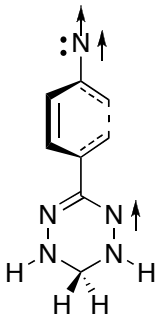
Planar doublet of NPhVerd model system, UB3LYP/6-31G*



$^2A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C8H8N5(2)\LAHTI\19-Mar-2004\0\\# T
 EST OPT B3LYP DIRECT 6-31G(D) GEOM=CHECK GUESS=(READ,MIX)\\Nitrenophen
 yl verdazyl model (no phenyl groups\\0,2\N,0.,0.,-4.653489236\C,0.,0.,
 -3.3278577391\C,0.,0.,-0.4828898252\C,-1.2272758034,0.,-2.5824468888\C
 ,1.2272758034,0.,-2.5824468888\C,1.2141783551,0.,-1.2023731718\C,-1.21
 41783551,0.,-1.2023731718\H,-2.1633609143,0.,-3.1318192125\H,2.1633609
 143,0.,-3.1318192125\H,2.1478844811,0.,-0.6507787959\H,-2.1478844811,0
 .,-0.6507787959\C,0.,0.,0.9988156803\C,0.,0.,3.8068789943\N,1.19102054
 46,0.,1.6118295199\N,-1.1910205446,0.,1.6118295199\N,-1.1746439117,0.,
 2.9529082212\N,1.1746439117,0.,2.9529082212\H,0.,-0.8903689962,4.45958
 67077\H,2.0867546559,0.,3.3811384719\H,-2.0867546559,0.,3.3811384719\H
 ,0.,0.8903689962,4.4595867077\\Version=SGI64-G03RevB.03\State=2-A1\HF=
 -583.2339946\S2=1.807373\S2-1=0.\S2A=0.950554\RMSD=8.516e-09\RMSF=1.35
 3e-04\Dipole=0.,0.,3.3056582\PG=C02V [C2(C1C1C1C1N1),SGV(C4H6N4),SGV'(
 H2)]\\@
```

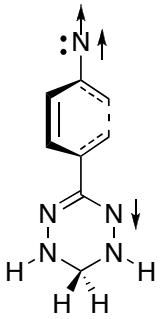
Twisted quartet of NPhVerd, UB3LYP/6-31G*



$^4A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C8H8N5(4)\LAHTI\11-Jan-2011\0\\#P
 UB3LYP/6-31G* GFINPUT IOP(6/7=3) TEST OPT\\Burak quartet p-nitrenophen
 yl-verdazyl, twisted\\0,4\N,0.,0.,-4.6502222132\C,0.,0.,-3.3235744819\
 C,0.,0.,-0.4874858937\C,-1.2306432931,0.,-2.5848597165\C,1.2306432931,
 0.,-2.5848597165\C,1.2134244577,0.,-1.2028460876\C,-1.2134244577,0.,-1
 .2028460876\H,-2.1643091657,0.,-3.1378087693\H,2.1643091657,0.,-3.1378
 087693\H,2.1495594258,0.,-0.6518056924\H,-2.1495594258,0.,-0.651805692
 4\C,0.,0.,1.0064045044\C,0.,0.,3.8092568092\N,0.,1.1947068722,1.607313
 9877\N,0.,-1.1947068722,1.6073139877\N,0.,-1.1762263516,2.9546377828\N
 ,0.,1.1762263516,2.9546377828\H,0.,2.0882332594,3.3823670658\H,0.,-2.0
 882332594,3.3823670658\H,-0.8902732859,0.,4.4617947596\H,0.8902732859,
 0.,4.4617947596\\Version=SGI64-G03RevB.03\State=4-A1\HF=-583.2241276\S
 2=3.829749\S2-1=0.\S2A=3.752704\RMSD=9.115e-09\RMSF=1.398e-04\Dipole=0
 .,0.,2.8079802\PG=C02V [C2(C1C1C1C1N1),SGV(C4H6),SGV'(H2N4)]\\@
```

Twisted doublet of NPhVerd, UB3LYP/6-31G*



$^2A_1$

```
1\1\GINC-GROND\FOpt\UB3LYP\6-31G(d)\C8H8N5(2)\LAHTI\19-Mar-2004\0\\# T
 EST OPT B3LYP DIRECT 6-31G(D) GEOM=CHECK GUESS=(READ,MIX)\\Nitrenophen
 yl verdazyl model (no phenyl groups\\0,2\N,0.,0.,-4.653489236\C,0.,0.,
 -3.3278577391\C,0.,0.,-0.4828898252\C,-1.2272758034,0.,-2.5824468888\C
 ,1.2272758034,0.,-2.5824468888\C,1.2141783551,0.,-1.2023731718\C,-1.21
 41783551,0.,-1.2023731718\H,-2.1633609143,0.,-3.1318192125\H,2.1633609
 143,0.,-3.1318192125\H,2.1478844811,0.,-0.6507787959\H,-2.1478844811,0
 .,-0.6507787959\C,0.,0.,0.9988156803\C,0.,0.,3.8068789943\N,1.19102054
 46,0.,1.6118295199\N,-1.1910205446,0.,1.6118295199\N,-1.1746439117,0.,
 2.9529082212\N,1.1746439117,0.,2.9529082212\H,0.,-0.8903689962,4.45958
 67077\H,2.0867546559,0.,3.3811384719\H,-2.0867546559,0.,3.3811384719\H
 ,0.,0.8903689962,4.4595867077\\Version=SGI64-G03RevB.03\State=2-A1\HF=
 -583.2339946\S2=1.807373\S2-1=0.\S2A=0.950554\RMSD=8.516e-09\RMSF=1.35
 3e-04\Dipole=0.,0.,3.3056582\PG=C02V [C2(C1C1C1C1N1),SGV(C4H6N4),SGV'(
 H2)]\\@
```

Planar quartet of NPhNN, UB97-D/DH* [Dunning-Hay double zeta basis set with polarization, as implemented in GAMESS version Oct2010R1 for Intel Apple Macintosh OS X]

```
 ***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 O           8.0   0.0000000000  -2.3485917501  -1.5017441478
 C           6.0   0.0000000000  -0.7630886626  -3.2830442262
 N           7.0   0.0000000000  -1.1173849870  -1.8334009047
 C           6.0   0.0000000000   0.0000000000   0.4242892293
 C           6.0   0.0000000000   0.0000000000  -1.0205640531
 C           6.0   0.0000000000   0.0000000000   3.2930007002
 C           6.0   0.0000000000  -1.2257640259   1.1623094725
 C           6.0   0.0000000000  -1.2339041435   2.5384822123
 N           7.0   0.0000000000   0.0000000000   4.6073650926
 H           1.0   0.0000000000  -2.1651733306   0.6242557064
 H           1.0   0.0000000000  -2.1741387111   3.0851677588
 H           1.0  -0.8924045553  -1.2094740267  -3.7341506779

NUCLEAR ENERGY    =      836.5532355617
          ELECTRONIC ENERGY =    -1498.5403354273
          TOTAL ENERGY      =     -662.0151998265

          SPIN SZ   =1.500
          S-SQUARED =3.810
```

Planar doublet of NPhNN, UB97-D/DH*

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***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 O           8.0   0.0000000000  -2.3467958609  -1.5012077940
 C           6.0   0.0000000000  -0.7630499268  -3.2851818213
 N           7.0   0.0000000000  -1.1156037329  -1.8342255539
 C           6.0   0.0000000000   0.0000000000   0.4293048129
 C           6.0   0.0000000000   0.0000000000  -1.0308627562
 C           6.0   0.0000000000   0.0000000000   3.2909626164
 C           6.0   0.0000000000  -1.2226460512   1.1611438323
 C           6.0   0.0000000000  -1.2306697911   2.5422474676
 N           7.0   0.0000000000   0.0000000000   4.6143613665
 H           1.0   0.0000000000  -2.1618444571   0.6226691833
 H           1.0   0.0000000000  -2.1713947541   3.0880835106
 H           1.0  -0.8924114429  -1.2109299718  -3.7348209222

NUCLEAR ENERGY    =      836.5895078449
          ELECTRONIC ENERGY =    -1498.5719601578
          TOTAL ENERGY      =     -662.0105167724

          SPIN SZ   =0.500
          S-SQUARED =1.787
```

Twisted quartet of NPhNN, UB97-D/DH*

```
***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 O           8.0  -2.3323465651   0.0000000000  -1.4171244473
 C           6.0  -0.7683034856   0.0000000000  -3.2672467667
 N           7.0  -1.1215205319   0.0000000000  -1.8087925984
 C           6.0   0.0000000000   0.0000000000   0.4271152072
 C           6.0   0.0000000000   0.0000000000  -1.0419831542
 C           6.0   0.0000000000   0.0000000000   3.2549699818
 C           6.0   0.0000000000  -1.2213347646   1.1324048753
 C           6.0   0.0000000000  -1.2374664714   2.5161758750
 N           7.0   0.0000000000   0.0000000000   4.5809838074
 H           1.0   0.0000000000  -2.1583729580   0.5785349077
 H           1.0   0.0000000000  -2.1739431519   3.0688977244
 H           1.0  -1.2133973799  -0.8926012240  -3.7188112456

NUCLEAR ENERGY    =      835.5852502906
          ELECTRONIC ENERGY =    -1497.5621074565
          TOTAL ENERGY      =     -662.0034558785

          SPIN SZ   =1.500
          S-SQUARED =3.803
```

Twisted doublet of NPhNN, UB97-D/DH*

```
***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 O           8.0  -2.3322647633   0.0000000000  -1.4169291037
 C           6.0  -0.7683317108   0.0000000000  -3.2673091001
 N           7.0  -1.1214478600   0.0000000000  -1.8088175514
 C           6.0   0.0000000000   0.0000000000   0.4272540822
 C           6.0   0.0000000000   0.0000000000  -1.0423755767
 C           6.0   0.0000000000   0.0000000000   3.2549439365
 C           6.0   0.0000000000  -1.2211773750   1.1323338247
 C           6.0   0.0000000000  -1.2373058519   2.5162651594
 N           7.0   0.0000000000   0.0000000000   4.5813395377
 H           1.0   0.0000000000  -2.1582290052   0.5785225734
 H           1.0   0.0000000000  -2.1738106875   3.0689144414
 H           1.0  -1.2134154163  -0.8926019463  -3.7188956168

NUCLEAR ENERGY    =      835.5896015606
          ELECTRONIC ENERGY =    -1497.5662452706
          TOTAL ENERGY      =     -662.0032417811

          SPIN SZ   =0.500
          S-SQUARED =1.801
```

Planar quartet of NPhVerd, UB97-D/DH*

```
***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0   0.0000000000   0.0000000000  -4.6346676766
 C           6.0   0.0000000000   0.0000000000  -3.3080765522
 C           6.0   0.0000000000   0.0000000000  -0.4294855738
 C           6.0   1.2421093381   0.0000000000  -2.5504985480
 C           6.0  -1.2273906601   0.0000000000  -1.1627621393
 H           1.0   2.1850300626   0.0000000000  -3.1030073088
 H           1.0  -2.1690004706   0.0000000000  -0.6105751848
 C           6.0   0.0000000000   0.0000000000   1.0403011857
 C           6.0   0.0000000000   0.0000000000   3.8741877442
 N           7.0  -1.2095872874   0.0000000000   1.6642376336
 N           7.0   1.1836239382   0.0000000000   3.0107066052
 H           1.0  -2.0970490266   0.0000000000   3.4505592183
 H           1.0   0.0000000000   0.8992018523   4.5256151602

NUCLEAR ENERGY    =      712.3126587057
          ELECTRONIC ENERGY =    -1295.2007835307
          TOTAL ENERGY      =     -582.9117445089

          SPIN SZ   =1.500
          S-SQUARED =3.804
```

Planar doublet of NPhVerd, UB97-D/DH*

```
***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0   0.0000000000   0.0000000000  -4.6424481630
 C           6.0   0.0000000000   0.0000000000  -3.3088159485
 C           6.0   0.0000000000   0.0000000000  -0.4346870814
 C           6.0   1.2394935734   0.0000000000  -2.5556156919
 C           6.0  -1.2247619490   0.0000000000  -1.1643245668
 H           1.0   2.1828675268   0.0000000000  -3.1073735392
 H           1.0  -2.1664293004   0.0000000000  -0.6122110297
 C           6.0   0.0000000000   0.0000000000   1.0474984137
 C           6.0   0.0000000000   0.0000000000   3.8785935178
 N           7.0  -1.2062990016   0.0000000000   1.6676429356
 N           7.0   1.1835083839   0.0000000000   3.0142468286
 H           1.0  -2.0972916164   0.0000000000   3.4529635509
 H           1.0   0.0000000000   0.8994820140   4.5300061433

NUCLEAR ENERGY    =      712.0996577245
          ELECTRONIC ENERGY =    -1294.9837614940
          TOTAL ENERGY      =     -582.9076822769

          SPIN SZ   =0.500
          S-SQUARED =1.786
```

Twisted quartet of NPhVerd, UB97-D/DH*

```
***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0   0.0000000000   0.0000000000  -4.6354446575
 C           6.0   0.0000000000   0.0000000000  -3.2991867841
 C           6.0   0.0000000000   0.0000000000  -0.4416737260
 C           6.0   1.2435084709   0.0000000000  -2.5548127803
 C           6.0  -1.2238673272   0.0000000000  -1.1596626244
 H           1.0   2.1841794586   0.0000000000  -3.1109741218
 H           1.0  -2.1646922791   0.0000000000  -0.6019389548
 C           6.0   0.0000000000   0.0000000000   1.0548539570
 C           6.0   0.0000000000   0.0000000000   3.8766625940
 N           7.0   0.0000000000  -1.2084138767   1.6567219698
 N           7.0   0.0000000000   1.1858349219   3.0112903042
 H           1.0   0.0000000000  -2.1002156958   3.4479321406
 H           1.0   0.8992795567   0.0000000000   4.5292433751

NUCLEAR ENERGY    =      710.4058474298
          ELECTRONIC ENERGY =    -1293.2794347321
          TOTAL ENERGY      =     -582.8966426408

          SPIN SZ   =1.500
          S-SQUARED =3.800
```

Twisted doublet of NPhVerd, UB97-D/DH*

```
***** EQUILIBRIUM GEOMETRY LOCATED *****
 COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)
   ATOM   CHARGE       X              Y              Z
 ------------------------------------------------------------
 N           7.0   0.0000000000   0.0000000000  -4.6366749670
 C           6.0   0.0000000000   0.0000000000  -3.2996524722
 C           6.0   0.0000000000   0.0000000000  -0.4421783321
 C           6.0   1.2431463406   0.0000000000  -2.5555397574
 C           6.0  -1.2235453011   0.0000000000  -1.1603228614
 H           1.0   2.1839031308   0.0000000000  -3.1115333433
 H           1.0  -2.1645161803   0.0000000000  -0.6028590477
 C           6.0   0.0000000000   0.0000000000   1.0555234724
 C           6.0   0.0000000000   0.0000000000   3.8775714660
 N           7.0   0.0000000000  -1.2083465934   1.6575139908
 N           7.0   0.0000000000   1.1856945009   3.0120950873
 H           1.0   0.0000000000  -2.1001343391   3.4485957688
 H           1.0   0.8992858835   0.0000000000   4.5301605794

NUCLEAR ENERGY    =      710.3376653531
          ELECTRONIC ENERGY =    -1293.2108284339
          TOTAL ENERGY      =     -582.8962078360

          SPIN SZ   =0.500
          S-SQUARED =1.796
```

Archive summaries for computations in Table 2, spin densities for optimized geometries.

Planar quartet of NPhNN, UB97-D/DH*, spin density of optimized geometry

```
ATOMIC SPIN POPULATION (ALPHA MINUS BETA)
       ATOM          MULL.POP.                      LOW.POP.
    1 O              0.364627                       0.350710
    2 O              0.364627                       0.350710
    3 C             -0.018963                      -0.010902
    4 C             -0.018963                      -0.010902
    5 N              0.279737                       0.277818
    6 N              0.279737                       0.277818
    7 C              0.261147                       0.208053
    8 C             -0.144287                      -0.099896
    9 C             -0.212365                      -0.104361
   10 C             -0.123468                      -0.082849
   11 C             -0.123468                      -0.082849
   12 C              0.287149                       0.246951
   13 C              0.287149                       0.246951
   14 N              1.467076                       1.392823
   15 H              0.005843                       0.004729
   16 H              0.005843                       0.004729
   17 H             -0.008259                      -0.008022
   18 H             -0.008259                      -0.008022
   19 H              0.013774                       0.011627
   20 H              0.013774                       0.011627
   21 H              0.013774                       0.011627
   22 H              0.013774                       0.011627
```

Twisted quartet of NPhNN, UB97-D/DH*, spin density of optimized geometry

```
ATOMIC SPIN POPULATION (ALPHA MINUS BETA)
       ATOM          MULL.POP.                      LOW.POP.
    1 O              0.327802                       0.314567
    2 O              0.327802                       0.314567
    3 C             -0.014563                      -0.008816
    4 C             -0.014563                      -0.008816
    5 N              0.237471                       0.237455
    6 N              0.237471                       0.237455
    7 C              0.302223                       0.234222
    8 C             -0.144535                      -0.092038
    9 C             -0.216951                      -0.103567
   10 C             -0.120283                      -0.080457
   11 C             -0.120283                      -0.080457
   12 C              0.306975                       0.264929
   13 C              0.306975                       0.264929
   14 N              1.550605                       1.477875
   15 H              0.005844                       0.004934
   16 H              0.005844                       0.004934
   17 H             -0.009626                      -0.008885
   18 H             -0.009626                      -0.008885
   19 H              0.010354                       0.009013
   20 H              0.010354                       0.009013
   21 H              0.010354                       0.009013
   22 H              0.010354                       0.009013
```

Planar quartet of NPhVerd, UB97-D/DH*, spin density of optimized geometry

ATOMIC SPIN POPULATION (ALPHA MINUS BETA)

	ATOM	MULL.POP.	LOW.POP.
1	N	1.566832	1.475636
2	C	-0.223559	-0.100461
3	C	0.303260	0.238854
4	C	0.307556	0.267332
5	C	0.307556	0.267332
6	C	-0.121963	-0.079444
7	C	-0.121963	-0.079444
8	H	-0.014050	-0.009202
9	H	-0.014050	-0.009202
10	H	0.008989	0.005021
11	H	0.008989	0.005021
12	C	-0.148572	-0.082172
13	C	-0.019252	-0.007092
14	N	0.385300	0.355000
15	N	0.385300	0.355000
16	N	0.204817	0.205838
17	N	0.204817	0.205838
18	H	-0.009350	-0.006233
19	H	-0.009350	-0.006233
20	H	-0.000654	-0.000694
21	H	-0.000654	-0.000694

Twisted quartet of NPhVerd, UB97-D/DH*, spin density of optimized geometry

ATOMIC SPIN POPULATION (ALPHA MINUS BETA)

	ATOM	MULL.POP.	LOW.POP.
1	N	1.486316	1.395264
2	C	-0.215580	-0.098060
3	C	0.284542	0.225994
4	C	0.284493	0.247544
5	C	0.284493	0.247544
6	C	-0.119722	-0.077944
7	C	-0.119722	-0.077944
8	H	-0.012827	-0.008435
9	H	-0.012827	-0.008435
10	H	0.008458	0.004979
11	H	0.008458	0.004979
12	C	-0.146328	-0.082431
13	C	-0.023866	-0.009149
14	N	0.421664	0.389323
15	N	0.421664	0.389323
16	N	0.230055	0.230704
17	N	0.230055	0.230704
18	H	-0.010754	-0.007285
19	H	-0.010754	-0.007285
20	H	0.006091	0.005305
21	H	0.006091	0.005305