

Supporting Information for

“On the Feasibility of Reactions through the Fullerene Wall: A Theoretical Study of $\text{NH}_x@\text{C}_{60}$ ”

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MINIMA

CH₄

UMP2/6-31G(d)//UB3LYP/6-31G(d)

1|1|UNPC-UNK|SP|RMP2-FC|6-31G(d)|C1H4|DRAL|17-Mar-2009|0|#P MP2/6-31G
 * SCF=TIGHT NAME=DRAL||CH4||0,1|C,0,0.,0.,0.|H,0,0.631077,-0.631077,0.
 631077|H,0,-0.631077,-0.631077,-0.631077|H,0,-0.631077,0.631077,0.6310
 77|H,0,0.631077,0.631077,-0.631077||Version=x86-Win32-G98RevA.6|HF=-40
 .19493|MP2=-40.3325287|RMSD=6.511e-010|PG=TD [O(C1),4C3(H1)]||@

UB3LYP/6-31G(d)

Zero-point correction=	0.045246 (Hartree/Particle)
Thermal correction to Energy=	0.048110
Thermal correction to Enthalpy=	0.049054
Thermal correction to Gibbs Free Energy=	0.027923
Sum of electronic and zero-point Energies=	-40.473143
Sum of electronic and thermal Energies=	-40.470279
Sum of electronic and thermal Enthalpies=	-40.469335
Sum of electronic and thermal Free Energies=	-40.490466

1|1|UNPC-UNK|Freq|RB3LYP|6-31G(d)|C1H4|DRAL|20-Dec-2007|0|#N GEOM=ALL
 CHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ||CH4_Td||0,1|C,-0.00000000008,-
 0.00000000008,-0.00000000008|H,0.6310768386,-0.6310768421,0.6310768386|H
 ,-0.6310768412,-0.6310768412,-0.6310768412|H,-0.6310768421,0.631076838
 6,0.6310768386|H,0.6310768386,0.6310768386,-0.6310768421||Version=x86-
 Win32-G98RevA.6|HF=-40.5183891|RMSD=8.846e-011|RMSF=7.245e-005|Dipole=
 0.,0.,0.|DipoleDeriv=0.0018121,-0.0001106,-0.000317,0.0003457,0.001096
 8,-0.0002495,0.0000433,-0.000176,0.0007055,-0.0005021,0.0734895,-0.073
 4876,0.0737509,-0.0005084,0.073453,-0.0736433,0.0735584,-0.0001628,-0.
 0006168,-0.0732194,-0.0732829,-0.0739413,-0.0000392,-0.0732774,-0.0739
 044,-0.0732621,0.0000616,-0.0001906,0.0733467,0.0734663,0.0736054,-0.0
 002151,-0.0735548,0.0736383,-0.0734591,-0.0002503,-0.0005027,-0.073506
 2,0.0736212,-0.0737608,-0.000334,0.0736288,0.0738661,0.0733388,-0.0003
 54|Polar=12.3762078,0.0020422,12.3792989,-0.0107564,0.0011635,12.36059
 86|PG=TD [O(C1),4C3(H1)]|NImag=0|



UMP2/6-31G(d)//UB3LYP/6-31G(d)

1|1|UNPC-UNK|SP|RMP2-FC|6-31G(d)|C1H5(1+)|DRAL|17-Mar-2009|0|#P MP2/6-31G* SCF=TIGHT NAME=DRAL||CH5+||1,1|C,0,0.,0.103909,0.|H,0,-0.778465,-0.764898,0.|H,0,-0.274448,0.58038,0.945335|H,0,0.214827,-1.049903,0.|H,0,-0.274448,0.58038,-0.945335|H,0,1.112533,0.030585,0.||Version=x86-Win32-G98RevA.6|State=1-A'|HF=-40.3842667|MP2=-40.5313584|RMSD=4.804e-009|PG=CS [SG(C1H3),X(H2)]||@

UB3LYP/6-31G(d)

Zero-point correction=	0.050504 (Hartree/Particle)
Thermal correction to Energy=	0.054238
Thermal correction to Enthalpy=	0.055183
Thermal correction to Gibbs Free Energy=	0.029640
Sum of electronic and zero-point Energies=	-40.672981
Sum of electronic and thermal Energies=	-40.669246
Sum of electronic and thermal Enthalpies=	-40.668302
Sum of electronic and thermal Free Energies=	-40.693845

1|1|UNPC-UNK|Freq|RB3LYP/6-31G(d)|C1H5(1+)|DRAL|12-Dec-2006|0|#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ||CH5+||1,1|C,0.0333395956,-0.0984154841,0.|H,0.4918873497,0.9742298119,0.|H,0.4461541905,-0.4616375348,0.945335357|H,-0.5403338362,0.9254657248,0.|H,0.4461541905,-0.4616375348,-0.945335357|H,-1.0438994684,-0.3859275624,0.||Version=x86-Win32-G98RevA.6|State=1-A'|HF=-40.7234847|RMSD=1.146e-009|RMSF=6.708e-005|Dipole=-0.2027712,0.6101999,0.|DipoleDeriv=-0.4717031,-0.2617974,0.,-0.2396258,-0.1621577,0.,0.,0.,-0.2123384,0.2578118,0.0302814,0.,0.1252748,0.2791902,0.,0.,0.,0.3367389,0.22221,0.0419079,0.0307608,0.0343252,0.1846329,-0.066317,0.0417453,-0.0735749,0.2089145,0.4450295,0.04712,0.,0.0389647,0.3050986,0.,0.,0.,0.1663375,0.22221,0.0419079,-0.0307608,0.0343252,0.1846329,0.066317,-0.0417453,0.0735749,0.2089145,0.3244424,0.1005802,0.0000001,0.006736,0.2086031,0.,0.0000001,0.,0.2914332|Polar=12.6774847,0.0598911,12.9517437,0.,-0.0000006,10.3630101|PG=CS [SG(C1H3),X(H2)]|NImag=0|



UMP2/6-31G(d)//UB3LYP/6-31G(d)

1|1|UNPC-UNK|SP|RMP2-FC|6-31G(d)|H2|DRAL|17-Mar-2009|0|#P MP2/6-31G* SCF=TIGHT NAME=DRAL||H2||0,1|H,0,0.,0.,0.371359|H,0,0.,0.,-0.371359||V

ersion=x86-Win32-G98RevA.6|State=1-SGG|HF=-1.1267114|MP2=-1.1441222|RM
SD=3.920e-012|PG=D*H [C*(H1.H1)]||@

UB3LYP/6-31G(d)

Zero-point correction=	0.010147 (Hartree/Particle)
Thermal correction to Energy=	0.012508
Thermal correction to Enthalpy=	0.013452
Thermal correction to Gibbs Free Energy=	-0.001340
Sum of electronic and zero-point Energies=	-1.165335
Sum of electronic and thermal Energies=	-1.162975
Sum of electronic and thermal Enthalpies=	-1.162031
Sum of electronic and thermal Free Energies=	-1.176822

1|1|UNPC-UNK|Freq|RB3LYP|6-31G(d)|H2|DRAL|17-Mar-2009|0|#P GEOM=ALLCH
ECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ||H2||0,1|H,-0.1827882421,-0.0566
571435,0.3182547137|H,0.1827882421,0.0566571435,-0.3182547137||Version
=x86-Win32-G98RevA.6|State=1-SGG|HF=-1.1754824|RMSD=2.603e-014|RMSF=2.
883e-005|Dipole=0.,0.,0.|DipoleDeriv=0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,
0.,0.,0.,0.,0.,0.|Polar=1.5449072,0.4788603,0.1484278,-2.6898558,-0
.8337492,4.6833389|PG=D*H [C*(H1.H1)]|NImag=0|

H₃⁺

UMP2/6-31G(d)//UB3LYP/6-31G(d)

1|1|UNPC-UNK|SP|RMP2-FC|6-31G(d)|H3(1+)|DRAL|17-Mar-2009|0|#P MP2/6-3
1G* SCF=TIGHT NAME=DRAL||H3+||1,1|H,0,-0.337668,-0.368247,0.|H,0,-0.15
022,0.476422,0.|H,0,0.487888,-0.108175,0.||Version=x86-Win32-G98RevA.6
|State=1-A'|HF=-1.2738724|MP2=-1.2962355|RMSD=1.337e-011|PG=CS [SG(H3)
]||@

UB3LYP/6-31G(d)

Zero-point correction=	0.020661 (Hartree/Particle)
Thermal correction to Energy=	0.023493
Thermal correction to Enthalpy=	0.024438
Thermal correction to Gibbs Free Energy=	0.006064
Sum of electronic and zero-point Energies=	-1.307697
Sum of electronic and thermal Energies=	-1.304864
Sum of electronic and thermal Enthalpies=	-1.303920
Sum of electronic and thermal Free Energies=	-1.322293

1|1|UNPC-UNK|Freq|RB3LYP|6-31G(d)|H3(1+)|DRAL|17-Mar-2009|0|#P GEOM=A
LLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ||H3+||1,1|H,-0.2239730349,-0
.4454893591,0.0316401262|H,0.2580831672,0.1210654224,-0.4102196264|H,-
0.0341101323,0.3244239367,0.3785795002||Version=x86-Win32-G98RevA.6|St
ate=1-A'|HF=-1.3283575|RMSD=2.356e-012|RMSF=3.243e-005|Dipole=-0.00005

57,0.0000603,0.0001709|DipoleDeriv=0.3595027,0.1443507,0.0842212,0.1442901,0.5562242,-0.0814533,0.0841635,-0.0815767,0.0841987,0.3991181,-0.0211249,-0.1543175,-0.0210877,0.1124344,-0.167428,-0.154282,-0.1673522,0.4879557,0.2413791,-0.1232259,0.0700963,-0.1232025,0.3313414,0.2488813,0.0701186,0.2489289,0.4278456|Polar=1.1635651,1.1834449,3.1400142,-1.241934,0.5818307,3.0835093|PG=CS [SG(H3)]|NImag=0|

N• (doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

Zero-point correction= 0.000000 (Hartree/Particle)
 Thermal correction to Energy= 0.001416
 Thermal correction to Enthalpy= 0.002360
 Thermal correction to Gibbs Free Energy= -0.014381
 Sum of electronic and zero-point Energies= -54.328615
 Sum of electronic and thermal Energies= -54.327199
 Sum of electronic and thermal Enthalpies= -54.326255
 Sum of electronic and thermal Free Energies= -54.342996

1\1\FAU-CCC-CCDN082\Freq\ROMP2-FC\6-31G(d)\N1(2)\DRAL\14-Jul-2010\0\#
 P ROMP2/6-31G* SCF=TIGHT Freq NAME=DRAL\N doublet\0,2\N,0.,0.,0.\Version=EM64L-G09RevA.02\HF=-54.2422865\MP2=-54.3286153\RMSD=8.881e-10\RMSF=0.000e+00\Thermal=0.0014163\PG=OH [O(N1)]\NImag=0\ -0.00000001,0.,-0.00000001,0.,0.,-0.00000001\0.,0.,0.\@

UB3LYP/6-31G(d)

Zero-point correction= 0.000000 (Hartree/Particle)
 Thermal correction to Energy= 0.001416
 Thermal correction to Enthalpy= 0.002360
 Thermal correction to Gibbs Free Energy= -0.014381
 Sum of electronic and zero-point Energies= -54.478999
 Sum of electronic and thermal Energies= -54.477582
 Sum of electronic and thermal Enthalpies= -54.476638
 Sum of electronic and thermal Free Energies= -54.493380

1\1\GINC-N01\Freq\UB3LYP/6-31G(d)\N1(2)\DRAL\10-Nov-2008\0\#P Geom=Al
 lCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq\N_doublet\0,2\N,0.,0.,0.\Version=AM64L-G03RevD.02\HF=-54.4789986\S2=0.75142\S2-1=0.\S2A=0.75\RMSD=1.155e-10\RMSF=0.000e+00\Thermal=0.0014163\Dipole=0.,0.,0.\DipoleDeriv=0.,0.,0.,0.,0.,0.,0.,0.,0.\Polar=2.438258,0.,3.6669446,0.,0.,3.9799702\PG=OH [O(N1)]\NImag=0\0.,0.,0.,0.,0.,0.\0.,0.,0.\@

N^{•••} (quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

Zero-point correction= 0.000000 (Hartree/Particle)
 Thermal correction to Energy= 0.001416
 Thermal correction to Enthalpy= 0.002360
 Thermal correction to Gibbs Free Energy= -0.015036
 Sum of electronic and zero-point Energies= -54.456551
 Sum of electronic and thermal Energies= -54.455135
 Sum of electronic and thermal Enthalpies= -54.454191
 Sum of electronic and thermal Free Energies= -54.471587

1\1\FAU-CCC-CCDN082\Freq\ROMP2-FC\6-31G(d)\N1(4)\DRAL\14-Jul-2010\0\#
 P ROMP2/6-31G* Freq SCF=TIGHT NAME=DRAL\N quartet\0,4\N,0.,0.,0.\Ve
 rsion=EM64L-G09RevA.02\State=4-A1G\HF=-54.3823113\MP2=-54.4565511\RMSD
 =2.257e-10\RMSF=0.000e+00\Thermal=0.0014163\PG=OH [O(N1)]\NImag=0\0.,
 0.,0.,0.,0.,0.\0.,0.,0.\@

UB3LYP/6-31G(d)

Zero-point correction= 0.000000 (Hartree/Particle)
 Thermal correction to Energy= 0.001416
 Thermal correction to Enthalpy= 0.002360
 Thermal correction to Gibbs Free Energy= -0.015036
 Sum of electronic and zero-point Energies= -54.584489
 Sum of electronic and thermal Energies= -54.583073
 Sum of electronic and thermal Enthalpies= -54.582129
 Sum of electronic and thermal Free Energies= -54.599525

1\1\GINC-N01\Freq\UB3LYP\6-31G(d)\N1(4)\DRAL\10-Nov-2008\0\#P Geom=Al
 lCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq\N_quartet\0
 ,4\N,0.,0.,0.\Version=AM64L-G03RevD.02\State=4-A1G\HF=-54.5844894\S2=
 3.752381\S2-1=0.\S2A=3.75\RMSD=3.151e-11\RMSF=0.000e+00\Thermal=0.0014
 163\Dipole=0.,0.,0.\DipoleDeriv=0.,0.,0.,0.,0.,0.,0.,0.,0.\Polar=3.929
 7388,0.,3.9297388,0.,0.,3.9297388\PG=OH [O(N1)]\NImag=0\0.,0.,0.,0
 .,0.\0.,0.,0.\@

NH^{••+} (quartet)***ROMP2/6-31G(d)//UB3LYP/6-31G(d)***

Zero-point correction= 0.005849 (Hartree/Particle)
 Thermal correction to Energy= 0.008209
 Thermal correction to Enthalpy= 0.009153
 Thermal correction to Gibbs Free Energy= -0.011796
 Sum of electronic and zero-point Energies= -54.577995
 Sum of electronic and thermal Energies= -54.575635
 Sum of electronic and thermal Enthalpies= -54.574691
 Sum of electronic and thermal Free Energies= -54.595641

1\1\FAU-CCC-ALTIX1\Freq\ROMP2-FC\6-31G(d)\H1N1(1+,4)\DRAL\26-Jul-2010\0\#P ROMP2/6-31G* FREQ=NORAMAN NAME=DRAL\NH(+)\1,4\N,0.,0.,-0.1389988866\H,0.,0.,0.9729922064\Version=IA64-Linux-G03RevB.03\State=4-SG\HF=-54.5157531\MP2=-54.5838441\RMSD=2.478e-09\RMSF=7.238e-03\PG=C*V [C*(H1N1)]\NImag=0\0.00599433,0.,0.00598668,0.,0.,0.23450757,-0.00599341,0.,0.23449537\0.,0.,-0.01253609,0.,0.,0.01253608\ \@

UB3LYP/6-31G(d)

Zero-point correction= 0.005787 (Hartree/Particle)
 Thermal correction to Energy= 0.008148
 Thermal correction to Enthalpy= 0.009092
 Thermal correction to Gibbs Free Energy= -0.011858
 Sum of electronic and zero-point Energies= -54.706109
 Sum of electronic and thermal Energies= -54.703749
 Sum of electronic and thermal Enthalpies= -54.702805
 Sum of electronic and thermal Free Energies= -54.723754

1\1\FAU-CCC-ALTIX1\FOpt\UB3LYP\6-31G(d)\H1N1(1+,4)\DRAL\26-Jul-2010\0\#P B3LYP/6-31G* OPT FREQ=NORAMAN NAME=DRAL\NH(+)\1,4\N,0.,0.,-0.1389988866\H,0.,0.,0.972992206\Version=IA64-Linux-G03RevB.03\State=4-SG\HF=-54.7118965\S2=3.751561\S2-1=0.\S2A=3.75\RMSD=1.639e-09\RMSF=1.755e-05\Dipole=0.,0.,0.6385664\PG=C*V [C*(H1N1)]\ \@

NH^{••} (triplet)***ROMP2/6-31G(d)//UB3LYP/6-31G(d)***

Zero-point correction= 0.007463 (Hartree/Particle)

Thermal correction to Energy= 0.009823
 Thermal correction to Enthalpy= 0.010767
 Thermal correction to Gibbs Free Energy= -0.009799
 Sum of electronic and zero-point Energies= -55.051022
 Sum of electronic and thermal Energies= -55.048662
 Sum of electronic and thermal Enthalpies= -55.047718
 Sum of electronic and thermal Free Energies= -55.068284

1\1\FAU-CCC-ALTIX1\Freq\ROMP2-FC\6-31G(d)\H1N1(3)\DRAL\26-Jul-2010\0\
 #P ROMP2/6-31G* FREQ=NORAMAN NAME=DRAL\NH\0,3\N,0,0,-0.1309808496\
 H,0,0,0.9168659474\Version=IA64-Linux-G03RevB.03\State=3-SG\HF=-54.
 9518252\MP2=-55.0584851\RMSD=6.600e-10\RMSF=3.931e-03\PG=C*V [C*(H1N1)
]\NImag=0\0.00348638,0,0.00348638,0,0,0.38177925,-0.00348649,0,0,
 38177940\0,0,-0.00680792,0,0,0.00680792\@

UB3LYP/6-31G(d)

Zero-point correction= 0.007377 (Hartree/Particle)
 Thermal correction to Energy= 0.009738
 Thermal correction to Enthalpy= 0.010682
 Thermal correction to Gibbs Free Energy= -0.009884
 Sum of electronic and zero-point Energies= -55.212060
 Sum of electronic and thermal Energies= -55.209700
 Sum of electronic and thermal Enthalpies= -55.208756
 Sum of electronic and thermal Free Energies= -55.229321

1\1\FAU-CCC-ALTIX1\FOpt\UB3LYP\6-31G(d)\H1N1(3)\DRAL\25-Jul-2010\0\#P
 B3LYP/6-31G* OPT FREQ=NORAMAN NAME=DRAL\N\0,3\N,0,0,-0.1309808496\
 H,0,0,0.9168659473\Version=IA64-Linux-G03RevB.03\State=3-SG\HF=-55
 .2194373\S2=2.005041\S2-1=0.\S2A=2.000006\RMSD=6.606e-09\RMSF=5.243e-0
 7\Dipole=0,0,0.6250546\PG=C*V [C*(H1N1)]\@

NH₂^{••+} (triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

Zero-point correction= 0.017173 (Hartree/Particle)
 Thermal correction to Energy= 0.020107
 Thermal correction to Enthalpy= 0.021051
 Thermal correction to Gibbs Free Energy= -0.000868
 Sum of electronic and zero-point Energies= -55.285563
 Sum of electronic and thermal Energies= -55.282630
 Sum of electronic and thermal Enthalpies= -55.281685
 Sum of electronic and thermal Free Energies= -55.303605

1\1\FAU-CCC-ALTIX1\Freq\ROMP2-FC\6-31G(d)\H2N1(1+,3)\DRAL\26-Jul-2010\0\#P ROMP2/6-31G* FREQ=NORAMAN NAME=DRAL\NH2(+)\1,3\N,-0.0406442076,0.,-0.0341045396\H,-0.5072848176,0.,0.8934569743\H,0.7917942707,0.,-0.6547251973\Version=IA64-Linux-G03RevB.03\State=3-B1\HF=-55.1981725\M P2=-55.3027362\RMSE=2.295e-09\RMSE=2.016e-03\PG=C02V [C2(N1),SGV(H2)]\NImag=0\0.37292051,0.,0.00052108,-0.35466057,0.,0.49799296,-0.0982790302584,0.,0.15430834\0.00018478,0.,-0.00015505,-0.00265584,0.,0.00334724,0.00283520,0.,-0.00319674\@

UB3LYP/6-31G(d)

Zero-point correction=	0.016973 (Hartree/Particle)
Thermal correction to Energy=	0.019918
Thermal correction to Enthalpy=	0.020862
Thermal correction to Gibbs Free Energy=	-0.001072
Sum of electronic and zero-point Energies=	-55.445797
Sum of electronic and thermal Energies=	-55.442852
Sum of electronic and thermal Enthalpies=	-55.441907
Sum of electronic and thermal Free Energies=	-55.463842

1\1\FAU-CCC-ALTIX1\FOpt\UB3LYP\6-31G(d)\H2N1(1+,3)\DRAL\26-Jul-2010\0\#P B3LYP/6-31G* OPT FREQ=NORAMAN NAME=DRAL\NH2(+)\1,3\N,-0.0406442075,0.,-0.0341045395\H,-0.5072848182,0.,0.8934569737\H,0.7917942705,0.,-0.6547251972\Version=IA64-Linux-G03RevB.03\State=3-B1\HF=-55.4627698\S2=2.007754\S2-1=0.\S2A=2.000016\RMSE=2.233e-09\RMSE=1.350e-06\Dipole=0.1910485,0.,0.1603088\PG=C02V [C2(N1),SGV(H2)]\@

NH₂• (doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

Zero-point correction=	0.019307 (Hartree/Particle)
Thermal correction to Energy=	0.022142
Thermal correction to Enthalpy=	0.023087
Thermal correction to Gibbs Free Energy=	0.000970
Sum of electronic and zero-point Energies=	-55.671469
Sum of electronic and thermal Energies=	-55.668634
Sum of electronic and thermal Enthalpies=	-55.667690
Sum of electronic and thermal Free Energies=	-55.689806

1\1\FAU-CCC-ALTIX1\Freq\ROMP2-FC\6-31G(d)\H2N1(2)\DRAL\26-Jul-2010\0\#P ROMP2/6-31G* FREQ=NORAMAN NAME=DRAL\NH2\0,2\N,-0.1107707316,0.,-0.09294768\H,-0.1292230967,0.,0.941358931\H,0.9046182183,0.,-0.2907251705\Version=IA64-Linux-G03RevB.03\State=2-B1\HF=-55.552525\MP2=-55.6907768\RMSE=7.657e-09\RMSE=3.384e-03\PG=C02V [C2(N1),SGV(H2)]\NImag=0\0

.,0.06995229\\-0.00605005,0.,-0.00507660,0.00162615,0.,0.00420794,0.00
442639,0.,0.00087074\\\\@

UB3LYP/6-31G(d)

Zero-point correction= 0.018970 (Hartree/Particle)
Thermal correction to Energy= 0.021805
Thermal correction to Enthalpy= 0.022749
Thermal correction to Gibbs Free Energy= 0.000633
Sum of electronic and zero-point Energies= -55.853649
Sum of electronic and thermal Energies= -55.850813
Sum of electronic and thermal Enthalpies= -55.849869
Sum of electronic and thermal Free Energies= -55.871986

1\\1\\FAU-CCC-ALTIX2\\FOpt\\UB3LYP\\6-31G(d)\\H2N1(2)\\DRAL\\25-Jul-2010\\0\\#P
B3LYP/6-31G* OPT FREQ=NORAMAN NAME=DRAL\\NH2\\0,2\\N,-0.1107707316,0.,
-0.09294768\\H,-0.1292230974,0.,0.9413589313\\H,0.9046182185,0.,-0.29072
51711\\Version=IA64L-G03RevC.02\\State=2-B1\\HF=-55.8726186\\S2=0.752804\\
S2-1=0.\\S2A=0.750004\\RMSD=3.470e-09\\RMSF=1.008e-04\\Dipole=0.6066537,0.,
0.5090429\\PG=C02V [C2(N1),SGV(H2)]\\\\@

NH₃⁺⁺ doublet

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

Zero-point correction= 0.033372 (Hartree/Particle)
Thermal correction to Energy= 0.036265
Thermal correction to Enthalpy= 0.037209
Thermal correction to Gibbs Free Energy= 0.014650
Sum of electronic and zero-point Energies= -55.970366
Sum of electronic and thermal Energies= -55.967473
Sum of electronic and thermal Enthalpies= -55.966529
Sum of electronic and thermal Free Energies= -55.989088

1\\1\\FAU-CCC-ALTIX1\\Freq\\ROMP2-FC\\6-31G(d)\\H3N1(1+,2)\\DRAL\\26-Jul-2010\\
0\\#P ROMP2/6-31G* FREQ=NORAMAN NAME=DRAL\\NH3(+))\\1,2\\N,0.,0.,-0.0002
295438\\H,-1.029087944,-0.0000000001,0.0005356022\\H,0.5145439719,0.8912
163023,0.0005356022\\H,0.5145439721,-0.8912163022,0.0005356022\\Version
=IA64-Linux-G03RevB.03\\State=2-A1\\HF=-55.8674276\\MP2=-56.0037378\\RMSD=
4.214e-09\\RMSF=1.237e-03\\PG=C03V [C3(N1),3SGV(H1)]\\NImag=0\\0.77883003
,0.00802578,0.00012722,-0.00018511,0.00933694\\-0.00009191,0.,-0.00011
527,-0.00214125,0.00003672\\\\@

B3LYP/6-31G(d)

Zero-point correction= 0.032875 (Hartree/Particle)
 Thermal correction to Energy= 0.035775
 Thermal correction to Enthalpy= 0.036719
 Thermal correction to Gibbs Free Energy= 0.014151
 Sum of electronic and zero-point Energies= -56.151503
 Sum of electronic and thermal Energies= -56.148602
 Sum of electronic and thermal Enthalpies= -56.147658
 Sum of electronic and thermal Free Energies= -56.170226

1\1\FAU-CCC-ALTIX1\FOpt\UB3LYP/6-31G(d)\H3N1(1+,2)\DRAL\26-Jul-2010\0\
 \#P B3LYP/6-31G* OPT FREQ=NORAMAN NAME=DRAL\NH3(+)\1,2\N,0.,0.,-0.00
 02295435\H,-1.0290879442,-0.0000000003,0.0005356015\H,0.5145439718,0.8
 912163025,0.0005356015\H,0.5145439724,-0.8912163022,0.0005356015\\Vers
 ion=IA64-Linux-G03RevB.03\State=2-A1\HF=-56.1843774\S2=0.753633\S2-1=0
 .\S2A=0.750008\RMSD=7.933e-09\RMSF=4.146e-05\Dipole=0.,0.,0.0010781\PG
 =C03V [C3(N1),3SGV(H1)]\@

NH₃**MP2/6-31G(d)//B3LYP/6-31G(d)**

Zero-point correction= 0.035188 (Hartree/Particle)
 Thermal correction to Energy= 0.038041
 Thermal correction to Enthalpy= 0.038985
 Thermal correction to Gibbs Free Energy= 0.017146
 Sum of electronic and zero-point Energies= -56.318999
 Sum of electronic and thermal Energies= -56.316146
 Sum of electronic and thermal Enthalpies= -56.315202
 Sum of electronic and thermal Free Energies= -56.337040

1\1\FAU-CCC-ALTIX1\Freq\RMP2-FC\6-31G(d)\H3N1\DRAL\26-Jul-2010\0\#P M
 P2/6-31G* FREQ=NORAMAN NAME=DRAL\NH3\0,1\N,0.,0.,-0.1192298682\H,-0.
 938872927,-0.0000000003,0.2782030258\H,0.4694364633,0.8130878059,0.278
 2030258\H,0.4694364637,-0.8130878056,0.2782030258\\Version=IA64-Linux-
 G03RevB.03\State=1-A1\HF=-56.1836003\MP2=-56.3541868\RMSD=2.176e-09\RM
 SF=1.284e-03\Dipole=0.,0.,0.7844142\DipoleDeriv=-0.3808086,0.,0.,0.,-0
 58735,0.0477026,0.0993951,0.0794553,-0.09364,0.1621893,0.2085712\Polar
 =9.3201458,0.,9.3201457,0.,0.,5.636387\PG=C03V [C3(N1),3SGV(H1)]\NImag
 =0\0.65302695,0.,0.65302696,0.,0.,0.25059157,-0.36857063,0.,0.1180196
 75922,0.00179906,0.07146224,-0.12377623,0.07993240\0.,0.,-0.00341820,
 -0.00102393,0.00113940\\@

B3LYP/6-31G(d)

Zero-point correction= 0.034524 (Hartree/Particle)
 Thermal correction to Energy= 0.037382
 Thermal correction to Enthalpy= 0.038326
 Thermal correction to Gibbs Free Energy= 0.016481
 Sum of electronic and zero-point Energies= -56.513424
 Sum of electronic and thermal Energies= -56.510566
 Sum of electronic and thermal Enthalpies= -56.509621
 Sum of electronic and thermal Free Energies= -56.531466

1\1\FAU-CCC-ALTIX2\FOpt\RB3LYP/6-31G(d)\H3N1\DRAL\25-Jul-2010\0\#P B3
 LYP/6-31G* OPT FREQ=NORAMAN NAME=DRAL\NH3\0,1\N,0,0,-0.1192298682\
 H,-0.9388729271,-0.0000000003,0.2782030257\H,0.4694364633,0.813087806,
 0.2782030257\H,0.4694364638,-0.8130878057,0.2782030257\Version=IA64L-
 G03RevC.02\State=1-A1\HF=-56.5479476\RMSD=1.334e-09\RMSF=5.840e-05\Dip
 ole=0,0,0.7517067\PG=C03V [C3(N1),3SGV(H1)]\@

NH₄⁺**MP2/6-31G(d)//B3LYP/6-31G(d)**

1\1\GINC-N01\SP\RMP2-FC\6-31G(d)\H4N1(1+)\DRAL\13-Nov-2008\0\#P MP2/6
 -31G* SCF=Tight Name=DrAl\NH4(+)\1,1\N,0,-1.921191391,0.073697243,0.
 617982363\H,0,-1.297242169,0.808205577,0.255955622\H,0,-2.589291054,0.
 488124335,1.282589435\H,0,-2.435746171,-0.355073347,-0.163732402\H,0,-
 1.362484727,-0.645966595,1.097006648\Version=AM64L-G03RevD.02\State=1
 -A\HF=-56.5299113\MP2=-56.7002924\RMSD=1.187e-09\Thermal=0.\PG=C01 [X(
 H4N1)]\@

B3LYP/6-31G(d)

Zero-point correction= 0.049859 (Hartree/Particle)
 Thermal correction to Energy= 0.052709
 Thermal correction to Enthalpy= 0.053653
 Thermal correction to Gibbs Free Energy= 0.030196
 Sum of electronic and zero-point Energies= -56.844029
 Sum of electronic and thermal Energies= -56.841180
 Sum of electronic and thermal Enthalpies= -56.840236
 Sum of electronic and thermal Free Energies= -56.863693

1\1\GINC-N01\Freq\RB3LYP/6-31G(d)\H4N1(1+)\DRAL\13-Nov-2008\0\#P Geom
 =AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq\NH4+\1,1
 \N,-1.9211913908,0.073697243,0.6179823628\H,-1.2972421689,0.8082055768

,0.2559556224\H,-2.5892910539,0.488124335,1.2825894351\H,-2.4357461707
 ,-0.355073347,-0.1637324021\H,-1.3624847267,-0.6459665949,1.0970066478
 \Version=AM64L-G03RevD.02\State=1-A\HF=-56.8938883\RMSD=1.810e-10\RMS
 F=4.934e-05\ZeroPoint=0.0498592\Thermal=0.0527086\Dipole=-0.0000019,0.
 0002267,-0.000047\DipoleDeriv=-0.3282509,0.0000556,-0.0000332,0.000011
 7,-0.3283544,0.0000635,-0.0000222,-0.0000182,-0.3284237,0.3351075,0.03
 87512,-0.0191203,0.0387711,0.347841,-0.0225091,-0.0190907,-0.022496,0.
 313283,0.339947,-0.0234352,-0.0376024,-0.0234186,0.3167534,0.0233091,-
 0.0375785,0.0233295,0.3395743,0.3245941,0.0186917,0.0340612,0.0186886,
 0.3177292,0.0283663,0.0340447,0.0283921,0.353932,0.3286023,-0.0340633,
 0.0226946,-0.0340527,0.3460307,-0.0292298,0.0226468,-0.0292074,0.32163
 44\Polar=7.1756989,0.0003346,7.1767346,-0.0007445,-0.0000121,7.1774986
 \PG=C01 [X(H4N1)]\NImag=0\

NH₄[•] (doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\GINC-N01\SP\ROMP2-FC\6-31G(d)\H4N1(2)\DRAL\12-Nov-2008\0\#P ROMP2
 /6-31G* SCF=TIGHT Name=Dral\NH4_doublet\0,2\N,0,0.052733756,0.045735
 372,0.100927998\H,0,0.8701551,-0.64692652,0.273250302\H,0,0.42262008,1
 .064805919,0.16087817\H,0,-0.713747897,-0.105721047,0.853741018\H,0,-0
 .368241039,-0.129553724,-0.883877488\Version=AM64L-G03RevD.02\State=2
 -A\HF=-56.604209\MP2=-56.7998633\RMSD=2.356e-09\Thermal=0.\PG=C01 [X(H
 4N1)]\@

UB3LYP/6-31G(d)

0 2

N	0.052733756	0.045735372	0.100927998
H	0.870155100	-0.646926520	0.273250302
H	0.422620080	1.064805919	0.160878170
H	-0.713747897	-0.105721047	0.853741018
H	-0.368241039	-0.129553724	-0.883877488

Zero-point correction=	0.031399 (Hartree/Particle)
Thermal correction to Energy=	0.034461
Thermal correction to Enthalpy=	0.035405
Thermal correction to Gibbs Free Energy=	0.010879
Sum of electronic and zero-point Energies=	-56.989209
Sum of electronic and thermal Energies=	-56.986147
Sum of electronic and thermal Enthalpies=	-56.985203
Sum of electronic and thermal Free Energies=	-57.009729

1\1\GINC-N01\Freq\UB3LYP\6-31G(d)\H4N1(2)\DRAL\12-Nov-2008\0\#N Geom=
 AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq\NH4_double
 t\0,2N,0.0527337558,0.0457353717,0.1009279977\H,0.8701550999,-0.6469
 265198,0.273250302\H,0.4226200798,1.0648059188,0.1608781701\H,-0.71374
 78969,-0.1057210467,0.853741018\H,-0.3682410386,-0.129553724,-0.883877
 4879\Version=AM64L-G03RevD.02\State=2-A\HF=-57.0206078\S2=0.750798\S2
 -1=0.\S2A=0.75\RMSD=9.808e-11\RMSF=4.074e-05\ZeroPoint=0.0313991\Therm
 al=0.0344608\Dipole=-0.0009704,-0.0016721,0.0005623\DipoleDeriv=1.4791
 897,0.0028386,0.0024899,0.0028162,1.4884617,0.0011009,0.0025047,0.0011
 388,1.479141,-0.7162123,0.7144166,-0.1776161,0.7133535,-0.4809581,0.15
 08926,-0.1772225,0.1508669,0.0867234,-0.048368,-0.4767179,-0.0280195,-
 0.4765468,-1.1891725,-0.0777626,-0.0279601,-0.0775657,0.1200048,-0.614
 9992,-0.1469675,0.7257488,-0.146352,0.0956914,0.143931,0.7261016,0.144
 6328,-0.5883653,-0.0996101,-0.0935699,-0.5226031,-0.0932709,0.0859775,
 -0.218162,-0.5234237,-0.2190728,-1.0975039\Polar=35.6384753,0.0286194,
 35.7367695,0.0269564,0.012691,35.6384598\PG=C01 [X(H4N1)]\NImag=0\

C60

B3LYP/6-311+G(d,p)//B3LYP/6-31G(d)

1\1\FAU-CCC-CCDN203\SP\RB3LYP\6-311+G(d,p)\C60\DRAL\24-Sep-2010\0\#P
 B3LYP/6-311+G(d,p) SCF=Tight SCFCyc=1200 Pop=None Name=Dral\C60\0,1\
 C,0,3.481142853,0.697421681,-0.000000001\C,0,3.481142853,-0.69742168,-
 0.000000002\C,0,-3.481142853,0.69742168,0.000000002\C,0,-3.481142853,-
 0.697421681,0.000000001\C,0,0.697421682,-0.000000003,3.481142853\C,0,-
 0.697421679,-0.000000003,3.481142853\C,0,0.697421679,0.000000003,-3.48
 1142853\C,0,-0.697421682,0.000000003,-3.481142853\C,0,0.,3.481142853,0
 .697421683\C,0,0.,3.481142854,-0.697421678\C,0,0.,-3.481142854,0.69742
 1678\C,0,0.,-3.481142853,-0.697421683\C,0,3.03181888,1.424443141,1.176
 345434\C,0,3.031818879,1.424443143,-1.176345435\C,0,3.03181888,-1.4244
 43142,1.176345432\C,0,3.031818879,-1.42444314,-1.176345437\C,0,-3.0318
 18879,1.42444314,1.176345437\C,0,-3.03181888,1.424443142,-1.176345432\
 C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141
 ,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-
 1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1
 .42444314,-1.176345437,3.031818879\C,0,1.42444314,1.176345437,-3.03181
 8879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.17634
 5437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.1763
 45435,3.031818879,1.424443143\C,0,-1.176345435,3.031818878,1.424443145
 \C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-
 1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-
 3.031818881,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-
 1.176345435,-3.031818879,-1.424443143\C,0,2.600788578,0.72702146,2.304
 797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727
 021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600

788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevA.02\State=1-AG\HF=-2286.609194\RMSD=1.948e-09\PG=IH [15SG(C4)]\\@

MP2/6-31G(d)//B3LYP/6-31G(d)

1\1\FAU-CCC-CCDN090\SP\RMP2-FC\6-31G(d)\C60\DRAL\14-Dec-2009\0\#P MP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Name=Dral\C60_FREQ\0,1\C,-0.577391081,-0.931649232,3.375994258\C,0.874374127,-0.904675356,3.318306361\C,1.296986021,0.484846288,3.269075027\C,0.105894172,1.317316341,3.294992344\C,-1.052826991,0.441963939,3.362271481\C,-1.284054796,-1.922034017,2.69315052\C,1.562159867,-1.870652424,2.582726796\C,2.388375139,0.853928863,2.481701151\C,0.054395763,2.487619086,2.536024345\C,-2.214952148,0.76938748,2.663033233\C,-0.56902665,-2.929566607,1.92698324\C,2.697968242,-1.484673532,1.762394212\C,2.335381097,2.070963431,1.690346826\C,-1.157270203,2.827686736,1.808133693\C,-2.95298083,-0.26204432,1.953340079\C,-2.495648909,-1.580338377,1.967100746\C,0.825282852,-2.901775711,1.870655851\C,3.105286333,-0.150937394,1.714897979\C,1.191687619,2.870421146,1.715302035\C,-2.269008358,1.986592348,1.871211447\C,-1.338102159,-3.206628489,0.724911883\C,2.665102101,-2.278506051,0.545981167\C,-0.682766097,-3.448105087,-0.483067868\C,3.01936321,1.819197703,0.432441947\C,-0.769205391,3.424532262,0.540839164\C,-3.460911926,0.317429212,0.721178444\C,-2.528443438,-2.373791572,0.75055245\C,1.507157145,-3.153480548,0.612151115\C,3.492905657,0.445001956,0.447248967\C,0.68245785,3.447375862,0.48298964\C,-3.03904786,1.707159066,0.670807317\C,-2.665368257,2.278671075,-0.54612409\C,0.577336948,0.932005008,-3.376828505\C,1.052167008,-0.441527006,-3.360958034\C,-0.105798222,-1.317304458,-3.295260468\C,-1.296697659,-0.484767328,-3.268297185\C,-0.87498352,0.905300922,-3.319966054\C,1.284333405,1.922178903,-2.69355619\C,2.21441389,-0.769149112,-2.662270946\C,-0.054234168,-2.486261398,-2.534380712\C,-2.389574989,-0.854356992,-2.483228044\C,-1.561811313,1.870103087,-2.582074761\C,2.496324679,1.580682602,-1.967590779\C,2.268964244,-1.986700115,-1.871136623\C,-1.191592452,-2.870221386,-1.715422387\C,-3.104938295,0.150883519,-1.714752243\C,-0.825098876,2.901156785,-1.870262412\C,0.569091362,2.928501833,-1.92630996\C,2.951998826,0.261881582,-1.95257774\C,1.15836053,-2.829715831,-1.809256542\C,-2.335615669,-2.071095316,-1.690578964\C,-2.699361151,1.485138886,-1.763134765\C,2.527729845,2.373066438,-0.75019426\C,3.039502137,-1.707343884,-0.670847072\C,-3.493488666,-0.445038497,-0.447301689\C,-1.5068

98532,3.152811645,-0.612098179\C,1.338309748,3.20728441,-0.72505024\C,
 3.462209128,-0.31752399,-0.721273948\C,0.768824866,-3.423376318,-0.540
 636478\C,-3.017245199,-1.817848064,-0.432306578\\Version=AM64L-G03RevD
 .02\State=1-A\HF=-2271.8153424\MP2=-2279.62772\RMSD=4.311e-09\Thermal=
 0.\PG=C01 [X(C60)]\@

B3LYP/6-31G(d)

0 1

C	-0.57739	-0.93165	3.37599
C	0.87437	-0.90468	3.31831
C	1.29699	0.48485	3.26908
C	0.10589	1.31732	3.29499
C	-1.05283	0.44196	3.36227
C	-1.28405	-1.92203	2.69315
C	1.56216	-1.87065	2.58273
C	2.38838	0.85393	2.48170
C	0.05440	2.48762	2.53602
C	-2.21495	0.76939	2.66303
C	-0.56903	-2.92957	1.92698
C	2.69797	-1.48467	1.76239
C	2.33538	2.07096	1.69035
C	-1.15727	2.82769	1.80813
C	-2.95298	-0.26204	1.95334
C	-2.49565	-1.58034	1.96710
C	0.82528	-2.90178	1.87066
C	3.10529	-0.15094	1.71490
C	1.19169	2.87042	1.71530
C	-2.26901	1.98659	1.87121
C	-1.33810	-3.20663	0.72491
C	2.66510	-2.27851	0.54598
C	-0.68277	-3.44811	-0.48307
C	3.01936	1.81920	0.43244
C	-0.76921	3.42453	0.54084
C	-3.46091	0.31743	0.72118
C	-2.52844	-2.37379	0.75055
C	1.50716	-3.15348	0.61215
C	3.49291	0.44500	0.44725
C	0.68246	3.44738	0.48299
C	-3.03905	1.70716	0.67081
C	-2.66537	2.27867	-0.54612
C	0.57734	0.93201	-3.37683
C	1.05217	-0.44153	-3.36096
C	-0.10580	-1.31730	-3.29526
C	-1.29670	-0.48477	-3.26830
C	-0.87498	0.90530	-3.31997
C	1.28433	1.92218	-2.69356
C	2.21441	-0.76915	-2.66227
C	-0.05423	-2.48626	-2.53438
C	-2.38957	-0.85436	-2.48323

C	-1.56181	1.87010	-2.58207
C	2.49632	1.58068	-1.96759
C	2.26896	-1.98670	-1.87114
C	-1.19159	-2.87022	-1.71542
C	-3.10494	0.15088	-1.71475
C	-0.82510	2.90116	-1.87026
C	0.56909	2.92850	-1.92631
C	2.95200	0.26188	-1.95258
C	1.15836	-2.82972	-1.80926
C	-2.33562	-2.07110	-1.69058
C	-2.69936	1.48514	-1.76313
C	2.52773	2.37307	-0.75019
C	3.03950	-1.70734	-0.67085
C	-3.49349	-0.44504	-0.44730
C	-1.50690	3.15281	-0.61210
C	1.33831	3.20728	-0.72505
C	3.46221	-0.31752	-0.72127
C	0.76882	-3.42338	-0.54064
C	-3.01725	-1.81785	-0.43231

Zero-point correction=	0.375080 (Hartree/Particle)
Thermal correction to Energy=	0.395830
Thermal correction to Enthalpy=	0.396774
Thermal correction to Gibbs Free Energy=	0.332004
Sum of electronic and zero-point Energies=	-2285.799134
Sum of electronic and thermal Energies=	-2285.778384
Sum of electronic and thermal Enthalpies=	-2285.777440
Sum of electronic and thermal Free Energies=	-2285.842211

1\1\FAU-CCC-CCDH153\Freq\RB3LYP\6-31G(d)\C60\DRAL\15-Nov-2008\0\#P B3
 LYP/6-31G* FREQ=NORAMAN NAME=DRAL\C60_FREQ\0,1\C,-0.577391081,-0.931
 649232,3.375994258\C,0.874374127,-0.904675356,3.318306361\C,1.29698602
 1,0.484846288,3.269075027\C,0.105894172,1.317316341,3.294992344\C,-1.0
 52826991,0.441963939,3.362271481\C,-1.284054796,-1.922034017,2.6931505
 2\C,1.562159867,-1.870652424,2.582726796\C,2.388375139,0.853928863,2.4
 81701151\C,0.054395763,2.487619086,2.536024345\C,-2.214952148,0.769387
 48,2.663033233\C,-0.56902665,-2.929566607,1.92698324\C,2.697968242,-1.
 484673532,1.762394212\C,2.335381097,2.070963431,1.690346826\C,-1.15727
 0203,2.827686736,1.808133693\C,-2.95298083,-0.26204432,1.953340079\C,-
 2.495648909,-1.580338377,1.967100746\C,0.825282852,-2.901775711,1.8706
 55851\C,3.105286333,-0.150937394,1.714897979\C,1.191687619,2.870421146
 ,1.715302035\C,-2.269008358,1.986592348,1.871211447\C,-1.338102159,-3.
 206628489,0.724911883\C,2.665102101,-2.278506051,0.545981167\C,-0.6827
 66097,-3.448105087,-0.483067868\C,3.01936321,1.819197703,0.432441947\C
 ,-0.769205391,3.424532262,0.540839164\C,-3.460911926,0.317429212,0.721
 178444\C,-2.528443438,-2.373791572,0.75055245\C,1.507157145,-3.1534805
 48,0.612151115\C,3.492905657,0.445001956,0.447248967\C,0.68245785,3.44
 7375862,0.48298964\C,-3.03904786,1.707159066,0.670807317\C,-2.66536825
 7,2.278671075,-0.54612409\C,0.577336948,0.932005008,-3.376828505\C,1.0

52167008,-0.441527006,-3.360958034\C,-0.105798222,-1.317304458,-3.2952
60468\C,-1.296697659,-0.484767328,-3.268297185\C,-0.87498352,0.9053009
22,-3.319966054\C,1.284333405,1.922178903,-2.69355619\C,2.21441389,-0.
769149112,-2.662270946\C,-0.054234168,-2.486261398,-2.534380712\C,-2.3
89574989,-0.854356992,-2.483228044\C,-1.561811313,1.870103087,-2.58207
4761\C,2.496324679,1.580682602,-1.967590779\C,2.268964244,-1.986700115
,-1.871136623\C,-1.191592452,-2.870221386,-1.715422387\C,-3.104938295,
0.150883519,-1.714752243\C,-0.825098876,2.901156785,-1.870262412\C,0.5
69091362,2.928501833,-1.92630996\C,2.951998826,0.261881582,-1.95257774
\C,1.15836053,-2.829715831,-1.809256542\C,-2.335615669,-2.071095316,-1
.690578964\C,-2.699361151,1.485138886,-1.763134765\C,2.527729845,2.373
066438,-0.75019426\C,3.039502137,-1.707343884,-0.670847072\C,-3.493488
666,-0.445038497,-0.447301689\C,-1.506898532,3.152811645,-0.612098179\
C,1.338309748,3.20728441,-0.72505024\C,3.462209128,-0.31752399,-0.7212
73948\C,0.768824866,-3.423376318,-0.540636478\C,-3.017245199,-1.817848
064,-0.432306578\\Version=AM64L-G03RevD.02\\State=1-A\\HF=-2286.1742144\
RMSD=3.870e-09\\RMSF=2.633e-04\\ZeroPoint=0.3750803\\Thermal=0.3958303\\ZP
E=235.366413\\Dipole=0.0001199,0.0001014,-0.000005\\DipoleDeriv=0.071102
9237,-0.025745,0.0755591,-0.0001776,-0.112776,0.0026898,-0.0136114\\Pol
ar=468.7230209,0.0233932,468.7805278,0.0290554,0.0456918,468.8311324\\P
G=C01 [X(C60)]\\NImag=0\\0.56279395,0.05593992,0.59759398,0.08569318,0.
875\\-0.00012731,-0.00015939,-0.00008512,-0.00023023,0.00032697,-0.000
320,0.00013877,0.00017576,0.00018657,0.00002615\\\\@

C₆₀⁻

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\\1\\GINC-I01R08C02S09\\SP\\UB3LYP\\6-311+G(d,p)\\C60(1-,2)\\DRAL\\25-Jan-201
3\\0\\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current
Name=DrAl GFINPUT GFPRINT\\C60(-) doublet\\-1,2\\C,0,3.481142853,0.6974
21681,-0.000000001\\C,0,3.481142853,-0.69742168,-0.000000002\\C,0,-3.481
142853,0.69742168,0.000000002\\C,0,-3.481142853,-0.697421681,0.00000000
1\\C,0,0.697421682,-0.000000003,3.481142853\\C,0,-0.697421679,-0.0000000
03,3.481142853\\C,0,0.697421679,0.000000003,-3.481142853\\C,0,-0.6974216
82,0.000000003,-3.481142853\\C,0,0.,3.481142853,0.697421683\\C,0,0.,3.48
1142854,-0.697421678\\C,0,0.,-3.481142854,0.697421678\\C,0,0.,-3.4811428
53,-0.697421683\\C,0,3.03181888,1.424443141,1.176345434\\C,0,3.031818879
,1.424443143,-1.176345435\\C,0,3.03181888,-1.424443142,1.176345432\\C,0,
3.031818879,-1.42444314,-1.176345437\\C,0,-3.031818879,1.42444314,1.176
345437\\C,0,-3.03181888,1.424443142,-1.176345432\\C,0,-3.031818879,-1.42
4443143,1.176345435\\C,0,-3.03181888,-1.424443141,-1.176345434\\C,0,1.42
4443143,1.176345433,3.03181888\\C,0,1.424443143,-1.176345437,3.03181887
8\\C,0,-1.42444314,1.176345432,3.031818881\\C,0,-1.42444314,-1.176345437
,3.031818879\\C,0,1.42444314,1.176345437,-3.031818879\\C,0,1.42444314,-1
.176345432,-3.031818881\\C,0,-1.424443143,1.176345437,-3.031818878\\C,0,
-1.424443143,-1.176345433,-3.03181888\\C,0,1.176345435,3.031818879,1.42
4443143\\C,0,-1.176345435,3.031818878,1.424443145\\C,0,1.176345434,3.031

818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.03181888,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.03181879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2286.7042204\S2=0.754465\S2-1=0.\S2A=0.750019\RMSE=9.654e-09\Dipole=0.,0.,0.\Quadrupole=-0.6614768,-0.2357452,0.897222,0.4330657,0.6926707,1.127596\PG=IH [15SG(C4)]\@

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN088\SP\ROMP2-FC\6-31G(d)\C60(1-,2)\DRAL\22-Mar-2010\0\#P ROMP2/6-31G* Geom=AllCheck Guess=Read Name=Dral\N@C60 doublet DFT SP\ -1,2\C,0,-1.397727,-1.246221,3.030203\C,0,-1.995587,0.067766,2.937043\C,0,-3.009431,0.035622,1.891483\C,0,-3.026946,-1.3043,1.332615\C,0,-2.023208,-2.091747,2.036004\C,0,-0.014818,-1.369896,3.283936\C,0,-1.213187,1.217783,3.102043\C,0,-3.197697,1.141984,1.061574\C,0,-3.231726,-1.489103,-0.035807\C,0,-1.267114,-3.034502,1.328585\C,0,0.796094,-0.181551,3.447151\C,0,-1.408831,2.364201,2.244126\C,0,-3.411378,0.950537,-0.363307\C,0,-2.445327,-2.469386,-0.768193\C,0,0.164115,-3.160443,1.590009\C,0,0.768563,-2.338482,2.547235\C,0,0.217889,1.089422,3.362326\C,0,-2.384666,2.335766,1.235779\C,0,-3.427597,-0.337346,-0.900514\C,0,-1.479739,-3.227001,-0.088236\C,0,2.097148,-0.423675,2.832927\C,0,-0.098125,2.939342,1.967561\C,0,2.757259,0.611757,2.16224\C,0,-2.722965,2.025456,-1.061795\C,0,-2.158205,-1.929058,-2.078448\C,0,0.832135,-3.441199,0.337804\C,0,2.079905,-1.759621,2.275316\C,0,0.90346,2.16194,2.674208\C,0,-2.097184,2.880314,-0.072312\C,0,-2.757259,-0.611757,-2.16224\C,0,-0.179407,-3.463293,-0.702952\C,0,0.098125,-2.939342,-1.967561\C,0,1.397727,1.246221,-3.030203\C,0,2.023208,2.091747,-2.036004\C,0,3.026946,1.3043,-1.332615\C,0,3.009431,-0.035622,-1.891483\C,0,1.995587,-0.067766,-2.937044\C,0,0.014818,1.369897,-3.283935\C,0,1.267114,3.034502,-1.328585\C,0,3.231726,1.489103,0.035807\C,0,3.197697,-1.141985,-1.061574\C,0,1.213187,-1.217783,-3.102043\C,0,-0.768563,2.338482,-2.547235\C,0,1.479739,3.227001,0.088236\C,0,3.427597,0.337346,0.900514\C,0,2.384666,-2.335766,-1.235779\C,0,-0.217889,-1.089422,-3.362326\C,0,-0.796094,0.181551,-3.447151\C,0,-0.164115,3.160443,-1.590009\C,0,2.445328,

2.469386,0.768193\C,0,3.411378,-0.950537,0.363307\C,0,1.408831,-2.364201,-2.244126\C,0,-2.079905,1.759621,-2.275316\C,0,0.179407,3.463294,0.702952\C,0,2.097184,-2.880314,0.072312\C,0,-0.90346,-2.16194,-2.674208\C,0,-2.097148,0.423675,-2.832928\C,0,-0.832135,3.441199,-0.337804\C,0,2.158205,1.929058,2.078448\C,0,2.722964,-2.025456,1.061795\\Version=A M64L-G03RevD.02\\State=2-A\\HF=-2271.8378457\\MP2=-2279.7181152\\RMSD=4.621e-09\\Thermal=0.\\PG=C01 [X(C60)]\\@

UB3LYP/6-31G(d)

Zero-point correction=	0.368307 (Hartree/Particle)
Thermal correction to Energy=	0.390549
Thermal correction to Enthalpy=	0.391493
Thermal correction to Gibbs Free Energy=	0.322040
Sum of electronic and zero-point Energies=	-2285.881819
Sum of electronic and thermal Energies=	-2285.859578
Sum of electronic and thermal Enthalpies=	-2285.858633
Sum of electronic and thermal Free Energies=	-2285.928086

1\\GINC-A02\Freq\UB3LYP\6-31G(d)\C60(1,2)\DRAL\01-Jan-2009\0\\#P UB3LYP/6-31G* Freq=NoRaman NAME=DRAL\C60 (1-)\-1,2\C,-1.397727,-1.246221,3.030203\C,-1.995587,0.067766,2.937043\C,-3.009431,0.035622,1.891483\C,-3.026946,-1.3043,1.332615\C,-2.023208,-2.091747,2.036004\C,-0.014818,-1.369896,3.283936\C,-1.213187,1.217783,3.102043\C,-3.197697,1.141984,1.061574\C,-3.231726,-1.489103,-0.035807\C,-1.267114,-3.034502,1.328585\C,0.796094,-0.181551,3.447151\C,-1.408831,2.364201,2.244126\C,-3.411378,0.950537,-0.363307\C,-2.445327,-2.469386,-0.768193\C,0.164115,-3.160443,1.590009\C,0.768563,-2.338482,2.547235\C,0.217889,1.089422,3.362326\C,-2.384666,2.335779\C,-3.427597,-0.337346,-0.900514\C,-1.479739,-3.227001,-0.088236\C,2.097148,-0.423675,2.832927\C,-0.098125,2.939342,1.967561\C,2.757259,0.611757,2.16224\C,-2.722965,2.025456,-1.061795\C,-2.158205,-1.929058,-2.078448\C,0.832135,-3.441199,0.337804\C,2.079905,-1.759621,2.275316\C,0.90346,2.16194,2.674208\C,-2.097184,-2.880314,-0.072312\C,-2.757259,-0.611757,-2.16224\C,-0.179407,-3.463293,-0.702952\C,0.098125,-2.939342,-1.967561\C,1.397727,1.246221,-3.030203\C,2.023208,2.091747,-2.036004\C,3.026946,1.3043,-1.332615\C,3.009431,-0.035622,-1.891483\C,1.995587,-0.067766,-2.937044\C,0.014818,1.369897,-3.283935\C,1.267114,3.034502,-1.328585\C,3.231726,1.489103,0.035807\C,3.197697,-1.141985,-1.061574\C,1.213187,-1.217783,-3.102043\C,-0.768563,2.338482,-2.547235\C,1.479739,3.227001,0.088236\C,3.427597,0.337346,0.900514\C,2.384666,-2.335779\C,-0.217889,-1.089422,-3.362326\C,-0.796094,0.181551,-3.447151\C,-0.164115,3.160443,-1.590009\C,-2.445328,2.469386,0.768193\C,3.411378,-0.950537,0.363307\C,1.408831,-2.364201,-2.244126\C,-2.079905,1.759621,-2.275316\C,0.179407,3.463294,0.702952\C,2.097184,-2.880314,0.072312\C,-0.90346,-2.16194,-2.674208\C,-2.097148,0.423675,-2.832928\C,-0.832135,3.441199,-0.337804\C,2.158205,1.929058,2.078448\C,2.722964,-2.025456,1.061795\\Version=IA64L-G03RevE.01\\State=2-A\\HF=-2286.2501263\\S2=0.754935\\S2-1=0.\\S2A=0.750023\\RMSD

=1.983e-09\RMSF=1.129e-04\ZeroPoint=0.3683071\Thermal=0.3905487\Dipole
 =-0.0000006,-0.0000008,0.\DipoleDeriv=-0.0803394,-0.261431,0.6179744,-
 0.0245198,-0.2179101,-0.0918356,0.0549668,-0.0703218,-0.0791009,-0.082
 7926,0.0055209,-0.0300698,-0.1013657,0.2188506,0.3602655,0.0954286,-0.
 0601384,-0.0299019,0.0008323,-0.0759718,0.1556565,-0.0546416,-0.017876
 8,0.1505154,0.108943,0.080344,0.0688971,-0.0025787,-0.0579887,0.160083
 8,-0.0365722,0.1442439,-0.0751527,0.1131679,-0.0077386,-0.1002499,-0.0
 762728,0.033715,-0.0205199,0.0080771,0.2384822,-0.0784954,0.143329,0.3
 220103,-0.041456,-0.0298758,0.2140217,-0.5152509,-0.0020229,-0.1892045
 ,0.0849967,-0.0030942,0.0646686,-0.3180056,0.0366247,-0.0738818,0.1192
 859,0.0204902,-0.2068348,-0.3724766,-0.0265553,-0.0269256,0.0286292,-0.
 .0431474,0.1313266,-0.0768323,0.1460329,0.1275463,-0.052207,-0.0201755
 ,0.0401432,0.0766095,-0.0505199,-0.033526,-0.1421863,-0.0857549,0.0898
 95,0.072457,-0.1177423,-0.0188596,0.1215814,0.0446457,-0.0453002,0.139
 1436,0.0018634,-0.2765745,0.0404539,-0.0277321,-0.2840707,0.1089906,0.
 0646408,0.1141362,0.1032052,0.0939724,0.07263,0.2917196,-0.1063691,-0.
 025027,-0.0023107,-0.0108233,0.0252793,-0.131744,-0.028925,0.0546862,0.
 .0196945,0.0405656,-0.3202007,-0.3544052,-0.0508529,0.1495549,0.035479
 9,0.1176244,0.037414,-0.0349746,0.0153083,-0.0699962,0.1029887,-0.1445
 198,-0.186152,0.1061129,-0.0297643,0.202532,-0.021207,-0.0648189,-0.41
 97721,-0.0230648,0.0907762,0.0707346,-0.1516148,-0.0799939,-0.1659528,
 0.0745372,0.0025194,-0.2423476,0.1353529,0.0566526,-0.1518331,-0.00405
 5,0.0128241,0.1723365,-0.1255691,-0.1396613,0.2121169,-0.1080714,0.102
 8139,0.0538818,-0.1589297,0.0523999,-0.1016673,-0.2918701,0.0529361,0.
 0025567,0.071003,-0.145099,0.057094,0.2070882,0.070134,-0.1391187,-0.1
 007896,-0.0237566,0.3166804,0.3069822,-0.0523194,-0.1303292,-0.0774075
 ,-0.0952331,0.0373588,-0.040003,-0.0745035,-0.0036754,0.1205232,-0.011
 3681,0.071802,-0.1112663,-0.0119277,-0.3035219,0.0420238,0.0444634,0.3
 617259,0.0042187,0.0249899,-0.0656857,-0.1180456,0.0393939,-0.1012536,
 0.3309207,-0.037953,0.1300793,-0.0666201,0.1739366,-0.1117535,0.014021
 4,0.0185373,0.1210406,0.0457324,0.0622305,-0.1035104,-0.1079015,-0.104
 5704,0.0148677,0.0269764,-0.132495,0.1742582,-0.3116327,-0.0211279,-0.
 0338303,0.0907686,-0.0956112,-0.0289134,0.025795,0.1139191,-0.0318082,
 0.1790448,0.0827665,-0.0979177,0.2950493,-0.1284785,-0.3116485,-0.4764
 096,-0.0336817,-0.1561616,0.0923743,-0.0485556,0.2685089,0.0961703,-0.
 0287426,-0.3818188,0.0621564,0.0243827,-0.4108781,0.0207425,-0.0344635
 ,0.1939406,-0.0758558,0.0304439,0.1338905,-0.0450941,0.0002117,0.14818
 46,-0.1185117,-0.0544233,0.082243,-0.3051039,-0.0313015,0.2162411,0.30
 74479,0.003063,-0.1345747,-0.0972631,-0.0392944,-0.2497127,-0.3458133,
 -0.1289767,0.5633016,-0.1164575,0.0580007,0.1344918,-0.0296751,-0.0108
 105,-0.2271258,-0.2110755,-0.1045693,0.0148699,0.0269758,-0.1324978,0.
 174253,-0.311633,-0.0211276,-0.0338285,0.0907703,0.1718291,0.0608619,0.
 .0954616,-0.0640239,-0.0206135,0.0361863,0.034415,0.1861484,0.0411618,
 0.173935,-0.1117568,0.0140235,0.0185378,0.1210428,0.0457316,0.0622295,
 -0.1035099,-0.1078967,-0.0803407,-0.2614311,0.6179735,-0.0245166,-0.21
 79114,-0.0918366,0.0549685,-0.0703227,-0.0791022,-0.076271,0.0337138,-
 0.0205233,0.0080748,0.2384818,-0.0784955,0.1433268,0.3220091,-0.041456
 ,-0.0025813,-0.0579881,0.1600854,-0.0365697,0.1442436,-0.0751532,0.113
 1672,-0.0077388,-0.1002517,0.0008329,-0.075972,0.1556566,-0.0546433,-0.
 .0178781,0.1505161,0.1089414,0.0803425,0.0688963,-0.0827927,0.0055217,

-0.0300687,-0.1013687,0.2188513,0.3602674,0.0954295,-0.0601382,-0.0299
045,-0.0298731,0.2140215,-0.5152524,-0.0020261,-0.1892073,0.0849974,-0
.003096,0.0646663,-0.3180037,0.0446446,-0.045302,0.1391433,0.0018661,-
0.2765739,0.0404545,-0.0277315,-0.2840727,0.1089893,-0.0505178,-0.0335
263,-0.1421882,-0.0857564,0.0898978,0.0724614,-0.117744,-0.0188604,0.1
215843,-0.0431471,0.1313265,-0.0768327,0.1460335,0.1275433,-0.0522109,
-0.0201761,0.0401415,0.0766082,0.036626,-0.0738837,0.1192855,0.0204926
,-0.2068343,-0.3724784,-0.0265562,-0.0269243,0.0286338,0.0566516,-0.15
18318,-0.004053,0.0128251,0.1723359,-0.125572,-0.1396568,0.2121173,-0.
1080725,-0.0113686,0.0718016,-0.1112734,-0.0119293,-0.3035231,0.042024
5,0.0444615,0.3617272,0.0042212,-0.0523191,-0.1303254,-0.0774067,-0.09
52347,0.0373567,-0.0400078,-0.0745046,-0.0036716,0.1205273,-0.1451009,
0.0570905,0.2070892,0.0701349,-0.1391157,-0.1007885,-0.0237602,0.31667
68,0.3069813,0.102814,0.0538822,-0.1589292,0.0523979,-0.1016652,-0.291
8693,0.0529369,0.0025564,0.0710023,0.0646431,0.114136,0.1032051,0.0939
736,0.0726314,0.2917192,-0.1063711,-0.0250247,-0.0023132,0.0907788,0.0
70736,-0.1516149,-0.0799961,-0.1659566,0.0745378,0.0025172,-0.2423472,
0.1353552,-0.1445215,-0.1861527,0.1061201,-0.029764,0.2025331,-0.02120
86,-0.064817,-0.4197759,-0.0230673,-0.0508537,0.1495516,0.0354801,0.11
76241,0.037413,-0.0349728,0.0153087,-0.0699947,0.1029924,-0.0108214,0.
0252819,-0.1317473,-0.0289246,0.0546862,0.0196945,0.0405697,-0.3201999
,-0.3544066,0.0304451,0.133891,-0.0450924,0.0002109,0.148186,-0.118507
2,-0.054426,0.0822415,-0.3051022,0.1718263,0.0608602,0.0954647,-0.0640
229,-0.020615,0.0361841,0.0344145,0.1861489,0.0411659,-0.1289772,0.563
3021,-0.1164591,0.0580009,0.134492,-0.0296766,-0.0108063,-0.2271231,-0
.2110737,-0.0312979,0.2162456,0.3074435,0.003061,-0.1345764,-0.0972624
,-0.0392965,-0.2497096,-0.3458143,0.0249888,-0.0656812,-0.1180455,0.03
93962,-0.101249,0.330919,-0.0379519,0.1300788,-0.0666187,-0.0287441,-0
.3818192,0.0621531,0.0243824,-0.4108733,0.0207414,-0.0344587,0.1939457
,-0.0758558,-0.1284752,-0.3116472,-0.4764137,-0.0336829,-0.1561614,0.0
923753,-0.0485571,0.2685141,0.0961699,-0.0956096,-0.0289108,0.0257953,
0.1139164,-0.0318071,0.1790476,0.0827631,-0.0979194,0.2950515\Polar=47
4.7036726,-0.1527557,512.4365586,-0.1512889,-0.1035798,512.5623642\PG=
C01 [X(C60)]\NImag=0\

C₆₀^{••2-} (triplet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I11R04A23\SP\UB3LYP\6-311+G(d,p)\C60(2-,3)\DRAL\25-Jan-2013\0
\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Nam
e=Dral GFINPUT GFPRINT\C60(2-) triplet\2,3\C,0,3.481142853,0.697421
681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.48114
2853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001\
C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000003
,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421682
,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.4811
42854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142853

, -0.697421683\C, 0, 3.03181888, 1.424443141, 1.176345434\C, 0, 3.031818879, 1.424443143, -1.176345435\C, 0, 3.03181888, -1.424443142, 1.176345432\C, 0, 3.031818879, -1.42444314, -1.176345437\C, 0, -3.031818879, 1.42444314, 1.176345437\C, 0, -3.03181888, 1.424443142, -1.176345432\C, 0, -3.031818879, -1.424443143, 1.176345435\C, 0, -3.03181888, -1.424443141, -1.176345434\C, 0, 1.424443143, 1.176345433, 3.03181888\C, 0, 1.424443143, -1.176345437, 3.031818878\C, 0, -1.42444314, 1.176345432, 3.031818881\C, 0, -1.42444314, -1.176345437, 3.031818879\C, 0, 1.42444314, 1.176345437, -3.031818879\C, 0, 1.42444314, -1.176345432, -3.031818881\C, 0, -1.424443143, 1.176345437, -3.031818878\C, 0, -1.424443143, -1.176345433, -3.03181888\C, 0, 1.176345435, 3.031818879, 1.424443143\C, 0, -1.176345435, 3.031818878, 1.424443145\C, 0, 1.176345434, 3.031818881, -1.42444314\C, 0, -1.176345436, 3.03181888, -1.424443139\C, 0, 1.176345436, -3.03181888, 1.424443139\C, 0, -1.176345434, -3.031818881, 1.42444314\C, 0, 1.176345435, -3.031818878, -1.424443145\C, 0, -1.176345435, -3.031818879, -1.424443143\C, 0, 2.600788578, 0.72702146, 2.304797418\C, 0, 2.600788575, 0.727021464, -2.304797419\C, 0, 2.600788578, -0.727021463, 2.304797416\C, 0, 2.600788576, -0.727021459, -2.30479742\C, 0, -2.600788576, 0.727021459, 2.30479742\C, 0, -2.600788578, 0.727021463, -2.304797416\C, 0, -2.600788575, -0.727021464, 2.304797419\C, 0, -2.600788578, -0.72702146, -2.304797418\C, 0, 0.727021462, 2.304797416, 2.600788578\C, 0, 0.727021463, -2.30479742, 2.600788574\C, 0, -0.72702146, 2.304797416, 2.600788579\C, 0, -0.72702146, -2.30479742, 2.600788575\C, 0, 0.72702146, 2.30479742, -2.600788575\C, 0, 0.72702146, -2.304797416, -2.600788579\C, 0, -0.727021463, 2.30479742, -2.600788574\C, 0, -0.727021462, -2.304797416, -2.600788578\C, 0, 2.304797418, 2.600788576, 0.727021462\C, 0, -2.304797418, 2.600788576, 0.727021464\C, 0, 2.304797418, 2.600788578, -0.72702146\C, 0, -2.304797419, 2.600788577, -0.727021458\C, 0, 2.304797419, -2.600788577, 0.727021458\C, 0, -2.304797418, -2.600788578, 0.72702146\C, 0, 2.304797418, -2.600788576, -0.727021464\C, 0, -2.304797418, -2.600788576, -0.727021462\\Version=EM64L-G09RevB.01\HF=-2286.6901679\S2=2.006003\S2-1=0.\S2A=2.000025\RMSE=7.261e-09\Dipole=0.,0.,0.\Quadrupole=-0.8576571,0.6370414,0.2206157,-0.6700682,1.0805859,0.4104857\PG=IH [15SG(C4)]\@

C₆₀²⁻ (singlet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I01R08C02S09\SP\RB3LYP\6-311+G(d,p)\C60(2-)\DRAL\25-Jan-2013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Name=DrAl GFINPUT GFPRINT\C60(2-) singlet\ -2,1\C, 0, 3.481142853, 0.697421681, -0.000000001\C, 0, 3.481142853, -0.69742168, -0.000000002\C, 0, -3.481142853, 0.69742168, 0.000000002\C, 0, -3.481142853, -0.697421681, 0.000000001\C, 0, 0.697421682, -0.000000003, 3.481142853\C, 0, -0.697421679, -0.000000003, 3.481142853\C, 0, 0.697421679, 0.000000003, -3.481142853\C, 0, -0.697421682, 0.000000003, -3.481142853\C, 0, 0., 3.481142853, 0.697421683\C, 0, 0., 3.481142854, -0.697421678\C, 0, 0., -3.481142854, 0.697421678\C, 0, 0., -3.481142853, -0.697421683\C, 0, 3.03181888, 1.424443141, 1.176345434\C, 0, 3.031818879, 1.424443143, -1.176345435\C, 0, 3.03181888, -1.424443142, 1.176345432\C, 0, 3.031818879, -1.42444314, -1.176345437\C, 0, -3.031818879, 1.42444314, 1.1763

45437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2286.6845501\RMSD=5.885e-09\Dipole=0.,0.,0.\Quadrupole=-1.2979397,-0.4961591,1.7940988,0.8982302,1.3572478,2.2546129\PG=IH [15SG(C4)]\@

C_{60}^{3-} (quartet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C_{60}

1\1\GINC-I11R04A23\SP\UB3LYP\6-311+G(d,p)\C60(3-,4)\DRAL\25-Jan-2013\0\\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Name=Dral GFINPUT GFPRINT\C60(3-) quartet\\-3,4\C,0,3.481142853,0.697421681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.481142853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001\C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000003,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421682,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142853,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3.031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.176345437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,3

.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevB.01\\State=4-AG\\HF=-2286.5685908\\S2=3.754803\\S2-1=0.\\S2A=3.750012\\RMSD=1.469e-09\\Dipole=0.,0.,0.\\Quadrupole=0.0041967,-0.0018239,-0.0023728,0.0031221,-0.0035043,-0.0019183\\PG=IH [15SG(C4)]\\@

C₆₀³⁻ (doublet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I01R08C02S09\SP\UB3LYP\6-311+G(d,p)\C60(3-,2)\DRAL\25-Jan-2013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Name=DrAl GFINPUT GFPRINT\C60(3-) doublet\\-3,2\C,0,3.481142853,0.697421681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.481142853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001\C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000003,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421682,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142853,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3.031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.176345437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.4

24443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2286.5620812\S2=0.754489\S2-1=0.\S2A=0.750019\RMSD=7.819e-09\Dipole=0.,0.,0.\Quadrupole=-1.4598835,0.3847752,1.0751083,-0.2211855,1.7093637,1.4844994\PG=IH [15SG (C4)]\@

C₆₀⁴⁻ (triplet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I11R05A35\SP\UB3LYP\6-311+G(d,p)\C60(4-,3)\DRAL\25-Jan-2013\0\\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Name=Dral GFINPUT GPRINT\C60(4-) triplet\\-4,3\C,0,3.481142853,0.697421681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.481142853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001\C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000003,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421682,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142853,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3.031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.176345437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\C

,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818879
 ,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0
 .727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2
 .600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.304
 79742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.72
 7021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.72
 7021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.60078857
 4\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,
 2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.3
 04797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.
 727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.7270
 21462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.60078
 8578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.30479
 7419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146
 \C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.6007885
 76,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2286.3342896\S2=2.006052
 \S2-1=0.\S2A=2.000025\RMSE=7.276e-09\Dipole=0.,0.,0.\Quadrupole=-0.627
 6362,-0.2258431,0.8534793,0.4222245,0.6653106,1.0808109\PG=IH [15SG(C4
)]\@

C₆₀⁴⁻ (singlet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I01R08C02S09\SP\RB3LYP\6-311+G(d,p)\C60(4-)\DRAL\25-Jan-2013\
 0\#\P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Na
 me=DrAl GFINPUT GFPRINT\C60(4-) singlet\ -4,1\C,0,3.481142853,0.69742
 1681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.4811
 42853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001
 \C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.00000000
 3,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.69742168
 2,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481
 142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.48114285
 3,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,
 1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3
 .031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.1763
 45437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424
 443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424
 443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878
 \C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,
 3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.
 176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-
 1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424
 443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.0318
 18881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.17634
 5436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\
 C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.03181887
 9,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,
 0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,

2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2286.3290603\RMSD=9.441e-09\Dipole=0.,0.,0.\Quadrupole=-1.6603618,1.2734173,0.3869445,-1.3354267,2.1139392,0.7641153\PG=IH [15SG(C4)]\@

C₆₀⁵⁻ (quartet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I11R05A35\SP\UB3LYP\6-311+G(d,p)\C60(5-,4)\DRAL\25-Jan-2013\0\\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Name=Dral GFINPUT GFPRINT\C60(5-) quartet\\-5,4\C,0,3.481142853,0.697421681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.481142853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001\C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000003,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421682,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142853,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3.031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.176345437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.60078857

4\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,
 2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.3
 04797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.
 727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.7270
 21462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.60078
 8578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.30479
 7419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146
 \C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.6007885
 76,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2285.9666405\S2=3.759641
 \S2-1=0.\S2A=3.750048\RMSD=7.555e-09\Dipole=0.,0.,0.\Quadrupole=0.9910
 063,-1.3060597,0.3150534,1.642065,-1.2357379,0.2846511\PG=IH [15SG(C4)
]\@

C₆₀⁵⁻ (doublet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I01R08C02S09\SP\UB3LYP\6-311+G(d,p)\C60(5-,2)\DRAL\25-Jan-201
 3\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current
 Name=DrAl GFINPUT GFPRINT\C60(5-) doublet\\-5,2\C,0,3.481142853,0.697
 421681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.48
 1142853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.0000000
 01\C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000
 003,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421
 682,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.4
 81142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142
 853,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.03181887
 9,1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0
 ,3.031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.17
 6345437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.4
 24443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.4
 24443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.0318188
 78\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.17634543
 7,3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-
 1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0
 ,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.4
 24443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.03
 1818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176
 345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.4244431
 4\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818
 879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.60078857
 5,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,
 0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.
 30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.
 727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.
 727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.60078
 8574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.304797
 42,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-
 2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,

-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.304797419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788576,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2285.9982208\S2=0.754504\S2-1=0.\S2A=0.75002\RMSE=1.561e-09\Dipole=0.,0.,0.\Quadrupole=-0.8226129,0.617327,0.2052859,-0.6374892,1.0511053,0.4001189\PG=IH [15SG(C4)]\@

C₆₀^{••6-} (triplet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I07R06A23\SP\UB3LYP\6-311+G(d,p)\C60(6-,3)\DRAL\26-Jan-2013\0\\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Name=Dral GFINPUT GFPRINT\C60(6-) triplet\\-6,3\C,0,3.481142853,0.697421681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.481142853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001\C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.000000003,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.697421682,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.481142853,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3.031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.176345437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878\C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.031818881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.176345436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.031818879,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.727021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.727021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.600788574\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0.727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.600788578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.30479

7419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.72702146
 \C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.6007885
 76,-0.727021462\\Version=EM64L-G09RevB.01\HF=-2285.5312684\S2=2.007581
 \S2-1=0.\S2A=2.000037\RMSD=9.331e-09\Dipole=0.,0.,0.\Quadrupole=1.6985
 088,-0.9100878,-0.788421,1.4735074,-1.4662286,-0.5992945\PG=IH [15SG(C
 4)]\@

C₆₀⁶⁻ (singlet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of C₆₀

1\1\GINC-I01R08C02S09\SP\RB3LYP\6-311+G(d,p)\C60(6-)\DRAL\25-Jan-2013\
 0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current Na
 me=DrAl GFINPUT GFPRINT\C60(6-) singlet\ -6,1\C,0,3.481142853,0.69742
 1681,-0.000000001\C,0,3.481142853,-0.69742168,-0.000000002\C,0,-3.4811
 42853,0.69742168,0.000000002\C,0,-3.481142853,-0.697421681,0.000000001
 \C,0,0.697421682,-0.000000003,3.481142853\C,0,-0.697421679,-0.00000000
 3,3.481142853\C,0,0.697421679,0.000000003,-3.481142853\C,0,-0.69742168
 2,0.000000003,-3.481142853\C,0,0.,3.481142853,0.697421683\C,0,0.,3.481
 142854,-0.697421678\C,0,0.,-3.481142854,0.697421678\C,0,0.,-3.48114285
 3,-0.697421683\C,0,3.03181888,1.424443141,1.176345434\C,0,3.031818879,
 1.424443143,-1.176345435\C,0,3.03181888,-1.424443142,1.176345432\C,0,3
 .031818879,-1.42444314,-1.176345437\C,0,-3.031818879,1.42444314,1.1763
 45437\C,0,-3.03181888,1.424443142,-1.176345432\C,0,-3.031818879,-1.424
 443143,1.176345435\C,0,-3.03181888,-1.424443141,-1.176345434\C,0,1.424
 443143,1.176345433,3.03181888\C,0,1.424443143,-1.176345437,3.031818878
 \C,0,-1.42444314,1.176345432,3.031818881\C,0,-1.42444314,-1.176345437,
 3.031818879\C,0,1.42444314,1.176345437,-3.031818879\C,0,1.42444314,-1.
 176345432,-3.031818881\C,0,-1.424443143,1.176345437,-3.031818878\C,0,-
 1.424443143,-1.176345433,-3.03181888\C,0,1.176345435,3.031818879,1.424
 443143\C,0,-1.176345435,3.031818878,1.424443145\C,0,1.176345434,3.0318
 18881,-1.42444314\C,0,-1.176345436,3.03181888,-1.424443139\C,0,1.17634
 5436,-3.03181888,1.424443139\C,0,-1.176345434,-3.031818881,1.42444314\
 C,0,1.176345435,-3.031818878,-1.424443145\C,0,-1.176345435,-3.03181887
 9,-1.424443143\C,0,2.600788578,0.72702146,2.304797418\C,0,2.600788575,
 0.727021464,-2.304797419\C,0,2.600788578,-0.727021463,2.304797416\C,0,
 2.600788576,-0.727021459,-2.30479742\C,0,-2.600788576,0.727021459,2.30
 479742\C,0,-2.600788578,0.727021463,-2.304797416\C,0,-2.600788575,-0.7
 27021464,2.304797419\C,0,-2.600788578,-0.72702146,-2.304797418\C,0,0.7
 27021462,2.304797416,2.600788578\C,0,0.727021463,-2.30479742,2.6007885
 74\C,0,-0.72702146,2.304797416,2.600788579\C,0,-0.72702146,-2.30479742
 ,2.600788575\C,0,0.72702146,2.30479742,-2.600788575\C,0,0.72702146,-2.
 304797416,-2.600788579\C,0,-0.727021463,2.30479742,-2.600788574\C,0,-0
 .727021462,-2.304797416,-2.600788578\C,0,2.304797418,2.600788576,0.727
 021462\C,0,-2.304797418,2.600788576,0.727021464\C,0,2.304797418,2.6007
 88578,-0.72702146\C,0,-2.304797419,2.600788577,-0.727021458\C,0,2.3047
 97419,-2.600788577,0.727021458\C,0,-2.304797418,-2.600788578,0.7270214
 6\C,0,2.304797418,-2.600788576,-0.727021464\C,0,-2.304797418,-2.600788
 576,-0.727021462\\Version=EM64L-G09RevB.01\State=1-AG\HF=-2285.565066\

RMSD=2.861e-09\Dipole=0.,0.,0.\Quadrupole=0.0104252,-0.0054351,-0.0049
901,0.0062712,-0.0115462,-0.0064226\PG=IH [15SG(C4)]\@

C₆₀H⁺

MP2/6-31G(d)//B3LYP/6-31G(d)

1\1\FAU-CCC-CCDH157\SP\RMP2-FC\6-31G(d)\C60H1(1+)\DRAL\07-Dec-2008\0\
#P MP2/6-31G* SCF=TIGHT NAME=DRAL\C60H(+)\1,1\C,0,1.335889335,2.9106
23993,1.946948593\C,0,-0.005201573,2.564702139,2.377565539\C,0,0.08890
6643,1.369973135,3.210710216\C,0,1.48331856,0.997272702,3.308546306\C,
0,2.257098769,1.943148782,2.520993948\C,0,1.544710472,3.391236367,0.65
2730732\C,0,-1.083807114,2.724070013,1.51542323\C,0,-0.901425845,0.382
896267,3.155596033\C,0,1.835879859,-0.355175632,3.321734306\C,0,3.3469
9199,1.496638061,1.777432466\C,0,0.418518758,3.540083027,-0.248978528\
C,0,-2.109642548,1.687603336,1.437092654\C,0,-0.531662723,-1.021075944
,3.181392464\C,0,2.977907706,-0.816100329,2.558960567\C,0,3.564392269,
1.997128254,0.429490855\C,0,2.683437521,2.924568245,-0.121710062\C,0,-
0.867225348,3.222583333,0.173111951\C,0,-2.00183667,0.53122576,2.23167
243\C,0,0.808202072,-1.385408583,3.265477706\C,0,3.716258631,0.0899966
05,1.79692642\C,0,0.862330353,3.150557851,-1.583804668\C,0,-2.49509195
2,1.558186458,0.073656296\C,0,0.00255347,2.463967628,-2.44839454\C,0,-
1.424698634,-1.740255459,2.285080156\C,0,2.652704705,-2.12732478,2.018
623287\C,0,4.067245791,0.898239616,-0.379730121\C,0,2.259916849,2.7850
90226,-1.505512021\C,0,-1.762230509,2.487295817,-0.716259957\C,0,-2.35
1384082,-0.788198759,1.706446072\C,0,1.317062312,-2.483475353,2.460391
064\C,0,4.161808086,-0.276354925,0.466047919\C,0,3.850295826,-1.536675
497,-0.052229255\C,0,-0.00749737,-2.892398982,-1.933539285\C,0,-0.9266
69527,-1.937906414,-2.513364764\C,0,-0.161241346,-1.004156763,-3.31140
1848\C,0,1.241091424,-1.381892213,-3.226018215\C,0,1.335347754,-2.5557
96384,-2.376598636\C,0,-0.216983206,-3.374572611,-0.63510056\C,0,-2.02
3810214,-1.481215569,-1.764707379\C,0,-0.520042687,0.342300489,-3.3229
06803\C,0,2.224225692,-0.395058964,-3.16345534\C,0,2.410979172,-2.6995
41529,-1.5009692\C,0,-1.354016136,-2.921673899,0.135758541\C,0,-2.4069
20916,-0.104956604,-1.811097395\C,0,0.507407074,1.371163576,-3.2604509
61\C,0,3.34107408,-0.542624379,-2.248672291\C,0,2.193425803,-3.2003165
7,-0.15251526\C,0,0.908399203,-3.538640552,0.270101923\C,0,-2.24157397
8,-1.982496336,-0.414626852\C,0,-1.663592891,0.794853722,-2.556531943\
C,0,1.848175034,1.008920118,-3.181994533\C,0,3.436854498,-1.674617532,
-1.436798132\C,0,-0.940145129,-2.797269715,1.517039555\C,0,-3.08074794
2,0.289147026,-0.49210782\C,0,3.66659656,0.769158747,-1.709977727\C,0,
3.085785888,-2.482906068,0.739689549\C,0,0.462074799,-3.175351233,1.60
3286568\C,0,-2.76209005,-0.922562958,0.390732005\C,0,-1.319931214,2.10
0829265,-1.994948504\C,0,2.739555264,1.725180224,-2.280299789\H,0,-4.1
71517436,0.417554455,-0.620297294\Version=AM64L-G03RevD.02\State=1-A\
HF=-2272.1599351\MP2=-2279.9518276\RMSD=9.128e-09\Thermal=0.\PG=C01 [X
(C60H1)]\@

B3LYP/6-31G(d)

Zero-point correction= 0.386256 (Hartree/Particle)
 Thermal correction to Energy= 0.407200
 Thermal correction to Enthalpy= 0.408144
 Thermal correction to Gibbs Free Energy= 0.343032
 Sum of electronic and zero-point Energies= -2286.135746
 Sum of electronic and thermal Energies= -2286.114803
 Sum of electronic and thermal Enthalpies= -2286.113859
 Sum of electronic and thermal Free Energies= -2286.178970

1\1\FAU-CCC-CCDH160\Freq\RB3LYP\6-31G(d)\C60H1(1+)\DRAL\06-Dec-2008\0\
 \#P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq\C
 60H(+)\1,1\C,1.335889335,2.9106239932,1.9469485934\C,-0.0052015732,2.
 5647021386,2.3775655394\C,0.0889066433,1.369973135,3.2107102162\C,1.48
 331856,0.9972727018,3.308546306\C,2.2570987687,1.9431487825,2.52099394
 85\C,1.5447104716,3.3912363666,0.6527307316\C,-1.0838071137,2.72407001
 26,1.5154232305\C,-0.9014258454,0.3828962666,3.1555960327\C,1.83587985
 92,-0.3551756325,3.3217343061\C,3.3469919899,1.4966380613,1.7774324657
 \C,0.4185187583,3.5400830266,-0.2489785281\C,-2.1096425482,1.687603335
 6,1.4370926541\C,-0.5316627231,-1.0210759441,3.1813924636\C,2.97790770
 62,-0.8161003288,2.5589605671\C,3.5643922693,1.9971282544,0.4294908547
 \C,2.6834375206,2.9245682446,-0.1217100616\C,-0.8672253484,3.222583333
 ,0.1731119511\C,-2.0018366705,0.5312257603,2.2316724298\C,0.8082020719
 ,-1.3854085828,3.2654777062\C,3.7162586314,0.0899966048,1.7969264201\C
 ,0.8623303527,3.150557851,-1.5838046675\C,-2.4950919519,1.5581864583,0
 .0736562955\C,0.0025534699,2.4639676284,-2.4483945403\C,-1.424698634,-
 1.7402554592,2.2850801565\C,2.6527047054,-2.12732478,2.018623287\C,4.0
 672457908,0.8982396157,-0.379730121\C,2.2599168486,2.785090226,-1.5055
 120214\C,-1.7622305087,2.4872958168,-0.7162599567\C,-2.3513840822,-0.7
 881987593,1.7064460719\C,1.3170623115,-2.4834753531,2.4603910638\C,4.1
 618080857,-0.2763549246,0.4660479191\C,3.8502958259,-1.5366754967,-0.0
 522292551\C,-0.0074973697,-2.8923989823,-1.9335392849\C,-0.9266695271,
 -1.9379064135,-2.5133647645\C,-0.1612413462,-1.0041567627,-3.311401848
 1\C,1.2410914236,-1.3818922126,-3.2260182153\C,1.3353477543,-2.5557963
 842,-2.3765986364\C,-0.2169832056,-3.3745726113,-0.6351005598\C,-2.023
 8102138,-1.4812155686,-1.764707379\C,-0.5200426866,0.3423004888,-3.322
 9068027\C,2.2242256917,-0.3950589635,-3.1634553397\C,2.4109791722,-2.6
 995415287,-1.5009692\C,-1.3540161364,-2.9216738986,0.1357585411\C,-2.4
 069209158,-0.1049566038,-1.8110973947\C,0.5074070735,1.3711635759,-3.2
 604509606\C,3.3410740805,-0.5426243786,-2.2486722906\C,2.1934258032,-3
 .2003165695,-0.1525152603\C,0.9083992031,-3.538640552,0.270101923\C,-2
 .2415739785,-1.9824963358,-0.4146268519\C,-1.6635928908,0.7948537219,-
 2.5565319433\C,1.8481750341,1.008920118,-3.1819945333\C,3.4368544976,-
 1.6746175318,-1.4367981322\C,-0.9401451286,-2.7972697154,1.5170395553\
 C,-3.0807479423,0.2891470256,-0.4921078196\C,3.6665965601,0.769158747,
 -1.7099777274\C,3.0857858883,-2.482906068,0.7396895486\C,0.4620747988,
 -3.1753512329,1.6032865684\C,-2.7620900498,-0.9225629578,0.390732005\C
 ,-1.319931214,2.1008292654,-1.9949485044\C,2.7395552641,1.7251802237,-

2.2802997893\H,-4.1715174363,0.4175544548,-0.6202972942\\Version=AM64L
 -G03RevD.02\State=1-A\HF=-2286.5220028\RMSD=7.547e-09\RMSF=1.289e-04\Z
 eroPoint=0.3862565\Thermal=0.4071997\ZPE=242.3795834\Dipole=-1.3225143
 ,0.3381731,-0.0875786\DipoleDeriv=0.0340084,0.03376,0.0533342,-0.04462
 ,0.1029411,-0.0012771,-0.0029744,0.0031844,0.0991442\Polar=494.6864842
 ,-4.0218731,474.5830444,1.4604566,-1.2830299,476.0469916\PG=C01 [X(C60
 H1)]\NImag=0\0.51963888,-0.03788030,0.33261909,-0.06057145,-0.2209834
 2,-0.00016903,0.03207444,-0.00244657,0.04666490\0.00031149,0.00002639
 618,0.00009581,-0.00013779,0.00011746,0.00002798\\@

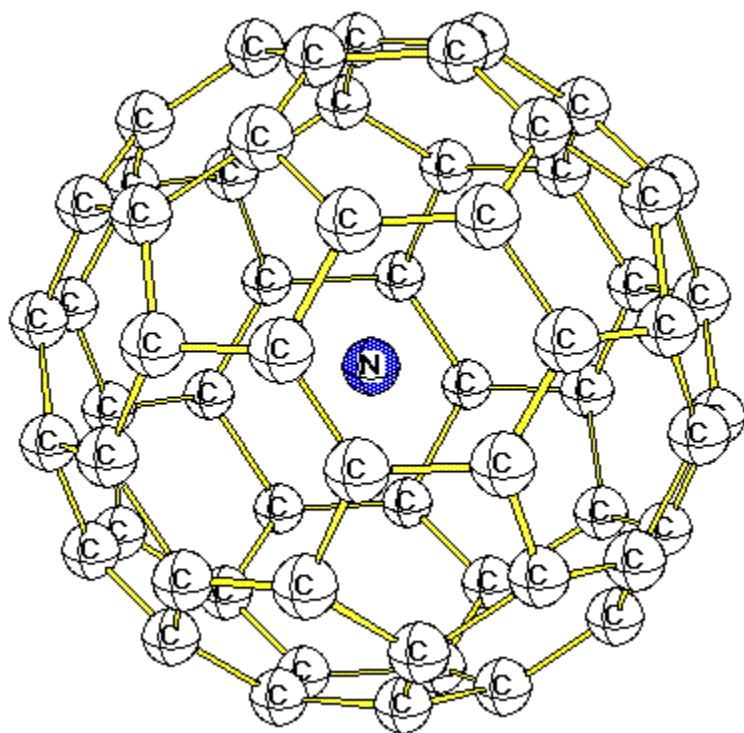
1^{...} (N@C₆₀, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN091\SP\ROMP2-FC\6-31G(d)\C60N1(4)\DRAL\20-Mar-2010\0\\
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 \C,0,3.0187238394,0.8145178169,1.6773646387\C,0,3.4995809282,0.4890290
 296,0.3450723739\C,0,3.1310756404,1.5789746039,-0.5431905251\C,0,2.426
 58377,2.5799544988,0.2407061545\C,0,2.3563819322,2.1062229581,1.613506
 5574\C,0,2.5108537438,-0.19026916,2.5012490273\C,0,3.4493277488,-0.828
 9252207,-0.1106067699\C,0,2.7289897123,1.3074733977,-1.8516760698\C,0,
 1.3469771651,3.2676816985,-0.3148428744\C,0,1.2119232545,2.3432638976,
 2.377798889\C,0,2.460350819,-1.5633435641,2.0272301381\C,0,3.032124541
 7,-1.1114674506,-1.4736210523\C,0,1.6050754042,2.0243427864,-2.4292876
 333\C,0,0.1540096667,3.5109219567,0.4787298858\C,0,0.681785962,1.29571
 30074,3.2359968418\C,0,1.3181402263,0.0546643871,3.2953237008\C,0,2.91
 95266546,-1.8754285584,0.7475097537\C,0,2.6792865501,-0.0646466924,-2.
 326983388\C,0,0.9285824444,2.9852973325,-1.6779118579\C,0,0.0878631614
 ,3.0598542974,1.7977876\C,0,1.2371857956,-2.1682216733,2.5287129905\C,
 0,2.2436791221,-2.3317804172,-1.4575961177\C,0,0.5216258889,-3.0615723
 78,1.7285556651\C,0,0.8610402591,1.0959172874,-3.2631670614\C,0,-1.001
 2522597,3.3805410633,-0.3936583251\C,0,-0.7697741861,1.364724172,3.184
 9272329\C,0,0.5308408706,-1.1673062957,3.3119849467\C,0,2.1745015312,-
 2.803841038,-0.0852808814\C,0,1.524557193,-0.1957726088,-3.1988888982\
 C,0,-0.52229595,3.0563103443,-1.7269508695\C,0,-1.1361822638,2.4539086
 394,2.2955514482\C,0,-2.2452594385,2.3287843801,1.4584653645\C,0,-3.02
 0238554,-0.8185609626,-1.6771134924\C,0,-2.3579856539,-2.1104894692,-1
 .6134329683\C,0,-2.4271431235,-2.5836351484,-0.2401883705\C,0,-3.13173
 18748,-1.5827576505,0.5438830283\C,0,-3.5003770024,-0.4927503023,-0.34
 43349539\C,0,-2.51073254,0.1863627112,-2.4996849083\C,0,-1.2121601038,
 -2.3454256233,-2.3758587854\C,0,-1.3475764456,-3.2716321528,0.31562427
 78\C,0,-2.7307714252,-1.3117857448,1.8532078182\C,0,-3.4519246597,0.82
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 0,-0.0885292009,-3.0611811729,-1.7955563832\C,0,-0.9297251682,-2.99016
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 2.0251883628\C,0,-0.682581441,-1.2991497307,-3.2352425853\C,0,-0.15464
 16347,-3.5170247983,-0.4780442964\C,0,-1.6073021579,-2.0298223758,2.43

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 ,1.1636929916,-3.3116611015\C,0,1.1350140077,-2.4567231799,-2.29437143
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 (C60N1)]\@

UB3LYP/6-31G(d)



0 4

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C	3.499580928	0.489029030	0.345072374
C	3.131075640	1.578974604	-0.543190525
C	2.426583770	2.579954499	0.240706154
C	2.356381932	2.106222958	1.613506557
C	2.510853744	-0.190269160	2.501249027
C	3.449327749	-0.828925221	-0.110606770
C	2.728989712	1.307473398	-1.851676070
C	1.346977165	3.267681698	-0.314842874
C	1.211923254	2.343263898	2.377798889
C	2.460350819	-1.563343564	2.027230138
C	3.032124542	-1.111467451	-1.473621052
C	1.605075404	2.024342786	-2.429287633
C	0.154009667	3.510921957	0.478729886
C	0.681785962	1.295713007	3.235996842
C	1.318140226	0.054664387	3.295323701

C 2.919526655 -1.875428558 0.747509754
 C 2.679286550 -0.064646692 -2.326983388
 C 0.928582444 2.985297332 -1.677911858
 C 0.087863161 3.059854297 1.797787600
 C 1.237185796 -2.168221673 2.528712990
 C 2.243679122 -2.331780417 -1.457596118
 C 0.521625889 -3.061572378 1.728555665
 C 0.861040259 1.095917287 -3.263167061
 C -1.001252260 3.380541063 -0.393658325
 C -0.769774186 1.364724172 3.184927233
 C 0.530840871 -1.167306296 3.311984947
 C 2.174501531 -2.803841038 -0.085280881
 C 1.524557193 -0.195772609 -3.198888898
 C -0.522295950 3.056310344 -1.726950870
 C -1.136182264 2.453908639 2.295551448
 C -2.245259438 2.328784380 1.458465364
 C -3.020238554 -0.818560963 -1.677113492
 C -2.357985654 -2.110489469 -1.613432968
 C -2.427143124 -2.583635148 -0.240188370
 C -3.131731875 -1.582757650 0.543883028
 C -3.500377002 -0.492750302 -0.344334954
 C -2.510732540 0.186362711 -2.499684908
 C -1.212160104 -2.345425623 -2.375858785
 C -1.347576446 -3.271632153 0.315624278
 C -2.730771425 -1.311785745 1.853207818
 C -3.451924660 0.825672948 0.111535220
 C -1.318921158 -0.058280769 -3.294711711
 C -0.088529201 -3.061181173 -1.795556383
 C -0.929725168 -2.990167603 1.679495177
 C -2.681576659 0.060865761 2.328566182
 C -2.921919082 1.872865512 -0.746792553
 C -2.459911358 1.558820467 -2.025188363
 C -0.682581441 -1.299149731 -3.235242585
 C -0.154641635 -3.517024798 -0.478044296
 C -1.607302158 -2.029822376 2.432179352
 C -3.034449211 1.108225841 1.474894120
 C -0.531889793 1.163692992 -3.311661102
 C 1.135014008 -2.456723180 -2.294371439
 C -1.526200480 0.192059796 3.200680417
 C -2.177831982 2.803026029 0.086256167
 C -1.237644872 2.163874875 -2.527351586
 C 0.768759622 -1.368316308 -3.184278191
 C 1.000714730 -3.386174943 0.394857154
 C -0.862639053 -1.100314341 3.265826353
 N -0.094452394 -0.020601474 0.063208183

Zero-point correction= 0.375218 (Hartree/Particle)
 Thermal correction to Energy= 0.398521
 Thermal correction to Enthalpy= 0.399465
 Thermal correction to Gibbs Free Energy= 0.325688

Sum of electronic and zero-point Energies= -2340.381492
 Sum of electronic and thermal Energies= -2340.358189
 Sum of electronic and thermal Enthalpies= -2340.357245
 Sum of electronic and thermal Free Energies= -2340.431022

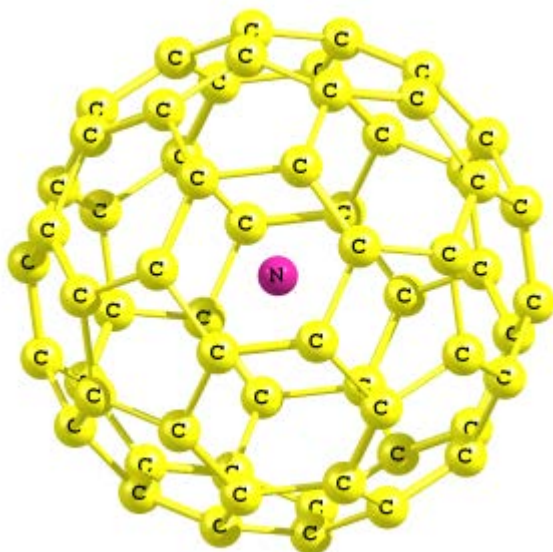
1\1\FAU-CCC-CCDH158\Freq\UB3LYP\6-31G(d)\C60N1(4)\DRAL\13-Nov-2008\0\N Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq\N@C60_quartet\0,4\C,3.0187238394,0.8145178169,1.6773646387\C,3.4995809282,0.4890290296,0.3450723739\C,3.1310756404,1.5789746039,-0.5431905251\C,2.42658377,2.5799544988,0.2407061545\C,2.3563819322,2.1062229581,1.6135065574\C,2.5108537438,-0.19026916,2.5012490273\C,3.4493277488,-0.8289252207,-0.1106067699\C,2.7289897123,1.3074733977,-1.8516760698\C,1.3469771651,3.2676816985,-0.3148428744\C,1.2119232545,2.3432638976,2.377798889\C,2.460350819,-1.5633435641,2.0272301381\C,3.0321245417,-1.1114674506,-1.4736210523\C,1.6050754042,2.0243427864,-2.4292876333\C,0.1540096667,3.5109219567,0.4787298858\C,0.681785962,1.2957130074,3.2359968418\C,1.3181402263,0.0546643871,3.2953237008\C,2.9195266546,-1.8754285584,0.7475097537\C,2.6792865501,-0.0646466924,-2.326983388\C,0.9285824444,2.9852973325,-1.6779118579\C,0.0878631614,3.0598542974,1.7977876\C,1.2371857956,-2.1682216733,2.5287129905\C,2.2436791221,-2.3317804172,-1.4575961177\C,0.5216258889,-3.061572378,1.7285556651\C,0.8610402591,1.0959172874,-3.2631670614\C,-1.0012522597,3.3805410633,-0.3936583251\C,-0.7697741861,1.364724172,3.1849272329\C,0.5308408706,-1.1673062957,3.3119849467\C,2.1745015312,-2.803841038,-0.0852808814\C,1.524557193,-0.1957726088,-3.1988888982\C,-0.52229595,3.0563103443,-1.7269508695\C,-1.1361822638,2.4539086394,2.2955514482\C,-2.2452594385,2.3287843801,1.4584653645\C,-3.020238554,-0.8185609626,-1.6771134924\C,-2.3579856539,-2.1104894692,-1.6134329683\C,-2.4271431235,-2.5836351484,-0.2401883705\C,-3.1317318748,-1.5827576505,0.5438830283\C,-3.5003770024,-0.4927503023,-0.3443349539\C,-2.51073254,0.1863627112,-2.4996849083\C,-1.2121601038,-2.3454256233,-2.3758587854\C,-1.3475764456,-3.2716321528,0.3156242778\C,-2.7307714252,-1.3117857448,1.8532078182\C,-3.4519246597,0.8256729479,0.1115352202\C,-1.3189211578,-0.0582807686,-3.2947117111\C,-0.0885292009,-3.0611811729,-1.7955563832\C,-0.9297251682,-2.9901676027,1.6794951774\C,-2.6815766593,0.0608657606,2.3285661817\C,-2.9219190815,1.8728655122,-0.7467925534\C,-2.4599113585,1.5588204671,-2.0251883628\C,-0.682581441,-1.2991497307,-3.2352425853\C,-0.1546416347,-3.5170247983,-0.4780442964\C,-1.6073021579,-2.0298223758,2.4321793523\C,-3.0344492106,1.1082258407,1.4748941195\C,-0.5318897932,1.1636929916,-3.3116611015\C,1.1350140077,-2.4567231799,-2.2943714394\C,-1.5262004802,0.1920597964,3.2006804169\C,-2.1778319823,2.8030260287,0.0862561672\C,-1.2376448721,2.1638748752,-2.5273515856\C,0.7687596216,-1.3683163081,-3.1842781912\C,1.0007147298,-3.3861749431,0.3948571538\C,-0.862639053,-1.1003143408,3.2658263527\N,-0.0944523944,-0.0206014737,0.0632081832\Version=AM64L-G03RevD.02\State=4-A\HF=-2340.75671\S2=3.752695\S2-1=0.\S2A=3.75\RMSD=6.365e-09\RMSF=2.872e-04\ZeroPoint=0.3752184\Thermal=0.3985211\ZPE=235.4530842\Dipole=0.0026969,0.0004788,-0.0040153\DipoleDeri,0.0000066,0.0076549\Polar=469.3684322,0.044374,469.4451644,0.0167194,-0.0216858,469.4104505\PG=C01 [X(C60N1)]\NImag=0\0.28556878,-0.0375580013796,-0.00008490,-0.00125894,0.00003334,0.00089127\0.00017575,-0.

016193,-0.00027711,0.00024958,-0.00009497,0.00005242,-0.00002745\\@

1• (N@C₆₀, doublet)

ROMP2/6-31G*//UB3LYP/6-31G*

```
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,0.748669202,-2.690941772\C,0.449182664,3.010905501,-1.828224435\C,1.7
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,-2.552458693\C,-1.556902891,1.980720262,-2.496024353\C,3.017284763,1.
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UB3LYP/6-31G(d)

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C	-0.078204835	-0.220090968	-3.537869340
C	0.574078561	1.062741678	-3.336343856
C	2.502975412	1.645309392	-1.912639620
C	2.871738046	-1.179303956	-1.749835503
C	0.434879340	-2.423398554	-2.553659051
C	-1.429231810	-0.374219128	-3.223264417
C	-0.150320274	2.140819061	-2.826278678
C	3.287438160	1.076097204	-0.829754764
C	2.409939492	-2.381993733	-1.075101770
C	-0.972067593	-2.584531391	-2.224468602
C	-2.183711588	0.748669202	-2.690941772
C	0.449182664	3.010905501	-1.828224435
C	1.749021541	2.768583451	-1.381236855
C	3.463418513	-0.305607122	-0.748775004
C	1.219241669	-2.993199074	-1.470921290
C	-1.885249416	-1.580869088	-2.552458693
C	-1.556902891	1.980720262	-2.496024353
C	3.017284763	1.847707086	0.371838546
C	2.726721773	-2.256216994	0.337416872
C	2.934577335	1.206029214	1.607929193
C	-1.057314862	-3.253231593	-0.936678109
C	-3.105811380	0.236185976	-1.690372840
C	-0.586685036	3.388350496	-0.881143342
C	2.066752872	2.893562931	0.031268828
C	3.380065002	-0.973717614	0.539242945
C	0.296849227	-3.505328495	-0.471287372
C	-2.921525354	-1.203569200	-1.604944316

C -1.826592488 2.751590535 -1.293459347
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 C -0.419840752 2.426305324 2.558976224
 C -2.850853999 1.178150921 1.750916668
 C -1.734549542 -2.767093612 1.385693620
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 C -0.434387233 -3.009035101 1.832381485
 C 2.197547424 -0.745461275 2.693025656
 C 0.986341317 2.587154744 2.228568039
 C -2.394561446 2.384469277 1.079763393
 C -2.052549591 -2.891639294 -0.027260405
 C 1.841224767 -2.748258744 1.297243406
 C -0.281578626 3.507904498 0.475446493
 C -3.365343442 0.976682528 -0.535474708
 C -3.003501165 -1.845824991 -0.367903755
 C 0.601880428 -3.385613441 0.885051019
 C 3.118251575 -0.232819601 1.692482419
 C 1.072010481 3.255789841 0.940818790
 N -0.376306531 -0.060315442 -0.103882641

Zero-point correction= 0.375631 (Hartree/Particle)
 Thermal correction to Energy= 0.398542
 Thermal correction to Enthalpy= 0.399486
 Thermal correction to Gibbs Free Energy= 0.329352
 Sum of electronic and zero-point Energies= -2340.340173
 Sum of electronic and thermal Energies= -2340.317263
 Sum of electronic and thermal Enthalpies= -2340.316318
 Sum of electronic and thermal Free Energies= -2340.386452

1\1\FAU-CCC-CCDH157\Freq\UB3LYP\6-31G(d)\C60N1(2)\DRAL\19-Apr-2009\0\
 #P UB3LYP/6-31G* scf=qc Freq=NoRaman Pop=None Name=DrAl scfcyc=600\N@
 C60 doublet\0,2\C,1.92803421,0.810094135,-2.870957611\C,2.111403207,-
 0.628603315,-2.78316135\C,0.872686181,-1.265424084,-3.197376137\C,-0.0
 78204835,-0.220090968,-3.53786934\C,0.574078561,1.062741678,-3.3363438
 56\C,2.502975412,1.645309392,-1.91263962\C,2.871738046,-1.179303956,-1
 .749835503\C,0.43487934,-2.423398554,-2.553659051\C,-1.42923181,-0.374
 219128,-3.223264417\C,-0.150320274,2.140819061,-2.826278678\C,3.287438
 16,1.076097204,-0.829754764\C,2.409939492,-2.381993733,-1.07510177\C,-

0.972067593,-2.584531391,-2.224468602\C,-2.183711588,0.748669202,-2.69
 0941772\C,0.449182664,3.010905501,-1.828224435\C,1.749021541,2.7685834
 51,-1.381236855\C,3.463418513,-0.305607122,-0.748775004\C,1.219241669,
 -2.993199074,-1.47092129\C,-1.885249416,-1.580869088,-2.552458693\C,-1
 .556902891,1.980720262,-2.496024353\C,3.017284763,1.847707086,0.371838
 546\C,2.726721773,-2.256216994,0.337416872\C,2.934577335,1.206029214,1
 .607929193\C,-1.057314862,-3.253231593,-0.936678109\C,-3.10581138,0.23
 6185976,-1.69037284\C,-0.586685036,3.388350496,-0.881143342\C,2.066752
 872,2.893562931,0.031268828\C,3.380065002,-0.973717614,0.539242945\C,0
 .296849227,-3.505328495,-0.471287372\C,-2.921525354,-1.2035692,-1.6049
 44316\C,-1.826592488,2.751590535,-1.293459347\C,-2.71215221,2.25979860
 2,-0.333173003\C,-1.91258384,-0.808286542,2.875808328\C,-0.559025093,-
 1.060574088,3.341342478\C,0.093188764,0.222718751,3.542956706\C,-0.857
 301362,1.268086225,3.202870847\C,-2.096945952,0.630992112,2.79034928\C
 ,-2.488849895,-1.644436574,1.918301612\C,0.164916077,-2.138277614,2.82
 9977777\C,1.443030626,0.377053637,3.225396216\C,-0.419840752,2.4263053
 24,2.558976224\C,-2.850853999,1.178150921,1.750916668\C,-1.734549542,-
 2.767093612,1.38569362\C,1.570989328,-1.977276241,2.498897388\C,1.8987
 54818,1.58312648,2.555045996\C,-1.203822844,2.995716255,1.475595971\C,
 -3.450673178,0.30776113,0.75278259\C,-3.273220232,-1.074802948,0.83480
 9617\C,-0.434387233,-3.009035101,1.832381485\C,2.197547424,-0.74546127
 5,2.693025656\C,0.986341317,2.587154744,2.228568039\C,-2.394561446,2.3
 84469277,1.079763393\C,-2.052549591,-2.891639294,-0.027260405\C,1.8412
 24767,-2.748258744,1.297243406\C,-0.281578626,3.507904498,0.475446493\
 C,-3.365343442,0.976682528,-0.535474708\C,-3.003501165,-1.845824991,-0
 .367903755\C,0.601880428,-3.385613441,0.885051019\C,3.118251575,-0.232
 819601,1.692482419\C,1.072010481,3.255789841,0.94081879\N,-0.376306531
 ,-0.060315442,-0.103882641\\Version=AM64L-G03RevD.02\\State=2-A\\HF=-
 2340.7158046\\S2=1.754141\\S2-1=0.\\S2A=0.76392\\RMSD=0.000e+00\\RMSF=3.709e-0
 4\\ZeroPoint=0.3756312\\Thermal=0.398542\\ZPE=235.7121642\\Dipole=-0.00841
 97,-0.0003049,-0.0033504\\DipoleDeriv=0.0700592,-0.0094194,0.0253929,-0
 2,-0.0000624,0.0143693,-0.0002301,0.0020373,-0.0002316,0.0144566\\Polar
 =469.9299074,-0.0056807,469.6053167,0.0224031,0.0162257,469.3591516\\PG
 =C01 [X(C60N1)]\\NImag=0\\0.46419510,0.01208087,0.57605404,0.20009556,0
 00013265,0.00048710,-0.00037586,0.00604482\\0.00030561,0.00004538,-0.0
 78,-0.00322704,-0.00043461,-0.00099072\\\\@

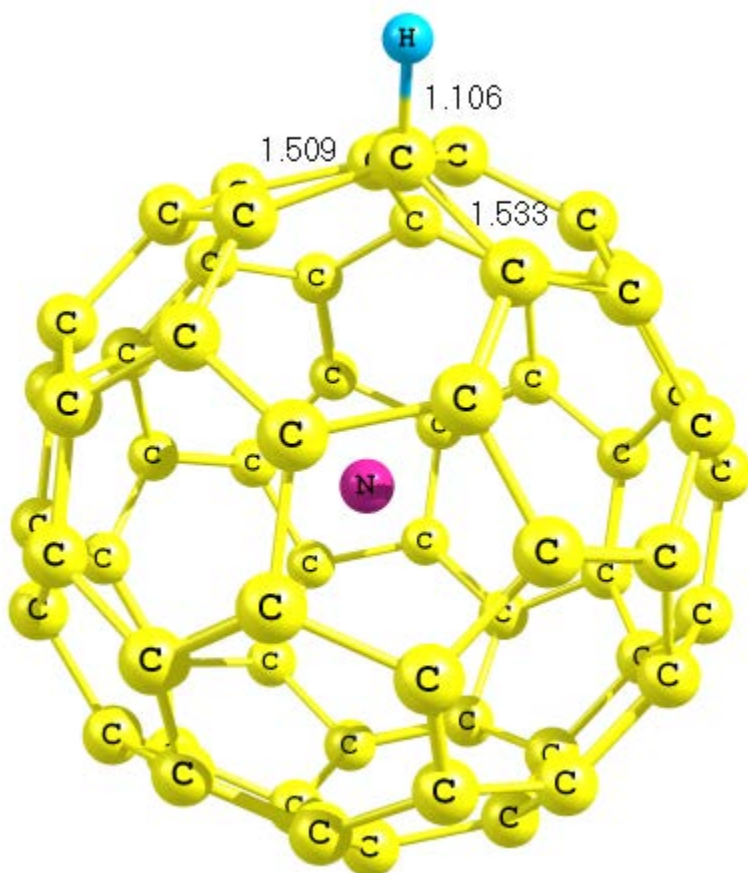
2a⁺ (N@C₆₀H⁺⁺⁺, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\\FAU-CCC-CCDN088\\SP\\ROMP2-FC\\6-31G(d)\\C60H1N1(1+,4)\\DRAL\\21-Mar-201
 0\\0\\#P ROMP2/6-31G* Geom=AllCheck Guess=Read Name=Dral\\N@C60H(+) qua
 rtet DFT SP\\1,4\\C,0,1.228022025,3.271684064,0.698267244\\C,0,-0.032041
 294,3.256580536,1.416802799\\C,0,0.132420816,2.398675082,2.586191692\\C,
 0,1.493281231,1.906858156,2.597005012\\C,0,2.171615479,2.43731919,1.425
 401197\\C,0,1.228022025,3.271684064,-0.698267244\\C,0,-1.237206658,3.259
 168364,0.724263522\\C,0,-0.915570475,1.580533653,3.022993829\\C,0,1.7511

60347,0.600393508,3.022315709\C,0,3.07488068,1.638708843,0.727118392\C,0,-0.032041294,3.256580536,-1.416802799\C,0,-2.326975555,2.391268608,1.161962719\C,0,-0.642058036,0.227657029,3.475020832\C,0,2.700696589,-0.22449235,2.302856259\C,0,3.07488068,1.638708843,-0.727118392\C,0,2.171615479,2.43731919,-1.425401197\C,0,-1.237206658,3.259168364,-0.724263522\C,0,-2.154379147,1.555079847,2.280556521\C,0,0.663356514,-0.25396673,3.478049227\C,0,3.346448357,0.281414527,1.174113684\C,0,0.132420816,2.398675082,-2.586191692\C,0,-2.963990775,1.872221401,0.\C,0,-0.915570475,1.580533653,-3.022993829\C,0,-1.73044014,-0.628062828,3.025439273\C,0,2.194588475,-1.58856281,2.301810553\C,0,3.346448357,0.281414527,-1.174113684\C,0,1.493281231,1.906858156,-2.597005012\C,0,-2.326975555,2.391268608,-1.161962719\C,0,-2.681319872,0.19045888,2.300016114\C,0,0.941509067,-1.61000729,3.033617514\C,0,3.515560507,-0.553658951,0.\C,0,3.031064958,-1.865117882,0.\C,0,-1.190007522,-3.268553368,-0.700589663\C,0,-2.133364425,-2.448710714,-1.429071364\C,0,-1.466433699,-1.930645328,-2.604633051\C,0,-0.100464952,-2.431953673,-2.605060372\C,0,0.06887034,-3.265440211,-1.427760974\C,0,-1.190007522,-3.268553368,0.700589663\C,0,-3.041239407,-1.637921574,-0.728263516\C,0,-1.73044014,-0.628062828,-3.025439273\C,0,0.941509067,-1.61000729,-3.033617514\C,0,1.274582484,-3.247463924,-0.727389761\C,0,-2.133364425,-2.448710714,1.429071364\C,0,-3.332807348,-0.315673096,-1.18765514\C,0,-0.642058036,0.227657029,-3.475020832\C,0,2.194588475,-1.58856281,-2.301810553\C,0,1.274582484,-3.247463924,0.727389761\C,0,0.06887034,-3.265440211,1.427760974\C,0,-3.041239407,-1.637921574,0.728263516\C,0,-2.681319872,0.19045888,-2.300016114\C,0,0.663356514,-0.25396673,-3.478049227\C,0,2.361245905,-2.394838027,-1.173963139\C,0,-1.466433699,-1.930645328,2.604633051\C,0,-3.725759595,0.570174761,0.\C,0,2.700696589,-0.22449235,-2.302856259\C,0,2.361245905,-2.394838027,1.173963139\C,0,-0.100464952,-2.431953673,2.605060372\C,0,-3.332807348,-0.315673096,1.18765514\C,0,-2.154379147,1.555079847,-2.280556521\C,0,1.751160347,0.600393508,-3.022315709\N,0,-0.142554427,0.080195955,0.\H,0,-4.810364938,0.785275544,0.\Versio
n=AM64L-G03RevD.02\State=4-A\"HF=-2326.5373498\MP2=-2334.4194086\RMSD=5.584e-09\Thermal=0.\PG=CS [SG(C4H1N1),X(C56)]\@

UB3LYP/6-31G(d)



1 4

C	1.228022025	3.271684064	0.698267244
C	-0.032041294	3.256580536	1.416802799
C	0.132420816	2.398675082	2.586191692
C	1.493281231	1.906858156	2.597005012
C	2.171615479	2.437319190	1.425401197
C	1.228022025	3.271684064	-0.698267244
C	-1.237206658	3.259168364	0.724263522
C	-0.915570475	1.580533653	3.022993829
C	1.751160347	0.600393508	3.022315709
C	3.074880680	1.638708843	0.727118392
C	-0.032041294	3.256580536	-1.416802799
C	-2.326975555	2.391268608	1.161962719
C	-0.642058036	0.227657029	3.475020832
C	2.700696589	-0.224492350	2.302856259
C	3.074880680	1.638708843	-0.727118392
C	2.171615479	2.437319190	-1.425401197
C	-1.237206658	3.259168364	-0.724263522
C	-2.154379147	1.555079847	2.280556521
C	0.663356514	-0.253966730	3.478049227
C	3.346448357	0.281414527	1.174113684
C	0.132420816	2.398675082	-2.586191692
C	-2.963990775	1.872221401	0.000000000

C	-0.915570475	1.580533653	-3.022993829
C	-1.730440140	-0.628062828	3.025439273
C	2.194588475	-1.588562810	2.301810553
C	3.346448357	0.281414527	-1.174113684
C	1.493281231	1.906858156	-2.597005012
C	-2.326975555	2.391268608	-1.161962719
C	-2.681319872	0.190458880	2.300016114
C	0.941509067	-1.610007290	3.033617514
C	3.515560507	-0.553658951	0.000000000
C	3.031064958	-1.865117882	0.000000000
C	-1.190007522	-3.268553368	-0.700589663
C	-2.133364425	-2.448710714	-1.429071364
C	-1.466433699	-1.930645328	-2.604633051
C	-0.100464952	-2.431953673	-2.605060372
C	0.068870340	-3.265440211	-1.427760974
C	-1.190007522	-3.268553368	0.700589663
C	-3.041239407	-1.637921574	-0.728263516
C	-1.730440140	-0.628062828	-3.025439273
C	0.941509067	-1.610007290	-3.033617514
C	1.274582484	-3.247463924	-0.727389761
C	-2.133364425	-2.448710714	1.429071364
C	-3.332807348	-0.315673096	-1.187655140
C	-0.642058036	0.227657029	-3.475020832
C	2.194588475	-1.588562810	-2.301810553
C	1.274582484	-3.247463924	0.727389761
C	0.068870340	-3.265440211	1.427760974
C	-3.041239407	-1.637921574	0.728263516
C	-2.681319872	0.190458880	-2.300016114
C	0.663356514	-0.253966730	-3.478049227
C	2.361245905	-2.394838027	-1.173963139
C	-1.466433699	-1.930645328	2.604633051
C	-3.725759595	0.570174761	0.000000000
C	2.700696589	-0.224492350	-2.302856259
C	2.361245905	-2.394838027	1.173963139
C	-0.100464952	-2.431953673	2.605060372
C	-3.332807348	-0.315673096	1.187655140
C	-2.154379147	1.555079847	-2.280556521
C	1.751160347	0.600393508	-3.022315709
N	-0.142554427	0.080195955	0.000000000
H	-4.810364938	0.785275544	0.000000000

Zero-point correction=	0.386533 (Hartree/Particle)
Thermal correction to Energy=	0.409835
Thermal correction to Enthalpy=	0.410779
Thermal correction to Gibbs Free Energy=	0.338566
Sum of electronic and zero-point Energies=	-2340.717945
Sum of electronic and thermal Energies=	-2340.694643
Sum of electronic and thermal Enthalpies=	-2340.693699
Sum of electronic and thermal Free Energies=	-2340.765912

1\1\FAU-CCC-CCDH156\Freq\UB3LYP/6-31G(d)\C60H1N1(1+,4)\DRAL\03-Dec-2008\0\#P Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Freq\N@C60H+\1,4\C,1.2280220251,3.2716840641,0.6982672445\C,-0.0320412943,3.2565805356,1.4168027991\C,0.1324208161,2.3986750818,2.586191692\C,1.493281231,1.906858156,2.5970050119\C,2.1716154789,2.4373191905,1.4254011971\C,1.2280220251,3.2716840641,-0.6982672445\C,-1.2372066577,3.2591683637,0.7242635221\C,-0.9155704746,1.5805336529,3.0229938288\C,1.7511603471,0.6003935077,3.0223157093\C,3.0748806803,1.6387088432,0.727183921\C,-0.0320412943,3.2565805356,-1.4168027991\C,-2.3269755546,2.3912686078,1.1619627194\C,-0.6420580356,0.2276570293,3.4750208321\C,2.7006965887,-0.2244923498,2.3028562594\C,3.0748806803,1.6387088432,-0.7271183921\C,2.1716154789,2.4373191905,-1.4254011971\C,-1.2372066577,3.2591683637,-0.7242635221\C,-2.1543791474,1.555079847,2.2805565206\C,0.663356514,-0.2539667301,3.4780492269\C,3.3464483573,0.2814145268,1.1741136845\C,0.1324208161,2.3986750818,-2.586191692\C,-2.9639907748,1.872221401,0.\C,-0.9155704746,1.5805336529,-3.0229938288\C,-1.7304401405,-0.6280628275,3.0254392731\C,2.1945884753,-1.5885628101,2.3018105527\C,3.3464483573,0.2814145268,-1.1741136845\C,1.493281231,1.906858156,-2.5970050119\C,-2.3269755546,2.3912686078,-1.1619627194\C,-2.6813198721,0.19045888,2.3000161143\C,0.9415090667,-1.6100072895,3.0336175144\C,3.5155605073,-0.5536589507,0.\C,3.0310649578,-1.8651178821,0.\C,-1.190007522,-3.2685533679,-0.7005896634\C,-2.1333644253,-2.4487107135,-1.429071364\C,-1.4664336993,-1.9306453275,-2.6046330508\C,-0.100464952,-2.4319536731,-2.605060372\C,0.0688703397,-3.2654402106,-1.4277609739\C,-1.190007522,-3.2685533679,0.7005896634\C,-3.0412394073,-1.6379215735,-0.7282635164\C,-1.7304401405,-0.6280628275,-3.0254392731\C,0.9415090667,-1.6100072895,-3.0336175144\C,1.2745824839,-3.247463924,-0.7273897608\C,-2.1333644253,-2.4487107135,1.429071364\C,-3.3328073475,-0.3156730961,-1.1876551401\C,-0.6420580356,0.2276570293,-3.4750208321\C,2.1945884753,-1.5885628101,-2.3018105527\C,1.2745824839,-3.247463924,0.7273897608\C,0.0688703397,-3.2654402106,1.4277609739\C,-3.0412394073,-1.6379215735,0.7282635164\C,-2.6813198721,0.19045888,-2.3000161143\C,0.663356514,-0.2539667301,-3.4780492269\C,2.3612459047,-2.394838027,-1.1739631393\C,-1.4664336993,-1.9306453275,2.6046330508\C,-3.7257595946,0.5701747612,0.\C,2.7006965887,-0.2244923498,-2.3028562594\C,2.3612459047,-2.394838027,1.1739631393\C,-0.100464952,-2.4319536731,2.605060372\C,-3.3328073475,-0.3156730961,1.1876551401\C,-2.1543791474,1.555079847,-2.2805565206\C,1.7511603471,0.6003935077,-3.0223157093\N,-0.1425544271,0.0801959552,0.\H,-4.8103649384,0.7852755437,0.\Version=AM64L-G03RevD.02\State=4-A\"HF=-2341.1044782\S2=3.752746\S2-1=0.\S2A=3.75\RMSD=5.161e-09\RMSE=1.491e-04\ZeroPoint=0.3865329\Thermal=0.4098348\ZPE=242.5530845\Dipole=-1.2856391,0.4525559,0.\DipoleDeriv=0.0472473,0.0227489,0.018159709562,0.009205,0.,-0.0205602,0.1042162,0.,0.,0.,0.0982356\Polar=494.5274646,-5.8695783,475.8028149,0.,-0.0000002,476.8859675\PG=CS [SG(C4H1N1),X(C56)]\NImag=0\0.48695983,-0.10472405,0.23770870,-0.03138918,-0.077,0.,0.,-0.00001615,0.,0.,0.04239496\0.00012239,0.00000356,-0.000164,-0.00006260,0.00025039,0.\@

2a⁺ (N@C₆₀H⁺, doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

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1\1\FAU-CCC-CCDN085\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,2)\DRAL\31-Mar-201
0\0\#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=(VShift,
Conver=5) Name=Dral\N@C60H(+)\1,2\C,0,-1.0997251898,3.3236578288,-0.
6956605092\C,0,0.1588415603,3.259107288,-1.413232763\C,0,-0.0388856693
,2.4101508777,-2.5843587125\C,0,-1.4178650591,1.9729511457,-2.59660097
41\C,0,-2.0752985855,2.5285031253,-1.4246049232\C,0,-1.1007594847,3.32
2206903,0.7011641364\C,0,1.3625704815,3.2125795693,-0.7195558866\C,0,0
.9762580939,1.5514494749,-3.0211186272\C,0,-1.7268379412,0.6780065297,
-3.0235656066\C,0,-3.0093349397,1.7655302071,-0.7274777016\C,0,0.15673
4872,3.2561782385,1.4204837135\C,0,2.4174067339,2.3025526726,-1.157204
8202\C,0,0.6500906254,0.211102968,-3.4751437807\C,0,-2.7085091289,-0.1
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,-2.0774028419,2.5255290075,1.426995132\C,0,1.3614903867,3.2110723104,
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985101\C,0,-0.0427334501,2.4047867022,2.5895469549\C,0,3.0319427263,1.
7570681243,0.0042117469\C,0,0.9717503934,1.5451856211,3.0260581155\C,0
,1.7035709506,-0.6874990249,-3.0253332305\C,0,-2.2565228264,-1.4923169
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-1.5628088933,-3.0363988728\C,0,-3.5381732,-0.4081899096,-0.0029278556
\C,0,-3.1055515858,-1.7379645172,-0.0039789388\C,0,1.056500804,-3.3073
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3840638282,-1.9841802228,2.60414149\C,0,-0.0006986311,-2.4312240986,2.
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C60H1N1)]\@

```

UB3LYP/6-31G(d)

Zero-point correction= 0.386179 (Hartree/Particle)
 Thermal correction to Energy= 0.409703
 Thermal correction to Enthalpy= 0.410647
 Thermal correction to Gibbs Free Energy= 0.337734
 Sum of electronic and zero-point Energies= -2340.678282
 Sum of electronic and thermal Energies= -2340.654758
 Sum of electronic and thermal Enthalpies= -2340.653814
 Sum of electronic and thermal Free Energies= -2340.726727

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 9\0\#P B3LYP/6-31G* Freq=NoRaman Geom=AllCheck SCF=QC SCFCYC=600 GUES
 S=READ POP=NONE NAME=DRAL\N@C60H(+)\1,2\C,-1.0997251898,3.3236578288
 ,-0.6956605092\C,0.1588415603,3.259107288,-1.413232763\C,-0.0388856693
 ,2.4101508777,-2.5843587125\C,-1.4178650591,1.9729511457,-2.5966009741
 \C,-2.0752985855,2.5285031253,-1.4246049232\C,-1.1007594847,3.32220690
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 9,1.5514494749,-3.0211186272\C,-1.7268379412,0.6780065297,-3.023565606
 6\C,-3.0093349397,1.7655302071,-0.7274777016\C,0.156734872,3.256178238
 5,1.4204837135\C,2.4174067339,2.3025526726,-1.1572048202\C,0.650090625
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 8\C,-3.0104037004,1.7640192885,0.726899032\C,-2.0774028419,2.525529007
 5,1.426995132\C,1.3614903867,3.2110723104,0.7284993457\C,2.2126675685,
 1.4760552482,-2.2780635716\C,-0.6733428083,-0.2183985803,-3.4795572675
 \C,-3.3348004484,0.420598292,-1.1760985101\C,-0.0427334501,2.404786702
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 C,-2.2565228264,-1.4923169745,-2.3049954151\C,-3.3365324993,0.41816763
 99,1.1722506532\C,-1.421720746,1.9675599391,2.5988192294\C,2.415665637
 8,2.3001299523,1.1658300902\C,2.6852550982,0.0919202285,-2.2979221555\
 C,-1.0050103219,-1.5628088933,-3.0363988728\C,-3.5381732,-0.4081899096
 ,-0.0029278556\C,-3.1055515858,-1.7379645172,-0.0039789388\C,1.0565008
 04,-3.3073202953,0.6982489232\C,2.0309648729,-2.5264063914,1.428307562
 6\C,1.3840638282,-1.9841802228,2.60414149\C,-0.0006986311,-2.431224098
 6,2.6031201609\C,-0.2018715947,-3.2558390734,1.4246952707\C,1.05754515
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 01\C,1.6990685275,-0.693775816,3.0267370286\C,-1.0095286504,-1.5690993
 114,3.0319323211\C,-1.405330072,-3.1895840775,0.7232569851\C,2.0330974
 83,-2.5234534014,-1.4302293467\C,3.3145073317,-0.4428316483,1.18984180
 94\C,0.6449105443,0.2038994101,3.4768172023\C,-2.25993159,-1.497079732
 4,2.298786116\C,-1.4042457434,-3.1880799523,-0.7316845198\C,-0.1997419
 893,-3.2528920287,-1.4314654879\C,2.9720021889,-1.749957691,-0.7279511
 107\C,2.6818236385,0.087147891,2.3023863581\C,-0.6785198499,-0.2256117
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 6964,-1.9787812884,-2.6058935376\C,3.7438688508,0.4275577626,0.0033701
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663102,-1.177933328\C,0.0031839063,-2.4258343537,-2.6078785272\C,3.316
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 0.00002769,-0.00001292,-0.00001012,0.00000062,-0.00000914,-0.00000005\
 \@

12a (N@C₆₀H, singlet)

MP2/6-31G(d)//B3LYP/6-31G(d)

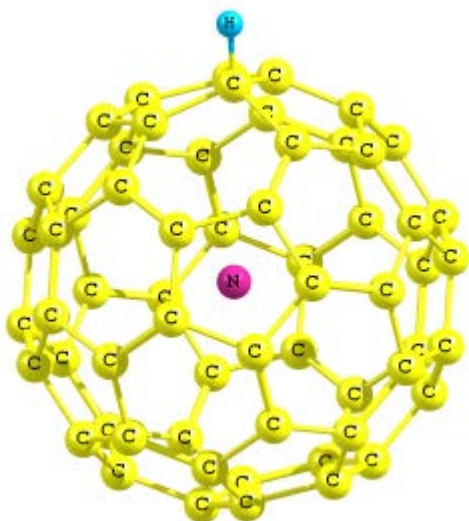
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 RMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=None N
 ame=Dral\N@C60H(dot) singlet\0,1\C,1.479046593,3.167291425,0.6982712
 79\C,0.223731555,3.253092399,1.422897886\C,0.318353041,2.395078021,2.5
 94952263\C,1.630683965,1.787890921,2.595338527\C,2.350411502,2.2594593
 14,1.423586058\C,1.479046593,3.167291425,-0.698271279\C,-0.976267357,3
 .344544069,0.724869196\C,-0.796571487,1.663062124,3.0306411\C,1.787833
 312,0.466022035,3.019270168\C,3.191853074,1.39369288,0.726629259\C,0.2
 23731555,3.253092399,-1.422897886\C,-2.119176097,2.554187324,1.1659530
 64\C,-0.625194298,0.286915799,3.469228902\C,2.669982343,-0.431595966,2
 .301208508\C,3.191853074,1.39369288,-0.726629259\C,2.350411502,2.25945
 9314,-1.423586058\C,-0.976267357,3.344544069,-0.724869196\C,-2.0417078
 01,1.747143377,2.310557334\C,0.63778766,-0.297354384,3.472070316\C,3.3
 58072593,0.02134139,1.174905087\C,0.318353041,2.395078021,-2.594952263
 \C,-2.777151758,2.068967298,0.\C,-0.796571487,1.663062124,-3.0306411\C
 ,-1.77272462,-0.479337703,3.018068076\C,2.06251468,-1.753212066,2.3057
 46081\C,3.358072593,0.02134139,-1.174905087\C,1.630683965,1.787890921,
 -2.595338527\C,-2.119176097,2.554187324,-1.165953064\C,-2.654622984,0.
 414623492,2.299763955\C,0.808665207,-1.671219421,3.029749241\C,3.45789
 3254,-0.82294633,0.\C,2.868294952,-2.089402387,0.\C,-1.447205484,-3.16
 555893,-0.69922679\C,-2.324543299,-2.271539582,-1.431296027\C,-1.61667
 5158,-1.802623383,-2.601257845\C,-0.296065651,-2.408076808,-2.60176323
 1\C,-0.192201151,-3.254812112,-1.426067491\C,-1.447205484,-3.16555893,
 0.69922679\C,-3.155568802,-1.389482856,-0.728085049\C,-1.77272462,-0.4
 79337703,-3.018068076\C,0.808665207,-1.671219421,-3.029749241\C,1.0124
 96694,-3.330878987,-0.726917732\C,-2.324543299,-2.271539582,1.43129602
 7\C,-3.335218452,-0.044559864,-1.185674448\C,-0.625194298,0.286915799,
 -3.469228902\C,2.06251468,-1.753212066,-2.305746081\C,1.012496694,-3.3
 30878987,0.726917732\C,-0.192201151,-3.254812112,1.426067491\C,-3.1555
 68802,-1.389482856,0.728085049\C,-2.654622984,0.414623492,-2.299763955


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\C,0.63778766,-0.297354384,-3.472070316\C,2.161534875,-2.565527851,-1.
17506005\C,-1.616675158,-1.802623383,2.601257845\C,-3.668623086,0.8618
96384,0\C,2.669982343,-0.431595966,-2.301208508\C,2.161534875,-2.5655
27851,1.17506005\C,-0.296065651,-2.408076808,2.601763231\C,-3.33521845
2,-0.044559864,1.185674448\C,-2.041707801,1.747143377,-2.310557334\C,1
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),X(C56)]\@

```

B3LYP/6-31G(d)



0 1

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C	0.223731555	3.253092399	1.422897886
C	0.318353041	2.395078021	2.594952263
C	1.630683965	1.787890921	2.595338527
C	2.350411502	2.259459314	1.423586058
C	1.479046593	3.167291425	-0.698271279
C	-0.976267357	3.344544069	0.724869196
C	-0.796571487	1.663062124	3.030641100
C	1.787833312	0.466022035	3.019270168
C	3.191853074	1.393692880	0.726629259
C	0.223731555	3.253092399	-1.422897886
C	-2.119176097	2.554187324	1.165953064
C	-0.625194298	0.286915799	3.469228902
C	2.669982343	-0.431595966	2.301208508
C	3.191853074	1.393692880	-0.726629259
C	2.350411502	2.259459314	-1.423586058
C	-0.976267357	3.344544069	-0.724869196
C	-2.041707801	1.747143377	2.310557334
C	0.637787660	-0.297354384	3.472070316
C	3.358072593	0.021341390	1.174905087
C	0.318353041	2.395078021	-2.594952263
C	-2.777151758	2.068967298	0.000000000

C	-0.796571487	1.663062124	-3.030641100
C	-1.772724620	-0.479337703	3.018068076
C	2.062514680	-1.753212066	2.305746081
C	3.358072593	0.021341390	-1.174905087
C	1.630683965	1.787890921	-2.595338527
C	-2.119176097	2.554187324	-1.165953064
C	-2.654622984	0.414623492	2.299763955
C	0.808665207	-1.671219421	3.029749241
C	3.457893254	-0.822946330	0.000000000
C	2.868294952	-2.089402387	0.000000000
C	-1.447205484	-3.165558930	-0.699226790
C	-2.324543299	-2.271539582	-1.431296027
C	-1.616675158	-1.802623383	-2.601257845
C	-0.296065651	-2.408076808	-2.601763231
C	-0.192201151	-3.254812112	-1.426067491
C	-1.447205484	-3.165558930	0.699226790
C	-3.155568802	-1.389482856	-0.728085049
C	-1.772724620	-0.479337703	-3.018068076
C	0.808665207	-1.671219421	-3.029749241
C	1.012496694	-3.330878987	-0.726917732
C	-2.324543299	-2.271539582	1.431296027
C	-3.335218452	-0.044559864	-1.185674448
C	-0.625194298	0.286915799	-3.469228902
C	2.062514680	-1.753212066	-2.305746081
C	1.012496694	-3.330878987	0.726917732
C	-0.192201151	-3.254812112	1.426067491
C	-3.155568802	-1.389482856	0.728085049
C	-2.654622984	0.414623492	-2.299763955
C	0.637787660	-0.297354384	-3.472070316
C	2.161534875	-2.565527851	-1.175060050
C	-1.616675158	-1.802623383	2.601257845
C	-3.668623086	0.861896384	0.000000000
C	2.669982343	-0.431595966	-2.301208508
C	2.161534875	-2.565527851	1.175060050
C	-0.296065651	-2.408076808	2.601763231
C	-3.335218452	-0.044559864	1.185674448
C	-2.041707801	1.747143377	-2.310557334
C	1.787833312	0.466022035	-3.019270168
N	-0.139451379	0.097489531	0.000000000
H	-4.733012735	1.159646859	0.000000000

Zero-point correction=	0.385075 (Hartree/Particle)
Thermal correction to Energy=	0.408715
Thermal correction to Enthalpy=	0.409659
Thermal correction to Gibbs Free Energy=	0.337764
Sum of electronic and zero-point Energies=	-2340.819208
Sum of electronic and thermal Energies=	-2340.795568
Sum of electronic and thermal Enthalpies=	-2340.794623
Sum of electronic and thermal Free Energies=	-2340.866519

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21,2.595338527\C,2.350411502,2.259459314,1.423586058\C,1.479046593,3.1
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71487,1.663062124,3.0306411\C,1.787833312,0.466022035,3.019270168\C,3.
191853074,1.39369288,0.726629259\C,0.223731555,3.253092399,-1.42289788
6\C,-2.119176097,2.554187324,1.165953064\C,-0.625194298,0.286915799,3.
469228902\C,2.669982343,-0.431595966,2.301208508\C,3.191853074,1.39369
288,-0.726629259\C,2.350411502,2.259459314,-1.423586058\C,-0.976267357
,3.344544069,-0.724869196\C,-2.041707801,1.747143377,2.310557334\C,0.6
3778766,-0.297354384,3.472070316\C,3.358072593,0.02134139,1.174905087\
C,0.318353041,2.395078021,-2.594952263\C,-2.777151758,2.068967298,0.\C
,-0.796571487,1.663062124,-3.0306411\C,-1.77272462,-0.479337703,3.0180
68076\C,2.06251468,-1.753212066,2.305746081\C,3.358072593,0.02134139,-
1.174905087\C,1.630683965,1.787890921,-2.595338527\C,-2.119176097,2.55
4187324,-1.165953064\C,-2.654622984,0.414623492,2.299763955\C,0.808665
207,-1.671219421,3.029749241\C,3.457893254,-0.82294633,0.\C,2.86829495
2,-2.089402387,0.\C,-1.447205484,-3.16555893,-0.69922679\C,-2.32454329
9,-2.271539582,-1.431296027\C,-1.616675158,-1.802623383,-2.601257845\C
,-0.296065651,-2.408076808,-2.601763231\C,-0.192201151,-3.254812112,-1
.426067491\C,-1.447205484,-3.16555893,0.69922679\C,-3.155568802,-1.389
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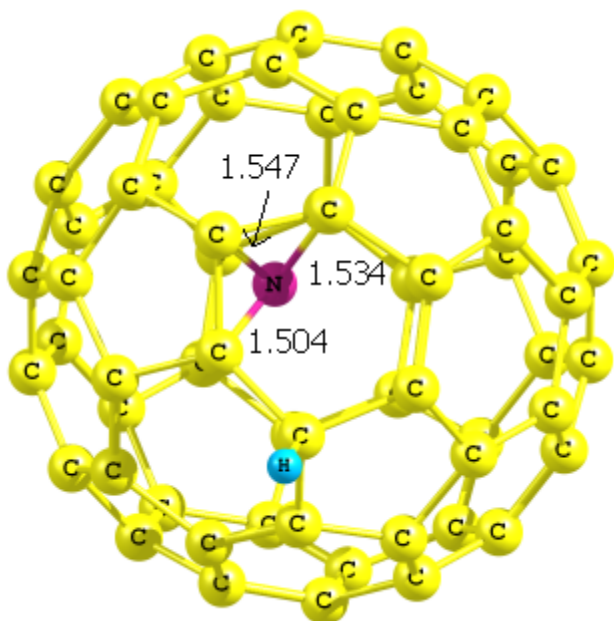
¹²e (N@C₆₀H, endohedrally bound, singlet)

MP2/6-31G(d)//UB3LYP/6-31G(d)

```

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\C,0,-1.0530880902,2.9522344772,-1.4604241113\C,0,1.6505464281,3.03348
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5285,2.3347635663,-0.0619302844\C,0,2.9334930288,-0.7041665534,-1.9361
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-0.8115803161,-3.148891417\C,0,-2.231513968,2.0924111423,-1.2308379751
\C,0,0.6684022932,3.4751508635,0.1769942882\C,0,3.3030415556,1.2141879
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UB3LYP/6-31G(d)

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C	0.934958149	-0.733084555	-3.391319874
C	-1.540079560	0.649042852	-3.248858116
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C	-0.299966320	-1.488516870	-3.245457422
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C	2.933493029	-0.704166553	-1.936184332
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C	-0.036023755	-2.635225949	-2.401307698
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C   -0.814361525 0.699981409 3.401095359
C   -2.812443372 -0.759769243 1.982989303
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```

```

Zero-point correction=          0.388922 (Hartree/Particle)
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Thermal correction to Enthalpy=  0.411439
Thermal correction to Gibbs Free Energy= 0.345361
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Sum of electronic and thermal Free Energies= -2340.995397

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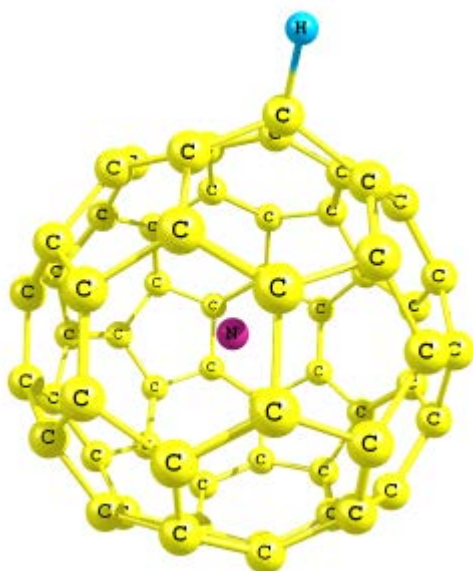
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³2a (N@C₆₀H[•],triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H1N1(3)\DRAL\02-Aug-2010\0
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 6060291\MP2=-2334.5194058\RMSD=1.208e-09\Thermal=0.\PG=CS [SG(C4H1N1),
 X(C56)]\\@

UB3LYP/6-31G(d)

0 3

C	1.484330850	3.165751476	0.698155922
C	0.228603419	3.249569424	1.424264657
C	0.326263274	2.401185748	2.600585854
C	1.637706743	1.787818970	2.599356164
C	2.356837529	2.259459292	1.425289242
C	1.484330850	3.165751476	-0.698155922
C	-0.971962495	3.329254461	0.723074276
C	-0.791708530	1.663259039	3.019262638
C	1.797949625	0.466941924	3.030593404
C	3.197218030	1.392629188	0.727199796
C	0.228603419	3.249569424	-1.424264657
C	-2.131358802	2.558173484	1.159378707
C	-0.622432576	0.287506927	3.462080156
C	2.673607965	-0.432465850	2.303908241
C	3.197218030	1.392629188	-0.727199796
C	2.356837529	2.259459292	-1.425289242
C	-0.971962495	3.329254461	-0.723074276
C	-2.042510097	1.754210528	2.304998357
C	0.643119112	-0.296484336	3.472998940
C	3.360520909	0.018991936	1.175174020
C	0.326263274	2.401185748	-2.600585854
C	-2.852159363	2.127205961	0.000000000
C	-0.791708530	1.663259039	-3.019262638
C	-1.771887301	-0.477691609	3.013846850
C	2.064754828	-1.754759145	2.304304867
C	3.360520909	0.018991936	-1.175174020
C	1.637706743	1.787818970	-2.599356164
C	-2.131358802	2.558173484	-1.159378707
C	-2.654601656	0.413863126	2.293193765
C	0.811427669	-1.672029853	3.028460459
C	3.460343607	-0.827774358	0.000000000

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C      2.877740347 -2.098387858 0.000000000
C      -1.443947587 -3.169501960 -0.697685630
C      -2.319956502 -2.268744807 -1.428395600
C      -1.613655898 -1.803462336 -2.597764481
C      -0.294291643 -2.410460434 -2.601335509
C      -0.189236589 -3.258418820 -1.425084504
C      -1.443947587 -3.169501960 0.697685630
C      -3.151617320 -1.383201011 -0.727817143
C      -1.771887301 -0.477691609 -3.013846850
C      0.811427669 -1.672029853 -3.028460459
C      1.017129686 -3.337274607 -0.727042867
C      -2.319956502 -2.268744807 1.428395600
C      -3.352601001 -0.038551362 -1.188043456
C      -0.622432576 0.287506927 -3.462080156
C      2.064754828 -1.754759145 -2.304304867
C      1.017129686 -3.337274607 0.727042867
C      -0.189236589 -3.258418820 1.425084504
C      -3.151617320 -1.383201011 0.727817143
C      -2.654601656 0.413863126 -2.293193765
C      0.643119112 -0.296484336 -3.472998940
C      2.166796333 -2.570940577 -1.174822204
C      -1.613655898 -1.803462336 2.597764481
C      -3.709827713 0.873544375 0.000000000
C      2.673607965 -0.432465850 -2.303908241
C      2.166796333 -2.570940577 1.174822204
C      -0.294291643 -2.410460434 2.601335509
C      -3.352601001 -0.038551362 1.188043456
C      -2.042510097 1.754210528 -2.304998357
C      1.797949625 0.466941924 -3.030593404
N      -0.136046768 0.096923257 0.000000000
H      -4.782516647 1.132048548 0.000000000

```

```

Zero-point correction=          0.384959 (Hartree/Particle)
Thermal correction to Energy=    0.408522
Thermal correction to Enthalpy=  0.409466
Thermal correction to Gibbs Free Energy= 0.336686
Sum of electronic and zero-point Energies= -2340.948545
Sum of electronic and thermal Energies= -2340.924982
Sum of electronic and thermal Enthalpies= -2340.924038
Sum of electronic and thermal Free Energies= -2340.996817

```

```

1\1\FAU-CCC-CCDN088\Freq\UB3LYP\6-31G(d)\C60H1N1(3)\DRAL\29-Oct-2009\0
\#P B3LYP/6-31G* Freq=NoRaman POP=NONE NAME=DRAL\N@C60H(dot) triplet
\0,3\C,1.48433085,3.165751476,0.698155922\C,0.228603419,3.249569424,1
.424264657\C,0.326263274,2.401185748,2.600585854\C,1.637706743,1.78781
897,2.599356164\C,2.356837529,2.259459292,1.425289242\C,1.48433085,3.1
65751476,-0.698155922\C,-0.971962495,3.329254461,0.723074276\C,-0.7917
0853,1.663259039,3.019262638\C,1.797949625,0.466941924,3.030593404\C,3
.19721803,1.392629188,0.727199796\C,0.228603419,3.249569424,-1.4242646
57\C,-2.131358802,2.558173484,1.159378707\C,-0.622432576,0.287506927,3

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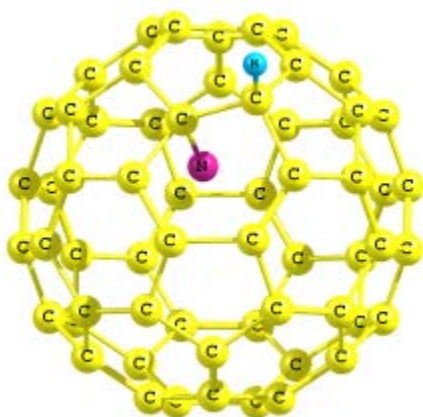
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 188,-0.727199796\C,2.356837529,2.259459292,-1.425289242\C,-0.971962495
 ,3.329254461,-0.723074276\C,-2.042510097,1.754210528,2.304998357\C,0.6
 43119112,-0.296484336,3.47299894\C,3.360520909,0.018991936,1.17517402\
 C,0.326263274,2.401185748,-2.600585854\C,-2.852159363,2.127205961,0.\C
 ,-0.79170853,1.663259039,-3.019262638\C,-1.771887301,-0.477691609,3.01
 384685\C,2.064754828,-1.754759145,2.304304867\C,3.360520909,0.01899193
 6,-1.17517402\C,1.637706743,1.78781897,-2.599356164\C,-2.131358802,2.5
 58173484,-1.159378707\C,-2.654601656,0.413863126,2.293193765\C,0.81142
 7669,-1.672029853,3.028460459\C,3.460343607,-0.827774358,0.\C,2.877740
 347,-2.098387858,0.\C,-1.443947587,-3.16950196,-0.69768563\C,-2.319956
 502,-2.268744807,-1.4283956\C,-1.613655898,-1.803462336,-2.597764481\C
 ,-0.294291643,-2.410460434,-2.601335509\C,-0.189236589,-3.25841882,-1.
 425084504\C,-1.443947587,-3.16950196,0.69768563\C,-3.15161732,-1.38320
 1011,-0.727817143\C,-1.771887301,-0.477691609,-3.01384685\C,0.81142766
 9,-1.672029853,-3.028460459\C,1.017129686,-3.337274607,-0.727042867\C,
 -2.319956502,-2.268744807,1.4283956\C,-3.352601001,-0.038551362,-1.188
 043456\C,-0.622432576,0.287506927,-3.462080156\C,2.064754828,-1.754759
 145,-2.304304867\C,1.017129686,-3.337274607,0.727042867\C,-0.189236589
 ,-3.25841882,1.425084504\C,-3.15161732,-1.383201011,0.727817143\C,-2.6
 54601656,0.413863126,-2.293193765\C,0.643119112,-0.296484336,-3.472998
 94\C,2.166796333,-2.570940577,-1.174822204\C,-1.613655898,-1.803462336
 ,2.597764481\C,-3.709827713,0.873544375,0.\C,2.673607965,-0.43246585,-
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 10460434,2.601335509\C,-3.352601001,-0.038551362,1.188043456\C,-2.0425
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 216\ZPE=241.5652263\Dipole=-0.5451767,0.1165135,0.\DipoleDeriv=0.06370
 ,0.,0.0666641\Polar=491.0243828,-7.1728356,472.5917283,0.0000002,-0.0
 000001,476.4824982\PG=CS [SG(C4H1N1),X(C56)]\NImag=0\0.46452262,-0.12
 24726\0.00010417,0.00006413,0.00005984,0.00010697,-0.00001170,-0.000
 000592,-0.00016248,-0.00014415,0.00030109,0.,0.00024820,0.00026011,0.\
 \@

³2b (N@C₆₀H[•], endohedrally bound, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN085\SP\ROMP2-FC\6-31G(d)\C60H1N1(3)\DRAL\06-Aug-2010\0
 \#P ROMP2/6-31G* SCF=Tight SCFCyc=1200 POP=NONE Guess=Read Geom=AllCh
 eck NAME=DRAL\endohedral-N@C60H triplet\0,3\C,0,0.8966868015,0.69260
 5653,-3.3808587763\C,0,-0.3600431381,1.4190081097,-3.2496620697\C,0,-0
 .1311978331,2.5983920421,-2.4371980552\C,0,1.2710127291,2.6075936518,-
 2.0675392787\C,0,1.9078949876,1.4373402247,-2.6531326282\C,0,0.9169797
 276,-0.705413497,-3.3728079539\C,0,-1.5496054901,0.6965468817,-3.09551

05954\C,0,-1.1008693566,3.0405773676,-1.512382432\C,0,1.6604845389,3.0
 471385366,-0.8000004579\C,0,2.9015023814,0.7571539839,-1.9479414579\C,
 0,-0.3181634727,-1.4664060942,-3.2330122139\C,0,-2.5053162903,1.165243
 5326,-2.1207748181\C,0,-0.6918417948,3.4687569142,-0.1823070801\C,0,2.
 6966991343,2.341215557,-0.0714064655\C,0,2.922568848,-0.6952060224,-1.
 9395563399\C,0,1.9492141709,-1.412031558,-2.6366648794\C,0,-1.52822003
 43,-0.7770154469,-3.0870208881\C,0,-2.3397918263,2.3184348004,-1.37038
 6546\C,0,0.658629718,3.4829414424,0.1598979641\C,0,3.3075770941,1.2191
 243492,-0.6327687832\C,0,-0.0553358661,-2.6292232273,-2.4070321685\C,0
 ,-2.8076576131,-0.0482421858,-1.2969508917\C,0,-1.0119204337,-3.088618
 521,-1.4770024447\C,0,-1.6803838802,3.0022037351,0.7835695441\C,0,2.34
 17720604,2.345037477,1.3401223633\C,0,3.3417052465,-1.1300070787,-0.61
 9218492\C,0,1.3465020593,-2.5934895622,-2.0375286638\C,0,-2.470048675,
 -1.2619095274,-2.1067164548\C,0,-2.7089222931,2.275107147,0.0819149875
 \C,0,1.0832749795,3.0482297513,1.482177146\C,0,3.5819411844,0.05299959
 96,0.1892235297\C,0,3.24155955,0.0558922846,1.5426214748\C,0,-0.799877
 2604,-0.6883159472,3.3916711526\C,0,-1.8193426995,-1.4387061372,2.6730
 224678\C,0,-1.1951984355,-2.5996888405,2.0886847439\C,0,0.213606813,-2
 .5793756556,2.4415004765\C,0,0.458543304,-1.3980900367,3.2508262462\C,
 0,-0.8200852234,0.7038306119,3.3836235198\C,0,-2.825702225,-0.76230630
 05,1.9689418905\C,0,-1.5926477761,-3.0404751626,0.8184502593\C,0,1.171
 0340811,-2.998270165,1.5170709988\C,0,1.6498442603,-0.6850154286,3.104
 727741\C,0,-1.8607571669,1.4159842968,2.65652735\C,0,-3.278223873,-1.2
 532621144,0.6972580395\C,0,-0.5908515676,-3.4893146744,-0.1421376798\C
 ,0,2.4086398901,-2.260568478,1.3667406966\C,0,1.6287342482,0.768308281
 1,3.0963109173\C,0,0.4172217915,1.4481535925,3.2343907996\C,0,-2.84697
 20397,0.7025944826,1.9604944146\C,0,-2.6417304695,-2.3517032499,0.1086
 293704\C,0,0.7594043492,-3.4604186881,0.1999816268\C,0,2.645318871,-1.
 1246869902,2.1443455064\C,0,-1.2705018494,2.5878077617,2.0587440399\C,
 0,-3.7778676256,-0.0556865416,-0.1436257043\C,0,2.7635105324,-2.262764
 8999,-0.0448161269\C,0,2.6111809396,1.225550526,2.1307403168\C,0,0.138
 2488591,2.6124449522,2.4115452566\C,0,-3.313390742,1.1655295506,0.6833
 248299\C,0,-2.271268688,-2.4010853515,-1.3431125985\C,0,1.7483573609,-
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 1 [X(C60H1N1)]\@

UB3LYP/6-31G(d)

0 3

C	0.896686802	0.692605653	-3.380858776
C	-0.360043138	1.419008110	-3.249662070
C	-0.131197833	2.598392042	-2.437198055
C	1.271012729	2.607593652	-2.067539279
C	1.907894988	1.437340225	-2.653132628
C	0.916979728	-0.705413497	-3.372807954
C	-1.549605490	0.696546882	-3.095510595
C	-1.100869357	3.040577368	-1.512382432
C	1.660484539	3.047138537	-0.800000458
C	2.901502381	0.757153984	-1.947941458
C	-0.318163473	-1.466406094	-3.233012214
C	-2.505316290	1.165243533	-2.120774818
C	-0.691841795	3.468756914	-0.182307080
C	2.696699134	2.341215557	-0.071406466
C	2.922568848	-0.695206022	-1.939556340
C	1.949214171	-1.412031558	-2.636664879
C	-1.528220034	-0.777015447	-3.087020888
C	-2.339791826	2.318434800	-1.370386546
C	0.658629718	3.482941442	0.159897964
C	3.307577094	1.219124349	-0.632768783
C	-0.055335866	-2.629223227	-2.407032168
C	-2.807657613	-0.048242186	-1.296950892
C	-1.011920434	-3.088618521	-1.477002445
C	-1.680383880	3.002203735	0.783569544
C	2.341772060	2.345037477	1.340122363
C	3.341705246	-1.130007079	-0.619218492
C	1.346502059	-2.593489562	-2.037528664
C	-2.470048675	-1.261909527	-2.106716455
C	-2.708922293	2.275107147	0.081914988
C	1.083274980	3.048229751	1.482177146
C	3.581941184	0.052999600	0.189223530
C	3.241559550	0.055892285	1.542621475
C	-0.799877260	-0.688315947	3.391671153
C	-1.819342700	-1.438706137	2.673022468
C	-1.195198436	-2.599688840	2.088684744

C	0.213606813	-2.579375656	2.441500476
C	0.458543304	-1.398090037	3.250826246
C	-0.820085223	0.703830612	3.383623520
C	-2.825702225	-0.762306300	1.968941890
C	-1.592647776	-3.040475163	0.818450259
C	1.171034081	-2.998270165	1.517070999
C	1.649844260	-0.685015429	3.104727741
C	-1.860757167	1.415984297	2.656527350
C	-3.278223873	-1.253262114	0.697258040
C	-0.590851568	-3.489314674	-0.142137680
C	2.408639890	-2.260568478	1.366740697
C	1.628734248	0.768308281	3.096310917
C	0.417221792	1.448153592	3.234390800
C	-2.846972040	0.702594483	1.960494415
C	-2.641730470	-2.351703250	0.108629370
C	0.759404349	-3.460418688	0.199981627
C	2.645318871	-1.124686990	2.144345506
C	-1.270501849	2.587807762	2.058744040
C	-3.777867626	-0.055686542	-0.143625704
C	2.763510532	-2.262764900	-0.044816127
C	2.611180940	1.225550526	2.130740317
C	0.138248859	2.612444952	2.411545257
C	-3.313390742	1.165529551	0.683324830
C	-2.271268688	-2.401085352	-1.343112598
C	1.748357361	-3.006863044	-0.765049669
N	-1.451691151	-0.024400742	-0.591816719
H	-4.837988715	-0.072720930	-0.422830339

Zero-point correction=	0.388161 (Hartree/Particle)
Thermal correction to Energy=	0.410042
Thermal correction to Enthalpy=	0.410986
Thermal correction to Gibbs Free Energy=	0.343356
Sum of electronic and zero-point Energies=	-2340.951128
Sum of electronic and thermal Energies=	-2340.929247
Sum of electronic and thermal Enthalpies=	-2340.928303
Sum of electronic and thermal Free Energies=	-2340.995933

1\1\FAU-CCC-CCDN086\Freq\UB3LYP\6-31G(d)\C60H1N1(3)\DRAL\04-Aug-2010\0
 \#P Geom=AllCheck Guess=TChech SCRF=Check GenChk UB3LYP/6-31G(d) Freq
 \endohedral-N@C60H triplet\0,3\C,0.8966868015,0.692605653,-3.3808587
 763\C,-0.3600431381,1.4190081097,-3.2496620697\C,-0.1311978331,2.59839
 20421,-2.4371980552\C,1.2710127291,2.6075936518,-2.0675392787\C,1.9078
 949876,1.4373402247,-2.6531326282\C,0.9169797276,-0.705413497,-3.37280
 79539\C,-1.5496054901,0.6965468817,-3.0955105954\C,-1.1008693566,3.040
 5773676,-1.512382432\C,1.6604845389,3.0471385366,-0.8000004579\C,2.901
 5023814,0.7571539839,-1.9479414579\C,-0.3181634727,-1.4664060942,-3.23
 30122139\C,-2.5053162903,1.1652435326,-2.1207748181\C,-0.6918417948,3.
 4687569142,-0.1823070801\C,2.6966991343,2.341215557,-0.0714064655\C,2.
 922568848,-0.6952060224,-1.9395563399\C,1.9492141709,-1.412031558,-2.6
 366648794\C,-1.5282200343,-0.7770154469,-3.0870208881\C,-2.3397918263,

2.3184348004,-1.370386546\C,0.658629718,3.4829414424,0.1598979641\C,3.3075770941,1.2191243492,-0.6327687832\C,-0.0553358661,-2.6292232273,-2.4070321685\C,-2.8076576131,-0.0482421858,-1.2969508917\C,-1.0119204337,-3.088618521,-1.4770024447\C,-1.6803838802,3.0022037351,0.7835695441\C,2.3417720604,2.345037477,1.3401223633\C,3.3417052465,-1.1300070787,-0.619218492\C,1.3465020593,-2.5934895622,-2.0375286638\C,-2.470048675,-1.2619095274,-2.1067164548\C,-2.7089222931,2.275107147,0.0819149875\C,1.0832749795,3.0482297513,1.482177146\C,3.5819411844,0.0529995996,0.1892235297\C,3.24155955,0.0558922846,1.5426214748\C,-0.7998772604,-0.6883159472,3.3916711526\C,-1.8193426995,-1.4387061372,2.6730224678\C,-1.1951984355,-2.5996888405,2.0886847439\C,0.213606813,-2.5793756556,2.4415004765\C,0.458543304,-1.3980900367,3.2508262462\C,-0.8200852234,0.7038306119,3.3836235198\C,-2.825702225,-0.7623063005,1.9689418905\C,-1.5926477761,-3.0404751626,0.8184502593\C,1.1710340811,-2.998270165,1.5170709988\C,1.6498442603,-0.6850154286,3.104727741\C,-1.8607571669,1.4159842968,2.65652735\C,-3.278223873,-1.2532621144,0.6972580395\C,-0.5908515676,-3.4893146744,-0.1421376798\C,2.4086398901,-2.260568478,1.3667406966\C,1.6287342482,0.7683082811,3.0963109173\C,0.4172217915,1.4481535925,3.2343907996\C,-2.8469720397,0.7025944826,1.9604944146\C,-2.6417304695,-2.3517032499,0.1086293704\C,0.7594043492,-3.4604186881,0.1999816268\C,2.645318871,-1.1246869902,2.1443455064\C,-1.2705018494,2.5878077617,2.0587440399\C,-3.7778676256,-0.0556865416,-0.1436257043\C,2.7635105324,-2.2627648999,-0.0448161269\C,2.6111809396,1.225550526,2.1307403168\C,0.1382488591,2.6124449522,2.4115452566\C,-3.313390742,1.1655295506,0.6833248299\C,-2.271268688,-2.4010853515,-1.3431125985\C,1.7483573609,-3.0068630442,-0.7650496689\C,-1.4516911511,-0.0244007425,-0.5918167191\H,-4.8379887154,-0.0727209301,-0.4228303388\\Version=EM64L-G09 RevA.02\State=3-A\HF=-2341.3392891\S2=2.013882\S2-1=0.\S2A=2.000114\RM SD=9.249e-09\RMSF=2.409e-05\ZeroPoint=0.3881611\Thermal=0.4100418\ZPE=243.5747784\Dipole=-0.6178492,-0.0100979,-0.1818046\DipoleDeriv=0.10720.0419968,-0.0003565,-0.0957116,-0.0012393,0.0679337\Polar=486.8658254,0.2350908,471.3896365,2.3665871,0.0334191,471.0140226\PG=C01 [X(C60H1N1)]\NImag=0\0.49687992,-0.02356535,0.66826177,0.08122035,0.08561832,180\0.00002567,-0.00006167,0.00000119,-0.00004100,-0.00000859,-0.0000.00001467,-0.00000373,-0.00000084,0.00002506\\@

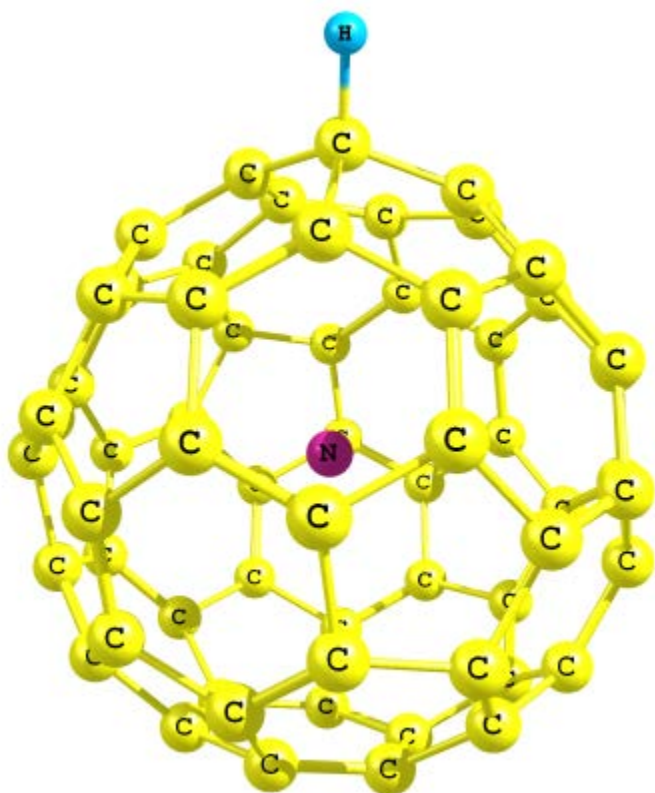
⁵2a (N@C₆₀H^{•••}, quintet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN086\SP\ROMP2-FC\6-31G(d)\C60H1N1(5)\DRAL\02-Aug-2010\0
 \#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=N
 one Name=DrAl\N@C60H(dot) quintet\0,5\C,1.484827421,3.166247283,0.69
 8193257\C,0.228903874,3.249454326,1.42396761\C,0.326564094,2.400737224
 ,2.600006141\C,1.638037837,1.787668333,2.599316356\C,2.357327385,2.259
 853366,1.425460921\C,1.484827421,3.166247283,-0.698193257\C,-0.9717187
 98,3.329120587,0.722912469\C,-0.791230934,1.662396191,3.018072415\C,1.
 798424813,0.466961567,3.031401014\C,3.197262159,1.392854788,0.72722675
 3\C,0.228903874,3.249454326,-1.42396761\C,-2.131690962,2.558210574,1.1

5867323\C,-0.622287293,0.287078746,3.462093562\C,2.673485663,-0.432333
 999,2.304016657\C,3.197262159,1.392854788,-0.727226753\C,2.357327385,2
 .259853366,-1.425460921\C,-0.971718798,3.329120587,-0.722912469\C,-2.0
 41900442,1.753294985,2.303661514\C,0.643424688,-0.29662254,3.473425484
 \C,3.360146692,0.019112966,1.175110082\C,0.326564094,2.400737224,-2.60
 0006141\C,-2.855950191,2.130837987,0.\C,-0.791230934,1.662396191,-3.01
 8072415\C,-1.77212586,-0.478026571,3.0144924\C,2.064677616,-1.75469553
 4,2.304163696\C,3.360146692,0.019112966,-1.175110082\C,1.638037837,1.7
 87668333,-2.599316356\C,-2.131690962,2.558210574,-1.15867323\C,-2.6545
 73121,0.413268196,2.292991762\C,0.811570891,-1.6721336,3.028600502\C,3
 .460106783,-0.827711874,0.\C,2.878090992,-2.098655314,0.\C,-1.44386105
 7,-3.169436651,-0.697696454\C,-2.319470228,-2.268312643,-1.428237553\C
 ,-1.613520885,-1.803587119,-2.597951767\C,-0.294157728,-2.410616049,-2
 .60149704\C,-0.189143629,-3.258464668,-1.425133102\C,-1.443861057,-3.1
 69436651,0.697696454\C,-3.15139802,-1.382672885,-0.727779094\C,-1.7721
 2586,-0.478026571,-3.0144924\C,0.811570891,-1.6721336,-3.028600502\C,1
 .017211972,-3.337372796,-0.727046218\C,-2.319470228,-2.268312643,1.428
 237553\C,-3.353561982,-0.038406331,-1.18820346\C,-0.622287293,0.287078
 746,-3.462093562\C,2.064677616,-1.754695534,-2.304163696\C,1.017211972
 ,-3.337372796,0.727046218\C,-0.189143629,-3.258464668,1.425133102\C,-3
 .15139802,-1.382672885,0.727779094\C,-2.654573121,0.413268196,-2.29299
 1762\C,0.643424688,-0.29662254,-3.473425484\C,2.16687908,-2.570993267,
 -1.174724035\C,-1.613520885,-1.803587119,2.597951767\C,-3.711695164,0.
 874294434,0.\C,2.673485663,-0.432333999,-2.304016657\C,2.16687908,-2.5
 70993267,1.174724035\C,-0.294157728,-2.410616049,2.60149704\C,-3.35356
 1982,-0.038406331,1.18820346\C,-2.041900442,1.753294985,-2.303661514\C
 ,1.798424813,0.466961567,-3.031401014\N,-0.135866567,0.096896741,0.\H,
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 N1),X(C56)]\@

UB3LYP/6-31G(d)



0 5

C	1.484827421	3.166247283	0.698193257
C	0.228903874	3.249454326	1.423967610
C	0.326564094	2.400737224	2.600006141
C	1.638037837	1.787668333	2.599316356
C	2.357327385	2.259853366	1.425460921
C	1.484827421	3.166247283	-0.698193257
C	-0.971718798	3.329120587	0.722912469
C	-0.791230934	1.662396191	3.018072415
C	1.798424813	0.466961567	3.031401014
C	3.197262159	1.392854788	0.727226753
C	0.228903874	3.249454326	-1.423967610
C	-2.131690962	2.558210574	1.158673230
C	-0.622287293	0.287078746	3.462093562
C	2.673485663	-0.432333999	2.304016657
C	3.197262159	1.392854788	-0.727226753
C	2.357327385	2.259853366	-1.425460921
C	-0.971718798	3.329120587	-0.722912469
C	-2.041900442	1.753294985	2.303661514
C	0.643424688	-0.296622540	3.473425484
C	3.360146692	0.019112966	1.175110082
C	0.326564094	2.400737224	-2.600006141
C	-2.855950191	2.130837987	0.000000000
C	-0.791230934	1.662396191	-3.018072415
C	-1.772125860	-0.478026571	3.014492400
C	2.064677616	-1.754695534	2.304163696

C	3.360146692	0.019112966	-1.175110082
C	1.638037837	1.787668333	-2.599316356
C	-2.131690962	2.558210574	-1.158673230
C	-2.654573121	0.413268196	2.292991762
C	0.811570891	-1.672133600	3.028600502
C	3.460106783	-0.827711874	0.000000000
C	2.878090992	-2.098655314	0.000000000
C	-1.443861057	-3.169436651	-0.697696454
C	-2.319470228	-2.268312643	-1.428237553
C	-1.613520885	-1.803587119	-2.597951767
C	-0.294157728	-2.410616049	-2.601497040
C	-0.189143629	-3.258464668	-1.425133102
C	-1.443861057	-3.169436651	0.697696454
C	-3.151398020	-1.382672885	-0.727779094
C	-1.772125860	-0.478026571	-3.014492400
C	0.811570891	-1.672133600	-3.028600502
C	1.017211972	-3.337372796	-0.727046218
C	-2.319470228	-2.268312643	1.428237553
C	-3.353561982	-0.038406331	-1.188203460
C	-0.622287293	0.287078746	-3.462093562
C	2.064677616	-1.754695534	-2.304163696
C	1.017211972	-3.337372796	0.727046218
C	-0.189143629	-3.258464668	1.425133102
C	-3.151398020	-1.382672885	0.727779094
C	-2.654573121	0.413268196	-2.292991762
C	0.643424688	-0.296622540	-3.473425484
C	2.166879080	-2.570993267	-1.174724035
C	-1.613520885	-1.803587119	2.597951767
C	-3.711695164	0.874294434	0.000000000
C	2.673485663	-0.432333999	-2.304016657
C	2.166879080	-2.570993267	1.174724035
C	-0.294157728	-2.410616049	2.601497040
C	-3.353561982	-0.038406331	1.188203460
C	-2.041900442	1.753294985	-2.303661514
C	1.798424813	0.466961567	-3.031401014
N	-0.135866567	0.096896741	0.000000000
H	-4.784419057	1.132007365	0.000000000

Zero-point correction= 0.384999 (Hartree/Particle)

Thermal correction to Energy= 0.408545

Thermal correction to Enthalpy= 0.409489

Thermal correction to Gibbs Free Energy= 0.336271

Sum of electronic and zero-point Energies= -2340.948394

Sum of electronic and thermal Energies= -2340.924848

Sum of electronic and thermal Enthalpies= -2340.923904

Sum of electronic and thermal Free Energies= -2340.997122

1\1\FAU-CCC-CCDN086\Freq\UB3LYP\6-31G(d)\C60H1N1(5)\DRAL\07-Nov-2009\0
 \#P B3LYP/6-31G* Freq=NoRaman POP=NONE NAME=DRAL\N@C60H(dot) quintet
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1.42396761\C,0.326564094,2.400737224,2.600006141\C,1.638037837,1.78766
8333,2.599316356\C,2.357327385,2.259853366,1.425460921\C,1.484827421,3
.166247283,-0.698193257\C,-0.971718798,3.329120587,0.722912469\C,-0.79
1230934,1.662396191,3.018072415\C,1.798424813,0.466961567,3.031401014\
C,3.197262159,1.392854788,0.727226753\C,0.228903874,3.249454326,-1.423
96761\C,-2.131690962,2.558210574,1.15867323\C,-0.622287293,0.287078746
,3.462093562\C,2.673485663,-0.432333999,2.304016657\C,3.197262159,1.39
2854788,-0.727226753\C,2.357327385,2.259853366,-1.425460921\C,-0.97171
8798,3.329120587,-0.722912469\C,-2.041900442,1.753294985,2.303661514\C
,0.643424688,-0.29662254,3.473425484\C,3.360146692,0.019112966,1.17511
0082\C,0.326564094,2.400737224,-2.600006141\C,-2.855950191,2.130837987
,0.\C,-0.791230934,1.662396191,-3.018072415\C,-1.77212586,-0.478026571
,3.0144924\C,2.064677616,-1.754695534,2.304163696\C,3.360146692,0.0191
12966,-1.175110082\C,1.638037837,1.787668333,-2.599316356\C,-2.1316909
62,2.558210574,-1.15867323\C,-2.654573121,0.413268196,2.292991762\C,0.
811570891,-1.6721336,3.028600502\C,3.460106783,-0.827711874,0.\C,2.878
090992,-2.098655314,0.\C,-1.443861057,-3.169436651,-0.697696454\C,-2.3
19470228,-2.268312643,-1.428237553\C,-1.613520885,-1.803587119,-2.5979
51767\C,-0.294157728,-2.410616049,-2.60149704\C,-0.189143629,-3.258464
668,-1.425133102\C,-1.443861057,-3.169436651,0.697696454\C,-3.15139802
,-1.382672885,-0.727779094\C,-1.77212586,-0.478026571,-3.0144924\C,0.8
11570891,-1.6721336,-3.028600502\C,1.017211972,-3.337372796,-0.7270462
18\C,-2.319470228,-2.268312643,1.428237553\C,-3.353561982,-0.038406331
,-1.18820346\C,-0.622287293,0.287078746,-3.462093562\C,2.064677616,-1.
754695534,-2.304163696\C,1.017211972,-3.337372796,0.727046218\C,-0.189
143629,-3.258464668,1.425133102\C,-3.15139802,-1.382672885,0.727779094
\C,-2.654573121,0.413268196,-2.292991762\C,0.643424688,-0.29662254,-3.
473425484\C,2.16687908,-2.570993267,-1.174724035\C,-1.613520885,-1.803
587119,2.597951767\C,-3.711695164,0.874294434,0.\C,2.673485663,-0.4323
33999,-2.304016657\C,2.16687908,-2.570993267,1.174724035\C,-0.29415772
8,-2.410616049,2.60149704\C,-3.353561982,-0.038406331,1.18820346\C,-2.
041900442,1.753294985,-2.303661514\C,1.798424813,0.466961567,-3.031401
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A=6.000682\RMSD=8.333e-09\RMSF=1.827e-04\ZeroPoint=0.3849993\Thermal=0
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000003,476.555464\PG=CS [SG(C4H1N1),X(C56)]\NImag=0\0.46447850,-0.125
94,0.,0.,-0.00001489,0.,0.,0.04630893\0.00011385,0.00008778,0.000088
1,0.,0.00027965,0.00036759,0.\@

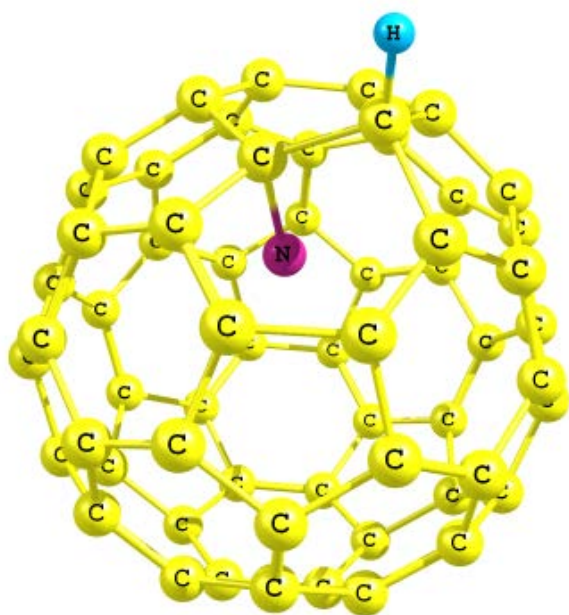
^{52b} (N@C₆₀H^{•••}, endohedrally bound, quintet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN086\SP\ROMP2-FC\6-31G(d)\C60H1N1(5)\DRAL\14-Aug-2010\0
\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCF=Tight SCFCyc=1
200 Name=Dral\endohedral-N@C60H quintet\0,5\C,0,0.8718725993,0.70603

58928,-3.3640349217\C,0,-0.3553180909,1.419352069,-3.2476864364\C,0,-0
 .1228922959,2.6054321974,-2.4126830806\C,0,1.2794888691,2.6274174922,-
 2.0557595778\C,0,1.8975817214,1.4495486935,-2.6354170793\C,0,0.9063299
 194,-0.7202423681,-3.3640959857\C,0,-1.5713748682,0.6931016093,-3.0872
 574955\C,0,-1.0795474377,3.0444874844,-1.4901165213\C,0,1.6785135466,3
 .0764670674,-0.7898669432\C,0,2.8879089155,0.768566938,-1.9366701307\C
 ,0,-0.3258055462,-1.4792844283,-3.227017267\C,0,-2.5113466939,1.148734
 796,-2.1335009722\C,0,-0.6715945344,3.4950257058,-0.1746412504\C,0,2.7
 122224026,2.3637223232,-0.0655979662\C,0,2.9105559455,-0.6919301552,-1
 .9282150665\C,0,1.930861519,-1.4113090507,-2.6340332764\C,0,-1.5371493
 237,-0.7917077007,-3.0772506636\C,0,-2.3316294614,2.3170753328,-1.3396
 640066\C,0,0.6835021287,3.5173334167,0.1691336049\C,0,3.3106832108,1.2
 338182929,-0.6296412192\C,0,-0.0653894727,-2.6450572703,-2.4020836933\
 C,0,-2.7947104046,-0.0575530967,-1.2994363123\C,0,-1.0206578503,-3.111
 2473929,-1.4727958268\C,0,-1.6597628287,3.0154965539,0.7804577014\C,0,
 2.358101889,2.3660878214,1.344657661\C,0,3.3325773676,-1.1214143021,-0
 .6236069505\C,0,1.3351856202,-2.5999400199,-2.0315364139\C,0,-2.470843
 325,-1.2745542481,-2.1023368527\C,0,-2.6944671392,2.280894887,0.062349
 1163\C,0,1.1037280094,3.077810207,1.4871600634\C,0,3.5744728176,0.0622
 05216,0.1875150894\C,0,3.2368726435,0.0650195704,1.5398605834\C,0,-0.7
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 .6615737544\C,0,-1.2012781651,-2.6173591551,2.0846695202\C,0,0.2087590
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 ,1.1626144668,-3.0038074225,1.5120417946\C,0,1.6479949169,-0.681597868
 9,3.0909014415\C,0,-1.8477774951,1.4138096564,2.646841486\C,0,-3.28885
 8291,-1.2709535573,0.6962124202\C,0,-0.5997497432,-3.5149591941,-0.140
 940048\C,0,2.4036091152,-2.2592056155,1.3554684873\C,0,1.626675852,0.7
 781753252,3.0832695284\C,0,0.4202921226,1.4601551067,3.2185940569\C,0,
 -2.8474897319,0.6965821918,1.9362054408\C,0,-2.6501208674,-2.375633935
 8,0.1069844439\C,0,0.7513797262,-3.4764640585,0.2005704481\C,0,2.63755
 1286,-1.1151959847,2.1426124078\C,0,-1.2530636008,2.5971947456,2.04533
 65035\C,0,-3.7675076042,-0.0655759642,-0.1426616849\C,0,2.7565014217,-
 2.2644638805,-0.0384509537\C,0,2.6177549534,1.2390601852,2.1303739111\
 C,0,0.1515201642,2.6325326394,2.4092675556\C,0,-3.323915705,1.15318765
 19,0.6888278175\C,0,-2.2752054378,-2.4198522287,-1.3333008509\C,0,1.73
 66011452,-3.0110715395,-0.762240057\N,0,-1.434424142,-0.0362865466,-0.
 5933980199\H,0,-4.8207327927,-0.0812318194,-0.4477664255\\Version=EM64
 L-G09RevA.02\State=5-A\HF=-2326.6017608\MP2=-2334.594259\RMSD=6.875e-0
 9\PG=C01 [X(C60H1N1)]\\@

UB3LYP/6-31G(d)



0 5

C	0.871872599	0.706035893	-3.364034922
C	-0.355318091	1.419352069	-3.247686436
C	-0.122892296	2.605432197	-2.412683081
C	1.279488869	2.627417492	-2.055759578
C	1.897581721	1.449548694	-2.635417079
C	0.906329919	-0.720242368	-3.364095986
C	-1.571374868	0.693101609	-3.087257496
C	-1.079547438	3.044487484	-1.490116521
C	1.678513547	3.076467067	-0.789866943
C	2.887908916	0.768566938	-1.936670131
C	-0.325805546	-1.479284428	-3.227017267
C	-2.511346694	1.148734796	-2.133500972
C	-0.671594534	3.495025706	-0.174641250
C	2.712222403	2.363722323	-0.065597966
C	2.910555946	-0.691930155	-1.928215066
C	1.930861519	-1.411309051	-2.634033276
C	-1.537149324	-0.791707701	-3.077250664
C	-2.331629461	2.317075333	-1.339664007
C	0.683502129	3.517333417	0.169133605
C	3.310683211	1.233818293	-0.629641219
C	-0.065389473	-2.645057270	-2.402083693
C	-2.794710405	-0.057553097	-1.299436312
C	-1.020657850	-3.111247393	-1.472795827
C	-1.659762829	3.015496554	0.780457701
C	2.358101889	2.366087821	1.344657661
C	3.332577368	-1.121414302	-0.623606950
C	1.335185620	-2.599940020	-2.031536414
C	-2.470843325	-1.274554248	-2.102336853
C	-2.694467139	2.280894887	0.062349116
C	1.103728009	3.077810207	1.487160063

C	3.574472818	0.062205216	0.187515089
C	3.236872644	0.065019570	1.539860583
C	-0.798634736	-0.700198394	3.372770749
C	-1.819391397	-1.449525783	2.661573754
C	-1.201278165	-2.617359155	2.084669520
C	0.208759073	-2.587795086	2.435699275
C	0.448792067	-1.399667062	3.243836374
C	-0.824777538	0.713948506	3.354869142
C	-2.826922684	-0.776247096	1.955071519
C	-1.601931226	-3.066482353	0.818882051
C	1.162614467	-3.003807422	1.512041795
C	1.647994917	-0.681597869	3.090901442
C	-1.847777495	1.413809656	2.646841486
C	-3.288858291	-1.270953557	0.696212420
C	-0.599749743	-3.514959194	-0.140940048
C	2.403609115	-2.259205616	1.355468487
C	1.626675852	0.778175325	3.083269528
C	0.420292123	1.460155107	3.218594057
C	-2.847489732	0.696582192	1.936205441
C	-2.650120867	-2.375633936	0.106984444
C	0.751379726	-3.476464058	0.200570448
C	2.637551286	-1.115195985	2.142612408
C	-1.253063601	2.597194746	2.045336504
C	-3.767507604	-0.065575964	-0.142661685
C	2.756501422	-2.264463880	-0.038450954
C	2.617754953	1.239060185	2.130373911
C	0.151520164	2.632532639	2.409267556
C	-3.323915705	1.153187652	0.688827818
C	-2.275205438	-2.419852229	-1.333300851
C	1.736601145	-3.011071540	-0.762240057
N	-1.434424142	-0.036286547	-0.593398020
H	-4.820732793	-0.081231819	-0.447766426

Zero-point correction= 0.384680 (Hartree/Particle)

Thermal correction to Energy= 0.406913

Thermal correction to Enthalpy= 0.407857

Thermal correction to Gibbs Free Energy= 0.339158

Sum of electronic and zero-point Energies= -2340.901873

Sum of electronic and thermal Energies= -2340.879641

Sum of electronic and thermal Enthalpies= -2340.878696

Sum of electronic and thermal Free Energies= -2340.947396

1\1\FAU-CCC-CCDN086\Freq\UB3LYP\6-31G(d)\C60H1N1(5)\DRAL\13-Aug-2010\0
 \#P B3LYP/6-31G* Freq=NoRaman Geom=AllCheck Guess=Read POP=NONE NAME=
 DRAL\endohedral-N@C60H quintet\0,5\C,0.8718725993,0.7060358928,-3.36
 40349217\C,-0.3553180909,1.419352069,-3.2476864364\C,-0.1228922959,2.6
 054321974,-2.4126830806\C,1.2794888691,2.6274174922,-2.0557595778\C,1.
 8975817214,1.4495486935,-2.6354170793\C,0.9063299194,-0.7202423681,-3.
 3640959857\C,-1.5713748682,0.6931016093,-3.0872574955\C,-1.0795474377,
 3.0444874844,-1.4901165213\C,1.6785135466,3.0764670674,-0.7898669432\C

,2.8879089155,0.768566938,-1.9366701307\C,-0.3258055462,-1.4792844283,
-3.227017267\C,-2.5113466939,1.148734796,-2.1335009722\C,-0.6715945344
,3.4950257058,-0.1746412504\C,2.7122224026,2.3637223232,-0.0655979662\
C,2.9105559455,-0.6919301552,-1.9282150665\C,1.930861519,-1.4113090507
,-2.6340332764\C,-1.5371493237,-0.7917077007,-3.0772506636\C,-2.331629
4614,2.3170753328,-1.3396640066\C,0.6835021287,3.5173334167,0.16913360
49\C,3.3106832108,1.2338182929,-0.6296412192\C,-0.0653894727,-2.645057
2703,-2.4020836933\C,-2.7947104046,-0.0575530967,-1.2994363123\C,-1.02
06578503,-3.1112473929,-1.4727958268\C,-1.6597628287,3.0154965539,0.78
04577014\C,2.358101889,2.3660878214,1.344657661\C,3.3325773676,-1.1214
143021,-0.6236069505\C,1.3351856202,-2.5999400199,-2.0315364139\C,-2.4
70843325,-1.2745542481,-2.1023368527\C,-2.6944671392,2.280894887,0.062
3491163\C,1.1037280094,3.077810207,1.4871600634\C,3.5744728176,0.06220
5216,0.1875150894\C,3.2368726435,0.0650195704,1.5398605834\C,-0.798634
7365,-0.7001983938,3.3727707494\C,-1.8193913967,-1.4495257829,2.661573
7544\C,-1.2012781651,-2.6173591551,2.0846695202\C,0.208759073,-2.58779
50861,2.4356992752\C,0.4487920672,-1.3996670624,3.2438363738\C,-0.8247
775377,0.7139485057,3.3548691423\C,-2.8269226836,-0.7762470957,1.95507
15192\C,-1.601931226,-3.0664823532,0.8188820511\C,1.1626144668,-3.0038
074225,1.5120417946\C,1.6479949169,-0.6815978689,3.0909014415\C,-1.847
7774951,1.4138096564,2.646841486\C,-3.288858291,-1.2709535573,0.696212
4202\C,-0.5997497432,-3.5149591941,-0.140940048\C,2.4036091152,-2.2592
056155,1.3554684873\C,1.626675852,0.7781753252,3.0832695284\C,0.420292
1226,1.4601551067,3.2185940569\C,-2.8474897319,0.6965821918,1.93620544
08\C,-2.6501208674,-2.3756339358,0.1069844439\C,0.7513797262,-3.476464
0585,0.2005704481\C,2.637551286,-1.1151959847,2.1426124078\C,-1.253063
6008,2.5971947456,2.0453365035\C,-3.7675076042,-0.0655759642,-0.142661
6849\C,2.7565014217,-2.2644638805,-0.0384509537\C,2.6177549534,1.23906
01852,2.1303739111\C,0.1515201642,2.6325326394,2.4092675556\C,-3.32391
5705,1.1531876519,0.6888278175\C,-2.2752054378,-2.4198522287,-1.333300
8509\C,1.7366011452,-3.0110715395,-0.762240057\N,-1.434424142,-0.03628
65466,-0.5933980199\H,-4.8207327927,-0.0812318194,-0.4477664255\\Versi
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=6.000271\RMSD=4.577e-09\RMSF=1.369e-05\ZeroPoint=0.3846804\Thermal=0.
4069129\ZPE=241.3906153\Dipole=-0.7205856,-0.0537456,-0.1468282\Dipole
-0.0117934,0.0608221,0.0028587,-0.0654533,0.0058356,0.0636281\Polar=52
1.7049034,-16.4478673,486.7781878,0.3576637,-4.1017427,517.3514996\PG=
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73,-0.00178458,0.07643044,0.00105665,0.06944844\0.00001166,0.0000319
00000605,0.00000503\\@

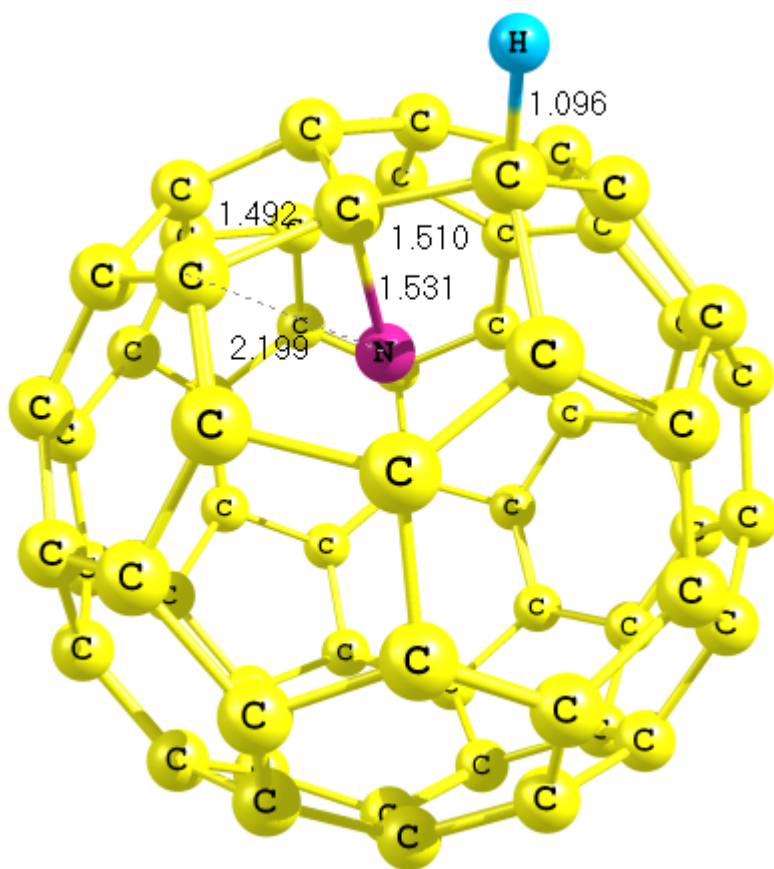
2b⁺ (N@C₆₀H⁺⁺⁺, endohedrally bound, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\21-Mar-201
0\0\#P ROMP2/6-31G* Geom=AllCheck Guess=Read Name=Dral\endohedral-N@
C60H(+) quartet DFT SP\1,4\C,0,0.882692973,0.700715512,-3.360328846\C

,0,-0.36321438,1.423726489,-3.242983813\C,0,-0.133367822,2.607835615,-
 2.428037082\C,0,1.271013064,2.61898417,-2.063170621\C,0,1.901318474,1.
 445342776,-2.645008578\C,0,0.903252541,-0.71364603,-3.352192124\C,0,-1
 .556023648,0.698631484,-3.090007479\C,0,-1.097676568,3.053853253,-1.50
 649414\C,0,1.658952656,3.056734702,-0.797510436\C,0,2.888662632,0.7608
 65179,-1.938500474\C,0,-0.321191176,-1.47105253,-3.226181135\C,0,-2.50
 2669873,1.162524086,-2.117378364\C,0,-0.689780136,3.48837546,-0.179862
 375\C,0,2.695775079,2.345510093,-0.068312524\C,0,2.90998698,-0.6992308
 63,-1.930152637\C,0,1.942958284,-1.420141888,-2.628513431\C,0,-1.53463
 326,-0.779251644,-3.081572782\C,0,-2.332971802,2.320484344,-1.35665522
 7\C,0,0.659954402,3.499066197,0.16207288\C,0,3.304110606,1.22038263,-0
 .630766762\C,0,-0.057213794,-2.638574152,-2.397754341\C,0,-2.801523426
 ,-0.04826794,-1.298488472\C,0,-1.008281505,-3.101513911,-1.470857879\C
 ,0,-1.677793197,3.01786685,0.78430633\C,0,2.341602753,2.348374955,1.33
 7205987\C,0,3.338360907,-1.131356422,-0.617211553\C,0,1.346814496,-2.6
 04716144,-2.032981854\C,0,-2.467421183,-1.259118916,-2.103283657\C,0,-
 2.70534718,2.282327097,0.078822689\C,0,1.084336728,3.060627914,1.48263
 2052\C,0,3.580245911,0.052990927,0.190052637\C,0,3.241211092,0.0558833
 55,1.540914853\C,0,-0.796954786,-0.696031047,3.362832548\C,0,-1.814010
 692,-1.442632423,2.660691091\C,0,-1.192030291,-2.611427483,2.082702132
 \C,0,0.217633344,-2.592549177,2.440744154\C,0,0.459961116,-1.406949172
 ,3.243249954\C,0,-0.817371223,0.711289432,3.35466551\C,0,-2.823945725,
 -0.764427988,1.956577571\C,0,-1.589630348,-3.056079855,0.819384318\C,0
 ,1.172422102,-3.010563634,1.517659647\C,0,1.6470091,-0.688828258,3.093
 908009\C,0,-1.855588773,1.419940554,2.644211713\C,0,-3.282010557,-1.25
 3270904,0.696449928\C,0,-0.588229327,-3.508772906,-0.139453805\C,0,2.4
 0856082,-2.263930296,1.363850115\C,0,1.625801261,0.771897495,3.0854447
 07\C,0,0.418399292,1.45693368,3.226620325\C,0,-2.84533523,0.704604878,
 1.948187186\C,0,-2.638013449,-2.358892182,0.105641841\C,0,0.761207592,
 -3.476449482,0.202358047\C,0,2.64472967,-1.125375972,2.14179512\C,0,-1
 .267649233,2.59950301,2.052575652\C,0,-3.773589958,-0.055648013,-0.142
 959946\C,0,2.76278912,-2.267052257,-0.0416717\C,0,2.610604159,1.226203
 841,2.128208608\C,0,0.141899421,2.625663731,2.410563184\C,0,-3.3168951
 94,1.165258994,0.682478308\C,0,-2.264561862,-2.402845643,-1.329432739\
 C,0,1.747081064,-3.016346315,-0.762410007\N,0,-1.439353874,-0.02466424
 ,-0.601006835\H,0,-4.828833161,-0.072326019,-0.437355479\\Version=AM64
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 9\Thermal=0.\PG=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)



1 4

C	0.882692973	0.700715512	-3.360328846
C	-0.363214380	1.423726489	-3.242983813
C	-0.133367822	2.607835615	-2.428037082
C	1.271013064	2.618984170	-2.063170621
C	1.901318474	1.445342776	-2.645008578
C	0.903252541	-0.713646030	-3.352192124
C	-1.556023648	0.698631484	-3.090007479
C	-1.097676568	3.053853253	-1.506494140
C	1.658952656	3.056734702	-0.797510436
C	2.888662632	0.760865179	-1.938500474
C	-0.321191176	-1.471052530	-3.226181135
C	-2.502669873	1.162524086	-2.117378364
C	-0.689780136	3.488375460	-0.179862375
C	2.695775079	2.345510093	-0.068312524
C	2.909986980	-0.699230863	-1.930152637
C	1.942958284	-1.420141888	-2.628513431
C	-1.534633260	-0.779251644	-3.081572782
C	-2.332971802	2.320484344	-1.356655227
C	0.659954402	3.499066197	0.162072880
C	3.304110606	1.220382630	-0.630766762
C	-0.057213794	-2.638574152	-2.397754341
C	-2.801523426	-0.048267940	-1.298488472
C	-1.008281505	-3.101513911	-1.470857879
C	-1.677793197	3.017866850	0.784306330

C	2.341602753	2.348374955	1.337205987
C	3.338360907	-1.131356422	-0.617211553
C	1.346814496	-2.604716144	-2.032981854
C	-2.467421183	-1.259118916	-2.103283657
C	-2.705347180	2.282327097	0.078822689
C	1.084336728	3.060627914	1.482632052
C	3.580245911	0.052990927	0.190052637
C	3.241211092	0.055883355	1.540914853
C	-0.796954786	-0.696031047	3.362832548
C	-1.814010692	-1.442632423	2.660691091
C	-1.192030291	-2.611427483	2.082702132
C	0.217633344	-2.592549177	2.440744154
C	0.459961116	-1.406949172	3.243249954
C	-0.817371223	0.711289432	3.354665510
C	-2.823945725	-0.764427988	1.956577571
C	-1.589630348	-3.056079855	0.819384318
C	1.172422102	-3.010563634	1.517659647
C	1.647009100	-0.688828258	3.093908009
C	-1.855588773	1.419940554	2.644211713
C	-3.282010557	-1.253270904	0.696449928
C	-0.588229327	-3.508772906	-0.139453805
C	2.408560820	-2.263930296	1.363850115
C	1.625801261	0.771897495	3.085444707
C	0.418399292	1.456933680	3.226620325
C	-2.845335230	0.704604878	1.948187186
C	-2.638013449	-2.358892182	0.105641841
C	0.761207592	-3.476449482	0.202358047
C	2.644729670	-1.125375972	2.141795120
C	-1.267649233	2.599503010	2.052575652
C	-3.773589958	-0.055648013	-0.142959946
C	2.762789120	-2.267052257	-0.041671700
C	2.610604159	1.226203841	2.128208608
C	0.141899421	2.625663731	2.410563184
C	-3.316895194	1.165258994	0.682478308
C	-2.264561862	-2.402845643	-1.329432739
C	1.747081064	-3.016346315	-0.762410007
N	-1.439353874	-0.024664240	-0.601006835
H	-4.828833161	-0.072326019	-0.437355479

Zero-point correction= 0.387136 (Hartree/Particle)

Thermal correction to Energy= 0.409160

Thermal correction to Enthalpy= 0.410104

Thermal correction to Gibbs Free Energy= 0.341879

Sum of electronic and zero-point Energies= -2340.700066

Sum of electronic and thermal Energies= -2340.678042

Sum of electronic and thermal Enthalpies= -2340.677098

Sum of electronic and thermal Free Energies= -2340.745323

1\1\FAU-CCC-CCDH154\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\18-Dec-200
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\1,4\C,0.882692973,0.700715512,-3.360328846\C,-0.36321438,1.423726489,
 -3.242983813\C,-0.133367822,2.607835615,-2.428037082\C,1.271013064,2.6
 1898417,-2.063170621\C,1.901318474,1.445342776,-2.645008578\C,0.903252
 541,-0.71364603,-3.352192124\C,-1.556023648,0.698631484,-3.090007479\C
 ,-1.097676568,3.053853253,-1.50649414\C,1.658952656,3.056734702,-0.797
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NBO Analysis

Summary of Natural Population Analysis:

Natural Population
 Natural -----

Atom	No	Charge	Core	Valence	Rydberg	Total

C	1	0.04206	1.99873	3.94488	0.01432	5.95794
C	2	0.01592	1.99867	3.97064	0.01477	5.98408
C	3	0.01791	1.99872	3.96890	0.01447	5.98209
C	4	0.00854	1.99870	3.97828	0.01447	5.99146
C	5	-0.00237	1.99869	3.98920	0.01448	6.00237
C	6	0.04202	1.99873	3.94493	0.01432	5.95798
C	7	0.01667	1.99868	3.96828	0.01636	5.98333
C	8	0.00752	1.99867	3.97903	0.01478	5.99248
C	9	0.01853	1.99871	3.96838	0.01439	5.98147
C	10	0.02960	1.99872	3.95731	0.01437	5.97040
C	11	0.01602	1.99867	3.97054	0.01477	5.98398
C	12	0.04716	1.99859	3.93627	0.01799	5.95284
C	13	0.01743	1.99871	3.96940	0.01446	5.98257
C	14	0.01794	1.99871	3.96900	0.01435	5.98206
C	15	0.02957	1.99872	3.95733	0.01437	5.97043
C	16	-0.00233	1.99869	3.98916	0.01448	6.00233
C	17	0.01662	1.99868	3.96834	0.01637	5.98338
C	18	0.03702	1.99864	3.94829	0.01605	5.96298
C	19	0.01366	1.99871	3.97323	0.01440	5.98634
C	20	0.00946	1.99870	3.97744	0.01440	5.99054
C	21	0.01782	1.99872	3.96899	0.01448	5.98218
C	22	0.00908	1.99897	3.96580	0.02615	5.99092
C	23	0.00760	1.99867	3.97895	0.01478	5.99240
C	24	0.00626	1.99871	3.98053	0.01451	5.99374
C	25	0.02028	1.99872	3.96666	0.01435	5.97972
C	26	0.00948	1.99870	3.97742	0.01440	5.99052
C	27	0.00855	1.99870	3.97827	0.01447	5.99145
C	28	0.04721	1.99859	3.93622	0.01799	5.95279
C	29	0.01106	1.99873	3.97503	0.01518	5.98894
C	30	0.01522	1.99871	3.97168	0.01439	5.98478
C	31	0.01340	1.99871	3.97342	0.01447	5.98660
C	32	0.01044	1.99870	3.97638	0.01448	5.98956
C	33	0.04175	1.99874	3.94516	0.01436	5.95825
C	34	0.00491	1.99870	3.98196	0.01443	5.99509
C	35	0.01624	1.99871	3.97061	0.01444	5.98376
C	36	0.01361	1.99870	3.97318	0.01451	5.98639
C	37	-0.00142	1.99869	3.98825	0.01448	6.00142
C	38	0.04174	1.99874	3.94516	0.01436	5.95826
C	39	0.01341	1.99871	3.97332	0.01457	5.98659
C	40	0.00625	1.99871	3.98054	0.01451	5.99375
C	41	0.01522	1.99871	3.97168	0.01439	5.98478
C	42	0.02725	1.99872	3.95963	0.01440	5.97275
C	43	0.00495	1.99870	3.98191	0.01443	5.99505
C	44	0.05508	1.99879	3.92952	0.01661	5.94492
C	45	0.01741	1.99871	3.96942	0.01446	5.98259
C	46	0.02028	1.99872	3.96666	0.01435	5.97972
C	47	0.02725	1.99872	3.95963	0.01440	5.97275
C	48	-0.00143	1.99869	3.98826	0.01448	6.00143

C	49	0.01334	1.99871	3.97339	0.01457	5.98666
C	50	0.01113	1.99873	3.97496	0.01518	5.98887
C	51	0.01368	1.99871	3.97321	0.01440	5.98632
C	52	0.01004	1.99870	3.97685	0.01441	5.98996
C	53	0.01623	1.99871	3.97062	0.01444	5.98377
C	54	-0.26839	1.99893	4.24916	0.02031	6.26839
C	55	0.01793	1.99871	3.96901	0.01435	5.98207
C	56	0.01003	1.99870	3.97685	0.01441	5.98997
C	57	0.01362	1.99870	3.97317	0.01451	5.98638
C	58	0.05516	1.99879	3.92944	0.01661	5.94484
C	59	0.03694	1.99864	3.94837	0.01605	5.96306
C	60	0.01850	1.99871	3.96840	0.01439	5.98150
N	61	-0.13569	1.99987	5.12538	0.01044	7.13569
H	62	0.30967	0.00000	0.68918	0.00115	0.69033

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* Total * 1.00000 121.92255 244.16102 0.91643 367.00000

NBO Analysis PCM (Benzene)

Summary of Natural Population Analysis:

Natural Population						
Natural -----						
Atom	No	Charge	Core	Valence	Rydberg	Total

C	1	0.04248	1.99873	3.94445	0.01433	5.95752
C	2	0.01627	1.99867	3.97028	0.01477	5.98373
C	3	0.01746	1.99872	3.96936	0.01447	5.98254
C	4	0.00803	1.99870	3.97881	0.01446	5.99197
C	5	-0.00261	1.99869	3.98945	0.01447	6.00261
C	6	0.04245	1.99873	3.94448	0.01433	5.95755
C	7	0.01729	1.99868	3.96766	0.01637	5.98271
C	8	0.00715	1.99867	3.97940	0.01477	5.99285
C	9	0.01772	1.99871	3.96919	0.01438	5.98228
C	10	0.02911	1.99872	3.95779	0.01437	5.97089
C	11	0.01642	1.99867	3.97014	0.01477	5.98358
C	12	0.05013	1.99859	3.93327	0.01801	5.94987
C	13	0.01710	1.99871	3.96974	0.01446	5.98290
C	14	0.01739	1.99871	3.96955	0.01434	5.98261
C	15	0.02904	1.99872	3.95787	0.01437	5.97096
C	16	-0.00261	1.99869	3.98944	0.01447	6.00261
C	17	0.01727	1.99868	3.96768	0.01637	5.98273
C	18	0.03761	1.99864	3.94770	0.01605	5.96239
C	19	0.01284	1.99871	3.97406	0.01440	5.98716
C	20	0.00881	1.99870	3.97809	0.01440	5.99119
C	21	0.01741	1.99872	3.96941	0.01447	5.98259
C	22	0.01024	1.99897	3.96454	0.02625	5.98976
C	23	0.00726	1.99867	3.97930	0.01477	5.99274
C	24	0.00584	1.99871	3.98096	0.01450	5.99416

C	25	0.01961	1.99872	3.96733	0.01434	5.98039
C	26	0.00881	1.99870	3.97809	0.01440	5.99119
C	27	0.00798	1.99870	3.97885	0.01446	5.99202
C	28	0.05012	1.99859	3.93328	0.01801	5.94988
C	29	0.01113	1.99873	3.97495	0.01519	5.98887
C	30	0.01439	1.99871	3.97252	0.01439	5.98561
C	31	0.01257	1.99871	3.97426	0.01446	5.98743
C	32	0.00960	1.99870	3.97722	0.01447	5.99040
C	33	0.04183	1.99874	3.94506	0.01437	5.95817
C	34	0.00483	1.99870	3.98204	0.01442	5.99517
C	35	0.01524	1.99871	3.97162	0.01443	5.98476
C	36	0.01290	1.99870	3.97391	0.01450	5.98710
C	37	-0.00186	1.99869	3.98870	0.01447	6.00186
C	38	0.04186	1.99874	3.94503	0.01437	5.95814
C	39	0.01388	1.99870	3.97285	0.01457	5.98612
C	40	0.00582	1.99871	3.98098	0.01450	5.99418
C	41	0.01435	1.99871	3.97255	0.01439	5.98565
C	42	0.02660	1.99872	3.96029	0.01440	5.97340
C	43	0.00488	1.99870	3.98199	0.01442	5.99512
C	44	0.05788	1.99879	3.92670	0.01663	5.94212
C	45	0.01706	1.99871	3.96978	0.01446	5.98294
C	46	0.01961	1.99872	3.96733	0.01435	5.98039
C	47	0.02659	1.99872	3.96029	0.01440	5.97341
C	48	-0.00186	1.99869	3.98870	0.01447	6.00186
C	49	0.01380	1.99870	3.97292	0.01457	5.98620
C	50	0.01130	1.99873	3.97479	0.01519	5.98870
C	51	0.01281	1.99871	3.97409	0.01439	5.98719
C	52	0.00925	1.99870	3.97764	0.01440	5.99075
C	53	0.01528	1.99871	3.97158	0.01444	5.98472
C	54	-0.26768	1.99893	4.24832	0.02043	6.26768
C	55	0.01734	1.99871	3.96960	0.01434	5.98266
C	56	0.00923	1.99870	3.97766	0.01440	5.99077
C	57	0.01293	1.99870	3.97387	0.01450	5.98707
C	58	0.05793	1.99879	3.92665	0.01663	5.94207
C	59	0.03761	1.99864	3.94770	0.01605	5.96239
C	60	0.01760	1.99871	3.96931	0.01438	5.98240
N	61	-0.13608	1.99987	5.12579	0.01041	7.13608
H	62	0.31477	0.00000	0.68413	0.00111	0.68523

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* Total * 1.00000 121.92254 244.16096 0.91650 367.00000

2c⁺ (N@C₆₀H⁺⁺⁺,endo-5,6-aza bridge, quartet)

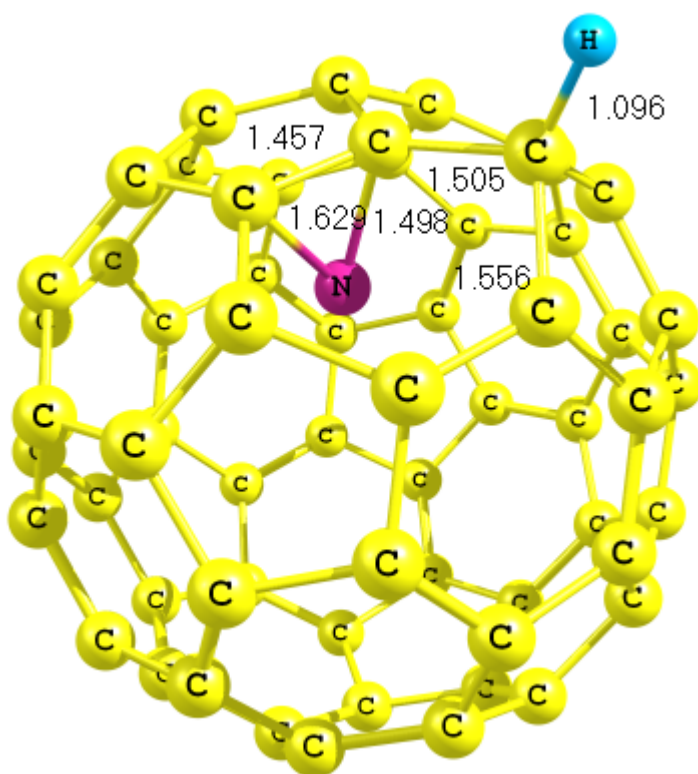
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 258406876,0.05841915\C,0,1.083437986,3.05732888,1.476708775\C,0,3.5796
 75741,0.057123495,0.190225082\C,0,3.2409698,0.062035842,1.541082889\C,
 0,-0.798108841,-0.70586767,3.356169023\C,0,-1.815928602,-1.461190604,2
 .657202607\C,0,-1.189899137,-2.631171038,2.086152677\C,0,0.22176634,-2
 .601069987,2.440748615\C,0,0.458784855,-1.410227414,3.239159896\C,0,-0
 .818946987,0.702195816,3.35439949\C,0,-2.81593436,-0.787527248,1.93817
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 76053,1.524320936\C,0,1.646236279,-0.68816241,3.092429043\C,0,-1.84958
 1339,1.400284896,2.63086808\C,0,-3.287335751,-1.281557853,0.681743106\
 C,0,-0.578624892,-3.52915915,-0.129644209\C,0,2.410663122,-2.266189058
 ,1.367063322\C,0,1.623201514,0.772089134,3.083379437\C,0,0.41479516,1.
 451822448,3.223800819\C,0,-2.831423247,0.679263305,1.928057976\C,0,-2.
 649378171,-2.405959255,0.105342106\C,0,0.773793478,-3.492457423,0.2098
 58675\C,0,2.640955086,-1.121512348,2.141077733\C,0,-1.26516762,2.58480
 8315,2.039399647\C,0,-3.811652112,-0.070604892,-0.142839274\C,0,2.7593
 7013,-2.270066331,-0.037816436\C,0,2.611982363,1.230635359,2.126885333
 \C,0,0.137627805,2.619816097,2.403695772\C,0,-3.297951018,1.135803008,
 0.664912286\C,0,-2.309755432,-2.500539722,-1.322164437\C,0,1.752774966
 ,-3.028609377,-0.753566978\N,0,-1.554433842,-0.34119265,-0.894089895\H
 ,0,-4.888852237,-0.069944148,-0.345787776\\Version=AM64L-G03RevD.02\St
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 G=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)

Zero-point correction=	0.386010 (Hartree/Particle)
Thermal correction to Energy=	0.408241
Thermal correction to Enthalpy=	0.409185
Thermal correction to Gibbs Free Energy=	0.340589
Sum of electronic and zero-point Energies=	-2340.688076
Sum of electronic and thermal Energies=	-2340.665845
Sum of electronic and thermal Enthalpies=	-2340.664900
Sum of electronic and thermal Free Energies=	-2340.733497

1\1\FAU-CCC-CCDH151\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\20-Jul-2009\0\#P UB3LYP/6-31G* Freq=NoRaman Name=Dral\endo-5-6-N@C60H (+) quar tet\1,4\C,0.892777826,0.701614083,-3.372756085\C,-0.349069233,1.423370721,-3.261339202\C,-0.123750089,2.602296616,-2.435221914\C,1.279619106,2.619041969,-2.068695576\C,1.909378489,1.444799052,-2.650497741\C,0.917373368,-0.719468353,-3.366401522\C,-1.548388358,0.700957006,-3.117425154\C,-1.092980452,3.035159362,-1.514395662\C,1.664372124,3.055350302,-0.801266228\C,2.893311658,0.761266771,-1.940299918\C,-0.306192882,-1.471950731,-3.245129781\C,-2.520360552,1.160392908,-2.149668522\C,-0.688003582,3.472931449,-0.189592461\C,2.701857854,2.348716032,-0.069327415\C,2.91041053,-0.699700832,-1.925878509\C,1.939114799,-1.421200843,-2.623228735\C,-1.492051867,-0.764410694,-3.099809008\C,-2.331664744,2.30523704,-1.369404758\C,0.66115552,3.493520269,0.156708442\C,3.308431541,1.223251429,-0.631683114\C,-0.056822855,-2.648625624,-2.387604994\C,-2.942370909,-0.040403756,-1.370900142\C,-1.005023278,-3.120082824,-1.455155047\C,-1.674500429,2.99725065,0.768325976\C,2.345792537,2.352154067,1.336071057\C,3.334681313,-1.128423171,-0.616009205\C,1.33639710

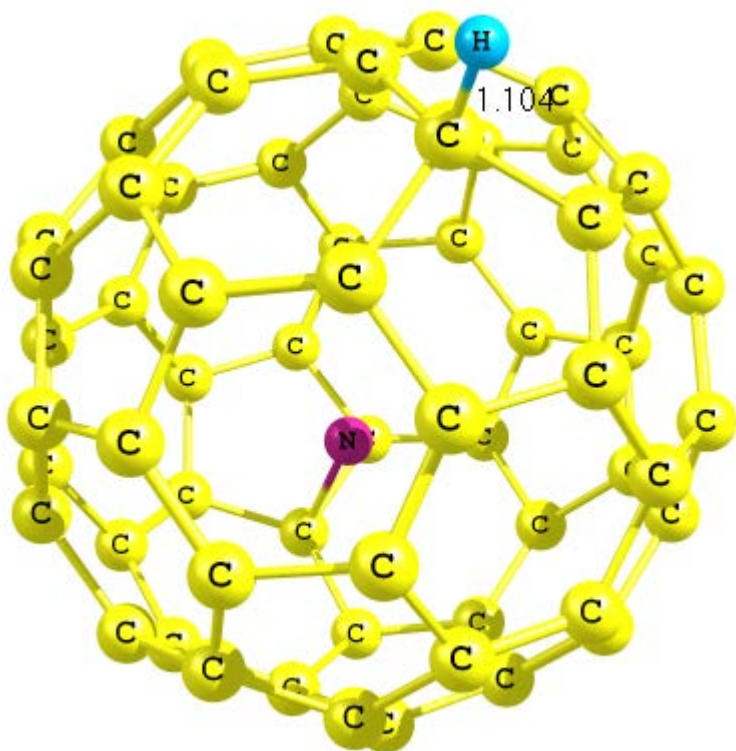
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 ,-2.695133248,2.258406876,0.05841915\C,1.083437986,3.05732888,1.476708
 775\C,3.579675741,0.057123495,0.190225082\C,3.2409698,0.062035842,1.54
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 ,-3.52915915,-0.129644209\C,2.410663122,-2.266189058,1.367063322\C,1.6
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 C,-2.831423247,0.679263305,1.928057976\C,-2.649378171,-2.405959255,0.1
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 -0.070604892,-0.142839274\C,2.75937013,-2.270066331,-0.037816436\C,2.6
 11982363,1.230635359,2.126885333\C,0.137627805,2.619816097,2.403695772
 \C,-3.297951018,1.135803008,0.664912286\C,-2.309755432,-2.500539722,-1
 .322164437\C,1.752774966,-3.028609377,-0.753566978\N,-1.554433842,-0.3
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 00024497,0.00023902,0.00033825,-0.00000071,0.00001202,-0.00001124\\@

2c⁺ (N@C₆₀H⁺⁺⁺, endo-5,6-aza bridge opposite to H⁺, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN088\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\23-Mar-201
 0\0\#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=VShift N
 ame=Dral\endo-opposite-5-6-N@C60H(+) quartet\1,4\C,0.103274781,3.577
 71277,0.778889026\C,-1.155953127,3.530981761,1.504508153\C,-0.98360709
 1,2.6770762,2.675195105\C,0.359353546,2.179503803,2.677493383\C,1.0487
 18435,2.760104218,1.50908711\C,0.104318066,3.569883534,-0.623597891\C,
 -2.35406132,3.509835241,0.807693972\C,-2.043401691,1.850088674,3.10166
 03\C,0.623646468,0.869379871,3.168876311\C,1.951683986,1.986553361,0.7
 88106667\C,-1.155039115,3.538114799,-1.342955787\C,-3.448041217,2.6421
 3196,1.245386155\C,-1.771876814,0.491780264,3.562846048\C,1.546047814,
 0.02890465,2.476691445\C,1.982808785,1.96410333,-0.674095742\C,1.05123
 6614,2.75009302,-1.367078744\C,-2.356654454,3.515625424,-0.639784031\C
 ,-3.288852227,1.839577745,2.392689819\C,-0.468313612,0.00860784,3.6002

54072\C,2.027662317,0.574806883,1.223767853\C,-0.987982067,2.693939822
 ,-2.514960703\C,-4.119734796,2.153198685,0.096525693\C,-2.038144045,1.
 863440448,-2.925905027\C,-2.854447175,-0.358551854,3.112286019\C,1.077
 293367,-1.345285531,2.439874221\C,2.239857071,0.602764383,-1.146311825
 \C,0.373131532,2.20167585,-2.528740828\C,-3.447370654,2.653338664,-1.0
 70726659\C,-3.801223848,0.460804903,2.388955304\C,-0.185540025,-1.3534
 91926,3.150999192\C,2.202176331,-0.268411395,0.049390998\C,1.941112195
 ,-1.693377472,0.087521837\C,-2.308486745,-3.00707078,-0.609464633\C,-3
 .251509593,-2.176912661,-1.338423779\C,-2.582743014,-1.657383283,-2.50
 6388577\C,-1.22038539,-2.157638737,-2.506674055\C,-1.052855578,-3.0029
 90782,-1.337718565\C,-2.308485964,-3.007180191,0.786031612\C,-4.153119
 387,-1.364210242,-0.637552766\C,-2.84645995,-0.348635956,-2.921694288\
 C,-0.174912213,-1.32739535,-2.925415402\C,0.156011449,-3.005882903,-0.
 642439108\C,-3.250624872,-2.181636366,1.516451873\C,-4.453493886,-0.03
 9204904,-1.094411542\C,-1.76109545,0.505755627,-3.367934859\C,1.078281
 592,-1.317357597,-2.208749353\C,0.155929294,-3.003123647,0.817666635\C
 ,-1.051243438,-2.997698372,1.513245646\C,-4.152006718,-1.366549031,0.8
 18431641\C,-3.796519733,0.466850733,-2.200274939\C,-0.453734272,0.0278
 39442,-3.382926794\C,1.246994542,-2.163755922,-1.094536742\C,-2.586044
 968,-1.66630172,2.691617632\C,-4.874619997,0.840112728,0.093537485\C,1
 .591554953,0.06946912,-2.253992009\C,1.24817529,-2.15528189,1.27107212
 8\C,-1.228307347,-2.166221621,2.702738858\C,-4.453813079,-0.042420915,
 1.279905551\C,-3.287116848,1.848440334,-2.202898384\C,0.639457786,0.88
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UB3LYP/6-31G(d)

Zero-point correction=	0.384603 (Hartree/Particle)
Thermal correction to Energy=	0.407147
Thermal correction to Enthalpy=	0.408091
Thermal correction to Gibbs Free Energy=	0.339034
Sum of electronic and zero-point Energies=	-2340.649130
Sum of electronic and thermal Energies=	-2340.626586
Sum of electronic and thermal Enthalpies=	-2340.625642
Sum of electronic and thermal Free Energies=	-2340.694699

1\1\FAU-CCC-CCDN085\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\21-Jul-2009\0\#P B3LYP/6-31G* Freq=NoRaman Pop=None NAME=DRAL\endo-opposite-5-6-N@C60H(+) quartet\1,4\C,0.103274781,3.57771277,0.778889026\C,-1.155953127,3.530981761,1.504508153\C,-0.983607091,2.6770762,2.675195105\C,0.359353546,2.179503803,2.677493383\C,1.048718435,2.760104218,1.50908711\C,0.104318066,3.569883534,-0.623597891\C,-2.35406132,3.509835241,0.807693972\C,-2.043401691,1.850088674,3.1016603\C,0.623646468,0.869379871,3.168876311\C,1.951683986,1.986553361,0.788106667\C,-1.155039115,3.538114799,-1.342955787\C,-3.448041217,2.64213196,1.245386155\C,-1.771876814,0.491780264,3.562846048\C,1.546047814,0.02890465,2.476691445\C,1.982808785,1.96410333,-0.674095742\C,1.051236614,2.75009302,-1.367078744\C,-2.356654454,3.515625424,-0.639784031\C,-3.288852227,1.839577745,2.392689819\C,-0.468313612,0.00860784,3.600254072\C,2.027662317,0.574806883,1.223767853\C,-0.987982067,2.693939822,-2.514960703\C,-4.119734796,2.153198685,0.096525693\C,-2.038144045,1.863440448,-2.925905027\C,-2.854447175,-0.358551854,3.112286019\C,1.077293367,-1.345285531,2.439874221\C,2.239857071,0.602764383,-1.146311825\C,0.373131532,2.20167585,

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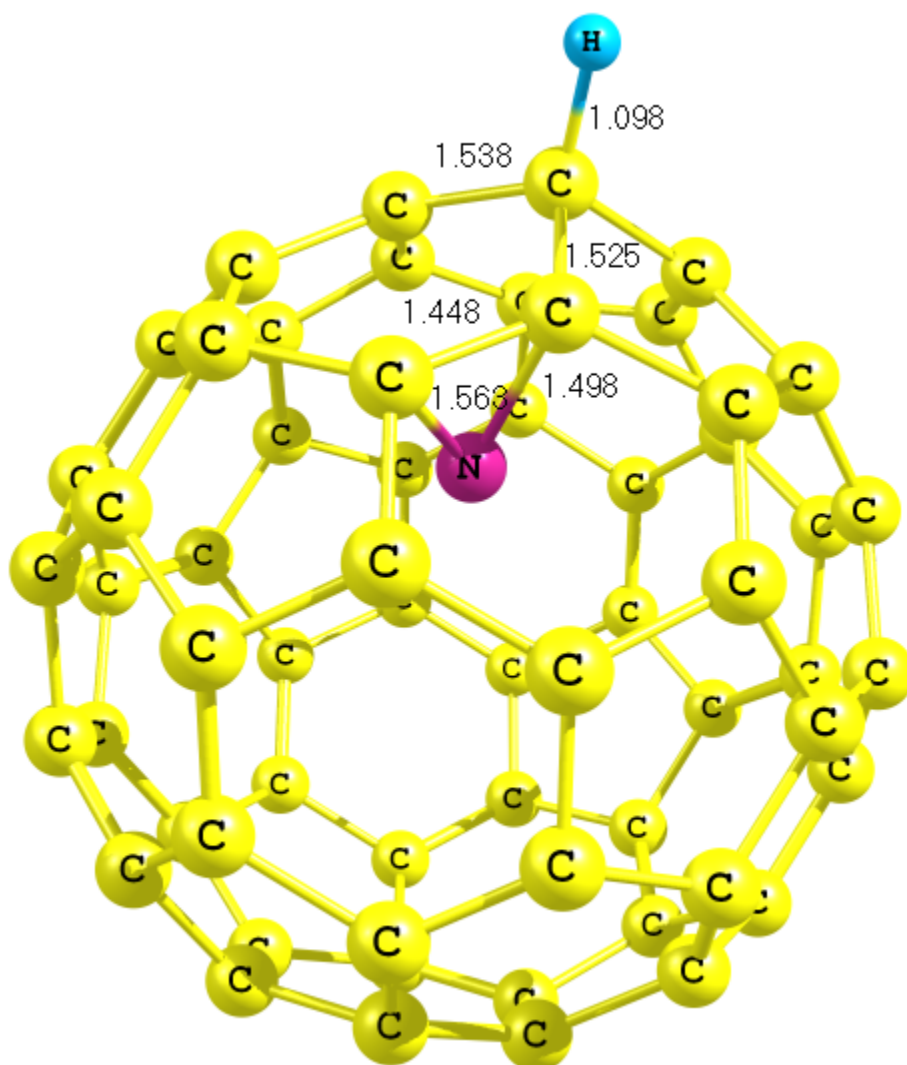
2d⁺ (N@C₆₀H⁺⁺⁺, endo-6,6-aza bridge, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN091\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\21-Mar-2010\0\#P ROMP2/6-31G* Geom=AllCheck Guess=Read Name=Dral\endo-6,6-N@C60H(+) quartet DFT SP\1,4\C,0,2.164326161,3.380530076,1.038861126\C,0,0.905154194,3.363664098,1.764933484\C,0,1.071389948,2.52211535,2.936670852\C,0,2.421032618,2.014183665,2.930432961\C,0,3.104091115,2.544583406,1.763399128\C,0,2.162631516,3.381437347,-0.35485258\C,0,-0.297903322,3.359341534,1.069517754\C,0,0.015400243,1.696994853,3.356346865\C,0,2.690774328,0.70567363,3.367961302\C,0,4.010906071,1.744439226,1.067243546\C,0,0.904322789,3.375720963,-1.083830148\C,0,-1.39446071,2.499195876,1.506783848\C,0,0.297679716,0.341519338,3.81037174\C,0,3.63950283,-0.118450617,2.649458602\C,0,4.011237021,1.748521356,-0.381230654\C,0,3.108127747,2.550129495,-1.079016918\C,0,-0.305126109,3.37986531,-0.378209522\C,0,-1.236124861,1.689728062,2.652217684\C,0,1.606231558,-0.14059739,3.82008301\C,0,4.28490913,0.386334325,1.517430687\C,0,1.0804400

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 528,-3.192224518,-0.33462542\C,0,-1.200524852,-2.365338619,-1.04522180
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 ,0,-0.733317108,-0.501289769,-2.702561904\C,0,1.881022692,-1.486123557
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 -1.955176467\C,0,2.211551644,-3.139720607,1.083070502\C,0,1.008205809,
 -3.163364783,1.788225568\C,0,-2.146897518,-1.567753064,1.136934422\C,0
 ,-1.588453189,0.354237364,-1.869419389\C,0,1.618025714,-0.124754785,-3
 .13441976\C,0,3.288803939,-2.278194671,-0.819119015\C,0,-0.522218987,-
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 10505531,1.591743451\C,0,-1.22368624,1.782584612,-1.995967923\C,0,2.70
 0643078,0.719989404,-2.688166132\N,0,-0.756607365,0.149442477,-0.56191
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 0.PG=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)



Zero-point correction=	0.386543 (Hartree/Particle)
Thermal correction to Energy=	0.408510
Thermal correction to Enthalpy=	0.409454
Thermal correction to Gibbs Free Energy=	0.341395
Sum of electronic and zero-point Energies=	-2340.678459
Sum of electronic and thermal Energies=	-2340.656493
Sum of electronic and thermal Enthalpies=	-2340.655548
Sum of electronic and thermal Free Energies=	-2340.723608

1\1\GINC-A05\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\14-Dec-2008\0\#P
 UB3LYP/6-31G* Freq=NoRaman Name=DrAl\6-6-N@C60H (+) (quartet)\1,4\C
 ,2.164326161,3.380530076,1.038861126\C,0.905154194,3.363664098,1.76493
 3484\C,1.071389948,2.52211535,2.936670852\C,2.421032618,2.014183665,2.
 930432961\C,3.104091115,2.544583406,1.763399128\C,2.162631516,3.381437
 347,-0.35485258\C,-0.297903322,3.359341534,1.069517754\C,0.015400243,1
 .696994853,3.356346865\C,2.690774328,0.70567363,3.367961302\C,4.010906
 071,1.744439226,1.067243546\C,0.904322789,3.375720963,-1.083830148\C,-

1.39446071,2.499195876,1.506783848\C,0.297679716,0.341519338,3.8103717
 4\C,3.63950283,-0.118450617,2.649458602\C,4.011237021,1.748521356,-0.3
 81230654\C,3.108127747,2.550129495,-1.079016918\C,-0.305126109,3.37986
 531,-0.378209522\C,-1.236124861,1.689728062,2.652217684\C,1.606231558,
 -0.14059739,3.82008301\C,4.28490913,0.386334325,1.517430687\C,1.080440
 076,2.552283823,-2.268247533\C,-2.115456665,2.044046072,0.366977042\C,
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 001385\C,3.140042834,-1.483160611,2.654307944\C,4.281156774,0.38963894
 1,-0.830001736\C,2.430904881,2.026268778,-2.251007181\C,-1.409691501,2
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 C,3.96865269,-1.760410513,0.3495732\C,-0.257453528,-3.192224518,-0.334
 62542\C,-1.200524852,-2.365338619,-1.045221807\C,-0.508005106,-1.82438
 586,-2.241064124\C,0.83246499,-2.324671742,-2.24457032\C,1.000944493,-
 3.164530173,-1.06622941\C,-0.252945627,-3.177587235,1.069722813\C,-2.1
 1183677,-1.592462166,-0.303120513\C,-0.733317108,-0.501289769,-2.70256
 1904\C,1.881022692,-1.486123557,-2.674244319\C,2.20643523,-3.137817341
 ,-0.370666487\C,-1.202119345,-2.362316768,1.815824236\C,-2.219157226,-
 0.157336929,-0.670730028\C,0.305790166,0.371935826,-3.168640928\C,3.12
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 1.136934422\C,-1.588453189,0.354237364,-1.869419389\C,1.618025714,-0.1
 24754785,-3.13441976\C,3.288803939,-2.278194671,-0.819119015\C,-0.5222
 18987,-1.828376768,2.965609716\C,-2.865536237,0.701701932,0.410286248\
 C,3.642556417,-0.110478097,-1.958443708\C,3.301174649,-2.288080375,1.5
 26222577\C,0.843348902,-2.327129643,2.965052294\C,-2.445287808,-0.2105
 05531,1.591743451\C,-1.22368624,1.782584612,-1.995967923\C,2.700643078
 ,0.719989404,-2.688166132\N,-0.756607365,0.149442477,-0.561913505\H,-3
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 29865,-0.0377974,-0.0728421,0.0728921,-0.046451,-0.0423929,-0.1489712,
 0.055599,-0.0255899,0.0763131,-0.01364,-0.0118267,-0.1114487,-0.022126
 3,0.0131835,-0.0170625,0.0165716,0.0880932,-0.2022969,-0.1027572,0.194
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 0273818,-0.004689,0.046785,-0.0340422,-0.0379296,0.0959345,-0.1366604,
 0.0302557,0.0526631,0.0323584,0.0187648,-0.0241102,0.0273271,0.0700996
 ,0.0739503,0.1451152,0.0060533,-0.1374287,0.16892,-0.0349692,0.0414485
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 419663,0.1654235,0.0443672,-0.1845952,-0.2704822,-0.2532819,-0.1991037
 ,-0.1023334,0.1038902,0.057851,-0.1010509,-0.0136768,-0.0122369,0.0659
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 .0563698,-0.0960877,0.0991001,0.0036687,-0.0160701,-0.0022251,-0.09899
 94,-0.0442611,-0.0953639,0.0951218,-0.052698,0.0192058,0.0088512,-0.04
 30109,0.0647647,0.0155983,0.0399372,-0.0439536,0.0691108,0.1332674,-0.

1475865,-0.0848654,-0.00028,0.0175306,0.0941359,0.1676199,0.0169446,0.
 0558174,0.0933247,0.1246625,0.0442201,-0.0046759,-0.0451065,-0.02172,-
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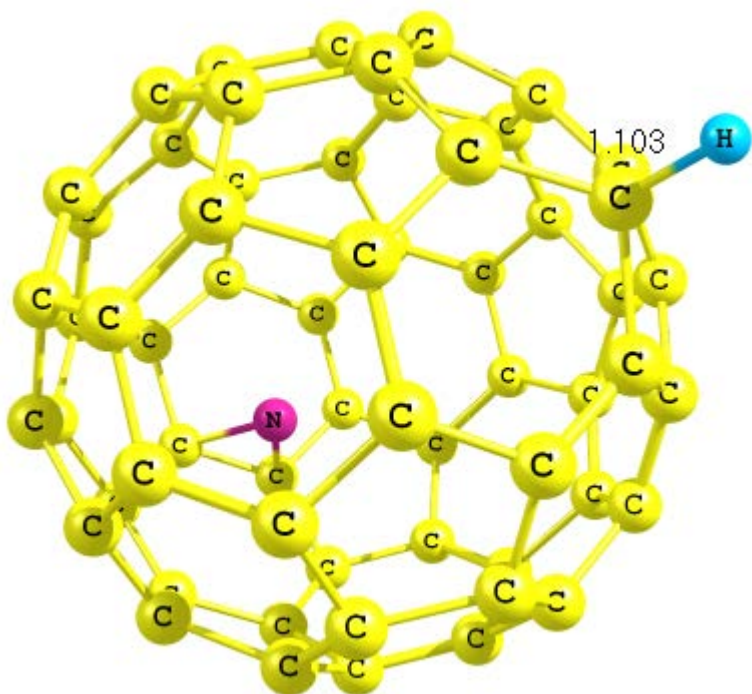
2d⁺ (N@C₆₀H⁺⁺⁺,endo-6,6-aza bridge opposite to H⁺, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN087\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\20-Mar-2010\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Name=Dral\endo-opposit-N@C60H (+) quartet\1,4\C,0.098774184,3.539332932,0.785445208\C,-1.15942858,3.522463396,1.511255485\C,-0.989664921,2.682715918,2.682656634\C,0.368795295,2.180463576,2.684362241\C,1.047000972,2.722574451,1.515788264\C,0.097833607,3.539250968,-0.615592054\C,-2.360522102,3.500858062,0.809864415\C,-2.040637676,1.856273405,3.098598154\C,0.636366521,0.876880749,3.136516595\C,1.986677759,1.949509776,0.820806086\C,-1.161223802,3.522975345,-1.339948197\C,-3.457419361,2.643623115,1.24470446\C,-1.761392556,0.499266437,3.544321508\C,1.584610834,0.060621639,2.422501794\C,1.985439021,1.949523702,-0.653830338\C,1.045402182,2.723132247,-1.347498249\C,-2.361445067,3.501133598,-0.637105423\C,-3.296813552,1.8461788,2.385715155\C,-0.456182611,0.019247516,3.573487066\C,2.244652956,0.615668511,1.30659283\C,-0.992907945,2.683836399,-2.511902466\C,-4.145352693,2.157805552,0.087173277\C,-2.044329797,1.857397894,-2.926824824\C,-2.846419743,-0.354320717,3.093534411\C,1.070580666,-1.337882837,2.424261578\C,2.24430549,0.616113307,-1.140878005\C,0.365335753,2.181314413,-2.515058086\C,-3.458925536,2.644128848,-1.071040024\C,-3.798718948,0.464588304,2.375194791\C,-0.18040462,-1.344486569,3.13639251\C,2.252359062,-0.208003416,0.082702512\C,1.742870014,-1.557210531,0.082769568\C,-2.314303571,-3.009542833,-0.615565514\C,-3.260216054,-2.181830663,-1.344013608\C,-2.591049569,-1.662338128,-2.51051577\C,-1.229119672,-2.165605634,-2.517958217\C,-1.065039599,-3.014282976,-1.347939622\C,-2.313387596,-3.00975768,0.785427116\C,-4.154482828,-1.363479382,-0.641935312\C,-2.850311713,-0.353057248,-2.922135101\C,-0.18415687,-1.343340812,-2.968838463\C,0.154580192,-3.036871767,-0.65453534\C,-3.258613292,-2.182599714,1.515444904\C,-4.465094611,-0.040481558,-1.098571627\C

, -1.765719116, 0.50067746, -3.373851445\C, 1.067890263, -1.337189791, -2.258448237\C, 0.155550678, -3.037105055, 0.821403184\C, -1.063186193, -3.01506942, 1.516371598\C, -4.153814632, -1.363937617, 0.814794566\C, -3.801715138, 0.465597841, -2.202203533\C, -0.460566075, 0.020685124, -3.404675681\C, 1.209970838, -2.1872535, -1.141192102\C, -2.587747043, -1.663382032, 2.681100668\C, -4.898563062, 0.839541572, 0.087333085\C, 1.58072855, 0.061675915, -2.25538592\C, 1.211782059, -2.187814937, 1.306990858\C, -1.225857643, -2.166815259, 2.686790102\C, -4.463558284, -0.041017469, 1.272257332\C, -3.299764941, 1.847155722, -2.212658095\C, 0.632496819, 0.878149878, -2.96845626\N, 0.681335864, -0.403587905, 0.083039362\H, -5.989195518, 1.005876838, 0.088118412\\Version=AM64L-G03RevD.02\State=4-A\HF=-2326.3538396\MP2=-2334.3336952\RMSD=3.720e-09\Thermal=0.\PG=C01 [X(C60H1N1)]\\@

UB3LYP/6-31G(d)



Zero-point correction=	0.385445 (Hartree/Particle)
Thermal correction to Energy=	0.407630
Thermal correction to Enthalpy=	0.408574
Thermal correction to Gibbs Free Energy=	0.340196
Sum of electronic and zero-point Energies=	-2340.657163
Sum of electronic and thermal Energies=	-2340.634978
Sum of electronic and thermal Enthalpies=	-2340.634034
Sum of electronic and thermal Free Energies=	-2340.702412

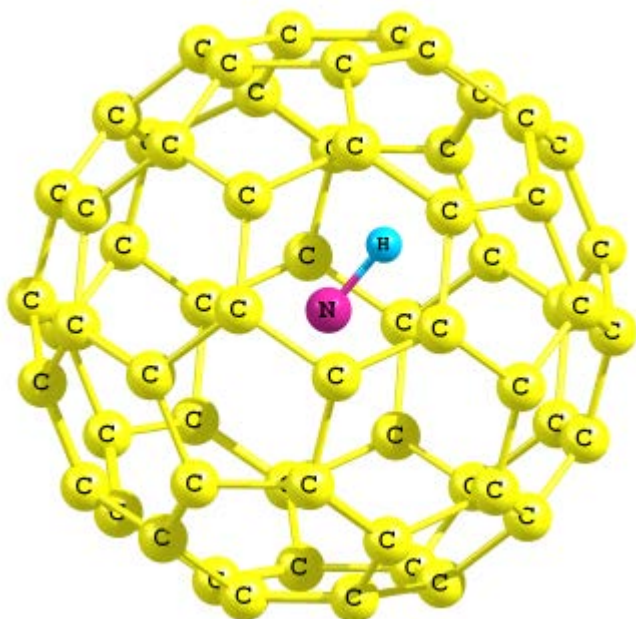
1\1\FAU-CCC-CCDH152\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\20-Jul-2009\0\\#P UB3LYP/6-31G* Freq=NoRaman Name=Dral\\endo-opposit-N@C60H (+) quartet\\1,4\C,0.098774184,3.539332932,0.785445208\C,-1.15942858,3.522

463396,1.511255485\C,-0.989664921,2.682715918,2.682656634\C,0.36879529
5,2.180463576,2.684362241\C,1.047000972,2.722574451,1.515788264\C,0.09
7833607,3.539250968,-0.615592054\C,-2.360522102,3.500858062,0.80986441
5\C,-2.040637676,1.856273405,3.098598154\C,0.636366521,0.876880749,3.1
36516595\C,1.986677759,1.949509776,0.820806086\C,-1.161223802,3.522975
345,-1.339948197\C,-3.457419361,2.643623115,1.24470446\C,-1.761392556,
0.499266437,3.544321508\C,1.584610834,0.060621639,2.422501794\C,1.9854
39021,1.949523702,-0.653830338\C,1.045402182,2.723132247,-1.347498249\
C,-2.361445067,3.501133598,-0.637105423\C,-3.296813552,1.8461788,2.385
715155\C,-0.456182611,0.019247516,3.573487066\C,2.244652956,0.61566851
1,1.30659283\C,-0.992907945,2.683836399,-2.511902466\C,-4.145352693,2.
157805552,0.087173277\C,-2.044329797,1.857397894,-2.926824824\C,-2.846
419743,-0.354320717,3.093534411\C,1.070580666,-1.337882837,2.424261578
\C,2.24430549,0.616113307,-1.140878005\C,0.365335753,2.181314413,-2.51
5058086\C,-3.458925536,2.644128848,-1.071040024\C,-3.798718948,0.46458
8304,2.375194791\C,-0.18040462,-1.344486569,3.13639251\C,2.252359062,-
0.208003416,0.082702512\C,1.742870014,-1.557210531,0.082769568\C,-2.31
4303571,-3.009542833,-0.615565514\C,-3.260216054,-2.181830663,-1.34401
3608\C,-2.591049569,-1.662338128,-2.51051577\C,-1.229119672,-2.1656056
34,-2.517958217\C,-1.065039599,-3.014282976,-1.347939622\C,-2.31338759
6,-3.00975768,0.785427116\C,-4.154482828,-1.363479382,-0.641935312\C,-
2.850311713,-0.353057248,-2.922135101\C,-0.18415687,-1.343340812,-2.96
8838463\C,0.154580192,-3.036871767,-0.65453534\C,-3.258613292,-2.18259
9714,1.515444904\C,-4.465094611,-0.040481558,-1.098571627\C,-1.7657191
16,0.50067746,-3.373851445\C,1.067890263,-1.337189791,-2.258448237\C,0
.155550678,-3.037105055,0.821403184\C,-1.063186193,-3.01506942,1.51637
1598\C,-4.153814632,-1.363937617,0.814794566\C,-3.801715138,0.46559784
1,-2.202203533\C,-0.460566075,0.020685124,-3.404675681\C,1.209970838,-
2.1872535,-1.141192102\C,-2.587747043,-1.663382032,2.681100668\C,-4.89
8563062,0.839541572,0.087333085\C,1.58072855,0.061675915,-2.25538592\C
,1.211782059,-2.187814937,1.306990858\C,-1.225857643,-2.166815259,2.68
6790102\C,-4.463558284,-0.041017469,1.272257332\C,-3.299764941,1.84715
5722,-2.212658095\C,0.632496819,0.878149878,-2.96845626\C,0.681335864,
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.6599907,-3.2269775,487.2095176,-0.0020071,0.0175199,488.4070526\PG=C0
1 [X(C60H1N1)]\NImag=0\0.48534845,-0.10550116,0.23420834,-0.02914131,
,0.00000239,-0.00013834,-0.00018747,0.00003144,0.04632894\0.00000089
.00000103,0.00000254\\@

3⁺ (NH⁺@C₆₀, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN088\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\31-Mar-201
 0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCFCyc=1200 Name=Dral\N
 H(+)\C60 (quartet)\1,4\C,-3.346961443,0.77927509,0.973219072\C,-3.340
 512963,1.192661828,-0.422130105\C,-3.346695186,-0.00669313,-1.24696768
 6\C,-3.357434292,-1.162098397,-0.360674501\C,-3.357577478,-0.675835599
 ,1.011978235\C,-2.604234396,1.494457569,1.9149248\C,-2.591572606,2.303
 835306,-0.815630564\C,-2.603311571,-0.04330257,-2.428919708\C,-2.62409
 4702,-2.303382252,-0.694743111\C,-2.624152534,-1.35205401,1.990019334\
 C,-1.825388555,2.648527634,1.500262517\C,-1.818249668,2.260319555,-2.0
 44282806\C,-1.840537173,-1.232093588,-2.770853646\C,-1.862204605,-3.00
 2432146,0.325980536\C,-1.851266466,-0.603104211,2.965956218\C,-1.84196
 6573,0.786876782,2.928863702\C,-1.819109338,3.044163696,0.167523433\C,
 -1.823450094,1.114177056,-2.83218862\C,-1.850969546,-2.335838142,-1.92
 471288\C,-1.862044966,-2.537603428,1.636953681\C,-0.580580415,2.647669
 36,2.261368531\C,-0.567327053,2.974117705,-1.814637196\C,0.621936672,3
 .05478677,1.656781823\C,-0.589699087,-0.802099794,-3.385835906\C,-0.61
 739685,-3.463692524,-0.279149782\C,-0.611164096,-1.33067143,3.21172312
 4\C,-0.590880505,1.508149779,3.136315655\C,-0.567787621,3.454346281,-0
 .460422074\C,-0.579240387,0.634462227,-3.422573838\C,-0.610505994,-3.0
 5523387,-1.657184808\C,-0.617543974,-2.515321622,2.398315962\C,0.57859
 3105,-2.970241245,1.815632768\C,3.349928944,-0.775379444,-0.971404393\
 C,3.360977871,0.677118276,-1.009779054\C,3.360457115,1.162415846,0.360
 234077\C,3.3498742,0.0096784,1.244999153\C,3.342932322,-1.187942569,0.
 421964699\C,2.614698729,-1.492651868,-1.914677634\C,2.634779744,1.3542
 84342,-1.988958837\C,2.63406352,2.304687735,0.694893514\C,2.613884628,
 0.046028852,2.42860284\C,2.600925122,-2.301409542,0.816196414\C,1.8529
 83038,-0.78435,-2.927485248\C,1.873348522,2.538734459,-1.63554951\C,1.
 862449495,2.3371474,1.924348689\C,1.835475499,-1.111362667,2.8322552\C
 ,1.828874222,-3.040909838,-0.16675132\C,1.83592065,-2.646235445,-1.499
 518651\C,1.863499025,0.605462841,-2.96459258\C,1.873132683,3.003095501
 ,-0.325223504\C,1.852084301,1.234255778,2.770228762\C,1.828841849,-2.2
 57357435,2.044681454\C,0.602462919,-1.504290698,-3.134913226\C,0.62902
 3672,2.516035033,-2.394991588\C,0.591195318,-0.632189125,3.421426911\C
 ,0.578683681,-3.451050251,0.460222548\C,0.591723057,-2.645232566,-2.25
 9831644\C,0.623143958,1.331716691,-3.208964742\C,0.628553734,3.4626236
 03,0.278865614\C,0.6014181,0.804913552,3.384077274\N,-0.101196657,-0.0
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UB3LYP/6-31G(d)

1 4

C	-3.346961443	0.779275090	0.973219072
C	-3.340512963	1.192661828	-0.422130105
C	-3.346695186	-0.006693130	-1.246967686
C	-3.357434292	-1.162098397	-0.360674501
C	-3.357577478	-0.675835599	1.011978235
C	-2.604234396	1.494457569	1.914924800
C	-2.591572606	2.303835306	-0.815630564
C	-2.603311571	-0.043302570	-2.428919708
C	-2.624094702	-2.303382252	-0.694743111
C	-2.624152534	-1.352054010	1.990019334
C	-1.825388555	2.648527634	1.500262517
C	-1.818249668	2.260319555	-2.044282806
C	-1.840537173	-1.232093588	-2.770853646
C	-1.862204605	-3.002432146	0.325980536
C	-1.851266466	-0.603104211	2.965956218
C	-1.841966573	0.786876782	2.928863702
C	-1.819109338	3.044163696	0.167523433
C	-1.823450094	1.114177056	-2.832188620
C	-1.850969546	-2.335838142	-1.924712880
C	-1.862044966	-2.537603428	1.636953681
C	-0.580580415	2.647669360	2.261368531
C	-0.567327053	2.974117705	-1.814637196
C	0.621936672	3.054786770	1.656781823
C	-0.589699087	-0.802099794	-3.385835906
C	-0.617396850	-3.463692524	-0.279149782
C	-0.611164096	-1.330671430	3.211723124
C	-0.590880505	1.508149779	3.136315655
C	-0.567787621	3.454346281	-0.460422074
C	-0.579240387	0.634462227	-3.422573838

C -0.610505994 -3.055233870 -1.657184808
 C -0.617543974 -2.515321622 2.398315962
 C 0.578593105 -2.970241245 1.815632768
 C 3.349928944 -0.775379444 -0.971404393
 C 3.360977871 0.677118276 -1.009779054
 C 3.360457115 1.162415846 0.360234077
 C 3.349874200 0.009678400 1.244999153
 C 3.342932322 -1.187942569 0.421964699
 C 2.614698729 -1.492651868 -1.914677634
 C 2.634779744 1.354284342 -1.988958837
 C 2.634063520 2.304687735 0.694893514
 C 2.613884628 0.046028852 2.428602840
 C 2.600925122 -2.301409542 0.816196414
 C 1.852983038 -0.784350000 -2.927485248
 C 1.873348522 2.538734459 -1.635549510
 C 1.862449495 2.337147400 1.924348689
 C 1.835475499 -1.111362667 2.832255200
 C 1.828874222 -3.040909838 -0.166751320
 C 1.835920650 -2.646235445 -1.499518651
 C 1.863499025 0.605462841 -2.964592580
 C 1.873132683 3.003095501 -0.325223504
 C 1.852084301 1.234255778 2.770228762
 C 1.828841849 -2.257357435 2.044681454
 C 0.602462919 -1.504290698 -3.134913226
 C 0.629023672 2.516035033 -2.394991588
 C 0.591195318 -0.632189125 3.421426911
 C 0.578683681 -3.451050251 0.460222548
 C 0.591723057 -2.645232566 -2.259831644
 C 0.623143958 1.331716691 -3.208964742
 C 0.628553734 3.462623603 0.278865614
 C 0.601418100 0.804913552 3.384077274
 N -0.101196657 -0.032082742 -0.008718088
 H -1.135496902 -0.174364802 -0.031237290

Zero-point correction= 0.382262 (Hartree/Particle)
 Thermal correction to Energy= 0.406371
 Thermal correction to Enthalpy= 0.407315
 Thermal correction to Gibbs Free Energy= 0.334568
 Sum of electronic and zero-point Energies= -2340.746262
 Sum of electronic and thermal Energies= -2340.722153
 Sum of electronic and thermal Enthalpies= -2340.721209
 Sum of electronic and thermal Free Energies= -2340.793956

1\1\FAU-CCC-CCDH159\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\22-Feb-200
 9\0\#P UB3LYP/6-31G* Freq=NoRaman Name=Dral\NH(+)\@C60 (quartet)\1,4
 \C,-3.346961443,0.77927509,0.973219072\C,-3.340512963,1.192661828,-0.4
 22130105\C,-3.346695186,-0.00669313,-1.246967686\C,-3.357434292,-1.162
 098397,-0.360674501\C,-3.357577478,-0.675835599,1.011978235\C,-2.60423
 4396,1.494457569,1.9149248\C,-2.591572606,2.303835306,-0.815630564\C,-
 2.603311571,-0.04330257,-2.428919708\C,-2.624094702,-2.303382252,-0.69

4743111\C,-2.624152534,-1.35205401,1.990019334\C,-1.825388555,2.648527
634,1.500262517\C,-1.818249668,2.260319555,-2.044282806\C,-1.840537173
,-1.232093588,-2.770853646\C,-1.862204605,-3.002432146,0.325980536\C,-
1.851266466,-0.603104211,2.965956218\C,-1.841966573,0.786876782,2.9288
63702\C,-1.819109338,3.044163696,0.167523433\C,-1.823450094,1.11417705
6,-2.83218862\C,-1.850969546,-2.335838142,-1.92471288\C,-1.862044966,-
2.537603428,1.636953681\C,-0.580580415,2.64766936,2.261368531\C,-0.567
327053,2.974117705,-1.814637196\C,0.621936672,3.05478677,1.656781823\C
,-0.589699087,-0.802099794,-3.385835906\C,-0.61739685,-3.463692524,-0.
279149782\C,-0.611164096,-1.33067143,3.211723124\C,-0.590880505,1.5081
49779,3.136315655\C,-0.567787621,3.454346281,-0.460422074\C,-0.5792403
87,0.634462227,-3.422573838\C,-0.610505994,-3.05523387,-1.657184808\C,
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76,-1.009779054\C,3.360457115,1.162415846,0.360234077\C,3.3498742,0.00
96784,1.244999153\C,3.342932322,-1.187942569,0.421964699\C,2.614698729
,-1.492651868,-1.914677634\C,2.634779744,1.354284342,-1.988958837\C,2.
63406352,2.304687735,0.694893514\C,2.613884628,0.046028852,2.42860284\
C,2.600925122,-2.301409542,0.816196414\C,1.852983038,-0.78435,-2.92748
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24348689\C,1.835475499,-1.111362667,2.8322552\C,1.828874222,-3.0409098
38,-0.16675132\C,1.83592065,-2.646235445,-1.499518651\C,1.863499025,0.
605462841,-2.96459258\C,1.873132683,3.003095501,-0.325223504\C,1.85208
4301,1.234255778,2.770228762\C,1.828841849,-2.257357435,2.044681454\C,
0.602462919,-1.504290698,-3.134913226\C,0.629023672,2.516035033,-2.394
991588\C,0.591195318,-0.632189125,3.421426911\C,0.578683681,-3.4510502
51,0.460222548\C,0.591723057,-2.645232566,-2.259831644\C,0.623143958,1
.331716691,-3.208964742\C,0.628553734,3.462623603,0.278865614\C,0.6014
181,0.804913552,3.384077274\N,-0.101196657,-0.032082742,-0.008718088\H
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MSF=4.187e-04\\ZeroPoint=0.3822621\\Thermal=0.4063709\\ZPE=239.8730921\\Di
pole=-0.1153737,-0.0013745,-0.0003367\\DipoleDeriv=-0.1042581,-0.022341
0000907,0.0244875\\Polar=465.767174,0.3821248,508.1401024,-0.1299352,-0
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.00818950,-0.00090746,-0.00083294,0.00831779,0.00061349,0.00274260\\0.
0.00505075,-0.00078565,-0.00011174\\\\@

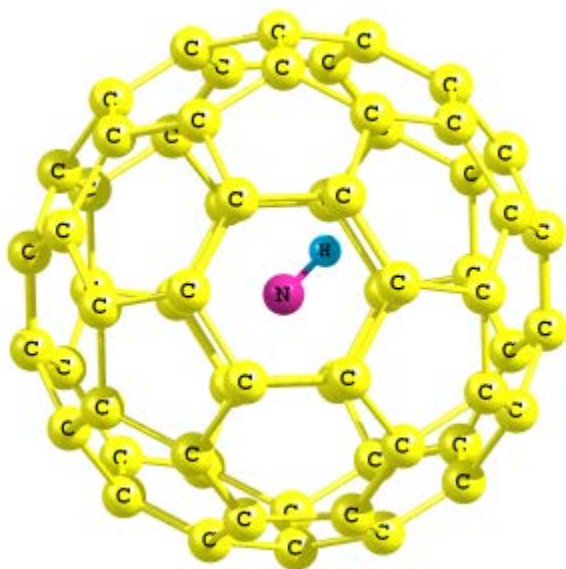
3⁺ (NH⁺@C₆₀, doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\\FAU-CCC-CCDN085\\SP\\ROMP2-FC\\6-31G(d)\\C60H1N1(1+,2)\\DRAL\\01-Apr-201
0\\0\\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCFCyc=1200 Name=Drall\\N
H(+)@C60 doublet DFT SP\\1,2\\C,0,-1.88879049,-2.944184562,0.616775079\
C,0,-0.645448379,-3.205918625,1.334064716\C,0,-0.632279703,-2.39301331
6,2.520237056\C,0,-1.867171928,-1.617022416,2.553601302\C,0,-2.6431506
65,-1.95925758,1.373164591\C,0,-1.889111207,-2.905785356,-0.774322383\
C,0,0.548600159,-3.429372271,0.62552716\C,0,0.57532284,-1.825755722,2.

965520504\C,0,-1.846368175,-0.305941282,3.017153108\C,0,-3.366710594,-
0.970143548,0.702934132\C,0,-0.646482501,-3.1280534,-1.506031079\C,0,1
.804276013,-2.856010123,1.094928012\C,0,0.596233608,-0.471068803,3.446
187254\C,0,-2.601554216,0.724897178,2.325687434\C,0,-3.367253557,-0.93
0355774,-0.751705289\C,0,-2.64433055,-1.881454483,-1.475437915\C,0,0.5
48053013,-3.390655206,-0.812154192\C,0,1.817574454,-2.069922546,2.2418
59266\C,0,-0.590425617,0.282988261,3.469114155\C,0,-3.345541837,0.4008
97,1.189749703\C,0,-0.63425468,-2.251345946,-2.645614239\C,0,2.5784134
86,-2.460772736,-0.06842835\C,0,0.572742366,-1.660908938,-3.061123166\
C,0,1.851906494,0.140820251,3.027322303\C,0,-1.813605686,1.944853708,2
.353271107\C,0,-3.346488612,0.465070948,-1.163274141\C,0,-1.869178704,
-1.475093826,-2.635808933\C,0,1.803186986,-2.792074468,-1.250854879\C,
0,2.605442966,-0.850808232,2.280573122\C,0,-0.570100812,1.660694664,3.
061267725\C,0,-3.333331499,1.287220545,0.036563442\C,0,-2.5773409,2.46
0266008,0.068310057\C,0,1.89132586,2.941826302,-0.615882102\C,0,2.6445
69824,1.957769637,-1.371787445\C,0,1.869400736,1.61585635,-2.551237832
\C,0,0.634850597,2.390879288,-2.517513722\C,0,0.648165186,3.202757596,
-1.331602299\C,0,1.891818308,2.903774775,0.773739183\C,0,3.364286938,0
.968923323,-0.701966016\C,0,1.849180151,0.306028417,-3.01685853\C,0,-0
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8572,-1.188744335\C,0,0.593410854,-0.281936656,-3.467836906\C,0,-1.815
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,0.750795036\C,0,2.603073633,-0.724845588,-2.325714208\C,0,-0.59320172
7,0.47216614,-3.447592871\C,0,-1.802431696,2.855767969,-1.09484134\C,0
,1.871373436,1.473817072,2.633396466\C,0,3.330261058,-1.286369158,-0.0
36725137\C,0,-2.603459372,0.850626063,-2.28047228\C,0,-1.801496842,2.7
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UB3LYP/6-31G(d)



1 2

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C	-0.645448379	-3.205918625	1.334064716
C	-0.632279703	-2.393013316	2.520237056
C	-1.867171928	-1.617022416	2.553601302
C	-2.643150665	-1.959257580	1.373164591
C	-1.889111207	-2.905785356	-0.774322383
C	0.548600159	-3.429372271	0.625527160
C	0.575322840	-1.825755722	2.965520504
C	-1.846368175	-0.305941282	3.017153108
C	-3.366710594	-0.970143548	0.702934132
C	-0.646482501	-3.128053400	-1.506031079
C	1.804276013	-2.856010123	1.094928012
C	0.596233608	-0.471068803	3.446187254
C	-2.601554216	0.724897178	2.325687434
C	-3.367253557	-0.930355774	-0.751705289
C	-2.644330550	-1.881454483	-1.475437915
C	0.548053013	-3.390655206	-0.812154192
C	1.817574454	-2.069922546	2.241859266
C	-0.590425617	0.282988261	3.469114155
C	-3.345541837	0.400897000	1.189749703
C	-0.634254680	-2.251345946	-2.645614239
C	2.578413486	-2.460772736	-0.068428350
C	0.572742366	-1.660908938	-3.061123166
C	1.851906494	0.140820251	3.027322303
C	-1.813605686	1.944853708	2.353271107
C	-3.346488612	0.465070948	-1.163274141
C	-1.869178704	-1.475093826	-2.635808933
C	1.803186986	-2.792074468	-1.250854879
C	2.605442966	-0.850808232	2.280573122
C	-0.570100812	1.660694664	3.061267725
C	-3.333331499	1.287220545	0.036563442

C	-2.577340900	2.460266008	0.068310057
C	1.891325860	2.941826302	-0.615882102
C	2.644569824	1.957769637	-1.371787445
C	1.869400736	1.615856350	-2.551237832
C	0.634850597	2.390879288	-2.517513722
C	0.648165186	3.202757596	-1.331602299
C	1.891818308	2.903774775	0.773739183
C	3.364286938	0.968923323	-0.701966016
C	1.849180151	0.306028417	-3.016858530
C	-0.572559476	1.825578011	-2.965705042
C	-0.546323727	3.429986872	-0.624400479
C	2.645768600	1.879931714	1.474182227
C	3.342528389	-0.400398572	-1.188744335
C	0.593410854	-0.281936656	-3.467836906
C	-1.815501591	2.070241749	-2.241865648
C	-0.545822867	3.391412563	0.811350878
C	0.649200905	3.125188195	1.503712495
C	3.364846551	0.929098699	0.750795036
C	2.603073633	-0.724845588	-2.325714208
C	-0.593201727	0.472166140	-3.447592871
C	-1.802431696	2.855767969	-1.094841340
C	1.871373436	1.473817072	2.633396466
C	3.330261058	-1.286369158	-0.036725137
C	-2.603459372	0.850626063	-2.280472280
C	-1.801496842	2.791925626	1.250768945
C	0.636810664	2.249174256	2.642852322
C	3.343760611	-0.464704323	1.162153134
C	1.815466868	-1.944428843	-2.353221629
C	-1.848910496	-0.140900916	-3.027812385
N	0.100625173	0.018977295	0.000890167
H	-0.891516620	-0.297395258	-0.008968311

Zero-point correction= 0.381742 (Hartree/Particle)

Thermal correction to Energy= 0.406304

Thermal correction to Enthalpy= 0.407248

Thermal correction to Gibbs Free Energy= 0.333465

Sum of electronic and zero-point Energies= -2340.748215

Sum of electronic and thermal Energies= -2340.723654

Sum of electronic and thermal Enthalpies= -2340.722709

Sum of electronic and thermal Free Energies= -2340.796492

1\1\GINC-A06\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,2)\DRAL\12-Dec-2008\0\#P
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 ,2.553601302\C,-2.643150665,-1.95925758,1.373164591\C,-1.889111207,-2.
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 ,-3.366710594,-0.970143548,0.702934132\C,-0.646482501,-3.1280534,-1.50
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 9266\C,-0.590425617,0.282988261,3.469114155\C,-3.345541837,0.400897,1.
 189749703\C,-0.63425468,-2.251345946,-2.645614239\C,2.578413486,-2.460
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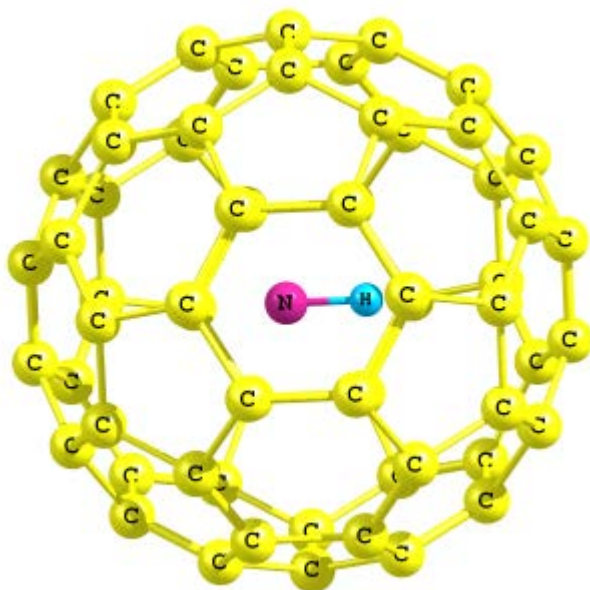
4 (NH@C₆₀, singlet)

MP2/6-31G(d)//B3LYP/6-31G(d)

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 1\C,0,0.140451845,-0.634289164,3.491421754\C,0,-0.845945841,-1.6076853
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B3LYP/6-31G(d)



0 1

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C	1.272712020	-2.348624157	2.344769034
C	1.449896616	-1.092447956	3.053837171
C	0.140451845	-0.634289164	3.491421754
C	-0.845945841	-1.607685317	3.050915522
C	-0.730033458	-3.252092516	1.218150995
C	2.051626214	-2.626505198	1.219750898
C	2.400849220	-0.169620418	2.612768690
C	-0.167044970	0.727538077	3.472091162
C	-2.099183763	-1.178283594	2.607324290
C	0.081713732	-3.539617172	0.047435953
C	3.041925942	-1.667761162	0.760554422
C	2.079573667	1.247662682	2.590603560
C	-1.473348340	1.173977684	3.012702782
C	-2.706600359	-1.792132527	1.437767266

C	-2.035542459	-2.809720846	0.757262810
C	1.444229184	-3.233702715	0.048539243
C	3.214629589	-0.463980497	1.444307528
C	0.823062893	1.689039669	3.013357374
C	-2.419965509	0.239337213	2.588345370
C	-0.721503858	-3.285564708	-1.136324959
C	3.049011049	-1.688572765	-0.693135442
C	-0.128567665	-2.727968770	-2.269852242
C	2.696344606	1.829667361	1.409838656
C	-1.290008149	2.410328846	2.271159772
C	-3.401869702	-0.753668606	0.695768429
C	-2.029736910	-2.829794614	-0.696856530
C	2.061699224	-2.658801509	-1.133452866
C	3.397017971	0.771068702	0.701314158
C	0.129402086	2.729534960	2.272954390
C	-3.224818944	0.501368189	1.406781729
C	-3.047748815	1.686539273	0.692564646
C	0.146655460	2.665018281	-2.341003651
C	0.844776726	1.604733632	-3.046472259
C	-0.140086298	0.632857431	-3.487164282
C	-1.448506986	1.090926304	-3.050907444
C	-1.271979080	2.346313499	-2.342431529
C	0.730855149	3.251910966	-1.217681988
C	2.097181743	1.175792112	-2.604349364
C	0.167628203	-0.726467822	-3.466676417
C	-2.399014604	0.169479155	-2.610843315
C	-2.052372749	2.626803133	-1.220085928
C	2.035921285	2.808932966	-0.756364722
C	2.419636417	-0.240135962	-2.587274478
C	-0.820801017	-1.686278858	-3.007692711
C	-3.212555034	0.463803413	-1.443279736
C	-1.443641936	3.232486683	-0.049238523
C	-0.081060290	3.538251057	-0.047318852
C	2.704038794	1.789505772	-1.435459414
C	1.472397494	-1.172946012	-3.009007276
C	-2.076964231	-1.245926564	-2.587643495
C	-3.042335232	1.667733464	-0.760971235
C	2.030921010	2.828646204	0.697552651
C	3.223725278	-0.502632202	-1.405958100
C	-3.394185466	-0.771168145	-0.699440032
C	-2.059796655	2.656770852	1.133045552
C	0.721764331	3.283515198	1.136606307
C	3.400067874	0.751454151	-0.693904085
C	1.290146391	-2.409016045	-2.268627658
C	-2.692702044	-1.828461604	-1.407560385
N	-0.009429223	0.011657966	-0.181828792
H	-0.010702719	0.028304321	0.857738968

Zero-point correction= 0.384128 (Hartree/Particle)
 Thermal correction to Energy= 0.408433
 Thermal correction to Enthalpy= 0.409377
 Thermal correction to Gibbs Free Energy= 0.336482

Sum of electronic and zero-point Energies= -2340.925120
 Sum of electronic and thermal Energies= -2340.900815
 Sum of electronic and thermal Enthalpies= -2340.899870
 Sum of electronic and thermal Free Energies= -2340.972765

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 08741,-0.0000869,0.0009663,0.0660828,-0.0014484,0.0001698,-0.0013974,-
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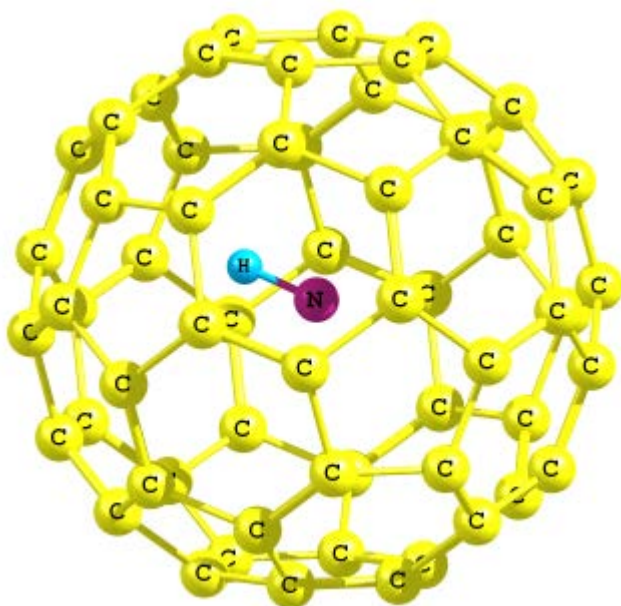
4 (NH⁺@C₆₀, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN091\SP\ROMP2-FC\6-31G(d)\C60H1N1(3)\DRAL\10-Aug-2010\0
 \#P ROMP2/6-31G* Geom=AllCheck Guess=Read Pop=None SCFCyc=1200 SCF=Ti
 ght Name=Dral\NH@C60 (triplet)\0,3\C,1.999308125,-1.247929968,-2.652
 219093\C,0.74817664,-0.95869723,-3.333811931\C,0.626890751,0.484579618
 ,-3.458601573\C,1.804294023,1.088933646,-2.855323613\C,2.653148155,0.0
 17422614,-2.356236546\C,2.06853781,-2.300039622,-1.73695876\C,-0.38338
 0352,-1.733332954,-3.072428837\C,-0.620816613,1.094395024,-3.31566953\
 C,1.685725057,2.278712316,-2.132824854\C,3.350928362,0.17971744,-1.155
 82436\C,0.890494992,-3.107776159,-1.46622018\C,-1.682749891,-1.0980965
 54,-2.926944979\C,-0.743414351,2.334204817,-2.566475849\C,2.411410252,
 2.447428917,-0.883423433\C,3.422615784,-0.917222609,-0.202922161\C,2.7
 93772341,-2.13103517,-0.488057181\C,-0.310726162,-2.829870595,-2.12065
 9842\C,-1.799238079,0.28759286,-3.046378098\C,0.386021802,2.914088089,
 -1.986611853\C,3.228234684,1.419996288,-0.404674037\C,0.887472785,-3.4
 37368298,-0.050859164\C,-2.412714454,-1.801392234,-1.885576754\C,-0.31
 6641114,-3.47549272,0.652983897\C,-1.997805337,2.292084055,-1.83343256
 3\C,1.55949229,3.18734144,0.033676924\C,3.345103502,-0.355033807,1.135

966955\C,2.063097309,-2.833414385,0.553781545\C,-1.564863422,-2.871108
512,-1.387228061\C,-2.650577475,1.027886311,-2.130446624\C,0.308754555
,3.475980294,-0.648125459\C,3.22459601,1.088575853,1.011502068\C,2.403
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,-2.658640597,-0.020289962,2.357582259\C,-1.810900135,-1.089938987,2.8
55636936\C,-0.63510457,-0.487324103,3.460505706\C,-0.755888988,0.95526
6876,3.335298961\C,-2.076661343,2.296364561,1.74122589\C,-3.354625334,
-0.182321048,1.159676858\C,-1.693993457,-2.279868242,2.137091341\C,0.6
11638051,-1.097420462,3.32142471\C,0.37484328,1.730742274,3.077366024\C
,-2.801095238,2.127304864,0.493249169\C,-3.231949882,-1.420817139,0.4
1009663\C,-0.39477168,-2.914189116,1.99111165\C,1.78972052,-0.28996935
3,3.05225927\C,0.302255607,2.827252217,2.126509429\C,-0.898694532,3.10
3696077,1.471627673\C,-3.427283817,0.913509659,0.208416384\C,-2.418135
029,-2.447866068,0.888543561\C,0.734416198,-2.336726605,2.572799572\C,
1.6737804,1.095422942,2.932458542\C,-2.071143936,2.829891171,-0.548125
649\C,-3.228589248,-1.090578474,-1.004917718\C,2.640881774,-1.02939039
2,2.135201829\C,1.556353748,2.86865507,1.392468205\C,-0.895225443,3.43
3421299,0.05625843\C,-3.349838703,0.352163517,-1.129685422\C,-1.567443
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UB3LYP/6-31G(d)



0 3

C	1.999308125	-1.247929968	-2.652219093
C	0.748176640	-0.958697230	-3.333811931
C	0.626890751	0.484579618	-3.458601573
C	1.804294023	1.088933646	-2.855323613
C	2.653148155	0.017422614	-2.356236546
C	2.068537810	-2.300039622	-1.736958760

C -0.383380352 -1.733332954 -3.072428837
 C -0.620816613 1.094395024 -3.315669530
 C 1.685725057 2.278712316 -2.132824854
 C 3.350928362 0.179717440 -1.155824360
 C 0.890494992 -3.107776159 -1.466220180
 C -1.682749891 -1.098096554 -2.926944979
 C -0.743414351 2.334204817 -2.566475849
 C 2.411410252 2.447428917 -0.883423433
 C 3.422615784 -0.917222609 -0.202922161
 C 2.793772341 -2.131035170 -0.488057181
 C -0.310726162 -2.829870595 -2.120659842
 C -1.799238079 0.287592860 -3.046378098
 C 0.386021802 2.914088089 -1.986611853
 C 3.228234684 1.419996288 -0.404674037
 C 0.887472785 -3.437368298 -0.050859164
 C -2.412714454 -1.801392234 -1.885576754
 C -0.316641114 -3.475492720 0.652983897
 C -1.997805337 2.292084055 -1.833432563
 C 1.559492290 3.187341440 0.033676924
 C 3.345103502 -0.355033807 1.135966955
 C 2.063097309 -2.833414385 0.553781545
 C -1.564863422 -2.871108512 -1.387228061
 C -2.650577475 1.027886311 -2.130446624
 C 0.308754555 3.475980294 -0.648125459
 C 3.224596010 1.088575853 1.011502068
 C 2.403988819 1.797834542 1.890383385
 C -2.006258908 1.243691480 2.653645194
 C -2.658640597 -0.020289962 2.357582259
 C -1.810900135 -1.089938987 2.855636936
 C -0.635104570 -0.487324103 3.460505706
 C -0.755888988 0.955266876 3.335298961
 C -2.076661343 2.296364561 1.741225890
 C -3.354625334 -0.182321048 1.159676858
 C -1.693993457 -2.279868242 2.137091341
 C 0.611638051 -1.097420462 3.321424710
 C 0.374843280 1.730742274 3.077366024
 C -2.801095238 2.127304864 0.493249169
 C -3.231949882 -1.420817139 0.410096630
 C -0.394771680 -2.914189116 1.991111650
 C 1.789720520 -0.289969353 3.052259270
 C 0.302255607 2.827252217 2.126509429
 C -0.898694532 3.103696077 1.471627673
 C -3.427283817 0.913509659 0.208416384
 C -2.418135029 -2.447866068 0.888543561
 C 0.734416198 -2.336726605 2.572799572
 C 1.673780400 1.095422942 2.932458542
 C -2.071143936 2.829891171 -0.548125649
 C -3.228589248 -1.090578474 -1.004917718
 C 2.640881774 -1.029390392 2.135201829
 C 1.556353748 2.868655070 1.392468205

C -0.895225443 3.433421299 0.056258430
 C -3.349838703 0.352163517 -1.129685422
 C -1.567443737 -3.187531488 -0.028440955
 C 1.987879479 -2.293638184 1.838290771
 N -0.042589496 -0.076263689 -0.116158685
 H 0.828981690 0.157205723 -0.639404180

Zero-point correction= 0.383966 (Hartree/Particle)
 Thermal correction to Energy= 0.408081
 Thermal correction to Enthalpy= 0.409025
 Thermal correction to Gibbs Free Energy= 0.335981
 Sum of electronic and zero-point Energies= -2341.007284
 Sum of electronic and thermal Energies= -2340.983168
 Sum of electronic and thermal Enthalpies= -2340.982224
 Sum of electronic and thermal Free Energies= -2341.055269

1\1\FAU-CCC-CCDH151\Freq\UB3LYP\6-31G(d)\C60H1N1(3)\DRAL\14-Dec-2008\0
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 39622,-1.73695876\C,-0.383380352,-1.733332954,-3.072428837\C,-0.620816
 613,1.094395024,-3.31566953\C,1.685725057,2.278712316,-2.132824854\C,3
 .350928362,0.17971744,-1.15582436\C,0.890494992,-3.107776159,-1.466220
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 ,-2.566475849\C,2.411410252,2.447428917,-0.883423433\C,3.422615784,-0.
 917222609,-0.202922161\C,2.793772341,-2.13103517,-0.488057181\C,-0.310
 726162,-2.829870595,-2.120659842\C,-1.799238079,0.28759286,-3.04637809
 8\C,0.386021802,2.914088089,-1.986611853\C,3.228234684,1.419996288,-0.
 404674037\C,0.887472785,-3.437368298,-0.050859164\C,-2.412714454,-1.80
 1392234,-1.885576754\C,-0.316641114,-3.47549272,0.652983897\C,-1.99780
 5337,2.292084055,-1.833432563\C,1.55949229,3.18734144,0.033676924\C,3.
 345103502,-0.355033807,1.135966955\C,2.063097309,-2.833414385,0.553781
 545\C,-1.564863422,-2.871108512,-1.387228061\C,-2.650577475,1.02788631
 1,-2.130446624\C,0.308754555,3.475980294,-0.648125459\C,3.22459601,1.0
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 908,1.24369148,2.653645194\C,-2.658640597,-0.020289962,2.357582259\C,-
 1.810900135,-1.089938987,2.855636936\C,-0.63510457,-0.487324103,3.4605
 05706\C,-0.755888988,0.955266876,3.335298961\C,-2.076661343,2.29636456
 1,1.74122589\C,-3.354625334,-0.182321048,1.159676858\C,-1.693993457,-2
 .279868242,2.137091341\C,0.611638051,-1.097420462,3.32142471\C,0.37484
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 3.231949882,-1.420817139,0.41009663\C,-0.39477168,-2.914189116,1.99111
 165\C,1.78972052,-0.289969353,3.05225927\C,0.302255607,2.827252217,2.1
 26509429\C,-0.898694532,3.103696077,1.471627673\C,-3.427283817,0.91350
 9659,0.208416384\C,-2.418135029,-2.447866068,0.888543561\C,0.734416198
 ,-2.336726605,2.572799572\C,1.6737804,1.095422942,2.932458542\C,-2.071
 143936,2.829891171,-0.548125649\C,-3.228589248,-1.090578474,-1.0049177
 18\C,2.640881774,-1.029390392,2.135201829\C,1.556353748,2.86865507,1.3
 92468205\C,-0.895225443,3.433421299,0.05625843\C,-3.349838703,0.352163

517,-1.129685422\C,-1.567443737,-3.187531488,-0.028440955\C,1.98787947
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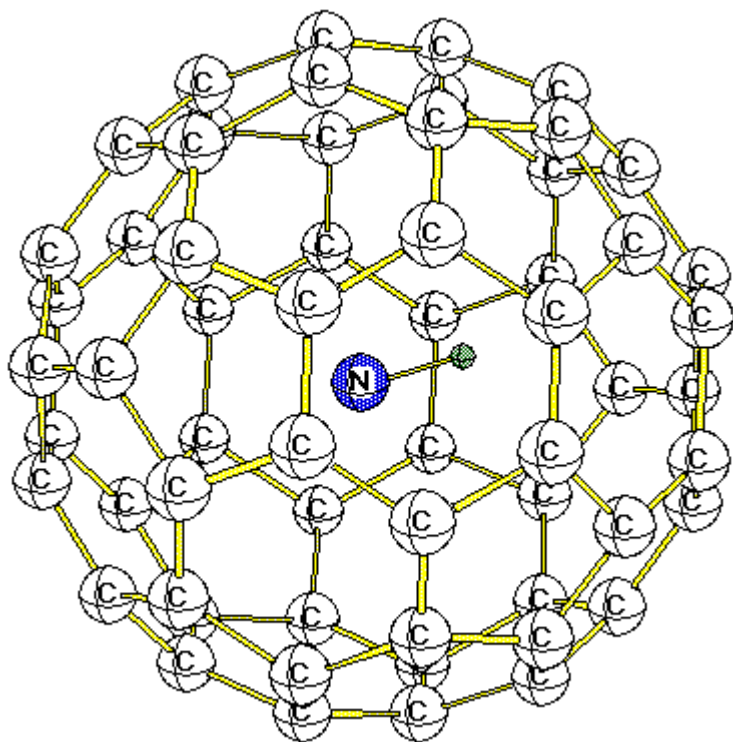
4 (NH⁺@C₆₀, quintet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN092\SP\ROMP2-FC\6-31G(d)\C60H1N1(5)\DRAL\20-Aug-2010\0
 \#P ROMP2/6-31G* Geom=AllCheck Guess=Read Pop=None SCFCyc=1200 SCF=Ti
 ght Name=Dral\NH@C60 quintet\0,5\C,1.892181396,2.166525146,-2.069839
 478\C,0.660385132,2.927236816,-1.863143921\C,0.665557861,3.42845752,-0
 .528182983\C,1.900375366,2.988134644,0.120178223\C,2.665740967,2.21466
 6626,-0.841720581\C,1.87210083,1.007247925,-2.834136963\C,-0.549468994
 ,2.48274231,-2.453399658\C,-0.539077759,3.485931396,0.218841553\C,1.88
 8671875,2.619857788,1.461288452\C,3.388809204,1.093460083,-0.422637939
 \C,0.621078491,0.546539307,-3.434661865\C,-1.795059204,2.545440674,-1.
 690322876\C,-0.550354004,3.106185913,1.59336853\C,2.642562866,1.459976
 196,1.901824951\C,3.36882019,-0.118637085,-1.222640991\C,2.626342773,-
 0.158065796,-2.408630371\C,-0.569046021,1.292160034,-3.23765564\C,-1.7
 89764404,3.033889771,-0.38848877\C,0.642791748,2.672302246,2.22567749\
 C,3.380426147,0.707183838,0.977539062\C,0.59437561,-0.877243042,-3.369
 674683\C,-2.591506958,1.380142212,-2.026412964\C,-0.622451782,-1.55764
 7705,-3.109283447\C,-1.808914185,2.413223267,1.864456177\C,1.850616455
 ,0.792266846,2.918991089\C,3.347985962,-1.253738403,-0.31690979\C,1.82
 9238892,-1.328292847,-2.729675293\C,-1.827713013,0.594924927,-2.977600
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 08,-2.21723938,0.843261719\C,-1.903518677,-2.989181519,-0.11781311\C,-
 0.66885376,-3.428161621,0.529663086\C,-0.663909912,-2.928314209,1.8636
 47461\C,-1.876083374,-1.008453369,2.835494995\C,-3.388793945,-1.094390
 869,0.424636841\C,-1.892242432,-2.619934082,-1.457351685\C,0.535751343
 ,-3.485931396,-0.216369629\C,0.545974731,-2.483612061,2.455154419\C,-2
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 38\C,1.792129517,-2.547332764,1.692611694\C,-1.831497192,1.325973511,2
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5215,0.875411987,3.372070312\C,-3.343841553,1.250839233,0.318984985\C,
 -1.853393555,-0.793365479,-2.914367676\C,1.805679321,-2.414169312,-1.8
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UB3LYP/6-31G(d)



0 5

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C	0.660385132	2.927236816	-1.863143921
C	0.665557861	3.428457520	-0.528182983
C	1.900375366	2.988134644	0.120178223
C	2.665740967	2.214666626	-0.841720581
C	1.872100830	1.007247925	-2.834136963
C	-0.549468994	2.482742310	-2.453399658
C	-0.539077759	3.485931396	0.218841553
C	1.888671875	2.619857788	1.461288452
C	3.388809204	1.093460083	-0.422637939
C	0.621078491	0.546539307	-3.434661865
C	-1.795059204	2.545440674	-1.690322876
C	-0.550354004	3.106185913	1.593368530
C	2.642562866	1.459976196	1.901824951
C	3.368820190	-0.118637085	-1.222640991
C	2.626342773	-0.158065796	-2.408630371
C	-0.569046021	1.292160034	-3.237655640
C	-1.789764404	3.033889771	-0.388488770
C	0.642791748	2.672302246	2.225677490
C	3.380426147	0.707183838	0.977539062
C	0.594375610	-0.877243042	-3.369674683

C	-2.591506958	1.380142212	-2.026412964
C	-0.622451782	-1.557647705	-3.109283447
C	-1.808914185	2.413223267	1.864456177
C	1.850616455	0.792266846	2.918991089
C	3.347985962	-1.253738403	-0.316909790
C	1.829238892	-1.328292847	-2.729675293
C	-1.827713013	0.594924927	-2.977600098
C	-2.581161499	2.379928589	0.636688232
C	0.619323730	1.556884766	3.114028931
C	3.353280762	-0.743438721	1.042755127
C	2.588790894	-1.381652832	2.028381348
C	-1.895355225	-2.168014526	2.069824219
C	-2.668243408	-2.217239380	0.843261719
C	-1.903518677	-2.989181519	-0.117813110
C	-0.668853760	-3.428161621	0.529663086
C	-0.663909912	-2.928314209	1.863647461
C	-1.876083374	-1.008453369	2.835494995
C	-3.388793945	-1.094390869	0.424636841
C	-1.892242432	-2.619934082	-1.457351685
C	0.535751343	-3.485931396	-0.216369629
C	0.545974731	-2.483612061	2.455154419
C	-2.628204346	0.156509399	2.409744263
C	-3.376754761	-0.708557129	-0.974227905
C	-0.645950317	-2.670944214	-2.219726562
C	1.786911011	-3.035278320	0.391113281
C	0.565719604	-1.294601440	3.240600586
C	-0.624420166	-0.548324585	3.434646606
C	-3.368865967	0.116851807	1.224014282
C	-2.644790649	-1.461090088	-1.898132324
C	0.547225952	-3.107192993	-1.589996338
C	1.792129517	-2.547332764	1.692611694
C	-1.831497192	1.325973511	2.730545044
C	-3.349578857	0.740905762	-1.039520264
C	2.581903198	-2.384027222	-0.634048462
C	1.823944092	-0.596557617	2.980010986
C	-0.597595215	0.875411987	3.372070312
C	-3.343841553	1.250839233	0.318984985
C	-1.853393555	-0.793365479	-2.914367676
C	1.805679321	-2.414169312	-1.861877441
N	-0.129182129	-0.054163574	-0.010568359
H	0.925143799	0.245403931	0.050513550

Zero-point correction=	0.380174 (Hartree/Particle)
Thermal correction to Energy=	0.403923
Thermal correction to Enthalpy=	0.404868
Thermal correction to Gibbs Free Energy=	0.332366
Sum of electronic and zero-point Energies=	-2340.948561
Sum of electronic and thermal Energies=	-2340.924811
Sum of electronic and thermal Enthalpies=	-2340.923867
Sum of electronic and thermal Free Energies=	-2340.996369

1\1\FAU-CCC-CCDN082\Freq\UB3LYP/6-31G(d)\C60H1N1(5)\DRAL\31-Jul-2010\0
 \#P UB3LYP/6-31G* SCFCYC=1200 FREQ=NORAMAN NAME=DRAL\NH@C60 quintet\
 \0,5\C,1.892181396,2.166525146,-2.069839478\C,0.660385132,2.927236816,
 -1.863143921\C,0.665557861,3.42845752,-0.528182983\C,1.900375366,2.988
 134644,0.120178223\C,2.665740967,2.214666626,-0.841720581\C,1.87210083
 ,1.007247925,-2.834136963\C,-0.549468994,2.48274231,-2.453399658\C,-0.
 539077759,3.485931396,0.218841553\C,1.888671875,2.619857788,1.46128845
 2\C,3.388809204,1.093460083,-0.422637939\C,0.621078491,0.546539307,-3.
 434661865\C,-1.795059204,2.545440674,-1.690322876\C,-0.550354004,3.106
 185913,1.59336853\C,2.642562866,1.459976196,1.901824951\C,3.36882019,-
 0.118637085,-1.222640991\C,2.626342773,-0.158065796,-2.408630371\C,-0.
 569046021,1.292160034,-3.23765564\C,-1.789764404,3.033889771,-0.388488
 77\C,0.642791748,2.672302246,2.22567749\C,3.380426147,0.707183838,0.97
 7539062\C,0.59437561,-0.877243042,-3.369674683\C,-2.591506958,1.380142
 212,-2.026412964\C,-0.622451782,-1.557647705,-3.109283447\C,-1.8089141
 85,2.413223267,1.864456177\C,1.850616455,0.792266846,2.918991089\C,3.3
 47985962,-1.253738403,-0.31690979\C,1.829238892,-1.328292847,-2.729675
 293\C,-1.827713013,0.594924927,-2.977600098\C,-2.581161499,2.379928589
 ,0.636688232\C,0.61932373,1.556884766,3.114028931\C,3.353280762,-0.743
 438721,1.042755127\C,2.588790894,-1.381652832,2.028381348\C,-1.8953552
 25,-2.168014526,2.069824219\C,-2.668243408,-2.21723938,0.843261719\C,-
 1.903518677,-2.989181519,-0.11781311\C,-0.66885376,-3.428161621,0.5296
 63086\C,-0.663909912,-2.928314209,1.863647461\C,-1.876083374,-1.008453
 369,2.835494995\C,-3.388793945,-1.094390869,0.424636841\C,-1.892242432
 ,-2.619934082,-1.457351685\C,0.535751343,-3.485931396,-0.216369629\C,0.
 545974731,-2.483612061,2.455154419\C,-2.628204346,0.156509399,2.40974
 4263\C,-3.376754761,-0.708557129,-0.974227905\C,-0.645950317,-2.670944
 214,-2.219726562\C,1.786911011,-3.03527832,0.391113281\C,0.565719604,-
 1.29460144,3.240600586\C,-0.624420166,-0.548324585,3.434646606\C,-3.36
 8865967,0.116851807,1.224014282\C,-2.644790649,-1.461090088,-1.8981323
 24\C,0.547225952,-3.107192993,-1.589996338\C,1.792129517,-2.547332764,
 1.692611694\C,-1.831497192,1.325973511,2.730545044\C,-3.349578857,0.74
 0905762,-1.039520264\C,2.581903198,-2.384027222,-0.634048462\C,1.82394
 4092,-0.596557617,2.980010986\C,-0.597595215,0.875411987,3.372070312\C
 ,-3.343841553,1.250839233,0.318984985\C,-1.853393555,-0.793365479,-2.9
 14367676\C,1.805679321,-2.414169312,-1.861877441\N,-0.129182129,-0.054
 163574,-0.010568359\H,0.925143799,0.245403931,0.05051355\Version=EM64
 L-G09RevA.02\State=5-A\HF=-2341.3287344\S2=6.014569\S2-1=0.\S2A=6.0000
 82\RMSD=5.364e-09\RMSF=3.619e-03\ZeroPoint=0.3801739\Thermal=0.4039233
 \ZPE=238.5627166\Dipole=0.1225862,-0.0019923,-0.0002898\DipoleDeriv=0.
 0070983,-0.0000501,-0.0041059,0.0000389,0.0070504\Polar=467.2649368,1.
 1748925,522.9703095,-0.035903,0.0418021,522.9798456\PG=C01 [X(C60H1N1)
]\NImag=0\0.41191346,-0.11000073,0.49456923,0.09803442,0.21701406,0.4
 6412,0.00389194,0.01744298\0.00017875,-0.00132122,-0.00100581,-0.0002
 949,-0.00939874,-0.00179151,0.03360775,0.00925376,0.00193294\@

5⁺ (NH⁺@C₆₀H⁺, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN087\SP\ROMP2-FC\6-31G(d)\C60H2N1(1+,3)\DRAL\10-Aug-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Po
p=None Name=Dral\NH@C60H+\1,3\C,0,1.6323492283,3.0917060474,0.698716
2042\C,0,1.6323492283,3.0917060474,-0.6987162042\C,0,0.3808105735,3.23
77084425,1.4175883625\C,0,0.3808105735,3.2377084425,-1.4175883625\C,0,
0.4351311272,2.3665351303,2.5878900985\C,0,0.4351311272,2.3665351303,-
2.5878900985\C,0,1.7228841433,1.7053275763,2.599028681\C,0,1.722884143
3,1.7053275763,-2.599028681\C,0,2.4638571469,2.1447079441,1.4266862447
\C,0,2.4638571469,2.1447079441,-1.4266862447\C,0,-0.8142626242,3.39278
63162,0.7242040857\C,0,-0.8142626242,3.3927863162,-0.7242040857\C,0,-0
.7081473518,1.6882772019,3.0226151211\C,0,-0.7081473518,1.6882772019,-
3.0226151211\C,0,1.8120653298,0.3762507635,3.0239222208\C,0,1.81206532
98,0.3762507635,-3.0239222208\C,0,3.260250403,1.2376051485,0.727971460
9\C,0,3.260250403,1.2376051485,-0.7279714609\C,0,-2.0071644831,2.67255
68358,1.161828936\C,0,-2.0071644831,2.6725568358,-1.161828936\C,0,-0.6
097982601,0.3124871804,3.4747439685\C,0,-0.6097982601,0.3124871804,-3.
4747439685\C,0,2.6491894124,-0.5634480054,2.303495688\C,0,2.6491894124
,-0.5634480054,-2.303495688\C,0,-1.9423200888,1.8208720477,2.280276114
\C,0,-1.9423200888,1.8208720477,-2.280276114\C,0,0.6238561991,-0.33195
98647,3.4789739919\C,0,0.6238561991,-0.3319598647,-3.4789739919\C,0,3.
3568025908,-0.1443302018,1.1749794582\C,0,3.3568025908,-0.1443302018,-
1.1749794582\C,0,-2.7038841221,2.2388334078,0.\C,0,-1.7990206094,-0.39
63840582,3.0253786762\C,0,-1.7990206094,-0.3963840582,-3.0253786762\C,
0,1.9721973663,-1.851296472,2.3024678988\C,0,1.9721973663,-1.851296472
,-2.3024678988\C,0,-2.6386375706,0.5366947468,2.3007184276\C,0,-2.6386
375706,0.5366947468,-2.3007184276\C,0,0.7263125448,-1.71184595,3.03424
7759\C,0,0.7263125448,-1.71184595,-3.034247759\C,0,3.418517129,-0.9944
303839,0.\C,0,2.7676895011,-2.2328979223,0.\C,0,-1.6002020388,-3.08058
68983,-0.7005412887\C,0,-1.6002020388,-3.0805868983,0.7005412887\C,0,-
2.4308385291,-2.1485137201,-1.4286322714\C,0,-2.4308385291,-2.14851372
01,1.4286322714\C,0,-1.7030075484,-1.7206450736,-2.6039842919\C,0,-1.7
030075484,-1.7206450736,2.6039842919\C,0,-0.4123021292,-2.3918744805,-
2.6041685639\C,0,-0.4123021292,-2.3918744805,2.6041685639\C,0,-0.35110
77654,-3.2394297353,-1.4271527888\C,0,-0.3511077654,-3.2394297353,1.42
71527888\C,0,-3.2286499091,-1.2292720206,-0.7281784887\C,0,-3.22864990
91,-1.2292720206,0.7281784887\C,0,0.8466226849,-3.3772322715,-0.727280
9935\C,0,0.8466226849,-3.3772322715,0.7272809935\C,0,-3.3484771774,0.1
178781792,-1.1872805417\C,0,-3.3484771774,0.1178781792,1.1872805417\C,
0,2.0340350484,-2.6715415769,-1.1738548612\C,0,2.0340350484,-2.6715415
769,1.1738548612\C,0,-3.6253150861,1.0459069064,0.\N,0,-0.1535815874,0
.0905299331,0.\H,0,0.8237523683,0.4530165707,0.\H,0,-4.674106624,1.395
7640213,0.\Version=AM64L-G03RevD.02\State=3-A"\HF=-2327.1080348\MP2=-
2335.0287082\RMSE=8.835e-09\Thermal=0.\PG=CS [SG(C4H2N1),X(C56)]\@
```

UB3LYP/6-31G(d)

Zero-point correction= 0.395233 (Hartree/Particle)
 Thermal correction to Energy= 0.419492
 Thermal correction to Enthalpy= 0.420436
 Thermal correction to Gibbs Free Energy= 0.347264
 Sum of electronic and zero-point Energies= -2341.345634
 Sum of electronic and thermal Energies= -2341.321375
 Sum of electronic and thermal Enthalpies= -2341.320431
 Sum of electronic and thermal Free Energies= -2341.393603

1\1\FAU-CCC-CCDH151\Freq\UB3LYP/6-31G(d)\C60H2N1(1+,3)\DRAL\07-Dec-200
 8\0\#P Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Fre
 q\NH@C60H+\1,3\C,1.6323492283,3.0917060474,0.6987162042\C,1.63234922
 83,3.0917060474,-0.6987162042\C,0.3808105735,3.2377084425,1.4175883625
 \C,0.3808105735,3.2377084425,-1.4175883625\C,0.4351311272,2.3665351303
 ,2.5878900985\C,0.4351311272,2.3665351303,-2.5878900985\C,1.7228841433
 ,1.7053275763,2.599028681\C,1.7228841433,1.7053275763,-2.599028681\C,2
 .4638571469,2.1447079441,1.4266862447\C,2.4638571469,2.1447079441,-1.4
 266862447\C,-0.8142626242,3.3927863162,0.7242040857\C,-0.8142626242,3.
 3927863162,-0.7242040857\C,-0.7081473518,1.6882772019,3.0226151211\C,-
 0.7081473518,1.6882772019,-3.0226151211\C,1.8120653298,0.3762507635,3.
 0239222208\C,1.8120653298,0.3762507635,-3.0239222208\C,3.260250403,1.2
 376051485,0.7279714609\C,3.260250403,1.2376051485,-0.7279714609\C,-2.0
 071644831,2.6725568358,1.161828936\C,-2.0071644831,2.6725568358,-1.161
 828936\C,-0.6097982601,0.3124871804,3.4747439685\C,-0.6097982601,0.312
 4871804,-3.4747439685\C,2.6491894124,-0.5634480054,2.303495688\C,2.649
 1894124,-0.5634480054,-2.303495688\C,-1.9423200888,1.8208720477,2.2802
 76114\C,-1.9423200888,1.8208720477,-2.280276114\C,0.6238561991,-0.3319
 598647,3.4789739919\C,0.6238561991,-0.3319598647,-3.4789739919\C,3.356
 8025908,-0.1443302018,1.1749794582\C,3.3568025908,-0.1443302018,-1.174
 9794582\C,-2.7038841221,2.2388334078,0.\C,-1.7990206094,-0.3963840582,
 3.0253786762\C,-1.7990206094,-0.3963840582,-3.0253786762\C,1.972197366
 3,-1.851296472,2.3024678988\C,1.9721973663,-1.851296472,-2.3024678988\
 C,-2.6386375706,0.5366947468,2.3007184276\C,-2.6386375706,0.5366947468
 ,-2.3007184276\C,0.7263125448,-1.71184595,3.034247759\C,0.7263125448,-
 1.71184595,-3.034247759\C,3.418517129,-0.9944303839,0.\C,2.7676895011,
 -2.2328979223,0.\C,-1.6002020388,-3.0805868983,-0.7005412887\C,-1.6002
 020388,-3.0805868983,0.7005412887\C,-2.4308385291,-2.1485137201,-1.428
 6322714\C,-2.4308385291,-2.1485137201,1.4286322714\C,-1.7030075484,-1.
 7206450736,-2.6039842919\C,-1.7030075484,-1.7206450736,2.6039842919\C,
 -0.4123021292,-2.3918744805,-2.6041685639\C,-0.4123021292,-2.391874480
 5,2.6041685639\C,-0.3511077654,-3.2394297353,-1.4271527888\C,-0.351107
 7654,-3.2394297353,1.4271527888\C,-3.2286499091,-1.2292720206,-0.72817
 84887\C,-3.2286499091,-1.2292720206,0.7281784887\C,0.8466226849,-3.377
 2322715,-0.7272809935\C,0.8466226849,-3.3772322715,0.7272809935\C,-3.3
 484771774,0.1178781792,-1.1872805417\C,-3.3484771774,0.1178781792,1.18
 72805417\C,2.0340350484,-2.6715415769,-1.1738548612\C,2.0340350484,-2.
 6715415769,1.1738548612\C,-3.6253150861,1.0459069064,0.\N,-0.153581587

4,0.0905299331,0.\H,0.8237523683,0.4530165707,0.\H,-4.674106624,1.3957
 640213,0.\Version=AM64L-G03RevD.02\State=3-A"\HF=-2341.7408672\S2=2.0
 05161\S2-1=0.\S2A=2.000007\RMSD=2.831e-09\RMSF=1.241e-04\ZeroPoint=0.3
 952331\Thermal=0.419492\ZPE=248.0125337\Dipole=-1.1342528,0.6482111,0.
 \DipoleDeriv=0.050668,0.0173922,0.0077564,-0.0370639,0.0151991,-0.0573
 531741,0.1198126,0.0071456,0.,-0.0189599,0.105369,0.,0.,0.,0.0991387\P
 olar=492.1691895,-7.1517235,477.9607787,0.,0.,476.459445\PG=CS [SG(C4H
 2N1),X(C56)]\NImag=0\0.45680332,-0.13216439,0.26845267,-0.04225765,-0
 -0.00002217,0.,0.,0.04219064\0.00002493,-0.00003164,0.00008578,0.0000
 1096,0.00108796,0.,0.00000891,-0.00000726,0.\@\@

6⁺ (NH₂⁺⁺@C₆₀, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN088\SP\ROMP2-FC\6-31G(d)\C60H2N1(1+,3)\DRAL\13-Aug-201
 0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCF=Tight SCFCy
 c=1200 Name=Dral\NH2(+)\@C60 triplet\1,3\C,0,3.363047979,-0.420589313
 ,1.135682789\C,0,3.367744394,-1.194442028,-0.096122736\C,0,3.351958408
 ,-0.261982121,-1.212784985\C,0,3.337123579,1.088554211,-0.671270497\C,
 0,3.34393342,0.990350764,0.780612202\C,0,2.634339107,-0.87090312,2.237
 832471\C,0,2.643209898,-2.3854108,-0.172996305\C,0,2.61290001,-0.56049
 1058,-2.358898418\C,0,2.585493514,2.083883335,-1.299084769\C,0,2.59823
 8496,1.891750418,1.543658303\C,0,1.879226736,-2.108991218,2.151775823\
 C,0,1.872173416,-2.689678146,-1.365544293\C,0,1.827736408,0.476394414,
 -3.006269329\C,0,1.807966088,3.017452648,-0.501966333\C,0,1.83882711,1
 .418251033,2.688154729\C,0,1.856076553,0.069186525,3.025871309\C,0,1.8
 83076912,-2.847767143,0.974622831\C,0,1.857764461,-1.799165487,-2.4328
 43868\C,0,1.814842668,1.768037805,-2.490178516\C,0,1.813962395,2.92331
 4447,0.886655974\C,0,0.632475501,-1.927495338,2.887876764\C,0,0.634646
 251,-3.337657479,-0.946654873\C,0,-0.560594925,-2.50615738,2.419531418
 \C,0,0.586633669,-0.128125105,-3.477899619\C,0,0.555654328,3.274126141
 ,-1.204952719\C,0,0.583980701,2.160797707,2.733886643\C,0,0.619094267,
 -0.5943804,3.423546155\C,0,0.64163366,-3.434495906,0.484131121\C,0,0.6
 04175833,-1.520604546,-3.125168577\C,0,0.559750238,2.508642497,-2.4236
 65204\C,0,0.568865201,3.083298573,1.629360808\C,0,-0.634743202,3.34562
 9039,0.950985913\C,0,-3.358993789,0.422558881,-1.134714912\C,0,-3.3429
 16482,-0.987387632,-0.77950791\C,0,-3.335959453,-1.085507696,0.6705608
 25\C,0,-3.347940642,0.264118867,1.212093637\C,0,-3.362472367,1.1964859
 18,0.09643485\C,0,-2.633668319,0.872719429,-2.2384848\C,0,-2.599397916
 ,-1.888459119,-1.541604051\C,0,-2.586365038,-2.080575608,1.297677908\C
 ,0,-2.611743854,0.562517571,2.35917088\C,0,-2.642362372,2.39037093,0.1
 73938872\C,0,-1.857095155,-0.068323787,-3.026935872\C,0,-1.816594792,-
 2.918975221,-0.884651955\C,0,-1.815293129,-1.764985839,2.487113447\C,0
 ,-1.856213631,1.800794524,2.433916414\C,0,-1.882738603,2.853696103,-0.
 975538663\C,0,-1.877527097,2.110019084,-2.152602081\C,0,-1.839348827,-
 1.415255658,-2.68469078\C,0,-1.810428721,-3.013368625,0.501215452\C,0,

-1.828240757,-0.475557253,3.006414849\C,0,-1.871873792,2.69599874,1.36
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UB3LYP/6-31G(d)

Zero-point correction=	0.394698 (Hartree/Particle)
Thermal correction to Energy=	0.419258
Thermal correction to Enthalpy=	0.420202
Thermal correction to Gibbs Free Energy=	0.347056
Sum of electronic and zero-point Energies=	-2341.387769
Sum of electronic and thermal Energies=	-2341.363209
Sum of electronic and thermal Enthalpies=	-2341.362265
Sum of electronic and thermal Free Energies=	-2341.435411

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7 (NH₂·@C₆₀)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

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 C 0.621215820 -3.365158081 -0.947937012
 C 3.387924194 -0.807037354 0.714904785
 C 1.377105713 2.500366211 2.113372803
 C -1.451431274 2.676620483 1.824829102
 C -3.532012939 -0.375274658 0.007446289
 C -0.823135376 -3.274627686 -1.095260620
 C 2.928924561 -2.013366699 0.043792725
 C 2.536010742 1.665420532 1.846847534
 C 3.099380493 1.641021729 0.570938110
 C 1.108749390 0.554275513 -3.325653076
 C -0.334182739 0.644348145 -3.473724365
 C -0.766647339 1.905334473 -2.895523071
 C 0.408752441 2.595031738 -2.391265869
 C 1.567565918 1.759765625 -2.656967163
 C 1.706924438 -0.674560547 -3.042205811
 C -1.123733521 -0.497741699 -3.331008911
 C -1.971588135 1.974792480 -2.195602417
 C 0.332992554 3.323318481 -1.204284668
 C 2.605133057 1.688964844 -1.726821899
 C 0.884521484 -1.863815308 -2.891113281
 C -2.378799438 -0.425918579 -2.601470947
 C -2.049957275 2.735534668 -0.959823608
 C 1.413040161 3.249404907 -0.235687256
 C 3.226974487 0.409362793 -1.428222656

C 2.788406372 -0.748458862 -2.073410034
 C -0.501953125 -1.776947021 -3.031921387
 C -2.792800903 0.785003662 -2.043640137
 C -0.920989990 3.394866943 -0.474349976
 C 2.526611328 2.449737549 -0.491806030
 C 1.457366943 -2.673599243 -1.827514648
 C -2.533584595 -1.661514282 -1.850341797
 C 0.827087402 3.275527954 1.093063354
 C 3.532012939 0.379501343 -0.007125854
 C 2.635086060 -1.984558105 -1.322052002
 C -1.372756958 -2.496932983 -2.116394043
 C -3.380523682 0.811141968 -0.713851929
 C -0.615600586 3.364807129 0.945709229
 N 0.053614014 0.105398438 -0.045227661
 H -0.911654053 -0.266129028 -0.167265381
 H 0.613569580 -0.782930664 0.129222046

Zero-point correction= 0.397494 (Hartree/Particle)
 Thermal correction to Energy= 0.420853
 Thermal correction to Enthalpy= 0.421797
 Thermal correction to Gibbs Free Energy= 0.351595
 Sum of electronic and zero-point Energies= -2341.645829
 Sum of electronic and thermal Energies= -2341.622470
 Sum of electronic and thermal Enthalpies= -2341.621526
 Sum of electronic and thermal Free Energies= -2341.691728

1\1\FAU-CCC-CCDH155\Freq\UB3LYP/6-31G(d)\C60H2N1(2)\DRAL\27-May-2009\0
 \#P B3LYP/6-31G* FREQ=NORAMAN POP=NONE NAME=DRAL\NH2@C60\0,2\C,-1.1
 04660034,-0.549942017,3.32635498\C,-1.564590454,-1.755264282,2.6573028
 56\C,-0.404602051,-2.591018677,2.390945435\C,0.771514893,-1.900772095,
 2.895706177\C,0.338348389,-0.63999939,3.473739624\C,-1.700653076,0.678
 787231,3.038696289\C,-2.6040802,-1.685287476,1.727920532\C,-0.32899475
 1,-3.322479248,1.204345703\C,1.977615356,-1.970581055,2.196044922\C,1.
 126647949,0.501876831,3.325668335\C,-2.781768799,0.752761841,2.0697326
 66\C,-2.525039673,-2.447250366,0.491394043\C,0.926696777,-3.394882202,
 0.473434448\C,2.800445557,-0.781387329,2.044754028\C,0.506256104,1.781
 112671,3.027603149\C,-0.878982544,1.868026733,2.887374878\C,-3.2260894
 78,-0.405456543,1.428573608\C,-1.410247803,-3.249084473,0.23475647\C,2
 .056427002,-2.732879639,0.959915161\C,2.381454468,0.430053711,2.596511
 841\C,-2.627548218,1.988098145,1.31942749\C,-3.098587036,-1.63734436,-
 0.572479248\C,-2.920578003,2.016952515,-0.044540405\C,0.62121582,-3.36
 5158081,-0.947937012\C,3.387924194,-0.807037354,0.714904785\C,1.377105
 713,2.500366211,2.113372803\C,-1.451431274,2.676620483,1.824829102\C,-
 3.532012939,-0.375274658,0.007446289\C,-0.823135376,-3.274627686,-1.09
 526062\C,2.928924561,-2.013366699,0.043792725\C,2.536010742,1.66542053
 2,1.846847534\C,3.099380493,1.641021729,0.57093811\C,1.10874939,0.5542
 75513,-3.325653076\C,-0.334182739,0.644348145,-3.473724365\C,-0.766647
 339,1.905334473,-2.895523071\C,0.408752441,2.595031738,-2.391265869\C,
 1.567565918,1.759765625,-2.656967163\C,1.706924438,-0.674560547,-3.042
 205811\C,-1.123733521,-0.497741699,-3.331008911\C,-1.971588135,1.97479

248,-2.195602417\C,0.332992554,3.323318481,-1.204284668\C,2.605133057,
 1.688964844,-1.726821899\C,0.884521484,-1.863815308,-2.891113281\C,-2.
 378799438,-0.425918579,-2.601470947\C,-2.049957275,2.735534668,-0.9598
 23608\C,1.413040161,3.249404907,-0.235687256\C,3.226974487,0.409362793
 ,-1.428222656\C,2.788406372,-0.748458862,-2.073410034\C,-0.501953125,-
 1.776947021,-3.031921387\C,-2.792800903,0.785003662,-2.043640137\C,-0.
 92098999,3.394866943,-0.474349976\C,2.526611328,2.449737549,-0.4918060
 3\C,1.457366943,-2.673599243,-1.827514648\C,-2.533584595,-1.661514282,
 -1.850341797\C,0.827087402,3.275527954,1.093063354\C,3.532012939,0.379
 501343,-0.007125854\C,2.63508606,-1.984558105,-1.322052002\C,-1.372756
 958,-2.496932983,-2.116394043\C,-3.380523682,0.811141968,-0.713851929\
 C,-0.615600586,3.364807129,0.945709229\N,0.053614014,0.105398438,-0.04
 5227661\H,-0.911654053,-0.266129028,-0.167265381\H,0.61356958,-0.78293
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 nt=0.397494\Thermal=0.4208531\ZPE=249.4312337\Dipole=-0.0460455,-0.128
 4089,0.0060697\DipoleDeriv=0.085093,0.0198359,-0.0007736,0.0102495,-0.
 071116,0.0062775,0.0576993\Polar=470.7921634,-0.159298,470.2995809,0.1
 302014,-0.04454,469.6775924\PG=C01 [X(C60H2N1)]\NImag=0\0.52932389,-0
 4,0.00535528,-0.00103677,0.03318118,-0.04177798,0.02263037\0.0000058
 2038,-0.00291218,-0.00118584,0.01376469,-0.02104640,0.00428703\\@

8⁺ (NH₂·@C₆₀H⁺)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H3N1(1+,2)\DRAL\12-Aug-201
 0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Po
 p=None Name=Dral\NH2@C60H(+)\1,2\C,3.33996582,-1.674835205,0.6976318
 36\C,3.33996582,-1.674835205,-0.697631836\C,3.247009277,-0.4190979,1.4
 15924072\C,3.247009277,-0.4190979,-1.415924072\C,2.401199341,-0.636245
 728,2.584655762\C,2.401199341,-0.636245728,-2.584655762\C,1.993988037,
 -2.024337769,2.595077515\C,1.993988037,-2.024337769,-2.595077515\C,2.5
 65551758,-2.667556763,1.424133301\C,2.565551758,-2.667556763,-1.424133
 301\C,3.175048828,0.782852173,0.723968506\C,3.175048828,0.782852173,-0
 .723968506\C,1.521087646,0.35887146,3.02432251\C,1.521087646,0.3588714
 6,-3.02432251\C,0.707626343,-2.363815308,3.023880005\C,0.707626343,-2.
 363815308,-3.023880005\C,1.8256073,-3.618927002,0.726715088\C,1.825607
 3,-3.618927002,-0.726715088\C,2.241699219,1.815002441,1.161834717\C,2.
 241699219,1.815002441,-1.161834717\C,0.186813354,0.00163269,3.47645568
 8\C,0.186813354,0.00163269,-3.476455688\C,-0.056625366,-3.365869263,2.
 304733276\C,-0.056625366,-3.365869263,-2.304733276\C,1.419616699,1.591
 751099,2.281021118\C,1.419616699,1.591751099,-2.281021118\C,-0.2130126
 95,-1.331268311,3.48046875\C,-0.213012695,-1.331268311,-3.48046875\C,0
 .488327026,-3.972961426,1.173995972\C,0.488327026,-3.972961426,-1.1739
 95972\C,1.681869507,2.415328979,0.\C,-0.735656738,1.034103394,3.025634
 766\C,-0.735656738,1.034103394,-3.025634766\C,-1.450256348,-2.94642041

,2.303192139\C,-1.450256348,-2.94642041,-2.303192139\C,0.023162842,2.0
 32363892,2.298812866\C,0.023162842,2.032363892,-2.298812866\C,-1.55050
 6592,-1.693969727,3.035919189\C,-1.550506592,-1.693969727,-3.035919189
 \C,-0.334701538,-4.193481445,0.\C,-1.674285889,-3.797540405,0.\C,-3.33
 996582,0.330978394,-0.700759888\C,-3.33996582,0.330978394,0.700759888\
 C,-2.576574585,1.323989868,-1.4296875\C,-2.576574585,1.323989868,1.429
 6875\C,-2.021942139,0.690750122,-2.606689453\C,-2.021942139,0.69075012
 2,2.606689453\C,-2.438415527,-0.705078125,-2.607788086\C,-2.438415527,
 -0.705078125,2.607788086\C,-3.259384155,-0.925933838,-1.428634644\C,-3
 .259384155,-0.925933838,1.428634644\C,-1.821813843,2.276327393,-0.7283
 3252\C,-1.821813843,2.276327393,0.72833252\C,-3.165008545,-2.129013062
 ,-0.727844238\C,-3.165008545,-2.129013062,0.727844238\C,-0.522262573,2
 .65171814,-1.187606812\C,-0.522262573,2.65171814,1.187606812\C,-2.2453
 46069,-3.163171509,-1.174835205\C,-2.245346069,-3.163171509,1.17483520
 5\C,0.337112427,3.094717285,0.\N,0.070409424,-0.43182666,0.\H,-0.53369
 4092,-0.770955566,0.810394287\H,-0.533694092,-0.770955566,-0.810394287
 \H,0.48324585,4.190481445,0.\Version=AM64L-G03RevD.02\State=2-A"\HF=-
 2327.7040418\MP2=-2335.6652617\RMSD=7.978e-10\Thermal=0.\PG=CS [SG(C4H
 1N1),X(C56H2)]\@

UB3LYP/6-31G(d)

1 2

C	3.339965820	-1.674835205	0.697631836
C	3.339965820	-1.674835205	-0.697631836
C	3.247009277	-0.419097900	1.415924072
C	3.247009277	-0.419097900	-1.415924072
C	2.401199341	-0.636245728	2.584655762
C	2.401199341	-0.636245728	-2.584655762
C	1.993988037	-2.024337769	2.595077515
C	1.993988037	-2.024337769	-2.595077515
C	2.565551758	-2.667556763	1.424133301
C	2.565551758	-2.667556763	-1.424133301
C	3.175048828	0.782852173	0.723968506
C	3.175048828	0.782852173	-0.723968506
C	1.521087646	0.358871460	3.024322510
C	1.521087646	0.358871460	-3.024322510
C	0.707626343	-2.363815308	3.023880005
C	0.707626343	-2.363815308	-3.023880005
C	1.825607300	-3.618927002	0.726715088
C	1.825607300	-3.618927002	-0.726715088
C	2.241699219	1.815002441	1.161834717
C	2.241699219	1.815002441	-1.161834717
C	0.186813354	0.001632690	3.476455688
C	0.186813354	0.001632690	-3.476455688
C	-0.056625366	-3.365869263	2.304733276
C	-0.056625366	-3.365869263	-2.304733276
C	1.419616699	1.591751099	2.281021118
C	1.419616699	1.591751099	-2.281021118

```

C    -0.213012695 -1.331268311 3.480468750
C    -0.213012695 -1.331268311 -3.480468750
C    0.488327026 -3.972961426 1.173995972
C    0.488327026 -3.972961426 -1.173995972
C    1.681869507 2.415328979 0.000000000
C    -0.735656738 1.034103394 3.025634766
C    -0.735656738 1.034103394 -3.025634766
C    -1.450256348 -2.946420410 2.303192139
C    -1.450256348 -2.946420410 -2.303192139
C    0.023162842 2.032363892 2.298812866
C    0.023162842 2.032363892 -2.298812866
C    -1.550506592 -1.693969727 3.035919189
C    -1.550506592 -1.693969727 -3.035919189
C    -0.334701538 -4.193481445 0.000000000
C    -1.674285889 -3.797540405 0.000000000
C    -3.339965820 0.330978394 -0.700759888
C    -3.339965820 0.330978394 0.700759888
C    -2.576574585 1.323989868 -1.429687500
C    -2.576574585 1.323989868 1.429687500
C    -2.021942139 0.690750122 -2.606689453
C    -2.021942139 0.690750122 2.606689453
C    -2.438415527 -0.705078125 -2.607788086
C    -2.438415527 -0.705078125 2.607788086
C    -3.259384155 -0.925933838 -1.428634644
C    -3.259384155 -0.925933838 1.428634644
C    -1.821813843 2.276327393 -0.728332520
C    -1.821813843 2.276327393 0.728332520
C    -3.165008545 -2.129013062 -0.727844238
C    -3.165008545 -2.129013062 0.727844238
C    -0.522262573 2.651718140 -1.187606812
C    -0.522262573 2.651718140 1.187606812
C    -2.245346069 -3.163171509 -1.174835205
C    -2.245346069 -3.163171509 1.174835205
C    0.337112427 3.094717285 0.000000000
N    0.070409424 -0.431826660 0.000000000
H    -0.533694092 -0.770955566 0.810394287
H    -0.533694092 -0.770955566 -0.810394287
H    0.483245850 4.190481445 0.000000000

```

```

Zero-point correction=          0.408638 (Hartree/Particle)
Thermal correction to Energy=    0.432074
Thermal correction to Enthalpy=   0.433018
Thermal correction to Gibbs Free Energy= 0.362536
Sum of electronic and zero-point Energies= -2341.983227
Sum of electronic and thermal Energies= -2341.959791
Sum of electronic and thermal Enthalpies= -2341.958847
Sum of electronic and thermal Free Energies= -2342.029329

```

```

1\1\FAU-CCC-CCDH154\Freq\UB3LYP\6-31G(d)\C60H3N1(1+,2)\DRAL\29-May-200
90\#P B3LYP/6-31G* FREQ=NORAMAN POP=NONE NAME=DRAL\NH2@C60H(+)\1,2

```

\C,3.33996582,-1.674835205,0.697631836\C,3.33996582,-1.674835205,-0.69
 7631836\C,3.247009277,-0.4190979,1.415924072\C,3.247009277,-0.4190979,
 -1.415924072\C,2.401199341,-0.636245728,2.584655762\C,2.401199341,-0.6
 36245728,-2.584655762\C,1.993988037,-2.024337769,2.595077515\C,1.99398
 8037,-2.024337769,-2.595077515\C,2.565551758,-2.667556763,1.424133301\
 C,2.565551758,-2.667556763,-1.424133301\C,3.175048828,0.782852173,0.72
 3968506\C,3.175048828,0.782852173,-0.723968506\C,1.521087646,0.3588714
 6,3.02432251\C,1.521087646,0.35887146,-3.02432251\C,0.707626343,-2.363
 815308,3.023880005\C,0.707626343,-2.363815308,-3.023880005\C,1.8256073
 ,-3.618927002,0.726715088\C,1.8256073,-3.618927002,-0.726715088\C,2.24
 1699219,1.815002441,1.161834717\C,2.241699219,1.815002441,-1.161834717
 \C,0.186813354,0.00163269,3.476455688\C,0.186813354,0.00163269,-3.4764
 55688\C,-0.056625366,-3.365869263,2.304733276\C,-0.056625366,-3.365869
 263,-2.304733276\C,1.419616699,1.591751099,2.281021118\C,1.419616699,1
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 2\C,0.488327026,-3.972961426,-1.173995972\C,1.681869507,2.415328979,0.
 \C,-0.735656738,1.034103394,3.025634766\C,-0.735656738,1.034103394,-3.
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 42041,-2.303192139\C,0.023162842,2.032363892,2.298812866\C,0.023162842
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 -1.674285889,-3.797540405,0.\C,-3.33996582,0.330978394,-0.700759888\C,
 -3.33996582,0.330978394,0.700759888\C,-2.576574585,1.323989868,-1.4296
 875\C,-2.576574585,1.323989868,1.4296875\C,-2.021942139,0.690750122,-2
 .606689453\C,-2.021942139,0.690750122,2.606689453\C,-2.438415527,-0.70
 5078125,-2.607788086\C,-2.438415527,-0.705078125,2.607788086\C,-3.2593
 84155,-0.925933838,-1.428634644\C,-3.259384155,-0.925933838,1.42863464
 4\C,-1.821813843,2.276327393,-0.72833252\C,-1.821813843,2.276327393,0.
 72833252\C,-3.165008545,-2.129013062,-0.727844238\C,-3.165008545,-2.12
 9013062,0.727844238\C,-0.522262573,2.65171814,-1.187606812\C,-0.522262
 573,2.65171814,1.187606812\C,-2.245346069,-3.163171509,-1.174835205\C,
 -2.245346069,-3.163171509,1.174835205\C,0.337112427,3.094717285,0.\N,0
 .070409424,-0.43182666,0.\H,-0.533694092,-0.770955566,0.810394287\H,-0
 .533694092,-0.770955566,-0.810394287\H,0.48324585,4.190481445,0.\Vers
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 0.4320742\ZPE=256.4244874\Dipole=0.2709166,1.2519171,0.\DipoleDeriv=0.
 0114414,0.1197416,0.,0.,0.,0.0975497\Polar=474.2646238,4.6763591,493.0
 52925,0.,0.,478.1342268\PG=CS [SG(C4H1N1),X(C56H2)]\NImag=0\0.2257723
 001665,-0.00000748,0.00001669,0.00001665,-0.00000748,0.,0.,0.04245237\
 -0.00011952,0.00001713,-0.00006745,-0.00011952,0.00001713,0.00006745,
 640161,-0.01658798,-0.00837155,-0.01640161,-0.00015445,-0.00016825,0.\
 \@

9⁺ (NH₃⁺@C₆₀)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN089\SP\ROMP2-FC\6-31G(d)\C60H3N1(1+,2)\DRAL\13-Aug-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Po
p=None Name=Dral\NH3(+)\C60\1,2\C,1.203460693,3.269073486,0.69613647
5\C,-0.053146362,3.268218994,1.425140381\C,0.113449097,2.423355103,2.5
96405029\C,1.475402832,1.903289795,2.585388184\C,2.143859863,2.4216766
36,1.420547485\C,1.203460693,3.269073486,-0.696136475\C,-1.263061523,3
.260421753,0.727554321\C,-0.932235718,1.610519409,3.022399902\C,1.7397
00317,0.591964722,3.020294189\C,3.057403564,1.615493774,0.719848633\C,
-0.053146362,3.268218994,-1.425140381\C,-2.356658936,2.412643433,1.176
361084\C,-0.658798218,0.246139526,3.460647583\C,2.69732666,-0.24226379
4,2.300888062\C,3.057403564,1.615493774,-0.719848633\C,2.143859863,2.4
21676636,-1.420547485\C,-1.263061523,3.260421753,-0.727554321\C,-2.194
595337,1.606155396,2.303436279\C,0.658218384,-0.248046875,3.46446228\C
,3.342437744,0.259857178,1.174224854\C,0.113449097,2.423355103,-2.5964
05029\C,-3.032302856,1.889358521,0.\C,-0.932235718,1.610519409,-3.0223
99902\C,-1.738204956,-0.5912323,3.01335144\C,2.196289062,-1.606628418,
2.306442261\C,3.342437744,0.259857178,-1.174224854\C,1.475402832,1.903
289795,-2.585388184\C,-2.356658936,2.412643433,-1.176361084\C,-2.69650
2686,0.24369812,2.297424316\C,0.933609009,-1.613357544,3.027313232\C,3
.515472412,-0.577789307,0.\C,3.030456543,-1.886123657,0.\C,-1.20043945
3,-3.269088745,-0.694763184\C,-2.140060425,-2.419876099,-1.41809082\C,
-1.47492981,-1.903625488,-2.580856323\C,-0.111785889,-2.422912598,-2.5
93780518\C,0.055511475,-3.266662598,-1.423156738\C,-1.200439453,-3.269
088745,0.694763184\C,-3.053741455,-1.611846924,-0.717041016\C,-1.73820
4956,-0.5912323,-3.01335144\C,0.933609009,-1.613357544,-3.027313232\C,
1.264892578,-3.260665894,-0.727172852\C,-2.140060425,-2.419876099,1.41
809082\C,-3.339981079,-0.256393433,-1.172317505\C,-0.658798218,0.24613
9526,-3.460647583\C,2.196289062,-1.606628418,-2.306442261\C,1.26489257
8,-3.260665894,0.727172852\C,0.055511475,-3.266662598,1.423156738\C,-3
.053741455,-1.611846924,0.717041016\C,-2.696502686,0.24369812,-2.29742
4316\C,0.658218384,-0.248062134,-3.46446228\C,2.356719971,-2.411636353
,-1.176773071\C,-1.47492981,-1.903625488,2.580856323\C,-3.515457153,0.
580841064,0.\C,2.69732666,-0.242263794,-2.300888062\C,2.356719971,-2.4
11636353,1.176773071\C,-0.111785889,-2.422912598,2.593780518\C,-3.3399
81079,-0.256393433,1.172317505\C,-2.194595337,1.606155396,-2.303436279
\C,1.739700317,0.591964722,-3.020294189\N,-0.135650635,-0.070068359,0.
018\H,-0.218200684,0.942474365,-0.174\H,0.417601929,-0.146764893,0.880
609009\H,0.44758667,-0.458764893,-0.736624268\Version=AM64L-G03RevD.0
2\State=2-A\HF=-2327.7134232\MP2=-2335.7536356\RMSD=1.620e-09\Thermal=
0.\PG=C01 [X(C60H3N1)]\@
```


UB3LYP/6-31G(d)

1 2

C	1.203460693	3.269073486	0.696136475
C	-0.053146362	3.268218994	1.425140381
C	0.113449097	2.423355103	2.596405029
C	1.475402832	1.903289795	2.585388184
C	2.143859863	2.421676636	1.420547485
C	1.203460693	3.269073486	-0.696136475
C	-1.263061523	3.260421753	0.727554321
C	-0.932235718	1.610519409	3.022399902
C	1.739700317	0.591964722	3.020294189
C	3.057403564	1.615493774	0.719848633
C	-0.053146362	3.268218994	-1.425140381
C	-2.356658936	2.412643433	1.176361084
C	-0.658798218	0.246139526	3.460647583
C	2.697326660	-0.242263794	2.300888062
C	3.057403564	1.615493774	-0.719848633
C	2.143859863	2.421676636	-1.420547485
C	-1.263061523	3.260421753	-0.727554321
C	-2.194595337	1.606155396	2.303436279
C	0.658218384	-0.248046875	3.464462280
C	3.342437744	0.259857178	1.174224854
C	0.113449097	2.423355103	-2.596405029
C	-3.032302856	1.889358521	0.000000000
C	-0.932235718	1.610519409	-3.022399902
C	-1.738204956	-0.591232300	3.013351440
C	2.196289062	-1.606628418	2.306442261
C	3.342437744	0.259857178	-1.174224854
C	1.475402832	1.903289795	-2.585388184
C	-2.356658936	2.412643433	-1.176361084
C	-2.696502686	0.243698120	2.297424316
C	0.933609009	-1.613357544	3.027313232
C	3.515472412	-0.577789307	0.000000000
C	3.030456543	-1.886123657	0.000000000
C	-1.200439453	-3.269088745	-0.694763184
C	-2.140060425	-2.419876099	-1.418090820
C	-1.474929810	-1.903625488	-2.580856323
C	-0.111785889	-2.422912598	-2.593780518
C	0.055511475	-3.266662598	-1.423156738
C	-1.200439453	-3.269088745	0.694763184
C	-3.053741455	-1.611846924	-0.717041016
C	-1.738204956	-0.591232300	-3.013351440
C	0.933609009	-1.613357544	-3.027313232
C	1.264892578	-3.260665894	-0.727172852
C	-2.140060425	-2.419876099	1.418090820
C	-3.339981079	-0.256393433	-1.172317505
C	-0.658798218	0.246139526	-3.460647583
C	2.196289062	-1.606628418	-2.306442261
C	1.264892578	-3.260665894	0.727172852

C 0.055511475 -3.266662598 1.423156738
 C -3.053741455 -1.611846924 0.717041016
 C -2.696502686 0.243698120 -2.297424316
 C 0.658218384 -0.248062134 -3.464462280
 C 2.356719971 -2.411636353 -1.176773071
 C -1.474929810 -1.903625488 2.580856323
 C -3.515457153 0.580841064 0.000000000
 C 2.697326660 -0.242263794 -2.300888062
 C 2.356719971 -2.411636353 1.176773071
 C -0.111785889 -2.422912598 2.593780518
 C -3.339981079 -0.256393433 1.172317505
 C -2.194595337 1.606155396 -2.303436279
 C 1.739700317 0.591964722 -3.020294189
 N -0.135650635 -0.070068359 0.018000000
 H -0.218200684 0.942474365 -0.174000000
 H 0.417601929 -0.146764893 0.880609009
 H 0.447586670 -0.458764893 -0.736624268

Zero-point correction= 0.410652 (Hartree/Particle)
 Thermal correction to Energy= 0.434381
 Thermal correction to Enthalpy= 0.435326
 Thermal correction to Gibbs Free Energy= 0.364620
 Sum of electronic and zero-point Energies= -2342.043812
 Sum of electronic and thermal Energies= -2342.020083
 Sum of electronic and thermal Enthalpies= -2342.019139
 Sum of electronic and thermal Free Energies= -2342.089845

1\1\FAU-CCC-CCDH158\Freq\UB3LYP/6-31G(d)\C60H3N1(1+,2)\DRAL\15-May-200
 9\0\#P B3LYP/6-31G* FREQ=NORAMAN POP=NONE NAME=DRAL\NH3(+)\@C60\1,2\
 C,1.203460693,3.269073486,0.696136475\C,-0.053146362,3.268218994,1.425
 140381\C,0.113449097,2.423355103,2.596405029\C,1.475402832,1.903289795
 ,2.585388184\C,2.143859863,2.421676636,1.420547485\C,1.203460693,3.269
 073486,-0.696136475\C,-1.263061523,3.260421753,0.727554321\C,-0.932235
 718,1.610519409,3.022399902\C,1.739700317,0.591964722,3.020294189\C,3.
 057403564,1.615493774,0.719848633\C,-0.053146362,3.268218994,-1.425140
 381\C,-2.356658936,2.412643433,1.176361084\C,-0.658798218,0.246139526,
 3.460647583\C,2.69732666,-0.242263794,2.300888062\C,3.057403564,1.6154
 93774,-0.719848633\C,2.143859863,2.421676636,-1.420547485\C,-1.2630615
 23,3.260421753,-0.727554321\C,-2.194595337,1.606155396,2.303436279\C,0
 .658218384,-0.248046875,3.46446228\C,3.342437744,0.259857178,1.1742248
 54\C,0.113449097,2.423355103,-2.596405029\C,-3.032302856,1.889358521,0
 .\C,-0.932235718,1.610519409,-3.022399902\C,-1.738204956,-0.5912323,3.
 01335144\C,2.196289062,-1.606628418,2.306442261\C,3.342437744,0.259857
 178,-1.174224854\C,1.475402832,1.903289795,-2.585388184\C,-2.356658936
 ,2.412643433,-1.176361084\C,-2.696502686,0.24369812,2.297424316\C,0.93
 3609009,-1.613357544,3.027313232\C,3.515472412,-0.577789307,0.\C,3.030
 456543,-1.886123657,0.\C,-1.200439453,-3.269088745,-0.694763184\C,-2.1
 40060425,-2.419876099,-1.41809082\C,-1.47492981,-1.903625488,-2.580856
 323\C,-0.111785889,-2.422912598,-2.593780518\C,0.055511475,-3.26666259
 8,-1.423156738\C,-1.200439453,-3.269088745,0.694763184\C,-3.053741455,

-1.611846924,-0.717041016\C,-1.738204956,-0.5912323,-3.01335144\C,0.93
 3609009,-1.613357544,-3.027313232\C,1.264892578,-3.260665894,-0.727172
 852\C,-2.140060425,-2.419876099,1.41809082\C,-3.339981079,-0.256393433
 ,-1.172317505\C,-0.658798218,0.246139526,-3.460647583\C,2.196289062,-1
 .606628418,-2.306442261\C,1.264892578,-3.260665894,0.727172852\C,0.055
 511475,-3.266662598,1.423156738\C,-3.053741455,-1.611846924,0.71704101
 6\C,-2.696502686,0.24369812,-2.297424316\C,0.658218384,-0.248062134,-3
 .46446228\C,2.356719971,-2.411636353,-1.176773071\C,-1.47492981,-1.903
 625488,2.580856323\C,-3.515457153,0.580841064,0.\C,2.69732666,-0.24226
 3794,-2.300888062\C,2.356719971,-2.411636353,1.176773071\C,-0.11178588
 9,-2.422912598,2.593780518\C,-3.339981079,-0.256393433,1.172317505\C,-
 2.194595337,1.606155396,-2.303436279\C,1.739700317,0.591964722,-3.0202
 94189\N,-0.135650635,-0.070068359,0.018\H,-0.218200684,0.942474365,-0.
 174\H,0.417601929,-0.146764893,0.880609009\H,0.44758667,-0.458764893,-
 0.736624268\\Version=AM64L-G03RevD.02\State=2-A\HF=-2342.4544644\S2=0.
 753944\S2-1=0.\S2A=0.750015\RMSD=9.992e-09\RMSF=1.799e-03\ZeroPoint=0.
 4106523\Thermal=0.4343815\ZPE=257.688232\Dipole=0.0243671,-0.0140608,-
 0.007677\DipoleDeriv=-0.0625959,-0.0876321,-0.1231207,0.0833283,0.0720
 ,0.0059201,0.0093756,-0.0027003,0.0066282\Polar=492.9098861,20.7714697
 ,482.366638,-0.1703661,-0.0906982,507.9741248\PG=C01 [X(C60H3N1)]\NIma
 g=0\\0.47350858,-0.10542387,0.23685341,-0.03626805,-0.08271497,0.67849
 514679,-0.01351960,-0.02382315,-0.14744271,0.10103724,0.25926432\\0.00
 5239,-0.00525359,-0.00970289\\@

10 (NH₃@C₆₀)

MP2/6-31G(d)//B3LYP/6-31G(d)

1\1\FAU-CCC-CCDN092\SP\RMP2-FC\6-31G(d)\C60H3N1\DRAL\12-Aug-2010\0\#P
 RMP2/6-31G* Guess=Read SCF=Tight SCFCyc=1200 Pop=None Geom=AllCheck N
 ame=Dral\NH3@C60_Cs\\0,1\C,1.215907,3.258231,0.697771\C,-0.04295,3.24
 3188,1.42426\C,0.126618,2.405773,2.599136\C,1.490493,1.902513,2.60046\
 C,2.164575,2.429603,1.424646\C,1.215907,3.258231,-0.697771\C,-1.250724
 ,3.226984,0.726302\C,-0.919197,1.588606,3.030104\C,1.755745,0.60187,3.
 032966\C,3.078075,1.634776,0.727639\C,-0.04295,3.243188,-1.42426\C,-2.
 339347,2.376534,1.174992\C,-0.643856,0.234001,3.479625\C,2.703839,-0.2
 2685,2.306115\C,3.078075,1.634776,-0.727639\C,2.164575,2.429603,-1.424
 646\C,-1.250724,3.226984,-0.726302\C,-2.17762,1.574519,2.304287\C,0.66
 6049,-0.249818,3.482599\C,3.352057,0.278615,1.176937\C,0.126618,2.4057
 73,-2.599136\C,-3.012818,1.851252,0.\C,-0.919197,1.588606,-3.030104\C,
 -1.733865,-0.617533,3.031213\C,2.19999,-1.590827,2.305512\C,3.352057,0
 .278615,-1.176937\C,1.490493,1.902513,-2.60046\C,-2.339347,2.376534,-1
 .174992\C,-2.681564,0.211831,2.305081\C,0.940946,-1.605546,3.033574\C,
 3.521602,-0.559088,0.\C,3.03792,-1.869006,0.\C,-1.195149,-3.275458,-0.
 698212\C,-2.143328,-2.446534,-1.425455\C,-1.470905,-1.920638,-2.602731
 \C,-0.105969,-2.424122,-2.602427\C,0.064273,-3.261534,-1.424983\C,-1.1
 95149,-3.275458,0.698212\C,-3.049719,-1.647382,-0.726574\C,-1.733865,-
 0.617533,-3.031213\C,0.940946,-1.605546,-3.033574\C,1.273816,-3.247107

, -0.726895\C, -2.143328, -2.446534, 1.425455\C, -3.32607, -0.293048, -1.175425\C, -0.643856, 0.234001, -3.479625\C, 2.19999, -1.590827, -2.305512\C, 1.273816, -3.247107, 0.726895\C, 0.064273, -3.261534, 1.424983\C, -3.049719, -1.647382, 0.726574\C, -2.681564, 0.211831, -2.305081\C, 0.666049, -0.249818, -3.482599\C, 2.363251, -2.394978, -1.17605\C, -1.470905, -1.920638, 2.602731\C, -3.495839, 0.543736, 0.\C, 2.703839, -0.22685, -2.306115\C, 2.363251, -2.394978, 1.17605\C, -0.105969, -2.424122, 2.602427\C, -3.32607, -0.293048, 1.175425\C, -2.17762, 1.574519, -2.304287\C, 1.755745, 0.60187, -3.032966\N, -0.136194, 0.084179, 0.\H, 0.764222, 0.553672, 0.\H, -0.128856, -0.529643, 0.809194\H, -0.128856, -0.529643, -0.809194\\Version=AM64L-G03RevD.02\State=1-A\HF=-2327.9888862\MP2=-2336.0085501\RMSD=3.665e-09\Thermal=0.\PG=CS [SG(C4H1N1),X(C56H2)]\\@

B3LYP/6-31G(d)

Zero-point correction=	0.412597 (Hartree/Particle)
Thermal correction to Energy=	0.436770
Thermal correction to Enthalpy=	0.437714
Thermal correction to Gibbs Free Energy=	0.366543
Sum of electronic and zero-point Energies=	-2342.304959
Sum of electronic and thermal Energies=	-2342.280786
Sum of electronic and thermal Enthalpies=	-2342.279842
Sum of electronic and thermal Free Energies=	-2342.351013

1\1\FAU-CCC-CCDH161\Freq\RB3LYP\6-31G(d)\C60H3N1\DRAL\27-Nov-2008\0\\#
P B3LYP/6-31G(d) Freq=NoRaman Name=Dral Pop=None\\NH3@C60_Cs\\0,1\C,1.
215907,3.258231,0.697771\C, -0.04295, 3.243188, 1.42426\C, 0.126618, 2.405773, 2.599136\C, 1.490493, 1.902513, 2.60046\C, 2.164575, 2.429603, 1.424646\C, 1.215907, 3.258231, -0.697771\C, -1.250724, 3.226984, 0.726302\C, -0.919197, 1.588606, 3.030104\C, 1.755745, 0.60187, 3.032966\C, 3.078075, 1.634776, 0.727639\C, -0.04295, 3.243188, -1.42426\C, -2.339347, 2.376534, 1.174992\C, -0.643856, 0.234001, 3.479625\C, 2.703839, -0.22685, 2.306115\C, 3.078075, 1.634776, -0.727639\C, 2.164575, 2.429603, -1.424646\C, -1.250724, 3.226984, -0.726302\C, -2.17762, 1.574519, 2.304287\C, 0.666049, -0.249818, 3.482599\C, 3.352057, 0.278615, 1.176937\C, 0.126618, 2.405773, -2.599136\C, -3.012818, 1.851252, 0.\C, -0.919197, 1.588606, -3.030104\C, -1.733865, -0.617533, 3.031213\C, 2.19999, -1.590827, 2.305512\C, 3.352057, 0.278615, -1.176937\C, 1.490493, 1.902513, -2.60046\C, -2.339347, 2.376534, -1.174992\C, -2.681564, 0.211831, 2.305081\C, 0.940946, -1.605546, 3.033574\C, 3.521602, -0.559088, 0.\C, 3.03792, -1.869006, 0.\C, -1.195149, -3.275458, -0.698212\C, -2.143328, -2.446534, -1.425455\C, -1.470905, -1.920638, -2.602731\C, -0.105969, -2.424122, -2.602427\C, 0.064273, -3.261534, -1.424983\C, -1.195149, -3.275458, 0.698212\C, -3.049719, -1.647382, -0.726574\C, -1.733865, -0.617533, -3.031213\C, 0.940946, -1.605546, -3.033574\C, 1.273816, -3.247107, -0.726895\C, -2.143328, -2.446534, 1.425455\C, -3.32607, -0.293048, -1.175425\C, -0.643856, 0.234001, -3.479625\C, 2.19999, -1.590827, -2.305512\C, 1.273816, -3.247107, 0.726895\C, 0.064273, -3.261534, 1.424983\C, -3.049719, -1.647382, 0.726574\C, -2.681564, 0.211831, -2.305081\C, 0.666049, -0.249818, -3.482599\C, 2.363251, -2.394978, -1

.17605\C,-1.470905,-1.920638,2.602731\C,-3.495839,0.543736,0.\C,2.7038
 39,-0.22685,-2.306115\C,2.363251,-2.394978,1.17605\C,-0.105969,-2.4241
 22,2.602427\C,-3.32607,-0.293048,1.175425\C,-2.17762,1.574519,-2.30428
 7\C,1.755745,0.60187,-3.032966\N,-0.136194,0.084179,0.\H,0.764222,0.55
 3672,0.\H,-0.128856,-0.529643,0.809194\H,-0.128856,-0.529643,-0.809194
 \\\Version=AM64L-G03RevD.02\State=1-A\HF=-2342.7175559\RMSD=1.770e-09\
 RMSF=1.657e-04\ZeroPoint=0.4125973\Thermal=0.4367697\ZPE=258.9087087\
 ipole=0.0985173,-0.079552,0.\DipoleDeriv=0.0819561,-0.0348932,-0.05056
 \Polar=470.4700173,0.3683133,470.5230196,0.,0.,470.8208647\PG=CS [SG(C
 4H1N1),X(C56H2)]\NImag=0\0.48261548,-0.10543527,0.23424846,-0.0319962
 15,-0.02553129,-0.02646227,-0.00168013,0.19439012,0.32047497\|-0.00002
 ,-0.00030934,0.00000646,-0.00036191,-0.00030934,-0.00000646\\\@

11⁺ (NH₃@C₆₀H⁺)

MP2/6-31G(d)//B3LYP/6-31G(d)

1\1\FAU-CCC-CCDN082\SP\RMP2-FC\6-31G(d)\C60H4N1(1+)\DRAL\13-Aug-2010\0
 \#P RMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Pop=No
 ne Name=Dral\NH3@C60H+\1,1\C,0,1.2266546595,3.272267957,0.6981432932
 \C,0,-0.0334396464,3.2568295168,1.4168100736\C,0,0.1307811492,2.398769
 8112,2.5854139074\C,0,1.4923045153,1.9073090872,2.597315882\C,0,2.1709
 684221,2.4381744242,1.4254416908\C,0,1.2266546595,3.272267957,-0.69814
 32932\C,0,-1.2376988679,3.25795934,0.7243520798\C,0,-0.9168464789,1.58
 16988235,3.0228831867\C,0,1.7512015789,0.6012518849,3.023744394\C,0,3.
 0774985555,1.6403688796,0.7276069559\C,0,-0.0334396464,3.2568295168,-1
 .4168100736\C,0,-2.3271743507,2.3919943037,1.1629858338\C,0,-0.6429653
 063,0.2286657973,3.4749473391\C,0,2.7015140342,-0.2241615546,2.3040783
 884\C,0,3.0774985555,1.6403688796,-0.7276069559\C,0,2.1709684221,2.438
 1744242,-1.4254416908\C,0,-1.2376988679,3.25795934,-0.7243520798\C,0,-
 2.1555271421,1.5562848938,2.2799038297\C,0,0.6632638551,-0.2532192382,
 3.4801529544\C,0,3.3481946408,0.2820204112,1.174876936\C,0,0.130781149
 2,2.3987698112,-2.5854139074\C,0,-2.9561202947,1.8680613051,0.\C,0,-0.
 9168464789,1.5816988235,-3.0228831867\C,0,-1.7320352112,-0.6275008646,
 3.0259536316\C,0,2.1958841261,-1.5891104522,2.3034411702\C,0,3.3481946
 408,0.2820204112,-1.174876936\C,0,1.4923045153,1.9073090872,-2.5973158
 82\C,0,-2.3271743507,2.3919943037,-1.1629858338\C,0,-2.6821907465,0.19
 12868375,2.2998404153\C,0,0.9418216409,-1.6102445275,3.0355563677\C,0,
 3.5173710598,-0.5537308293,0.\C,0,3.0320167676,-1.865471309,0.\C,0,-1.
 1918555979,-3.2708053377,-0.7008503812\C,0,-2.1354634865,-2.4502784691
 ,-1.4297993512\C,0,-1.4686144306,-1.9318348315,-2.6064107526\C,0,-0.10
 14761228,-2.4331516931,-2.606911692\C,0,0.0680064335,-3.2666216292,-1.
 4281298377\C,0,-1.1918555979,-3.2708053377,0.7008503812\C,0,-3.0416900
 695,-1.6380001133,-0.7281341359\C,0,-1.7320352112,-0.6275008646,-3.025
 9536316\C,0,0.9418216409,-1.6102445275,-3.0355563677\C,0,1.2748403138,
 -3.2488889229,-0.7277300477\C,0,-2.1354634865,-2.4502784691,1.42979935
 12\C,0,-3.3303805774,-0.3150599889,-1.1871124852\C,0,-0.6429653063,0.2

286657973,-3.4749473391\C,0,2.1958841261,-1.5891104522,-2.3034411702\C,0,1.2748403138,-3.2488889229,0.7277300477\C,0,0.0680064335,-3.2666216292,1.4281298377\C,0,-3.0416900695,-1.6380001133,0.7281341359\C,0,-2.6821907465,0.1912868375,-2.2998404153\C,0,0.6632638551,-0.2532192382,-3.4801529544\C,0,2.3618198948,-2.3952976129,-1.1746526794\C,0,-1.4686144306,-1.9318348315,2.6064107526\C,0,-3.7198420531,0.5698874233,0.\C,0,2.7015140342,-0.2241615546,-2.3040783884\C,0,2.3618198948,-2.3952976129,1.1746526794\C,0,-0.1014761228,-2.4331516931,2.606911692\C,0,-3.3303805774,-0.3150599889,1.1871124852\C,0,-2.1555271421,1.5562848938,-2.2799038297\C,0,1.7512015789,0.6012518849,-3.023744394\N,0,-0.1434345003,0.0808186539,0.\H,0,0.7563123245,0.5534281541,0.\H,0,-0.1245861979,-0.5388051715,0.8053510244\H,0,-0.1245861979,-0.5388051715,-0.8053510244\H,0,-4.8040200716,0.7870594145,0.\Version=AM64L-G03RevD.02\State=1-A'\HF=-2328.3381994\MP2=-2336.3352413\RMSD=1.998e-09\Thermal=0.\PG=CS [S G(C4H2N1),X(C56H2)]\@

B3LYP/6-31G(d)

Zero-point correction=	0.424164 (Hartree/Particle)
Thermal correction to Energy=	0.448325
Thermal correction to Enthalpy=	0.449269
Thermal correction to Gibbs Free Energy=	0.378306
Sum of electronic and zero-point Energies=	-2342.644188
Sum of electronic and thermal Energies=	-2342.620027
Sum of electronic and thermal Enthalpies=	-2342.619083
Sum of electronic and thermal Free Energies=	-2342.690046

1\1\FAU-CCC-CCDH152\Freq\RB3LYP\6-31G(d)\C60H4N1(1+)\DRAL\17-Nov-2008\0\#P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq\NH3@C60H+\1,1\C,1.2266546595,3.272267957,0.6981432932\C,-0.0334396464,3.2568295168,1.4168100736\C,0.1307811492,2.3987698112,2.5854139074\C,1.4923045153,1.9073090872,2.597315882\C,2.1709684221,2.4381744242,1.4254416908\C,1.2266546595,3.272267957,-0.6981432932\C,-1.2376988679,3.25795934,0.7243520798\C,-0.9168464789,1.5816988235,3.0228831867\C,1.7512015789,0.6012518849,3.023744394\C,3.0774985555,1.6403688796,0.7276069559\C,-0.0334396464,3.2568295168,-1.4168100736\C,-2.3271743507,2.3919943037,1.1629858338\C,-0.6429653063,0.2286657973,3.4749473391\C,2.7015140342,-0.2241615546,2.3040783884\C,3.0774985555,1.6403688796,-0.7276069559\C,2.1709684221,2.4381744242,-1.4254416908\C,-1.2376988679,3.25795934,-0.7243520798\C,-2.1555271421,1.5562848938,2.2799038297\C,0.6632638551,-0.2532192382,3.4801529544\C,3.3481946408,0.2820204112,1.174876936\C,0.1307811492,2.3987698112,-2.5854139074\C,-2.9561202947,1.8680613051,0.\C,-0.9168464789,1.5816988235,-3.0228831867\C,-1.7320352112,-0.6275008646,3.0259536316\C,2.1958841261,-1.5891104522,2.3034411702\C,3.3481946408,0.2820204112,-1.174876936\C,1.4923045153,1.9073090872,-2.597315882\C,-2.3271743507,2.3919943037,-1.1629858338\C,-2.6821907465,0.1912868375,2.2998404153\C,0.9418216409,-1.6102445275,3.0355563677\C,3.5173710598,-0.5537308293,0.\C,3.0320167676,-1.865471309,0.\C,-1.191855597

9,-3.2708053377,-0.7008503812\C,-2.1354634865,-2.4502784691,-1.4297993
 512\C,-1.4686144306,-1.9318348315,-2.6064107526\C,-0.1014761228,-2.433
 1516931,-2.606911692\C,0.0680064335,-3.2666216292,-1.4281298377\C,-1.1
 918555979,-3.2708053377,0.7008503812\C,-3.0416900695,-1.6380001133,-0.
 7281341359\C,-1.7320352112,-0.6275008646,-3.0259536316\C,0.9418216409,
 -1.6102445275,-3.0355563677\C,1.2748403138,-3.2488889229,-0.7277300477
 \C,-2.1354634865,-2.4502784691,1.4297993512\C,-3.3303805774,-0.3150599
 889,-1.1871124852\C,-0.6429653063,0.2286657973,-3.4749473391\C,2.19588
 41261,-1.5891104522,-2.3034411702\C,1.2748403138,-3.2488889229,0.72773
 00477\C,0.0680064335,-3.2666216292,1.4281298377\C,-3.0416900695,-1.638
 0001133,0.7281341359\C,-2.6821907465,0.1912868375,-2.2998404153\C,0.66
 32638551,-0.2532192382,-3.4801529544\C,2.3618198948,-2.3952976129,-1.1
 746526794\C,-1.4686144306,-1.9318348315,2.6064107526\C,-3.7198420531,0
 .5698874233,0.\C,2.7015140342,-0.2241615546,-2.3040783884\C,2.36181989
 48,-2.3952976129,1.1746526794\C,-0.1014761228,-2.4331516931,2.60691169
 2\C,-3.3303805774,-0.3150599889,1.1871124852\C,-2.1555271421,1.5562848
 938,-2.2799038297\C,1.7512015789,0.6012518849,-3.023744394\N,-0.143434
 5003,0.0808186539,0.\H,0.7563123245,0.5534281541,0.\H,-0.1245861979,-0
 .5388051715,0.8053510244\H,-0.1245861979,-0.5388051715,-0.8053510244\H
 ,-4.8040200716,0.7870594145,0.\Version=AM64L-G03RevD.02\State=1-A\HF
 =-2343.0683518\RMSD=9.982e-09\RMSF=1.530e-04\ZeroPoint=0.4241639\Therm
 al=0.4483247\ZPE=266.1668594\Dipole=-1.2094384,0.3908325,0.\DipoleDeri
 10641,0.,-0.0172741,0.1018198,0.,0.,0.097173\Polar=492.6321455,-5.0
 128233,475.2949856,0.,0.,477.6880091\PG=CS [SG(C4H2N1),X(C56H2)]\NImag
 =0\0.48715209,-0.10474548,0.23816517,-0.03206965,-0.08471080,0.671773
 0001194,0.,0.,0.04229978\0.00003973,0.00002485,0.00000913,-0.00005325
 .00000035,-0.00000237,0.\@

12⁺ (NH₄⁺@C₆₀)

UB3LYP/6-311+G(d,p)//UB3LYP/6-31G(d)

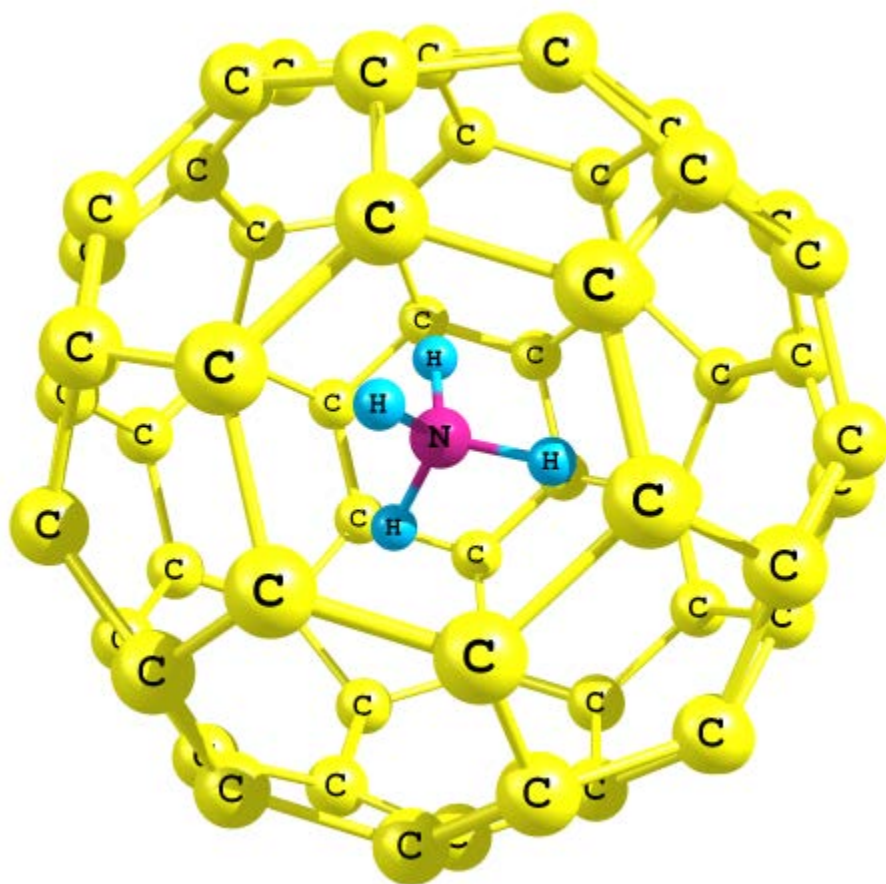
1\1\GINC-I01R11C01S09\SP\RB3LYP\6-311+G(d,p)\C60H4N1(1+)\DRAL\23-Jan-2
 013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Curren
 t Name=DrAl GFINPUT GFPRINT\NH4(+)@C60 singlet\1,1\C,0,-1.47092,2.36
 026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-0.030
 85\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,0,-1.
 58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2.9122
 8,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49338\C,0
 ,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792,2.81
 584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26303\C
 ,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2.4584
 7,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-1.685
 39\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C,0,-2
 .04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914,2.01
 942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3.3925
 3\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0,2.04
 112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.24036,-0
 .92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\C,0,0

.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Version=EM64L-G09RevB.01\State=1-A\HF=-2343.5339491\RMSD=9.751e-09\Dipole=-0.0062402,0.0122575,-0.0019111\Quadrupole=0.0122356,0.0054647,-0.0177003,0.0151352,-0.0242458,0.0257308\PG=C01 [X(C60H4N1)]\\@

MP2/6-31G(d)//B3LYP/6-31G(d)

1\1\FAU-CCC-CCDN090\SP\RMP2-FC\6-31G(d)\C60H4N1(1+)\DRAL\13-Aug-2010\0\\#P RMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Pop=No ne Name=Dral\NH4(+)\@C60\1,1\C,-1.47092,2.36026,-2.21132\C,-2.26764,2.54384,-1.00861\C,-1.44943,3.24567,-0.03085\C,-0.14616,3.49559,-0.62985\C,-0.16013,2.94835,-1.97762\C,-1.58699,1.18077,-2.9516\C,-3.14793,1.54092,-0.59558\C,-1.5423,2.91228,1.32213\C,1.01129,3.40378,0.14713\C,0.98389,2.33258,-2.49338\C,-2.50363,0.136,-2.5224\C,-3.24155,1.19384,0.81528\C,-0.33792,2.81584,2.13264\C,2.20241,2.76273,-0.39084\C,0.86246,1.1031,-3.26303\C,-0.39619,0.53938,-3.48827\C,-3.26817,0.31279,-1.36713\C,-2.45847,1.8685,1.75496\C,0.91153,3.0558,1.55615\C,2.19037,2.23878,-1.68539\C,-1.87907,-1.15002,-2.79309\C,-3.42119,-0.24787,0.91414\C,-2.04411,-2.20915,-1.89888\C,-0.51038,1.71405,3.06728\C,2.83914,2.01942,0.68559\C,1.99394,0.25073,-2.93282\C,-0.57698,-0.90076,-3.39253\C,-3.43874,-0.79105,-0.43497\C,-1.82072,1.12718,2.83313\C,2.04112,2.19998,1.88895\C,2.81351,0.9516,-1.95576\C,3.42754,0.24036,-0.92223\C,1.47035,-2.36472,2.20738\C,0.16017,-2.95152,1.97305\C,0.14485,-3.49559,0.62375\C,1.44702,-3.24425,0.02499\C,2.26726,-2.54585,1.00381\C,1.5865,-1.18768,2.95076\C,-0.98247,-2.33746,2.48964\C,-1.01099,-3.40569,-0.15561\C,1.54102,-2.91353,-1.32964\C,3.14793,-1.54395,0.58797\C,0.39537,-0.54762,3.48827\C,-2.1862,-2.24342,1.67863\C,-0.91371,-3.06261,-1.56635\C,2.45935,-1.87144,-1.76247\C,3.26778,-0.31754,1.36087\C,2.50264,-0.1441,2.51717\C,-0.86201,-1.11086,3.26266\C,-2.201,-2.76662,0.38316\C,0.33675,-2.82159,-2.14166\C,3.24605,-1.19969,-0.82289\C,0.57367,0.89287,3.38768\C,-2.80771,-0.95634,1.94885\C,1.8208,-1.13225,-2.84073\C,3.43874,0.78506,0.42653\C,1.87537,1.14124,2.78554\C,-1.99051,-0.25568,2.92744\C,-2.83978,-2.02647,-0.69466\C,0.50946,-1.71938,-3.07497\N,-0.00657,0.02455,-0.00859\H,-0.97351,0.09818,0.38126\H,0.65589,0.54851,0.59986\H,0.01,0.43145,-0.95482\H,0.27297,-0.97749,-0.06544\\Version=AM64L-G03RevD.02\State=1-A\HF=-2328.3509855\MP2=-2336.3667368\RMSD=3.811e-09\Thermal=0.PG=C01 [X(C60H4N1)]\\@

B3LYP/6-31G(d)



1 1

C	-1.470920000	2.360260000	-2.211320000
C	-2.267640000	2.543840000	-1.008610000
C	-1.449430000	3.245670000	-0.030850000
C	-0.146160000	3.495590000	-0.629850000
C	-0.160130000	2.948350000	-1.977620000
C	-1.586990000	1.180770000	-2.951600000
C	-3.147930000	1.540920000	-0.595580000
C	-1.542300000	2.912280000	1.322130000
C	1.011290000	3.403780000	0.147130000
C	0.983890000	2.332580000	-2.493380000
C	-2.503630000	0.136000000	-2.522400000
C	-3.241550000	1.193840000	0.815280000
C	-0.337920000	2.815840000	2.132640000
C	2.202410000	2.762730000	-0.390840000
C	0.862460000	1.103100000	-3.263030000
C	-0.396190000	0.539380000	-3.488270000
C	-3.268170000	0.312790000	-1.367130000
C	-2.458470000	1.868500000	1.754960000
C	0.911530000	3.055800000	1.556150000
C	2.190370000	2.238780000	-1.685390000

C	-1.879070000	-1.150020000	-2.793090000
C	-3.421190000	-0.247870000	0.914140000
C	-2.044110000	-2.209150000	-1.898880000
C	-0.510380000	1.714050000	3.067280000
C	2.839140000	2.019420000	0.685590000
C	1.993940000	0.250730000	-2.932820000
C	-0.576980000	-0.900760000	-3.392530000
C	-3.438740000	-0.791050000	-0.434970000
C	-1.820720000	1.127180000	2.833130000
C	2.041120000	2.199980000	1.888950000
C	2.813510000	0.951600000	-1.955760000
C	3.427540000	0.240360000	-0.922230000
C	1.470350000	-2.364720000	2.207380000
C	0.160170000	-2.951520000	1.973050000
C	0.144850000	-3.495590000	0.623750000
C	1.447020000	-3.244250000	0.024990000
C	2.267260000	-2.545850000	1.003810000
C	1.586500000	-1.187680000	2.950760000
C	-0.982470000	-2.337460000	2.489640000
C	-1.010990000	-3.405690000	-0.155610000
C	1.541020000	-2.913530000	-1.329640000
C	3.147930000	-1.543950000	0.587970000
C	0.395370000	-0.547620000	3.488270000
C	-2.186200000	-2.243420000	1.678630000
C	-0.913710000	-3.062610000	-1.566350000
C	2.459350000	-1.871440000	-1.762470000
C	3.267780000	-0.317540000	1.360870000
C	2.502640000	-0.144100000	2.517170000
C	-0.862010000	-1.110860000	3.262660000
C	-2.201000000	-2.766620000	0.383160000
C	0.336750000	-2.821590000	-2.141660000
C	3.246050000	-1.199690000	-0.822890000
C	0.573670000	0.892870000	3.387680000
C	-2.807710000	-0.956340000	1.948850000
C	1.820800000	-1.132250000	-2.840730000
C	3.438740000	0.785060000	0.426530000
C	1.875370000	1.141240000	2.785540000
C	-1.990510000	-0.255680000	2.927440000
C	-2.839780000	-2.026470000	-0.694660000
C	0.509460000	-1.719380000	-3.074970000
N	-0.006570000	0.024550000	-0.008590000
H	-0.973510000	0.098180000	0.381260000
H	0.655890000	0.548510000	0.599860000
H	0.010000000	0.431450000	-0.954820000
H	0.272970000	-0.977490000	-0.065440000

Zero-point correction=	0.427258 (Hartree/Particle)
Thermal correction to Energy=	0.450995
Thermal correction to Enthalpy=	0.451940
Thermal correction to Gibbs Free Energy=	0.381297

Sum of electronic and zero-point Energies= -2342.654952
 Sum of electronic and thermal Energies= -2342.631215
 Sum of electronic and thermal Enthalpies= -2342.630271
 Sum of electronic and thermal Free Energies= -2342.700913

1\1\FAU-CCC-CCDH155\Freq\RB3LYP\6-31G(d)\C60H4N1(1+)\DRAL\22-May-2009\
 0\#P B3LYP/6-31G* FREQ=NORAMAN NAME=DRAL\NH4(+)\@C60\1,1\C,-1.47092,
 2.36026,-2.21132\C,-2.26764,2.54384,-1.00861\C,-1.44943,3.24567,-0.030
 85\C,-0.14616,3.49559,-0.62985\C,-0.16013,2.94835,-1.97762\C,-1.58699,
 1.18077,-2.9516\C,-3.14793,1.54092,-0.59558\C,-1.5423,2.91228,1.32213\
 C,1.01129,3.40378,0.14713\C,0.98389,2.33258,-2.49338\C,-2.50363,0.136,
 -2.5224\C,-3.24155,1.19384,0.81528\C,-0.33792,2.81584,2.13264\C,2.2024
 1,2.76273,-0.39084\C,0.86246,1.1031,-3.26303\C,-0.39619,0.53938,-3.488
 27\C,-3.26817,0.31279,-1.36713\C,-2.45847,1.8685,1.75496\C,0.91153,3.0
 558,1.55615\C,2.19037,2.23878,-1.68539\C,-1.87907,-1.15002,-2.79309\C,
 -3.42119,-0.24787,0.91414\C,-2.04411,-2.20915,-1.89888\C,-0.51038,1.71
 405,3.06728\C,2.83914,2.01942,0.68559\C,1.99394,0.25073,-2.93282\C,-0.
 57698,-0.90076,-3.39253\C,-3.43874,-0.79105,-0.43497\C,-1.82072,1.1271
 8,2.83313\C,2.04112,2.19998,1.88895\C,2.81351,0.9516,-1.95576\C,3.4275
 4,0.24036,-0.92223\C,1.47035,-2.36472,2.20738\C,0.16017,-2.95152,1.973
 05\C,0.14485,-3.49559,0.62375\C,1.44702,-3.24425,0.02499\C,2.26726,-2.
 54585,1.00381\C,1.5865,-1.18768,2.95076\C,-0.98247,-2.33746,2.48964\C,
 -1.01099,-3.40569,-0.15561\C,1.54102,-2.91353,-1.32964\C,3.14793,-1.54
 395,0.58797\C,0.39537,-0.54762,3.48827\C,-2.1862,-2.24342,1.67863\C,-0
 .91371,-3.06261,-1.56635\C,2.45935,-1.87144,-1.76247\C,3.26778,-0.3175
 4,1.36087\C,2.50264,-0.1441,2.51717\C,-0.86201,-1.11086,3.26266\C,-2.2
 01,-2.76662,0.38316\C,0.33675,-2.82159,-2.14166\C,3.24605,-1.19969,-0.
 82289\C,0.57367,0.89287,3.38768\C,-2.80771,-0.95634,1.94885\C,1.8208,-
 1.13225,-2.84073\C,3.43874,0.78506,0.42653\C,1.87537,1.14124,2.78554\C
 ,-1.99051,-0.25568,2.92744\C,-2.83978,-2.02647,-0.69466\C,0.50946,-1.7
 1938,-3.07497\N,-0.00657,0.02455,-0.00859\H,-0.97351,0.09818,0.38126\H
 ,0.65589,0.54851,0.59986\H,0.01,0.43145,-0.95482\H,0.27297,-0.97749,-0
 .06544\Version=AM64L-G03RevD.02\State=1-A\HF=-2343.0822103\RMSD=2.872
 e-09\RMSF=1.447e-03\ZeroPoint=0.4272581\Thermal=0.4509954\ZPE=268.1085
 042\Dipole=-0.0045998,0.0089886,-0.0013888\DipoleDeriv=0.0822566,0.036
 6143,0.0044776,0.0680776\Polar=468.9633712,0.0230664,468.944929,-0.033
 4295,0.0646758,468.8025216\PG=C01 [X(C60H4N1)]\NImag=0\0.46662618,0.1
 2492,0.03391651,0.00826033,-0.00440230,0.01598502,0.06099239\0.000262
 040729,0.00010175,-0.00064400,0.00240061,-0.00939463,-0.00174381\ \@

13 (NH₄@C₆₀)

*UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12**

1\1\GINC-I01R12C01S09\SP\UB3LYP\6-311+G(d,p)\C60H4N1(2)\DRAL\27-Jan-20
 13\0\#P B3LYP/6-311+G(d,p) SCF=XQC Pop=(NBO,Full) Density=Current Nam
 e=DrAl GFINPUT GFPRINT\NH4(+)\@C60(-) doublet\0,2\C,0,-1.47092,2.3602
 6,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-0.03085
 \C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,0,-1.58

699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2.91228,
 1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49338\C,0,-
 2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792,2.8158
 4,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26303\C,0
 ,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2.45847,
 1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-1.68539
 \C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C,0,-2.0
 4411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914,2.0194
 2,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3.39253\
 C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0,2.0411
 2,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.24036,-0.9
 2223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\C,0,0.1
 4485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,-2.5458
 5,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.48964\C,
 0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,3.14793
 ,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.24342,1.
 67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76247\C,0
 ,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,-1.
 11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.1416
 6\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0,-2.807
 71,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.78506,0
 .42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92744\C,0,-
 2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.00657,0
 .02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54851,0.599
 86\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Version=EM
 64L-G09RevB.01\State=2-A\HF=-2343.7438397\S2=0.754492\S2-1=0.\S2A=0.75
 0019\RMSD=9.616e-06\Dipole=-0.0087431,0.0079689,-0.0003257\Quadrupole=
 1.3289542,-0.8832279,-0.4457263,-0.2703233,1.0240499,-0.1167737\PG=C01
 [X(C60H4N1)]\@

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN086\SP\ROMP2-FC\6-31G(d)\C60H4N1(2)\DRAL\01-Feb-2010\0
 \#P ROMP2/6-31G* SCF=Tight Geom=AllCheck Guess=Read SCFCyc=600 Pop=No
 ne Name=Dral\NH4@C60 DFT SP\0,2\C,0,2.377914429,-2.114059448,-1.5788
 57422\C,0,1.199462891,-2.320999146,-2.412017822\C,0,1.007196167,-1.139
 49585,-3.220849731\C,0,2.056015015,-0.191223145,-2.889627197\C,0,2.915
 466309,-0.796035767,-1.878540039\C,0,2.410272339,-2.597747803,-0.26867
 6758\C,0,0.097970703,-3.012313843,-1.88142395\C,0,-0.29914856,-0.66719
 0552,-3.480819702\C,0,1.782867432,1.178192139,-2.830780029\C,0,3.46118
 1641,-0.009689331,-0.857696533\C,0,1.266397217,-3.316680908,0.27784729
 \C,0,-1.253601074,-2.519638062,-2.148178101\C,0,-0.583953857,0.7459869
 38,-3.420776367\C,0,2.352401733,1.99220874,-1.774917603\C,0,3.49252319
 3,-0.51399231,0.506546021\C,0,2.976776123,-1.782485962,0.792984009\C,0
 ,0.129464844,-3.51399231,-0.527908325\C,0,-1.440603516,-1.375457764,-2
 .928512573\C,0,0.4324646,1.663833618,-3.10333252\C,0,3.177642822,1.414
 825439,-0.801757812\C,0,1.122827271,-2.944976807,1.665267944\C,0,-2.05
 8929443,-2.730316162,-0.957244873\C,0,-0.16305542,-2.778634766,2.22557
 0679\C,0,-1.913650513,0.919509888,-2.840164185\C,0,1.343054077,2.96983

9355,-1.384811401\C,0,3.22869873,0.600997925,1.401550293\C,0,2.1716766
 36,-1.995584229,1.988006592\C,0,-1.201248169,-3.33241272,0.050170898\C
 ,0,-2.45211792,-0.392751953,-2.545288086\C,0,0.167205811,2.772369385,-
 2.216094971\C,0,3.033599854,1.790481567,0.592422485\C,0,2.066299438,2.
 737091064,0.965682983\C,0,-2.37912915,2.117196777,1.583206177\C,0,-2.9
 13955688,0.799981812,1.883499146\C,0,-2.053314209,0.193567017,2.890060
 425\C,0,-1.000350952,1.138839722,3.219116211\C,0,-1.195617676,2.324060
 181,2.413543701\C,0,-2.409890869,2.601129272,0.274719238\C,0,-3.460906
 982,0.012298584,0.864608765\C,0,-1.777801514,-1.178268433,2.836364746\
 C,0,0.302398682,0.669732788,3.480819702\C,0,-0.089859009,3.012268066,1
 .886428833\C,0,-2.978134155,1.784210205,-0.786224365\C,0,-3.174850464,
 -1.412109375,0.809936523\C,0,-0.428115845,-1.666137695,3.107107422\C,0
 ,1.447219849,1.377624512,2.932052612\C,0,-0.122116089,3.51399231,0.533
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 01 [X(C60H4N1)]\@

UB3LYP/6-31G(d)

%chk=nh4atc60_freq_30
 #P B3LYP FREQ=readfc geom=allcheck guess=read pop=none NAME=DRAL
 NH4(+)@C60(dot-)

0 2

C	2.377914429	-2.114059448	-1.578857422
C	1.199462891	-2.320999146	-2.412017822
C	1.007196167	-1.139495850	-3.220849731
C	2.056015015	-0.191223145	-2.889627197
C	2.915466309	-0.796035767	-1.878540039
C	2.410272339	-2.597747803	-0.268676758
C	0.097970703	-3.012313843	-1.881423950
C	-0.299148560	-0.667190552	-3.480819702
C	1.782867432	1.178192139	-2.830780029
C	3.461181641	-0.009689331	-0.857696533
C	1.266397217	-3.316680908	0.277847290
C	-1.253601074	-2.519638062	-2.148178101
C	-0.583953857	0.745986938	-3.420776367
C	2.352401733	1.992208740	-1.774917603

C	3.492523193	-0.513992310	0.506546021
C	2.976776123	-1.782485962	0.792984009
C	0.129464844	-3.513992310	-0.527908325
C	-1.440603516	-1.375457764	-2.928512573
C	0.432464600	1.663833618	-3.103332520
C	3.177642822	1.414825439	-0.801757812
C	1.122827271	-2.944976807	1.665267944
C	-2.058929443	-2.730316162	-0.957244873
C	-0.163055420	-2.778634766	2.225570679
C	-1.913650513	0.919509888	-2.840164185
C	1.343054077	2.969839355	-1.384811401
C	3.228698730	0.600997925	1.401550293
C	2.171676636	-1.995584229	1.988006592
C	-1.201248169	-3.332412720	0.050170898
C	-2.452117920	-0.392751953	-2.545288086
C	0.167205811	2.772369385	-2.216094971
C	3.033599854	1.790481567	0.592422485
C	2.066299438	2.737091064	0.965682983
C	-2.379129150	2.117196777	1.583206177
C	-2.913955688	0.799981812	1.883499146
C	-2.053314209	0.193567017	2.890060425
C	-1.000350952	1.138839722	3.219116211
C	-1.195617676	2.324060181	2.413543701
C	-2.409890869	2.601129272	0.274719238
C	-3.460906982	0.012298584	0.864608765
C	-1.777801514	-1.178268433	2.836364746
C	0.302398682	0.669732788	3.480819702
C	-0.089859009	3.012268066	1.886428833
C	-2.978134155	1.784210205	-0.786224365
C	-3.174850464	-1.412109375	0.809936523
C	-0.428115845	-1.666137695	3.107107422
C	1.447219849	1.377624512	2.932052612
C	-0.122116089	3.513992310	0.533721924
C	-1.260635376	3.315551758	-0.269226074
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C	-2.344640991	-1.990484497	1.780456543
C	0.586944580	-0.747360229	3.420889160
C	1.259140015	2.522567749	2.153732300
C	-2.170043945	1.990753174	-1.979934692
C	-3.029739380	-1.785614014	-0.584609985
C	2.453018188	0.396850586	2.549484253
C	1.206680298	3.334167480	-0.042587280
C	-1.117126465	2.942153931	-1.656280518
C	-3.225906372	-0.597015381	-1.394134521
C	-1.337118408	-2.971328735	1.392059326
C	1.918802002	-0.919586182	2.844940186
N	0.013695801	-0.014621216	-0.109362427
H	-0.607963745	-0.752476074	-0.488592773
H	-0.142662231	0.872843506	-0.637509399
H	0.997161255	-0.327695679	-0.229084473

H -0.180686157 0.135174194 0.903567505

SCF Done: E(UB+HF-LYP) = -2343.280582560 A.U. after 29 cycles

Zero-point correction= 0.420997 (Hartree/Particle)
 Thermal correction to Energy= 0.446004
 Thermal correction to Enthalpy= 0.446948
 Thermal correction to Gibbs Free Energy= 0.372612
 Sum of electronic and zero-point Energies= -2342.859586
 Sum of electronic and thermal Energies= -2342.834579
 Sum of electronic and thermal Enthalpies= -2342.833634
 Sum of electronic and thermal Free Energies= -2342.907970

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NBO Analysis PCM

Summary of Natural Population Analysis:

Natural Population
Natural -----

Atom	No	Charge	Core	Valence	Rydberg	Total

C	1	-0.01122	1.99872	3.99786	0.01465	6.01122
C	2	-0.01795	1.99871	4.00446	0.01477	6.01795
C	3	-0.02837	1.99871	4.01479	0.01487	6.02837
C	4	-0.00489	1.99872	3.99153	0.01465	6.00489
C	5	-0.02019	1.99871	4.00672	0.01476	6.02019
C	6	-0.00878	1.99872	3.99548	0.01458	6.00878
C	7	-0.02560	1.99871	4.01211	0.01478	6.02560
C	8	-0.03322	1.99871	4.01959	0.01492	6.03322
C	9	-0.01000	1.99872	3.99667	0.01461	6.01000
C	10	-0.01248	1.99871	3.99901	0.01476	6.01248
C	11	-0.01805	1.99871	4.00460	0.01474	6.01805
C	12	-0.01505	1.99873	4.00152	0.01479	6.01505
C	13	-0.01627	1.99872	4.00286	0.01469	6.01627
C	14	-0.02235	1.99871	4.00894	0.01470	6.02235
C	15	-0.01139	1.99871	3.99799	0.01469	6.01139
C	16	-0.01657	1.99871	4.00323	0.01463	6.01657
C	17	-0.02483	1.99872	4.01140	0.01472	6.02483
C	18	-0.00660	1.99872	3.99327	0.01460	6.00660
C	19	-0.01996	1.99872	4.00647	0.01477	6.01996
C	20	-0.01072	1.99870	3.99730	0.01472	6.01072
C	21	-0.02415	1.99871	4.01071	0.01472	6.02415
C	22	-0.03898	1.99872	4.02528	0.01498	6.03898
C	23	-0.03025	1.99871	4.01675	0.01479	6.03025
C	24	-0.01155	1.99872	3.99823	0.01460	6.01155
C	25	-0.00734	1.99873	3.99403	0.01457	6.00734
C	26	-0.00815	1.99871	3.99480	0.01465	6.00815
C	27	-0.00444	1.99871	3.99118	0.01454	6.00444
C	28	-0.00825	1.99872	3.99495	0.01458	6.00825
C	29	-0.02323	1.99871	4.00981	0.01471	6.02323
C	30	-0.04300	1.99871	4.02919	0.01510	6.04300
C	31	-0.01322	1.99871	3.99984	0.01467	6.01322
C	32	-0.02592	1.99871	4.01251	0.01471	6.02592
C	33	-0.00464	1.99871	3.99143	0.01450	6.00464
C	34	-0.01301	1.99871	3.99978	0.01453	6.01301
C	35	-0.00726	1.99872	3.99401	0.01452	6.00726
C	36	-0.03479	1.99871	4.02123	0.01484	6.03479
C	37	-0.01687	1.99872	4.00351	0.01464	6.01687
C	38	-0.00421	1.99871	3.99095	0.01454	6.00421
C	39	-0.00247	1.99871	3.98922	0.01454	6.00247
C	40	-0.01150	1.99872	3.99828	0.01451	6.01150
C	41	-0.03710	1.99871	4.02355	0.01484	6.03710
C	42	-0.02233	1.99871	4.00898	0.01464	6.02233
C	43	-0.01262	1.99870	3.99933	0.01458	6.01262
C	44	-0.00982	1.99870	3.99647	0.01465	6.00982
C	45	-0.01657	1.99872	4.00329	0.01456	6.01657
C	46	-0.00511	1.99872	3.99191	0.01448	6.00511
C	47	-0.02473	1.99871	4.01134	0.01468	6.02473
C	48	-0.02093	1.99872	4.00749	0.01473	6.02093

C	49	-0.00350	1.99870	3.99020	0.01459	6.00350
C	50	-0.02059	1.99871	4.00728	0.01459	6.02059
C	51	-0.01747	1.99872	4.00415	0.01460	6.01747
C	52	-0.00334	1.99873	3.99017	0.01445	6.00334
C	53	-0.00695	1.99872	3.99360	0.01462	6.00695
C	54	-0.01986	1.99871	4.00635	0.01479	6.01986
C	55	-0.01868	1.99871	4.00538	0.01459	6.01868
C	56	-0.00362	1.99872	3.99042	0.01448	6.00362
C	57	-0.03646	1.99872	4.02269	0.01505	6.03646
C	58	-0.00939	1.99871	3.99605	0.01463	6.00939
C	59	-0.00160	1.99872	3.98841	0.01447	6.00160
C	60	-0.00732	1.99872	3.99410	0.01450	6.00732
N	61	-0.96487	1.99969	5.96138	0.00380	7.96487
H	62	0.48182	0.00000	0.51610	0.00207	0.51818
H	63	0.48443	0.00000	0.51347	0.00210	0.51557
H	64	0.48131	0.00000	0.51669	0.00200	0.51869
H	65	0.48300	0.00000	0.51538	0.00162	0.51700

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* Total *   0.00000   121.92256  248.18569   0.89175  371.00000
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Natural Population

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Core           121.92256 ( 99.9365% of 122)
Valence        248.18569 ( 99.6730% of 249)
Natural Minimal Basis  370.10825 ( 99.7596% of 371)
Natural Rydberg Basis   0.89175 (  0.2404% of 371)
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NBO Analysis PCM (Benzene)

Summary of Natural Population Analysis:

Natural Population						
Natural -----						
Atom	No	Charge	Core	Valence	Rydberg	Total

C	1	-0.01185	1.99872	3.99849	0.01463	6.01185
C	2	-0.01756	1.99871	4.00407	0.01478	6.01756
C	3	-0.02746	1.99871	4.01388	0.01487	6.02746
C	4	-0.00518	1.99872	3.99183	0.01464	6.00518
C	5	-0.02095	1.99871	4.00750	0.01474	6.02095
C	6	-0.00938	1.99872	3.99610	0.01457	6.00938
C	7	-0.02499	1.99871	4.01150	0.01478	6.02499
C	8	-0.03225	1.99871	4.01861	0.01493	6.03225
C	9	-0.01009	1.99872	3.99677	0.01460	6.01009
C	10	-0.01367	1.99871	4.00022	0.01474	6.01367
C	11	-0.01753	1.99871	4.00408	0.01475	6.01753
C	12	-0.01519	1.99873	4.00168	0.01479	6.01519
C	13	-0.01582	1.99872	4.00240	0.01470	6.01582
C	14	-0.02237	1.99871	4.00896	0.01470	6.02237

C	15	-0.01258	1.99871	3.99919	0.01467	6.01258
C	16	-0.01731	1.99871	4.00399	0.01461	6.01731
C	17	-0.02408	1.99872	4.01064	0.01472	6.02408
C	18	-0.00672	1.99873	3.99339	0.01460	6.00672
C	19	-0.01961	1.99872	4.00612	0.01477	6.01961
C	20	-0.01126	1.99870	3.99785	0.01471	6.01126
C	21	-0.02325	1.99871	4.00981	0.01473	6.02325
C	22	-0.03895	1.99872	4.02525	0.01498	6.03895
C	23	-0.02914	1.99871	4.01564	0.01479	6.02914
C	24	-0.01171	1.99872	3.99840	0.01460	6.01171
C	25	-0.00748	1.99873	3.99418	0.01457	6.00748
C	26	-0.00877	1.99871	3.99542	0.01464	6.00877
C	27	-0.00474	1.99871	3.99149	0.01454	6.00474
C	28	-0.00827	1.99872	3.99497	0.01458	6.00827
C	29	-0.02333	1.99871	4.00992	0.01470	6.02333
C	30	-0.04244	1.99871	4.02862	0.01510	6.04244
C	31	-0.01336	1.99871	3.99999	0.01467	6.01336
C	32	-0.02551	1.99871	4.01210	0.01471	6.02551
C	33	-0.00500	1.99871	3.99179	0.01449	6.00500
C	34	-0.01346	1.99871	4.00023	0.01452	6.01346
C	35	-0.00755	1.99872	3.99431	0.01452	6.00755
C	36	-0.03405	1.99871	4.02049	0.01485	6.03405
C	37	-0.01642	1.99872	4.00306	0.01464	6.01642
C	38	-0.00468	1.99871	3.99143	0.01453	6.00468
C	39	-0.00336	1.99871	3.99012	0.01453	6.00336
C	40	-0.01151	1.99872	3.99829	0.01450	6.01151
C	41	-0.03619	1.99871	4.02263	0.01484	6.03619
C	42	-0.02164	1.99871	4.00828	0.01464	6.02164
C	43	-0.01324	1.99871	3.99996	0.01457	6.01324
C	44	-0.01030	1.99870	3.99696	0.01464	6.01030
C	45	-0.01602	1.99872	4.00274	0.01456	6.01602
C	46	-0.00511	1.99872	3.99191	0.01448	6.00511
C	47	-0.02402	1.99871	4.01063	0.01468	6.02402
C	48	-0.02056	1.99872	4.00712	0.01473	6.02056
C	49	-0.00443	1.99871	3.99115	0.01458	6.00443
C	50	-0.02049	1.99871	4.00719	0.01459	6.02049
C	51	-0.01697	1.99872	4.00364	0.01460	6.01697
C	52	-0.00319	1.99873	3.99002	0.01444	6.00319
C	53	-0.00740	1.99872	3.99406	0.01462	6.00740
C	54	-0.02020	1.99871	4.00671	0.01479	6.02020
C	55	-0.01866	1.99871	4.00537	0.01458	6.01866
C	56	-0.00351	1.99872	3.99031	0.01448	6.00351
C	57	-0.03603	1.99872	4.02225	0.01506	6.03603
C	58	-0.00997	1.99871	3.99664	0.01462	6.00997
C	59	-0.00155	1.99872	3.98836	0.01447	6.00155
C	60	-0.00735	1.99872	3.99413	0.01449	6.00735
N	61	-0.96488	1.99969	5.96139	0.00381	7.96488
H	62	0.48182	0.00000	0.51610	0.00208	0.51818
H	63	0.48442	0.00000	0.51347	0.00211	0.51558
H	64	0.48131	0.00000	0.51670	0.00200	0.51869

H 65 0.48299 0.00000 0.51538 0.00162 0.51701

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* Total * 0.00000 121.92257 248.18587 0.89156 371.00000

13a ((NH₂+H₂)@C₆₀)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN089\SP\ROMP2-FC\6-31G(d)\C60H4N1(2)\DRAL\30-Jan-2010\0
 \#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCF=Tight SCFCyc=600 Pop=No
 ne Name=Dral\((NH2+H2)@C60\0,2\C,3.018435913,-1.384942749,-1.31592126
 5\C,3.481826782,-0.832345703,-0.047113159\C,2.966064453,-1.679168701,1
 .022161743\C,2.191604614,-2.753051758,0.416525146\C,2.222177246,-2.571
 817139,-1.023828247\C,2.620730835,-0.530755737,-2.34836145\C,3.5296750
 49,0.558721802,0.131613037\C,2.527136108,-1.111740112,2.222967407\C,1.
 029220581,-3.223022461,1.038864136\C,1.083474854,-2.858779907,-1.77784
 729\C,2.672464111,0.914245605,-2.160424927\C,3.067730469,1.14644458,1.
 386663696\C,1.31791687,-1.600112915,2.868667603\C,-0.151885986,-3.5319
 97681,0.24836731\C,0.680261353,-1.974685669,-2.856231689\C,1.431573608
 ,-0.832641602,-3.133584717\C,3.120849609,1.449584961,-0.950113037\C,2.
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 3\C,-0.123663208,-3.350753784,-1.133621216\C,1.518441895,1.493347168,-
 2.834390381\C,2.378933472,2.391882202,1.078253052\C,0.848373413,2.5820
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 2.273468018\C,-1.271780273,-2.770217896,-1.811737061\C,-2.404012939,-2
 .393737793,-1.085464478\C,-3.025772095,1.385467529,1.307800293\C,-2.24
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UB3LYP/6-31G(d)

Zero-point correction= 0.414691 (Hartree/Particle)
 Thermal correction to Energy= 0.438910
 Thermal correction to Enthalpy= 0.439854
 Thermal correction to Gibbs Free Energy= 0.368143
 Sum of electronic and zero-point Energies= -2342.765710
 Sum of electronic and thermal Energies= -2342.741490
 Sum of electronic and thermal Enthalpies= -2342.740546
 Sum of electronic and thermal Free Energies= -2342.812257

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NBO Analysis PCM

Summary of Natural Population Analysis:

Natural Population						
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.00071	1.99870	3.98613	0.01445	5.99929
C	2	-0.00561	1.99871	3.99202	0.01488	6.00561
C	3	0.00012	1.99871	3.98678	0.01439	5.99988
C	4	0.00121	1.99872	3.98579	0.01428	5.99879
C	5	-0.00024	1.99871	3.98722	0.01431	6.00024
C	6	0.00348	1.99871	3.98354	0.01426	5.99652
C	7	-0.00245	1.99872	3.98898	0.01475	6.00245
C	8	-0.00015	1.99872	3.98718	0.01425	6.00015
C	9	-0.00251	1.99872	3.98953	0.01425	6.00251
C	10	0.00199	1.99872	3.98505	0.01424	5.99801
C	11	0.00485	1.99872	3.98219	0.01424	5.99515
C	12	-0.00049	1.99871	3.98742	0.01436	6.00049
C	13	-0.00174	1.99872	3.98868	0.01434	6.00174
C	14	-0.00334	1.99871	3.99037	0.01425	6.00334
C	15	0.00410	1.99872	3.98294	0.01423	5.99590
C	16	0.00079	1.99872	3.98623	0.01426	5.99921
C	17	-0.00090	1.99870	3.98776	0.01443	6.00090
C	18	0.00040	1.99872	3.98665	0.01423	5.99960
C	19	-0.00156	1.99872	3.98852	0.01432	6.00156
C	20	0.00318	1.99872	3.98387	0.01423	5.99682
C	21	0.00109	1.99872	3.98594	0.01425	5.99891
C	22	0.00181	1.99873	3.98520	0.01426	5.99819
C	23	0.00364	1.99872	3.98341	0.01422	5.99636
C	24	0.00072	1.99872	3.98623	0.01433	5.99928
C	25	-0.00785	1.99872	3.99478	0.01435	6.00785
C	26	0.00310	1.99872	3.98383	0.01435	5.99690
C	27	0.00144	1.99872	3.98559	0.01424	5.99856
C	28	0.00027	1.99872	3.98671	0.01430	5.99973
C	29	-0.00161	1.99871	3.98852	0.01438	6.00161
C	30	-0.00934	1.99872	3.99607	0.01455	6.00934

C	31	0.00457	1.99872	3.98237	0.01434	5.99543
C	32	0.00331	1.99872	3.98347	0.01451	5.99669
C	33	0.00072	1.99871	3.98612	0.01445	5.99928
C	34	-0.00492	1.99872	3.99178	0.01442	6.00492
C	35	0.00001	1.99872	3.98688	0.01439	5.99999
C	36	0.00458	1.99871	3.98213	0.01458	5.99542
C	37	0.00495	1.99871	3.98165	0.01469	5.99505
C	38	-0.00408	1.99871	3.99094	0.01443	6.00408
C	39	-0.01145	1.99872	3.99813	0.01460	6.01145
C	40	0.00114	1.99872	3.98587	0.01427	5.99886
C	41	0.01457	1.99872	3.97233	0.01438	5.98543
C	42	0.00716	1.99871	3.97946	0.01467	5.99284
C	43	-0.00244	1.99872	3.98930	0.01443	6.00244
C	44	-0.00604	1.99872	3.99299	0.01433	6.00604
C	45	0.00016	1.99871	3.98677	0.01435	5.99984
C	46	0.01431	1.99871	3.97268	0.01430	5.98569
C	47	0.00180	1.99871	3.98511	0.01438	5.99820
C	48	-0.00555	1.99871	3.99241	0.01443	6.00555
C	49	-0.00656	1.99872	3.99331	0.01453	6.00656
C	50	0.00075	1.99872	3.98633	0.01421	5.99925
C	51	0.00976	1.99872	3.97718	0.01434	5.99024
C	52	0.00931	1.99871	3.97748	0.01449	5.99069
C	53	-0.00490	1.99872	3.99173	0.01445	6.00490
C	54	-0.00406	1.99872	3.99104	0.01430	6.00406
C	55	0.01124	1.99872	3.97573	0.01431	5.98876
C	56	-0.00038	1.99872	3.98735	0.01431	6.00038
C	57	-0.00636	1.99872	3.99312	0.01452	6.00636
C	58	-0.00058	1.99872	3.98751	0.01435	6.00058
C	59	-0.00015	1.99872	3.98719	0.01425	6.00015
C	60	0.00741	1.99873	3.97957	0.01430	5.99259
N	61	-0.76221	1.99981	5.74473	0.01767	7.76221
H	62	-0.01709	0.00000	1.01405	0.00304	1.01709
H	63	0.34378	0.00000	0.65407	0.00215	0.65622
H	64	0.05815	0.00000	0.93900	0.00285	0.94185
H	65	0.34399	0.00000	0.65389	0.00212	0.65601

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* Total * 0.00000 121.92283 248.18683 0.89034 371.00000

Natural Population

Core	121.92283 (99.9367% of 122)
Valence	248.18683 (99.6734% of 249)
Natural Minimal Basis	370.10966 (99.7600% of 371)
Natural Rydberg Basis	0.89034 (0.2400% of 371)

NBO Analysis PCM (Benzene)

Summary of Natural Population Analysis:

Natural Population

Natural -----						
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.00055	1.99870	3.98629	0.01445	5.99945
C	2	-0.00567	1.99871	3.99208	0.01488	6.00567
C	3	0.00013	1.99871	3.98676	0.01439	5.99987
C	4	0.00121	1.99872	3.98578	0.01428	5.99879
C	5	-0.00031	1.99871	3.98729	0.01431	6.00031
C	6	0.00334	1.99871	3.98368	0.01426	5.99666
C	7	-0.00247	1.99872	3.98899	0.01475	6.00247
C	8	0.00009	1.99872	3.98694	0.01425	5.99991
C	9	-0.00243	1.99872	3.98946	0.01426	6.00243
C	10	0.00194	1.99872	3.98510	0.01424	5.99806
C	11	0.00477	1.99872	3.98227	0.01424	5.99523
C	12	-0.00045	1.99871	3.98737	0.01436	6.00045
C	13	-0.00151	1.99871	3.98845	0.01434	6.00151
C	14	-0.00327	1.99871	3.99031	0.01425	6.00327
C	15	0.00401	1.99872	3.98304	0.01423	5.99599
C	16	0.00063	1.99872	3.98639	0.01426	5.99937
C	17	-0.00097	1.99870	3.98784	0.01443	6.00097
C	18	0.00065	1.99872	3.98640	0.01423	5.99935
C	19	-0.00141	1.99872	3.98837	0.01433	6.00141
C	20	0.00314	1.99872	3.98390	0.01423	5.99686
C	21	0.00096	1.99872	3.98607	0.01425	5.99904
C	22	0.00188	1.99873	3.98513	0.01427	5.99812
C	23	0.00360	1.99872	3.98345	0.01423	5.99640
C	24	0.00097	1.99872	3.98597	0.01433	5.99903
C	25	-0.00775	1.99872	3.99468	0.01435	6.00775
C	26	0.00297	1.99872	3.98396	0.01435	5.99703
C	27	0.00130	1.99872	3.98573	0.01424	5.99870
C	28	0.00031	1.99872	3.98667	0.01430	5.99969
C	29	-0.00140	1.99871	3.98831	0.01438	6.00140
C	30	-0.00918	1.99872	3.99590	0.01456	6.00918
C	31	0.00448	1.99872	3.98246	0.01434	5.99552
C	32	0.00316	1.99872	3.98361	0.01451	5.99684
C	33	0.00070	1.99871	3.98614	0.01445	5.99930
C	34	-0.00493	1.99872	3.99180	0.01442	6.00493
C	35	-0.00011	1.99872	3.98700	0.01439	6.00011
C	36	0.00440	1.99871	3.98231	0.01458	5.99560
C	37	0.00485	1.99871	3.98175	0.01469	5.99515
C	38	-0.00397	1.99871	3.99084	0.01443	6.00397
C	39	-0.01124	1.99872	3.99792	0.01460	6.01124
C	40	0.00110	1.99872	3.98591	0.01427	5.99890
C	41	0.01436	1.99872	3.97254	0.01438	5.98564
C	42	0.00703	1.99871	3.97959	0.01467	5.99297
C	43	-0.00228	1.99872	3.98913	0.01443	6.00228
C	44	-0.00589	1.99872	3.99283	0.01434	6.00589
C	45	0.00008	1.99871	3.98686	0.01435	5.99992
C	46	0.01406	1.99871	3.97292	0.01430	5.98594
C	47	0.00175	1.99871	3.98515	0.01438	5.99825

C	48	-0.00548	1.99871	3.99233	0.01443	6.00548
C	49	-0.00636	1.99872	3.99311	0.01454	6.00636
C	50	0.00077	1.99872	3.98630	0.01421	5.99923
C	51	0.00963	1.99872	3.97731	0.01434	5.99037
C	52	0.00911	1.99871	3.97768	0.01449	5.99089
C	53	-0.00473	1.99871	3.99156	0.01446	6.00473
C	54	-0.00392	1.99872	3.99090	0.01431	6.00392
C	55	0.01107	1.99872	3.97590	0.01431	5.98893
C	56	-0.00044	1.99872	3.98742	0.01431	6.00044
C	57	-0.00619	1.99872	3.99295	0.01452	6.00619
C	58	-0.00038	1.99872	3.98731	0.01436	6.00038
C	59	-0.00013	1.99872	3.98717	0.01425	6.00013
C	60	0.00726	1.99873	3.97971	0.01430	5.99274
N	61	-0.76225	1.99981	5.74477	0.01768	7.76225
H	62	-0.01706	0.00000	1.01402	0.00304	1.01706
H	63	0.34380	0.00000	0.65405	0.00215	0.65620
H	64	0.05812	0.00000	0.93903	0.00285	0.94188
H	65	0.34401	0.00000	0.65387	0.00212	0.65599

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* Total * 0.00000 121.92283 248.18674 0.89044 371.00000

13c ((H+H₃N)@C₆₀)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN089\SP\ROMP2-FC\6-31G(d)\C60H4N1(2)\DRAL\27-Jan-2010\0
 \#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCF=Tight SCFCyc=600 Pop=None
 Name=DRAL\((NH3+H)@C60\0,2\C,-1.948669434,1.189254761,-2.797073364
 \C,-0.632614136,1.707427979,-3.094360352\C,0.214538574,0.506408691,-3.
 318435669\C,-0.656204224,-0.689605713,-3.466583252\C,-1.962966919,-0.2
 61611938,-3.022613525\C,-2.639175415,1.73538208,-1.699447632\C,-0.0352
 32544,2.726135254,-2.356491089\C,1.689285278,0.482254028,-3.259689331\
 C,-0.080780029,-1.895584106,-3.075271606\C,-2.667404175,-1.102615356,-
 2.141281128\C,-2.03616333,2.792404175,-0.913650513\C,1.400695801,2.612
 640381,-1.991149902\C,2.191146851,-0.790588379,-2.774719238\C,-0.81185
 9131,-2.750869751,-2.174087524\C,-3.386856079,-0.52545166,-1.013656616
 \C,-3.373016357,0.856399536,-0.798553467\C,-0.752365112,3.280105591,-1
 .235351562\C,2.214828491,1.538269043,-2.412231445\C,1.355697632,-1.926
 818848,-2.697769165\C,-2.086700439,-2.359573364,-1.715438843\C,-2.3956
 90918,2.573852539,0.47644043\C,1.533233643,3.127761841,-0.648834229\C,
 -1.472015381,2.837387085,1.491653442\C,3.133071899,-0.512390137,-1.697
 158813\C,0.145553589,-3.331665039,-1.244903564\C,-3.253067017,-1.43714
 9048,0.111175537\C,-3.225143433,1.380493164,0.549636841\C,0.213424683,
 3.53112793,-0.176452637\C,3.147491455,0.927459717,-1.472869873\C,1.474
 334717,-2.828018188,-1.575927734\C,-2.446105957,-2.56703186,-0.3235931

4\C,-1.530761719,-3.144287109,0.560577393\C,1.920944214,-1.183959961,2.705993652\C,1.935531616,0.251556396,2.929763794\C,0.616470337,0.644256592,3.397155762\C,-0.210769653,-0.546218872,3.466598511\C,0.593460083,-1.675231934,3.036651611\C,2.624603271,-1.729614258,1.632141113\C,2.652954102,1.084655762,2.070510864\C,0.065292358,1.856262207,2.977813721\C,-1.561630249,-0.478240967,3.115997314\C,0.020507812,-2.691665649,2.27015686\C,3.372680664,-0.862075806,0.737579346\C,2.07673645,2.345581055,1.631729126\C,-1.342010498,1.928085327,2.614517212\C,-2.160018921,-1.536941528,2.323165894\C,0.747024536,-3.256057739,1.149841309\C,2.026016235,-2.786499023,0.83291626\C,3.386856079,0.516189575,0.952301025\C,0.805831909,2.720397949,2.079986572\C,-2.13710022,0.782363892,2.684204102\C,-1.386978149,-2.622528076,1.906448364\C,3.236618042,-1.387481689,-0.612945557\C,2.453765869,2.557235718,0.24798584\C,-3.108703613,-0.932296753,1.404327393\C,-0.208633423,-3.531112671,0.089752197\C,2.402145386,-2.573822021,-0.550582886\C,3.266159058,1.430343628,-0.174255371\C,-0.141067505,3.323547363,1.156677246\C,-3.094711304,0.503921509,1.627838135\N,-0.014383545,-0.016871826,0.100100952\H,0.430536133,0.889155029,-0.047224854\H,0.562587646,-0.745279297,-0.322065063\H,-0.932116943,-0.01053772,-0.345285645\H,0.19142041,0.33680835,-2.20489502\\Version=AM64L-G03RevD.02\State=2-A\HF=-2328.4366541\MP2=-2336.4733954\RMSE=2.489e-09\Thermal=0\PG=C01 [X(C60H4N1)]\@

UB3LYP/6-31G(d)

Zero-point correction=	0.421902 (Hartree/Particle)
Thermal correction to Energy=	0.445692
Thermal correction to Enthalpy=	0.446636
Thermal correction to Gibbs Free Energy=	0.375865
Sum of electronic and zero-point Energies=	-2342.787979
Sum of electronic and thermal Energies=	-2342.764189
Sum of electronic and thermal Enthalpies=	-2342.763245
Sum of electronic and thermal Free Energies=	-2342.834016

1\1\FAU-CCC-CCDN086\Freq\UB3LYP\6-31G(d)\C60H4N1(2)\DRAL\28-Aug-2009\0\\#P B3LYP/6-31G* Freq=NoRaman Pop=None NAME=DRAL\\(NH3+H)@C60\0,2\C,-1.948669434,1.189254761,-2.797073364\C,-0.632614136,1.707427979,-3.094360352\C,0.214538574,0.506408691,-3.318435669\C,-0.656204224,-0.689605713,-3.466583252\C,-1.962966919,-0.261611938,-3.022613525\C,-2.639175415,1.73538208,-1.699447632\C,-0.035232544,2.726135254,-2.356491089\C,1.689285278,0.482254028,-3.259689331\C,-0.080780029,-1.895584106,-3.075271606\C,-2.667404175,-1.102615356,-2.141281128\C,-2.03616333,2.792404175,-0.913650513\C,1.400695801,2.612640381,-1.991149902\C,2.191146851,-0.790588379,-2.774719238\C,-0.811859131,-2.750869751,-2.174087524\C,-3.386856079,-0.52545166,-1.013656616\C,-3.373016357,0.856399536,-0.798553467\C,-0.752365112,3.280105591,-1.235351562\C,2.214828491,1.538269043,-2.412231445\C,1.355697632,-1.926818848,-2.697769165\C,-2.086700439,-2.359573364,-1.715438843\C,-2.395690918,2.573852539,0.47644043\C,1.533233643,3.127761841,-0.648834229\C,-1.472015381,2.837387085,1.491653442\C,3.133071899,-0.512390137,-1.697158813\C,0.145553589,-3.331665039

, -1.244903564\C, -3.253067017, -1.437149048, 0.111175537\C, -3.225143433, 1.380493164, 0.549636841\C, 0.213424683, 3.53112793, -0.176452637\C, 3.147491455, 0.927459717, -1.472869873\C, 1.474334717, -2.828018188, -1.575927734\C, -2.446105957, -2.56703186, -0.32359314\C, -1.530761719, -3.144287109, 0.560577393\C, 1.920944214, -1.183959961, 2.705993652\C, 1.935531616, 0.251556396, 2.929763794\C, 0.616470337, 0.644256592, 3.397155762\C, -0.210769653, -0.546218872, 3.466598511\C, 0.593460083, -1.675231934, 3.036651611\C, 2.624603271, -1.729614258, 1.632141113\C, 2.652954102, 1.084655762, 2.070510864\C, 0.065292358, 1.856262207, 2.977813721\C, -1.561630249, -0.478240967, 3.115997314\C, 0.020507812, -2.691665649, 2.27015686\C, 3.372680664, -0.862075806, 0.737579346\C, 2.07673645, 2.345581055, 1.631729126\C, -1.342010498, 1.928085327, 2.614517212\C, -2.160018921, -1.536941528, 2.323165894\C, 0.747024536, -3.256057739, 1.149841309\C, 2.026016235, -2.786499023, 0.83291626\C, 3.386856079, 0.516189575, 0.952301025\C, 0.805831909, 2.720397949, 2.079986572\C, -2.13710022, 0.782363892, 2.684204102\C, -1.386978149, -2.622528076, 1.906448364\C, 3.236618042, -1.387481689, -0.612945557\C, 2.453765869, 2.557235718, 0.24798584\C, -3.108703613, -0.932296753, 1.404327393\C, -0.208633423, -3.531112671, 0.089752197\C, 2.402145386, -2.573822021, -0.550582886\C, 3.266159058, 1.430343628, -0.174255371\C, -0.141067505, 3.323547363, 1.156677246\C, -3.094711304, 0.503921509, 1.627838135\N, -0.014383545, -0.016871826, 0.100100952\H, 0.430536133, 0.889155029, -0.047224854\H, 0.562587646, -0.745279297, -0.322065063\H, -0.932116943, -0.01053772, -0.345285645\H, 0.19142041, 0.33680835, -2.20489502\\Version=AM64L-G03RevD.02\\State=2-A\\HF=-2343.2098813\\S2=0.775478\\S2-1=0.\\S2A=0.750489\\RMSD=7.923e-09\\RMSF=8.461e-04\\ZeroPoint=0.4219024\\Thermal=0.4456918\\ZPE=264.7477246\\Dipole=-0.048011, 0.0349236, -0.2028657\\DipoleDeriv=0.0529275, 0.0110382, 0.0541341, 0.028069, -0.0185857, 0.0861877\\Polar=479.0349967, 0.671608, 482.2322899, -4.1738091, -0.5927916, 486.1989155\\PG=C01 [X(C60H4N1)]\\NImag=0\\0.48963300293340, -0.00229729, -0.02811190, 0.24135892\\0.00008936, -0.00007741, 0.380, -0.00168466, -0.00015317, 0.00021166, -0.00080549\\\\@

NBO Analysis PCM

Summary of Natural Population Analysis:

Natural Population						
Natural -----						
Atom	No	Charge	Core	Valence	Rydberg	Total

C	1	-0.01915	1.99869	4.00554	0.01492	6.01915
C	2	0.04606	1.99868	3.93846	0.01681	5.95394
C	3	-0.31758	1.99876	4.29742	0.02141	6.31758
C	4	0.04546	1.99868	3.93906	0.01680	5.95454
C	5	-0.01929	1.99869	4.00568	0.01492	6.01929
C	6	-0.00079	1.99872	3.98749	0.01458	6.00079
C	7	-0.01029	1.99866	3.99671	0.01492	6.01029
C	8	0.03297	1.99858	3.94942	0.01903	5.96703
C	9	-0.00974	1.99866	3.99618	0.01490	6.00974
C	10	-0.00209	1.99872	3.98876	0.01461	6.00209
C	11	-0.01436	1.99872	4.00127	0.01437	6.01436
C	12	-0.00967	1.99876	3.99589	0.01501	6.00967

C	13	-0.01117	1.99871	3.99754	0.01492	6.01117
C	14	-0.01035	1.99870	3.99713	0.01452	6.01035
C	15	-0.00535	1.99872	3.99226	0.01436	6.00535
C	16	-0.00427	1.99872	3.99122	0.01433	6.00427
C	17	-0.01107	1.99870	3.99783	0.01455	6.01107
C	18	-0.01046	1.99871	3.99683	0.01492	6.01046
C	19	-0.01012	1.99876	3.99636	0.01500	6.01012
C	20	-0.01471	1.99872	4.00164	0.01436	6.01471
C	21	-0.00094	1.99872	3.98788	0.01434	6.00094
C	22	-0.02435	1.99873	4.01112	0.01450	6.02435
C	23	-0.00244	1.99872	3.98938	0.01434	6.00244
C	24	-0.01001	1.99871	3.99672	0.01458	6.01001
C	25	-0.00120	1.99873	3.98822	0.01426	6.00120
C	26	-0.00803	1.99871	3.99503	0.01429	6.00803
C	27	-0.00733	1.99871	3.99432	0.01430	6.00733
C	28	-0.00345	1.99873	3.99043	0.01429	6.00345
C	29	-0.00908	1.99871	3.99580	0.01457	6.00908
C	30	-0.02314	1.99873	4.00994	0.01446	6.02314
C	31	-0.00129	1.99872	3.98823	0.01433	6.00129
C	32	-0.00190	1.99872	3.98885	0.01434	6.00190
C	33	0.00752	1.99872	3.97935	0.01441	5.99248
C	34	0.00749	1.99872	3.97939	0.01440	5.99251
C	35	0.00840	1.99872	3.97849	0.01439	5.99160
C	36	0.00521	1.99872	3.98170	0.01438	5.99479
C	37	0.00833	1.99872	3.97856	0.01439	5.99167
C	38	-0.00062	1.99871	3.98752	0.01438	6.00062
C	39	-0.00052	1.99871	3.98740	0.01440	6.00052
C	40	0.00324	1.99872	3.98357	0.01446	5.99676
C	41	0.00420	1.99872	3.98261	0.01447	5.99580
C	42	0.00375	1.99872	3.98307	0.01446	5.99625
C	43	-0.00007	1.99872	3.98703	0.01432	6.00007
C	44	-0.00271	1.99872	3.98967	0.01432	6.00271
C	45	0.00393	1.99872	3.98293	0.01442	5.99607
C	46	0.00516	1.99872	3.98168	0.01444	5.99484
C	47	-0.00556	1.99872	3.99248	0.01436	6.00556
C	48	-0.00273	1.99872	3.98968	0.01433	6.00273
C	49	0.00051	1.99872	3.98644	0.01433	5.99949
C	50	-0.00653	1.99872	3.99348	0.01433	6.00653
C	51	0.00511	1.99872	3.98172	0.01445	5.99489
C	52	0.00430	1.99872	3.98257	0.01441	5.99570
C	53	-0.00078	1.99872	3.98777	0.01429	6.00078
C	54	-0.01000	1.99872	3.99691	0.01437	6.01000
C	55	0.00703	1.99872	3.97995	0.01430	5.99297
C	56	0.00426	1.99873	3.98279	0.01422	5.99574
C	57	-0.01161	1.99872	3.99849	0.01440	6.01161
C	58	0.00060	1.99872	3.98638	0.01430	5.99940
C	59	0.00276	1.99873	3.98430	0.01421	5.99724
C	60	0.00708	1.99872	3.97990	0.01430	5.99292
N	61	-1.10697	1.99977	6.09234	0.01486	8.10697
H	62	0.38208	0.00000	0.61616	0.00175	0.61792

H	63	0.38200	0.00000	0.61628	0.00171	0.61800
H	64	0.38047	0.00000	0.61781	0.00172	0.61953
H	65	0.36377	0.00000	0.63114	0.00509	0.63623

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* Total * 0.00000 121.92262 248.16819 0.90919 371.00000
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NBO Analysis PCM (Benzene)

Summary of Natural Population Analysis:

Natural Population						
Natural -----						
Atom	No	Charge	Core	Valence	Rydberg	Total

C	1	-0.01887	1.99869	4.00526	0.01492	6.01887
C	2	0.04742	1.99867	3.93708	0.01682	5.95258
C	3	-0.31636	1.99875	4.29613	0.02148	6.31636
C	4	0.04686	1.99868	3.93765	0.01681	5.95314
C	5	-0.01901	1.99869	4.00540	0.01492	6.01901
C	6	-0.00045	1.99872	3.98715	0.01459	6.00045
C	7	-0.01042	1.99866	3.99685	0.01491	6.01042
C	8	0.03246	1.99858	3.94993	0.01904	5.96754
C	9	-0.00987	1.99866	3.99631	0.01489	6.00987
C	10	-0.00175	1.99872	3.98842	0.01461	6.00175
C	11	-0.01459	1.99872	4.00151	0.01436	6.01459
C	12	-0.00941	1.99876	3.99563	0.01501	6.00941
C	13	-0.01128	1.99871	3.99765	0.01492	6.01128
C	14	-0.01047	1.99870	3.99725	0.01452	6.01047
C	15	-0.00505	1.99872	3.99196	0.01437	6.00505
C	16	-0.00396	1.99872	3.99091	0.01434	6.00396
C	17	-0.01115	1.99870	3.99791	0.01455	6.01115
C	18	-0.01058	1.99871	3.99695	0.01491	6.01058
C	19	-0.00985	1.99876	3.99608	0.01500	6.00985
C	20	-0.01499	1.99872	4.00191	0.01436	6.01499
C	21	-0.00100	1.99872	3.98794	0.01434	6.00100
C	22	-0.02448	1.99873	4.01125	0.01450	6.02448
C	23	-0.00267	1.99872	3.98961	0.01434	6.00267
C	24	-0.00990	1.99871	3.99661	0.01458	6.00990
C	25	-0.00116	1.99873	3.98818	0.01426	6.00116
C	26	-0.00799	1.99871	3.99499	0.01429	6.00799
C	27	-0.00729	1.99871	3.99428	0.01430	6.00729
C	28	-0.00337	1.99873	3.99036	0.01429	6.00337
C	29	-0.00896	1.99871	3.99567	0.01458	6.00896
C	30	-0.02325	1.99873	4.01006	0.01446	6.02325
C	31	-0.00136	1.99872	3.98831	0.01433	6.00136
C	32	-0.00214	1.99872	3.98908	0.01434	6.00214
C	33	0.00742	1.99872	3.97946	0.01441	5.99258
C	34	0.00739	1.99872	3.97949	0.01440	5.99261
C	35	0.00817	1.99872	3.97872	0.01439	5.99183

C	36	0.00479	1.99872	3.98212	0.01438	5.99521
C	37	0.00809	1.99872	3.97880	0.01439	5.99191
C	38	-0.00070	1.99871	3.98760	0.01438	6.00070
C	39	-0.00058	1.99871	3.98746	0.01440	6.00058
C	40	0.00302	1.99872	3.98379	0.01446	5.99698
C	41	0.00392	1.99872	3.98289	0.01447	5.99608
C	42	0.00353	1.99872	3.98329	0.01446	5.99647
C	43	-0.00003	1.99872	3.98699	0.01432	6.00003
C	44	-0.00292	1.99872	3.98989	0.01432	6.00292
C	45	0.00375	1.99872	3.98310	0.01442	5.99625
C	46	0.00502	1.99872	3.98182	0.01444	5.99498
C	47	-0.00579	1.99872	3.99271	0.01436	6.00579
C	48	-0.00294	1.99872	3.98988	0.01433	6.00294
C	49	0.00056	1.99872	3.98639	0.01434	5.99944
C	50	-0.00679	1.99872	3.99374	0.01433	6.00679
C	51	0.00498	1.99872	3.98185	0.01445	5.99502
C	52	0.00413	1.99872	3.98274	0.01441	5.99587
C	53	-0.00078	1.99872	3.98777	0.01429	6.00078
C	54	-0.01020	1.99872	3.99712	0.01437	6.01020
C	55	0.00707	1.99872	3.97990	0.01430	5.99293
C	56	0.00422	1.99873	3.98283	0.01422	5.99578
C	57	-0.01180	1.99872	3.99869	0.01440	6.01180
C	58	0.00061	1.99872	3.98637	0.01430	5.99939
C	59	0.00272	1.99873	3.98434	0.01421	5.99728
C	60	0.00712	1.99872	3.97986	0.01431	5.99288
N	61	-1.10703	1.99977	6.09240	0.01487	8.10703
H	62	0.38207	0.00000	0.61618	0.00175	0.61793
H	63	0.38199	0.00000	0.61629	0.00171	0.61801
H	64	0.38049	0.00000	0.61779	0.00172	0.61951
H	65	0.36340	0.00000	0.63153	0.00507	0.63660

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* Total * 0.00000 121.92261 248.16805 0.90933 371.00000

Natural Population

Core	121.92261 (99.9366% of 122)
Valence	248.16805 (99.6659% of 249)
Natural Minimal Basis	370.09067 (99.7549% of 371)
Natural Rydberg Basis	0.90933 (0.2451% of 371)

12³⁻ (triplet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12³⁻

1\1\GINC-I01R10C03S05\SP\UB3LYP\6-311+G(d,p)\C60H4N1(1-,3)\DRAL\25-Jan
-2013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Curr

ent Name=DrAl GFINPUT GFPRINT\NH4(+)@C60(2-) triplet\ -1,3\C,0,-1.470
 92,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567
 ,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\
 C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423
 ,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49
 338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.337
 92,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.
 26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,
 -2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878
 ,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414
 \C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.839
 14,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,
 -3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C
 ,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.2
 4036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.9730
 5\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.2672
 6,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2
 .48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,
 0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2
 .24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.
 76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.
 86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.8215
 9,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C
 ,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,
 0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92
 744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-
 0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54
 851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\V
 ersion=EM64L-G09RevB.01\State=3-A\HF=-2343.8433074\S2=2.006006\S2-1=0.
 \S2A=2.000025\RMSD=7.614e-09\Dipole=-0.0082035,0.0079172,0.0013257\Qua
 drupole=0.6483934,-1.0772504,0.428857,-0.6836061,0.3093974,0.9641472\P
 G=C01 [X(C60H4N1)]\@

12⁻ (singlet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

1\1\GINC-I01R05C01S09\SP\RB3LYP\6-311+G(d,p)\C60H4N1(1-)\DRAL\03-Feb-2
 013\0\#P B3LYP/6-311+G(d,p) SCF=XQC Pop=(NBO,Full) Density=Current Na
 me=DrAl GFINPUT GFPRINT\NH4(+)@C60(2-) singlet\ -1,1\C,0,-1.47092,2.3
 6026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-0.03
 085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,0,-1
 .58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2.912
 28,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49338\C,
 0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792,2.8
 1584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26303\
 C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2.458
 47,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-1.68
 539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C,0,-

2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914,2.0
 1942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3.392
 53\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0,2.0
 4112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.24036,-
 0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\C,0,
 0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,-2.5
 4585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.48964
 \C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,3.14
 793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.24342
 ,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76247\
 C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,
 -1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.1
 4166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0,-2.
 80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.7850
 6,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92744\C,
 0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.0065
 7,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54851,0.
 59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Version
 =EM64L-G09RevB.01\State=1-A\HF=-2343.837618\RMSD=1.546e-05\Dipole=-0.0
 103298,0.0060417,0.0006981\Quadrupole=2.6721006,-1.7399172,-0.9321834,
 -0.4359099,2.0270653,-0.2057308\PG=C01 [X(C60H4N1)]\\@

12^{••2-} (quartet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

1\1\GINC-I01R10C03S05\SP\UB3LYP\6-311+G(d,p)\C60H4N1(2-,4)\DRAL\25-Jan
 -2013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Curr
 ent Name=Dral GFINPUT GFPRINT\NH4(+)@C60(3-) quartet\ -2,4\C,0,-1.470
 92,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567
 ,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\
 C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423
 ,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49
 338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.337
 92,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.
 26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,
 -2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878
 ,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414
 \C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.839
 14,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,
 -3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C
 ,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.2
 4036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.9730
 5\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.2672
 6,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.
 48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,
 0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.
 24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.

76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Version=EM64L-G09RevB.01\State=4-A\HF=-2343.8336154\S2=3.754725\S2-1=0.\S2A=3.750012\RMSD=8.724e-09\Dipole=-0.0068154,0.0082946,0.0022841\Quadrupole=0.0026645,-0.0080095,0.005345,0.0137061,-0.0156036,0.0225789\PG=C01 [X(C60H4N1)]\@

12²⁻ (doublet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12²⁻

1\1\GINC-I01R03C03S03\SP\UB3LYP\6-311+G(d,p)\C60H4N1(2-,2)\DRAL\05-Feb-2013\0\#P B3LYP/6-311+G(d,p) SCF=(Restart,XQC) Pop=(NBO,Full) Density=Current GFINPUT GFPRINT Name=DrAl\NH4(+)\@C60(3-) doublet\2-,2\C,0,-1.47092,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.24036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Version=EM64L-G09RevB.01\State=2-A\HF=-2343.8270173\S2=0.754547\S

2-1=0.\S2A=0.75002\RMSD=3.361e-09\Dipole=-0.009724,0.0070122,0.001543\
 Quadrupole=2.0166675,-1.7887637,-0.2279038,-0.9297473,1.2489446,0.9292
 515\PG=C01 [X(C60H4N1)]\@

12^{•3-} (triplet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

1\1\GINC-I01R10C03S05\SP\UB3LYP/6-311+G(d,p)\C60H4N1(3-,3)\DRAL\26-Jan
 -2013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Curr
 ent Name=Dral GFINPUT GFPRINT\NH4(+)\@C60(4-) triplet\ -3,3\C,0,-1.470
 92,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567
 ,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\
 C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423
 ,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49
 338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.337
 92,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.
 26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,
 -2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878
 ,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414
 \C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.839
 14,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,
 -3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C
 ,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.2
 4036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.9730
 5\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.2672
 6,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2
 .48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,
 0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2
 .24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.
 76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.
 86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.8215
 9,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C
 ,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,
 0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92
 744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-
 0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54
 851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\V
 ersion=EM64L-G09RevB.01\State=3-A\HF=-2343.7089289\S2=2.006119\S2-1=0.
 \S2A=2.000026\RMSD=4.945e-09\Dipole=-0.0084558,0.0075707,0.0021474\Qua
 drupole=1.3965057,-0.8483393,-0.5481664,-0.322378,0.851162,-0.1135426\
 PG=C01 [X(C60H4N1)]\@

12³⁻ (singlet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

```
1\1\GINC-I01R03C03S03\SP\RB3LYP\6-311+G(d,p)\C60H4N1(3-)\DRAL\23-Jan-2
013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Current
Name=DrAl GFINPUT GFPRINT\NH4(+)\@C60(4-) singlet\|-3,1\C,0,-1.47092
,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-
0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,
0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2
.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.4933
8\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792
,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26
303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2
.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-
1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C
,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914
,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3
.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0
,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.240
36,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\
C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,
-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.4
8964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,
3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.2
4342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76
247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86
201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,
-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0
,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.
78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.9274
4\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.
00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.5485
1,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\Ver
sion=EM64L-G09RevB.01\State=1-A\HF=-2343.7035406\RMSD=6.537e-09\Dipole
=-0.0101339,0.0079274,0.0019166\Quadrupole=1.2686039,-1.6917248,0.4231
209,-1.2310484,0.7814079,2.1391658\PG=C01 [X(C60H4N1)]\@\@
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12³⁺⁴⁻ (quartet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

```
1\1\GINC-I01R07C02S01\SP\UB3LYP\6-311+G(d,p)\C60H4N1(4-,4)\DRAL\09-Feb
-2013\0\#P B3LYP/6-311+G(d,p) SCF=XQC Pop=(NBO,Full) Density=Current
Name=DrAl GFINPUT GFPRINT SCF=Restart\NH4(+)\@C60(5-) quartet\|-4,4\C,
0,-1.47092,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943
,3.24567,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-
```

1.97762\C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0
 ,-1.5423,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.332
 58,-2.49338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,
 0,-0.33792,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.
 1031,-3.26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36
 713\C,0,-2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037
 ,2.23878,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787
 ,0.91414\C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C
 ,0,2.83914,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-
 0.90076,-3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2
 .83313\C,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.4
 2754,0.24036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.9515
 2,1.97305\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,
 0,2.26726,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2
 .33746,2.48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.
 32964\C,0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2
 .1862,-2.24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.8
 7144,-1.76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717
 \C,0,-0.86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675
 ,-2.82159,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3
 .38768\C,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,
 3.43874,0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25
 568,2.92744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.074
 97\N,0,-0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65
 589,0.54851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.
 06544\\Version=EM64L-G09RevB.01\State=4-A\HF=-2343.447657\S2=3.75956\S
 2-1=0.\S2A=3.750047\RMSD=1.074e-04\Dipole=-0.00976,0.0101725,0.0031382
 \Quadrupole=0.5673625,-1.7098903,1.1425278,0.377881,-0.5538759,-1.3189
 854\PG=C01 [X(C60H4N1)]\@

12⁴⁻ (doublet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁴⁻

1\1\GINC-I01R03C03S03\SP\UB3LYP/6-311+G(d,p)\C60H4N1(4-,2)\DRAL\24-Jan
 -2013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Curr
 ent Name=Dral GFINPUT GFPRINT\NH4(+)\@C60(5-) doublet\|-4,2\C,0,-1.470
 92,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567
 ,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\
 C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423
 ,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49
 338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.337
 92,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.
 26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,
 -2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878
 ,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414
 \C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.839
 14,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,
 -3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C

,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.24036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.92744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.54851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Version=EM64L-G09RevB.01\State=2-A\HF=-2343.4793217\S2=0.754595\S2-1=0.\S2A=0.75002\RMSD=4.726e-09\Dipole=-0.0090724,0.0082383,0.0027307\Quadrupole=0.6434618,-1.0543412,0.4108794,-0.6431443,0.3084462,0.9692392\P G=C01 [X(C60H4N1)]\@

12^{•5-} (triplet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

1\1\GINC-I01R02C03S03\SP\UB3LYP\6-311+G(d,p)\C60H4N1(5-,3)\DRAL\08-Feb-2013\0\#P B3LYP/6-311+G(d,p) SCF=XQC Pop=(NBO,Full) Density=Current Name=DrAl GFINPUT GFPRINT SCF=Restart\NH4(+)\@C60(6-) triplet\ -5,3\C,0,-1.47092,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2.91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.49338\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2.45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3.39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.24036,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,-2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.48964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.24342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,-2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3

.38768\C,0,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,
 3.43874,0.78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25
 568,2.92744\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.074
 97\N,0,-0.00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65
 589,0.54851,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.
 06544\\Version=EM64L-G09RevB.01\State=3-A\HF=-2343.119294\S2=2.004729\
 S2-1=0.\S2A=2.000015\RMSD=4.334e-07\Dipole=0.5137212,0.3831436,2.03861
 98\Quadrupole=-4.7343696,2.8050561,1.9293135,-3.7450663,-3.6845379,-5.
 5297663\PG=C01 [X(C60H4N1)]\@

12⁵⁻ (singlet)

UB3LYP/6-311+G(d,p) on UB3LYP/6-31G(d) geometry of 12⁺

1\1\GINC-I01R03C03S03\SP\RB3LYP\6-311+G(d,p)\C60H4N1(5-)\DRAL\24-Jan-2
 013\0\#P B3LYP/6-311+G(d,p) SCFCyc=1200 Pop=(NBO,Full) Density=Curren
 t Name=DrAl GFINPUT GFPRINT\NH4(+)\@C60(6-) singlet\5,1\C,0,-1.47092
 ,2.36026,-2.21132\C,0,-2.26764,2.54384,-1.00861\C,0,-1.44943,3.24567,-
 0.03085\C,0,-0.14616,3.49559,-0.62985\C,0,-0.16013,2.94835,-1.97762\C,
 0,-1.58699,1.18077,-2.9516\C,0,-3.14793,1.54092,-0.59558\C,0,-1.5423,2
 .91228,1.32213\C,0,1.01129,3.40378,0.14713\C,0,0.98389,2.33258,-2.4933
 8\C,0,-2.50363,0.136,-2.5224\C,0,-3.24155,1.19384,0.81528\C,0,-0.33792
 ,2.81584,2.13264\C,0,2.20241,2.76273,-0.39084\C,0,0.86246,1.1031,-3.26
 303\C,0,-0.39619,0.53938,-3.48827\C,0,-3.26817,0.31279,-1.36713\C,0,-2
 .45847,1.8685,1.75496\C,0,0.91153,3.0558,1.55615\C,0,2.19037,2.23878,-
 1.68539\C,0,-1.87907,-1.15002,-2.79309\C,0,-3.42119,-0.24787,0.91414\C
 ,0,-2.04411,-2.20915,-1.89888\C,0,-0.51038,1.71405,3.06728\C,0,2.83914
 ,2.01942,0.68559\C,0,1.99394,0.25073,-2.93282\C,0,-0.57698,-0.90076,-3
 .39253\C,0,-3.43874,-0.79105,-0.43497\C,0,-1.82072,1.12718,2.83313\C,0
 ,2.04112,2.19998,1.88895\C,0,2.81351,0.9516,-1.95576\C,0,3.42754,0.240
 36,-0.92223\C,0,1.47035,-2.36472,2.20738\C,0,0.16017,-2.95152,1.97305\
 C,0,0.14485,-3.49559,0.62375\C,0,1.44702,-3.24425,0.02499\C,0,2.26726,
 -2.54585,1.00381\C,0,1.5865,-1.18768,2.95076\C,0,-0.98247,-2.33746,2.4
 8964\C,0,-1.01099,-3.40569,-0.15561\C,0,1.54102,-2.91353,-1.32964\C,0,
 3.14793,-1.54395,0.58797\C,0,0.39537,-0.54762,3.48827\C,0,-2.1862,-2.2
 4342,1.67863\C,0,-0.91371,-3.06261,-1.56635\C,0,2.45935,-1.87144,-1.76
 247\C,0,3.26778,-0.31754,1.36087\C,0,2.50264,-0.1441,2.51717\C,0,-0.86
 201,-1.11086,3.26266\C,0,-2.201,-2.76662,0.38316\C,0,0.33675,-2.82159,
 -2.14166\C,0,3.24605,-1.19969,-0.82289\C,0,0.57367,0.89287,3.38768\C,0
 ,-2.80771,-0.95634,1.94885\C,0,1.8208,-1.13225,-2.84073\C,0,3.43874,0.
 78506,0.42653\C,0,1.87537,1.14124,2.78554\C,0,-1.99051,-0.25568,2.9274
 4\C,0,-2.83978,-2.02647,-0.69466\C,0,0.50946,-1.71938,-3.07497\N,0,-0.
 00657,0.02455,-0.00859\H,0,-0.97351,0.09818,0.38126\H,0,0.65589,0.5485
 1,0.59986\H,0,0.01,0.43145,-0.95482\H,0,0.27297,-0.97749,-0.06544\\Ver
 sion=EM64L-G09RevB.01\State=1-A\HF=-2343.1479264\RMSD=6.086e-10\Dipole
 =-0.008444,0.0092287,0.0035402\Quadrupole=-0.0040602,-0.0242348,0.0282
 95,0.0068924,-0.0035893,0.0248456\PG=C01 [X(C60H4N1)]\@

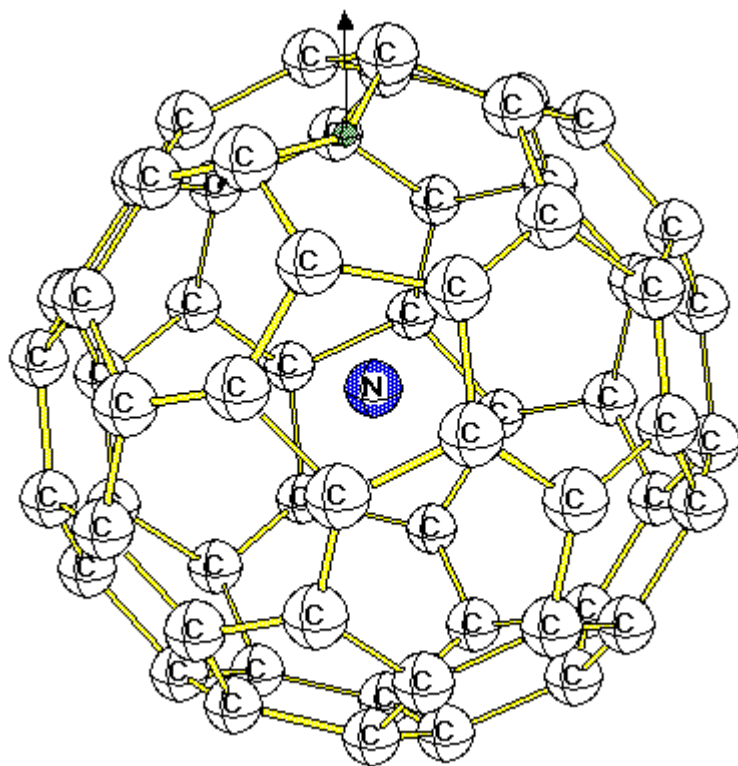
TRANSITION STATES

TS1a⁺ (TS of N^{•••}@C₆₀H⁺ → NH^{•••+}@C₆₀ by breaking [5,6]-bond, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN089\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\23-Mar-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCFCyc=1200 Nam
e=Dral\TS_NatC60_prot_hex_pent\1,4\C,0.892535,1.174305,3.222573\C,-0
.47865,0.722551,3.403736\C,-0.479402,-0.722073,3.403733\C,0.89131,-1.1
75252,3.222562\C,1.737361,-0.000914,3.101632\C,1.153592,2.303196,2.448
936\C,-1.53652,1.421077,2.820805\C,-1.538001,-1.419493,2.8208\C,1.1511
88,-2.304413,2.448923\C,2.804186,-0.001468,2.201706\C,0.053459,3.03705
4,1.846999\C,-2.645878,0.706071,2.206824\C,-1.261901,-2.621344,2.04877
3\C,2.260032,-2.307332,1.512171\C,3.069707,1.174031,1.388663\C,2.26244
3,2.304969,1.512187\C,-1.259162,2.622639,2.048784\C,-2.646613,-0.70332
7,2.20682\C,0.05029,-3.037117,1.84698\C,3.06848,-1.177239,1.388658\C,0
.482005,3.489537,0.530007\C,-3.096884,1.564086,1.078196\C,-0.417247,3.
509941,-0.537902\C,-2.208411,-2.686695,0.952107\C,1.841448,-3.035271,0
.326025\C,3.494253,0.724996,0.074\C,1.844613,3.033346,0.326043\C,-2.20
5608,2.688989,0.952122\C,-3.098515,-1.560865,1.078188\C,0.478364,-3.49
0043,0.529988\C,3.493491,-0.728637,0.073996\C,3.09187,-1.42624,-1.0655
76\C,-0.863797,-1.171947,-3.193594\C,-1.705318,0.000897,-3.029962\C,-0
.862573,1.172863,-3.193582\C,0.501258,0.724435,-3.424425\C,0.500503,-0
.724937,-3.424429\C,-1.104769,-2.318824,-2.441259\C,-2.786276,0.001457
,-2.13535\C,-1.102354,2.31999,-2.441247\C,1.564981,1.422479,-2.853678\
C,1.563496,-1.424092,-2.853684\C,-2.213348,-2.345987,-1.515147\C,-3.06
1038,1.229155,-1.39201\C,0.005448,3.050721,-1.848528\C,2.670524,0.6955
97,-2.252033\C,1.307559,-2.604228,-2.043717\C,0.002268,-3.05072,-1.848
549\C,-3.062307,-1.225954,-1.392013\C,-2.210904,2.3483,-1.515133\C,1.3
10273,2.602877,-2.043703\C,2.669794,-0.698366,-2.252035\C,-1.79141,-3.
076585,-0.33041\C,-3.631647,1.077075,-0.102098\C,3.09336,1.423026,-1.0
65571\C,2.248986,-2.601434,-0.937634\C,-0.420907,-3.509502,-0.537922\C
,-3.632765,-1.073291,-0.102105\C,-1.788202,3.078452,-0.330392\C,2.2516
97,2.599095,-0.93762\N,-0.114544,0.000075,-0.019591\H,-3.400391,0.0017
7,0.247378\Version=AM64L-G03RevD.02\State=4-A\HF=-2326.3597835\MP2=-2
334.2720192\RMSD=8.567e-09\Thermal=0.\PG=C01 [X(C60H1N1)]\@
```

UB3LYP/6-31G(d)



Zero-point correction= 0.382687 (Hartree/Particle)
 Thermal correction to Energy= 0.406369
 Thermal correction to Enthalpy= 0.407313
 Thermal correction to Gibbs Free Energy= 0.333880
 Sum of electronic and zero-point Energies= -2340.574507
 Sum of electronic and thermal Energies= -2340.550825
 Sum of electronic and thermal Enthalpies= -2340.549881
 Sum of electronic and thermal Free Energies= -2340.623314

1\1\FAU-CCC-CCDH152\Freq\UB3LYP\6-31G(d)\C60H11N1(1+,4)\DRAL\02-Dec-200
 8\0\#P UB3LYP/6-31G* FREQ=NORAMAN NAME=DRAL\TS_NatC60_prot_hex_pent\
 \1,4C,0.892535,1.174305,3.222573\C,-0.47865,0.722551,3.403736\C,-0.47
 9402,-0.722073,3.403733\C,0.89131,-1.175252,3.222562\C,1.737361,-0.000
 914,3.101632\C,1.153592,2.303196,2.448936\C,-1.53652,1.421077,2.820805
 \C,-1.538001,-1.419493,2.8208\C,1.151188,-2.304413,2.448923\C,2.804186
 ,-0.001468,2.201706\C,0.053459,3.037054,1.846999\C,-2.645878,0.706071,
 2.206824\C,-1.261901,-2.621344,2.048773\C,2.260032,-2.307332,1.512171\
 C,3.069707,1.174031,1.388663\C,2.262443,2.304969,1.512187\C,-1.259162,
 2.622639,2.048784\C,-2.646613,-0.703327,2.20682\C,0.05029,-3.037117,1.
 84698\C,3.06848,-1.177239,1.388658\C,0.482005,3.489537,0.530007\C,-3.0
 96884,1.564086,1.078196\C,-0.417247,3.509941,-0.537902\C,-2.208411,-2.
 686695,0.952107\C,1.841448,-3.035271,0.326025\C,3.494253,0.724996,0.07
 4\C,1.844613,3.033346,0.326043\C,-2.205608,2.688989,0.952122\C,-3.0985
 15,-1.560865,1.078188\C,0.478364,-3.490043,0.529988\C,3.493491,-0.7286
 37,0.073996\C,3.09187,-1.42624,-1.065576\C,-0.863797,-1.171947,-3.1935
 94\C,-1.705318,0.000897,-3.029962\C,-0.862573,1.172863,-3.193582\C,0.5
 01258,0.724435,-3.424425\C,0.500503,-0.724937,-3.424429\C,-1.104769,-2

.318824,-2.441259\C,-2.786276,0.001457,-2.13535\C,-1.102354,2.31999,-2.441247\C,1.564981,1.422479,-2.853678\C,1.563496,-1.424092,-2.853684\C,-2.213348,-2.345987,-1.515147\C,-3.061038,1.229155,-1.39201\C,0.005448,3.050721,-1.848528\C,2.670524,0.695597,-2.252033\C,1.307559,-2.604228,-2.043717\C,0.002268,-3.05072,-1.848549\C,-3.062307,-1.225954,-1.392013\C,-2.210904,2.3483,-1.515133\C,1.310273,2.602877,-2.043703\C,2.669794,-0.698366,-2.252035\C,-1.79141,-3.076585,-0.33041\C,-3.631647,1.077075,-0.102098\C,3.09336,1.423026,-1.065571\C,2.248986,-2.601434,-0.937634\C,-0.420907,-3.509502,-0.537922\C,-3.632765,-1.073291,-0.102105\C,-1.788202,3.078452,-0.330392\C,2.251697,2.599095,-0.93762\N,-0.114544,0.000075,-0.019591\H,-3.400391,0.00177,0.247378\\Version=AM64L-G03Rev D.02\State=4-A\HF=-2340.9571938\S2=3.752731\S2-1=0.\S2A=3.75\RMSD=4.419e-09\RMSF=2.539e-05\ZeroPoint=0.3826872\Thermal=0.4063687\ZPE=240.1398292\Dipole=-1.0305566,0.0005274,0.0445211\DipoleDeriv=0.068712,-0.0143\Polar=484.6863303,-0.0059123,473.0699713,-0.0824721,-0.0000617,465.7953174\PG=C01 [X(C60H1N1)]\NImag=1\\0.51077036,0.00641201,0.61981847,-7,-0.00000054,0.00002409,0.03411169,-0.00001119,0.08202425\\-0.000050194,-0.00000055,-0.00005073\\@

Vibrational Normal Modes

62

C	0.892518	1.174318	3.222573
C	-0.478660	0.722544	3.403736
C	-0.479392	-0.722080	3.403733
C	0.891327	-1.175239	3.222562
C	1.737361	-0.000889	3.101632
C	1.153559	2.303213	2.448936
C	-1.536541	1.421055	2.820805
C	-1.537981	-1.419515	2.820800
C	1.151221	-2.304396	2.448923
C	2.804186	-0.001427	2.201706
C	0.053415	3.037055	1.846999
C	-2.645888	0.706033	2.206824
C	-1.261863	-2.621362	2.048773
C	2.260065	-2.307299	1.512171
C	3.069690	1.174075	1.388663
C	2.262410	2.305002	1.512187
C	-1.259200	2.622621	2.048784
C	-2.646603	-0.703365	2.206820
C	0.050334	-3.037116	1.846980
C	3.068497	-1.177195	1.388658
C	0.481955	3.489544	0.530007
C	-3.096907	1.564041	1.078196
C	-0.417298	3.509935	-0.537902
C	-2.208372	-2.686727	0.952107
C	1.841492	-3.035244	0.326025
C	3.494243	0.725046	0.074000

C	1.844569	3.033373	0.326043
C	-2.205647	2.688957	0.952122
C	-3.098492	-1.560910	1.078188
C	0.478414	-3.490036	0.529988
C	3.493502	-0.728587	0.073996
C	3.091891	-1.426195	-1.065576
C	-0.863780	-1.171959	-3.193594
C	-1.705318	0.000872	-3.029962
C	-0.862590	1.172851	-3.193582
C	0.501248	0.724442	-3.424425
C	0.500513	-0.724930	-3.424429
C	-1.104736	-2.318840	-2.441259
C	-2.786276	0.001417	-2.135350
C	-1.102388	2.319974	-2.441247
C	1.564960	1.422502	-2.853678
C	1.563517	-1.424069	-2.853684
C	-2.213314	-2.346019	-1.515147
C	-3.061056	1.229111	-1.392010
C	0.005404	3.050721	-1.848528
C	2.670514	0.695636	-2.252033
C	1.307597	-2.604209	-2.043717
C	0.002312	-3.050720	-1.848549
C	-3.062289	-1.225998	-1.392013
C	-2.210938	2.348268	-1.515133
C	1.310235	2.602896	-2.043703
C	2.669804	-0.698327	-2.252035
C	-1.791366	-3.076611	-0.330410
C	-3.631663	1.077023	-0.102098
C	3.093339	1.423071	-1.065571
C	2.249024	-2.601402	-0.937634
C	-0.420856	-3.509508	-0.537922
C	-3.632750	-1.073343	-0.102105
C	-1.788246	3.078426	-0.330392
C	2.251659	2.599128	-0.937620
N	-0.114544	0.000073	-0.019591
H	-3.400391	0.001721	0.247378

NORMALMODES 180

[illegible]

C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	0.08	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	-0.08	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	0.00	0.00	0.00
H	-0.98	0.00	0.17

-1028.1408

[illegible]


```

C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.01 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.01 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.01 0.00 0.02
C 0.01 0.00 0.02
C 0.01 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.00 0.00 0.02
C 0.01 0.00 0.02
N -0.18 0.01 -0.97
H 0.00 0.00 0.02

```

TS1b⁺ (TS of N^{•••}@C₆₀H⁺ → NH^{•••+}@C₆₀ by breaking [6,6]-bond, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

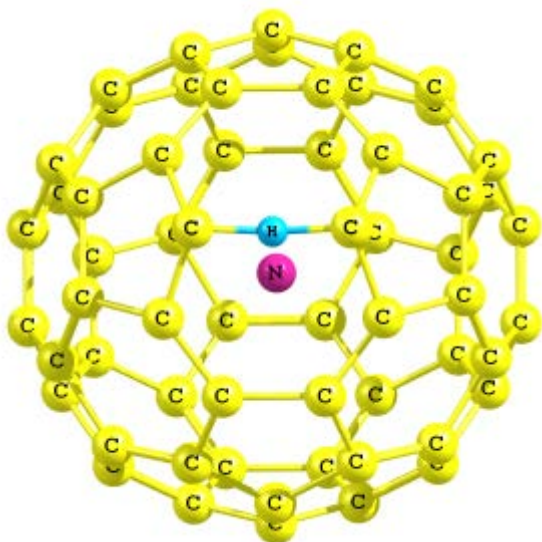
```

1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\26-Mar-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCFCyc=1200 Nam
e=Dral\TS N@C60H(+) -> NH(+)@C60 (quartet)\1,4\C,0,-0.9988788547,-3.
3611532801,-0.7062155359\C,0,-1.9943252087,-2.6039337883,-1.4276319096
\C,0,-1.3495742616,-1.9937829915,-2.5829885401\C,0,0.0388305136,-2.424
9005881,-2.5972091637\C,0,0.258011027,-3.2642713241,-1.4304197419\C,0,
-1.0027214164,-3.3624210934,0.6965372557\C,0,-2.9792752645,-1.90800296
12,-0.7356284749\C,0,-1.6840595412,-0.6959790658,-2.9651105891\C,0,1.0
346739546,-1.5467334617,-3.018856152\C,0,1.4562353434,-3.1758649391,-0
.7258668843\C,0,-2.0023013511,-2.6067824833,1.4133428086\C,0,-3.389239
8016,-0.5779347487,-1.1878447914\C,0,-0.6496979378,0.2064961328,-3.418
4213201\C,0,2.2967432034,-1.4702605995,-2.295879804\C,0,1.4521365468,-
3.1769845343,0.7306377982\C,0,0.249995493,-3.2663712357,1.4280519141\C
,0,-2.9836462899,-1.9102564216,0.716748185\C,0,-2.6890600709,0.0761724

```

493,-2.2309251156\C,0,0.6833594216,-0.207898889,-3.451131015\C,0,2.501
 0338534,-2.2671048636,-1.1688038268\C,0,-1.3643983903,-1.9978044588,2.
 5729474505\C,0,-3.9070613221,0.0221849985,-0.0107597228\C,0,-1.7013041
 426,-0.7004241181,2.9546067862\C,0,-0.9896243299,1.5348712122,-2.96255
 48519\C,0,2.7267294408,-0.0856012087,-2.2930459389\C,0,2.4942307912,-2
 .2688258619,1.1807944091\C,0,0.0238543977,-2.4286942876,2.5945318028\C
 ,0,-3.3982101724,-0.5826669392,1.1697035389\C,0,-2.2544621681,1.467029
 0876,-2.2294428426\C,0,1.7317046817,0.6951885818,-3.0149558376\C,0,3.1
 425230219,-1.7087261454,0.0082343667\C,0,3.5573092515,-0.3753126031,0.
 0103309121\C,0,1.0811181337,3.3356541659,0.7066859506\C,0,-0.172266091
 1,3.2781711723,1.4214542931\C,0,0.0063925181,2.4095218475,2.5783907339
 \C,0,1.3937149348,1.9778105271,2.6004372281\C,0,2.0568229896,2.5429743
 298,1.4363902478\C,0,1.0848749307,3.3364726355,-0.6954171719\C,0,-1.37
 5353751,3.2686619618,0.7252783671\C,0,-1.0069916415,1.5305099135,2.959
 2093964\C,0,1.7140969222,0.6906214762,3.0261951111\C,0,2.9976559465,1.
 7902312751,0.7383368245\C,0,-0.1644542644,3.2797251162,-1.4173261104\C
 ,0,-2.4688099037,2.40532087,1.1767719015\C,0,-0.6696121434,0.201343064
 9,3.414922997\C,0,2.7133959432,-0.0890858025,2.3092108197\C,0,3.001728
 2736,1.7913034377,-0.7179966109\C,0,2.064895896,2.5450136766,-1.420535
 0276\C,0,-1.3716014809,3.2686123408,-0.7279716551\C,0,-2.2681302024,1.
 4646245112,2.2192767631\C,0,0.6632143062,-0.2131187536,3.4549469704\C,
 0,3.3402521158,0.449584332,1.1851160845\C,0,0.0213295982,2.4132076281,
 -2.5745351568\C,0,-3.2078333155,2.172219087,-0.0073384195\C,0,2.283235
 7938,-1.4736374379,2.3075390779\C,0,3.3469190783,0.4513761444,-1.16460
 56385\C,0,1.40888296,1.9816519351,-2.5892404327\C,0,-2.4617258401,2.40
 32942295,-1.1856170194\C,0,-2.7030609003,0.0724979604,2.2162846691\C,0
 ,1.0170918826,-1.5512573318,3.0231263678\N,0,-0.0582331091,0.049251460
 1,-0.0215589168\H,0,-3.4042468761,1.0559164785,0.0203180324\\Version=A
 M64L-G03RevD.02\State=4-A\HF=-2326.3045194\MP2=-2334.2426483\RMSE=1.19
 2e-09\Thermal=0.\PG=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)



C -0.998878855 -3.361153280 -0.706215536
C -1.994325209 -2.603933788 -1.427631910
C -1.349574262 -1.993782992 -2.582988540
C 0.038830514 -2.424900588 -2.597209164
C 0.258011027 -3.264271324 -1.430419742
C -1.002721416 -3.362421093 0.696537256
C -2.979275264 -1.908002961 -0.735628475
C -1.684059541 -0.695979066 -2.965110589
C 1.034673955 -1.546733462 -3.018856152
C 1.456235343 -3.175864939 -0.725866884
C -2.002301351 -2.606782483 1.413342809
C -3.389239802 -0.577934749 -1.187844791
C -0.649697938 0.206496133 -3.418421320
C 2.296743203 -1.470260600 -2.295879804
C 1.452136547 -3.176984534 0.730637798
C 0.249995493 -3.266371236 1.428051914
C -2.983646290 -1.910256422 0.716748185
C -2.689060071 0.076172449 -2.230925116
C 0.683359422 -0.207898889 -3.451131015
C 2.501033853 -2.267104864 -1.168803827
C -1.364398390 -1.997804459 2.572947450
C -3.907061322 0.022184998 -0.010759723
C -1.701304143 -0.700424118 2.954606786
C -0.989624330 1.534871212 -2.962554852
C 2.726729441 -0.085601209 -2.293045939
C 2.494230791 -2.268825862 1.180794409
C 0.023854398 -2.428694288 2.594531803
C -3.398210172 -0.582666939 1.169703539
C -2.254462168 1.467029088 -2.229442843
C 1.731704682 0.695188582 -3.014955838
C 3.142523022 -1.708726145 0.008234367
C 3.557309252 -0.375312603 0.010330912
C 1.081118134 3.335654166 0.706685951
C -0.172266091 3.278171172 1.421454293
C 0.006392518 2.409521848 2.578390734
C 1.393714935 1.977810527 2.600437228
C 2.056822990 2.542974330 1.436390248
C 1.084874931 3.336472636 -0.695417172
C -1.375353751 3.268661962 0.725278367
C -1.006991642 1.530509914 2.959209396
C 1.714096922 0.690621476 3.026195111
C 2.997655946 1.790231275 0.738336824
C -0.164454264 3.279725116 -1.417326110
C -2.468809904 2.405320870 1.176771902
C -0.669612143 0.201343065 3.414922997
C 2.713395943 -0.089085802 2.309210820
C 3.001728274 1.791303438 -0.717996611
C 2.064895896 2.545013677 -1.420535028
C -1.371601481 3.268612341 -0.727971655
C -2.268130202 1.464624511 2.219276763

C 0.663214306 -0.213118754 3.454946970
 C 3.340252116 0.449584332 1.185116084
 C 0.021329598 2.413207628 -2.574535157
 C -3.207833316 2.172219087 -0.007338420
 C 2.283235794 -1.473637438 2.307539078
 C 3.346919078 0.451376144 -1.164605638
 C 1.408882960 1.981651935 -2.589240433
 C -2.461725840 2.403294230 -1.185617019
 C -2.703060900 0.072497960 2.216284669
 C 1.017091883 -1.551257332 3.023126368
 N -0.058233109 0.049251460 -0.021558917
 H -3.404246876 1.055916478 0.020318032

Zero-point correction= 0.378480 (Hartree/Particle)
 Thermal correction to Energy= 0.402517
 Thermal correction to Enthalpy= 0.403461
 Thermal correction to Gibbs Free Energy= 0.328515
 Sum of electronic and zero-point Energies= -2340.539387
 Sum of electronic and thermal Energies= -2340.515350
 Sum of electronic and thermal Enthalpies= -2340.514405
 Sum of electronic and thermal Free Energies= -2340.589352

1\1\FAU-CCC-CCDH159\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\29-Jun-200
 9\0\#P B3LYP/6-31G* SCFCYC=1200 FREQ=NORAMAN Geom=AllCheck NAME=DRAL\
 \TS N@C60H(+) -> NH(+)@C60 (quartet)\1,4\C,-0.9988788547,-3.361153280
 1,-0.7062155359\C,-1.9943252087,-2.6039337883,-1.4276319096\C,-1.34957
 42616,-1.9937829915,-2.5829885401\C,0.0388305136,-2.4249005881,-2.5972
 091637\C,0.258011027,-3.2642713241,-1.4304197419\C,-1.0027214164,-3.36
 24210934,0.6965372557\C,-2.9792752645,-1.9080029612,-0.7356284749\C,-1
 .6840595412,-0.6959790658,-2.9651105891\C,1.0346739546,-1.5467334617,-
 3.018856152\C,1.4562353434,-3.1758649391,-0.7258668843\C,-2.0023013511
 ,-2.6067824833,1.4133428086\C,-3.3892398016,-0.5779347487,-1.187844791
 4\C,-0.6496979378,0.2064961328,-3.4184213201\C,2.2967432034,-1.4702605
 995,-2.295879804\C,1.4521365468,-3.1769845343,0.7306377982\C,0.2499954
 93,-3.2663712357,1.4280519141\C,-2.9836462899,-1.9102564216,0.71674818
 5\C,-2.6890600709,0.0761724493,-2.2309251156\C,0.6833594216,-0.2078988
 89,-3.451131015\C,2.5010338534,-2.2671048636,-1.1688038268\C,-1.364398
 3903,-1.9978044588,2.5729474505\C,-3.9070613221,0.0221849985,-0.010759
 7228\C,-1.7013041426,-0.7004241181,2.9546067862\C,-0.9896243299,1.5348
 712122,-2.9625548519\C,2.7267294408,-0.0856012087,-2.2930459389\C,2.49
 42307912,-2.2688258619,1.1807944091\C,0.0238543977,-2.4286942876,2.594
 5318028\C,-3.3982101724,-0.5826669392,1.1697035389\C,-2.2544621681,1.4
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 1425230219,-1.7087261454,0.0082343667\C,3.5573092515,-0.3753126031,0.0
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 37149348,1.9778105271,2.6004372281\C,2.0568229896,2.5429743298,1.43639
 02478\C,1.0848749307,3.3364726355,-0.6954171719\C,-1.375353751,3.26866
 19618,0.7252783671\C,-1.0069916415,1.5305099135,2.9592093964\C,1.71409
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45\C,-0.1644542644,3.2797251162,-1.4173261104\C,-2.4688099037,2.405320
87,1.1767719015\C,-0.6696121434,0.2013430649,3.414922997\C,2.713395943
2,-0.0890858025,2.3092108197\C,3.0017282736,1.7913034377,-0.7179966109
\C,2.064895896,2.5450136766,-1.4205350276\C,-1.3716014809,3.2686123408
,-0.7279716551\C,-2.2681302024,1.4646245112,2.2192767631\C,0.663214306
2,-0.2131187536,3.4549469704\C,3.3402521158,0.449584332,1.1851160845\C
,0.0213295982,2.4132076281,-2.5745351568\C,-3.2078333155,2.172219087,-
0.0073384195\C,2.2832357938,-1.4736374379,2.3075390779\C,3.3469190783,
0.4513761444,-1.1646056385\C,1.40888296,1.9816519351,-2.5892404327\C,-
2.4617258401,2.4032942295,-1.1856170194\C,-2.7030609003,0.0724979604,2
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4025172\ZPE=237.4999979\Dipole=-0.8362628,0.2710054,-0.003077\DipoleDe
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)]\NImag=2\0.50285082,-0.09310341,0.22929248,-0.02425442,-0.08878175,
0.00690557\0.00001115,0.00014170,-0.00011302,-0.00028162,-0.00019783
-0.00007043,-0.00004064,0.00021835,0.00000302,0.00015378\\@

Vibrational Normal Modes

62

C	-0.998879	-3.361153	-0.706216
C	-1.994325	-2.603934	-1.427632
C	-1.349574	-1.993783	-2.582989
C	0.038831	-2.424901	-2.597209
C	0.258011	-3.264271	-1.430420
C	-1.002721	-3.362421	0.696537
C	-2.979275	-1.908003	-0.735628
C	-1.684060	-0.695979	-2.965111
C	1.034674	-1.546733	-3.018856
C	1.456235	-3.175865	-0.725867
C	-2.002301	-2.606782	1.413343
C	-3.389240	-0.577935	-1.187845
C	-0.649698	0.206496	-3.418421
C	2.296743	-1.470261	-2.295880
C	1.452137	-3.176985	0.730638
C	0.249995	-3.266371	1.428052
C	-2.983646	-1.910256	0.716748
C	-2.689060	0.076172	-2.230925
C	0.683359	-0.207899	-3.451131
C	2.501034	-2.267105	-1.168804
C	-1.364398	-1.997804	2.572947
C	-3.907061	0.022185	-0.010760
C	-1.701304	-0.700424	2.954607

[illegible]

C 0.00 0.00 0.00
N 0.00 0.00 0.00
H -0.95 0.30 0.03
-1207.7308
C 0.00 -0.01 0.01
C -0.01 -0.01 0.02
C 0.01 0.02 0.03
C -0.01 0.01 0.01
C 0.00 0.00 0.01
C 0.00 -0.02 0.00
C -0.07 -0.07 0.00
C 0.01 0.01 -0.04
C 0.00 0.01 0.02
C 0.00 0.00 0.00
C -0.01 -0.01 -0.02
C 0.01 -0.02 -0.04
C 0.01 0.02 -0.01
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.07 -0.08 0.01
C 0.05 0.01 -0.02
C 0.01 0.02 -0.01
C 0.00 0.00 0.00
C 0.01 0.01 -0.02
C 0.64 0.15 0.01
C 0.01 0.01 0.04
C 0.00 0.01 0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.01 0.01 -0.01
C 0.00 -0.04 0.05
C -0.04 0.02 0.00
C 0.01 0.01 -0.02
C 0.00 -0.01 0.00
C 0.00 -0.01 0.00
C -0.03 -0.03 0.01
C -0.01 -0.03 0.02
C 0.00 0.01 0.04
C 0.01 0.00 0.02
C -0.01 -0.01 0.01
C -0.03 -0.03 -0.01
C 0.00 -0.12 -0.01
C 0.00 0.01 -0.02
C 0.01 0.00 0.02
C -0.01 -0.01 0.00
C -0.01 -0.03 -0.02
C -0.03 -0.05 -0.04
C 0.00 0.02 0.01
C 0.00 0.00 0.00

```

C -0.01 -0.01 0.00
C -0.01 -0.01 -0.01
C 0.00 -0.12 0.01
C -0.04 0.02 -0.01
C 0.01 0.02 0.01
C 0.00 0.00 0.00
C 0.00 0.01 -0.04
C -0.46 0.47 -0.01
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.01 0.00 -0.02
C -0.03 -0.06 0.04
C 0.04 0.00 0.02
C -0.01 0.01 -0.01
N 0.06 -0.01 -0.04
H -0.03 0.10 0.12
-6.3384

```

TS1c⁺ (TS of N^{•••}@C₆₀H⁺ → NH^{•••+}@C₆₀ by breaking two bonds)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

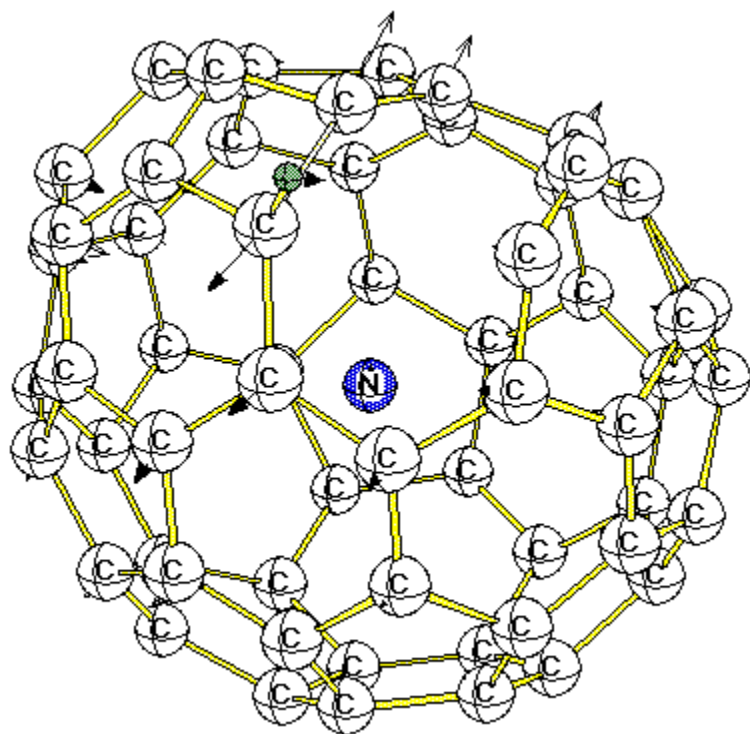
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0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCFCyc=1200 Nam
e=Dral\TS of N@C60H(+) -> NH(+)@C60 via breacking of two bonds\1,4\C
,0,-1.0977730808,3.5477499233,0.6533203564\C,0,-1.1668542118,3.5566312
889,-0.7451820948\C,0,-2.3455715779,2.8370840203,-1.1684542196\C,0,-3.
0277987271,2.4030414732,0.0560756702\C,0,-2.1940842755,2.8474344518,1.
1855091846\C,0,0.3547084458,3.3907402375,0.9125550649\C,0,0.1452748586
,3.1513870538,-0.9771812561\C,0,-2.127020608,1.9020540284,-2.163015737
7\C,0,-3.584593427,1.1280645168,0.1130442559\C,0,-1.8723885521,1.95476
68523,2.1995549822\C,0,3.0958246398,3.1458300937,0.4438731087\C,0,0.41
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1733703228\C,0,-3.4035843822,0.2893184652,1.3006497517\C,0,-0.48314206
,1.7722962121,2.6396319853\C,0,0.6421098458,2.3375330626,1.9908610565\C
,0,2.9926294825,3.1145320546,-0.7941067927\C,0,-0.772535033,1.6810306
138,-2.6832295767\C,0,-3.5385103455,0.2441603056,-1.0386655254\C,0,-2.
5835198444,0.7154219528,2.3539050535\C,0,3.0299977881,2.005327538,1.25
85426575\C,0,1.6975959508,1.5729710588,-2.3382424831\C,0,3.6337001146,
0.9106754016,0.5537109426\C,0,-1.9888822502,-0.3196963025,-2.879198714
8\C,0,-3.3551385657,-1.097532248,0.8867239622\C,0,-0.4356036187,0.4737
353349,3.2630852908\C,0,1.9331288553,1.6735958168,2.1613763909\C,0,2.8
683661977,1.9525111723,-1.565415849\C,0,-0.7536444285,0.3591850762,-3.
2494017\C,0,-3.4275704142,-1.1271332107,-0.5651269584\C,0,-1.701879531
4,-0.2105054982,3.026091411\C,0,-1.6974514844,-1.5538853567,2.67535344
46\C,0,0.5929697073,-3.4553774769,-0.6925409498\C,0,1.813498227,-2.857
6936601,-1.2054646121\C,0,2.6466936049,-2.4925673105,-0.0728298125\C,0

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,1.9209178406,-2.8197197157,1.1416342234\C,0,0.6612873103,-3.434910629
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230657,-2.0150962648,-2.3197143698\C,0,3.4249363415,-1.3409000299,-0.1
270845598\C,0,1.9651000377,-1.9411939111,2.2301569129\C,0,-0.497402762
9,-3.192802055,1.5010674631\C,0,-0.6855630762,-2.3842492758,-2.5048470
095\C,0,2.528318375,-0.7847209757,-2.3435121185\C,0,3.4982075672,-0.44
90949326,1.0138381621\C,0,0.7505427326,-1.6599378296,2.9643776698\C,0,
-1.7748322446,-2.9972374129,0.8296434951\C,0,-1.838360231,-3.022655221
7,-0.5661733383\C,0,0.4768441093,-1.7602312864,-2.9544571701\C,0,3.389
5299289,-0.4876699515,-1.2991900307\C,0,2.7349043344,-0.7108248254,2.1
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96,-1.6477135513,-2.4669272281\C,0,1.6706768088,0.2696149631,-2.875264
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,0,0.4401048478,-0.3511384568,-3.2825488177\C,0,3.5559021802,0.8871916
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UB3LYP/6-31G(d)



1 4

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C	-2.345571578	2.837084020	-1.168454220
C	-3.027798727	2.403041473	0.056075670
C	-2.194084276	2.847434452	1.185509185
C	0.354708446	3.390740238	0.912555065

C	0.145274859	3.151387054	-0.977181256
C	-2.127020608	1.902054028	-2.163015738
C	-3.584593427	1.128064517	0.113044256
C	-1.872388552	1.954766852	2.199554982
C	3.095824640	3.145830094	0.443873109
C	0.411766832	2.240790652	-2.080639132
C	-2.818054868	0.634833899	-2.173370323
C	-3.403584382	0.289318465	1.300649752
C	-0.483142060	1.772296212	2.639631985
C	0.642109846	2.337533063	1.990861056
C	2.992629482	3.114532055	-0.794106793
C	-0.772535033	1.681030614	-2.683229577
C	-3.538510346	0.244160306	-1.038665525
C	-2.583519844	0.715421953	2.353905054
C	3.029997788	2.005327538	1.258542658
C	1.697595951	1.572971059	-2.338242483
C	3.633700115	0.910675402	0.553710943
C	-1.988882250	-0.319696302	-2.879198715
C	-3.355138566	-1.097532248	0.886723962
C	-0.435603619	0.473735335	3.263085291
C	1.933128855	1.673595817	2.161376391
C	2.868366198	1.952511172	-1.565415849
C	-0.753644428	0.359185076	-3.249401700
C	-3.427570414	-1.127133211	-0.565126958
C	-1.701879531	-0.210505498	3.026091411
C	-1.697451484	-1.553885357	2.675353445
C	0.592969707	-3.455377477	-0.692540950
C	1.813498227	-2.857693660	-1.205464612
C	2.646693605	-2.492567310	-0.072829812
C	1.920917841	-2.819719716	1.141634223
C	0.661287310	-3.434910630	0.759725427
C	-0.629121454	-3.244898318	-1.339343538
C	1.753923066	-2.015096265	-2.319714370
C	3.424936342	-1.340900030	-0.127084560
C	1.965100038	-1.941193911	2.230156913
C	-0.497402763	-3.192802055	1.501067463
C	-0.685563076	-2.384249276	-2.504847010
C	2.528318375	-0.784720976	-2.343512118
C	3.498207567	-0.449094933	1.013838162
C	0.750542733	-1.659937830	2.964377670
C	-1.774832245	-2.997237413	0.829643495
C	-1.838360231	-3.022655222	-0.566173338
C	0.476844109	-1.760231286	-2.954457170
C	3.389529929	-0.487669952	-1.299190031
C	2.734904334	-0.710824825	2.142814979
C	-0.447718193	-2.293710335	2.636709012
C	-1.939039270	-1.647713551	-2.466927228
C	1.670676809	0.269614963	-2.875264884
C	0.750701616	-0.238201364	3.256959289
C	-2.527634437	-2.000972172	1.562763415

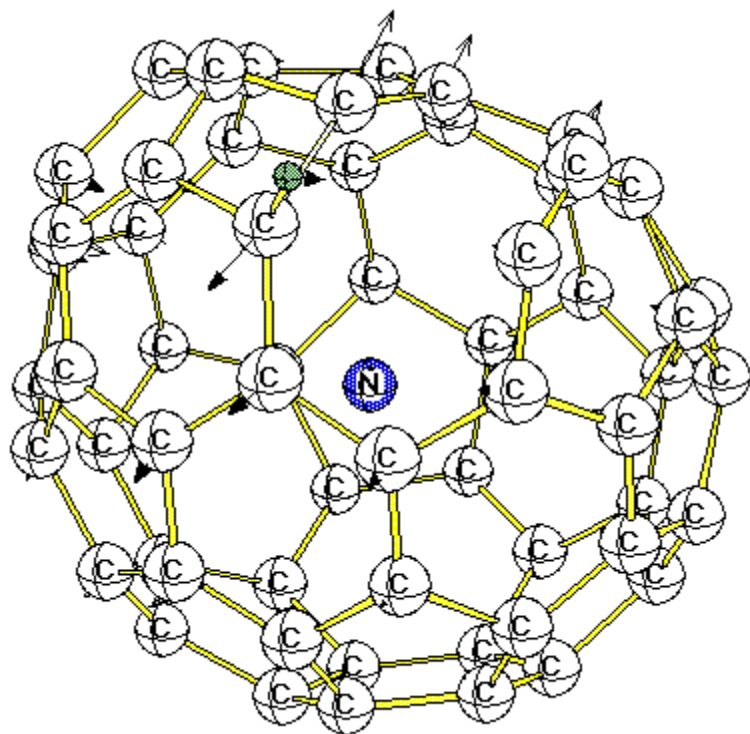
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 C 0.440104848 -0.351138457 -3.282548818
 C 3.555902180 0.887191617 -0.892434768
 C 1.937296248 0.366368036 2.719650069
 H 0.963698887 4.290210537 0.957956889
 N -0.086242953 -0.114681759 0.036631188

Zero-point correction= 0.379828 (Hartree/Particle)
 Thermal correction to Energy= 0.404297
 Thermal correction to Enthalpy= 0.405241
 Thermal correction to Gibbs Free Energy= 0.330954
 Sum of electronic and zero-point Energies= -2340.443729
 Sum of electronic and thermal Energies= -2340.419261
 Sum of electronic and thermal Enthalpies= -2340.418316
 Sum of electronic and thermal Free Energies= -2340.492603

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 H(+) -> NH(+)@C60 via breacking of two bonds\1,4\C,-1.0977730808,3.54
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 3455715779,2.8370840203,-1.1684542196\C,-3.0277987271,2.4030414732,0.0
 560756702\C,-2.1940842755,2.8474344518,1.1855091846\C,0.3547084458,3.3
 907402375,0.9125550649\C,0.1452748586,3.1513870538,-0.9771812561\C,-2.
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 0442559\C,-1.8723885521,1.9547668523,2.1995549822\C,3.0958246398,3.145
 8300937,0.4438731087\C,0.4117668318,2.2407906517,-2.0806391325\C,-2.81
 80548681,0.6348338989,-2.1733703228\C,-3.4035843822,0.2893184652,1.300
 6497517\C,-0.48314206,1.7722962121,2.6396319853\C,0.6421098458,2.33753
 30626,1.9908610565\C,2.9926294825,3.1145320546,-0.7941067927\C,-0.7725
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 7148\C,-3.3551385657,-1.097532248,0.8867239622\C,-0.4356036187,0.47373
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 3435121185\C,3.4982075672,-0.4490949326,1.0138381621\C,0.7505427326,-1.
 6599378296,2.9643776698\C,-1.7748322446,-2.9972374129,0.8296434951\C,
 -1.838360231,-3.0226552217,-0.5661733383\C,0.4768441093,-1.7602312864,
 -2.9544571701\C,3.3895299289,-0.4876699515,-1.2991900307\C,2.734904334
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 69833\C,0.4401048478,-0.3511384568,-3.2825488177\C,3.5559021802,0.8871
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Vibrational Normal Modes



62

C	-1.097773	3.547750	0.653320
C	-1.166854	3.556631	-0.745182
C	-2.345572	2.837084	-1.168454
C	-3.027799	2.403041	0.056076
C	-2.194084	2.847434	1.185509
C	0.354708	3.390740	0.912555
C	0.145275	3.151387	-0.977181
C	-2.127021	1.902054	-2.163016
C	-3.584593	1.128065	0.113044
C	-1.872389	1.954767	2.199555

C	3.095825	3.145830	0.443873
C	0.411767	2.240791	-2.080639
C	-2.818055	0.634834	-2.173370
C	-3.403584	0.289318	1.300650
C	-0.483142	1.772296	2.639632
C	0.642110	2.337533	1.990861
C	2.992629	3.114532	-0.794107
C	-0.772535	1.681031	-2.683230
C	-3.538510	0.244160	-1.038666
C	-2.583520	0.715422	2.353905
C	3.029998	2.005328	1.258543
C	1.697596	1.572971	-2.338242
C	3.633700	0.910675	0.553711
C	-1.988882	-0.319696	-2.879199
C	-3.355139	-1.097532	0.886724
C	-0.435604	0.473735	3.263085
C	1.933129	1.673596	2.161376
C	2.868366	1.952511	-1.565416
C	-0.753644	0.359185	-3.249402
C	-3.427570	-1.127133	-0.565127
C	-1.701880	-0.210505	3.026091
C	-1.697451	-1.553885	2.675353
C	0.592970	-3.455377	-0.692541
C	1.813498	-2.857694	-1.205465
C	2.646694	-2.492567	-0.072830
C	1.920918	-2.819720	1.141634
C	0.661287	-3.434911	0.759725
C	-0.629121	-3.244898	-1.339344
C	1.753923	-2.015096	-2.319714
C	3.424936	-1.340900	-0.127085
C	1.965100	-1.941194	2.230157
C	-0.497403	-3.192802	1.501067
C	-0.685563	-2.384249	-2.504847
C	2.528318	-0.784721	-2.343512
C	3.498208	-0.449095	1.013838
C	0.750543	-1.659938	2.964378
C	-1.774832	-2.997237	0.829643
C	-1.838360	-3.022655	-0.566173
C	0.476844	-1.760231	-2.954457
C	3.389530	-0.487670	-1.299190
C	2.734904	-0.710825	2.142815
C	-0.447718	-2.293710	2.636709
C	-1.939039	-1.647714	-2.466927
C	1.670677	0.269615	-2.875265
C	0.750702	-0.238201	3.256959
C	-2.527634	-2.000972	1.562763
C	-2.662185	-2.054847	-1.272037
C	0.440105	-0.351138	-3.282549
C	3.555902	0.887192	-0.892435
C	1.937296	0.366368	2.719650

H	0.963699	4.290211	0.957957
N	-0.086243	-0.114682	0.036631

NORMALMODES 180

C	0.16	-0.07	0.00
C	0.12	-0.02	-0.02
C	0.09	-0.02	0.00
C	0.11	-0.04	0.00
C	0.12	-0.08	-0.03
C	-0.01	0.08	0.51
C	0.07	0.19	-0.48
C	0.02	-0.01	-0.03
C	0.05	-0.01	0.00
C	0.01	-0.02	0.05
C	-0.05	0.02	0.01
C	-0.01	0.05	-0.29
C	0.00	-0.01	-0.01
C	0.01	-0.01	0.01
C	-0.02	-0.02	0.14
C	0.00	0.11	0.29
C	-0.06	-0.01	0.01
C	-0.03	-0.04	-0.13
C	0.02	-0.01	0.00
C	-0.01	-0.02	0.03
C	-0.04	0.03	0.03
C	0.01	0.02	-0.15
C	-0.07	0.02	0.00
C	-0.03	-0.03	-0.03
C	0.00	-0.01	0.00
C	-0.03	-0.04	0.07
C	0.02	0.04	0.13
C	-0.05	0.01	-0.03
C	-0.03	-0.05	-0.08
C	0.00	-0.01	0.00
C	-0.03	-0.03	0.03
C	-0.02	-0.02	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.01	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	-0.01	0.00
C	-0.01	-0.01	0.00
C	-0.03	0.02	0.00
C	-0.01	0.01	0.00
C	0.00	-0.01	0.00
C	-0.01	-0.01	0.00
C	-0.02	0.00	-0.01
C	-0.04	0.02	0.00
C	-0.01	-0.01	0.01

C -0.01 -0.01 0.00
C -0.01 -0.01 0.00
C -0.01 -0.02 -0.01
C -0.04 0.02 0.00
C -0.02 0.01 0.01
C -0.01 -0.01 0.00
C -0.02 -0.02 0.00
C 0.00 -0.01 -0.06
C -0.01 -0.02 0.03
C -0.01 -0.02 0.00
C -0.01 -0.01 0.00
C -0.01 -0.03 -0.05
C -0.08 0.02 0.00
C 0.00 0.01 0.04
H 0.15 -0.02 -0.04
N 0.02 0.06 0.00
-103.8116
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 0.00 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 0.00 0.00
C 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00
C 0.02 -0.01 0.00

```

C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02  0.00  0.00
C  0.02  0.00  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02  0.00  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02 -0.01  0.00
C  0.02  0.00  0.00
C  0.02 -0.01  0.00
C  0.02  0.00  0.00
H  0.02 -0.01  0.00
N -0.95  0.26 -0.01
61.3357

```

TS1d⁺ (TS of N^{•••}@C₆₀H⁺ → NH^{•••+}@C₆₀ by breaking three bonds)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

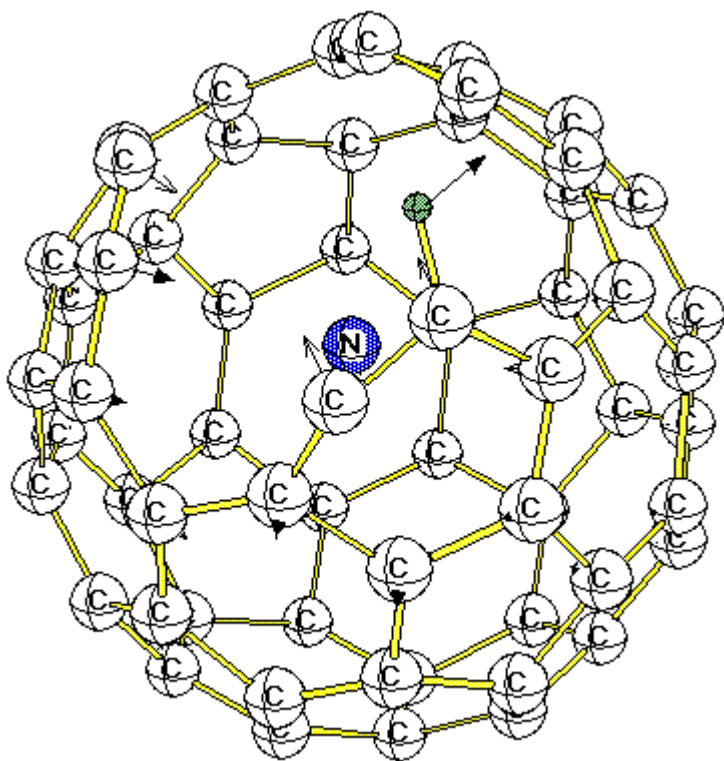
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1\1\FAU-CCC-CCDN092\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\27-Mar-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCFCyc=1200 Nam
e=DrAl\open TS of N@C60H(+) -> NH(+)@C60 via 3-bonds breacking\1,4\C
,0,0.402954,2.885427,-2.012482\C,0,-0.630829,3.341429,-1.102746\C,0,0.
003257,3.542889,0.18464\C,0,1.410192,3.265801,0.060101\C,0,1.660498,2.
856243,-1.318902\C,0,0.12456,1.904137,-2.953255\C,0,-1.91419,2.814643,
-1.177468\C,0,-0.662326,3.195298,1.352477\C,0,2.147349,2.710796,1.1562
71\C,0,2.669101,1.898143,-1.650333\C,0,-1.224024,1.369571,-3.05051\C,0
,-2.627483,2.474085,0.040505\C,0,0.05202,2.509157,2.414217\C,0,3.34877
2,2.192609,0.622637\C,0,2.335731,0.782387,-2.541419\C,0,1.078491,0.834
077,-3.184333\C,0,-2.222175,1.809303,-2.179808\C,0,-2.013445,2.668302,
1.281122\C,0,1.429754,2.225575,2.32806\C,0,3.574072,1.864055,-0.559979

```

\C,0,-1.121805,-0.035288,-3.37753\C,0,-3.389007,1.265078,-0.210603\C,0
 ,-2.013164,-0.956308,-2.813636\C,0,-0.888418,1.588317,3.026072\C,0,3.0
 67448,0.266584,2.584276\C,0,2.8649,-0.573822,-2.232721\C,0,0.283835,-0
 .359707,-3.472225\C,0,-3.137604,0.851508,-1.583313\C,0,-2.152839,1.669
 349,2.318065\C,0,1.910086,0.992821,2.946549\C,0,3.802683,-0.82455,-1.1
 9529\C,0,3.668445,-1.977758,-0.487597\C,0,-0.55383,-2.852598,2.00842\C
 ,0,-1.81619,-2.79937,1.292473\C,0,-1.568427,-3.208831,-0.074545\C,0,-0
 .154312,-3.507086,-0.196743\C,0,0.489163,-3.259095,1.087444\C,0,-0.271
 647,-1.895778,2.976998\C,0,-2.727886,-1.774791,1.557181\C,0,-2.244908,
 -2.580835,-1.126278\C,0,0.50703,-3.223117,-1.382437\C,0,1.815103,-2.79
 934,1.203636\C,0,-1.217855,-0.837155,3.259004\C,0,-3.417303,-1.112467,
 0.464153\C,0,-1.532686,-2.246098,-2.345132\C,0,1.827026,-2.648297,-1.3
 1747\C,0,2.139107,-1.882162,2.304493\C,0,1.068856,-1.375254,3.100699\C
 ,0,-2.417985,-0.769963,2.560128\C,0,-3.184913,-1.50923,-0.851819\C,0,-
 0.189066,-2.572876,-2.480583\C,0,2.511374,-2.571897,-0.047851\C,0,-0.4
 43387,0.363204,3.501597\C,0,-3.523741,0.3033,0.791342\C,0,1.966783,-1.
 675881,-2.366998\C,0,3.207101,-0.948885,2.314475\C,0,0.958925,0.0381,3
 .429282\C,0,-2.903746,0.51341,2.084238\C,0,-3.041497,-0.504666,-1.8986
 51\C,0,0.72594,-1.613645,-3.072297\H,0,4.335346,-0.019052,-0.676278\N,
 0,1.228779,-0.082005,0.108954\\Version=AM64L-G03RevD.02\\State=4-A\\HF=-
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 N1)]\\@

UB3LYP/6-31G(d)



1 4

C	0.402954000	2.885427000	-2.012482000
C	-0.630829000	3.341429000	-1.102746000

C	0.003257000	3.542889000	0.184640000
C	1.410192000	3.265801000	0.060101000
C	1.660498000	2.856243000	-1.318902000
C	0.124560000	1.904137000	-2.953255000
C	-1.914190000	2.814643000	-1.177468000
C	-0.662326000	3.195298000	1.352477000
C	2.147349000	2.710796000	1.156271000
C	2.669101000	1.898143000	-1.650333000
C	-1.224024000	1.369571000	-3.050510000
C	-2.627483000	2.474085000	0.040505000
C	0.052020000	2.509157000	2.414217000
C	3.348772000	2.192609000	0.622637000
C	2.335731000	0.782387000	-2.541419000
C	1.078491000	0.834077000	-3.184333000
C	-2.222175000	1.809303000	-2.179808000
C	-2.013445000	2.668302000	1.281122000
C	1.429754000	2.225575000	2.328060000
C	3.574072000	1.864055000	-0.559979000
C	-1.121805000	-0.035288000	-3.377530000
C	-3.389007000	1.265078000	-0.210603000
C	-2.013164000	-0.956308000	-2.813636000
C	-0.888418000	1.588317000	3.026072000
C	3.067448000	0.266584000	2.584276000
C	2.864900000	-0.573822000	-2.232721000
C	0.283835000	-0.359707000	-3.472225000
C	-3.137604000	0.851508000	-1.583313000
C	-2.152839000	1.669349000	2.318065000
C	1.910086000	0.992821000	2.946549000
C	3.802683000	-0.824550000	-1.195290000
C	3.668445000	-1.977758000	-0.487597000
C	-0.553830000	-2.852598000	2.008420000
C	-1.816190000	-2.799370000	1.292473000
C	-1.568427000	-3.208831000	-0.074545000
C	-0.154312000	-3.507086000	-0.196743000
C	0.489163000	-3.259095000	1.087444000
C	-0.271647000	-1.895778000	2.976998000
C	-2.727886000	-1.774791000	1.557181000
C	-2.244908000	-2.580835000	-1.126278000
C	0.507030000	-3.223117000	-1.382437000
C	1.815103000	-2.799340000	1.203636000
C	-1.217855000	-0.837155000	3.259004000
C	-3.417303000	-1.112467000	0.464153000
C	-1.532686000	-2.246098000	-2.345132000
C	1.827026000	-2.648297000	-1.317470000
C	2.139107000	-1.882162000	2.304493000
C	1.068856000	-1.375254000	3.100699000
C	-2.417985000	-0.769963000	2.560128000
C	-3.184913000	-1.509230000	-0.851819000
C	-0.189066000	-2.572876000	-2.480583000
C	2.511374000	-2.571897000	-0.047851000

```

C      -0.443387000 0.363204000 3.501597000
C      -3.523741000 0.303300000 0.791342000
C      1.966783000 -1.675881000 -2.366998000
C      3.207101000 -0.948885000 2.314475000
C      0.958925000 0.038100000 3.429282000
C      -2.903746000 0.513410000 2.084238000
C      -3.041497000 -0.504666000 -1.898651000
C      0.725940000 -1.613645000 -3.072297000
H      4.335346000 -0.019052000 -0.676278000
N      1.228779000 -0.082005000 0.108954000

```

```

Zero-point correction=          0.374248 (Hartree/Particle)
Thermal correction to Energy=    0.400063
Thermal correction to Enthalpy=  0.401007
Thermal correction to Gibbs Free Energy= 0.325196
Sum of electronic and zero-point Energies= -2340.380720
Sum of electronic and thermal Energies= -2340.354906
Sum of electronic and thermal Enthalpies= -2340.353962
Sum of electronic and thermal Free Energies= -2340.429772

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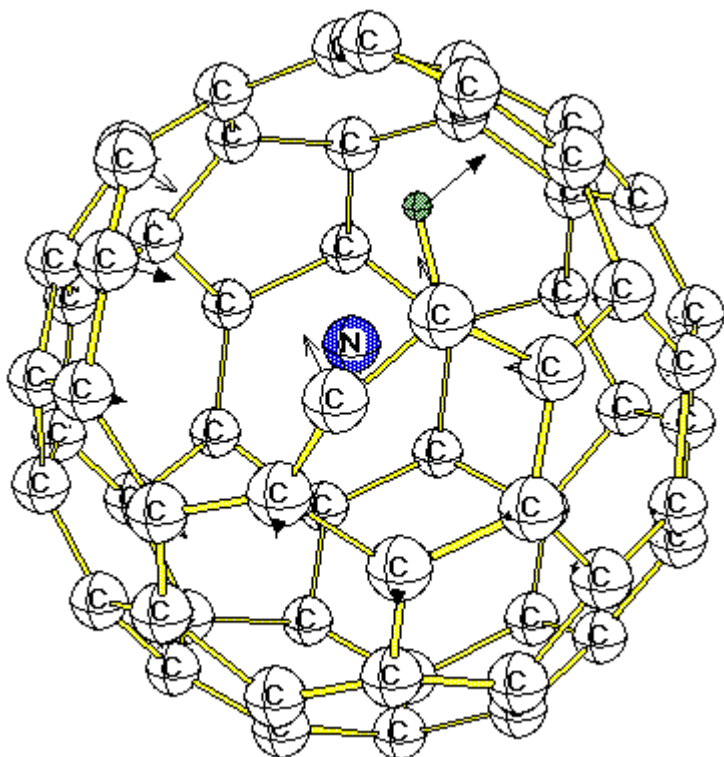
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UB3LYP/6-31G* Freq=NoRaman Pop=None Name=Dral\openTS of N@C60H(+)->
NH(+ )@C60 via breaking 3 bonds (quartet)\1,4\C,0.402954,2.885427,-2.
012482\C,-0.630829,3.341429,-1.102746\C,0.003257,3.542889,0.18464\C,1.
410192,3.265801,0.060101\C,1.660498,2.856243,-1.318902\C,0.12456,1.904
137,-2.953255\C,-1.91419,2.814643,-1.177468\C,-0.662326,3.195298,1.352
477\C,2.147349,2.710796,1.156271\C,2.669101,1.898143,-1.650333\C,-1.22
4024,1.369571,-3.05051\C,-2.627483,2.474085,0.040505\C,0.05202,2.50915
7,2.414217\C,3.348772,2.192609,0.622637\C,2.335731,0.782387,-2.541419\
C,1.078491,0.834077,-3.184333\C,-2.22175,1.809303,-2.179808\C,-2.0134
45,2.668302,1.281122\C,1.429754,2.225575,2.32806\C,3.574072,1.864055,-
0.559979\C,-1.121805,-0.035288,-3.37753\C,-3.389007,1.265078,-0.210603
\C,-2.013164,-0.956308,-2.813636\C,-0.888418,1.588317,3.026072\C,3.067
448,0.266584,2.584276\C,2.8649,-0.573822,-2.232721\C,0.283835,-0.35970
7,-3.472225\C,-3.137604,0.851508,-1.583313\C,-2.152839,1.669349,2.3180
65\C,1.910086,0.992821,2.946549\C,3.802683,-0.82455,-1.19529\C,3.66844
5,-1.977758,-0.487597\C,-0.55383,-2.852598,2.00842\C,-1.81619,-2.79937
,1.292473\C,-1.568427,-3.208831,-0.074545\C,-0.154312,-3.507086,-0.196
743\C,0.489163,-3.259095,1.087444\C,-0.271647,-1.895778,2.976998\C,-2.
727886,-1.774791,1.557181\C,-2.244908,-2.580835,-1.126278\C,0.50703,-3
.223117,-1.382437\C,1.815103,-2.79934,1.203636\C,-1.217855,-0.837155,3
.259004\C,-3.417303,-1.112467,0.464153\C,-1.532686,-2.246098,-2.345132
\C,1.827026,-2.648297,-1.31747\C,2.139107,-1.882162,2.304493\C,1.06885
6,-1.375254,3.100699\C,-2.417985,-0.769963,2.560128\C,-3.184913,-1.509
23,-0.851819\C,-0.189066,-2.572876,-2.480583\C,2.511374,-2.571897,-0.0
47851\C,-0.443387,0.363204,3.501597\C,-3.523741,0.3033,0.791342\C,1.96
6783,-1.675881,-2.366998\C,3.207101,-0.948885,2.314475\C,0.958925,0.03
81,3.429282\C,-2.903746,0.51341,2.084238\C,-3.041497,-0.504666,-1.8986
51\C,0.72594,-1.613645,-3.072297\H,4.335346,-0.019052,-0.676278\N,1.22
8779,-0.082005,0.108954\Version=IA64L-G03RevE.01\State=4-A\HF=-2340.7

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575,-0.005328,-0.0624768,-0.0255385,0.0109007,0.0394044,0.0775927,0.06
14196,0.1077037,-0.0311431,0.0597364,0.0386769,-0.0459668,0.0181417,-0
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1,-0.0012273,-0.0806313,0.0072992,0.0740029,0.0876991,0.077549,0.06822
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48,-0.0011824,-0.0679365,0.0231376,0.0129137,0.0710389,0.0559688,-0.11
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Vibrational Normal Modes



62

C	0.402953	2.885427	-2.012482
C	-0.630830	3.341429	-1.102746
C	0.003256	3.542889	0.184640
C	1.410191	3.265801	0.060101
C	1.660497	2.856243	-1.318902
C	0.124560	1.904137	-2.953255
C	-1.914191	2.814643	-1.177468
C	-0.662327	3.195298	1.352477
C	2.147348	2.710796	1.156271
C	2.669101	1.898143	-1.650333
C	-1.224024	1.369571	-3.050510
C	-2.627483	2.474085	0.040505
C	0.052020	2.509157	2.414217
C	3.348772	2.192610	0.622637
C	2.335731	0.782387	-2.541419
C	1.078491	0.834077	-3.184333
C	-2.222175	1.809303	-2.179808
C	-2.013446	2.668302	1.281122
C	1.429754	2.225575	2.328060
C	3.574072	1.864056	-0.559979
C	-1.121805	-0.035288	-3.377530
C	-3.389007	1.265077	-0.210603
C	-2.013164	-0.956308	-2.813636
C	-0.888418	1.588317	3.026072
C	3.067448	0.266585	2.584276
C	2.864900	-0.573821	-2.232721

C	0.283835	-0.359707	-3.472225
C	-3.137604	0.851507	-1.583313
C	-2.152839	1.669349	2.318065
C	1.910086	0.992821	2.946549
C	3.802683	-0.824549	-1.195290
C	3.668445	-1.977757	-0.487597
C	-0.553829	-2.852598	2.008420
C	-1.816189	-2.799370	1.292473
C	-1.568426	-3.208831	-0.074545
C	-0.154311	-3.507086	-0.196743
C	0.489164	-3.259095	1.087444
C	-0.271647	-1.895778	2.976998
C	-2.727886	-1.774792	1.557181
C	-2.244908	-2.580835	-1.126278
C	0.507031	-3.223117	-1.382437
C	1.815104	-2.799340	1.203636
C	-1.217855	-0.837155	3.259004
C	-3.417303	-1.112468	0.464153
C	-1.532686	-2.246098	-2.345132
C	1.827026	-2.648297	-1.317470
C	2.139107	-1.882162	2.304493
C	1.068856	-1.375254	3.100699
C	-2.417985	-0.769963	2.560128
C	-3.184913	-1.509231	-0.851819
C	-0.189066	-2.572876	-2.480583
C	2.511374	-2.571897	-0.047851
C	-0.443387	0.363204	3.501597
C	-3.523741	0.303299	0.791342
C	1.966783	-1.675881	-2.366998
C	3.207101	-0.948884	2.314475
C	0.958925	0.038100	3.429282
C	-2.903746	0.513409	2.084238
C	-3.041497	-0.504667	-1.898651
C	0.725940	-1.613645	-3.072297
H	4.335346	-0.019051	-0.676278
N	1.228779	-0.082005	0.108954

NORMALMODES 180

C	0.01	0.00	0.00
C	0.01	0.00	0.00
C	0.01	0.01	0.00
C	0.01	0.02	0.00
C	0.01	0.01	0.01
C	0.01	-0.01	0.01
C	0.01	0.00	0.00
C	0.01	0.01	0.00
C	0.01	0.02	0.00
C	-0.01	-0.01	0.02
C	0.01	-0.01	0.01
C	0.01	0.00	0.00

C 0.01 0.01 0.00
C 0.00 -0.06 0.06
C 0.00 -0.02 0.03
C 0.01 -0.02 0.01
C 0.01 -0.01 0.00
C 0.01 0.01 0.00
C 0.00 0.02 -0.01
C -0.03 0.01 0.03
C 0.01 -0.01 0.01
C 0.01 0.00 0.01
C 0.00 -0.01 0.00
C 0.02 0.00 0.00
C -0.06 -0.02 -0.19
C -0.07 0.00 0.16
C 0.01 -0.02 0.02
C 0.00 0.00 0.00
C 0.01 0.01 0.00
C 0.01 0.00 -0.07
C 0.07 0.17 0.15
C -0.14 0.36 0.30
C -0.01 -0.01 0.00
C -0.01 0.00 0.00
C -0.02 -0.01 0.00
C -0.03 -0.02 -0.01
C -0.02 -0.03 -0.01
C 0.01 -0.01 -0.01
C 0.00 0.01 0.00
C -0.01 0.00 0.00
C -0.02 0.00 0.01
C -0.04 -0.01 -0.05
C 0.02 0.00 -0.01
C 0.00 0.01 0.01
C -0.01 0.00 0.00
C 0.07 -0.18 -0.05
C -0.01 0.01 -0.09
C 0.02 -0.01 -0.04
C 0.02 0.00 0.00
C -0.01 0.01 0.00
C 0.00 0.01 0.02
C 0.03 -0.15 -0.04
C 0.03 0.00 -0.01
C 0.00 0.01 0.01
C 0.04 -0.06 0.05
C 0.03 -0.01 -0.29
C 0.03 -0.01 -0.04
C 0.02 0.00 0.00
C 0.00 0.01 0.00
C 0.01 0.00 0.04
H 0.50 0.18 -0.36
N -0.12 -0.02 -0.02

-129.2208

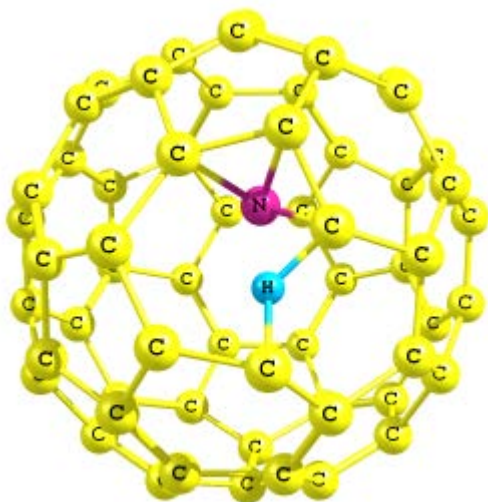
¹TS1j (TS of endohedrally bound N@C₆₀H → NH@C₆₀ by breaking [5,6]-bond, singlet)

MP2/6-31G(d)//B3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN082\SP\RMP2-FC\6-31G(d)\C60H1N1\DRAL\03-Aug-2010\0\#P
RMP2/6-31G*  Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=None N
ame=Dral\TS1f N@C60H -> NH@C60 via breaking 6,6-bond\0,1\C,0.9039214
63,-1.163347375,-3.153945611\C,-0.451768119,-0.722911108,-3.338634817\
C,-0.414748372,0.756653318,-3.362060646\C,0.947210057,1.197346168,-3.1
89154921\C,1.764878187,0.008826154,-3.042202695\C,1.188673723,-2.31639
6886,-2.406561884\C,-1.521557322,-1.438627277,-2.779598662\C,-1.444778
901,1.482385928,-2.811218404\C,1.209444857,2.341310052,-2.415656722\C,
2.831591517,0.003809509,-2.144402737\C,0.097549132,-3.054719229,-1.819
716355\C,-2.742830404,-0.819221806,-2.25553994\C,-1.21105223,2.732388
898,-2.077385144\C,2.304682455,2.323429714,-1.467370376\C,3.098588772,
-1.173158557,-1.336120752\C,2.290690792,-2.303535652,-1.465759671\C,-1
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\C,3.51132846,-0.720109943,-0.018790604\C,1.872373941,-3.038858906,-0.
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9041,-2.316056775,2.451909584\C,1.563032251,-1.419297919,2.890913924\C
,1.557784202,1.430162514,2.881995028\C,-2.204879856,2.374681722,1.5132
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\C,-1.781822219,3.194209375,0.317361017\C,-3.799390865,-1.13849457,0.1
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64,0.978730522\C,-0.396223946,3.547842224,0.54409144\C,-3.240011062,0.
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0H1N1)]\@

B3LYP/6-31G(d)



0 1

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C	-0.451768119	-0.722911108	-3.338634817
C	-0.414748372	0.756653318	-3.362060646
C	0.947210057	1.197346168	-3.189154921
C	1.764878187	0.008826154	-3.042202695
C	1.188673723	-2.316396886	-2.406561884
C	-1.521557322	-1.438627277	-2.779598662
C	-1.444778901	1.482385928	-2.811218404
C	1.209444857	2.341310052	-2.415656722
C	2.831591517	0.003809509	-2.144402737
C	0.097549132	-3.054719229	-1.819716355
C	-2.742830404	-0.819221806	-2.255553994
C	-1.211052230	2.732388898	-2.077385144
C	2.304682455	2.323429714	-1.467370376
C	3.098588772	-1.173158557	-1.336120752
C	2.290690792	-2.303535652	-1.465759671
C	-1.224305291	-2.641632015	-2.019896484
C	-2.480949164	0.677834981	-2.073081128
C	0.126059750	3.105927206	-1.840327128
C	3.098128543	1.182679198	-1.333921147
C	0.513986260	-3.499221820	-0.501566549
C	-3.155633545	-1.623014466	-1.120719624
C	-0.404155676	-3.502388729	0.552434953
C	-2.176713540	2.886774027	-0.995106004
C	1.880728852	3.057664989	-0.284877914
C	3.511328460	-0.720109943	-0.018790604
C	1.872373941	-3.038858906	-0.279987107
C	-2.186902976	-2.711690580	-0.948071807
C	-3.033878912	1.671587121	-1.118004403
C	0.529120485	3.539641653	-0.512713657

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C    3.515413815  0.731525810 -0.019812448
C    3.101323057  1.431888564  1.117314433
C    -0.868570668  1.171943807  3.196581007
C    -1.699405811 -0.014089157  3.054179972
C    -0.866743032 -1.182817815  3.236810823
C    0.490061719 -0.725853115  3.453318747
C    0.485553212  0.730506133  3.441412307
C    -1.105178319  2.332280456  2.438676443
C    -2.760521069 -0.026097373  2.134281374
C    -1.109609041 -2.316056775  2.451909584
C    1.563032251 -1.419297919  2.890913924
C    1.557784202  1.430162514  2.881995028
C    -2.204879856  2.374681722  1.513290787
C    -3.079049214 -1.269949777  1.375057122
C    0.005733287 -3.036158161  1.864322022
C    2.668894530 -0.691902254  2.297119218
C    1.311210699  2.610331048  2.069529287
C    0.009835769  3.058905258  1.855192400
C    -2.980556147  1.206395854  1.409293527
C    -2.220895456 -2.365455985  1.530864186
C    1.312891658 -2.598150602  2.078588330
C    2.670741764  0.708280431  2.298917770
C    -1.781822219  3.194209375  0.317361017
C    -3.799390865 -1.138494570  0.101745452
C    3.103521849 -1.418280580  1.120191086
C    2.270115932  2.612987364  0.978730522
C    -0.396223946  3.547842224  0.544091440
C    -3.240011062  0.863313616  0.041072267
C    -1.778930241 -3.093185763  0.331598503
C    2.266554151 -2.600056275  0.983773727
N    -1.888201387  0.710373836 -0.645506383
H    -3.078632681 -0.254516193 -0.246098866

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Zero-point correction= 0.382436 (Hartree/Particle)

Thermal correction to Energy= 0.404349

Thermal correction to Enthalpy= 0.405294

Thermal correction to Gibbs Free Energy= 0.338670

Sum of electronic and zero-point Energies= -2340.739536

Sum of electronic and thermal Energies= -2340.717623

Sum of electronic and thermal Enthalpies= -2340.716678

Sum of electronic and thermal Free Energies= -2340.783302

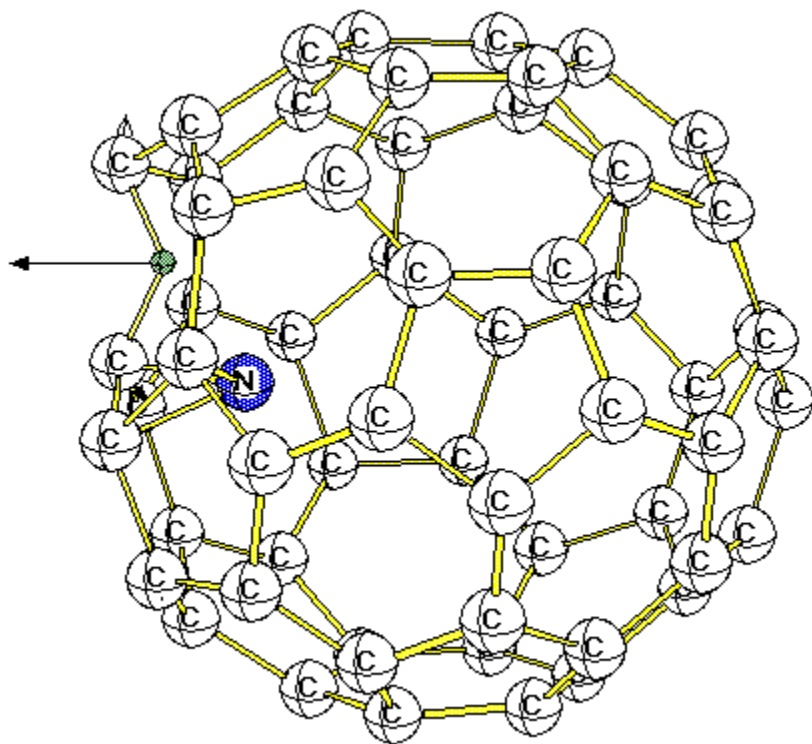
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0.451768119,-0.722911108,-3.338634817\C,-0.414748372,0.756653318,-3.36
2060646\C,0.947210057,1.197346168,-3.189154921\C,1.764878187,0.0088261
54,-3.042202695\C,1.188673723,-2.316396886,-2.406561884\C,-1.521557322
,-1.438627277,-2.779598662\C,-1.444778901,1.482385928,-2.811218404\C,1
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 0690792,-2.303535652,-1.465759671\C,-1.224305291,-2.641632015,-2.01989
 6484\C,-2.480949164,0.677834981,-2.073081128\C,0.12605975,3.105927206,
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Vibrational Normal Modes



62

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C	0.590982	-0.907927	-3.284470
C	-0.830241	-1.287601	-3.120147
C	-1.641857	-0.095939	-3.136236
C	-0.742648	1.030673	-3.294108
C	1.688922	1.266190	-2.876120
C	1.631426	-1.596873	-2.642558
C	-1.174430	-2.339927	-2.304537
C	-2.751905	-0.005397	-2.278730
C	-0.988872	2.219790	-2.609038
C	2.759273	0.569282	-2.206249
C	1.443328	-2.804753	-1.832965
C	-2.379868	-2.313743	-1.466753
C	-2.990646	1.224559	-1.551183
C	0.111676	2.964444	-2.022397
C	1.418349	2.492437	-2.153054
C	2.744192	-0.826755	-2.112091
C	-0.046233	-2.935428	-1.505569
C	-3.115450	-1.113434	-1.424647
C	-2.130706	2.312413	-1.711657
C	3.155635	1.357630	-1.053024
C	2.414708	-2.733041	-0.757969
C	3.509099	0.716856	0.137936
C	-2.160183	-3.036808	-0.219124
C	-3.476597	0.870040	-0.226308
C	-0.345363	3.500725	-0.751773

C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.02
C	0.00	0.00	0.00
C	-0.01	0.00	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	-0.03	-0.01	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	-0.02
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.15	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.11	0.07	-0.02
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	0.00	-0.02	0.02
H	0.00	-0.98	0.06

-1047.6217

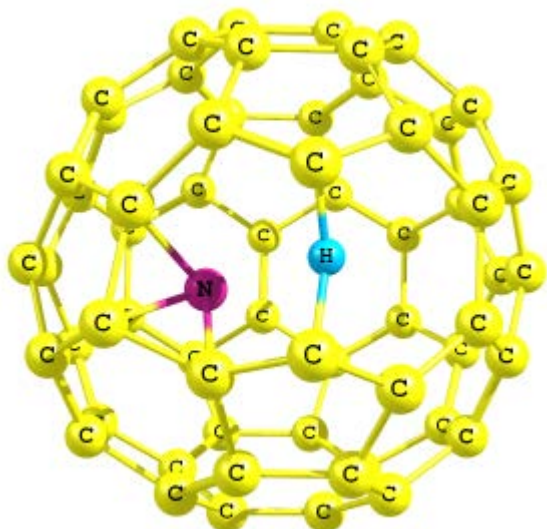
¹TS1k (TS of endohedrally bound N@C₆₀H → NH@C₆₀ by breaking [6,6]-bond, singlet)

MP2/6-31G(d)//B3LYP/6-31G(d)

```
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,2.4927140852,-0.1072758492,2.5905012092\C,0,3.0025841674,1.930718575,
-0.2989322439\C,0,2.1006757098,2.6757461372,-1.0534865283\C,0,-1.43428
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71,-1.7478331623\C,0,-0.9487816347,-1.9550945922,-2.8767540305\C,0,0.4
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B3LYP/6-31G(d)



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C	1.012512453	3.381712539	-0.391102756
C	-1.560115721	3.175582201	0.794060778
C	-1.335283311	1.353346086	2.935576228
C	1.400039059	0.599059533	3.240276483
C	2.856475619	1.858658707	1.148261080
C	-0.158137668	3.287667225	-1.219025239
C	-2.668947382	2.289146601	1.102477046
C	-0.989254676	0.008026227	3.341954178
C	2.492714085	-0.107275849	2.590501209
C	3.002584167	1.930718575	-0.298932244
C	2.100675710	2.675746137	-1.053486528
C	-1.434280185	3.231063827	-0.654223817
C	-2.522351918	1.303376769	2.096068910
C	0.347563367	-0.362810498	3.508525210
C	3.207938942	0.510067833	1.562092236
C	0.215588654	2.504124802	-2.415765776
C	-3.307612075	2.015081700	-0.175422018
C	-0.677314404	1.595982383	-2.944299229
C	-1.937251816	-0.901653137	2.737219348
C	2.121435224	-1.504434335	2.478425180
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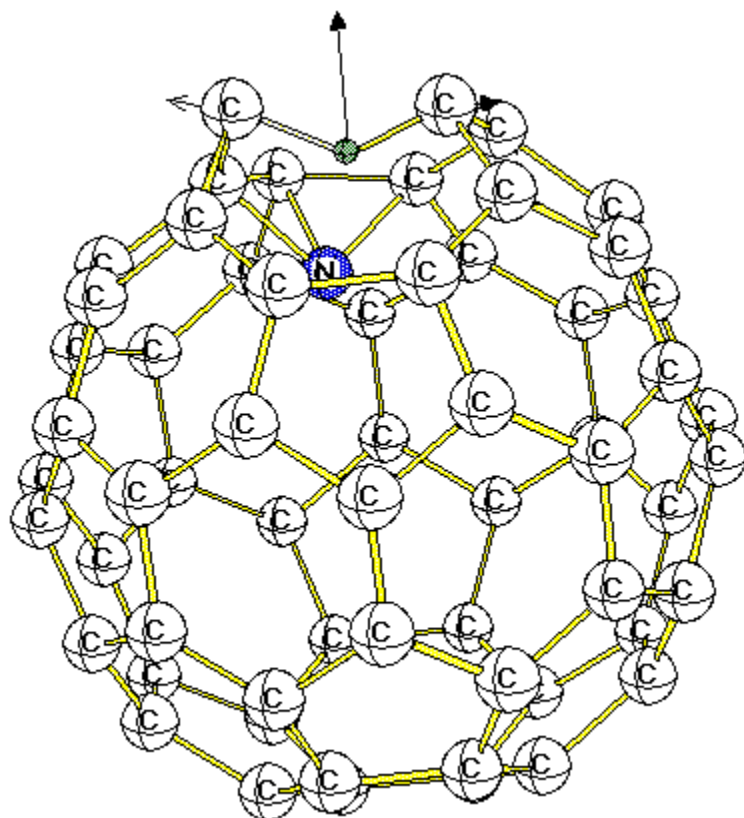
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 C 0.446017529 -2.297198775 -2.697088965
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 C 1.687500002 -3.077493947 -0.703421673
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 C 2.040725129 0.898939216 -2.778382103
 N -1.661375716 0.184165710 -1.279487184
 H -3.273765962 0.901747958 -0.047589171

Zero-point correction= 0.382899 (Hartree/Particle)
 Thermal correction to Energy= 0.404865
 Thermal correction to Enthalpy= 0.405809
 Thermal correction to Gibbs Free Energy= 0.339103
 Sum of electronic and zero-point Energies= -2340.749607
 Sum of electronic and thermal Energies= -2340.727641
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Vibrational Normal Modes



62

C	-0.415815	3.496190	-0.712608
C	-1.580773	3.244880	0.096952
C	-1.142777	3.048899	1.464629
C	0.295612	3.243446	1.510471
C	0.749781	3.517352	0.154722
C	-0.318514	2.922190	-1.989668
C	-2.627527	2.464978	-0.400663
C	-1.736833	2.047366	2.243093
C	1.083325	2.468204	2.358780
C	1.962624	2.998697	-0.292585
C	-1.371686	2.073271	-2.474319
C	-3.326368	1.518790	0.451830
C	-0.914346	1.247647	3.125548
C	2.359130	1.942553	1.899359
C	2.068713	2.427572	-1.628052
C	0.952943	2.389454	-2.459593
C	-2.534090	1.873096	-1.726328
C	-2.821666	1.223793	1.731951
C	0.464785	1.459790	3.198640
C	2.791387	2.201568	0.596919
C	-0.735517	0.992265	-3.256951
C	-3.819615	0.485762	-0.445716
C	-1.227428	-0.293121	-3.172381
C	-1.456967	-0.092771	3.153159

C	2.534120	0.622187	2.472484
C	2.967806	1.286503	-1.561552
C	0.689176	1.206437	-3.263421
C	-3.205722	0.565668	-1.690746
C	-2.647158	-0.140753	2.313072
C	1.368614	0.328266	3.284771
C	3.411814	1.150111	-0.186359
C	3.580426	-0.123952	0.365221
C	0.550861	-3.436860	0.745514
C	-0.603991	-3.492717	-0.122175
C	-0.158072	-3.263501	-1.522614
C	1.264211	-3.002641	-1.460632
C	1.706280	-3.131515	-0.076519
C	0.442447	-2.889906	2.036634
C	-1.791715	-2.971817	0.371647
C	-0.944316	-2.532873	-2.416468
C	1.857730	-2.038005	-2.287595
C	2.710627	-2.301483	0.421151
C	-0.822739	-2.376274	2.519199
C	-2.605705	-2.070585	-0.482801
C	-0.364925	-1.459408	-3.206387
C	2.899937	-1.175036	-1.763338
C	2.599379	-1.737032	1.757721
C	1.483122	-2.023126	2.545418
C	-1.940466	-2.427023	1.690281
C	-2.249885	-1.997859	-1.898425
C	1.027600	-1.241527	-3.170628
C	3.321660	-1.303327	-0.438428
C	-0.582746	-1.180617	3.296236
C	-3.733332	-1.528517	0.404284
C	2.716665	0.150865	-2.334406
C	3.138924	-0.392061	1.721334
C	0.849114	-0.965714	3.326189
C	-2.935075	-1.342795	1.638198
C	-2.344714	-0.550119	-2.209118
C	1.555129	0.103975	-3.201120
N	-1.612434	-0.993790	-0.915383
H	-3.373734	-0.356532	0.144817

NORMALMODES 180

C	0.01	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.00
C	0.02	0.02	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00

C	0.00	0.00	0.00
C	0.01	0.03	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.02	-0.01
C	0.00	0.00	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.02	0.16	-0.07
C	0.00	0.00	0.00
C	0.00	0.00	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.00
C	0.00	-0.01	-0.02
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.01	0.01	0.02
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	0.00	0.00
C	-0.01	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.02	-0.24	0.08
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	-0.02	0.00
C	0.00	0.00	0.01
C	0.00	0.00	0.00

N -0.02 0.01 0.01
 H -0.94 -0.07 0.07
 -685.8948

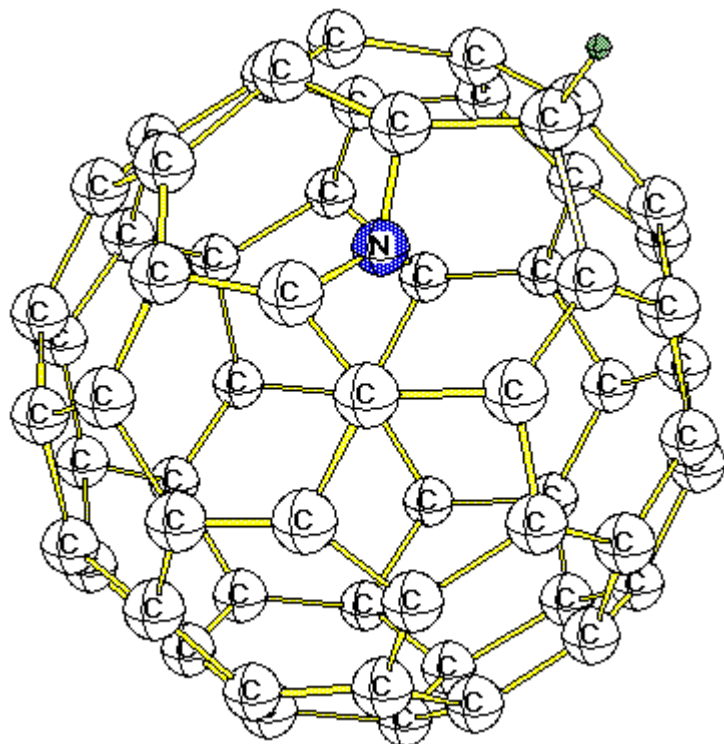
¹TS1h (TS of N-escape from singlet N@C₆₀H by breaking [5,6]-bond)

MP2/6-31G(d)//B3LYP/6-31G(d)

```
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RMP2/6-31G* SCF=Tight SCFCyc=1200 Guess=Read Geom=AllCheck Pop=None N
AME=DRAL\TS N-escape from N@C60H via breaking 5,6-bond singlet\0,1\C
,0,0.9746240559,0.399938221,-3.5233208335\C,0,-0.3042039103,1.10119516
58,-3.3805955472\C,0,-0.0650009543,2.2979090386,-2.5776240707\C,0,1.33
41194823,2.3271905468,-2.2213018581\C,0,1.9756375659,1.1605005946,-2.8
013690085\C,0,1.0568255397,-0.9961088795,-3.5613523125\C,0,-1.49780855
41,0.3985660447,-3.2750072363\C,0,-1.0331399614,2.7370792107,-1.669648
3334\C,0,1.7335420065,2.7881003376,-0.9608315953\C,0,2.9841113552,0.49
41088151,-2.1013533606\C,0,-0.1618269748,-1.7752533867,-3.4691547896\C
,0,-2.6073772299,0.9909381947,-2.4188881311\C,0,-0.6203209386,3.187841
0406,-0.3564171784\C,0,2.7754736988,2.0883758926,-0.2297469307\C,0,3.0
298724434,-0.9561425944,-2.0924725645\C,0,2.0807442436,-1.6882731243,-
2.8046348966\C,0,-1.3837632521,-1.0909052931,-3.3766938317\C,0,-2.3288
663897,2.0863635463,-1.5712523471\C,0,0.7352987991,3.2241112966,-0.010
9159451\C,0,3.3905752445,0.9662794385,-0.7860980143\C,0,0.0961596658,-
2.9634330019,-2.6207391246\C,0,-3.2278035874,0.0045561005,-1.488256777
1\C,0,-0.8702240672,-3.4635804893,-1.6978399848\C,0,-1.6093187099,2.74
30121853,0.5987992518\C,0,2.420663073,2.0978250991,1.1801789287\C,0,3.
4450649539,-1.3837836464,-0.768621185\C,0,1.4762520701,-2.877526665,-2
.2128189005\C,0,-2.1167639329,-1.6668636602,-2.3120595904\C,0,-2.67448
73426,2.051117209,-0.0983024434\C,0,1.1555975825,2.7986569249,1.312441
6845\C,0,3.668729547,-0.1952519097,0.0376011987\C,0,3.3231087332,-0.19
06962535,1.3916213416\C,0,-0.7309495906,-0.9437567615,3.1865183603\C,0
,-1.7439193333,-1.6895652334,2.4357285068\C,0,-1.1242665465,-2.8410292
927,1.8681458116\C,0,0.2831333875,-2.8210895243,2.2407404518\C,0,0.523
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6455106\C,0,-2.7645202231,-1.0135433992,1.7349677263\C,0,-1.5224072847
,-3.2936410635,0.5897479274\C,0,1.2579201343,-3.2425952498,1.340938971
8\C,0,1.7224141748,-0.9350295742,2.9394678651\C,0,-1.7915945396,1.1604
95914,2.4802248748\C,0,-3.248982953,-1.488539393,0.4716978066\C,0,-0.4
815563665,-3.7758906235,-0.3379545659\C,0,2.4965065019,-2.5086429427,1
.2085413318\C,0,1.6999435467,0.516436604,2.9332400031\C,0,0.4848219242
,1.1932999096,3.0606210788\C,0,-2.7777849641,0.4614413623,1.7886021074
\C,0,-2.5853646406,-2.6571933913,-0.1334933719\C,0,0.8661479949,-3.721
2958171,0.0212663263\C,0,2.7269788797,-1.3707697888,1.9907236766\C,0,-
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 6165,0.9785333935,1.9715672028\C,0,0.2054803404,2.3578040053,2.2350382
 65\C,0,-3.3189669896,0.9937521717,0.5701432619\C,0,-2.1916295868,-2.86
 64105052,-1.618228352\C,0,1.8667138725,-3.2827502188,-0.9284889221\N,0
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 11,-0.2136011951\\Version=EM64L-G09RevA.02\State=1-A\HF=-2326.4852953\
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B3LYP/6-31G(d)



0 1

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C	-0.304203910	1.101195166	-3.380595547
C	-0.065000954	2.297909039	-2.577624071
C	1.334119482	2.327190547	-2.221301858
C	1.975637566	1.160500595	-2.801369008
C	1.056825540	-0.996108880	-3.561352312
C	-1.497808554	0.398566045	-3.275007236
C	-1.033139961	2.737079211	-1.669648333
C	1.733542006	2.788100338	-0.960831595
C	2.984111355	0.494108815	-2.101353361
C	-0.161826975	-1.775253387	-3.469154790
C	-2.607377230	0.990938195	-2.418888131
C	-0.620320939	3.187841041	-0.356417178
C	2.775473699	2.088375893	-0.229746931
C	3.029872443	-0.956142594	-2.092472564
C	2.080744244	-1.688273124	-2.804634897
C	-1.383763252	-1.090905293	-3.376693832

C	-2.328866390	2.086363546	-1.571252347
C	0.735298799	3.224111297	-0.010915945
C	3.390575244	0.966279438	-0.786098014
C	0.096159666	-2.963433002	-2.620739125
C	-3.227803587	0.004556100	-1.488256777
C	-0.870224067	-3.463580489	-1.697839985
C	-1.609318710	2.743012185	0.598799252
C	2.420663073	2.097825099	1.180178929
C	3.445064954	-1.383783646	-0.768621185
C	1.476252070	-2.877526665	-2.212818900
C	-2.116763933	-1.666863660	-2.312059590
C	-2.674487343	2.051117209	-0.098302443
C	1.155597582	2.798656925	1.312441684
C	3.668729547	-0.195251910	0.037601199
C	3.323108733	-0.190696254	1.391621342
C	-0.730949591	-0.943756762	3.186518360
C	-1.743919333	-1.689565233	2.435728507
C	-1.124266546	-2.841029293	1.868145812
C	0.283133388	-2.821089524	2.240740452
C	0.523557336	-1.648829297	3.064328765
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C	1.722414175	-0.935029574	2.939467865
C	-1.791594540	1.160495914	2.480224875
C	-3.248982953	-1.488539393	0.471697807
C	-0.481556366	-3.775890624	-0.337954566
C	2.496506502	-2.508642943	1.208541332
C	1.699943547	0.516436604	2.933240003
C	0.484821924	1.193299910	3.060621079
C	-2.777784964	0.461441362	1.788602107
C	-2.585364641	-2.657193391	-0.133493372
C	0.866147995	-3.721295817	0.021266326
C	2.726978880	-1.370769789	1.990723677
C	-1.201448818	2.330367974	1.875494138
C	-3.980925149	-0.146680361	-0.187503939
C	2.864327626	-2.516637040	-0.197497028
C	2.686474616	0.978533394	1.971567203
C	0.205480340	2.357804005	2.235038265
C	-3.318966990	0.993752172	0.570143262
C	-2.191629587	-2.866410505	-1.618228352
C	1.866713872	-3.282750219	-0.928488922
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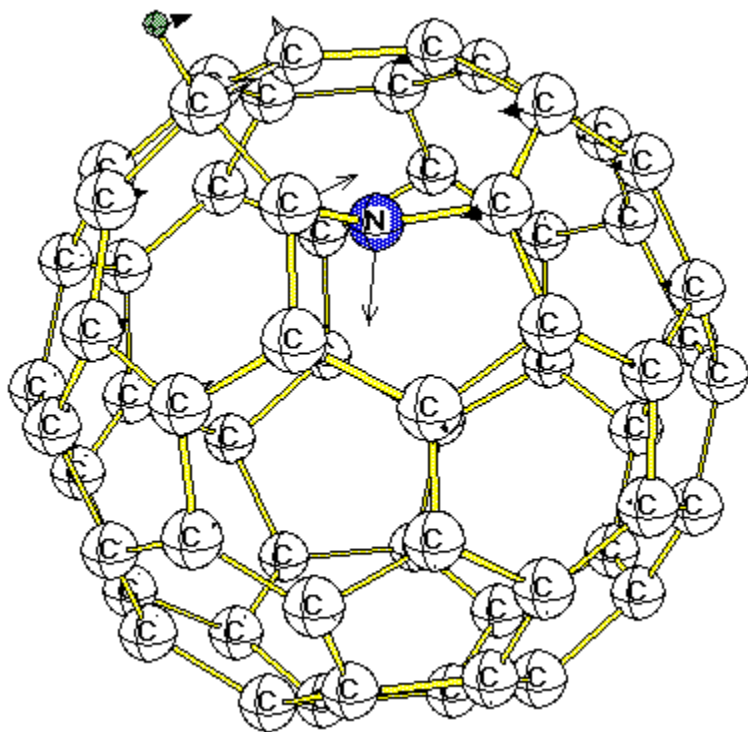
Zero-point correction=	0.384178 (Hartree/Particle)
Thermal correction to Energy=	0.406276
Thermal correction to Enthalpy=	0.407220
Thermal correction to Gibbs Free Energy=	0.340075

Sum of electronic and zero-point Energies= -2340.838550
 Sum of electronic and thermal Energies= -2340.816451
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 Sum of electronic and thermal Free Energies= -2340.882653

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 2\C,-0.0650009543,2.2979090386,-2.5776240707\C,1.3341194823,2.32719054
 68,-2.2213018581\C,1.9756375659,1.1605005946,-2.8013690085\C,1.0568255
 397,-0.9961088795,-3.5613523125\C,-1.4978085541,0.3985660447,-3.275007
 2363\C,-1.0331399614,2.7370792107,-1.6696483334\C,1.7335420065,2.78810
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 36604,2.9332400031\C,0.4848219242,1.1932999096,3.0606210788\C,-2.77778
 49641,0.4614413623,1.7886021074\C,-2.5853646406,-2.6571933913,-0.13349
 33719\C,0.8661479949,-3.7212958171,0.0212663263\C,2.7269788797,-1.3707
 697888,1.9907236766\C,-1.2014488177,2.330367974,1.8754941377\C,-3.9809
 251487,-0.1466803607,-0.187503939\C,2.8643276261,-2.5166370399,-0.1974
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-0.00014236,0.00011982,-0.00000349,0.00000818,-0.00000645\\\\@

Vibrational Normal Modes



62

C	0.520586	1.645850	3.071916
C	-0.821207	1.075285	3.218817
C	-0.669902	-0.363016	3.424977
C	0.739661	-0.675251	3.393301
C	1.473997	0.558683	3.175712
C	0.782114	2.719512	2.214009
C	-1.897376	1.583581	2.502559
C	-1.601148	-1.250703	2.877825
C	1.187470	-1.865707	2.807602
C	2.620684	0.560920	2.378076
C	-0.309918	3.295262	1.454630
C	-2.993106	0.620169	2.071050
C	-1.133998	-2.468669	2.248134
C	2.374389	-1.860085	1.970398
C	2.857629	1.646116	1.444476
C	1.952579	2.703343	1.359683
C	-1.597879	2.768127	1.637098
C	-2.785614	-0.772694	2.184594
C	0.230723	-2.777318	2.222338
C	3.078926	-0.674252	1.759675
C	0.178086	3.623573	0.093674
C	-3.391342	0.777861	0.642591

C	-0.626387	3.433865	-1.069349
C	-1.965150	-2.720356	1.093029
C	2.150653	-2.778005	0.865302
C	3.443752	1.083024	0.241467
C	1.566085	3.235578	0.056867
C	-2.149145	2.533148	0.355164
C	-2.988682	-1.698655	1.004917
C	0.821554	-3.341939	1.021897
C	3.581090	-0.350618	0.437518
C	3.362005	-1.228539	-0.627424
C	-0.378126	-1.675390	-3.084229
C	-1.347895	-0.579938	-3.158767
C	-0.636017	0.635212	-3.379286
C	0.784424	0.319006	-3.427888
C	0.942022	-1.114444	-3.252735
C	-0.577711	-2.728716	-2.200728
C	-2.507889	-0.588454	-2.356247
C	-1.085278	1.831126	-2.774613
C	1.720647	1.187750	-2.874455
C	2.020158	-1.618724	-2.514031
C	-1.766218	-2.754935	-1.363915
C	-3.038044	0.617880	-1.790677
C	-0.078369	2.761290	-2.229179
C	2.834665	0.671628	-2.110981
C	1.806285	-2.707514	-1.578034
C	0.529201	-3.252196	-1.425494
C	-2.710347	-1.734616	-1.448527
C	-2.283909	1.868889	-1.987290
C	1.277368	2.430149	-2.254677
C	2.983216	-0.708340	-1.928492
C	-1.392504	-3.263513	-0.066125
C	-3.997001	0.068710	-0.545813
C	3.071405	1.585377	-1.005848
C	2.632144	-2.464505	-0.407352
C	0.025302	-3.576786	-0.100195
C	-3.425073	-1.314475	-0.276552
C	-2.002223	2.984864	-0.948786
C	2.121262	2.682521	-1.105921
N	-2.285560	1.180625	0.155193
H	-5.076821	0.135936	-0.700457

NORMALMODES 180

C	0.00	0.00	0.02
C	0.00	0.00	0.03
C	0.00	0.01	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	-0.03	-0.01	0.01
C	0.00	0.03	0.06
C	-0.01	0.03	0.00

C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.06 -0.02 0.02
C 0.10 0.07 -0.12
C -0.02 0.02 0.01
C 0.00 0.01 0.00
C -0.01 0.01 0.00
C -0.03 0.00 0.00
C -0.05 0.03 0.07
C 0.01 0.06 -0.04
C -0.01 0.01 0.00
C 0.00 0.01 0.00
C -0.05 -0.06 0.00
C 0.17 0.24 -0.22
C -0.08 -0.07 0.04
C -0.02 0.03 0.00
C -0.01 0.01 0.00
C -0.01 0.00 -0.01
C -0.03 0.00 0.00
C -0.11 -0.10 0.10
C 0.01 0.07 -0.01
C -0.01 0.01 0.00
C 0.00 0.01 0.00
C -0.01 0.01 0.00
C 0.00 0.00 0.00
C -0.01 -0.01 -0.02
C -0.01 -0.01 0.01
C -0.01 0.00 0.00
C 0.00 0.00 0.00
C -0.01 0.00 0.00
C -0.02 -0.02 -0.04
C -0.03 -0.03 0.03
C -0.02 0.01 0.00
C 0.00 0.00 0.00
C -0.01 0.02 0.01
C -0.07 -0.03 -0.10
C -0.06 -0.04 0.04
C -0.01 0.01 0.00
C 0.00 0.00 0.00
C -0.01 0.01 0.00
C -0.01 0.03 0.00
C -0.04 -0.10 0.04
C -0.03 0.00 0.01
C -0.01 0.00 0.00
C -0.01 0.02 0.00
C 0.05 0.19 -0.09
C -0.01 0.00 -0.01
C 0.00 0.00 0.00
C -0.01 0.01 0.00
C 0.01 0.10 0.00

C -0.13 -0.12 0.09
 C -0.03 0.00 0.00
 N 0.66 -0.39 0.07
 H 0.04 0.15 -0.03
 -382.3343

¹TS1i (TS of N-escape from singlet N@C₆₀H by breaking [6,6]-bond)

MP2/6-31G(d)//B3LYP/6-31G(d)

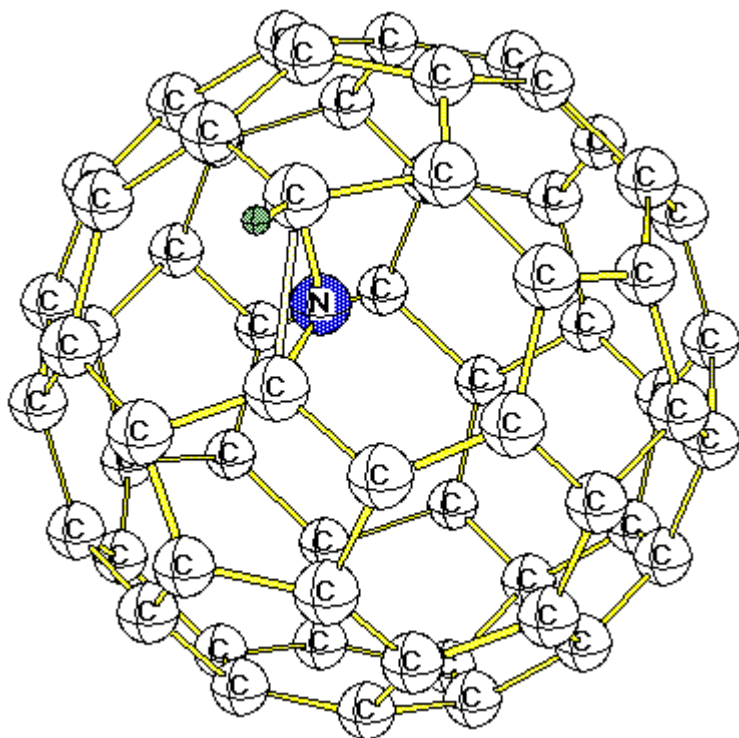
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RMP2/6-31G* SCF=Tight SCFCyc=1200 Guess=Read Geom=AllCheck Pop=None N
AME=DRAL\TS N-escape from N@C60H via breaking 6,6-bond singlet\0,1\C
,0,2.3629500302,-2.6282856698,-0.6154039214\C,0,1.1885295756,-3.088092
0922,-1.3498929866\C,0,1.0213403566,-2.2601221567,-2.5248422434\C,0,2.
1122155431,-1.3093220547,-2.5405524891\C,0,2.938777294,-1.5321577599,-
1.3637755509\C,0,2.3534051483,-2.5930108231,0.7809001913\C,0,0.0565363
378,-3.5338329901,-0.6656042311\C,0,-0.263488056,-1.8725897339,-2.9885
983081\C,0,1.9036515319,-0.0079736509,-3.003326323\C,0,3.5064342271,-0
.4457255137,-0.6926246193\C,0,1.175421975,-3.0225465492,1.527850434\C,
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72702,-3.4534985736\C,0,2.5007644623,1.1134739266,-2.3149351014\C,0,3.
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51,-2.3141204498,-2.3201401424\C,0,0.5825013611,0.3953656579,-3.466300
2615\C,0,3.285695079,0.9034089057,-1.1762503353\C,0,0.9948398948,-2.13
49728585,2.6568915286\C,0,-1.6984102126,-2.6247623255,0.07163024\C,0,-
0.2934361085,-1.7257988153,3.0885296022\C,0,-1.8088967876,-0.089495733
6,-3.0371360059\C,0,1.5498716026,2.2163707009,-2.3485343156\C,0,3.2720
128197,0.9624422897,1.172579268\C,0,2.0844087808,-1.1801467575,2.63408
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0,3.1460427457,1.7767335839,-0.0243198795\C,0,2.2308075716,2.829863848
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476829,1.6338045021,1.3662531191\C,0,-2.0347734075,1.3747536591,2.5509
264771\C,0,-0.9291997008,2.3057393543,2.5272770032\C,0,-1.0432685869,3
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.3409082776,3.4717947665\C,0,1.5194603478,2.3302616382,2.2540596046\C,
0,0.1111671141,3.4935670722,-0.815614268\C,0,-1.0243758242,3.074346712
6,-1.5112547694\C,0,-3.4497416428,0.5493502924,-0.7871441805\C,0,-2.49
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C,0,2.4725356402,1.228607573,2.2882993426\C,0,1.4273980505,3.064948925
5,-1.2444183359\C,0,-0.8950680861,2.185647152,-2.6573938241\C,0,-3.300
7109077,-0.8071714083,-1.2703682187\C,0,-1.47367211,-2.2059741458,2.42
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B3LYP/6-31G(d)



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C	2.362950030	-2.628285670	-0.615403921
C	1.188529576	-3.088092092	-1.349892987
C	1.021340357	-2.260122157	-2.524842243
C	2.112215543	-1.309322055	-2.540552489
C	2.938777294	-1.532157760	-1.363775551
C	2.353405148	-2.593010823	0.780900191
C	0.056536338	-3.533832990	-0.665604231
C	-0.263488056	-1.872589734	-2.988598308
C	1.903651532	-0.007973651	-3.003326323
C	3.506434227	-0.445725514	-0.692624619
C	1.175421975	-3.022546549	1.527850434
C	-1.243458930	-3.174684340	-1.201569820
C	-0.473867604	-0.509797270	-3.453498574
C	2.500764462	1.113473927	-2.314935101
C	3.497456925	-0.409347135	0.759617546
C	2.923131300	-1.460430046	1.479173066

C	0.048528019	-3.501978831	0.854992968
C	-1.450996065	-2.314120450	-2.320140142
C	0.582501361	0.395365658	-3.466300262
C	3.285695079	0.903408906	-1.176250335
C	0.994839895	-2.134972858	2.656891529
C	-1.698410213	-2.624762326	0.071630240
C	-0.293436108	-1.725798815	3.088529602
C	-1.808896788	-0.089495734	-3.037136006
C	1.549871603	2.216370701	-2.348534316
C	3.272012820	0.962442290	1.172579268
C	2.084408781	-1.180146758	2.634088960
C	-1.258375675	-3.131263376	1.367026056
C	-2.473302931	-1.185581965	-2.378796323
C	0.375478139	1.777265628	-3.070421033
C	3.146042746	1.776733584	-0.024319880
C	2.230807572	2.829863848	-0.056052583
C	-2.221873624	2.717265255	0.613466808
C	-2.828447683	1.633804502	1.366253119
C	-2.034773408	1.374753659	2.550926477
C	-0.929199701	2.305739354	2.527277003
C	-1.043268587	3.139968575	1.338118658
C	-2.213342776	2.684202642	-0.783965798
C	-3.446923058	0.580266930	0.696547809
C	-1.844319877	0.049656416	3.007338378
C	0.337566998	1.925882158	2.981858716
C	0.101475271	3.528665729	0.640065088
C	-2.818579395	1.573585038	-1.496341881
C	-3.273805100	-0.758464463	1.232928399
C	-0.514006582	-0.340908278	3.471794766
C	1.519460348	2.330261638	2.254059605
C	0.111167114	3.493567072	-0.815614268
C	-1.024375824	3.074346713	-1.511254769
C	-3.449741643	0.549350292	-0.787144180
C	-2.495897337	-1.084581627	2.405775140
C	0.539787159	0.567576887	3.450222697
C	1.412122574	3.123451488	1.107688538
C	-2.005675410	1.255419410	-2.651041854
C	-3.320029759	-1.618247352	-0.001687001
C	2.472535640	1.228607573	2.288299343
C	1.427398050	3.064948926	-1.244418336
C	-0.895068086	2.185647152	-2.657393824
C	-3.300710908	-0.807171408	-1.270368219
C	-1.473672110	-2.205974146	2.429765398
C	1.867465909	0.142175562	3.025955678
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H	-3.744821559	-2.627988027	0.024805995

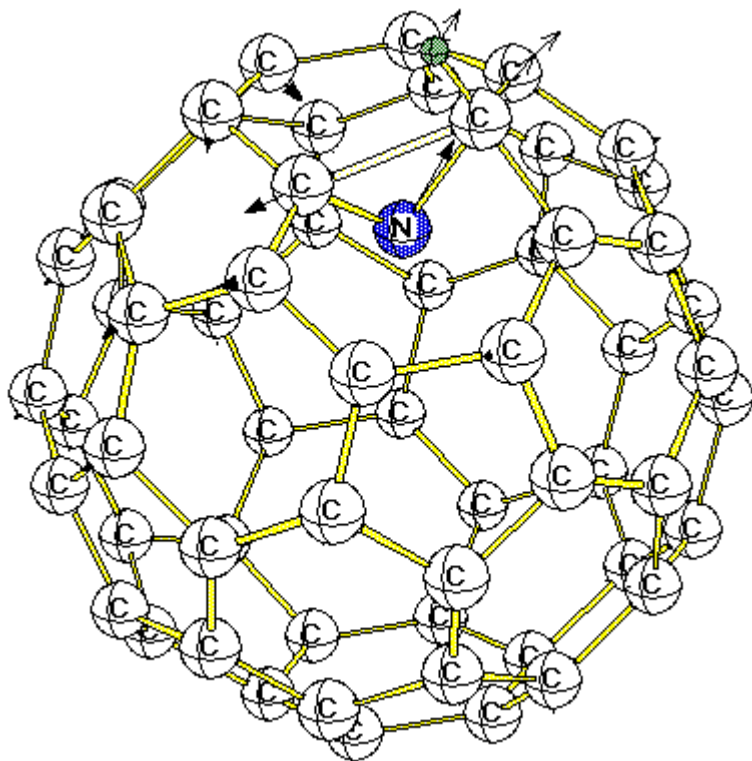
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Thermal correction to Energy=	0.405366
Thermal correction to Enthalpy=	0.406310

Thermal correction to Gibbs Free Energy= 0.338132
 Sum of electronic and zero-point Energies= -2340.841219
 Sum of electronic and thermal Energies= -2340.818806
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 Sum of electronic and thermal Free Energies= -2340.886039

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 20547,-2.5405524891\C,2.938777294,-1.5321577599,-1.3637755509\C,2.3534
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Vibrational Normal Modes



62

C	1.391827	-3.055398	-1.260106
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C	0.174398	-1.943331	-2.952025
C	1.508290	-1.384141	-2.903903
C	2.259614	-2.065629	-1.860470
C	1.438503	-3.283134	0.117195
C	-1.082814	-3.190374	-1.256662
C	-0.936884	-1.103338	-3.226797
C	1.705917	-0.018202	-3.119126
C	3.161945	-1.350390	-1.068483
C	0.209673	-3.467130	0.882834
C	-2.219735	-2.358644	-1.605759
C	-0.721677	0.320930	-3.433541
C	2.647775	0.717524	-2.306919
C	3.211294	-1.587828	0.363858
C	2.358211	-2.530552	0.943433
C	-1.031788	-3.445235	0.241916
C	-2.181036	-1.280822	-2.539378
C	0.565193	0.847445	-3.387209
C	3.362422	0.067808	-1.294993
C	0.354260	-2.796558	2.157416

C	-2.437216	-1.947172	-0.222348
C	-0.724864	-2.104329	2.765448
C	-1.842125	1.040645	-2.834441
C	2.092473	2.042800	-2.068192
C	3.443094	-0.316292	1.021606
C	1.687955	-2.231872	2.199375
C	-2.138135	-2.798432	0.924008
C	-2.796790	0.094838	-2.314522
C	0.817106	2.126047	-2.746160
C	3.542068	0.708312	-0.004015
C	3.004959	1.975924	0.224932
C	-1.232408	3.097982	1.260796
C	-2.125223	2.128555	1.870386
C	-1.416256	1.421758	2.918374
C	-0.074923	1.959476	2.954035
C	0.041872	2.997618	1.938325
C	-1.279384	3.328306	-0.117147
C	-3.065339	1.459209	1.089927
C	-1.638750	0.040349	3.124950
C	1.021354	1.133872	3.222716
C	1.227864	3.144353	1.216732
C	-2.226300	2.609689	-0.950336
C	-3.306018	0.055243	1.374232
C	-0.485260	-0.816435	3.395832
C	2.246574	1.289573	2.471265
C	1.179486	3.383418	-0.218829
C	-0.051926	3.468468	-0.871140
C	-3.125159	1.711269	-0.371303
C	-2.633524	-0.707155	2.400665
C	0.799934	-0.284379	3.434348
C	2.358183	2.279270	1.489999
C	-1.592467	2.283444	-2.210174
C	-3.660337	-0.500502	0.020997
C	2.804358	-0.035327	2.233182
C	2.279085	2.664000	-0.829869
C	-0.246046	2.815659	-2.158113
C	-3.426867	0.490482	-1.088602
C	-2.016703	-2.069573	2.143002
C	1.911550	-1.005130	2.827283
N	-2.117719	-0.701139	-0.034476
H	-4.380700	-1.319250	-0.086029

NORMALMODES 180

C	0.05	-0.02	0.00
C	0.04	-0.02	0.01
C	0.01	0.01	0.03
C	0.01	0.00	0.01
C	0.02	0.00	0.01
C	0.04	0.00	0.00
C	0.07	-0.05	0.00

C 0.00 0.02 0.05
C 0.01 0.00 0.01
C 0.02 0.00 0.00
C 0.05 -0.05 0.01
C 0.06 -0.03 0.09
C 0.01 0.01 0.01
C 0.01 0.00 -0.01
C 0.02 0.01 0.00
C 0.02 0.01 0.00
C 0.06 -0.08 0.02
C 0.03 0.07 0.12
C 0.01 0.01 0.00
C 0.01 0.00 0.00
C 0.03 0.01 -0.01
C 0.09 -0.27 0.08
C 0.04 0.00 0.01
C 0.02 0.03 0.01
C 0.01 0.00 0.00
C 0.01 0.00 0.00
C 0.03 0.00 0.00
C 0.01 -0.15 0.03
C -0.02 0.05 0.01
C 0.01 0.01 -0.01
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.02 0.01 -0.01
C 0.04 -0.01 -0.04
C 0.02 -0.02 0.00
C 0.00 -0.02 0.00
C 0.01 -0.01 0.00
C 0.02 0.02 -0.02
C 0.05 0.04 -0.05
C 0.01 -0.03 -0.04
C 0.02 0.00 0.02
C 0.01 -0.01 0.00
C 0.02 0.06 -0.02
C 0.08 -0.03 -0.14
C 0.03 -0.01 0.00
C 0.01 0.00 0.00
C 0.01 0.00 0.00
C 0.02 0.01 -0.01
C -0.02 0.10 -0.03
C 0.00 -0.09 0.02
C 0.02 0.01 0.01
C 0.01 0.00 0.01
C 0.01 0.04 -0.03
C -0.29 0.18 -0.11
C 0.02 0.00 0.00
C 0.01 0.00 0.00
C 0.02 0.02 -0.02

C -0.17 0.16 -0.07
 C 0.04 0.03 -0.01
 C 0.02 0.01 -0.01
 N -0.69 -0.04 0.08
 H -0.18 0.10 -0.12
 -232.9897

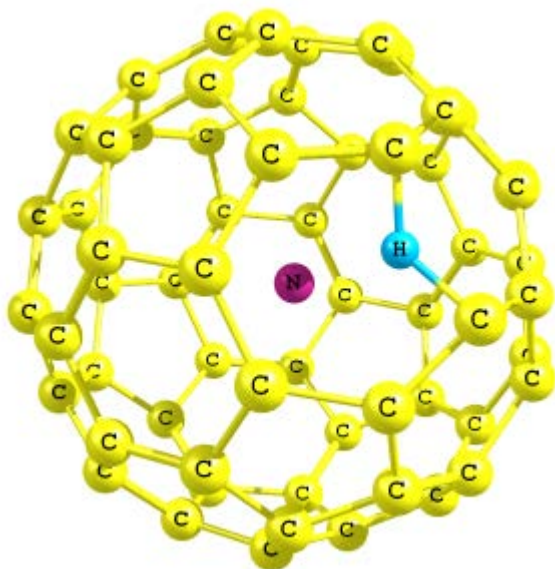
³TS1a (TS of N@C₆₀H[•] → NH[•]@C₆₀ by breaking [5,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN087\SP\ROMP2-FC\6-31G(d)\C60H1N1(3)\DRAL\10-Aug-2010\0
 \#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=N
 one SCF=(Conver=5) Name=Drall\TS N@C60H -> NH@C60 triplet via 5,6-bond
 breaking\0,3\C,0.887443496,1.177799326,3.21697933\C,-0.482034064,0.7
 25275851,3.393882123\C,-0.481310013,-0.726487074,3.40317226\C,0.882395
 675,-1.175845879,3.219176491\C,1.728505367,-0.000407197,3.094195494\C,
 1.159062737,2.31399939,2.452429095\C,-1.534880857,1.418522204,2.803725
 585\C,-1.54378303,-1.414021926,2.81109452\C,1.154712193,-2.314954673,2
 .451866034\C,2.799667055,-0.001077419,2.19855096\C,0.064781151,3.05058
 5289,1.851348306\C,-2.673318214,0.719295688,2.194641069\C,-1.256599145
 ,-2.618013773,2.040380761\C,2.260125696,-2.309289443,1.513708566\C,3.0
 70214993,1.175394473,1.388885797\C,2.266851392,2.309295381,1.51398537\
 C,-1.249114866,2.617961121,2.040743728\C,-2.675035,-0.715712385,2.2189
 40229\C,0.057927142,-3.043728972,1.849623688\C,3.068567637,-1.17772294
 5,1.38735886\C,0.490532788,3.501979039,0.53873897\C,-3.119285755,1.558
 994806,1.090629697\C,-0.417964467,3.508803497,-0.52750426\C,-2.2023382
 93,-2.68687293,0.953339458\C,1.84585315,-3.039086908,0.324647431\C,3.4
 92648826,0.724277434,0.073207652\C,1.84991766,3.040518981,0.327946212\
 C,-2.192663552,2.668038552,0.949008797\C,-3.098568302,-1.556035727,1.0
 85069605\C,0.483029371,-3.494503225,0.530886132\C,3.492925305,-0.72897
 9537,0.073405999\C,3.094371486,-1.427430975,-1.069926169\C,-0.86339264
 8,-1.176668344,-3.192853096\C,-1.701824646,0.003431054,-3.023060854\C,
 -0.866151455,1.171754485,-3.201345252\C,0.495001407,0.724090766,-3.420
 728141\C,0.497370057,-0.729006412,-3.41977754\C,-1.106299484,-2.324560
 272,-2.440531988\C,-2.774666408,0.005652382,-2.113808473\C,-1.11003778
 9,2.318084062,-2.433999065\C,1.564106988,1.420849224,-2.851464716\C,1.
 566194848,-1.427443219,-2.853694796\C,-2.216597422,-2.35874559,-1.5180
 21851\C,-3.06276145,1.237165172,-1.373096138\C,0.001246889,3.042173366
 ,-1.837816835\C,2.669008623,0.696681008,-2.254020844\C,1.310764705,-2.
 608400427,-2.044912744\C,0.004101946,-3.052650107,-1.847236751\C,-3.04
 9541694,-1.228486757,-1.376314934\C,-2.215278588,2.350175997,-1.517107
 335\C,1.308347681,2.601149097,-2.038551155\C,2.672382138,-0.702548818,
 -2.25416176\C,-1.790340784,-3.08007856,-0.329375566\C,-3.731614158,1.0
 90065131,-0.107515157\C,3.089858051,1.422288062,-1.066379259\C,2.25217
 1938,-2.604952404,-0.938643183\C,-0.418206504,-3.511722992,-0.53602150
 5\C,-3.628505219,-1.04493293,-0.091903536\C,-1.785817692,3.082078834,-
 0.320127917\C,2.253641845,2.603965566,-0.936757388\C,-0.089159955,-0.0

14071956,-0.051296591\H,-3.311208785,0.015521539,0.205802583\\Version=
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 61e-06\Thermal=0.\PG=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)



0 3

C	0.887443496	1.177799326	3.216979330
C	-0.482034064	0.725275851	3.393882123
C	-0.481310013	-0.726487074	3.403172260
C	0.882395675	-1.175845879	3.219176491
C	1.728505367	-0.000407197	3.094195494
C	1.159062737	2.313999390	2.452429095
C	-1.534880857	1.418522204	2.803725585
C	-1.543783030	-1.414021926	2.811094520
C	1.154712193	-2.314954673	2.451866034
C	2.799667055	-0.001077419	2.198550960
C	0.064781151	3.050585289	1.851348306
C	-2.673318214	0.719295688	2.194641069
C	-1.256599145	-2.618013773	2.040380761
C	2.260125696	-2.309289443	1.513708566
C	3.070214993	1.175394473	1.388885797
C	2.266851392	2.309295381	1.513985370
C	-1.249114866	2.617961121	2.040743728
C	-2.675035000	-0.715712385	2.218940229
C	0.057927142	-3.043728972	1.849623688
C	3.068567637	-1.177722945	1.387358860
C	0.490532788	3.501979039	0.538738970
C	-3.119285755	1.558994806	1.090629697
C	-0.417964467	3.508803497	-0.527504260
C	-2.202338293	-2.686872930	0.953339458
C	1.845853150	-3.039086908	0.324647431
C	3.492648826	0.724277434	0.073207652

C	1.849917660	3.040518981	0.327946212
C	-2.192663552	2.668038552	0.949008797
C	-3.098568302	-1.556035727	1.085069605
C	0.483029371	-3.494503225	0.530886132
C	3.492925305	-0.728979537	0.073405999
C	3.094371486	-1.427430975	-1.069926169
C	-0.863392648	-1.176668344	-3.192853096
C	-1.701824646	0.003431054	-3.023060854
C	-0.866151455	1.171754485	-3.201345252
C	0.495001407	0.724090766	-3.420728141
C	0.497370057	-0.729006412	-3.419777540
C	-1.106299484	-2.324560272	-2.440531988
C	-2.774666408	0.005652382	-2.113808473
C	-1.110037789	2.318084062	-2.433999065
C	1.564106988	1.420849224	-2.851464716
C	1.566194848	-1.427443219	-2.853694796
C	-2.216597422	-2.358745590	-1.518021851
C	-3.062761450	1.237165172	-1.373096138
C	0.001246889	3.042173366	-1.837816835
C	2.669008623	0.696681008	-2.254020844
C	1.310764705	-2.608400427	-2.044912744
C	0.004101946	-3.052650107	-1.847236751
C	-3.049541694	-1.228486757	-1.376314934
C	-2.215278588	2.350175997	-1.517107335
C	1.308347681	2.601149097	-2.038551155
C	2.672382138	-0.702548818	-2.254161760
C	-1.790340784	-3.080078560	-0.329375566
C	-3.731614158	1.090065131	-0.107515157
C	3.089858051	1.422288062	-1.066379259
C	2.252171938	-2.604952404	-0.938643183
C	-0.418206504	-3.511722992	-0.536021505
C	-3.628505219	-1.044932930	-0.091903536
C	-1.785817692	3.082078834	-0.320127917
C	2.253641845	2.603965566	-0.936757388
N	-0.089159955	-0.014071956	-0.051296591
H	-3.311208785	0.015521539	0.205802583

Zero-point correction=	0.379711 (Hartree/Particle)
Thermal correction to Energy=	0.403818
Thermal correction to Enthalpy=	0.404762
Thermal correction to Gibbs Free Energy=	0.330300
Sum of electronic and zero-point Energies=	-2340.787644
Sum of electronic and thermal Energies=	-2340.763537
Sum of electronic and thermal Enthalpies=	-2340.762593
Sum of electronic and thermal Free Energies=	-2340.837056

1\1\FAU-CCC-CCDN089\Freq\UB3LYP/6-31G(d)\C60H1N1(3)\DRAL\16-Nov-2009\0
 \#P B3LYP/6-31G* FREQ=NORAMAN POP=NONE SCFCYC=600 NAME=DRAL\TS N@C60
 H -> NH@C60 triplet via 5,6-bond breaking\0,3\C,0.887443496,1.1777993
 26,3.21697933\C,-0.482034064,0.725275851,3.393882123\C,-0.481310013,-0

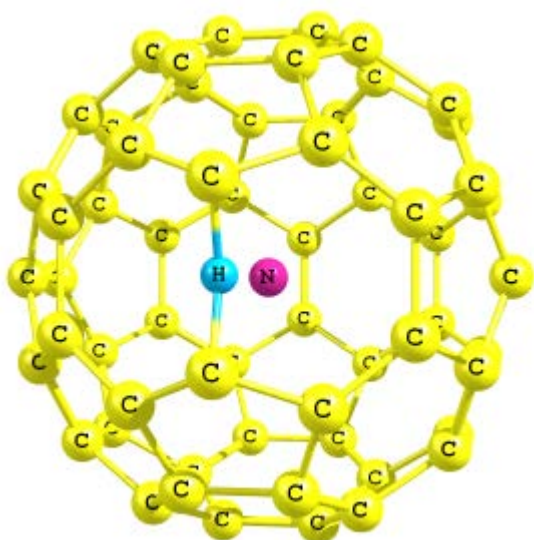
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³TS1b (TS of N@C₆₀H[•] → NH^{••}@C₆₀ by breaking [6,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\\1\\FAU-CCC-CCDN086\\SP\\ROMP2-FC\\6-31G(d)\\C60H1N1(3)\\DRAL\\03-Aug-2010\\0
\\#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=N
one Name=Dral\\TS N@C60H -> NH@C60 triplet via 6,6\\0,3\\C,-0.994650069

, -3.375551657, -0.703876537\C, -1.990231416, -2.609141418, -1.426596554\C, -1.352900718, -2.001064803, -2.577986052\C, 0.035890738, -2.42579043, -2.592527313\C, 0.260400681, -3.269446659, -1.427849645\C, -0.99844309, -3.376628787, 0.694285441\C, -2.965775797, -1.900283406, -0.734383686\C, -1.691838278, -0.694241796, -2.943178554\C, 1.032824212, -1.547190881, -3.015529931\C, 1.462854443, -3.182879648, -0.725637804\C, -1.997932364, -2.611319074, 1.412765315\C, -3.396006991, -0.576805702, -1.177512757\C, -0.655510696, 0.209203678, -3.392829975\C, 2.29269062, -1.470416152, -2.295559926\C, 1.458908162, -3.183998388, 0.729669763\C, 0.252662524, -3.271642729, 1.425218382\C, -2.969714528, -1.901399853, 0.716359746\C, -2.707146494, 0.068982828, -2.22248378\C, 0.678104827, -0.205471348, -3.440264769\C, 2.502220718, -2.268831262, -1.169512936\C, -1.366858625, -2.005014401, 2.568525925\C, -3.95244616, 0.068785186, -0.010178732\C, -1.707771696, -0.698748091, 2.933858158\C, -0.997080551, 1.539718093, -2.939581226\C, 2.724269098, -0.08269385, -2.293319453\C, 2.495845004, -2.270633592, 1.180571432\C, 0.021835071, -2.42976891, 2.5899506\C, -3.402352385, -0.578602128, 1.159173322\C, -2.266831426, 1.484830924, -2.220206802\C, 1.730824427, 0.697164126, -3.01192266\C, 3.143768891, -1.709282476, 0.007706732\C, 3.558613887, -0.375402723, 0.009852934\C, 1.091976658, 3.345024718, 0.705102242\C, -0.16591174, 3.279465799, 1.422249909\C, 0.008930903, 2.41879438, 2.575649283\C, 1.39356544, 1.980980142, 2.597052993\C, 2.062191027, 2.546854842, 1.434579866\C, 1.09576691, 3.346092498, -0.693061616\C, -1.368277782, 3.247953434, 0.72464735\C, -1.013015434, 1.535209231, 2.937449303\C, 1.714456412, 0.69253922, 3.023306731\C, 3.006638017, 1.79264202, 0.737678678\C, -0.158211023, 3.281642254, -1.417122524\C, -2.475233717, 2.40254749, 1.163972174\C, -0.67390249, 0.204001589, 3.390503672\C, 2.711784887, -0.08622083, 2.308908135\C, 3.010581774, 1.79375442, -0.717630806\C, 2.069925802, 2.549035583, -1.418486575\C, -1.364342192, 3.249060643, -0.726098444\C, -2.278841989, 1.481430909, 2.211116935\C, 0.659434334, -0.210749978, 3.444548004\C, 3.342268375, 0.450961565, 1.184945981\C, 0.022887402, 2.422735615, -2.570871504\C, -3.294390168, 2.18475192, -0.00677448\C, 2.280205242, -1.473942627, 2.306681943\C, 3.348641701, 0.452760458, -1.165129178\C, 1.407617924, 1.984947218, -2.585432291\C, -2.468892023, 2.40433082, -1.172718387\C, -2.719155919, 0.065582661, 2.2088374\C, 1.016454506, -1.55181828, 3.01969022\N, -0.074751559, 0.023092435, -0.002537628\H, -3.253787298, 1.011826175, -0.007534046\\Version=AM64L-G03RevD.02\\State=3-A\\HF=-2326.3918552\\MP2=-2334.4022682\\RMSD=2.773e-09\\Thermal=0.\\PG=C01 [X(C60H1N1)]\\@

UB3LYP/6-31G(d)

0 3

C	-0.994650069	-3.375551657	-0.703876537
C	-1.990231416	-2.609141418	-1.426596554
C	-1.352900718	-2.001064803	-2.577986052
C	0.035890738	-2.425790430	-2.592527313
C	0.260400681	-3.269446659	-1.427849645
C	-0.998443090	-3.376628787	0.694285441
C	-2.965775797	-1.900283406	-0.734383686
C	-1.691838278	-0.694241796	-2.943178554
C	1.032824212	-1.547190881	-3.015529931
C	1.462854443	-3.182879648	-0.725637804
C	-1.997932364	-2.611319074	1.412765315
C	-3.396006991	-0.576805702	-1.177512757
C	-0.655510696	0.209203678	-3.392829975
C	2.292690620	-1.470416152	-2.295559926
C	1.458908162	-3.183998388	0.729669763
C	0.252662524	-3.271642729	1.425218382
C	-2.969714528	-1.901399853	0.716359746
C	-2.707146494	0.068982828	-2.222483780
C	0.678104827	-0.205471348	-3.440264769
C	2.502220718	-2.268831262	-1.169512936
C	-1.366858625	-2.005014401	2.568525925
C	-3.952446160	0.068785186	-0.010178732
C	-1.707771696	-0.698748091	2.933858158
C	-0.997080551	1.539718093	-2.939581226
C	2.724269098	-0.082693850	-2.293319453
C	2.495845004	-2.270633592	1.180571432
C	0.021835071	-2.429768910	2.589950600
C	-3.402352385	-0.578602128	1.159173322
C	-2.266831426	1.484830924	-2.220206802
C	1.730824427	0.697164126	-3.011922660
C	3.143768891	-1.709282476	0.007706732

C	3.558613887	-0.375402723	0.009852934
C	1.091976658	3.345024718	0.705102242
C	-0.165911740	3.279465799	1.422249909
C	0.008930903	2.418794380	2.575649283
C	1.393565440	1.980980142	2.597052993
C	2.062191027	2.546854842	1.434579866
C	1.095766910	3.346092498	-0.693061616
C	-1.368277782	3.247953434	0.724647350
C	-1.013015434	1.535209231	2.937449303
C	1.714456412	0.692539220	3.023306731
C	3.006638017	1.792642020	0.737678678
C	-0.158211023	3.281642254	-1.417122524
C	-2.475233717	2.402547490	1.163972174
C	-0.673902490	0.204001589	3.390503672
C	2.711784887	-0.086220830	2.308908135
C	3.010581774	1.793754420	-0.717630806
C	2.069925802	2.549035583	-1.418486575
C	-1.364342192	3.249060643	-0.726098444
C	-2.278841989	1.481430909	2.211116935
C	0.659434334	-0.210749978	3.444548004
C	3.342268375	0.450961565	1.184945981
C	0.022887402	2.422735615	-2.570871504
C	-3.294390168	2.184751920	-0.006774480
C	2.280205242	-1.473942627	2.306681943
C	3.348641701	0.452760458	-1.165129178
C	1.407617924	1.984947218	-2.585432291
C	-2.468892023	2.404330820	-1.172718387
C	-2.719155919	0.065582661	2.208837400
C	1.016454506	-1.551818280	3.019690220
N	-0.074751559	0.023092435	-0.002537628
H	-3.253787298	1.011826175	-0.007534046

Zero-point correction= 0.379873 (Hartree/Particle)

Thermal correction to Energy= 0.403673

Thermal correction to Enthalpy= 0.404618

Thermal correction to Gibbs Free Energy= 0.331501

Sum of electronic and zero-point Energies= -2340.778255

Sum of electronic and thermal Energies= -2340.754454

Sum of electronic and thermal Enthalpies= -2340.753510

Sum of electronic and thermal Free Energies= -2340.826626

1\1\FAU-CCC-CCDN086\Freq\UB3LYP\6-31G(d)\C60H1N1(3)\DRAL\13-Nov-2009\0
 \#P B3LYP/6-31G* FREQ=NORAMAN Pop=None SCFCyc=600 Name=DrAl\TS N@C60
 H -> NH@C60 triplet via 6,6\0,3\C,-0.994650069,-3.375551657,-0.703876
 537\C,-1.990231416,-2.609141418,-1.426596554\C,-1.352900718,-2.0010648
 03,-2.577986052\C,0.035890738,-2.42579043,-2.592527313\C,0.260400681,-
 3.269446659,-1.427849645\C,-0.99844309,-3.376628787,0.694285441\C,-2.9
 65775797,-1.900283406,-0.734383686\C,-1.691838278,-0.694241796,-2.9431
 78554\C,1.032824212,-1.547190881,-3.015529931\C,1.462854443,-3.1828796
 48,-0.725637804\C,-1.997932364,-2.611319074,1.412765315\C,-3.396006991

, -0.576805702, -1.177512757\C, -0.655510696, 0.209203678, -3.392829975\C, 2.29269062, -1.470416152, -2.295559926\C, 1.458908162, -3.183998388, 0.729669763\C, 0.252662524, -3.271642729, 1.425218382\C, -2.969714528, -1.901399853, 0.716359746\C, -2.707146494, 0.068982828, -2.22248378\C, 0.678104827, -0.205471348, -3.440264769\C, 2.502220718, -2.268831262, -1.169512936\C, -1.366858625, -2.005014401, 2.568525925\C, -3.95244616, 0.068785186, -0.010178732\C, -1.707771696, -0.698748091, 2.933858158\C, -0.997080551, 1.539718093, -2.939581226\C, 2.724269098, -0.08269385, -2.293319453\C, 2.495845004, -2.270633592, 1.180571432\C, 0.021835071, -2.42976891, 2.5899506\C, -3.402352385, -0.578602128, 1.159173322\C, -2.266831426, 1.484830924, -2.220206802\C, 1.730824427, 0.697164126, -3.01192266\C, 3.143768891, -1.709282476, 0.007706732\C, 3.558613887, -0.375402723, 0.009852934\C, 1.091976658, 3.345024718, 0.705102242\C, -0.16591174, 3.279465799, 1.422249909\C, 0.008930903, 2.41879438, 2.575649283\C, 1.39356544, 1.980980142, 2.597052993\C, 2.062191027, 2.546854842, 1.434579866\C, 1.09576691, 3.346092498, -0.693061616\C, -1.368277782, 3.247953434, 0.72464735\C, -1.013015434, 1.535209231, 2.937449303\C, 1.714456412, 0.69253922, 3.023306731\C, 3.006638017, 1.79264202, 0.737678678\C, -0.158211023, 3.281642254, -1.417122524\C, -2.475233717, 2.40254749, 1.163972174\C, -0.67390249, 0.204001589, 3.390503672\C, 2.711784887, -0.08622083, 2.308908135\C, 3.010581774, 1.79375442, -0.717630806\C, 2.069925802, 2.549035583, -1.418486575\C, -1.364342192, 3.249060643, -0.726098444\C, -2.278841989, 1.481430909, 2.211116935\C, 0.659434334, -0.210749978, 3.444548004\C, 3.342268375, 0.450961565, 1.184945981\C, 0.022887402, 2.422735615, -2.570871504\C, -3.294390168, 2.18475192, -0.00677448\C, 2.280205242, -1.473942627, 2.306681943\C, 3.348641701, 0.452760458, -1.165129178\C, 1.407617924, 1.984947218, -2.585432291\C, -2.468892023, 2.40433082, -1.172718387\C, -2.719155919, 0.065582661, 2.2088374\C, 1.016454506, -1.55181828, 3.01969022\N, -0.074751559, 0.023092435, -0.002537628\H, -3.253787298, 1.011826175, -0.007534046\\Version=AM64L-G03RevD.02\\State=3-A\\HF=-2341.1581276\\S2=3.023714\\S2-1=0.\\S2A=2.052946\\RMSD=3.164e-09\\RMSF=3.084e-06\\ZeroPoint=0.3798726\\Thermal=0.4036735\\ZPE=238.3736736\\Dipole=0.4106838, -0.1277175, 0.0009833\\DipoleDeriv=0.0864577, -0.0116562, -0.0248456, -0.0203138, -0.0321263, -0.082\\Polar=498.7059056, -4.0440578, 486.9540738, 0.0802835, 0.0039667, 468.211766\\PG=C01 [X(C60H1N1)]\\NImag=1\\0.50015353, -0.08936942, 0.22587151, 0.000204, -0.00023755, 0.00008405, 0.00036696, 0.02617002\\-0.00000143, -0.000000249\\\\@

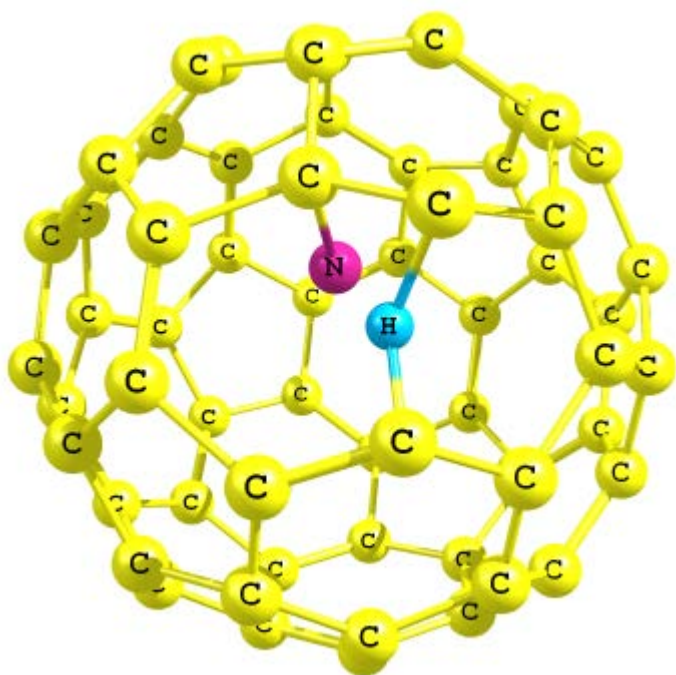
³TS1e (TS of endohedrally bound N@C₆₀H[•] → NH[•]@C₆₀ by breaking [5,6]-bond, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

\\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCFCyc=1200 SCF=Tight Pop=N
one Name=Drall\\TS endo-N@C60H -> NH@C60 triplet\\0,3\C,0,0.9582917733,
0.7060298343, -3.3226955455\C,0, -0.3197235788, 1.4044048153, -3.264349120

5\C,0,-0.1483374224,2.6135871331,-2.484898501\C,0,1.2390007111,2.67024
 43046,-2.066247096\C,0,1.9274724952,1.5015981943,-2.5915855188\C,0,1.0
 120595994,-0.687494148,-3.2611598434\C,0,-1.4985383352,0.6572875507,-3
 .1261710826\C,0,-1.1594373745,3.0641155814,-1.6049928094\C,0,1.5746394
 205,3.1583258306,-0.8004945544\C,0,2.9182053545,0.8741806854,-1.835524
 7571\C,0,-0.2100203583,-1.4720852307,-3.1144296248\C,0,-2.5104602412,1
 .1586824609,-2.2336030324\C,0,-0.8055514961,3.5335908261,-0.2744107043
 \C,0,2.6066406507,2.5074281517,-0.0179284508\C,0,2.9804256509,-0.57601
 68856,-1.7793623899\C,0,2.0432614124,-1.3404501396,-2.4765904789\C,0,-
 1.4439929701,-0.8169392693,-3.0303054998\C,0,-2.3876851046,2.326337680
 4,-1.4865583663\C,0,0.5293261867,3.5908815712,0.1137687095\C,0,3.27034
 14741,1.3887486031,-0.524515549\C,0,0.0669042592,-2.5988047434,-2.2503
 147042\C,0,-2.8647637735,-0.0154170313,-1.3884685522\C,0,-0.8983655321
 ,-3.0554523407,-1.3310162341\C,0,-1.8162094019,3.0596318413,0.66943324
 48\C,0,2.2040692672,2.54227385,1.3809433586\C,0,3.3750329275,-0.955982
 9552,-0.4346710018\C,0,1.4591039127,-2.5180423782,-1.8552291096\C,0,-2
 .4131446246,-1.2896674855,-2.054570032\C,0,-2.8072799471,2.3186552388,
 -0.0405535258\C,0,0.9216507926,3.2104543546,1.4618291214\C,0,3.5561465
 433,0.2584342735,0.3415346393\C,0,3.1724012683,0.2934894618,1.68380330
 43\C,0,-0.8951105207,-0.5353336502,3.443109486\C,0,-1.8721951332,-1.35
 27638122,2.7482812309\C,0,-1.1888972096,-2.5118933737,2.2121092278\C,0
 ,0.2101808635,-2.4193529851,2.5912635382\C,0,0.392056807,-1.2031329551
 ,3.3627559945\C,0,-0.9674157319,0.8505048206,3.3594119007\C,0,-2.90256
 79969,-0.7397028633,2.0070772486\C,0,-1.5323881811,-3.0547801454,0.953
 4695535\C,0,1.2057073952,-2.8308969495,1.7025040365\C,0,1.5589064837,-
 0.4524216984,3.2220413505\C,0,-2.003472596,1.4932971634,2.5561901028\C
 ,0,-3.3246212128,-1.4442768407,0.841008\C,0,-0.4876945276,-3.441892005
 8,0.0134045563\C,0,2.4209326684,-2.055583546,1.5596452799\C,0,1.486741
 1284,0.9977375701,3.1620590922\C,0,0.2472215901,1.635101096,3.23263301
 52\C,0,-2.9652362873,0.7281543633,1.8686704419\C,0,-2.5983039065,-2.45
 73440373,0.2100048766\C,0,0.8484573407,-3.3457350288,0.386567769\C,0,2
 .5959376053,-0.8871017503,2.3044820591\C,0,-1.4367028732,2.6795033891,
 1.9687566982\C,0,-3.9785559396,0.1536383388,-0.3532004866\C,0,2.817425
 3292,-2.0896033349,0.1591840617\C,0,2.4868095017,1.4582095785,2.215088
 8959\C,0,-0.0442641667,2.7609064,2.3642196214\C,0,-3.4117532564,1.1830
 733603,0.5542681747\C,0,-2.1860536742,-2.4114790465,-1.2424614101\C,0,
 1.8455453686,-2.8835948079,-0.5634942281\N,0,-1.5048482713,0.048586283
 7,-0.6208403017\H,0,-3.1415344358,-0.6631369885,0.0876867667\\Version=
 EM64L-G09RevA.02\State=3-A\HF=-2326.4488267\MP2=-2334.423958\RMSE=6.41
 8e-09\PG=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)



0 3

C	0.958291773	0.706029834	-3.322695546
C	-0.319723579	1.404404815	-3.264349120
C	-0.148337422	2.613587133	-2.484898501
C	1.239000711	2.670244305	-2.066247096
C	1.927472495	1.501598194	-2.591585519
C	1.012059599	-0.687494148	-3.261159843
C	-1.498538335	0.657287551	-3.126171083
C	-1.159437374	3.064115581	-1.604992809
C	1.574639420	3.158325831	-0.800494554
C	2.918205354	0.874180685	-1.835524757
C	-0.210020358	-1.472085231	-3.114429625
C	-2.510460241	1.158682461	-2.233603032
C	-0.805551496	3.533590826	-0.274410704
C	2.606640651	2.507428152	-0.017928451
C	2.980425651	-0.576016886	-1.779362390
C	2.043261412	-1.340450140	-2.476590479
C	-1.443992970	-0.816939269	-3.030305500
C	-2.387685105	2.326337680	-1.486558366
C	0.529326187	3.590881571	0.113768710
C	3.270341474	1.388748603	-0.524515549
C	0.066904259	-2.598804743	-2.250314704
C	-2.864763774	-0.015417031	-1.388468552
C	-0.898365532	-3.055452341	-1.331016234
C	-1.816209402	3.059631841	0.669433245
C	2.204069267	2.542273850	1.380943359
C	3.375032928	-0.955982955	-0.434671002
C	1.459103913	-2.518042378	-1.855229110
C	-2.413144625	-1.289667486	-2.054570032

```

C   -2.807279947 2.318655239 -0.040553526
C   0.921650793 3.210454355 1.461829121
C   3.556146543 0.258434273 0.341534639
C   3.172401268 0.293489462 1.683803304
C   -0.895110521 -0.535333650 3.443109486
C   -1.872195133 -1.352763812 2.748281231
C   -1.188897210 -2.511893374 2.212109228
C   0.210180864 -2.419352985 2.591263538
C   0.392056807 -1.203132955 3.362755994
C   -0.967415732 0.850504821 3.359411901
C   -2.902567997 -0.739702863 2.007077249
C   -1.532388181 -3.054780145 0.953469554
C   1.205707395 -2.830896950 1.702504036
C   1.558906484 -0.452421698 3.222041350
C   -2.003472596 1.493297163 2.556190103
C   -3.324621213 -1.444276841 0.841008000
C   -0.487694528 -3.441892006 0.013404556
C   2.420932668 -2.055583546 1.559645280
C   1.486741128 0.997737570 3.162059092
C   0.247221590 1.635101096 3.232633015
C   -2.965236287 0.728154363 1.868670442
C   -2.598303906 -2.457344037 0.210004877
C   0.848457341 -3.345735029 0.386567769
C   2.595937605 -0.887101750 2.304482059
C   -1.436702873 2.679503389 1.968756698
C   -3.978555940 0.153638339 -0.353200487
C   2.817425329 -2.089603335 0.159184062
C   2.486809502 1.458209578 2.215088896
C   -0.044264167 2.760906400 2.364219621
C   -3.411753256 1.183073360 0.554268175
C   -2.186053674 -2.411479046 -1.242461410
C   1.845545369 -2.883594808 -0.563494228
N   -1.504848271 0.048586284 -0.620840302
H   -3.141534436 -0.663136988 0.087686767

```

```

Zero-point correction=          0.382942 (Hartree/Particle)
Thermal correction to Energy=    0.405111
Thermal correction to Enthalpy=  0.406055
Thermal correction to Gibbs Free Energy= 0.337988
Sum of electronic and zero-point Energies= -2340.750605
Sum of electronic and thermal Energies= -2340.728436
Sum of electronic and thermal Enthalpies= -2340.727492
Sum of electronic and thermal Free Energies= -2340.795558

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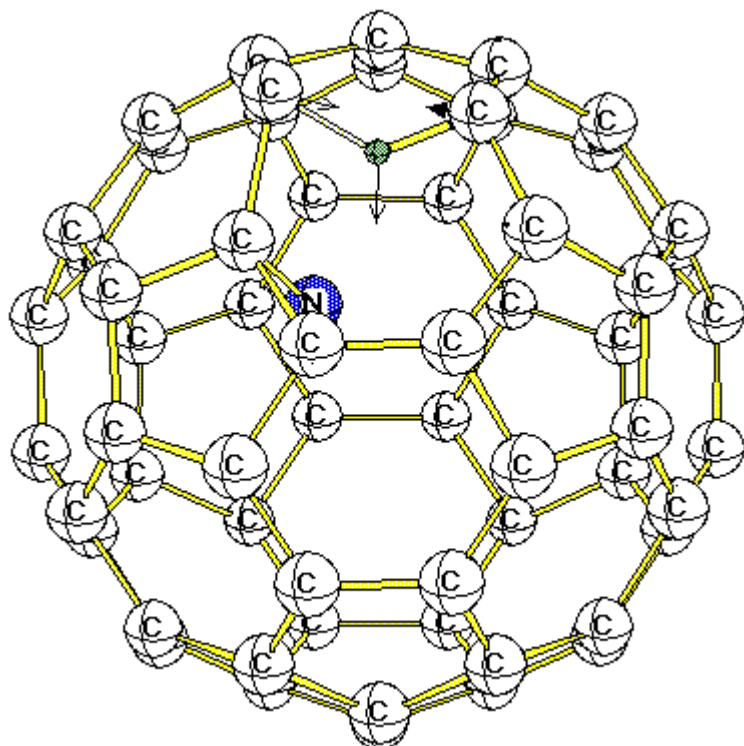
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\TS endo-N@C60H -> NH@C60 triplet\0,3\C,0.9582917733,0.7060298343,-3
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Vibrational Normal Modes



62

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C	-0.383701	-3.535473	-0.433513
C	-1.720052	-3.129460	-0.042996
C	-2.339568	-2.441656	-1.164973
C	-1.285278	-1.271218	-3.061544
C	1.080873	-2.590416	-2.172269
C	0.662167	-3.492259	0.517184
C	-1.971795	-2.691041	1.259856
C	-3.181445	-1.352032	-0.939594
C	0.016873	-0.741454	-3.454412
C	2.123818	-2.579268	-1.180200
C	0.400792	-2.997228	1.859838
C	-2.849509	-1.561142	1.492343
C	-3.094094	-0.177959	-1.790488
C	-2.161793	-0.138604	-2.828769
C	1.182232	-1.374465	-3.006955
C	1.962923	-3.017130	0.130890
C	-0.886790	-2.617661	2.225796
C	-3.447533	-0.904353	0.415510
C	-0.058101	0.703231	-3.466293
C	2.676447	-1.197872	-1.248321
C	1.036005	1.484459	-3.044396
C	1.544033	-2.193904	2.289462
C	-2.312195	-0.791733	2.605637
C	-3.310448	0.993919	-0.960923

C	-1.404042	1.076755	-3.079308
C	2.287508	-0.546821	-2.550713
C	2.526082	-2.188197	1.254621
C	-1.100497	-1.443690	3.057680
C	-3.530746	0.545564	0.403098
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C	1.269352	2.430969	2.265308
C	2.246649	2.507515	1.195399
C	1.630213	3.180562	0.070689
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C	0.052969	3.083621	1.814009
C	1.195541	1.288883	3.054595
C	3.130694	1.432581	0.972068
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C	-0.760524	3.454942	-0.481297
C	-1.190551	2.576192	2.189614
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C	3.499497	1.211672	-0.387879
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C	-1.268442	1.398422	3.037292
C	-0.097214	0.770238	3.463004
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C	2.816407	1.719005	-1.496033
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C	3.867569	-0.854797	-0.351426
C	-2.586119	2.161936	-1.205399
C	-2.400187	0.602223	2.596673
C	-0.008173	-0.678402	3.470665
C	3.297095	-1.024644	1.008799
C	2.256090	0.855319	-2.601386
C	-1.619122	2.203947	-2.282612
N	1.402003	-0.588608	-0.579510
H	3.164504	0.168708	-0.493712

NORMALMODES 180

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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00

C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	-0.01	-0.03
C	0.00	0.00	0.00
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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	-0.01
C	0.01	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.01	-0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	0.00	0.01
C	0.02	-0.02	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.03	-0.17	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.02
C	0.01	-0.04	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.08	0.26	-0.02
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	0.01	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	-0.03	-0.02	-0.01
H	-0.83	-0.05	0.44

-658.5400

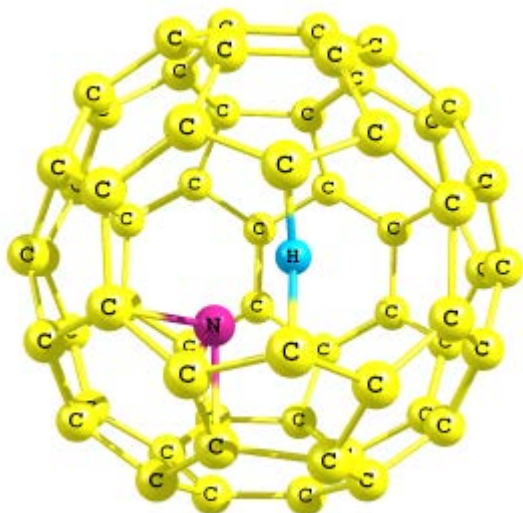
³TS1f (TS of endohedrally bound N@C₆₀H^{••} → NH^{••}@C₆₀ by breaking [6,6]-bond, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
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one Name=Dral\TS endo-N@C60H -> NH@C60 via breaking 6,6-bond triplet\
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UB3LYP/6-31G(d)



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C	-0.323487968	2.281647508	2.692211854
C	1.064954100	1.893184442	2.829510284
C	1.828618558	2.541349077	1.773824177
C	1.056999257	3.408476127	-0.402522980
C	-1.538018469	3.155016383	0.749949565
C	-1.347174258	1.352740659	2.925492558
C	1.394271006	0.596172765	3.227687146
C	2.876507163	1.859994932	1.149177055
C	-0.109181973	3.336822492	-1.257911530
C	-2.650167753	2.248292212	1.047298094
C	-0.998435749	0.011043258	3.341594684
C	2.491474772	-0.106850210	2.585522200
C	3.034900655	1.938528094	-0.292988312
C	2.141745182	2.692684388	-1.055523552
C	-1.388238000	3.234322050	-0.693958386
C	-2.538336158	1.293174302	2.092649386
C	0.340023346	-0.360324705	3.498707379
C	3.217319821	0.511771050	1.563759216
C	0.239503241	2.559465072	-2.424254760
C	-3.290368655	1.988552164	-0.200265677
C	-0.692363436	1.652665431	-2.949820214
C	-1.952605081	-0.897897552	2.749004163
C	2.119543082	-1.503337281	2.468137549
C	3.474338197	0.638202562	-0.768135705

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C    3.590822885  -0.242193822  0.379924492
C    3.231222534  -1.586725552  0.263352084
C    -0.737922658 -3.330642741 -0.980315653
C    -1.673199794 -2.621023495 -1.810087171
C    -0.924476301 -1.952834461 -2.881489370
C    0.469366314  -2.299069318 -2.720203844
C    0.590043394  -3.168751606 -1.556522375
C    -0.889917308 -3.391010978  0.420316632
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C    1.698637670  -3.073560414 -0.716544993
C    -1.996457721 -2.707880775  1.104680502
C    -3.289212861 -0.554097384 -1.443024480
C    -0.255261257  0.349168187  -3.461531914
C    2.628275585  -1.259021143 -2.105787616
C    1.539217124  -3.149332668  0.725716871
C    0.258984771  -3.299217922  1.278513832
C    -2.920864753 -1.986645085  0.388338963
C    -2.287962855  0.069556021  -2.351629170
C    1.105182317  -0.005823464 -3.370225440
C    2.747075994  -2.104618395 -1.001126868
C    -1.517383782 -2.172100428  2.353543118
C    -4.168052416 -0.053216985 -0.293841668
C    2.996742409  0.141057487  -1.983312820
C    2.480415998  -2.231423424  1.330399998
C    -0.117467398 -2.544926687  2.469013885
C    -3.538296025 -0.749317297  0.858059714
C    -1.995539380  1.542118743  -2.355548004
C    2.053229343  0.916989612  -2.765789373
N    -1.871057482 -0.370205142 -0.972916724
H    -3.296680235  0.867886002  -0.121731521

```

```

Zero-point correction=          0.380235 (Hartree/Particle)
Thermal correction to Energy=    0.402624
Thermal correction to Enthalpy=  0.403569
Thermal correction to Gibbs Free Energy=  0.335030
Sum of electronic and zero-point Energies= -2340.735851
Sum of electronic and thermal Energies= -2340.713462
Sum of electronic and thermal Enthalpies= -2340.712518
Sum of electronic and thermal Free Energies= -2340.781056

```

```

1\1\FAU-CCC-CCDN085\Freq\UB3LYP/6-31G(d)\C60H1N1(3)\DRAL\25-Aug-2010\0
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\TS endo-N@C60H -> NH@C60 via breaking 6,6-bond triplet\0,3\C,0.9087
983563,3.3371285224,0.9852761891\C,-0.4148396408,3.188341667,1.5631185

```

188\C,-0.323487968,2.2816475084,2.6922118542\C,1.0649540995,1.89318444
 19,2.8295102843\C,1.8286185584,2.541349077,1.7738241771\C,1.0569992568
 ,3.4084761271,-0.40252298\C,-1.5380184691,3.1550163829,0.7499495647\C,
 -1.347174258,1.3527406589,2.9254925582\C,1.3942710056,0.5961727652,3.2
 276871457\C,2.8765071626,1.8599949321,1.1491770554\C,-0.1091819733,3.3
 368224922,-1.2579115301\C,-2.6501677531,2.2482922123,1.0472980937\C,-0
 .9984357489,0.0110432578,3.3415946845\C,2.4914747719,-0.1068502102,2.5
 855221997\C,3.0349006547,1.9385280943,-0.2929883121\C,2.1417451823,2.6
 926843879,-1.0555235523\C,-1.3882380003,3.2343220501,-0.6939583858\C,-
 2.5383361576,1.2931743019,2.092649386\C,0.3400233461,-0.3603247051,3.4
 987073788\C,3.2173198207,0.5117710499,1.563759216\C,0.2395032406,2.559
 4650717,-2.4242547598\C,-3.2903686554,1.9885521638,-0.2002656772\C,-0.
 6923634364,1.6526654311,-2.9498202135\C,-1.9526050807,-0.8978975518,2.
 7490041626\C,2.1195430817,-1.5033372806,2.468137549\C,3.4743381968,0.6
 382025615,-0.7681357048\C,1.636353273,2.1682877166,-2.3108268537\C,-2.
 3800814377,2.3612883829,-1.2856056983\C,-2.9366846272,-0.1333402269,1.
 988042767\C,0.7933374774,-1.6619663579,3.0414295053\C,3.5908228847,-0.
 242193822,0.379924492\C,3.2312225343,-1.5867255523,0.2633520836\C,-0.7
 379226581,-3.3306427412,-0.9803156529\C,-1.6731997936,-2.621023495,-1.
 8100871711\C,-0.9244763014,-1.9528344609,-2.8814893703\C,0.4693663138,
 -2.2990693176,-2.7202038435\C,0.5900433937,-3.1687516061,-1.5565223754
 \C,-0.8899173076,-3.391010978,0.4203166322\C,-2.6124255217,-1.79294674
 14,-1.0531531763\C,-1.2680331499,-0.6396362529,-3.2348677805\C,1.46869
 17853,-1.3491273501,-2.9788697891\C,1.69863767,-3.0735604145,-0.716544
 9927\C,-1.9964577212,-2.7078807752,1.1046805021\C,-3.2892128612,-0.554
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 57168709\C,0.2589847706,-3.2992179223,1.278513832\C,-2.9208647529,-1.9
 866450849,0.3883389627\C,-2.2879628546,0.069556021,-2.3516291703\C,1.1
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 0011268679\C,-1.5173837824,-2.1721004279,2.3535431178\C,-4.1680524155,
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 C,2.4804159982,-2.2314234243,1.3303999984\C,-0.1174673984,-2.544926686
 6,2.4690138847\C,-3.5382960254,-0.7493172971,0.8580597144\C,-1.9955393
 799,1.5421187431,-2.3555480039\C,2.0532293432,0.9169896119,-2.76578937
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 \\S2=2.063005\\S2-1=0.\\S2A=2.002611\\RMSD=6.606e-09\\RMSF=5.042e-05\\ZeroPo
 int=0.3802349\\Thermal=0.4026245\\ZPE=238.6010208\\Dipole=0.2964959,-0.15
 37554,-0.0392801\\DipoleDeriv=0.0241972,-0.0719275,0.0049789,0.0026001,
 \\Polar=516.9052268,4.3826121,491.0464462,7.9852479,0.952509,476.264969
 \\PG=C01 [X(C60H1N1)]\\NImag=1\\0.50912041,-0.07424580,0.23361483,-0.045
 3,0.00541351,0.03789570\\-0.00000984,0.00001634,-0.00002624,-0.0000380
 019542,-0.00032275,0.00004713,-0.00008918,-0.00001771\\\\@

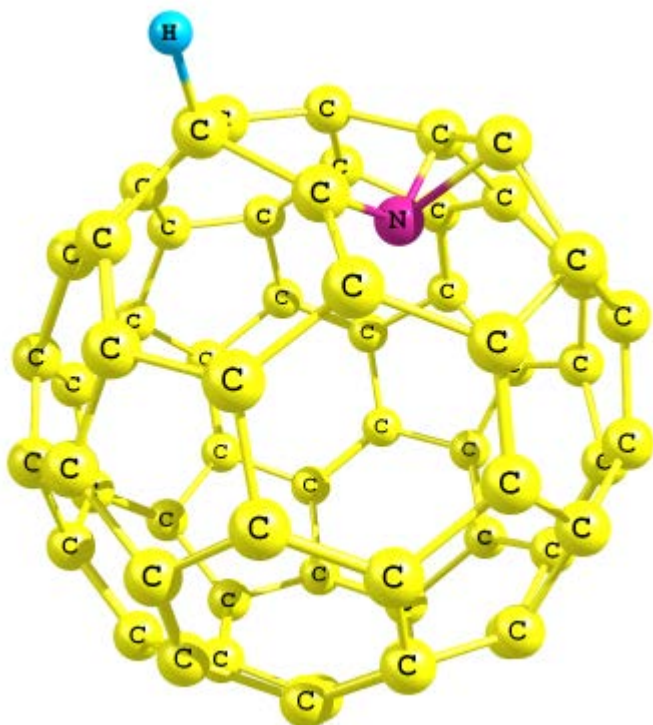
³TS1m (TS of N-escape from triplet N@C₆₀H^{••} by displacing carbon atom)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN087\SP\ROMP2-FC\6-31G(d)\C60H1N1(3)\DRAL\21-Aug-2010\0
\#P ROMP2/6-31G* SCF=Tight SCFCyc=1200 Guess=Read Geom=AllCheck Pop=N
one NAME=DRAL\TS N-escape from N@C60H via breaking 5,6-bond triplet\
0,3\C,0,0.9773851604,0.4374065098,-3.563991438\C,0,-0.2975797024,1.113
9784594,-3.3964917108\C,0,-0.0730512775,2.3033082378,-2.568491343\C,0,
1.3225156074,2.3372141419,-2.2162560197\C,0,1.9688728016,1.1766453664,
-2.8148258661\C,0,1.0215293101,-0.9676437692,-3.5775493283\C,0,-1.4927
582151,0.3997145694,-3.3208948963\C,0,-1.0438311138,2.7370611726,-1.65
21472397\C,0,1.7287719274,2.7946113442,-0.9555015559\C,0,2.9723236862,
0.5050124148,-2.1088647428\C,0,-0.196873066,-1.7299669978,-3.554374603
8\C,0,-2.5034412484,0.8595530133,-2.3039364563\C,0,-0.621893575,3.2039
288197,-0.3375667306\C,0,2.7677925889,2.093296313,-0.2308469151\C,0,2.
9965731834,-0.9478367421,-2.0983535775\C,0,2.028964679,-1.6633904104,-
2.801259381\C,0,-1.4207328389,-1.0657953993,-3.5711796723\C,0,-2.29991
47236,2.0452273654,-1.5149929704\C,0,0.7297987341,3.2310037995,0.00167
30525\C,0,3.3774153776,0.9674052631,-0.7960268774\C,0,0.0266263167,-2.
8676309131,-2.5876783078\C,0,-2.9308474024,-0.2057305718,-1.4740295868
\C,0,-0.8983412084,-3.2722799978,-1.6171897381\C,0,-1.6039189787,2.750
2635394,0.6284660704\C,0,2.4164119757,2.0961812567,1.1789058095\C,0,3.
4096174372,-1.3826824653,-0.7756599646\C,0,1.4137940801,-2.8365192448,
-2.2000766274\C,0,-2.4712738388,-1.7505316948,-2.7566600339\C,0,-2.641
4501896,2.0308718537,-0.0743835773\C,0,1.1581786863,2.8048531984,1.324
777291\C,0,3.6478491428,-0.1980906273,0.0281382707\C,0,3.3102865777,-0
.1947498665,1.3841333468\C,0,-0.7316411012,-0.9359833517,3.2371262729\
C,0,-1.7541695168,-1.6792486713,2.5201606697\C,0,-1.1415436468,-2.8313
043717,1.917895378\C,0,0.2737859567,-2.818319348,2.269624628\C,0,0.522
9625153,-1.6430654029,3.0848578399\C,0,-0.7433645127,0.4624992235,3.23
29894458\C,0,-2.7665428893,-1.0009244523,1.8203491371\C,0,-1.566237358
6,-3.2723687619,0.6495817216\C,0,1.2380139952,-3.2448131828,1.35926645
33\C,0,1.720401618,-0.9326488623,2.9449271323\C,0,-1.7818124751,1.1769
238226,2.5161378107\C,0,-3.2700568733,-1.4958420961,0.5783155452\C,0,-
0.5284204203,-3.6872177784,-0.3057155021\C,0,2.4809935421,-2.513597962
6,1.2113198192\C,0,1.7032818454,0.5200430731,2.9384168165\C,0,0.491935
8182,1.2018091318,3.079968594\C,0,-2.7670634884,0.4671846683,1.8207870
898\C,0,-2.6986700278,-2.6504729887,-0.0100769913\C,0,0.8290037144,-3.
701328666,0.0423202031\C,0,2.7156784488,-1.3728538192,1.9871401706\C,0
,-1.1945649874,2.3480392001,1.9067448365\C,0,-3.7597084554,-0.25883813
15,-0.2346137213\C,0,2.831814525,-2.5152548821,-0.1977130379\C,0,2.684
8009284,0.9772468568,1.9724243312\C,0,0.2145301574,2.3686437827,2.2541
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20237\C,0,-3.2516892969,0.9415901646,0.5652883404\C,0,-2.2249566298,-2
 .5848960641,-1.4954707036\C,0,1.807120788,-3.2513580442,-0.9166791987\
 N,0,-1.951858562,-1.1772005341,-1.5365891452\H,0,-4.8354403066,-0.2449
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UB3LYP/6-31G(d)



0 3

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C	-0.297579702	1.113978459	-3.396491711
C	-0.073051278	2.303308238	-2.568491343
C	1.322515607	2.337214142	-2.216256020
C	1.968872802	1.176645366	-2.814825866
C	1.021529310	-0.967643769	-3.577549328
C	-1.492758215	0.399714569	-3.320894896
C	-1.043831114	2.737061173	-1.652147240
C	1.728771927	2.794611344	-0.955501556
C	2.972323686	0.505012415	-2.108864743
C	-0.196873066	-1.729966998	-3.554374604
C	-2.503441248	0.859553013	-2.303936456
C	-0.621893575	3.203928820	-0.337566731
C	2.767792589	2.093296313	-0.230846915
C	2.996573183	-0.947836742	-2.098353578
C	2.028964679	-1.663390410	-2.801259381
C	-1.420732839	-1.065795399	-3.571179672
C	-2.299914724	2.045227365	-1.514992970
C	0.729798734	3.231003800	0.001673052
C	3.377415378	0.967405263	-0.796026877

C	0.026626317	-2.867630913	-2.587678308
C	-2.930847402	-0.205730572	-1.474029587
C	-0.898341208	-3.272279998	-1.617189738
C	-1.603918979	2.750263539	0.628466070
C	2.416411976	2.096181257	1.178905810
C	3.409617437	-1.382682465	-0.775659965
C	1.413794080	-2.836519245	-2.200076627
C	-2.471273839	-1.750531695	-2.756660034
C	-2.641450190	2.030871854	-0.074383577
C	1.158178686	2.804853198	1.324777291
C	3.647849143	-0.198090627	0.028138271
C	3.310286578	-0.194749866	1.384133347
C	-0.731641101	-0.935983352	3.237126273
C	-1.754169517	-1.679248671	2.520160670
C	-1.141543647	-2.831304372	1.917895378
C	0.273785957	-2.818319348	2.269624628
C	0.522962515	-1.643065403	3.084857840
C	-0.743364513	0.462499224	3.232989446
C	-2.766542889	-1.000924452	1.820349137
C	-1.566237359	-3.272368762	0.649581722
C	1.238013995	-3.244813183	1.359266453
C	1.720401618	-0.932648862	2.944927132
C	-1.781812475	1.176923823	2.516137811
C	-3.270056873	-1.495842096	0.578315545
C	-0.528420420	-3.687217778	-0.305715502
C	2.480993542	-2.513597963	1.211319819
C	1.703281845	0.520043073	2.938416816
C	0.491935818	1.201809132	3.079968594
C	-2.767063488	0.467184668	1.820787090
C	-2.698670028	-2.650472989	-0.010076991
C	0.829003714	-3.701328666	0.042320203
C	2.715678449	-1.372853819	1.987140171
C	-1.194564987	2.348039200	1.906744836
C	-3.759708455	-0.258838132	-0.234613721
C	2.831814525	-2.515254882	-0.197713038
C	2.684800928	0.977246857	1.972424331
C	0.214530157	2.368643783	2.254120237
C	-3.251689297	0.941590165	0.565288340
C	-2.224956630	-2.584896064	-1.495470704
C	1.807120788	-3.251358044	-0.916679199
N	-1.951858562	-1.177200534	-1.536589145
H	-4.835440307	-0.244966507	-0.454992987

Zero-point correction=	0.383465 (Hartree/Particle)
Thermal correction to Energy=	0.405356
Thermal correction to Enthalpy=	0.406301
Thermal correction to Gibbs Free Energy=	0.338609
Sum of electronic and zero-point Energies=	-2340.820808
Sum of electronic and thermal Energies=	-2340.798917
Sum of electronic and thermal Enthalpies=	-2340.797973

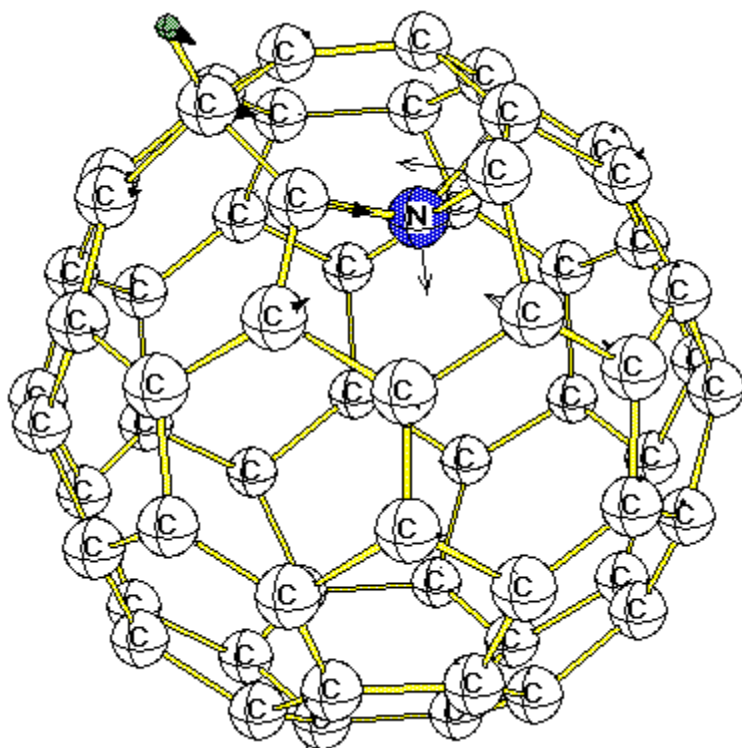
Sum of electronic and thermal Free Energies= -2340.865664

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1\1\FAU-CCC-CCDN089\Freq\UB3LYP\6-31G(d)\C60H1N1(3)\DRAL\19-Aug-2010\
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\TS N-escape from N@C60H via breaking 5,6-bond triplet\0,3\C,0.97738
51604,0.4374065098,-3.563991438\C,-0.2975797024,1.1139784594,-3.396491
7108\C,-0.0730512775,2.3033082378,-2.568491343\C,1.3225156074,2.337214
1419,-2.2162560197\C,1.9688728016,1.1766453664,-2.8148258661\C,1.02152
93101,-0.9676437692,-3.5775493283\C,-1.4927582151,0.3997145694,-3.3208
948963\C,-1.0438311138,2.7370611726,-1.6521472397\C,1.7287719274,2.794
6113442,-0.9555015559\C,2.9723236862,0.5050124148,-2.1088647428\C,-0.1
96873066,-1.7299669978,-3.5543746038\C,-2.5034412484,0.8595530133,-2.3
039364563\C,-0.621893575,3.2039288197,-0.3375667306\C,2.7677925889,2.0
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8665,1.3841333468\C,-0.7316411012,-0.9359833517,3.2371262729\C,-1.7541
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95378\C,0.2737859567,-2.818319348,2.269624628\C,0.5229625153,-1.643065
4029,3.0848578399\C,-0.7433645127,0.4624992235,3.2329894458\C,-2.76654
28893,-1.0009244523,1.8203491371\C,-1.5662373586,-3.2723687619,0.64958
17216\C,1.2380139952,-3.2448131828,1.3592664533\C,1.720401618,-0.93264
88623,2.9449271323\C,-1.7818124751,1.1769238226,2.5161378107\C,-3.2700
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7155021\C,2.4809935421,-2.5135979626,1.2113198192\C,1.7032818454,0.520
0430731,2.9384168165\C,0.4919358182,1.2018091318,3.079968594\C,-2.7670
634884,0.4671846683,1.8207870898\C,-2.6986700278,-2.6504729887,-0.0100
769913\C,0.8290037144,-3.701328666,0.0423202031\C,2.7156784488,-1.3728
538192,1.9871401706\C,-1.1945649874,2.3480392001,1.9067448365\C,-3.759
7084554,-0.2588381315,-0.2346137213\C,2.831814525,-2.5152548821,-0.197
7130379\C,2.6848009284,0.9772468568,1.9724243312\C,0.2145301574,2.3686
437827,2.254120237\C,-3.2516892969,0.9415901646,0.5652883404\C,-2.2249
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00240,-0.00004852,-0.00000796\@

```

Vibrational Normal Modes



62

C	1.078174	-2.956680	1.692241
C	1.734880	-1.877006	2.409444
C	0.723104	-1.191241	3.219715
C	-0.542624	-1.833980	2.979615
C	-0.328645	-2.912333	2.023399
C	1.473563	-3.258426	0.377358
C	2.802036	-1.177259	1.847420
C	0.783448	0.196000	3.425047
C	-1.726412	-1.085095	2.939913
C	-1.296717	-3.171691	1.047716
C	2.603390	-2.591133	-0.209488
C	2.825357	0.314867	2.047801
C	-0.446620	0.976057	3.374423
C	-2.723316	-1.359405	1.926272
C	-0.886234	-3.451728	-0.317770
C	0.468342	-3.473145	-0.644915
C	3.333843	-1.682650	0.552310
C	1.853429	0.984878	2.870066
C	-1.669699	0.351032	3.137123
C	-2.511765	-2.382791	0.995345
C	2.207333	-2.238285	-1.622772
C	2.977073	1.004237	0.819794
C	2.452370	-0.997978	-2.225058
C	-0.141428	2.241044	2.734054

C	-3.289566	-0.092895	1.494770
C	-1.844484	-2.828724	-1.213783
C	0.927946	-2.850058	-1.876424
C	3.848805	-0.527814	-0.245881
C	1.266791	2.264457	2.410998
C	-2.642313	0.965986	2.247419
C	-2.850898	-2.170572	-0.401335
C	-3.396039	-0.952525	-0.815900
C	-1.227937	2.902679	-1.685915
C	0.184462	2.901472	-2.028224
C	0.423406	1.843946	-2.971522
C	-0.850608	1.184057	-3.233201
C	-1.869176	1.841751	-2.434531
C	-1.635305	3.169075	-0.374812
C	1.153615	3.172415	-1.047361
C	1.620602	1.104556	-2.911972
C	-0.911725	-0.193157	-3.433028
C	-2.899031	1.092476	-1.854775
C	-0.647346	3.451208	0.648413
C	2.410681	2.493577	-1.038334
C	1.527156	-0.351437	-3.093933
C	-1.977301	-0.974075	-2.836139
C	-3.317176	1.370786	-0.491563
C	-2.694550	2.390937	0.232199
C	0.714299	3.447921	0.326117
C	2.673214	1.472615	-1.984153
C	0.306925	-0.981430	-3.373348
C	-2.951466	-0.342410	-2.054940
C	-1.080541	2.839876	1.883867
C	2.886478	2.445684	0.445619
C	-1.411422	-2.239461	-2.403667
C	-3.623071	0.106821	0.152158
C	-2.349590	2.182268	1.631464
C	1.674949	2.928351	1.244483
C	3.171572	0.083650	-1.476695
C	0.001637	-2.239390	-2.738365
N	2.569242	0.139195	-0.175929
H	3.820072	2.986231	0.650971

NORMALMODES 180

C	0.03	0.01	0.01
C	0.01	-0.04	-0.02
C	-0.04	0.03	-0.02
C	0.00	0.01	0.02
C	0.01	0.02	0.00
C	0.05	0.01	-0.02
C	0.02	-0.03	0.02
C	-0.02	0.01	-0.04
C	-0.02	0.01	0.00
C	0.02	0.01	0.00

C 0.01 0.10 0.00
C 0.14 -0.08 -0.03
C -0.02 0.01 0.01
C -0.01 0.00 0.01
C 0.02 0.00 0.00
C 0.04 0.01 0.01
C -0.03 0.16 0.02
C -0.01 0.05 -0.02
C -0.02 0.00 0.01
C 0.00 0.01 0.01
C 0.03 0.02 -0.01
C 0.10 -0.30 -0.10
C 0.08 -0.01 -0.03
C 0.00 -0.01 0.01
C -0.01 0.00 0.00
C 0.02 -0.01 0.01
C 0.02 0.01 0.00
C -0.13 0.43 0.20
C 0.04 -0.04 0.02
C -0.01 0.00 0.01
C 0.01 0.00 0.01
C 0.01 0.00 0.00
C 0.01 0.00 -0.01
C 0.01 -0.01 0.00
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C 0.01 0.00 0.00
C 0.01 0.01 0.01
C 0.03 0.01 0.01
C 0.03 -0.02 -0.01
C 0.01 0.00 -0.01
C 0.02 0.00 0.01
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C 0.03 -0.01 -0.02
C 0.04 0.00 -0.01
C 0.02 -0.01 0.01
C 0.01 0.00 0.01
C 0.02 0.00 0.01
C 0.05 -0.04 0.00
C -0.01 -0.02 0.01
C 0.03 0.01 0.01
C 0.00 0.01 0.01
C 0.01 -0.02 0.01
C 0.05 -0.14 -0.04
C 0.01 0.00 0.00
C 0.00 0.00 0.01
C 0.00 0.00 0.01
C 0.06 -0.07 -0.03
C -0.09 0.03 0.08
C 0.02 0.01 0.01

N -0.65 -0.11 -0.11
 H 0.06 -0.18 0.03
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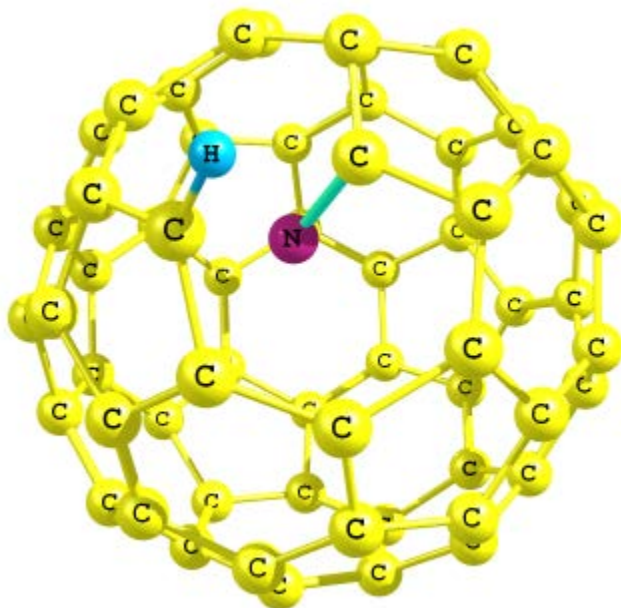
³TS1i (TS of N-escape from triplet N@C₆₀H^{••} by breaking [6,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
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one NAME=DRAL\TS N-escape from N@C60H via breaking 6,6-bond triplet\
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0,2.1176837159,-1.3108412663,-2.5339870006\C,0,2.9532913209,-1.5313671
19,-1.3628200348\C,0,2.3821080144,-2.6005794716,0.7786859844\C,0,0.110
1071396,-3.6006645659,-0.6710182116\C,0,-0.2559238035,-1.8830799594,-2
.9681079326\C,0,1.8998289406,-0.0111296485,-2.9955900002\C,0,3.5157451
229,-0.4425508212,-0.6909158104\C,0,1.2059485934,-3.0515547774,1.52747
21206\C,0,-1.1905277027,-3.2059072454,-1.1900321748\C,0,-0.4798156867,
-0.5220325047,-3.4084753494\C,0,2.5019138892,1.1173165038,-2.309822491
1\C,0,3.5060748761,-0.4062543519,0.7588023246\C,0,2.9343509397,-1.4602
721362,1.4767914774\C,0,0.099951523,-3.5625453937,0.851563815\C,0,-1.4
337720741,-2.3322713345,-2.2727250797\C,0,0.5777036353,0.3883065724,-3
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44,-2.1436463166,2.6418872456\C,0,-1.6354288037,-2.6417698141,0.055134
5461\C,0,-0.2960965904,-1.7322883451,3.0547430991\C,0,-1.8066291627,-0
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C,0,3.2727960875,0.9660121562,1.1716705114\C,0,2.0832775754,-1.1816960
725,2.6242117286\C,0,-1.2073552026,-3.142747762,1.3327898703\C,0,-2.46
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2.8378620793,-0.0562381557\C,0,-2.223916404,2.7460615498,0.6119844803\
C,0,-2.847201281,1.6608751057,1.3604098323\C,0,-2.0378432283,1.3809880
174,2.5171341231\C,0,-0.9287120082,2.3165675339,2.515740774\C,0,-1.041
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0,0.1058650267,3.5475184785,0.6383795999\C,0,-2.8282578945,1.589766263
2,-1.479859024\C,0,-3.418155328,-0.7358847656,1.2213354934\C,0,-0.5253
854979,-0.3509843848,3.4234252332\C,0,1.5236243886,2.3346693157,2.2505
028676\C,0,0.1155517366,3.5111598343,-0.8138327723\C,0,-1.0224885205,3
.0894438031,-1.506734321\C,0,-3.4764389521,0.5793019966,-0.7755446194\
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429045,1.2526169932,-2.6102343127\C,0,-3.5660626132,-1.5686098799,0.01
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 692534362,-1.2422494588\C,0,-0.8943155762,2.1874637218,-2.640871742\C,
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UB3LYP/6-31G(d)



0 3

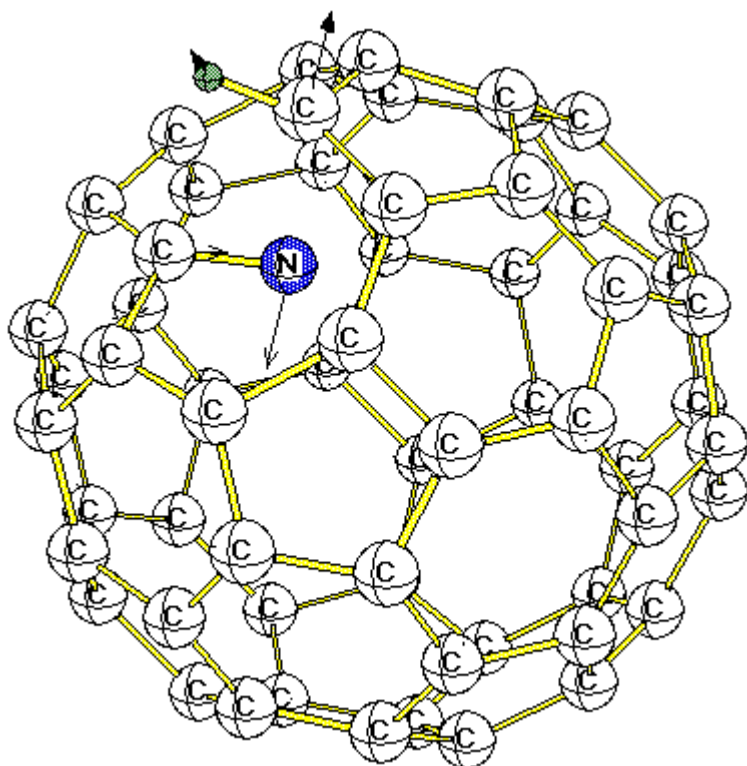
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C	1.225186544	-3.123767946	-1.356845540
C	1.034897163	-2.272830949	-2.517936660
C	2.117683716	-1.310841266	-2.533987001
C	2.953291321	-1.531367119	-1.362820035
C	2.382108014	-2.600579472	0.778685984
C	0.110107140	-3.600664566	-0.671018212
C	-0.255923804	-1.883079959	-2.968107933
C	1.899828941	-0.011129648	-2.995590000
C	3.515745123	-0.442550821	-0.690915810
C	1.205948593	-3.051554777	1.527472121
C	-1.190527703	-3.205907245	-1.190032175
C	-0.479815687	-0.522032505	-3.408475349
C	2.501913889	1.117316504	-2.309822491
C	3.506074876	-0.406254352	0.758802325
C	2.934350940	-1.460272136	1.476791477
C	0.099951523	-3.562545394	0.851563815
C	-1.433772074	-2.332271334	-2.272725080
C	0.577703635	0.388306572	-3.442740290
C	3.288449175	0.907258552	-1.175008389
C	1.000481064	-2.143646317	2.641887246

C	-1.635428804	-2.641769814	0.055134546
C	-0.296096590	-1.732288345	3.054743099
C	-1.806629163	-0.100403438	-2.968064163
C	1.554272650	2.219632473	-2.344200350
C	3.272796088	0.966012156	1.171670511
C	2.083277575	-1.181696072	2.624211729
C	-1.207355203	-3.142747762	1.332789870
C	-2.461697428	-1.172342229	-2.264581952
C	0.371559606	1.769298002	-3.052114798
C	3.148642676	1.781117566	-0.023692470
C	2.235924418	2.837862079	-0.056238156
C	-2.223916404	2.746061550	0.611984480
C	-2.847201281	1.660875106	1.360409832
C	-2.037843228	1.380988017	2.517134123
C	-0.928712008	2.316567534	2.515740774
C	-1.041452481	3.160622827	1.336281460
C	-2.214642360	2.711250732	-0.778429267
C	-3.486272271	0.616217990	0.698961652
C	-1.846068243	0.047634340	2.944815216
C	0.331428635	1.919927724	2.964234282
C	0.105865027	3.547518478	0.638379600
C	-2.828257894	1.589766263	-1.479859024
C	-3.418155328	-0.735884766	1.221335493
C	-0.525385498	-0.350984385	3.423425233
C	1.523624389	2.334669316	2.250502868
C	0.115551737	3.511159834	-0.813832772
C	-1.022488521	3.089443803	-1.506734321
C	-3.476438952	0.579301997	-0.775544619
C	-2.492056361	-1.058383475	2.287185405
C	0.531886280	0.560282490	3.426189464
C	1.414485181	3.128042751	1.105860578
C	-2.003642904	1.252616993	-2.610234313
C	-3.566062613	-1.568609880	0.015381671
C	2.471271868	1.232330523	2.283964740
C	1.430147923	3.069253436	-1.242249459
C	-0.894315576	2.187463722	-2.640871742
C	-3.401819144	-0.797222536	-1.228652220
C	-1.464719514	-2.216108673	2.367069076
C	1.859722386	0.139412963	3.017253802
N	-1.625752350	-1.352208268	0.022910111
H	-3.817068845	-2.624783435	0.040148987

Zero-point correction=	0.383174 (Hartree/Particle)
Thermal correction to Energy=	0.405483
Thermal correction to Enthalpy=	0.406427
Thermal correction to Gibbs Free Energy=	0.337852
Sum of electronic and zero-point Energies=	-2340.828510
Sum of electronic and thermal Energies=	-2340.806200
Sum of electronic and thermal Enthalpies=	-2340.805256
Sum of electronic and thermal Free Energies=	-2340.873831

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 \#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d) Freq
 \TS N-escape from N@C60H via breaking 6,6-bond triplet\0,3\C,2.39141
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 455405\C,1.0348971632,-2.272830949,-2.5179366602\C,2.1176837159,-1.310
 8412663,-2.5339870006\C,2.9532913209,-1.531367119,-1.3628200348\C,2.38
 21080144,-2.6005794716,0.7786859844\C,0.1101071396,-3.6006645659,-0.67
 10182116\C,-0.2559238035,-1.8830799594,-2.9681079326\C,1.8998289406,-0
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 1147982\C,3.1486426762,1.7811175665,-0.02369247\C,2.2359244176,2.83786
 20793,-0.0562381557\C,-2.223916404,2.7460615498,0.6119844803\C,-2.8472
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 ,0.6383795999\C,-2.8282578945,1.5897662632,-1.479859024\C,-3.418155328
 ,-0.7358847656,1.2213354934\C,-0.5253854979,-0.3509843848,3.4234252332
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 ,-2.2161086728,2.3670690765\C,1.8597223857,0.1394129626,3.0172538017N
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 =0.3831736\Thermal=0.4054833\ZPE=240.4450664\Dipole=-0.4752099,-0.5960
 831,0.0117618\DipoleDeriv=0.0503226,0.1162281,-0.0006592,0.0166177,0.0
 0568995\Polar=509.6974149,7.3886322,497.1884955,-0.0526663,-0.1334855,
 489.8958626\PG=C01 [X(C60H1N1)]\NImag=1\\0.35847423,0.16378714,0.34669
 177,-0.00015088,-0.00200940,-0.00168718,-0.00693021,0.04980992\\0.0000
 00002168,-0.00001676,0.00000047\\@

Vibrational Normal Modes



62

C	-2.644341	-2.355311	0.697596
C	-1.528554	-2.944613	1.442681
C	-1.239880	-2.090344	2.580806
C	-2.216313	-1.020444	2.579992
C	-3.081152	-1.180794	1.420318
C	-2.644353	-2.355325	-0.697510
C	-0.475644	-3.551800	0.761581
C	0.088641	-1.826730	3.012451
C	-1.859923	0.260204	3.007443
C	-3.533254	-0.055782	0.725131
C	-1.528579	-2.944641	-1.442605
C	0.863796	-3.282566	1.261855
C	0.457231	-0.486244	3.417097
C	-2.347437	1.428420	2.297670
C	-3.533266	-0.055796	-0.725073
C	-3.081176	-1.180819	-1.420247
C	-0.475657	-3.551815	-0.761512
C	1.206775	-2.413156	2.320686
C	-0.499288	0.530106	3.435617
C	-3.162046	1.274234	1.173747
C	-1.239924	-2.090393	-2.580750
C	1.353532	-2.798275	0.000011
C	0.088591	-1.826787	-3.012422
C	1.816631	-0.216250	2.957420
C	-1.289792	2.426264	2.298111
C	-3.162065	1.274212	-1.173719

C	-2.216355	-1.020491	-2.579938
C	0.863775	-3.282593	-1.261814
C	2.349874	-1.367443	2.276641
C	-0.153957	1.872161	3.009168
C	-2.942581	2.100592	0.000005
C	-1.924434	3.056729	-0.000012
C	2.495176	2.483586	-0.695483
C	2.995014	1.321453	-1.420646
C	2.150227	1.099693	-2.564571
C	1.144706	2.145731	-2.579200
C	1.355709	3.001701	-1.422023
C	2.495188	2.483600	0.695398
C	3.527818	0.232093	-0.737529
C	1.816581	-0.216306	-2.957443
C	-0.154006	1.872105	-3.009200
C	0.261470	3.523063	-0.726384
C	2.995039	1.321481	1.420576
C	3.314322	-1.117751	-1.225418
C	0.457175	-0.486307	-3.417096
C	-1.289829	2.426222	-2.298134
C	0.261481	3.523076	0.726316
C	1.355732	3.001728	1.421947
C	3.527833	0.232107	0.737472
C	2.349834	-1.367488	-2.276654
C	-0.499344	0.530043	-3.435619
C	-1.088011	3.231335	-1.174470
C	2.150269	1.099742	2.564518
C	3.385785	-1.931933	-0.000007
C	-2.347474	1.428378	-2.297659
C	-1.087992	3.231356	1.174428
C	1.144748	2.145780	2.579143
C	3.314348	-1.117727	1.225392
C	1.206735	-2.413202	-2.320665
C	-1.859973	0.260149	-3.007419
N	1.478609	-1.514353	0.000001
H	3.525106	-3.008831	0.000004

NORMALMODES 180

C	0.01	-0.01	0.01
C	0.00	0.02	0.00
C	-0.01	-0.01	0.00
C	-0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.01	-0.01	-0.01
C	0.03	0.00	-0.01
C	0.00	-0.01	0.00
C	0.00	0.00	-0.01
C	0.01	0.00	0.01
C	0.00	0.02	0.00
C	0.01	0.03	0.03

C 0.00 0.00 -0.01
C 0.00 -0.01 0.00
C 0.01 0.00 -0.01
C 0.00 0.00 0.00
C 0.03 0.00 0.01
C -0.01 -0.01 0.00
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C -0.01 -0.01 0.00
C 0.05 0.23 0.00
C 0.00 -0.01 0.00
C 0.01 -0.01 -0.02
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C -0.01 0.00 0.00
C 0.01 0.03 -0.03
C 0.03 -0.01 -0.03
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 -0.01 0.01
C 0.00 0.00 -0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.03 0.00 0.02
C 0.02 -0.01 0.02
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 -0.01 -0.01
C 0.01 -0.08 0.10
C 0.00 0.00 0.01
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.03 0.00 -0.02
C 0.03 -0.01 0.03
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.01
C 0.62 -0.07 0.00
C 0.00 -0.01 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.01 -0.08 -0.10
C -0.01 -0.01 0.00
C 0.00 0.00 0.01
N -0.69 0.09 0.00
H 0.13 -0.12 0.00

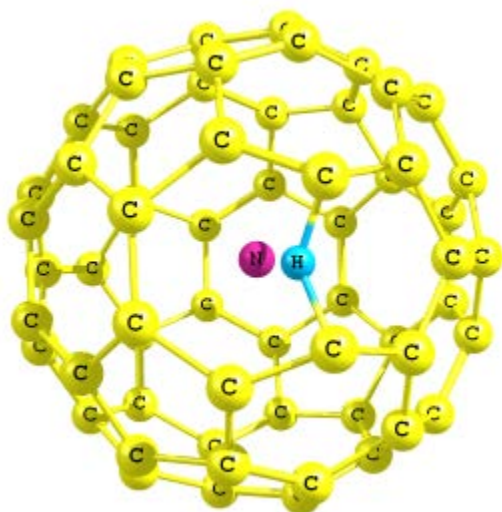
-722.3639

⁵TS1a (TS of N^{••}@C₆₀H[•] → NH^{••}@C₆₀^{••} by breaking [5,6]-bond)***ROMP2/6-31G(d)//UB3LYP/6-31G(d)***

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1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H1N1(5)\DRAL\03-Aug-2010\0
\#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=N
one Name=Dral\TS N@C60H -> NH@C60 via 5,6-bond quintet\0,5\C,0.88714
7597,1.178720377,3.216576558\C,-0.481993773,0.726741973,3.393239535\C,
-0.481377527,-0.725681914,3.400872746\C,0.882462341,-1.175264541,3.217
998004\C,1.728294521,0.000444454,3.093448922\C,1.159201319,2.315166964
,2.451840973\C,-1.535252519,1.419777278,2.803427015\C,-1.54330993,-1.4
1346251,2.809357022\C,1.155181771,-2.31498342,2.451565391\C,2.79968168
7,-0.000243561,2.198067363\C,0.06504362,3.051402025,1.850921876\C,-2.6
74219913,0.72110256,2.195716687\C,-1.256078509,-2.617755678,2.03980621
9\C,2.260814375,-2.309110612,1.513550343\C,3.070502999,1.176275392,1.3
8849169\C,2.266929906,2.310112802,1.513551059\C,-1.249181094,2.6197944
79,2.040512545\C,-2.675584869,-0.715335183,2.216871983\C,0.058650139,-
3.04405379,1.849538273\C,3.068535684,-1.177016362,1.387005693\C,0.4905
87797,3.502158599,0.537810532\C,-3.117613505,1.559309542,1.090630712\C
,-0.417202782,3.509681167,-0.528356402\C,-2.201278155,-2.685252614,0.9
52617361\C,1.846476586,-3.038560764,0.324351817\C,3.492523898,0.725176
636,0.072832256\C,1.850343846,3.041052607,0.327230897\C,-2.192484031,2
.670722112,0.949073868\C,-3.098885323,-1.554119275,1.084752621\C,0.483
657992,-3.494291983,0.530880804\C,3.492562837,-0.728167455,0.072925396
\C,3.094323325,-1.42652428,-1.070389406\C,-0.863333874,-1.175833337,-3
.19396978\C,-1.701201138,0.003862524,-3.022386482\C,-0.865588401,1.172
98023,-3.200735686\C,0.495233737,0.72511835,-3.420584954\C,0.497306092
,-0.72819182,-3.420244197\C,-1.106498672,-2.323418788,-2.440370093\C,-
2.774462864,0.005970769,-2.113830197\C,-1.109997528,2.320001715,-2.434
841611\C,1.564579274,1.421887026,-2.851833042\C,1.566356702,-1.4265364
34,-2.854058301\C,-2.216506004,-2.357625938,-1.518620672\C,-3.06150038
8,1.237822688,-1.373435632\C,0.001741014,3.043895258,-1.838815137\C,2.
669419129,0.697648726,-2.25444976\C,1.310832493,-2.607565532,-2.045149
741\C,0.004140364,-3.051496461,-1.847145428\C,-3.050430372,-1.22798360
6,-1.376481452\C,-2.215751087,2.352723691,-1.518397814\C,1.308733194,2
.602317782,-2.039238266\C,2.67254875,-0.701856253,-2.254789775\C,-1.78
9671354,-3.078683261,-0.329156771\C,-3.724369818,1.088616152,-0.106887
472\C,3.090159241,1.422983395,-1.067006478\C,2.252408263,-2.604450285,
-0.939002501\C,-0.417666153,-3.510714067,-0.535963598\C,-3.634400755,-
1.046764994,-0.09349789\C,-1.785381515,3.082076375,-0.32078158\C,2.253
898678,2.60489446,-0.937316642\N,-0.101458516,-0.062930948,-0.02441379
5\H,-3.312168795,0.014864558,0.206100394\Version=AM64L-G03RevD.02\Sta
te=5-A\HF=-2326.5338108\MP2=-2334.4791868\RMSE=2.271e-09\Thermal=0.\PG
=C01 [X(C60H1N1)]\@@

```

UB3LYP/6-31G(d)

0 5

C	0.887147597	1.178720377	3.216576558
C	-0.481993773	0.726741973	3.393239535
C	-0.481377527	-0.725681914	3.400872746
C	0.882462341	-1.175264541	3.217998004
C	1.728294521	0.000444454	3.093448922
C	1.159201319	2.315166964	2.451840973
C	-1.535252519	1.419777278	2.803427015
C	-1.543309930	-1.413462510	2.809357022
C	1.155181771	-2.314983420	2.451565391
C	2.799681687	-0.000243561	2.198067363
C	0.065043620	3.051402025	1.850921876
C	-2.674219913	0.721102560	2.195716687
C	-1.256078509	-2.617755678	2.039806219
C	2.260814375	-2.309110612	1.513550343
C	3.070502999	1.176275392	1.388491690
C	2.266929906	2.310112802	1.513551059
C	-1.249181094	2.619794479	2.040512545
C	-2.675584869	-0.715335183	2.216871983
C	0.058650139	-3.044053790	1.849538273
C	3.068535684	-1.177016362	1.387005693
C	0.490587797	3.502158599	0.537810532
C	-3.117613505	1.559309542	1.090630712
C	-0.417202782	3.509681167	-0.528356402
C	-2.201278155	-2.685252614	0.952617361
C	1.846476586	-3.038560764	0.324351817
C	3.492523898	0.725176636	0.072832256
C	1.850343846	3.041052607	0.327230897
C	-2.192484031	2.670722112	0.949073868
C	-3.098885323	-1.554119275	1.084752621
C	0.483657992	-3.494291983	0.530880804
C	3.492562837	-0.728167455	0.072925396
C	3.094323325	-1.426524280	-1.070389406

C -0.863333874 -1.175833337 -3.193969780
 C -1.701201138 0.003862524 -3.022386482
 C -0.865588401 1.172980230 -3.200735686
 C 0.495233737 0.725118350 -3.420584954
 C 0.497306092 -0.728191820 -3.420244197
 C -1.106498672 -2.323418788 -2.440370093
 C -2.774462864 0.005970769 -2.113830197
 C -1.109997528 2.320001715 -2.434841611
 C 1.564579274 1.421887026 -2.851833042
 C 1.566356702 -1.426536434 -2.854058301
 C -2.216506004 -2.357625938 -1.518620672
 C -3.061500388 1.237822688 -1.373435632
 C 0.001741014 3.043895258 -1.838815137
 C 2.669419129 0.697648726 -2.254449760
 C 1.310832493 -2.607565532 -2.045149741
 C 0.004140364 -3.051496461 -1.847145428
 C -3.050430372 -1.227983606 -1.376481452
 C -2.215751087 2.352723691 -1.518397814
 C 1.308733194 2.602317782 -2.039238266
 C 2.672548750 -0.701856253 -2.254789775
 C -1.789671354 -3.078683261 -0.329156771
 C -3.724369818 1.088616152 -0.106887472
 C 3.090159241 1.422983395 -1.067006478
 C 2.252408263 -2.604450285 -0.939002501
 C -0.417666153 -3.510714067 -0.535963598
 C -3.634400755 -1.046764994 -0.093497890
 C -1.785381515 3.082076375 -0.320781580
 C 2.253898678 2.604894460 -0.937316642
 N -0.101458516 -0.062930948 -0.024413795
 H -3.312168795 0.014864558 0.206100394

Zero-point correction= 0.379725 (Hartree/Particle)
 Thermal correction to Energy= 0.403820
 Thermal correction to Enthalpy= 0.404764
 Thermal correction to Gibbs Free Energy= 0.330197
 Sum of electronic and zero-point Energies= -2340.787667
 Sum of electronic and thermal Energies= -2340.763572
 Sum of electronic and thermal Enthalpies= -2340.762628
 Sum of electronic and thermal Free Energies= -2340.837194

1\1\FAU-CCC-CCDN092\Freq\UB3LYP/6-31G(d)\C60H1N1(5)\DRAL\07-Nov-2009\0
 \#P B3LYP/6-31G* FREQ=NORAMAN POP=NONE SCFCyc=600 Name=Dral\TS N@C60
 H -> NH@C60 via 5,6-bond quintet\0,5\C,0.887147597,1.178720377,3.2165
 76558\C,-0.481993773,0.726741973,3.393239535\C,-0.481377527,-0.7256819
 14,3.400872746\C,0.882462341,-1.175264541,3.217998004\C,1.728294521,0.
 000444454,3.093448922\C,1.159201319,2.315166964,2.451840973\C,-1.53525
 2519,1.419777278,2.803427015\C,-1.54330993,-1.41346251,2.809357022\C,1
 .155181771,-2.31498342,2.451565391\C,2.799681687,-0.000243561,2.198067
 363\C,0.06504362,3.051402025,1.850921876\C,-2.674219913,0.72110256,2.1
 95716687\C,-1.256078509,-2.617755678,2.039806219\C,2.260814375,-2.3091

10612,1.513550343\C,3.070502999,1.176275392,1.38849169\C,2.266929906,2.310112802,1.513551059\C,-1.249181094,2.619794479,2.040512545\C,-2.675584869,-0.715335183,2.216871983\C,0.058650139,-3.04405379,1.849538273\C,3.068535684,-1.177016362,1.387005693\C,0.490587797,3.502158599,0.537810532\C,-3.117613505,1.559309542,1.090630712\C,-0.417202782,3.509681167,-0.528356402\C,-2.201278155,-2.685252614,0.952617361\C,1.846476586,-3.038560764,0.324351817\C,3.492523898,0.725176636,0.072832256\C,1.850343846,3.041052607,0.327230897\C,-2.192484031,2.670722112,0.949073868\C,-3.098885323,-1.554119275,1.084752621\C,0.483657992,-3.494291983,0.530880804\C,3.492562837,-0.728167455,0.072925396\C,3.094323325,-1.42652428,-1.070389406\C,-0.863333874,-1.175833337,-3.19396978\C,-1.701201138,0.003862524,-3.022386482\C,-0.865588401,1.17298023,-3.200735686\C,0.495233737,0.72511835,-3.420584954\C,0.497306092,-0.72819182,-3.420244197\C,-1.106498672,-2.323418788,-2.440370093\C,-2.774462864,0.005970769,-2.113830197\C,-1.109997528,2.320001715,-2.434841611\C,1.564579274,1.421887026,-2.851833042\C,1.566356702,-1.426536434,-2.854058301\C,-2.216506004,-2.357625938,-1.518620672\C,-3.061500388,1.237822688,-1.373435632\C,0.001741014,3.043895258,-1.838815137\C,2.669419129,0.697648726,-2.25444976\C,1.310832493,-2.607565532,-2.045149741\C,0.004140364,-3.051496461,-1.847145428\C,-3.050430372,-1.227983606,-1.376481452\C,-2.215751087,2.352723691,-1.518397814\C,1.308733194,2.602317782,-2.039238266\C,2.67254875,-0.701856253,-2.254789775\C,-1.789671354,-3.078683261,-0.329156771\C,-3.724369818,1.088616152,-0.106887472\C,3.090159241,1.422983395,-1.067006478\C,2.252408263,-2.604450285,-0.939002501\C,-0.417666153,-3.510714067,-0.535963598\C,-3.634400755,-1.046764994,-0.09349789\C,-1.785381515,3.082076375,-0.32078158\C,2.253898678,2.60489446,-0.937316642\N,-0.101458516,-0.062930948,-0.024413795\H,-3.312168795,0.014864558,0.206100394\\Version=AM64L-G03RevD.02\\State=5-A\\HF=-2341.1673917\\S2=6.023733\\S2-1=0.\\S2A=6.000187\\RMSD=7.080e-09\\RMSF=1.675e-05\\ZeroPoint=0.379725\\Thermal=0.4038199\\ZPE=238.2810209\\Dipole=-0.0240746,-0.1300154,-0.0846901\\DipoleDeriv=0.1216578,-0.173504,0.039436,-0.0158001,-4,0.0454746,-0.0188185\\Polar=509.3538726,-2.3960675,487.3508641,-3.1871125,-3.5896143,480.7984094\\PG=C01 [X(C60H1N1)]\\NImag=1\\0.50903217,0.21,0.03508091,0.00716334,0.07393004\\-0.00002900,0.00001592,0.000002120002947\\@

Vibrational Normal Modes

62

C	-0.298725	-1.446048	3.215875
C	0.831108	-0.544369	3.359039
C	0.322334	0.815478	3.398532
C	-1.118398	0.759991	3.268762
C	-1.503112	-0.636425	3.145263
C	-0.184017	-2.598447	2.435387
C	2.037561	-0.818465	2.721173
C	1.053430	1.837516	2.788967
C	-1.801243	1.738909	2.536507

C	-2.539531	-1.002996	2.284426
C	1.075427	-2.898552	1.784183
C	2.836342	0.240941	2.093229
C	0.334279	2.871846	2.055471
C	-2.869008	1.354589	1.634007
C	-2.411312	-2.192066	1.458214
C	-1.257579	-2.973267	1.532918
C	2.161473	-2.035329	1.941554
C	2.335523	1.586384	2.145821
C	-1.052610	2.811846	1.916250
C	-3.233395	0.012398	1.508266
C	0.785969	-3.457467	0.475612
C	3.503586	-0.378080	0.956566
C	1.598512	-3.136113	-0.618626
C	1.154788	3.276769	0.940689
C	-2.780919	2.194222	0.448586
C	-3.013300	-1.905172	0.166760
C	-0.656008	-3.500468	0.318281
C	3.021508	-1.741930	0.819988
C	2.395852	2.531006	1.019551
C	-1.657204	3.096915	0.621875
C	-3.522137	-0.544189	0.198720
C	-3.436519	0.260247	-0.941024
C	0.276317	1.433320	-3.193632
C	1.479938	0.620759	-3.074528
C	1.100475	-0.765393	-3.251965
C	-0.338209	-0.821082	-3.418816
C	-0.848928	0.539153	-3.386544
C	0.130254	2.586126	-2.423114
C	2.519100	0.986533	-2.200616
C	1.759359	-1.761071	-2.519514
C	-1.073945	-1.853922	-2.831960
C	-2.072901	0.812907	-2.771672
C	1.191587	2.998668	-1.536385
C	3.246630	-0.073397	-1.496853
C	0.994457	-2.834435	-1.904659
C	-2.339318	-1.568764	-2.184215
C	-2.217042	2.000842	-1.945544
C	-1.142047	2.872885	-1.779257
C	2.372897	2.231876	-1.445481
C	2.839944	-1.412647	-1.639420
C	-0.390919	-2.877318	-2.053937
C	-2.832216	-0.259280	-2.153769
C	0.584001	3.512991	-0.318499
C	3.862052	0.286788	-0.248925
C	-2.434906	-2.406771	-1.000255
C	-3.055992	1.657301	-0.810520
C	-0.859121	3.438431	-0.472310
C	3.030763	2.254810	-0.185880
C	2.737130	-2.257889	-0.445078

C	-1.233575	-3.221573	-0.923010
N	0.071034	0.094009	-0.026741
H	3.112003	1.144814	0.100405

NORMALMODES 180

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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	-0.01	0.00
C	0.01	0.00	0.00
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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.02	0.02
C	0.00	0.00	0.00
C	0.01	0.00	0.00
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C	0.01	0.00	0.00
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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	-0.01
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.02	-0.01
C	0.00	0.00	0.00

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C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.01 -0.01 -0.01
C  0.00  0.00 -0.01
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00 -0.01  0.00
C -0.06  0.14  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.05 -0.13  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
N  0.00  0.00  0.00
H -0.89 -0.38 -0.13
-968.6815

```

⁵TS1b (TS of N^{••}@C₆₀H[•] → NH^{••}@C₆₀^{••} by breaking [6,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

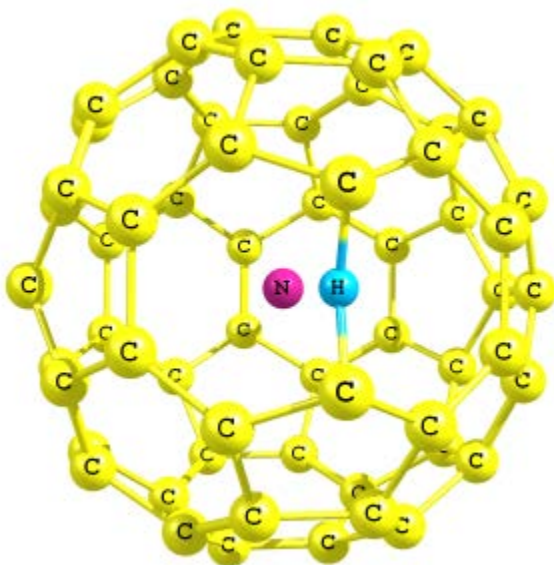
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\#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Pop=N
one Name=Dral\TS N@C60H -> NH@C60 quintet via 6,6\0,5\C,-0.994850606
,-3.375785714,-0.703909223\C,-1.990237847,-2.608775735,-1.426278711\C,
-1.352892275,-2.000604786,-2.577561568\C,0.035810111,-2.425582807,-2.5
92377804\C,0.260215038,-3.269581701,-1.427915279\C,-0.998640499,-3.376
856246,0.694220529\C,-2.966142982,-1.900044108,-0.734393978\C,-1.69216
294,-0.69403434,-2.943133399\C,1.032713006,-1.54714333,-3.015692518\C,
1.462648169,-3.18286235,-0.725701339\C,-1.997933369,-2.610950456,1.412
358607\C,-3.396553562,-0.576696246,-1.177602081\C,-0.655793307,0.20929
3179,-3.392888056\C,2.292573998,-1.470395702,-2.295701743\C,1.45870370
2,-3.18397719,0.72962971\C,0.252481455,-3.271766539,1.425180062\C,-2.9
70076027,-1.901155631,0.716280007\C,-2.707651706,0.069041709,-2.222561
905\C,0.67787304,-0.205398674,-3.440363618\C,2.50201541,-2.268774366,-
1.169587037\C,-1.366839962,-2.004545597,2.568008446\C,-3.953032322,0.0
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463935,1.53973606,-2.939537944\C,2.724158948,-0.082653044,-2.29347055\
C,2.495645956,-2.270574678,1.180544729\C,0.021762723,-2.429552683,2.58
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99012\C,2.062138673,2.547093694,1.434545056\C,1.095744202,3.346425009,
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 \C,2.711682202,-0.086179059,2.308964404\C,3.010390729,1.793835583,-0.7
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 8309,-0.72610734\C,-2.279280404,1.481669158,2.211120622\C,0.659209535,
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 \C,2.280096658,-1.473921506,2.306729068\C,3.348419648,0.452813792,-1.1
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 1864,-1.172802764\C,-2.71966433,0.065647218,2.20884389\C,1.016351484,-
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UB3LYP/6-31G(d)



0 5

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C	-1.352892275	-2.000604786	-2.577561568
C	0.035810111	-2.425582807	-2.592377804
C	0.260215038	-3.269581701	-1.427915279
C	-0.998640499	-3.376856246	0.694220529
C	-2.966142982	-1.900044108	-0.734393978
C	-1.692162940	-0.694034340	-2.943133399
C	1.032713006	-1.547143330	-3.015692518
C	1.462648169	-3.182862350	-0.725701339
C	-1.997933369	-2.610950456	1.412358607
C	-3.396553562	-0.576696246	-1.177602081
C	-0.655793307	0.209293179	-3.392888056
C	2.292573998	-1.470395702	-2.295701743
C	1.458703702	-3.183977190	0.729629710

C	0.252481455	-3.271766539	1.425180062
C	-2.970076027	-1.901155631	0.716280007
C	-2.707651706	0.069041709	-2.222561905
C	0.677873040	-0.205398674	-3.440363618
C	2.502015410	-2.268774366	-1.169587037
C	-1.366839962	-2.004545597	2.568008446
C	-3.953032322	0.069093444	-0.010217126
C	-1.708093057	-0.698536229	2.933739428
C	-0.997463935	1.539736060	-2.939537944
C	2.724158948	-0.082653044	-2.293470550
C	2.495645956	-2.270574678	1.180544729
C	0.021762723	-2.429552683	2.589701090
C	-3.402888444	-0.578486445	1.159175587
C	-2.267267763	1.485064022	-2.220281036
C	1.730694847	0.697193106	-3.012081408
C	3.143571244	-1.709227078	0.007655567
C	3.558402398	-0.375344008	0.009802164
C	1.091954467	3.345354931	0.705037970
C	-0.166116342	3.279170688	1.421835694
C	0.008695009	2.418419188	2.575125343
C	1.393394861	1.980863281	2.596799012
C	2.062138673	2.547093694	1.434545056
C	1.095744202	3.346425009	-0.693091036
C	-1.368711103	3.247956320	0.724565535
C	-1.013394644	1.535233975	2.937333962
C	1.714333930	0.692569192	3.023371266
C	3.006445502	1.792720216	0.737638532
C	-0.158420970	3.281344512	-1.416798323
C	-2.475725722	2.402751646	1.163971379
C	-0.674180815	0.204096580	3.390488438
C	2.711682202	-0.086179059	2.308964404
C	3.010390729	1.793835583	-0.717691851
C	2.069872895	2.549279144	-1.418550583
C	-1.364778372	3.249068309	-0.726107340
C	-2.279280404	1.481669158	2.211120622
C	0.659209535	-0.210673359	3.444556520
C	3.342050979	0.451013097	1.184925504
C	0.022643248	2.422360659	-2.570441936
C	-3.295043055	2.184844587	-0.006811572
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C	3.348419648	0.452813792	-1.165208246
C	1.407441889	1.984832506	-2.585278565
C	-2.469390973	2.404541864	-1.172802764
C	-2.719664330	0.065647218	2.208843890
C	1.016351484	-1.551767805	3.019760785
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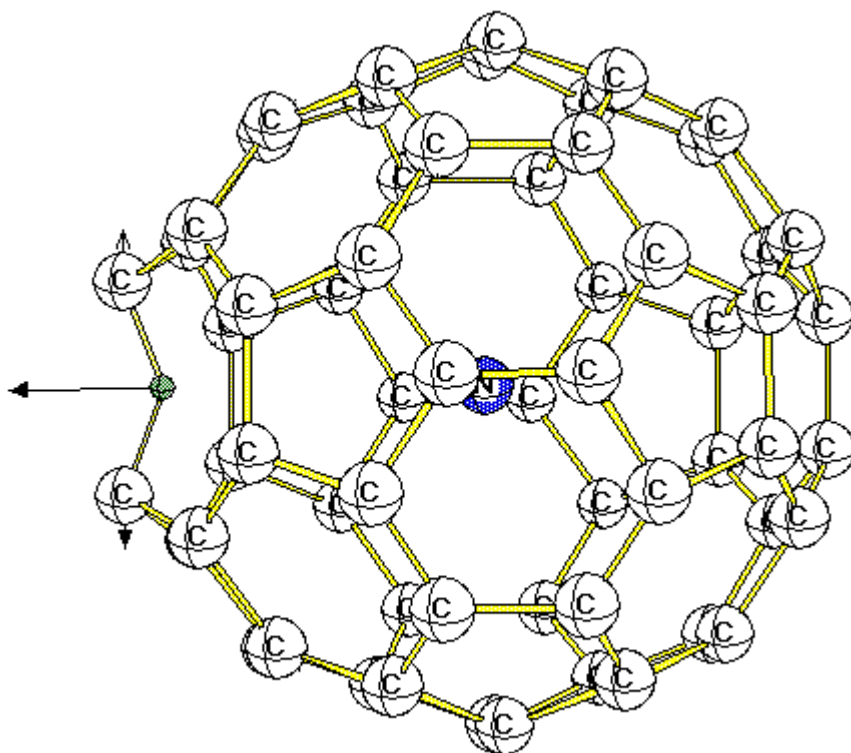
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Thermal correction to Energy=	0.403680

Thermal correction to Enthalpy= 0.404624
 Thermal correction to Gibbs Free Energy= 0.330941
 Sum of electronic and zero-point Energies= -2340.778231
 Sum of electronic and thermal Energies= -2340.754425
 Sum of electronic and thermal Enthalpies= -2340.753481
 Sum of electronic and thermal Free Energies= -2340.827164

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 \#P B3LYP/6-31G* FREQ=NORAMAN Pop=None SCFCyc=600 Name=Dral\TS N@C60
 H -> NH@C60 quintet via 6,6\0,5\C,-0.994850606,-3.375785714,-0.703909
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26,-0.00000099,-0.00000012,-0.00000062,-0.00000133,0.00000051\\\\@

Vibrational Normal Modes



62

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C	-1.126576	-3.084342	-1.419318
C	-0.701402	-2.316057	-2.572791
C	0.750818	-2.309304	-2.591038
C	1.218577	-3.046734	-1.426537
C	0.053432	-3.519886	0.699081
C	-2.267343	-2.696474	-0.725341
C	-1.414384	-1.169835	-2.938450
C	1.440734	-1.175011	-3.017727
C	2.342606	-2.605621	-0.727647
C	-1.126591	-3.084333	1.419330
C	-3.072516	-1.561428	-1.168403
C	-0.694239	-0.000094	-3.391704
C	2.622603	-0.726331	-2.301208
C	2.342599	-2.605616	0.727690
C	1.218562	-3.046723	1.426570
C	-2.267351	-2.696469	0.725339
C	-2.609025	-0.741791	-2.215721
C	0.702297	0.000080	-3.442470
C	3.062430	-1.424706	-1.175049
C	-0.701429	-2.316038	2.572800
C	-3.792976	-1.108321	-0.000014

C	-1.414414	-1.169814	2.938446
C	-1.414676	1.169470	-2.938457
C	2.622421	0.726975	-2.301215
C	3.062419	-1.424697	1.175092
C	0.750790	-2.309286	2.591061
C	-3.072529	-1.561420	1.168384
C	-2.609207	0.741132	-2.215724
C	1.440438	1.175358	-3.017735
C	3.511555	-0.698011	0.000021
C	3.511376	0.698890	0.000016
C	0.052551	3.519917	0.699057
C	-1.127362	3.084068	1.419308
C	-0.702007	2.315891	2.572784
C	0.750214	2.309501	2.591047
C	1.217802	3.047051	1.426551
C	0.052559	3.519911	-0.699078
C	-2.268024	2.695914	0.725320
C	-1.414706	1.169491	2.938438
C	1.440406	1.175379	3.017742
C	2.341946	2.606206	0.727672
C	-1.127346	3.084058	-1.419337
C	-3.072916	1.560668	1.168372
C	-0.694274	-0.000071	3.391699
C	2.622396	0.726991	2.301238
C	2.341954	2.606202	-0.727664
C	1.217818	3.047041	-1.426556
C	-2.268017	2.695910	-0.725359
C	-2.609230	0.741147	2.215696
C	0.702261	0.000103	3.442477
C	3.062059	1.425471	1.175084
C	-0.701979	2.315873	-2.572804
C	-3.793258	1.107387	-0.000021
C	2.622577	-0.726316	2.301241
C	3.062070	1.425463	-1.175060
C	0.750241	2.309483	-2.591052
C	-3.072904	1.560660	-1.168411
C	-2.609048	-0.741776	2.215702
C	1.440702	-1.174992	3.017751
N	-0.061206	-0.000199	-0.000054
H	-3.405089	-0.000423	-0.000005

NORMALMODES 180

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C	0.00	0.01	0.00
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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	-0.01	0.00
C	0.00	0.00	0.00

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C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 -0.02 0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
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C -0.01 0.01 0.01
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C 0.00 -0.02 -0.01
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C 0.00 0.00 0.00
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C 0.00 0.00 0.00
C 0.00 0.00 0.00
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C 0.00 0.00 0.00
C 0.01 0.01 0.00
C -0.01 -0.01 -0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 -0.01 0.00
C 0.00 0.16 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.02 0.01

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 C 0.00 0.00 0.00
 N 0.00 0.00 0.00
 H -0.97 0.00 0.00
 -920.2922

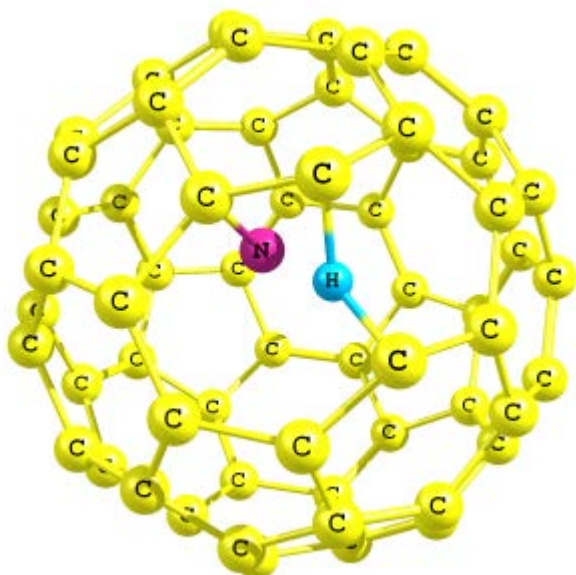
⁵TS1e (TS of endohedrally bound N^{••}@C₆₀H[•] → NH^{••}@C₆₀^{••} by breaking [5,6]-bond, quintet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN086\SP\ROMP2-FC\6-31G(d)\C60H1N1(5)\DRAL\24-Aug-2010\0
 \#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCFCyc=1200 SCF=Tight Pop=N
 one Name=Drall\TS endo-N@C60H -> NH@C60 quintet\0,5\C,0,0.9591825073,
 0.7124226359,-3.3262648682\C,0,-0.3144452886,1.3969637617,-3.253295905
 6\C,0,-0.1441296057,2.6160510656,-2.4713991426\C,0,1.2436686117,2.6768
 585834,-2.062424951\C,0,1.9257223536,1.5027027702,-2.5910156334\C,0,0.
 9996959918,-0.6913529653,-3.2538866165\C,0,-1.4966025975,0.6532067785,
 -3.1273969046\C,0,-1.1503176212,3.0714843759,-1.5972738281\C,0,1.58210
 20611,3.1671748403,-0.7979913232\C,0,2.9165178356,0.8773981402,-1.8327
 61056\C,0,-0.2115414425,-1.4706846764,-3.1181706053\C,0,-2.5025405553,
 1.1558153204,-2.2367401579\C,0,-0.79641284,3.5566358403,-0.2730674813\
 C,0,2.6157048401,2.5180596162,-0.0134879403\C,0,2.9754844178,-0.575106
 6303,-1.7763170418\C,0,2.0385219661,-1.3408799241,-2.4709543151\C,0,-1.
 4594107165,-0.8241336244,-3.0335189854\C,0,-2.3769858135,2.3263955859
 ,-1.4744743209\C,0,0.5391268638,3.6071281744,0.1136943629\C,0,3.270669
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 ,-3.0423352521,-1.3186784369\C,0,-1.803855417,3.0831952199,0.669981401
 1\C,0,2.213258455,2.5506129107,1.3800200434\C,0,3.3766991102,-0.955383
 1365,-0.4343074107\C,0,1.4625421559,-2.5191642817,-1.8474675435\C,0,-2.
 4523062038,-1.2989822765,-2.0953745083\C,0,-2.7896556062,2.3280393463
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 5767,0.2615122657,0.3412802265\C,0,3.1673612405,0.293466148,1.68303692
 12\C,0,-0.9040236928,-0.5348888076,3.4275234899\C,0,-1.8728281118,-1.3
 423059144,2.7443131845\C,0,-1.1782382105,-2.5186975206,2.200527067\C,0
 ,0.2108071236,-2.4255093241,2.5821412596\C,0,0.3850607513,-1.201426748
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.4661638372,0.1897202797\C,0,0.8650648372,-3.3575999118,0.3909333508\C
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 98736,-2.0907382411,0.1615354737\C,0,2.4826516799,1.4606179962,2.21422
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 ,0,1.856317978,-2.8913255258,-0.5613254096\N,0,-1.5017959825,0.0430991
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UB3LYP/6-31G(d)



0 5

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C	-0.144129606	2.616051066	-2.471399143
C	1.243668612	2.676858583	-2.062424951
C	1.925722354	1.502702770	-2.591015633
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C	-1.496602598	0.653206778	-3.127396905
C	-1.150317621	3.071484376	-1.597273828
C	1.582102061	3.167174840	-0.797991323
C	2.916517836	0.877398140	-1.832761056
C	-0.211541442	-1.470684676	-3.118170605
C	-2.502540555	1.155815320	-2.236740158
C	-0.796412840	3.556635840	-0.273067481
C	2.615704840	2.518059616	-0.013487940
C	2.975484418	-0.575106630	-1.776317042
C	2.038521966	-1.340879924	-2.470954315
C	-1.459410716	-0.824133624	-3.033518985
C	-2.376985814	2.326395586	-1.474474321
C	0.539126864	3.607128174	0.113694363
C	3.270669915	1.391397765	-0.524416462

C	0.064406393	-2.591223364	-2.237161683
C	-2.902103350	-0.023485965	-1.444637211
C	-0.891172364	-3.042335252	-1.318678437
C	-1.803855417	3.083195220	0.669981401
C	2.213258455	2.550612911	1.380020043
C	3.376699110	-0.955383136	-0.434307411
C	1.462542156	-2.519164282	-1.847467544
C	-2.452306204	-1.298982276	-2.095374508
C	-2.789655606	2.328039346	-0.050675814
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C	3.552775577	0.261512266	0.341280226
C	3.167361240	0.293466148	1.683036921
C	-0.904023693	-0.534888808	3.427523490
C	-1.872828112	-1.342305914	2.744313184
C	-1.178238210	-2.518697521	2.200527067
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C	0.385060751	-1.201426748	3.345277269
C	-0.974246142	0.865123838	3.361540400
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C	1.481726140	1.002043516	3.156640087
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C	-2.962705881	0.722024535	1.874916456
C	-2.609209673	-2.466163837	0.189720280
C	0.865064837	-3.357599912	0.390933351
C	2.597995146	-0.888019769	2.305327844
C	-1.427611712	2.685289961	1.956931636
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C	2.826299874	-2.090738241	0.161535474
C	2.482651680	1.460617996	2.214225230
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C	-3.396688566	1.189323227	0.562788922
C	-2.196658569	-2.398023272	-1.219517384
C	1.856317978	-2.891325526	-0.561325410
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H	-3.229797080	-0.748981142	0.078530960

Zero-point correction=	0.379968 (Hartree/Particle)
Thermal correction to Energy=	0.402719
Thermal correction to Enthalpy=	0.403663
Thermal correction to Gibbs Free Energy=	0.334102
Sum of electronic and zero-point Energies=	-2340.722805
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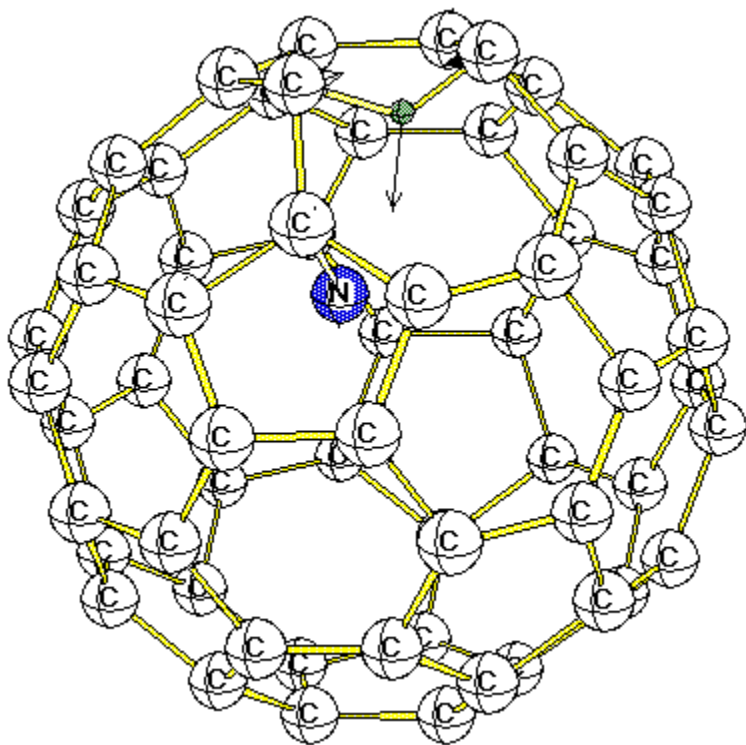
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Vibrational Normal Modes



62

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C	-0.984978	-2.713727	-2.094305
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C	-2.608414	-2.404668	-0.435100
C	-2.881234	-1.471517	-1.520478
C	-1.350575	-0.554720	-3.231434
C	0.388699	-2.621700	-2.360880
C	-0.516611	-3.547272	0.214578
C	-2.818548	-2.011172	0.889568
C	-3.355322	-0.191367	-1.230497
C	0.065096	-0.444177	-3.508074
C	1.292468	-3.019248	-1.320229
C	-0.725217	-3.114079	1.586792
C	-3.315818	-0.681274	1.188272
C	-2.832247	0.955453	-1.956878
C	-1.852707	0.777065	-2.934379
C	0.949243	-1.447831	-3.068377
C	0.896694	-3.475644	-0.054474
C	-1.852664	-2.367961	1.915383
C	-3.578880	0.212558	0.143639
C	0.449725	0.948391	-3.364036
C	2.284090	-1.927476	-1.269748
C	1.684472	1.304591	-2.808370
C	0.570058	-2.752390	2.152363
C	-2.657071	-0.212146	2.392788

C	-2.743623	2.069736	-1.031085
C	-0.741406	1.707684	-3.022687
C	2.230959	-1.080948	-2.507986
C	1.583339	-2.973183	1.159427
C	-1.747918	-1.250030	2.840667
C	-3.199556	1.607512	0.269625
C	-2.567376	2.059691	1.429693
C	1.784608	1.705875	2.543530
C	2.811324	1.550114	1.554149
C	2.524764	2.483208	0.454479
C	1.331764	3.218629	0.800409
C	0.871891	2.744163	2.094440
C	1.289820	0.588917	3.234117
C	3.337692	0.278634	1.262603
C	2.743371	2.110073	-0.878647
C	0.394977	3.558840	-0.187952
C	-0.492083	2.636382	2.357340
C	1.785477	-0.728139	2.907893
C	3.856029	0.089097	-0.064905
C	1.762685	2.431892	-1.899553
C	-1.021068	3.440966	0.087693
C	-1.005343	1.484988	3.086414
C	-0.128567	0.485354	3.513561
C	2.791211	-0.911088	1.937850
C	3.334597	0.831869	-1.192042
C	0.618315	3.153515	-1.562849
C	-1.461015	2.995100	1.338543
C	0.675541	-1.662619	3.022651
C	3.320887	-1.959006	-0.213487
C	-1.678021	2.966122	-1.120434
C	-2.288885	1.131879	2.513593
C	-0.509324	-0.910018	3.386957
C	2.704827	-2.091072	1.084291
C	2.624255	0.283873	-2.356477
C	-0.661763	2.785529	-2.139718
N	1.195050	-0.942711	-0.545455
H	3.198894	-0.791735	-0.360355

NORMALMODES 180

[illegible]

C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	0.00	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.02	0.00	0.01
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.05	-0.14	-0.02
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.00	-0.01	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.05	0.13	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	-0.02	0.00	-0.01

H -0.85 0.31 0.36
-896.3776

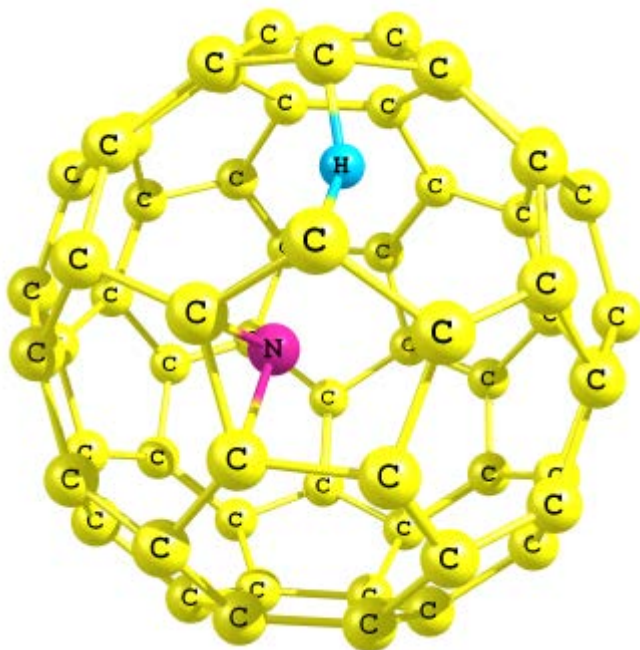
⁵TS1f (TS of endohedrally bound N^{•••}@C₆₀H[•] → NH^{••}@C₆₀^{••} by breaking [6,6]-bond, quintet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN085\SP\ROMP2-FC\6-31G(d)\C60H1N1(5)\DRAL\26-Aug-2010\0
\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCFCyc=1200 SCF=Tight Pop=N
one Name=Dral\TS endo-N@C60H -> NH@C60 via breaking 6,6-bond quintet\
\0,5\C,0,0.9069960082,3.3398651005,0.9846027872\C,0,-0.4156091265,3.18
48544713,1.5573671211\C,0,-0.3292715704,2.2780174916,2.6863457688\C,0,
1.0601166881,1.8911021717,2.8276583066\C,0,1.8240262134,2.5419384134,1
.7728567627\C,0,1.0533733356,3.4140851471,-0.4052851762\C,0,-1.5332763
871,3.143228795,0.7371865127\C,0,-1.351516267,1.3474400322,2.914393939
7\C,0,1.3875106382,0.594281847,3.2245737945\C,0,2.8698483406,1.8593649
618,1.1472344542\C,0,-0.1085316362,3.3450362804,-1.2645743067\C,0,-2.6
473154342,2.2518942003,1.0360078469\C,0,-1.0061572256,0.0067023226,3.3
376224465\C,0,2.4856763757,-0.1096453405,2.5839856001\C,0,3.0274708224
,1.940290078,-0.2964056653\C,0,2.136344255,2.6965009872,-1.0580879951\
C,0,-1.3830233154,3.2098585829,-0.7074797384\C,0,-2.5413334378,1.28958
59408,2.0775770632\C,0,0.333010378,-0.3622653588,3.4941614879\C,0,3.20
97088733,0.5111108566,1.5610430232\C,0,0.2367960052,2.5675214186,-2.43
61386865\C,0,-3.3114385482,2.0473042724,-0.2260682543\C,0,-0.696506397
8,1.681304798,-2.982093287\C,0,-1.9617228593,-0.9086456866,2.755822029
3\C,0,2.1122268838,-1.5048905032,2.4680524898\C,0,3.4652414704,0.63895
1318,-0.7723800463\C,0,1.6315225625,2.1770731189,-2.3177435739\C,0,-2.
3869614954,2.3587564789,-1.3149242273\C,0,-2.9387953113,-0.138978068,1
.9921898874\C,0,0.7848189527,-1.6638907108,3.0390158699\C,0,3.57998887
87,-0.2427756524,0.3771387929\C,0,3.2189100142,-1.5861339986,0.2625561
776\C,0,-0.7457114511,-3.3623795115,-0.9696322739\C,0,-1.6836665729,-2
.6518929386,-1.7912136762\C,0,-0.9538399273,-1.8958863297,-2.819729590
9\C,0,0.4374434187,-2.2631883247,-2.6898142572\C,0,0.5719007278,-3.160
838128,-1.5472083504\C,0,-0.9061696363,-3.4336821269,0.4363387243\C,0,
-2.5977241242,-1.8443158708,-1.028873073\C,0,-1.3138616865,-0.57294773
46,-3.1964342329\C,0,1.446034506,-1.3320428986,-2.9652539188\C,0,1.686
4077016,-3.0706200763,-0.7143596578\C,0,-2.0190070331,-2.7636078746,1.
1259835688\C,0,-3.0118994979,-0.4988360516,-1.4345330011\C,0,-0.260265
4605,0.3827107569,-3.4613963601\C,0,2.6117148803,-1.253536718,-2.10601
72986\C,0,1.5289119837,-3.1536020761,0.7282681072\C,0,0.2503687326,-3.
3133780867,1.2847225822\C,0,-2.9505547857,-2.0423060178,0.4001737577\C
,0,-2.4645649142,0.1639232634,-2.6376536371\C,0,1.0887140362,0.0128951
65,-3.3643930184\C,0,2.7305040835,-2.101803496,-1.0013837004\C,0,-1.52
77946526,-2.1881419335,2.3581765054\C,0,-3.9498785351,-0.0401309481,-0
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 03459329,-2.4269840809\C,0,2.0474887314,0.926099383,-2.7716208452\N,0,
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UB3LYP/6-31G(d)



0 5

C	0.906996008	3.339865100	0.984602787
C	-0.415609126	3.184854471	1.557367121
C	-0.329271570	2.278017492	2.686345769
C	1.060116688	1.891102172	2.827658307
C	1.824026213	2.541938413	1.772856763
C	1.053373336	3.414085147	-0.405285176
C	-1.533276387	3.143228795	0.737186513
C	-1.351516267	1.347440032	2.914393940
C	1.387510638	0.594281847	3.224573794
C	2.869848341	1.859364962	1.147234454
C	-0.108531636	3.345036280	-1.264574307
C	-2.647315434	2.251894200	1.036007847
C	-1.006157226	0.006702323	3.337622446
C	2.485676376	-0.109645340	2.583985600
C	3.027470822	1.940290078	-0.296405665
C	2.136344255	2.696500987	-1.058087995
C	-1.383023315	3.209858583	-0.707479738
C	-2.541333438	1.289585941	2.077577063
C	0.333010378	-0.362265359	3.494161488
C	3.209708873	0.511110857	1.561043023
C	0.236796005	2.567521419	-2.436138686
C	-3.311438548	2.047304272	-0.226068254

C	-0.696506398	1.681304798	-2.982093287
C	-1.961722859	-0.908645687	2.755822029
C	2.112226884	-1.504890503	2.468052490
C	3.465241470	0.638951318	-0.772380046
C	1.631522562	2.177073119	-2.317743574
C	-2.386961495	2.358756479	-1.314924227
C	-2.938795311	-0.138978068	1.992189887
C	0.784818953	-1.663890711	3.039015870
C	3.579988879	-0.242775652	0.377138793
C	3.218910014	-1.586133999	0.262556178
C	-0.745711451	-3.362379512	-0.969632274
C	-1.683666573	-2.651892939	-1.791213676
C	-0.953839927	-1.895886330	-2.819729591
C	0.437443419	-2.263188325	-2.689814257
C	0.571900728	-3.160838128	-1.547208350
C	-0.906169636	-3.433682127	0.436338724
C	-2.597724124	-1.844315871	-1.028873073
C	-1.313861686	-0.572947735	-3.196434233
C	1.446034506	-1.332042899	-2.965253919
C	1.686407702	-3.070620076	-0.714359658
C	-2.019007033	-2.763607875	1.125983569
C	-3.011899498	-0.498836052	-1.434533001
C	-0.260265460	0.382710757	-3.461396360
C	2.611714880	-1.253536718	-2.106017299
C	1.528911984	-3.153602076	0.728268107
C	0.250368733	-3.313378087	1.284722582
C	-2.950554786	-2.042306018	0.400173758
C	-2.464564914	0.163923263	-2.637653637
C	1.088714036	0.012895165	-3.364393018
C	2.730504084	-2.101803496	-1.001383700
C	-1.527794653	-2.188141934	2.358176505
C	-3.949878535	-0.040130948	-0.363898501
C	2.988379073	0.144663510	-1.986927647
C	2.470051117	-2.232867927	1.329632495
C	-0.125594810	-2.551203573	2.471032634
C	-3.494402083	-0.758788177	0.843813694
C	-2.039144050	1.550345933	-2.426984081
C	2.047488731	0.926099383	-2.771620845
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H	-3.305720327	0.907800827	-0.063252354

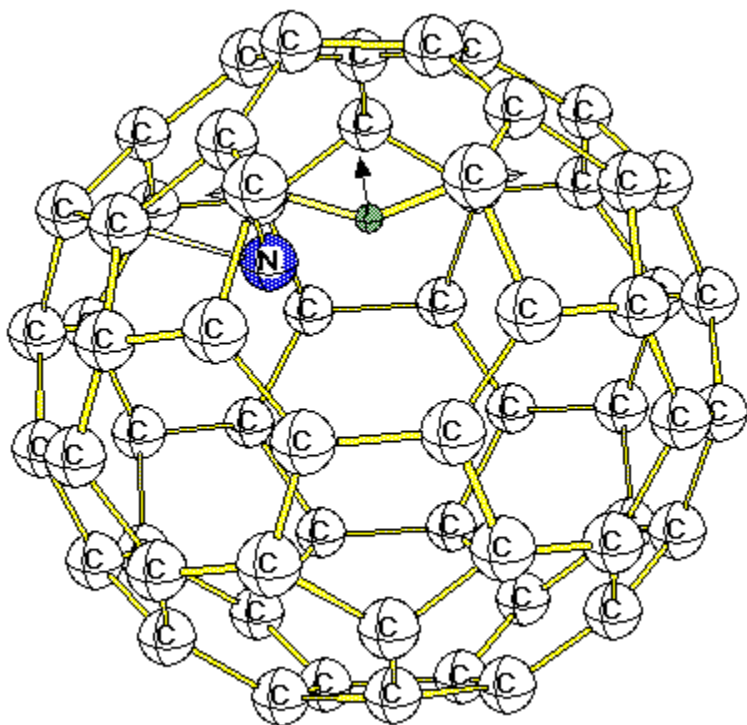
Zero-point correction=	0.378692 (Hartree/Particle)
Thermal correction to Energy=	0.401623
Thermal correction to Enthalpy=	0.402567
Thermal correction to Gibbs Free Energy=	0.332557
Sum of electronic and zero-point Energies=	-2340.705318
Sum of electronic and thermal Energies=	-2340.682388
Sum of electronic and thermal Enthalpies=	-2340.681443
Sum of electronic and thermal Free Energies=	-2340.751453

```

1\1\FAU-CCC-CCDN089\Freq\UB3LYP/6-31G(d)\C60H1N1(5)\DRAL\24-Aug-2010\0
\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d) Freq
\TS endo-N@C60H -> NH@C60 via breaking 6,6-bond quintet\0,5\C,0.9069
960082,3.3398651005,0.9846027872\C,-0.4156091265,3.1848544713,1.557367
1211\C,-0.3292715704,2.2780174916,2.6863457688\C,1.0601166881,1.891102
1717,2.8276583066\C,1.8240262134,2.5419384134,1.7728567627\C,1.0533733
356,3.4140851471,-0.4052851762\C,-1.5332763871,3.143228795,0.737186512
7\C,-1.351516267,1.3474400322,2.9143939397\C,1.3875106382,0.594281847,
3.2245737945\C,2.8698483406,1.8593649618,1.1472344542\C,-0.1085316362,
3.3450362804,-1.2645743067\C,-2.6473154342,2.2518942003,1.0360078469\C
,-1.0061572256,0.0067023226,3.3376224465\C,2.4856763757,-0.1096453405,
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.2427756524,0.3771387929\C,3.2189100142,-1.5861339986,0.2625561776\C,-
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,-1.7912136762\C,-0.9538399273,-1.8958863297,-2.8197295909\C,0.4374434
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504\C,-0.9061696363,-3.4336821269,0.4363387243\C,-2.5977241242,-1.8443
158708,-1.028873073\C,-1.3138616865,-0.5729477346,-3.1964342329\C,1.44
6034506,-1.3320428986,-2.9652539188\C,1.6864077016,-3.0706200763,-0.71
43596578\C,-2.0190070331,-2.7636078746,1.1259835688\C,-3.0118994979,-0
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,2.6117148803,-1.253536718,-2.1060172986\C,1.5289119837,-3.1536020761,
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,-2.0423060178,0.4001737577\C,-2.4645649142,0.1639232634,-2.6376536371
\C,1.0887140362,0.012895165,-3.3643930184\C,2.7305040835,-2.101803496,
-1.0013837004\C,-1.5277946526,-2.1881419335,2.3581765054\C,-3.94987853
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68\C,2.4700511174,-2.2328679271,1.3296324948\C,-0.1255948101,-2.551203
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Vibrational Normal Modes



62

C	1.135803	3.238751	1.080785
C	-0.188987	3.153187	1.663007
C	-0.153115	2.206298	2.761422
C	1.208619	1.723709	2.874819
C	2.004680	2.356502	1.832893
C	1.274295	3.348375	-0.307568
C	-1.314275	3.212522	0.854418
C	-1.233001	1.338610	2.971013
C	1.452433	0.395785	3.226451
C	2.997029	1.626847	1.174181
C	0.102690	3.384570	-1.155626
C	-2.482496	2.387749	1.137019
C	-0.973952	-0.035160	3.347340
C	2.495450	-0.358149	2.551517
C	3.146704	1.744164	-0.267805
C	2.301131	2.582227	-0.994977
C	-1.172914	3.316105	-0.588968
C	-2.431507	1.387087	2.146083
C	0.339008	-0.497017	3.477089
C	3.250006	0.246253	1.540915
C	0.384894	2.624478	-2.355195
C	-3.170099	2.268899	-0.123470
C	-0.610256	1.820366	-2.918738
C	-1.993578	-0.865679	2.747290
C	2.028836	-1.721039	2.395259
C	3.492494	0.432874	-0.789938
C	1.751513	2.138758	-2.264874

C	-2.236753	2.553700	-1.212057
C	-2.924024	-0.008434	2.019557
C	0.698973	-1.810204	2.975607
C	3.558569	-0.491528	0.329490
C	3.107767	-1.803537	0.176101
C	-0.977317	-3.271879	-1.067932
C	-1.873198	-2.474358	-1.855907
C	-1.103899	-1.735278	-2.867825
C	0.260931	-2.198062	-2.765212
C	0.345548	-3.139424	-1.653421
C	-1.129519	-3.378184	0.336746
C	-2.724522	-1.633235	-1.058032
C	-1.378345	-0.379803	-3.198060
C	1.326806	-1.327357	-3.021998
C	1.471035	-3.150503	-0.830585
C	-2.188988	-2.658638	1.059791
C	-3.051757	-0.250745	-1.415882
C	-0.265839	0.512022	-3.444093
C	2.502807	-1.354369	-2.173733
C	1.321340	-3.269847	0.610323
C	0.040048	-3.362553	1.175601
C	-3.076894	-1.853878	0.367806
C	-2.472321	0.413135	-2.603249
C	1.056319	0.050610	-3.373982
C	2.574740	-2.244206	-1.098141
C	-1.649462	-2.157486	2.304182
C	-3.947421	0.233995	-0.320763
C	2.972853	0.011152	-2.014261
C	2.327107	-2.433638	1.230258
C	-0.273612	-2.616209	2.389758
C	-3.529999	-0.552272	0.858236
C	-1.953589	1.760692	-2.353169
C	2.079103	0.878420	-2.763071
N	-1.704067	-0.431119	-0.648766
H	-3.238855	1.126823	0.002803

NORMALMODES 180

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C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
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C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.01	-0.01
C	0.00	0.00	0.00

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C 0.00 0.00 0.00
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C 0.00 0.00 0.00
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N -0.01 0.01 0.01
H -0.93 0.28 0.08
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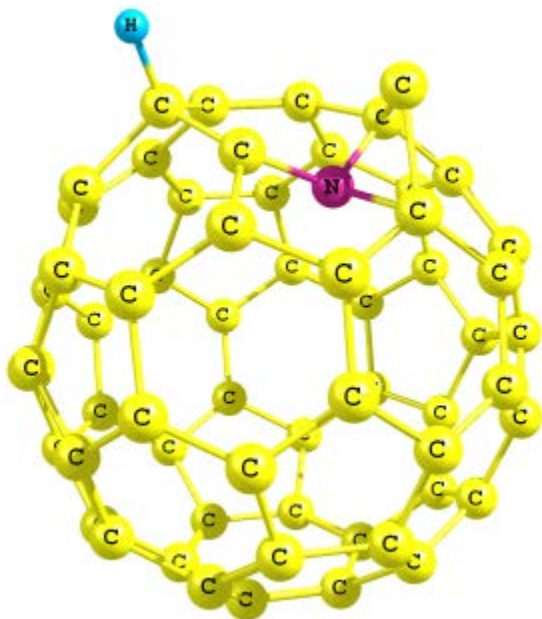
⁵TS1m (TS of N-escape from quintet N^{•••}@C₆₀H[•] by displacing carbon atom)

ROMP2/6-31G(d)//UB3LYP/6-31G(d) using DFT checkpoint

```
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one NAME=DRAL\\TS N-escape from N@C60H via breaking 5,6-bond quintet\\
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0,1.3344442688,2.3514273944,-2.2065334802\C,0,1.9639697797,1.180988813
1,-2.7857746253\C,0,0.9895661325,-0.9781608778,-3.4797165478\C,0,-1.56
71256248,0.4453585175,-3.2883791665\C,0,-1.0295675023,2.783064585,-1.6
402620458\C,0,1.7456880653,2.8140866573,-0.9542808159\C,0,2.9804874593
,0.5140172231,-2.0993763291\C,0,-0.2154746917,-1.7538710787,-3.3658237
117\C,0,-2.5030168894,0.9060336732,-2.2845657752\C,0,-0.6032292906,3.2
399185506,-0.3343758639\C,0,2.787806197,2.1074828271,-0.2290882327\C,0
,3.01949302,-0.9423825888,-2.0849292322\C,0,2.0396219597,-1.670611536,
-2.7850581648\C,0,-1.5139030779,-1.076307976,-3.1559131009\C,0,-2.2939
77673,2.0879617101,-1.4901581535\C,0,0.7552484736,3.260100029,0.008748
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028625327,-2.5560873138\C,0,-2.9662537018,-0.2097885616,-1.562774707\C
,0,-0.9038928634,-3.32939751,-1.6227509834\C,0,-1.582614424,2.77151692
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177,-1.3705898353,-0.7768913345\C,0,1.453369878,-2.8625736938,-2.18312
41236\C,0,-2.8279471438,-1.9374945118,-2.8434671815\C,0,-2.6224108621,
2.0461581283,-0.0835683237\C,0,1.179378335,2.8250612919,1.3222568775\C
,0,3.665793585,-0.1856021862,0.0310196536\C,0,3.3245249721,-0.18053149
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,0,-2.7593357306,-1.0067338331,1.7794647207\C,0,-1.5550465513,-3.27321
62711,0.6215009422\C,0,1.2297082252,-3.2506367147,1.3417362918\C,0,1.7
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14,-3.7235483261,-0.3185271233\C,0,2.4827405916,-2.501943754,1.1967998
515\C,0,1.707707769,0.5227795675,2.9247725168\C,0,0.499548617,1.210906
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8135563,-2.6208287188,-0.0746478487\C,0,0.8378400873,-3.7273812162,0.0
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6,2.3519403112,1.8945997115\C,0,-3.7281122377,-0.2728484131,-0.2905197
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28\C,0,2.8570011099,-2.5178334381,-0.1870044914\C,0,2.6994403043,0.987
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 -1.5647960664\C,0,1.8353723782,-3.2664618659,-0.9087935401\N,0,-1.9216
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UB3LYP/6-31G(d)



0 5

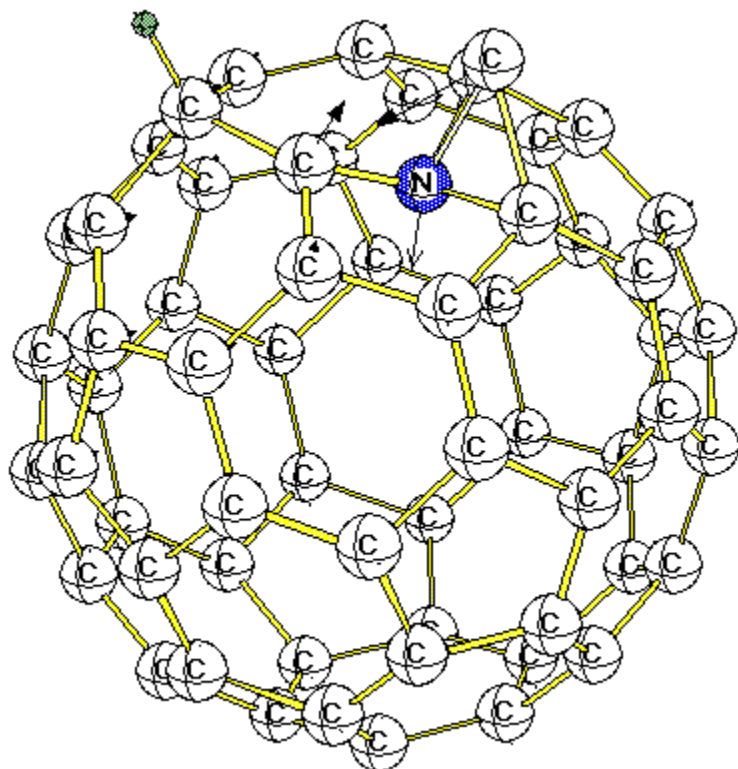
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C	1.334444269	2.351427394	-2.206533480
C	1.963969780	1.180988813	-2.785774625
C	0.989566132	-0.978160878	-3.479716548
C	-1.567125625	0.445358518	-3.288379166
C	-1.029567502	2.783064585	-1.640262046
C	1.745688065	2.814086657	-0.954280816
C	2.980487459	0.514017223	-2.099376329
C	-0.215474692	-1.753871079	-3.365823712
C	-2.503016889	0.906033673	-2.284565775
C	-0.603229291	3.239918551	-0.334375864
C	2.787806197	2.107482827	-0.229088233
C	3.019493020	-0.942382589	-2.084929232
C	2.039621960	-1.670611536	-2.785058165
C	-1.513903078	-1.076307976	-3.155913101
C	-2.293977673	2.087961710	-1.490158154
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C	0.053644733	-2.902862533	-2.556087314

C	-2.966253702	-0.209788562	-1.562774707
C	-0.903892863	-3.329397510	-1.622750983
C	-1.582614424	2.771516925	0.631397300
C	2.434417395	2.112108541	1.179226317
C	3.433666818	-1.370589835	-0.776891334
C	1.453369878	-2.862573694	-2.183124124
C	-2.827947144	-1.937494512	-2.843467182
C	-2.622410862	2.046158128	-0.083568324
C	1.179378335	2.825061292	1.322256878
C	3.665793585	-0.185602186	0.031019654
C	3.324524972	-0.180531497	1.384156548
C	-0.733664768	-0.947208446	3.205079126
C	-1.761391489	-1.688780415	2.486292216
C	-1.149783176	-2.844423202	1.896827237
C	0.264306402	-2.823071938	2.258980953
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C	-2.759335731	-1.006733833	1.779464721
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C	1.722654338	-0.926649861	2.928837644
C	-1.772243376	1.168052553	2.493227154
C	-3.221600909	-1.489114170	0.510976716
C	-0.533305121	-3.723548326	-0.318527123
C	2.482740592	-2.501943754	1.196799852
C	1.707707769	0.522779568	2.924772517
C	0.499548617	1.210906560	3.056260000
C	-2.771899059	0.456739650	1.782755416
C	-2.643813556	-2.620828719	-0.074647849
C	0.837840087	-3.727381216	0.045300760
C	2.712488999	-1.359728988	1.983384075
C	-1.175287158	2.351940311	1.894599712
C	-3.728112238	-0.272848413	-0.290519728
C	2.857001110	-2.517833438	-0.187004491
C	2.699440304	0.987955109	1.969403688
C	0.232028622	2.383249408	2.257907733
C	-3.234391055	0.923885596	0.534208047
C	-2.214520200	-2.595042236	-1.564796066
C	1.835372378	-3.266461866	-0.908793540
N	-1.921664824	-1.165545995	-1.724105228
H	-4.813702550	-0.275784864	-0.460891505

Zero-point correction=	0.381035 (Hartree/Particle)
Thermal correction to Energy=	0.403121
Thermal correction to Enthalpy=	0.404065
Thermal correction to Gibbs Free Energy=	0.335609
Sum of electronic and zero-point Energies=	-2340.791724
Sum of electronic and thermal Energies=	-2340.769638
Sum of electronic and thermal Enthalpies=	-2340.768694
Sum of electronic and thermal Free Energies=	-2340.837149

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 \#P Geom=AllCheck Guess=TChef SCRF=Check GenChk UB3LYP/6-31G(d) Freq
 \TS N-escape from N@C60H via breaking 5,6-bond quintet\0,5\C,0.94085
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Vibrational Normal Modes



62

C	-0.387729	-1.350427	-3.208543
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C	1.171963	0.394726	-3.326954
C	1.032189	-1.044277	-3.219799
C	-0.849265	-2.408867	-2.388554
C	-2.386925	0.074141	-2.653057
C	-0.406065	2.204093	-2.751154
C	2.205508	1.045304	-2.648836
C	1.926067	-1.784182	-2.443380
C	-2.085972	-2.292764	-1.664747
C	-2.580980	1.332484	-1.964093
C	0.660404	2.865023	-2.028912
C	3.122657	0.279039	-1.822471
C	1.439226	-2.870140	-1.602838
C	0.066833	-3.181808	-1.596100
C	-2.836091	-1.017585	-1.682369
C	-1.648035	2.426235	-2.035197
C	1.943633	2.304571	-1.975788
C	2.987583	-1.107265	-1.723619
C	-1.937415	-2.939095	-0.396493
C	-3.067731	1.061625	-0.671677
C	-2.499058	-2.351669	0.747803
C	0.079015	3.446912	-0.831121
C	3.418857	1.063773	-0.637265
C	2.177169	-2.852937	-0.369545

C	-0.600068	-3.494032	-0.337311
C	-4.111441	-0.822837	-0.732879
C	-1.348503	3.162860	-0.828642
C	2.689698	2.313779	-0.735728
C	3.136112	-1.763476	-0.435132
C	3.419495	-1.008112	0.703547
C	0.521757	1.346902	3.239188
C	-0.903147	1.042914	3.246011
C	-1.056795	-0.380021	3.339246
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C	2.461184	-0.056405	2.623082
C	0.121314	3.153176	1.615387
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C	-1.786758	-2.287920	1.965282
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C	2.266043	2.218080	1.690337
C	-1.265795	2.860076	1.607183
C	-3.046234	-0.255230	1.857559
C	-0.492973	-2.864019	2.046858
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C	1.529352	-3.142428	0.852423
C	3.564778	0.429634	0.601651
C	2.132005	2.885543	0.417605
C	-2.005082	2.922220	0.406939
C	-3.302422	-1.092341	0.577281
C	0.105730	-3.456105	0.859928
N	-2.609249	-0.263171	-0.415993
H	-4.170626	2.457044	0.539932

NORMALMODES 180

C	-0.01	0.01	0.00
C	0.01	0.01	0.02
C	0.00	0.00	-0.02
C	0.01	0.00	-0.01
C	0.01	0.00	0.00
C	-0.02	0.01	0.03
C	0.00	0.02	-0.06
C	-0.02	-0.03	0.01
C	0.00	0.00	-0.01
C	0.00	0.01	-0.01
C	-0.05	-0.04	0.00
C	-0.10	0.00	-0.05

C -0.02 -0.01 0.00
C -0.01 0.00 0.00
C -0.01 0.01 0.01
C -0.02 0.02 0.01
C -0.02 0.00 0.06
C -0.03 -0.09 0.03
C -0.01 0.00 0.00
C 0.01 0.00 -0.01
C -0.02 -0.03 0.01
C -0.33 -0.14 -0.06
C -0.03 -0.02 -0.01
C -0.01 -0.02 0.00
C -0.01 0.00 0.00
C 0.00 0.01 -0.01
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C 0.32 0.61 -0.02
C -0.01 -0.06 0.00
C -0.01 0.00 -0.01
C 0.01 0.00 -0.01
C 0.00 0.00 -0.01
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N 0.55 0.00 0.12
H -0.01 0.02 0.05

-386.6179

⁵TS1i (TS of N-escape from quintet N^{•••}@C₆₀H[•] by breaking [6,6]-bond)***ROMP2/6-31G(d)//UB3LYP/6-31G(d)***

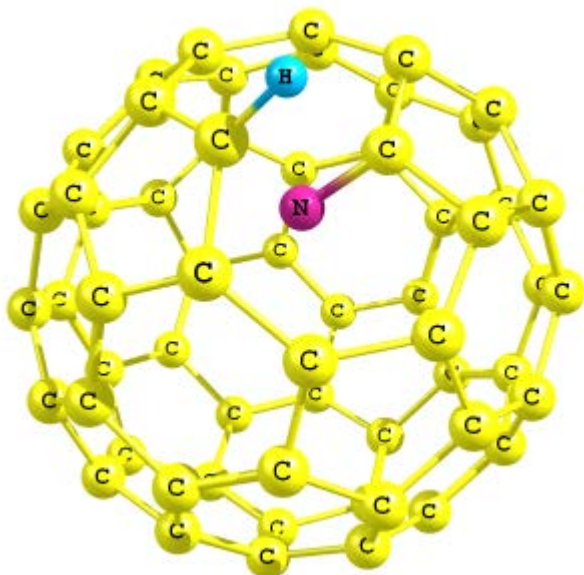
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,2.1165860329,-1.3058272597,-2.544679751\C,0,2.9394433778,-1.533177048
,-1.3648617993\C,0,2.363708098,-2.6051624154,0.7888444558\C,0,0.094404
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9\C,0,-1.1974880948,-3.1976750882,-1.1805896812\C,0,-0.4683586636,-0.5
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,0,-0.289917718,-1.7149085938,3.0616149237\C,0,-1.7905531087,-0.096310
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UB3LYP/6-31G(d)



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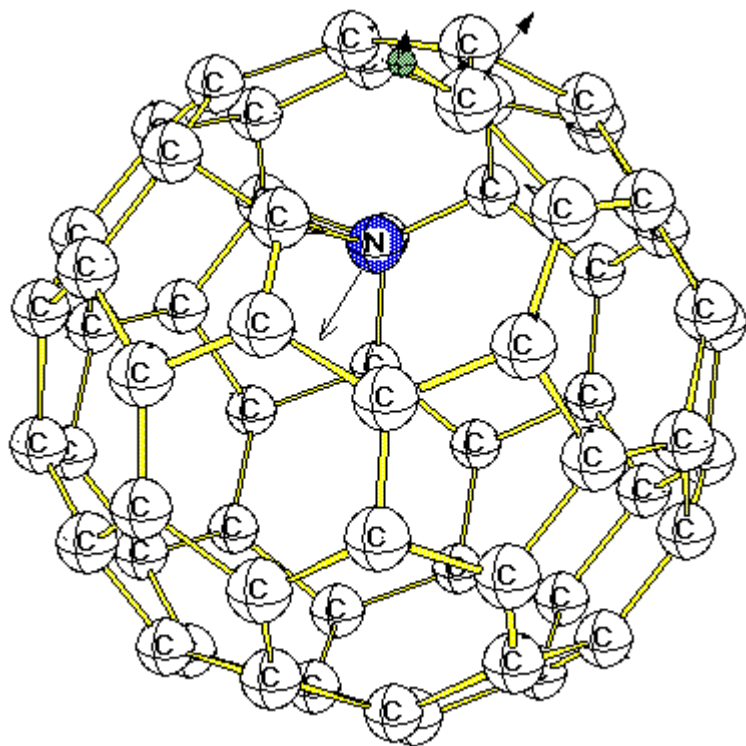
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C	2.939443378	-1.533177048	-1.364861799
C	2.363708098	-2.605162415	0.788844456
C	0.094404670	-3.595384728	-0.672965269
C	-0.249661608	-1.866086648	-2.975766544
C	1.906543778	-0.005691978	-3.009480656
C	3.501851593	-0.444831597	-0.693335486
C	1.202527062	-3.050518551	1.528007002
C	-1.197488095	-3.197675088	-1.180589681
C	-0.468358664	-0.512480772	-3.432262418
C	2.506077892	1.121607306	-2.318636329
C	3.492135513	-0.408413107	0.761141586
C	2.920455142	-1.461961319	1.478728564
C	0.084215034	-3.557206881	0.853040744
C	-1.439928441	-2.300005892	-2.273754325
C	0.589864106	0.397498753	-3.468242840
C	3.286085606	0.903140391	-1.176530035
C	0.993747097	-2.130916648	2.648323926
C	-1.622932859	-2.615922176	0.054623810
C	-0.289917718	-1.714908594	3.061614924
C	-1.790553109	-0.096310285	-2.983656182
C	1.560685524	2.219767444	-2.352360120
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C	2.082043052	-1.176144904	2.634631830
C	-1.214211217	-3.135121524	1.322897782
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C	0.379952250	1.772818157	-3.069571167
C	3.141985021	1.774246923	-0.023559557
C	2.228305232	2.829889936	-0.056090067
C	-2.229570004	2.721472191	0.624398629
C	-2.842076924	1.653937872	1.357006262
C	-2.024273019	1.372551681	2.530916020
C	-0.923821075	2.314552401	2.532637495
C	-1.044713378	3.144445292	1.343424393
C	-2.220134762	2.686072662	-0.789657658
C	-3.482830837	0.600630416	0.697735201
C	-1.830171628	0.052517600	2.960387105
C	0.339601172	1.924339964	2.981621406
C	0.099277200	3.527760039	0.642531043
C	-2.823191475	1.582997617	-1.476043556
C	-3.439079761	-0.745181127	1.215957552
C	-0.514225906	-0.340230666	3.446862093
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C	1.410248005	3.122229227	1.107921312
C	-1.989916142	1.243511027	-2.623415145
C	-3.583437474	-1.573234393	0.015285282
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C	1.425931274	3.063342954	-1.244061648
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C	-3.422969931	-0.806261360	-1.223207463
C	-1.470868479	-2.183850097	2.366436003
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Vibrational Normal Modes



62

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C	-2.910236	-1.531110	1.422521
C	-2.336262	-2.650186	-0.707572
C	-0.046349	-3.577819	0.763128
C	0.292850	-1.787575	3.019612
C	-1.884225	0.048662	3.021423
C	-3.489398	-0.466346	0.727830
C	-1.174883	-3.100815	-1.443219
C	1.244177	-3.152976	1.251896
C	0.499010	-0.420573	3.440647
C	-2.501080	1.151463	2.306698
C	-3.489534	-0.466289	-0.727135
C	-2.910510	-1.530983	-1.422024
C	-0.046495	-3.577791	-0.763389
C	1.483422	-2.225513	2.320620
C	-0.569294	0.478038	3.461040
C	-3.285931	0.895660	1.175715
C	-0.983905	-2.207289	-2.587556
C	1.654920	-2.597610	-0.000322
C	0.292211	-1.787331	-3.019796
C	1.813421	-0.000904	2.972839
C	-1.568109	2.260708	2.306566
C	-3.286182	0.895762	-1.174976

C	-2.082936	-1.264800	-2.590359
C	1.243944	-3.153009	-1.252428
C	2.464926	-1.103327	2.280125
C	-0.377714	1.845211	3.026711
C	-3.159284	1.739162	0.000386
C	-2.257544	2.805518	0.000339
C	2.196772	2.730324	-0.707396
C	2.816682	1.651732	-1.417228
C	1.994551	1.331811	-2.578175
C	0.883411	2.261011	-2.595985
C	1.002517	3.121761	-1.428729
C	2.196915	2.730275	0.707134
C	3.473702	0.622569	-0.736194
C	1.812776	-0.000677	-2.973199
C	-0.378352	1.845453	-3.026513
C	-0.141212	3.509607	-0.729904
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C	3.441983	-0.736217	-1.220314
C	0.498280	-0.420301	-3.440786
C	-1.568595	2.260894	-2.306078
C	-0.141063	3.509548	0.730185
C	1.002824	3.121649	1.428739
C	3.473865	0.622521	0.735546
C	2.464408	-1.103191	-2.280698
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C	1.995108	1.331628	2.577886
C	3.603586	-1.532235	-0.000328
C	-2.501573	1.151640	-2.306109
C	-1.450203	3.077703	1.176645
C	0.883965	2.260803	2.595961
C	3.442396	-0.736317	1.219669
C	1.482932	-2.225361	-2.321127
C	-1.884865	0.048910	-3.021046
N	1.639199	-1.289941	-0.000317
H	3.826545	-2.595658	-0.000411

NORMALMODES 180

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C	0.01	0.01	-0.01
C	0.00	-0.01	-0.01
C	-0.01	-0.01	0.00
C	0.00	0.00	0.00
C	0.00	-0.01	0.00
C	0.02	0.00	-0.01
C	0.01	-0.01	0.01
C	0.00	-0.01	-0.01
C	0.00	0.00	0.00
C	0.01	0.01	0.01
C	0.01	0.04	0.01

C 0.01 0.00 -0.01
C 0.00 -0.01 0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.02 0.00 0.01
C -0.02 0.01 -0.01
C 0.02 0.00 -0.01
C 0.00 0.00 0.00
C 0.00 -0.01 0.01
C 0.00 0.21 0.00
C 0.01 -0.01 -0.01
C 0.02 -0.01 -0.02
C 0.01 -0.01 0.00
C 0.00 0.00 0.00
C -0.01 -0.01 0.00
C 0.01 0.03 -0.01
C 0.05 0.00 -0.02
C 0.00 0.01 0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.01 -0.01 0.00
C -0.02 -0.01 0.01
C 0.01 0.00 -0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.01 -0.01 0.00
C -0.02 -0.02 0.02
C 0.02 -0.01 0.02
C 0.00 0.01 -0.01
C 0.01 0.00 -0.01
C -0.02 -0.01 -0.01
C -0.02 -0.08 0.10
C 0.01 0.00 0.01
C 0.01 -0.01 0.00
C 0.01 0.00 0.01
C 0.00 0.00 0.00
C -0.02 -0.02 -0.02
C 0.05 0.00 0.02
C 0.02 0.00 0.01
C 0.00 0.00 0.00
C 0.01 0.00 0.01
C 0.61 -0.03 0.00
C 0.00 -0.01 -0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.02 -0.08 -0.10
C -0.02 0.01 0.01
C 0.00 -0.01 0.01
N -0.69 0.10 0.00
H 0.18 -0.11 0.00

-591.9921

TS1a⁺ (TS of N@C₆₀H⁺ → NH⁺@C₆₀ by breaking [5,6]-bond, doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN092\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,2)\DRAL\30-Mar-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCFCyc=1200 SCF
=(VShift,Conver=5) Name=Dral\TS N@C60H(+) -> NH(+)@C60 via breaking 5
,6-bond (doublet)\1,2\C,1.412953,0.344074,3.234568\C,0.053055,0.82949
3,3.413124\C,-0.839378,-0.308738,3.398131\C,-0.038448,-1.505435,3.2057
49\C,1.356784,-1.101857,3.097213\C,2.316597,1.079656,2.471091\C,-0.347
123,2.035233,2.837633\C,-2.103141,-0.20162,2.811984\C,-0.525245,-2.545
952,2.420472\C,2.196181,-1.745291,2.193871\C,1.90299,2.340813,1.878277
\C,-1.65946,2.161425,2.220834\C,-2.622629,-1.308175,2.025847\C,0.34994
9,-3.219673,1.481921\C,3.138066,-0.977237,1.394956\C,3.197253,0.409789
,1.532934\C,0.61235,2.818497,2.077202\C,-2.531409,1.050463,2.208475\C,
-1.842479,-2.439781,1.813796\C,1.685528,-2.824618,1.367831\C,2.525378,
2.446073,0.565516\C,-1.48505,3.122254,1.101772\C,1.833934,3.026816,-0.
499446\C,-3.403099,-0.763573,0.928952\C,-0.422233,-3.526967,0.289372\C
,3.201755,-1.578751,0.075116\C,3.320845,1.251967,0.35342\C,-0.089407,3
.464398,0.984784\C,-3.409617,0.670126,1.069856\C,-1.776423,-3.047225,0
.491668\C,2.304425,-2.723329,0.059659\C,1.562688,-3.013284,-1.087231\C
,-1.388484,-0.360522,-3.206744\C,-1.330289,1.080061,-3.029139\C,0.0590
91,1.484866,-3.178414\C,0.858921,0.296621,-3.419198\C,-0.036345,-0.845
89,-3.434153\C,-2.288891,-1.120446,-2.464117\C,-2.181885,1.733894,-2.1
29621\C,0.570171,2.528876,-2.41301\C,2.125893,0.188128,-2.843925\C,0.3
66804,-2.054388,-2.870087\C,-3.183827,-0.468415,-1.535921\C,-1.650878,
2.860092,-1.372476\C,1.892139,2.417703,-1.815254\C,2.546175,-1.070535,
-2.250121\C,-0.565021,-2.833014,-2.071925\C,-1.869038,-2.383967,-1.879
817\C,-3.161659,0.935335,-1.399259\C,-0.290198,3.222005,-1.485162\C,2.
647456,1.266343,-2.020954\C,1.684326,-2.171473,-2.263903\C,-3.306391,-
1.314864,-0.358345\C,-2.206631,3.067662,-0.082681\C,3.321499,-0.770628
,-1.0571\C,0.172979,-3.421051,-0.969069\C,-2.491595,-2.497202,-0.57368
\C,-3.511455,1.40251,-0.104778\C,0.486613,3.527954,-0.293453\C,3.38154
7,0.672324,-0.91516\N,-0.075075,0.056715,-0.022492\H,-2.634179,2.05370
7,0.266152\Version=AM64L-G03RevD.02\State=2-A\HF=-2326.2200616\MP2=-
2334.1479394\RMSD=7.064e-06\Thermal=0.\PG=C01 [X(C60H1N1)]\@
```

UB3LYP/6-31G(d)

1 2

C 1.412953000 0.344074000 3.234568000

C	0.053055000	0.829493000	3.413124000
C	-0.839378000	-0.308738000	3.398131000
C	-0.038448000	-1.505435000	3.205749000
C	1.356784000	-1.101857000	3.097213000
C	2.316597000	1.079656000	2.471091000
C	-0.347123000	2.035233000	2.837633000
C	-2.103141000	-0.201620000	2.811984000
C	-0.525245000	-2.545952000	2.420472000
C	2.196181000	-1.745291000	2.193871000
C	1.902990000	2.340813000	1.878277000
C	-1.659460000	2.161425000	2.220834000
C	-2.622629000	-1.308175000	2.025847000
C	0.349949000	-3.219673000	1.481921000
C	3.138066000	-0.977237000	1.394956000
C	3.197253000	0.409789000	1.532934000
C	0.612350000	2.818497000	2.077202000
C	-2.531409000	1.050463000	2.208475000
C	-1.842479000	-2.439781000	1.813796000
C	1.685528000	-2.824618000	1.367831000
C	2.525378000	2.446073000	0.565516000
C	-1.485050000	3.122254000	1.101772000
C	1.833934000	3.026816000	-0.499446000
C	-3.403099000	-0.763573000	0.928952000
C	-0.422233000	-3.526967000	0.289372000
C	3.201755000	-1.578751000	0.075116000
C	3.320845000	1.251967000	0.353420000
C	-0.089407000	3.464398000	0.984784000
C	-3.409617000	0.670126000	1.069856000
C	-1.776423000	-3.047225000	0.491668000
C	2.304425000	-2.723329000	0.059659000
C	1.562688000	-3.013284000	-1.087231000
C	-1.388484000	-0.360522000	-3.206744000
C	-1.330289000	1.080061000	-3.029139000
C	0.059091000	1.484866000	-3.178414000
C	0.858921000	0.296621000	-3.419198000
C	-0.036345000	-0.845890000	-3.434153000
C	-2.288891000	-1.120446000	-2.464117000
C	-2.181885000	1.733894000	-2.129621000
C	0.570171000	2.528876000	-2.413010000
C	2.125893000	0.188128000	-2.843925000
C	0.366804000	-2.054388000	-2.870087000
C	-3.183827000	-0.468415000	-1.535921000
C	-1.650878000	2.860092000	-1.372476000
C	1.892139000	2.417703000	-1.815254000
C	2.546175000	-1.070535000	-2.250121000
C	-0.565021000	-2.833014000	-2.071925000
C	-1.869038000	-2.383967000	-1.879817000
C	-3.161659000	0.935335000	-1.399259000
C	-0.290198000	3.222005000	-1.485162000
C	2.647456000	1.266343000	-2.020954000

C 1.684326000 -2.171473000 -2.263903000
 C -3.306391000 -1.314864000 -0.358345000
 C -2.206631000 3.067662000 -0.082681000
 C 3.321499000 -0.770628000 -1.057100000
 C 0.172979000 -3.421051000 -0.969069000
 C -2.491595000 -2.497202000 -0.573680000
 C -3.511455000 1.402510000 -0.104778000
 C 0.486613000 3.527954000 -0.293453000
 C 3.381547000 0.672324000 -0.915160000
 N -0.075075000 0.056715000 -0.022492000
 H -2.634179000 2.053707000 0.266152000

Zero-point correction= 0.382818 (Hartree/Particle)
 Thermal correction to Energy= 0.406475
 Thermal correction to Enthalpy= 0.407419
 Thermal correction to Gibbs Free Energy= 0.334773
 Sum of electronic and zero-point Energies= -2340.534597
 Sum of electronic and thermal Energies= -2340.510939
 Sum of electronic and thermal Enthalpies= -2340.509995
 Sum of electronic and thermal Free Energies= -2340.582641

1\1\FAU-CCC-CCDH156\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,2)\DRAL\18-Jul-200
 9\0\#P scf=qc UB3LYP/6-31G(d) Freq=NoRaman SCFCYC=1200 Name=Dral\TS
 N@C60H(+)-> NH(+)\C60 via breaking 5,6-bond (doublet)\1,2\C,1.412953
 ,0.344074,3.234568\C,0.053055,0.829493,3.413124\C,-0.839378,-0.308738,
 3.398131\C,-0.038448,-1.505435,3.205749\C,1.356784,-1.101857,3.097213\
 C,2.316597,1.079656,2.471091\C,-0.347123,2.035233,2.837633\C,-2.103141
 ,-0.20162,2.811984\C,-0.525245,-2.545952,2.420472\C,2.196181,-1.745291
 ,2.193871\C,1.90299,2.340813,1.878277\C,-1.65946,2.161425,2.220834\C,-
 2.622629,-1.308175,2.025847\C,0.349949,-3.219673,1.481921\C,3.138066,-
 0.977237,1.394956\C,3.197253,0.409789,1.532934\C,0.61235,2.818497,2.07
 7202\C,-2.531409,1.050463,2.208475\C,-1.842479,-2.439781,1.813796\C,1.
 685528,-2.824618,1.367831\C,2.525378,2.446073,0.565516\C,-1.48505,3.12
 2254,1.101772\C,1.833934,3.026816,-0.499446\C,-3.403099,-0.763573,0.92
 8952\C,-0.422233,-3.526967,0.289372\C,3.201755,-1.578751,0.075116\C,3.
 320845,1.251967,0.35342\C,-0.089407,3.464398,0.984784\C,-3.409617,0.67
 0126,1.069856\C,-1.776423,-3.047225,0.491668\C,2.304425,-2.723329,0.05
 9659\C,1.562688,-3.013284,-1.087231\C,-1.388484,-0.360522,-3.206744\C,
 -1.330289,1.080061,-3.029139\C,0.059091,1.484866,-3.178414\C,0.858921,
 0.296621,-3.419198\C,-0.036345,-0.84589,-3.434153\C,-2.288891,-1.12044
 6,-2.464117\C,-2.181885,1.733894,-2.129621\C,0.570171,2.528876,-2.4130
 1\C,2.125893,0.188128,-2.843925\C,0.366804,-2.054388,-2.870087\C,-3.18
 3827,-0.468415,-1.535921\C,-1.650878,2.860092,-1.372476\C,1.892139,2.4
 17703,-1.815254\C,2.546175,-1.070535,-2.250121\C,-0.565021,-2.833014,-
 2.071925\C,-1.869038,-2.383967,-1.879817\C,-3.161659,0.935335,-1.39925
 9\C,-0.290198,3.222005,-1.485162\C,2.647456,1.266343,-2.020954\C,1.684
 326,-2.171473,-2.263903\C,-3.306391,-1.314864,-0.358345\C,-2.206631,3.
 067662,-0.082681\C,3.321499,-0.770628,-1.0571\C,0.172979,-3.421051,-0.
 969069\C,-2.491595,-2.497202,-0.57368\C,-3.511455,1.40251,-0.104778\C,
 0.486613,3.527954,-0.293453\C,3.381547,0.672324,-0.91516\N,-0.075075,0

.056715,-0.022492\H,-2.634179,2.053707,0.266152\\Version=AM64L-G03RevD
 .02\State=2-A\HF=-2340.9174142\S2=1.754197\S2-1=0.\S2A=0.763983\RMSD=0
 .000e+00\RMSF=1.142e-03\ZeroPoint=0.3828176\Thermal=0.4064747\ZPE=240.
 2216508\Dipole=-0.7991378,0.6226074,0.0496021\DipoleDeriv=0.0347461,0.
 ,-0.0066525,-0.008331\Polar=480.3389009,-5.3079779,476.9038397,-0.2801
 034,0.1386873,466.0907315\PG=C01 [X(C60H1N1)]\NImag=1\\0.56082588,0.05
 ,0.00004994,0.03465264,-0.02414975,0.08431419\\0.00031744,0.00089128,0
 ,0.00087887\\@

Vibrational Normal Modes

62

C	1.412953	0.344073	3.234568
C	0.053056	0.829493	3.413124
C	-0.839378	-0.308737	3.398131
C	-0.038450	-1.505435	3.205749
C	1.356783	-1.101858	3.097213
C	2.316598	1.079654	2.471091
C	-0.347121	2.035233	2.837633
C	-2.103141	-0.201618	2.811984
C	-0.525248	-2.545951	2.420472
C	2.196179	-1.745293	2.193871
C	1.902992	2.340811	1.878277
C	-1.659458	2.161427	2.220834
C	-2.622630	-1.308172	2.025847
C	0.349946	-3.219673	1.481921
C	3.138065	-0.977240	1.394956
C	3.197253	0.409786	1.532934
C	0.612353	2.818496	2.077202
C	-2.531408	1.050466	2.208475
C	-1.842481	-2.439779	1.813796
C	1.685525	-2.824620	1.367831
C	2.525380	2.446070	0.565516
C	-1.485047	3.122255	1.101772
C	1.833937	3.026814	-0.499446
C	-3.403100	-0.763570	0.928952
C	-0.422237	-3.526967	0.289372
C	3.201753	-1.578754	0.075116
C	3.320846	1.251964	0.353420
C	-0.089403	3.464398	0.984784
C	-3.409616	0.670129	1.069856
C	-1.776426	-3.047223	0.491668
C	2.304422	-2.723331	0.059659
C	1.562685	-3.013286	-1.087231
C	-1.388484	-0.360521	-3.206744
C	-1.330288	1.080062	-3.029139
C	0.059093	1.484866	-3.178414
C	0.858921	0.296620	-3.419198

C	-0.036346	-0.845890	-3.434153
C	-2.288892	-1.120444	-2.464117
C	-2.181883	1.733896	-2.129621
C	0.570174	2.528875	-2.413010
C	2.125893	0.188126	-2.843925
C	0.366802	-2.054388	-2.870087
C	-3.183827	-0.468412	-1.535921
C	-1.650875	2.860094	-1.372476
C	1.892141	2.417701	-1.815254
C	2.546174	-1.070538	-2.250121
C	-0.565024	-2.833013	-2.071925
C	-1.869040	-2.383965	-1.879817
C	-3.161658	0.935338	-1.399259
C	-0.290195	3.222005	-1.485162
C	2.647457	1.266340	-2.020954
C	1.684324	-2.171475	-2.263903
C	-3.306392	-1.314861	-0.358345
C	-2.206628	3.067664	-0.082681
C	3.321498	-0.770631	-1.057100
C	0.172976	-3.421051	-0.969069
C	-2.491598	-2.497199	-0.573680
C	-3.511454	1.402514	-0.104778
C	0.486617	3.527953	-0.293453
C	3.381548	0.672321	-0.915160
N	-0.075075	0.056715	-0.022492
H	-2.634177	2.053710	0.266152

NORMALMODES 180

C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00

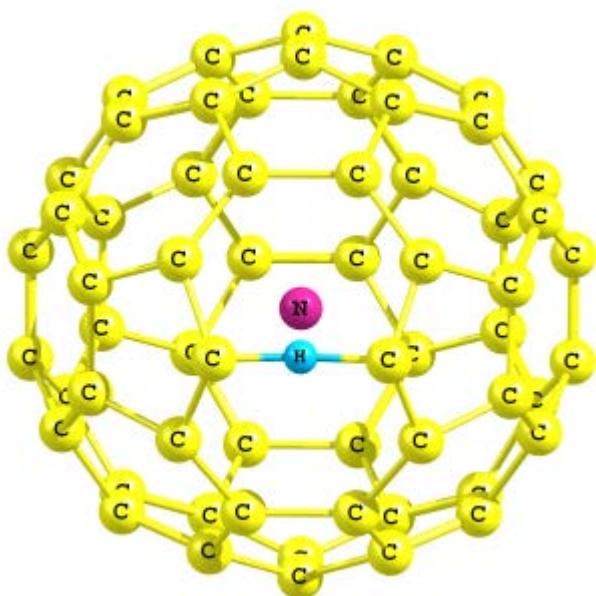
C	0.00	0.00	0.00
C	0.00	-0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	-0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	-0.01	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.08	0.07	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.05	-0.09	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	0.00	0.00	0.00
H	-0.76	0.60	0.21
	-971.9290		

TS1b⁺ (TS of N@C₆₀H⁺ → NH⁺@C₆₀ by breaking [6,6]-bond, doublet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,2)\DRAL\02-Aug-201
0\0\#P ROMP2/6-31G* Geom=AllCheck Guess=Read SCFCyc=1200 SCF=Tight Po
p=None Name=Dral\TS N@C60H+ -> NH(+ )@C60 via 6-6\1,2\C,-2.407452,2.5
52412,-0.704477\C,-1.250561,3.035453,-1.421829\C,-1.042796,2.171147,-2
.576626\C,-2.112501,1.187879,-2.596497\C,-2.951068,1.416754,-1.431396\
C,-2.408364,2.553767,0.696745\C,-0.157981,3.545232,-0.730255\C,0.24835
5,1.809475,-2.960069\C,-1.852035,-0.113467,-3.020967\C,-3.478841,0.335
18,-0.730744\C,-1.252455,3.038197,1.414715\C,1.199065,3.229049,-1.1838
47\C,0.510729,0.462636,-3.414167\C,-2.421097,-1.244155,-2.301931\C,-3.
47983,0.336623,0.725801\C,-2.95295,1.419543,1.425094\C,-0.158925,3.546
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,0.000856\C,-2.424198,-1.23959,2.301286\C,-1.28856,-3.118982,-1.172497
\C,1.009919,-2.211275,-2.592409\C,3.318957,0.923468,-1.177271\C,1.4137
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UB3LYP/6-31G(d)



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C	-1.042796000	2.171147000	-2.576626000
C	-2.112501000	1.187879000	-2.596497000
C	-2.951068000	1.416754000	-1.431396000
C	-2.408364000	2.553767000	0.696745000
C	-0.157981000	3.545232000	-0.730255000
C	0.248355000	1.809475000	-2.960069000
C	-1.852035000	-0.113467000	-3.020967000
C	-3.478841000	0.335180000	-0.730744000
C	-1.252455000	3.038197000	1.414715000
C	1.199065000	3.229049000	-1.183847000
C	0.510729000	0.462636000	-3.414167000
C	-2.421097000	-1.244155000	-2.301931000
C	-3.479830000	0.336623000	0.725801000
C	-2.952950000	1.419543000	1.425094000
C	-0.158925000	3.546585000	0.723635000
C	1.416874000	2.288989000	-2.222935000
C	-0.516631000	-0.481721000	-3.452530000
C	-3.214678000	-1.023624000	-1.175689000
C	-1.046334000	2.176222000	2.571457000
C	1.967209000	3.329768000	-0.001611000
C	0.244283000	1.815295000	2.957273000
C	1.829227000	0.088895000	-2.955372000
C	-1.439516000	-2.311601000	-2.300328000
C	-3.216247000	-1.021284000	1.173629000
C	-2.116045000	1.192981000	2.591738000
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C	-0.263740000	-1.842978000	-3.019776000

C -3.057361000 -1.861165000 -0.000142000
 C -2.110518000 -2.887421000 0.001437000
 C 2.340170000 -2.612730000 0.705149000
 C 2.917745000 -1.501042000 1.423522000
 C 2.077107000 -1.222847000 2.579272000
 C 1.006415000 -2.206055000 2.598035000
 C 1.163587000 -3.060446000 1.432358000
 C 2.341118000 -2.614131000 -0.696935000
 C 3.511412000 -0.452453000 0.729402000
 C 1.825195000 0.094758000 2.957882000
 C -0.267822000 -1.836986000 3.023113000
 C 0.040995000 -3.493842000 0.731648000
 C 2.919704000 -1.503954000 -1.416622000
 C 3.317025000 0.925970000 1.180025000
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 C -1.442618000 -2.307055000 2.302999000
 C 0.041966000 -3.495253000 -0.724833000
 C 1.165491000 -3.063278000 -1.424876000
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 C -0.521331000 -0.474881000 3.453013000
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 C 3.530150000 1.690835000 0.000856000
 C -2.424198000 -1.239590000 2.301286000
 C -1.288560000 -3.118982000 -1.172497000
 C 1.009919000 -2.211275000 -2.592409000
 C 3.318957000 0.923468000 -1.177271000
 C 1.413761000 2.293289000 2.220736000
 C -1.856155000 -0.107502000 3.018997000
 N 0.083708000 0.093951000 -0.005857000
 H 2.621674000 2.405149000 -0.002548000

Zero-point correction= 0.378842 (Hartree/Particle)

Thermal correction to Energy= 0.403433

Thermal correction to Enthalpy= 0.404377

Thermal correction to Gibbs Free Energy= 0.329610

Sum of electronic and zero-point Energies= -2340.499483

Sum of electronic and thermal Energies= -2340.474892

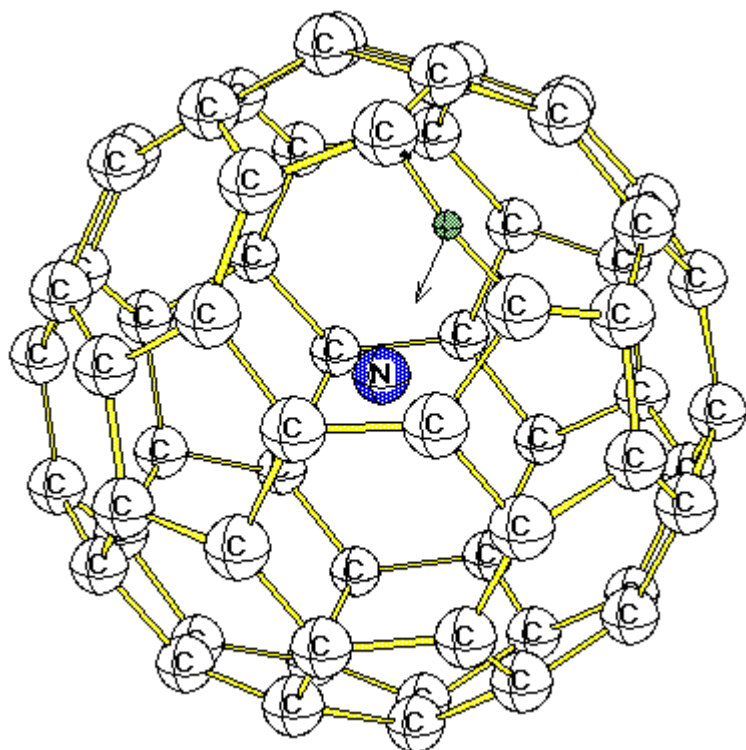
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Sum of electronic and thermal Free Energies= -2340.548715

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 501,1.187879,-2.596497\C,-2.951068,1.416754,-1.431396\C,-2.408364,2.55
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 935\C,3.511412,-0.452453,0.729402\C,1.825195,0.094758,2.957882\C,-0.26
 7822,-1.836986,3.023113\C,0.040995,-3.493842,0.731648\C,2.919704,-1.50
 3954,-1.416622\C,3.317025,0.92597,1.180025\C,0.506067,0.469395,3.41424
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 24198,-1.23959,2.301286\C,-1.28856,-3.118982,-1.172497\C,1.009919,-2.2
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VIBRATIONAL NORMAL MODES



62

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C	-2.408141	2.553977	0.696745
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C	-1.252189	3.038306	1.414715
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C	0.510769	0.462591	-3.414167
C	-2.421206	-1.243943	-2.301931
C	-3.479801	0.336927	0.725801
C	-2.952826	1.419801	1.425094
C	-0.158615	3.546599	0.723635
C	1.417074	2.288865	-2.222935
C	-0.516673	-0.481676	-3.452530
C	-3.214767	-1.023343	-1.175689
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C	0.244442	1.815274	2.957273
C	1.829235	0.088735	-2.955372
C	-1.439718	-2.311475	-2.300328
C	-3.216336	-1.021003	1.173629

-1208.2783

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C 0.01 -0.03 -0.02
C -0.01 0.00 -0.03
C -0.01 -0.01 -0.01
C 0.00 -0.01 -0.01
C 0.02 -0.02 0.00
C 0.04 -0.11 0.01
C 0.00 0.01 0.03
C -0.01 0.00 -0.02
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H -0.04 0.07 -0.08
35.5361

```

TS1e⁺ (TS of endohedrally bound N^{•••}@C₆₀H⁺ → NH^{•••+}@C₆₀ by breaking [5,6]-bond, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

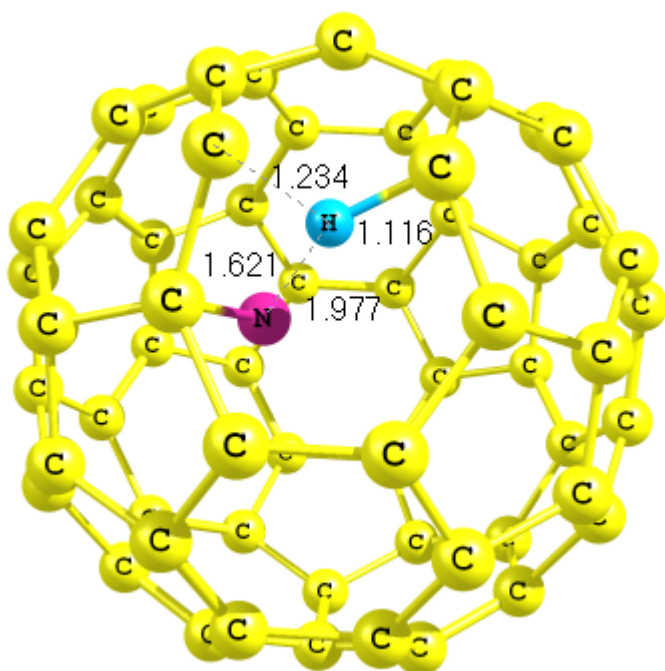
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UB3LYP/6-31G(d)



1 4

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C	1.241094645	2.674354599	-2.062230577
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C	-1.504961430	0.656100432	-3.134654786
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C	1.577862404	3.163611500	-0.798642681
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 C -2.427476964 -1.291105598 -2.070893130
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 C -1.871643183 -1.339991944 2.743470601
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 C 0.390524637 -1.200305469 3.364740305
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 C -2.901699995 -0.723264038 2.008453869
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 C 1.200456711 -2.826164576 1.701803980
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 C -2.000550473 1.496826978 2.567982313
 C -3.346332332 -1.441729471 0.862428401
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 C 2.418933323 -2.053180957 1.559371907
 C 1.485580038 1.002028251 3.161486148
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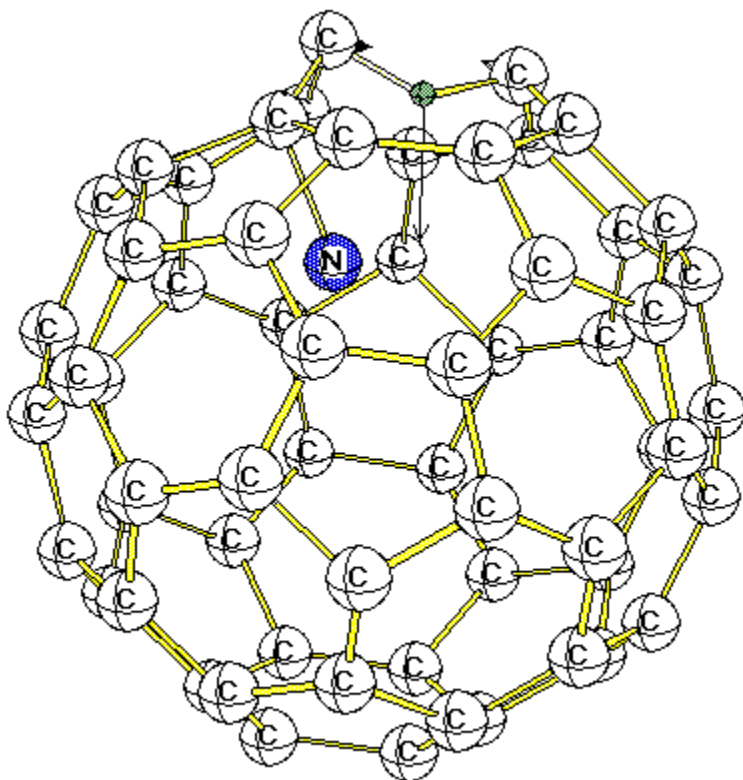
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Thermal correction to Energy= 0.405263
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Thermal correction to Gibbs Free Energy= 0.337499
Sum of electronic and zero-point Energies= -2340.510598
Sum of electronic and thermal Energies= -2340.488219
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VIBRATIONAL NORMAL MODES



62

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[illegible]

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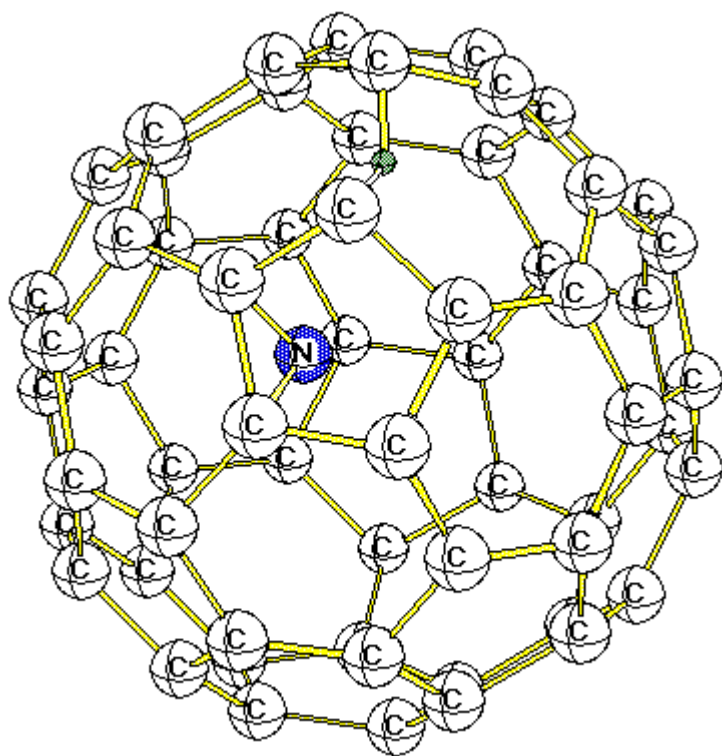
TS1f⁺ (TS of endohedrally bound N^{•••}@C₆₀H⁺ → NH^{•••+}@C₆₀ by breaking [6,6]-bond, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN091\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\27-Mar-201
 0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCFCyc=1200 Nam
 e=Dral\TS endo-N@C60H(+) -> NH(+)@C60 via breaking 6-6 bond\1,4\C,0.
 90338156,3.33678071,0.985028023\C,-0.417173477,3.191586712,1.563145102
 \C,-0.328962832,2.280864109,2.687677197\C,1.062815889,1.89275668,2.828
 837989\C,1.825172828,2.540905053,1.775399562\C,1.052278661,3.413181737
 ,-0.402096241\C,-1.536699851,3.157499393,0.745594024\C,-1.348211827,1.
 349722205,2.913877936\C,1.38715695,0.595185774,3.223804914\C,2.8666488
 32,1.859090138,1.145841544\C,-0.115436704,3.335140808,-1.256006759\C,-
 2.642697505,2.257195876,1.042512306\C,-1.00624427,0.008425084,3.334126
 066\C,2.484088537,-0.107833588,2.581296732\C,3.02154683,1.938839326,-0
 .298947703\C,2.132377219,2.696618752,-1.058227034\C,-1.384817834,3.224
 360374,-0.697581622\C,-2.537277519,1.294187087,2.073485203\C,0.3308976
 8,-0.361208209,3.490530637\C,3.208107828,0.511057494,1.559865779\C,0.2
 34575723,2.565780975,-2.442495829\C,-3.285812886,2.025718358,-0.230349
 535\C,-0.6957761,1.691803363,-3.003945739\C,-1.962438959,-0.905277171,
 2.747814079\C,2.110653418,-1.504719622,2.464703828\C,3.458676057,0.637
 185547,-0.774254479\C,1.625007374,2.177762538,-2.317687521\C,-2.381597
 527,2.345223675,-1.30283663\C,-2.940447747,-0.141228684,1.985956596\C,
 0.78288019,-1.663545091,3.034937541\C,3.578467328,-0.243789056,0.37590
 086\C,3.224362796,-1.587783456,0.26540062\C,-0.732256684,-3.3673964,-0
 .971280767\C,-1.665195059,-2.624095556,-1.791713359\C,-0.954601638,-1.
 905561602,-2.809456229\C,0.447207044,-2.283761611,-2.692998424\C,0.583
 394694,-3.180848558,-1.551431942\C,-0.89779097,-3.4155894,0.423993644\C,
 -2.598868947,-1.83571616,-1.023853364\C,-1.314037932,-0.571288785,-3

.206093634\C,1.43597998,-1.339216084,-2.950791695\C,1.694646621,-3.082090488,-0.714935244\C,-2.020070869,-2.752219261,1.120450264\C,-3.053930058,-0.505927626,-1.437985491\C,-0.260545028,0.389943492,-3.479365808\C,2.60932631,-1.256717442,-2.101611752\C,1.531416935,-3.153636283,0.726406218\C,0.256486688,-3.309016194,1.283008176\C,-2.965890802,-2.044042745,0.4016199\C,-2.393528012,0.158589448,-2.572937335\C,1.079201774,0.01772059,-3.362302951\C,2.730401893,-2.104944725,-0.998531434\C,-1.527559236,-2.186150818,2.349216508\C,-3.974771175,-0.034805196,-0.362479888\C,2.98143378,0.141697149,-1.986677428\C,2.475863296,-2.231974123,1.330702141\C,-0.124523923,-2.552095379,2.468292234\C,-3.513784052,-0.762995386,0.849008678\C,-2.03360243,1.558901203,-2.437017373\C,2.039751116,0.923461651,-2.771446162\N,-1.705867338,-0.557985199,-0.656250098\H,-3.277385138,0.893136042,-0.070925867\\Version=AM64L-G03RevD.02\State=4-A\HF=-2326.1330634\MP2=-2334.1622691\RMSD=9.015e-09\Thermal=0.\PG=C01 [X(C60H1N1)]\@

UB3LYP/6-31G(d)



1 4

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C	-0.417173477	3.191586712	1.563145102
C	-0.328962832	2.280864109	2.687677197
C	1.062815889	1.892756680	2.828837989
C	1.825172828	2.540905053	1.775399562
C	1.052278661	3.413181737	-0.402096241
C	-1.536699851	3.157499393	0.745594024
C	-1.348211827	1.349722205	2.913877936
C	1.387156950	0.595185774	3.223804914

C	2.866648832	1.859090138	1.145841544
C	-0.115436704	3.335140808	-1.256006759
C	-2.642697505	2.257195876	1.042512306
C	-1.006244270	0.008425084	3.334126066
C	2.484088537	-0.107833588	2.581296732
C	3.021546830	1.938839326	-0.298947703
C	2.132377219	2.696618752	-1.058227034
C	-1.384817834	3.224360374	-0.697581622
C	-2.537277519	1.294187087	2.073485203
C	0.330897680	-0.361208209	3.490530637
C	3.208107828	0.511057494	1.559865779
C	0.234575723	2.565780975	-2.442495829
C	-3.285812886	2.025718358	-0.230349535
C	-0.695776100	1.691803363	-3.003945739
C	-1.962438959	-0.905277171	2.747814079
C	2.110653418	-1.504719622	2.464703828
C	3.458676057	0.637185547	-0.774254479
C	1.625007374	2.177762538	-2.317687521
C	-2.381597527	2.345223675	-1.302836630
C	-2.940447747	-0.141228684	1.985956596
C	0.782880190	-1.663545091	3.034937541
C	3.578467328	-0.243789056	0.375900860
C	3.224362796	-1.587783456	0.265400620
C	-0.732256684	-3.367396400	-0.971280767
C	-1.665195059	-2.624095556	-1.791713359
C	-0.954601638	-1.905561602	-2.809456229
C	0.447207044	-2.283761611	-2.692998424
C	0.583394694	-3.180848558	-1.551431942
C	-0.897790970	-3.415589400	0.423993644
C	-2.598868947	-1.835716160	-1.023853364
C	-1.314037932	-0.571288785	-3.206093634
C	1.435979980	-1.339216084	-2.950791695
C	1.694646621	-3.082090488	-0.714935244
C	-2.020070869	-2.752219261	1.120450264
C	-3.053930058	-0.505927626	-1.437985491
C	-0.260545028	0.389943492	-3.479365808
C	2.609326310	-1.256717442	-2.101611752
C	1.531416935	-3.153636283	0.726406218
C	0.256486688	-3.309016194	1.283008176
C	-2.965890802	-2.044042745	0.401619900
C	-2.393528012	0.158589448	-2.572937335
C	1.079201774	0.017720590	-3.362302951
C	2.730401893	-2.104944725	-0.998531434
C	-1.527559236	-2.186150818	2.349216508
C	-3.974771175	-0.034805196	-0.362479888
C	2.981433780	0.141697149	-1.986677428
C	2.475863296	-2.231974123	1.330702141
C	-0.124523923	-2.552095379	2.468292234
C	-3.513784052	-0.762995386	0.849008678
C	-2.033602430	1.558901203	-2.437017373

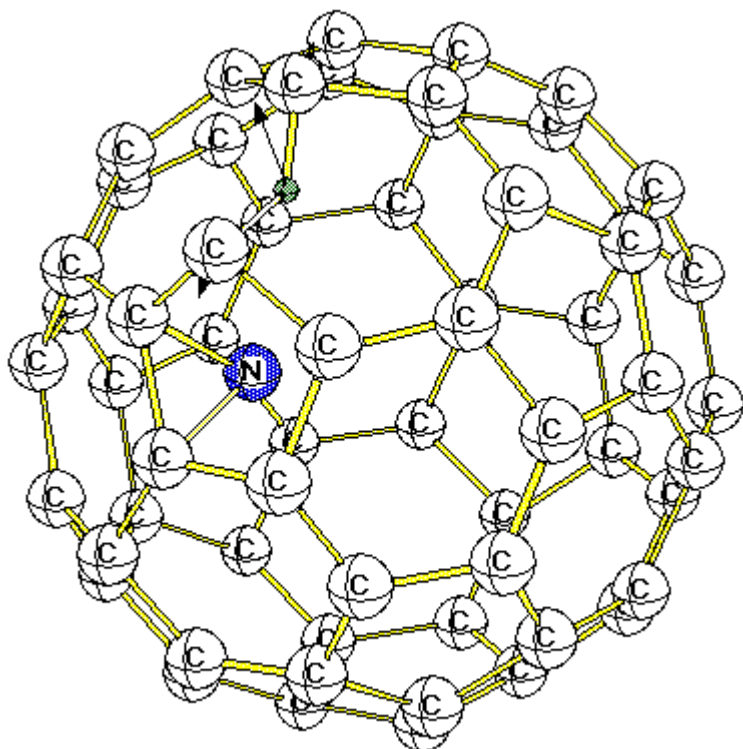
C 2.039751116 0.923461651 -2.771446162
 N -1.705867338 -0.557985199 -0.656250098
 H -3.277385138 0.893136042 -0.070925867

Zero-point correction= 0.379780 (Hartree/Particle)
 Thermal correction to Energy= 0.402533
 Thermal correction to Enthalpy= 0.403477
 Thermal correction to Gibbs Free Energy= 0.334082
 Sum of electronic and zero-point Energies= -2340.479930
 Sum of electronic and thermal Energies= -2340.457177
 Sum of electronic and thermal Enthalpies= -2340.456233
 Sum of electronic and thermal Free Energies= -2340.525628

1\1\FAU-CCC-CCDN089\Freq\UB3LYP/6-31G(d)\C60H1N1(1+,4)\DRAL\09-Sep-200
 9\0\#P POP=NONE SCFCYC=600 B3LYP/6-31G* Freq=NoRaman NAME=DRAL\TS en
 do-N@C60H(+) -> NH(+)@C60 via breaking 6-6 bond\1,4\C,0.90338156,3.33
 678071,0.985028023\C,-0.417173477,3.191586712,1.563145102\C,-0.3289628
 32,2.280864109,2.687677197\C,1.062815889,1.89275668,2.828837989\C,1.82
 5172828,2.540905053,1.775399562\C,1.052278661,3.413181737,-0.402096241
 \C,-1.536699851,3.157499393,0.745594024\C,-1.348211827,1.349722205,2.9
 13877936\C,1.38715695,0.595185774,3.223804914\C,2.866648832,1.85909013
 8,1.145841544\C,-0.115436704,3.335140808,-1.256006759\C,-2.642697505,2
 .257195876,1.042512306\C,-1.00624427,0.008425084,3.334126066\C,2.48408
 8537,-0.107833588,2.581296732\C,3.02154683,1.938839326,-0.298947703\C,
 2.132377219,2.696618752,-1.058227034\C,-1.384817834,3.224360374,-0.697
 581622\C,-2.537277519,1.294187087,2.073485203\C,0.33089768,-0.36120820
 9,3.490530637\C,3.208107828,0.511057494,1.559865779\C,0.234575723,2.56
 5780975,-2.442495829\C,-3.285812886,2.025718358,-0.230349535\C,-0.6957
 761,1.691803363,-3.003945739\C,-1.962438959,-0.905277171,2.747814079\C
 ,2.110653418,-1.504719622,2.464703828\C,3.458676057,0.637185547,-0.774
 254479\C,1.625007374,2.177762538,-2.317687521\C,-2.381597527,2.3452236
 75,-1.30283663\C,-2.940447747,-0.141228684,1.985956596\C,0.78288019,-1
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 -1.665195059,-2.624095556,-1.791713359\C,-0.954601638,-1.905561602,-2.
 809456229\C,0.447207044,-2.283761611,-2.692998424\C,0.583394694,-3.180
 848558,-1.551431942\C,-0.89779097,-3.4155894,0.423993644\C,-2.59886894
 7,-1.83571616,-1.023853364\C,-1.314037932,-0.571288785,-3.206093634\C,
 1.43597998,-1.339216084,-2.950791695\C,1.694646621,-3.082090488,-0.714
 935244\C,-2.020070869,-2.752219261,1.120450264\C,-3.053930058,-0.50592
 7626,-1.437985491\C,-0.260545028,0.389943492,-3.479365808\C,2.60932631
 ,-1.256717442,-2.101611752\C,1.531416935,-3.153636283,0.726406218\C,0.
 256486688,-3.309016194,1.283008176\C,-2.965890802,-2.044042745,0.40161
 99\C,-2.393528012,0.158589448,-2.572937335\C,1.079201774,0.01772059,-3
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 3378,0.141697149,-1.986677428\C,2.475863296,-2.231974123,1.330702141\C
 ,-0.124523923,-2.552095379,2.468292234\C,-3.513784052,-0.762995386,0.8
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 \\0.00000549,0.00000971,-0.00001249,0.00000785,0.00000921,-0.00001329,
 69,-0.00012008,0.00000257,0.00008150\\\\@

Vibrational Normal Modes



62

C	0.891704	3.339913	0.985132
C	-0.428338	3.190121	1.563249
C	-0.336956	2.279711	2.687781
C	1.056166	1.896453	2.828942
C	1.816261	2.547252	1.775503
C	1.040334	3.416832	-0.401993
C	-1.547739	3.152136	0.745698
C	-1.352957	1.345026	2.913981
C	1.385023	0.600019	3.223908
C	2.860105	1.869068	1.145945
C	-0.127103	3.334725	-1.255903
C	-2.650594	2.247986	1.042616
C	-1.006320	0.004928	3.334230
C	2.484396	-0.099176	2.581400
C	3.014724	1.949356	-0.298844
C	2.122921	2.704034	-1.058123

C	-1.396090	3.219525	-0.697478
C	-2.541822	1.285351	2.073589
C	0.332101	-0.360047	3.490634
C	3.206256	0.522232	1.559969
C	0.225587	2.566589	-2.442392
C	-3.292900	2.014271	-0.230246
C	-0.701716	1.689377	-3.003842
C	-1.959328	-0.912099	2.747918
C	2.115827	-1.497354	2.464807
C	3.456383	0.649232	-0.774151
C	1.617361	2.183415	-2.317584
C	-2.389803	2.336923	-1.302733
C	-2.939991	-0.151460	1.986060
C	0.788615	-1.660802	3.035041
C	3.579242	-0.231320	0.376004
C	3.229819	-1.576539	0.265504
C	-0.720579	-3.369919	-0.971177
C	-1.656100	-2.629872	-1.791610
C	-0.948013	-1.908868	-2.809353
C	0.455104	-2.282184	-2.692895
C	0.594415	-3.178791	-1.551328
C	-0.885945	-3.418688	0.424097
C	-2.592514	-1.844748	-1.023750
C	-1.312094	-0.575854	-3.205990
C	1.440582	-1.334201	-2.950688
C	1.705316	-3.076164	-0.714832
C	-2.010528	-2.759230	1.120554
C	-3.052203	-0.516552	-1.437882
C	-0.261954	0.389040	-3.479262
C	2.613634	-1.247617	-2.101508
C	1.542336	-3.148278	0.726510
C	0.267955	-3.308096	1.283112
C	-2.958808	-2.054352	0.401723
C	-2.394119	0.150260	-2.572834
C	1.079081	0.021485	-3.362199
C	2.737662	-2.095418	-0.998428
C	-1.519990	-2.191450	2.349320
C	-3.974679	-0.048639	-0.362376
C	2.980869	0.152085	-1.986574
C	2.483568	-2.223333	1.330806
C	-0.115689	-2.552507	2.468396
C	-3.511159	-0.775220	0.849112
C	-2.039071	1.551817	-2.436914
C	2.036470	0.930565	-2.771343
N	-1.703967	-0.563915	-0.656147
H	-3.280528	0.881725	-0.070822

NORMALMODES 180

C 0.00 0.00 0.00

C 0.00 0.00 0.00

[illegible]

```

C 0.00 0.00 0.00
C -0.03 -0.16 -0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 -0.02 -0.01
C 0.00 0.00 0.01
C 0.00 0.00 0.00
N -0.02 0.01 0.01
H -0.94 0.22 0.07
-895.2452

```

TS1g⁺ (TS of N@C₆₀H⁺ → endohedrally bound N@C₆₀H⁺, quartet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

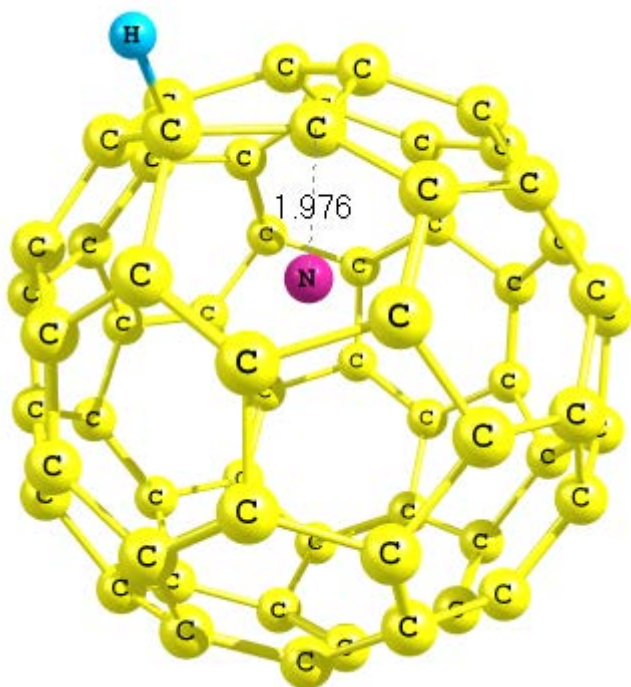
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S of N@C60H(+) -> endo-N@C60H(+) quartet DFT SP\1,4\C,0,1.028393221,0
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088508\C,0,2.026786486,1.429553558,-2.566748681\C,0,1.02841442,-0.7025
53419,-3.33377681\C,0,-1.426499203,0.731399584,-3.161783628\C,0,-0.995
479811,3.057320482,-1.523619383\C,0,1.729723905,3.028111524,-0.7119566
16\C,0,2.97590092,0.728931189,-1.827367854\C,0,-0.218000364,-1.4310257
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57,3.491869869,-0.184301179\C,0,2.730239398,2.304650996,0.050630689\C,
0,2.975922829,-0.728871003,-1.827355809\C,0,2.026829712,-1.429534358,-
2.566725106\C,0,-1.426477213,-0.731495154,-3.161771833\C,0,-2.23819432
4,2.330295302,-1.42192669\C,0,0.699918598,3.482962557,0.211048385\C,0,
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3.332297264\C,0,-1.944635529,-1.430843687,2.580669128\C,0,-1.314897835
,-2.60530359,2.019470384\C,0,0.080671304,-2.605519415,2.431320876\C,0,
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2285908\C,0,-2.910461387,-0.732349852,1.83862527\C,0,-1.665819592,-3.0
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626728,-0.728196478,3.156961652\C,0,-1.944678868,1.430826833,2.5806456
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UB3LYP/6-31G(d)

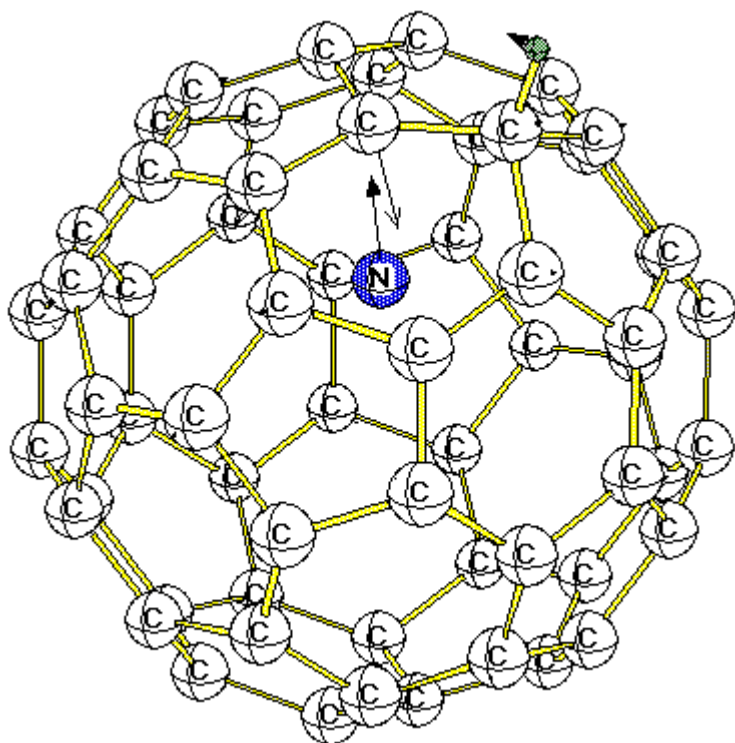


Zero-point correction=	0.386014 (Hartree/Particle)
Thermal correction to Energy=	0.408035
Thermal correction to Enthalpy=	0.408979
Thermal correction to Gibbs Free Energy=	0.340688
Sum of electronic and zero-point Energies=	-2340.687006
Sum of electronic and thermal Energies=	-2340.664985
Sum of electronic and thermal Enthalpies=	-2340.664041
Sum of electronic and thermal Free Energies=	-2340.732332

1\1\FAU-CCC-CCDH151\Freq\UB3LYP/6-31G(d)\C60H1N1(1+,4)\DRAL\07-Jan-200
 9\0\#P Geom=AllCheck Guess=Read SCRF=Check GenChk UB3LYP/6-31G(d) Fre
 q\TS (N@C60H(+)->endo-N@C60H(+)) quartet\1,4\C,1.0283932207,0.7025
 296937,-3.3337883682\C,-0.2180436697,1.43096555,-3.2449520084\C,-0.002
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VIBRATIONAL NORMAL MODES



62

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C	1.386156	2.604017	-1.997824
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C	1.026580	-0.702565	-3.334318
C	-1.428211	0.731431	-3.160943
C	-0.996231	3.057341	-1.523016
C	1.729427	3.028083	-0.712884
C	2.974937	0.728883	-1.829000
C	-0.219797	-1.431015	-3.244771
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C	-0.634318	3.491881	-0.183900
C	2.730358	2.304603	0.049140
C	2.974934	-0.728919	-1.828990
C	2.025414	-1.429564	-2.567828
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C	-2.238901	2.330337	-1.420627
C	0.700148	3.482950	0.210700
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C	-0.003409	-2.605258	-2.407454
C	-2.886487	-0.000003	-1.531875
C	-0.996245	-3.057356	-1.522978
C	-1.665393	3.034045	0.739678
C	2.316663	2.302832	1.441459
C	3.341390	-1.175411	-0.497140

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C	1.066918	3.034230	1.544164
C	3.565323	-0.000006	0.325020
C	3.172521	0.000003	1.664979
C	-0.944990	-0.701624	3.332865
C	-1.943160	-1.430815	2.581796
C	-1.313758	-2.605285	2.020241
C	0.082042	-2.605526	2.431308
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C	-2.909391	-0.732303	1.840296
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C	-1.943154	1.430856	2.581778
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NORMALMODES 180

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C	-0.01	-0.02	0.02
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C	0.01	0.02	-0.01
C	0.00	0.01	0.00
C	0.00	0.01	0.01
C	0.02	-0.04	-0.01
C	0.09	0.07	0.01

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C 0.00 -0.01 0.01
C 0.00 -0.01 0.01
C -0.02 -0.02 0.02
C -0.01 0.07 -0.03
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C 0.00 0.00 0.00
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C 0.51 0.00 0.43
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C 0.01 0.01 0.00
C -0.03 -0.01 0.02
C 0.00 0.00 0.00
C 0.01 0.00 0.00
C 0.00 0.01 -0.01
C 0.00 0.01 0.00
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C 0.00 0.01 0.00
C -0.03 0.01 0.02
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 C -0.09 -0.11 -0.10
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 C 0.07 0.09 0.06
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 C -0.05 0.08 -0.06
 C -0.03 0.07 -0.05
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 C -0.02 0.07 -0.03
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 C -0.08 0.10 -0.05
 C 0.02 0.07 0.03
 C 0.03 0.07 0.05
 C 0.03 -0.01 0.00

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 C -0.07 0.07 -0.05
 C -0.04 0.08 -0.04
 C 0.05 0.04 0.04
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 C -0.07 0.08 -0.03
 C 0.04 0.08 0.04
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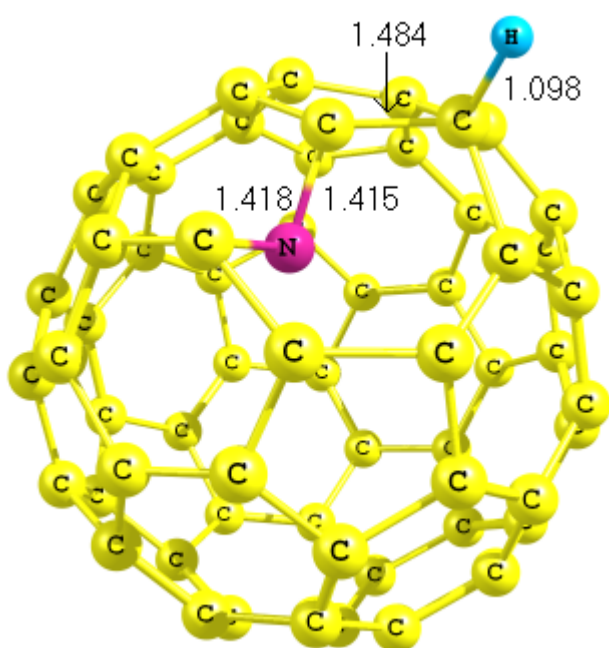
TS1h⁺ (TS of N-escape from quartet N@C₆₀H⁺ by breaking [5,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN085\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\30-Mar-201
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 .754579838,-1.655111907\C,1.729283343,2.78529005,-0.959198131\C,2.9837
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UB3LYP/6-31G(d)



1 4

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C	-0.073337313	2.298595263	-2.572948512
C	1.328851250	2.330607051	-2.218344120
C	1.973938013	1.171466731	-2.807330283
C	1.036835000	-0.973625294	-3.557882358
C	-1.514083102	0.401219250	-3.280536268
C	-1.036085798	2.754579838	-1.655111907
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C	0.734067942	3.228512086	0.001484220
C	3.384992291	0.966681100	-0.793081633
C	0.064997154	-2.889608385	-2.586401248
C	-3.159075944	-0.115314250	-1.543082525
C	-0.884337568	-3.373712345	-1.644148320
C	-1.599561576	2.757309804	0.630101045
C	2.416419527	2.091989080	1.179583126
C	3.423974342	-1.379314031	-0.770143851
C	1.450750919	-2.846610619	-2.202017330
C	-2.425401077	-1.830340637	-2.661942846
C	-2.640213938	2.045495642	-0.067001050
C	1.161998935	2.800746410	1.323426913
C	3.661218448	-0.196953437	0.033772377
C	3.313665841	-0.194326445	1.386143299
C	-0.734558237	-0.933891943	3.219382957
C	-1.747147079	-1.668391575	2.477317858
C	-1.127180580	-2.821073717	1.885166050
C	0.276738674	-2.818356152	2.260746358
C	0.520881961	-1.645906371	3.081452914
C	-0.743557639	0.459191668	3.223760279
C	-2.754918299	-0.994758437	1.773012525
C	-1.533806608	-3.256187152	0.614984341
C	1.250803747	-3.249693403	1.359451372
C	1.716207192	-0.936485495	2.944734165
C	-1.782249539	1.176386878	2.506768012
C	-3.248258346	-1.469831989	0.507587650
C	-0.500232186	-3.714180338	-0.306320423
C	2.493426002	-2.515322158	1.216155146
C	1.702892186	0.516790623	2.939174640
C	0.494175329	1.199976626	3.078531467
C	-2.767388429	0.472141096	1.811077152
C	-2.628597142	-2.617728636	-0.094035894
C	0.848482112	-3.707249070	0.049520710
C	2.717227642	-1.376395866	1.987412390
C	-1.192895976	2.350586823	1.908120688
C	-3.843385432	-0.201931178	-0.228603813
C	2.853631069	-2.518287182	-0.193487270
C	2.685563283	0.973265111	1.974273195
C	0.216062351	2.365297999	2.254467517
C	-3.255760884	0.964897299	0.563034006
C	-2.206442538	-2.803529639	-1.601876114
C	1.835747752	-3.249469954	-0.913626469
N	-2.080204913	-1.031253590	-1.542032087
H	-4.939300014	-0.198890181	-0.289021695

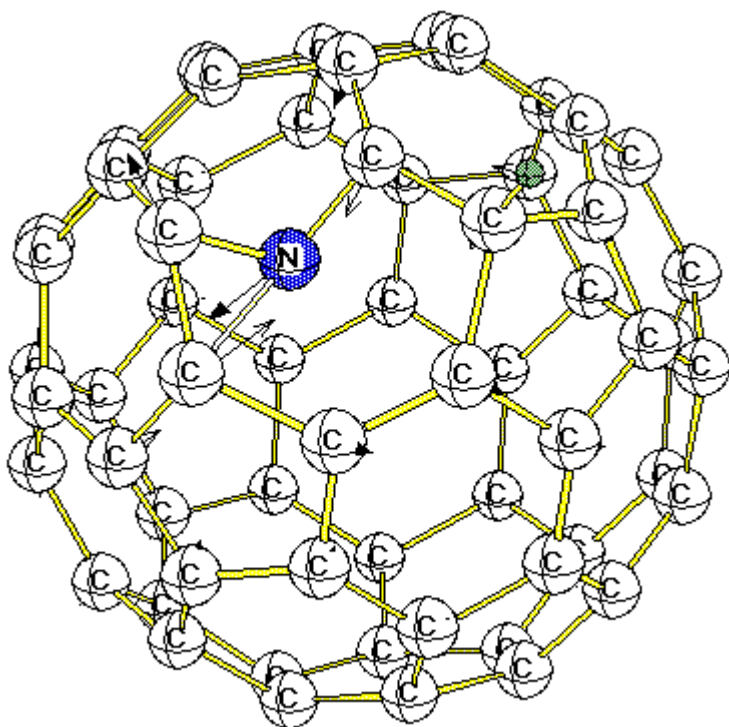
Zero-point correction=	0.382514 (Hartree/Particle)
Thermal correction to Energy=	0.404885
Thermal correction to Enthalpy=	0.405829

Thermal correction to Gibbs Free Energy= 0.336530
 Sum of electronic and zero-point Energies= -2340.563521
 Sum of electronic and thermal Energies= -2340.541150
 Sum of electronic and thermal Enthalpies= -2340.540206
 Sum of electronic and thermal Free Energies= -2340.609505

1\1\FAU-CCC-CCDH154\Freq\UB3LYP\6-31G(d)\C60H1N1(1+,4)\DRAL\19-Jul-2009\0\#P B3LYP/6-31G* Freq=NoRaman Pop=None Name=Dral\TS of N-escape from NatC60H(+) quartet\1,4\C,0.972969846,0.421299603,-3.534236218\C,-0.312248794,1.109731097,-3.375552299\C,-0.073337313,2.298595263,-2.572948512\C,1.32885125,2.330607051,-2.21834412\C,1.973938013,1.171466731,-2.807330283\C,1.036835,-0.973625294,-3.557882358\C,-1.514083102,0.40121925,-3.280536268\C,-1.036085798,2.754579838,-1.655111907\C,1.729283343,2.78529005,-0.959198131\C,2.98377274,0.503681415,-2.107578412\C,-0.178778672,-1.74275259,-3.491163675\C,-2.542351356,0.929238281,-2.312300835\C,-0.6147591,3.209190672,-0.337213569\C,2.770642298,2.087753356,-0.231722861\C,3.017902448,-0.947959542,-2.097398214\C,2.059337289,-1.669429111,-2.80035688\C,-1.418506748,-1.093605001,-3.459290148\C,-2.287448901,2.066608844,-1.520879248\C,0.734067942,3.228512086,0.00148422\C,3.384992291,0.9666811,-0.793081633\C,0.064997154,-2.889608385,-2.586401248\C,-3.159075944,-0.11531425,-1.543082525\C,-0.884337568,-3.373712345,-1.64414832\C,-1.599561576,2.757309804,0.630101045\C,2.416419527,2.09198908,1.179583126\C,3.423974342,-1.379314031,-0.770143851\C,1.450750919,-2.846610619,-2.20201733\C,-2.425401077,-1.830340637,-2.661942846\C,-2.640213938,2.045495642,-0.06700105\C,1.161998935,2.80074641,1.323426913\C,3.661218448,-0.196953437,0.033772377\C,3.313665841,-0.194326445,1.386143299\C,-0.734558237,-0.933891943,3.219382957\C,-1.747147079,-1.668391575,2.477317858\C,-1.12718058,-2.821073717,1.88516605\C,0.276738674,-2.818356152,2.260746358\C,0.520881961,-1.645906371,3.081452914\C,-0.743557639,0.459191668,3.223760279\C,-2.754918299,-0.994758437,1.773012525\C,-1.533806608,-3.256187152,0.614984341\C,1.250803747,-3.249693403,1.359451372\C,1.716207192,-0.936485495,2.944734165\C,-1.782249539,1.176386878,2.506768012\C,-3.248258346,-1.469831989,0.50758765\C,-0.500232186,-3.714180338,-0.306320423\C,2.493426002,-2.515322158,1.216155146\C,1.702892186,0.516790623,2.93917464\C,0.494175329,1.199976626,3.078531467\C,-2.767388429,0.472141096,1.811077152\C,-2.628597142,-2.617728636,-0.094035894\C,0.848482112,-3.70724907,0.04952071\C,2.717227642,-1.376395866,1.98741239\C,-1.192895976,2.350586823,1.908120688\C,-3.843385432,-0.201931178,-0.228603813\C,2.853631069,-2.518287182,-0.19348727\C,2.685563283,0.973265111,1.974273195\C,0.216062351,2.365297999,2.254467517\C,-3.255760884,0.964897299,0.563034006\C,-2.206442538,-2.803529639,-1.601876114\C,1.835747752,-3.249469954,-0.913626469\C,-2.080204913,-1.03125359,-1.542032087\C,-4.939300014,-0.198890181,-0.289021695\Version=AM64L-G03RevD.02\State=4-A\HF=-2340.9460347\S2=3.826665\S2-1=0.\S2A=3.75263\RMSD=6.833e-09\RMSF=3.157e-05\ZeroPoint=0.3825139\Thermal=0.4048846\ZPE=240.0310728\Dipole=-1.1744382,-0.6561409,-0.7086594\DipoleDeriv=0.1050475,-0.0078095,0.074562,0.0822634,0.024026,0.06158,-0.0082849,0.0622228,0.0078922,-0.0334011,-0.0145408,0.097778\Polar=509.8668484,7.5905933,482.2699015,7.036172,6.2676471,492.1899994\PG=C01[X(C60H1N1)]\NImag=1\0.48596540,-0.02279086,0.66507458,0.08053077,0.

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00011462,0.00004494,-0.00004037,-0.00000422,-0.00000230,0.00002038\\\\@

Vibrational Normal Modes



62

C	0.468343	-2.375314	2.580504
C	1.397909	-1.294724	2.925666
C	0.608155	-0.191123	3.448162
C	-0.786878	-0.571389	3.401452
C	-0.874298	-1.916403	2.862987
C	0.701107	-3.188755	1.469383
C	2.560411	-1.065554	2.183040
C	0.977037	1.142249	3.196612
C	-1.766276	0.372063	3.080189
C	-1.929519	-2.260749	2.012522
C	1.899923	-3.006320	0.692671
C	2.951318	0.372716	1.954582
C	-0.045752	2.116992	2.843311
C	-2.855153	0.016163	2.192558
C	-1.673522	-3.068149	0.833072
C	-0.384234	-3.514086	0.564014
C	2.851055	-2.056641	1.083559
C	2.162499	1.432834	2.443304
C	-1.384376	1.743203	2.790471
C	-2.934789	-1.274511	1.666089
C	1.529824	-3.119042	-0.736881
C	3.378065	0.617653	0.605127
C	2.064591	-2.292128	-1.763367

C	0.503235	2.995416	1.825119
C	-3.142774	1.164915	1.347028
C	-2.509547	-2.567389	-0.245291
C	0.134453	-3.464951	-0.793445
C	3.548744	-1.443245	-0.069417
C	1.860578	2.596633	1.552761
C	-2.238162	2.232181	1.720149
C	-3.297085	-1.465684	0.271017
C	-3.565238	-0.361956	-0.541131
C	-0.621833	2.370732	-2.581872
C	0.734372	1.915224	-2.843991
C	0.669183	0.583113	-3.377760
C	-0.730427	0.200548	-3.460176
C	-1.529206	1.305326	-2.960954
C	-0.894484	3.144494	-1.455935
C	1.788535	2.258666	-1.985959
C	1.654822	-0.354411	-3.034840
C	-1.121259	-1.112939	-3.197137
C	-2.668427	1.050589	-2.194107
C	0.183652	3.517289	-0.558174
C	2.856709	1.342355	-1.686361
C	1.225283	-1.723884	-2.776234
C	-2.304437	-1.380287	-2.401802
C	-2.945091	1.852533	-1.014038
C	-2.073808	2.881579	-0.654744
C	1.489868	3.098118	-0.819976
C	2.794855	0.006418	-2.210806
C	-0.118045	-2.092492	-2.849035
C	-3.057543	-0.319058	-1.903099
C	-0.317328	3.475147	0.795231
C	3.441188	1.800772	-0.289234
C	-2.023059	-2.529931	-1.555639
C	-3.494140	0.979299	0.006281
C	-1.711369	3.076492	0.739906
C	2.352622	2.724203	0.254627
C	3.099835	-1.340762	-1.450272
C	-0.672157	-2.965900	-1.828238
N	2.608349	-0.381897	-0.036235
H	4.433828	2.264452	-0.355221

NORMALMODES 180

C	0.00	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.02	0.01
C	0.00	0.01	0.00
C	0.01	0.01	0.00
C	0.00	0.01	-0.01
C	-0.01	0.00	0.02
C	0.01	0.00	0.00
C	0.00	0.01	0.00

C 0.00 0.01 0.00
C -0.03 0.02 0.01
C -0.04 -0.05 -0.11
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 -0.01
C 0.00 0.00 -0.01
C -0.02 0.02 0.02
C 0.01 0.00 -0.04
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.02 -0.01
C -0.18 -0.14 -0.15
C -0.12 0.14 0.15
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.01 -0.01 -0.01
C -0.01 0.00 -0.02
C 0.46 -0.12 0.20
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.01 0.01 -0.01
C 0.01 0.01 0.00
C 0.01 0.00 0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.03 -0.01
C 0.03 0.02 0.01
C 0.01 -0.01 0.01
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.01 0.07 -0.04
C 0.03 0.02 0.05
C 0.00 -0.01 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.01 0.00
C 0.05 0.11 -0.07
C -0.01 -0.02 0.01
C 0.00 0.00 0.01
C 0.00 0.00 0.00
C -0.07 -0.07 -0.03
C -0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 -0.01
C -0.12 0.39 0.31

C 0.00 -0.02 -0.02
 N -0.04 -0.41 -0.25
 H -0.01 -0.17 0.07
 -442.3826

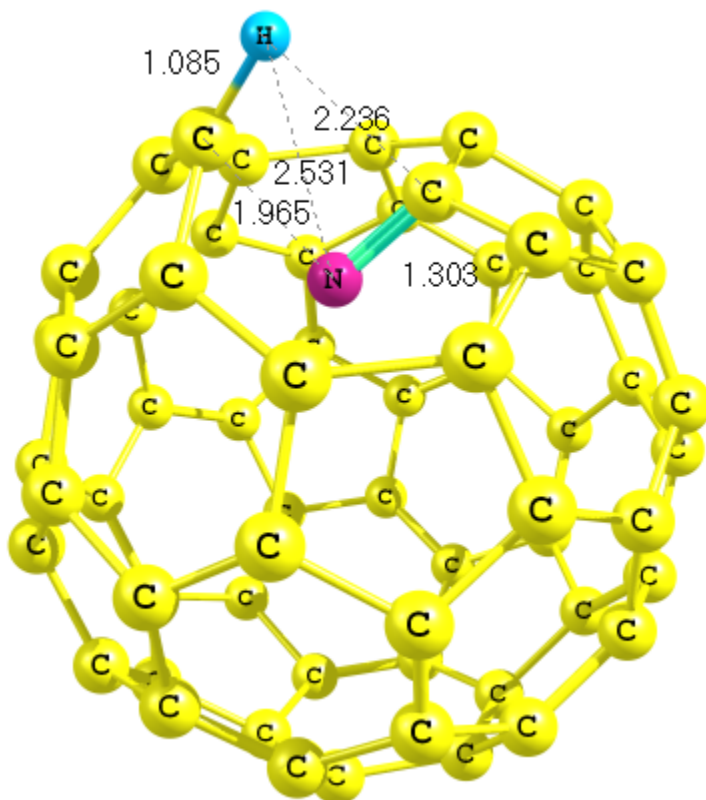
TS1i⁺ (TS of N-escape from quartet N@C₆₀H⁺ by breaking [6,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN085\SP\ROMP2-FC\6-31G(d)\C60H1N1(1+,4)\DRAL\30-Mar-201
 0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCF=VShift SCFC
 yc=1200 Name=Dral\TS N-escape from N@C60H(+) via 6,6-bond quartet ROM
 P2//DFT\1,4\C,0,2.388912796,-2.62810888,-0.619402425\C,0,1.229721231,
 -3.119095534,-1.354154693\C,0,1.038078915,-2.266008232,-2.51969927\C,0,
 2.125164025,-1.3059406,-2.538895654\C,0,2.957350249,-1.526650144,-1.3
 66130324\C,0,2.379530943,-2.592943657,0.781738587\C,0,0.119157736,-3.6
 05498479,-0.667037859\C,0,-0.246197184,-1.876541267,-2.96897175\C,0,1.
 905543174,-0.008895125,-2.999438242\C,0,3.514465692,-0.439278748,-0.69
 2155357\C,0,1.210543245,-3.046949568,1.5245935\C,0,-1.176637866,-3.193
 485142,-1.175373766\C,0,-0.47157875,-0.519335395,-3.418520164\C,0,2.50
 5410512,1.121353371,-2.310406921\C,0,3.5048087,-0.402916496,0.75992035
 5\C,0,2.938401078,-1.455361384,1.479961405\C,0,0.109068278,-3.56748836
 3,0.847845582\C,0,-1.424274514,-2.318321015,-2.264779187\C,0,0.5839038
 29,0.38987771,-3.45149874\C,0,3.290612348,0.910811144,-1.174554231\C,0,
 1.003661617,-2.136692505,2.643324489\C,0,-1.666258574,-2.663798988,0.
 055292111\C,0,-0.286328729,-1.725617114,3.05528994\C,0,-1.794565906,-0
 .099949001,-2.971123718\C,0,1.558897112,2.220441031,-2.344638861\C,0,3
 .275013785,0.969562025,1.171152754\C,0,2.090756807,-1.176518292,2.6290
 29572\C,0,-1.193204297,-3.130987758,1.317545142\C,0,-2.444033198,-1.18
 0522653,-2.257033652\C,0,0.375939908,1.769663336,-3.056964512\C,0,3.15
 0094884,1.78377456,-0.023714822\C,0,2.236543152,2.839683414,-0.0562420
 63\C,0,-2.21767816,2.728789656,0.617250696\C,0,-2.837810598,1.6531365,
 1.355344573\C,0,-2.026113912,1.373647904,2.521353473\C,0,-0.923057083,
 2.317473009,2.52440772\C,0,-1.038640393,3.156885051,1.343518521\C,0,-2
 .208359653,2.69372709,-0.782757597\C,0,-3.488758182,0.615405225,0.6949
 64281\C,0,-1.83398759,0.04829818,2.948019198\C,0,0.335788518,1.9205794
 74,2.969191505\C,0,0.103499978,3.53817217,0.641296288\C,0,-2.818986113
 ,1.582243999,-1.474332369\C,0,-3.424293388,-0.741121753,1.20443677\C,0
 ,-0.517240788,-0.347737872,3.433444482\C,0,1.528291108,2.335540396,2.2
 51044119\C,0,0.11321388,3.501649797,-0.816263197\C,0,-1.019612712,3.08
 534629,-1.513727794\C,0,-3.478982957,0.578636927,-0.771570225\C,0,-2.4
 74212285,-1.066810204,2.280187687\C,0,0.538011091,0.56232704,3.4350561
 82\C,0,1.415450235,3.126942474,1.105965975\C,0,-1.991926659,1.24504818
 2,-2.613928746\C,0,-3.664535249,-1.570396563,0.014869021\C,0,2.4748211
 29,1.236426486,2.284476965\C,0,1.431082901,3.068125686,-1.242218571\C,
 0,-0.888579214,2.187914032,-2.649476549\C,0,-3.407968965,-0.801770196,
 -1.211521095\C,0,-1.455022697,-2.202385321,2.358322466\C,0,1.86544797,

0.141860869,3.021153654\N,0,-1.710540874,-1.361489328,0.02234735\H,0,-
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 [X(C60H1N1)]\\@

UB3LYP/6-31G(d)



1 4

C	2.388912796	-2.628108880	-0.619402425
C	1.229721231	-3.119095534	-1.354154693
C	1.038078915	-2.266008232	-2.519699270
C	2.125164025	-1.305940600	-2.538895654
C	2.957350249	-1.526650144	-1.366130324
C	2.379530943	-2.592943657	0.781738587
C	0.119157736	-3.605498479	-0.667037859
C	-0.246197184	-1.876541267	-2.968971750
C	1.905543174	-0.008895125	-2.999438242
C	3.514465692	-0.439278748	-0.692155357
C	1.210543245	-3.046949568	1.524593500
C	-1.176637866	-3.193485142	-1.175373766
C	-0.471578750	-0.519335395	-3.418520164
C	2.505410512	1.121353371	-2.310406921
C	3.504808700	-0.402916496	0.759920355
C	2.938401078	-1.455361384	1.479961405
C	0.109068278	-3.567488363	0.847845582
C	-1.424274514	-2.318321015	-2.264779187

C	0.583903829	0.389877710	-3.451498740
C	3.290612348	0.910811144	-1.174554231
C	1.003661617	-2.136692505	2.643324489
C	-1.666258574	-2.663798988	0.055292111
C	-0.286328729	-1.725617114	3.055289940
C	-1.794565906	-0.099949001	-2.971123718
C	1.558897112	2.220441031	-2.344638861
C	3.275013785	0.969562025	1.171152754
C	2.090756807	-1.176518292	2.629029572
C	-1.193204297	-3.130987758	1.317545142
C	-2.444033198	-1.180522653	-2.257033652
C	0.375939908	1.769663336	-3.056964512
C	3.150094884	1.783774560	-0.023714822
C	2.236543152	2.839683414	-0.056242063
C	-2.217678160	2.728789656	0.617250696
C	-2.837810598	1.653136500	1.355344573
C	-2.026113912	1.373647904	2.521353473
C	-0.923057083	2.317473009	2.524407720
C	-1.038640393	3.156885051	1.343518521
C	-2.208359653	2.693727090	-0.782757597
C	-3.488758182	0.615405225	0.694964281
C	-1.833987590	0.048298180	2.948019198
C	0.335788518	1.920579474	2.969191505
C	0.103499978	3.538172170	0.641296288
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C	-3.424293388	-0.741121753	1.204436770
C	-0.517240788	-0.347737872	3.433444482
C	1.528291108	2.335540396	2.251044119
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C	-1.019612712	3.085346290	-1.513727794
C	-3.478982957	0.578636927	-0.771570225
C	-2.474212285	-1.066810204	2.280187687
C	0.538011091	0.562327040	3.435056182
C	1.415450235	3.126942474	1.105965975
C	-1.991926659	1.245048182	-2.613928746
C	-3.664535249	-1.570396563	0.014869021
C	2.474821129	1.236426486	2.284476965
C	1.431082901	3.068125686	-1.242218571
C	-0.888579214	2.187914032	-2.649476549
C	-3.407968965	-0.801770196	-1.211521095
C	-1.455022697	-2.202385321	2.358322466
C	1.865447970	0.141860869	3.021153654
N	-1.710540874	-1.361489328	0.022347350
H	-3.901730334	-2.628740454	0.039832989

Zero-point correction=	0.382930 (Hartree/Particle)
Thermal correction to Energy=	0.405222
Thermal correction to Enthalpy=	0.406166
Thermal correction to Gibbs Free Energy=	0.337404
Sum of electronic and zero-point Energies=	-2340.587555

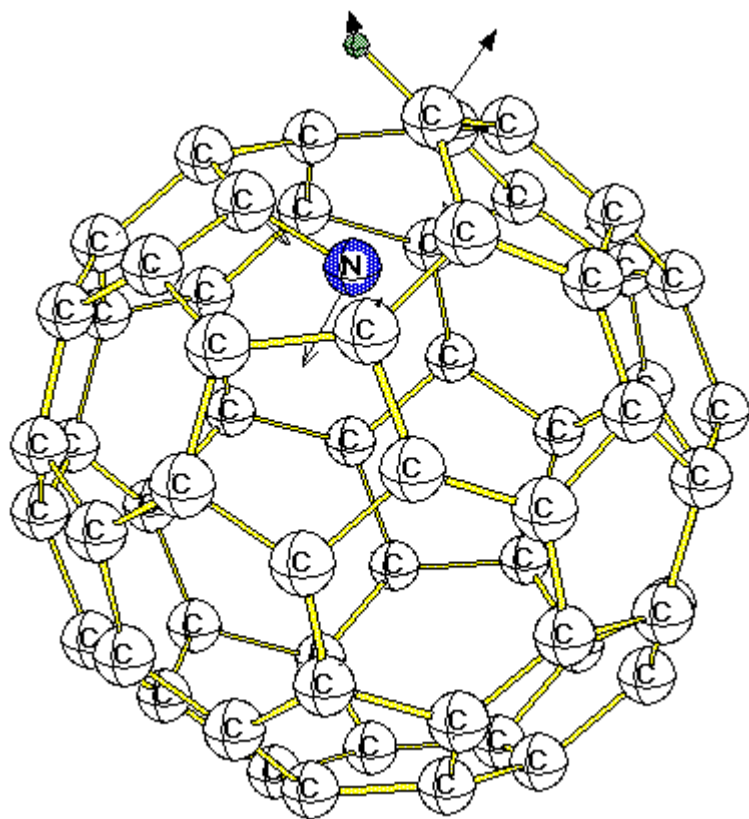
Sum of electronic and thermal Energies= -2340.565262
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VIBRATIONAL NORMAL MODES



62

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C	-3.485473	-0.564951	0.727003
C	-1.089314	-3.130100	-1.441041
C	1.317841	-3.111593	1.245071
C	0.516580	-0.413807	3.426772
C	-2.531959	1.075408	2.299433
C	-3.485930	-0.564246	-0.725560
C	-2.880946	-1.610106	-1.423477
C	0.036653	-3.588078	-0.759388
C	1.535686	-2.200260	2.310930
C	-0.575232	0.451887	3.444760
C	-3.314545	0.804732	1.174566
C	-0.926724	-2.240148	-2.583177
C	1.777932	-2.592953	-0.001590
C	0.342781	-1.786850	-3.014051
C	1.818500	0.048268	2.960046

C	-1.631318	2.212905	2.300116
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C	1.317041	-3.110312	-1.248686
C	2.507666	-1.022134	2.268191
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C	2.763008	1.734833	-1.415271
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C	0.815627	2.290876	-2.586960
C	0.903547	3.163350	-1.427852
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C	1.816693	0.051167	-2.961083
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C	0.904421	3.161972	1.430352
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NORMALMODES 180

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C	0.00	0.00	-0.01
C	0.00	0.00	0.00

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C 0.02 0.00 0.04
C 0.01 0.00 -0.01
C 0.00 -0.01 0.00
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C -0.02 0.01 0.00
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C -0.03 -0.02 -0.01
C 0.05 -0.01 0.02
C 0.01 0.00 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.01
C 0.62 0.02 0.00
C 0.00 -0.01 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
C -0.01 -0.09 -0.10
C -0.02 0.01 0.00
C 0.00 0.00 0.01

N -0.69 0.06 0.00
 H 0.12 -0.11 0.00
 -650.7913
 C -0.06 0.00 0.00
 C -0.04 0.00 -0.03
 C -0.02 0.01 -0.06
 C -0.02 0.02 -0.03
 C -0.05 0.02 -0.01
 C -0.06 0.00 0.00
 C -0.04 -0.04 -0.01
 C 0.00 0.00 -0.11
 C -0.01 0.01 -0.05
 C -0.05 0.03 0.00
 C -0.04 0.00 0.03
 C 0.00 -0.13 0.01
 C 0.00 0.00 -0.13
 C -0.03 0.02 -0.02
 C -0.05 0.03 0.00
 C -0.05 0.02 0.01
 C -0.04 -0.04 0.01
 C 0.00 -0.05 -0.05
 C 0.00 0.00 -0.08
 C -0.05 0.03 0.00
 C -0.02 0.01 0.06
 C 0.21 -0.29 0.00
 C 0.00 0.00 0.11
 C 0.00 -0.01 -0.11
 C -0.02 0.03 -0.02
 C -0.05 0.03 0.00
 C -0.02 0.02 0.03
 C 0.00 -0.13 -0.01
 C 0.05 -0.02 -0.06
 C -0.01 0.01 -0.04
 C -0.05 0.04 0.00
 C -0.04 0.05 0.00
 C -0.01 0.05 0.00
 C -0.02 0.04 0.02
 C -0.02 0.01 0.05
 C -0.02 0.02 0.03
 C -0.02 0.04 0.01
 C -0.01 0.05 0.00
 C 0.00 0.03 0.01
 C 0.00 -0.01 0.11
 C -0.01 0.01 0.04
 C -0.03 0.05 0.00
 C -0.02 0.04 -0.02
 C 0.09 0.02 0.03
 C 0.00 0.00 0.13
 C -0.02 0.03 0.02
 C -0.03 0.05 0.00

```

C -0.02 0.04 -0.01
C 0.00 0.03 -0.01
C 0.05 -0.02 0.06
C 0.00 0.00 0.08
C -0.03 0.05 0.00
C -0.02 0.01 -0.05
C 0.42 0.06 0.00
C -0.03 0.02 0.02
C -0.03 0.05 0.00
C -0.02 0.02 -0.03
C 0.09 0.02 -0.03
C 0.00 -0.05 0.05
C -0.01 0.01 0.05
N 0.21 -0.31 0.00
H 0.51 0.09 0.00

```

TS2a⁺ (TS of NH^{••}@C₆₀H⁺ → NH₂^{••+}@C₆₀ by breaking [5,6]-bond, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```

1\1\FAU-CCC-CCDN090\SP\ROMP2-FC\6-31G(d)\C60H2N1(1+,3)\DRAL\11-Aug-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck Pop=None SCF=Tight SCFCy
c=1200 Name=Dral\TS of NH@C60H(+) -> NH2(+ )@C60 vis breaking 5-6 bond
(triplet)\1,3\C,1.422927856,0.643539429,3.245651245\C,-0.00958252,0.
836807251,3.415390015\C,-0.642745972,-0.461273193,3.404342651\C,0.3931
427,-1.467681885,3.228378296\C,1.669509888,-0.782424927,3.122314453\C,
2.160568237,1.54788208,2.484848022\C,-0.649124146,1.92980957,2.8305358
89\C,-1.893814087,-0.622390747,2.808578491\C,0.140014648,-2.593200684,
2.448043823\C,2.637817383,-1.246185303,2.230163574\C,1.498519897,2.691
78772,1.88130188\C,-1.954071045,1.775436401,2.204391479\C,-2.163665771
,-1.820556641,2.029067993\C,1.144866943,-3.07661438,1.518829346\C,3.40
0558472,-0.30241394,1.429031372\C,3.168777466,1.068161011,1.556030273\
C,0.134246826,2.891052246,2.06980896\C,-2.570800781,0.50944519,2.19277
9541\C,-1.164703369,-2.76789856,1.833267212\C,2.369171143,-2.416122437
,1.410507202\C,2.094543457,2.916748047,0.570663452\C,-1.971542358,2.74
7314453,1.07913208\C,1.304748535,3.33215332,-0.503341675\C,-3.03236389
2,-1.461044312,0.925964355\C,0.461105347,-3.543762207,0.324813843\C,3.
597976685,-0.88684082,0.113143921\C,3.123703003,1.91166687,0.371932983
\C,-0.676727295,3.369644165,0.967468262\C,-3.339874268,-0.059646606,1.
054351807\C,-0.965530396,-3.356430054,0.51612854\C,2.960098267,-2.1936
49292,0.101837158\C,2.304031372,-2.640075684,-1.045883179\C,-1.1226959
23,-0.670776367,-3.198074341\C,-1.36756897,0.751480103,-3.031524658\C,
-0.09463501,1.436737061,-3.179748535\C,0.937835693,0.437316895,-3.4040

```

83252\C,0.302200317,-0.865158081,-3.415405273\C,-1.847579956,-1.598846
 436,-2.455932617\C,-2.346633911,1.220794678,-2.1434021\C,0.185470581,2
 .570343018,-2.420913696\C,2.196594238,0.597625732,-2.823730469\C,0.946
 929932,-1.961776733,-2.843688965\C,-2.866226196,-1.142974854,-1.538253
 784\C,-2.06237793,2.442153931,-1.393081665\C,1.496276855,2.739685059,-
 1.815063477\C,2.867523193,-0.543212891,-2.220336914\C,0.192932129,-2.9
 14413452,-2.044921875\C,-1.177474976,-2.743209839,-1.860900879\C,-3.14
 0655518,0.234848022,-1.412994385\C,-0.807449341,3.077148438,-1.5018768
 31\C,2.477355957,1.768280029,-2.006744385\C,2.254348755,-1.796020508,-
 2.229751587\C,-2.817550659,-1.98890686,-0.35635376\C,-2.652877808,2.54
 9743652,-0.108016968\C,3.555801392,-0.078826904,-1.024505615\C,1.02986
 145,-3.32762146,-0.9324646\C,-1.771820068,-2.975921631,-0.557449341\C,
 -3.597976685,0.614593506,-0.12538147\C,-0.119171143,3.543777466,-0.308
 853149\C,3.31211853,1.348327637,-0.894714355\N,-0.004568359,-0.0119808
 35,0.065994873\H,0.913593628,0.05872229,-0.501219116\H,-2.920852661,1.
 479812622,0.227890015\\Version=AM64L-G03RevD.02\State=3-A\HF=-2326.928
 7773\MP2=-2334.8802566\RMSD=6.437e-09\Thermal=0.\PG=C01 [X(C60H2N1)]\\

UB3LYP/6-31G(d)

Zero-point correction=	0.392398 (Hartree/Particle)
Thermal correction to Energy=	0.416080
Thermal correction to Enthalpy=	0.417024
Thermal correction to Gibbs Free Energy=	0.345275
Sum of electronic and zero-point Energies=	-2341.200839
Sum of electronic and thermal Energies=	-2341.177158
Sum of electronic and thermal Enthalpies=	-2341.176214
Sum of electronic and thermal Free Energies=	-2341.247963

1\1\FAU-CCC-CCDH154\Freq\UB3LYP\6-31G(d)\C60H2N1(1+,3)\DRAL\04-Jun-200
 9\0\#P B3LYP/6-31G* FREQ=NORAMAN POP=NONE NAME=DRAL\TS of NH@C60H(+)
 -> NH2(+)\@C60 vis breaking 5-6 bond (triplet)\1,3\C,1.422927856,0.64
 3539429,3.245651245\C,-0.00958252,0.836807251,3.415390015\C,-0.6427459
 72,-0.461273193,3.404342651\C,0.3931427,-1.467681885,3.228378296\C,1.6
 69509888,-0.782424927,3.122314453\C,2.160568237,1.54788208,2.484848022
 \C,-0.649124146,1.92980957,2.830535889\C,-1.893814087,-0.622390747,2.8
 08578491\C,0.140014648,-2.593200684,2.448043823\C,2.637817383,-1.24618
 5303,2.230163574\C,1.498519897,2.69178772,1.88130188\C,-1.954071045,1.
 775436401,2.204391479\C,-2.163665771,-1.820556641,2.029067993\C,1.1448
 66943,-3.07661438,1.518829346\C,3.400558472,-0.30241394,1.429031372\C,
 3.168777466,1.068161011,1.556030273\C,0.134246826,2.891052246,2.069808
 96\C,-2.570800781,0.50944519,2.192779541\C,-1.164703369,-2.76789856,1.
 833267212\C,2.369171143,-2.416122437,1.410507202\C,2.094543457,2.91674
 8047,0.570663452\C,-1.971542358,2.747314453,1.07913208\C,1.304748535,3
 .33215332,-0.503341675\C,-3.032363892,-1.461044312,0.925964355\C,0.461
 105347,-3.543762207,0.324813843\C,3.597976685,-0.88684082,0.113143921\
 C,3.123703003,1.91166687,0.371932983\C,-0.676727295,3.369644165,0.9674
 68262\C,-3.339874268,-0.059646606,1.054351807\C,-0.965530396,-3.356430

054,0.51612854\C,2.960098267,-2.193649292,0.101837158\C,2.304031372,-2.640075684,-1.045883179\C,-1.122695923,-0.670776367,-3.198074341\C,-1.36756897,0.751480103,-3.031524658\C,-0.09463501,1.436737061,-3.179748535\C,0.937835693,0.437316895,-3.404083252\C,0.302200317,-0.865158081,-3.415405273\C,-1.847579956,-1.598846436,-2.455932617\C,-2.346633911,1.220794678,-2.1434021\C,0.185470581,2.570343018,-2.420913696\C,2.196594238,0.597625732,-2.823730469\C,0.946929932,-1.961776733,-2.843688965\C,-2.866226196,-1.142974854,-1.538253784\C,-2.06237793,2.442153931,-1.393081665\C,1.496276855,2.739685059,-1.815063477\C,2.867523193,-0.543212891,-2.220336914\C,0.192932129,-2.914413452,-2.044921875\C,-1.177474976,-2.743209839,-1.860900879\C,-3.140655518,0.234848022,-1.412994385\C,-0.807449341,3.077148438,-1.501876831\C,2.477355957,1.768280029,-2.006744385\C,2.254348755,-1.796020508,-2.229751587\C,-2.817550659,-1.98890686,-0.35635376\C,-2.652877808,2.549743652,-0.108016968\C,3.555801392,-0.078826904,-1.024505615\C,1.02986145,-3.32762146,-0.9324646\C,-1.771820068,-2.975921631,-0.557449341\C,-3.597976685,0.614593506,-0.12538147\C,-0.119171143,3.543777466,-0.308853149\C,3.31211853,1.348327637,-0.894714355\N,-0.004568359,-0.011980835,0.065994873\H,0.913593628,0.05872229,-0.501219116\H,-2.920852661,1.479812622,0.227890015\\Version=AM64L-G03RevD.02\State=3-A\HF=-2341.5932376\S2=2.005546\S2-1=0.\S2A=2.000008\RMSD=4.241e-09\RMSF=2.724e-03\ZeroPoint=0.3923983\Thermal=0.4160798\ZPE=246.2336643\Dipole=-0.8346605,0.4587719,-0.023339\DipoleDeriv=0.1538192,-0.1340592,-0.00817,0.0055218,-0.0043548,-0.0032456\Polar=482.7004074,-4.3656282,475.2100648,-0.1576848,-0.0700405,465.908641\PG=C01[X(C60H2N1)]\NImag=1\\0.54059817,0.04930430,0.59538865,-0.15148360,-0.562,0.08062775\\0.00024248,-0.00006594,0.00003200,-0.00014691,-0.00005868,-0.00072844\\@

Vibrational Normal Modes

63

C	1.243930	0.704198	3.240491
C	-0.195802	0.840110	3.404653
C	-0.776542	-0.482238	3.391696
C	0.299404	-1.446492	3.220112
C	1.547769	-0.710804	3.118673
C	1.947770	1.637107	2.482163
C	-0.876251	1.906539	2.816911
C	-2.017869	-0.693367	2.791198
C	0.094460	-2.581419	2.439263
C	2.537263	-1.135721	2.230432
C	1.242870	2.753494	1.875622
C	-2.171565	1.699988	2.185824
C	-2.236624	-1.901551	2.011138
C	1.121397	-3.024522	1.514106
C	3.264762	-0.162422	1.431855
C	2.977912	1.197827	1.557414
C	-0.128991	2.898129	2.058811

C	-2.737166	0.410361	2.172352
C	-1.199858	-2.808266	1.819553
C	2.318739	-2.315661	1.410219
C	1.834472	3.001768	0.567191
C	-2.223524	2.670114	1.060116
C	1.032851	3.385016	-0.510004
C	-3.114739	-1.577312	0.904564
C	0.461452	-3.518915	0.317662
C	3.490442	-0.738818	0.116969
C	2.903729	2.038566	0.372815
C	-0.954190	3.343660	0.953174
C	-3.478495	-0.189290	1.031209
C	-0.972256	-3.388694	0.503424
C	2.905340	-2.070075	0.103738
C	2.272061	-2.542645	-1.046313
C	-1.222306	-0.712383	-3.212430
C	-1.524455	0.698993	-3.047392
C	-0.279358	1.434533	-3.191003
C	0.793080	0.477114	-3.410973
C	0.210046	-0.849724	-3.424213
C	-1.912379	-1.668495	-2.472705
C	-2.524904	1.129029	-2.163222
C	-0.047699	2.578614	-2.431553
C	2.042183	0.687738	-2.825857
C	0.895874	-1.919562	-2.849587
C	-2.951955	-1.253466	-1.559125
C	-2.292571	2.360957	-1.412305
C	1.252951	2.800350	-1.820744
C	2.755834	-0.425230	-2.219436
C	0.177474	-2.901370	-2.053338
C	-1.199379	-2.785020	-1.874647
C	-3.281702	0.112321	-1.435472
C	-1.063609	3.045564	-1.516537
C	2.272794	1.868878	-2.008268
C	2.193251	-1.701542	-2.230702
C	-2.874068	-2.096485	-0.376708
C	-2.891844	2.445181	-0.129560
C	3.420395	0.066584	-1.021157
C	1.025955	-3.280530	-0.937511
C	-1.788966	-3.040974	-0.573393
C	-3.758787	0.473806	-0.149776
C	-0.399126	3.539619	-0.321068
C	3.119381	1.482893	-0.892874
N	-0.143975	-0.008627	0.055642
H	0.772806	0.098569	-0.508072
H	-3.118143	1.365480	0.205745

NORMALMODES 183

C 0.00 0.00 0.00

C 0.00 0.00 0.00

[illegible]

```

C  0.00  0.00  0.00
C  0.05  0.07 -0.01
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C -0.01 -0.08 -0.01
C  0.00  0.00  0.00
C  0.00  0.00  0.00
N  0.00  0.00  0.00
H  0.00  0.00  0.00
H -0.90  0.39  0.16
-1050.0916

```

TS2b⁺ (TS of NH^{••}@C₆₀H⁺ → NH₂^{••+}@C₆₀ by breaking [6,6]-bond, triplet)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```

1\1\FAU-CCC-CCDN089\SP\ROMP2-FC\6-31G(d)\C60H2N1(1+,3)\DRAL\13-Aug-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Na
me=Dral\TS NH@C60H(+) -> NH2(+ )@C60 via breaking 6,6-bond triplet\1,
3\C,0,-3.266196,1.273864,-0.729892\C,0,-2.423188,2.208153,-1.43891\C,0
,-1.851816,1.517068,-2.587876\C,0,-2.395937,0.170519,-2.613642\C,0,-3.
262326,0.015828,-1.457109\C,0,-3.278229,1.27317,0.669938\C,0,-1.665543
,3.139714,-0.74216\C,0,-0.527417,1.745492,-2.964038\C,0,-1.59964,-0.89
2643,-3.034442\C,0,-3.280754,-1.187948,-0.75831\C,0,-2.447891,2.206399
,1.394728\C,0,-0.300042,3.434656,-1.187342\C,0,0.291768,0.641519,-3.41
0003\C,0,-1.634759,-2.159521,-2.318332\C,0,-3.294634,-1.188582,0.69741
7\C,0,-3.288314,0.014912,1.396576\C,0,-1.677931,3.138794,0.712575\C,0,
0.314039,2.67883,-2.219904\C,0,-0.230841,-0.651715,-3.454423\C,0,-2.45
4772,-2.301179,-1.198272\C,0,-1.899875,1.51468,2.55491\C,0,0.348234,3.
813748,0.004288\C,0,-0.58362,1.742931,2.956838\C,0,1.639957,0.870419,-
2.939477\C,0,-0.289388,-2.702307,-2.30502\C,0,-2.477476,-2.302315,1.15
2009\C,0,-2.444833,0.169022,2.569888\C,0,-0.319069,3.429572,1.181178\C
,0,1.672603,2.139276,-2.204867\C,0,0.577705,-1.77335,-3.016741\C,0,-1.
961486,-2.989422,-0.018499\C,0,-0.667433,-3.513972,-0.006363\C,0,3.228
633,-1.352005,0.730653\C,0,3.266079,-0.101068,1.451289\C,0,2.379533,-0
.212164,2.600397\C,0,1.83359,-1.559484,2.612633\C,0,2.352182,-2.262724
,1.450881\C,0,3.243746,-1.353764,-0.671678\C,0,3.352961,1.100724,0.757
739\C,0,1.583039,0.86854,2.970702\C,0,0.520507,-1.774024,3.026002\C,0,
1.530976,-3.138927,0.743049\C,0,3.296891,-0.102067,-1.392538\C,0,2.582
937,2.262324,1.199973\C,0,0.226814,0.639371,3.416977\C,0,-0.332515,-2.
702633,2.297914\C,0,1.544854,-3.139945,-0.71372\C,0,2.37966,-2.267127,
-1.404822\C,0,3.367966,1.100066,-0.695567\C,0,1.628012,2.136219,2.2370
3\C,0,-0.295916,-0.653676,3.450085\C,0,0.16287,-3.37002,1.176488\C,0,2

```

.431947,-0.211644,-2.55747\C,0,2.486627,3.064538,0.025043\C,0,-1.67776
 4,-2.160201,2.286314\C,0,0.184706,-3.370218,-1.17372\C,0,1.884027,-1.5
 59848,-2.579481\C,0,2.610347,2.263147,-1.152626\C,0,0.27195,2.67456,2.
 228253\C,0,-1.656043,-0.894183,3.003599\N,0,-0.032457,0.124898,0.04797
 \H,0,0.631906,-0.566997,-0.359396\H,0,1.338226,3.296438,-0.025106\\Ver
 sion=EM64L-G09RevA.02\State=3-A\HF=-2326.8761732\MP2=-2334.8463976\RMS
 D=7.070e-09\PG=C01 [X(C60H2N1)]\@

UB3LYP/6-31G(d)

Zero-point correction=	0.387413 (Hartree/Particle)
Thermal correction to Energy=	0.413059
Thermal correction to Enthalpy=	0.414003
Thermal correction to Gibbs Free Energy=	0.337780
Sum of electronic and zero-point Energies=	-2341.166810
Sum of electronic and thermal Energies=	-2341.141164
Sum of electronic and thermal Enthalpies=	-2341.140219
Sum of electronic and thermal Free Energies=	-2341.216443

1\1\FAU-CCC-CCDH154\Freq\UB3LYP\6-31G(d)\C60H2N1(1+,3)\DRAL\13-Jul-200
 9\0\#P scf=qc UB3LYP/6-31G(d) Freq=NoRaman SCFCYC=600 Name=Dral\TS N
 H@C60H(+)->NH2(+)\@C60 via breaking 6,6-bond (triplet)\1,3\C,-3.2661
 97,1.273862,-0.729892\C,-2.423189,2.208152,-1.43891\C,-1.851817,1.5170
 67,-2.587876\C,-2.395937,0.170518,-2.613642\C,-3.262326,0.015826,-1.45
 7109\C,-3.27823,1.273168,0.669938\C,-1.665545,3.139713,-0.74216\C,-0.5
 27418,1.745492,-2.964038\C,-1.59964,-0.892644,-3.034442\C,-3.280753,-1
 .18795,-0.75831\C,-2.447892,2.206398,1.394728\C,-0.300044,3.434656,-1.
 187342\C,0.291768,0.641519,-3.410003\C,-1.634758,-2.159522,-2.318332\C
 ,-3.294633,-1.188584,0.697417\C,-3.288314,0.01491,1.396576\C,-1.677933
 ,3.138793,0.712575\C,0.314038,2.67883,-2.219904\C,-0.230841,-0.651715,
 -3.454423\C,-2.454771,-2.30118,-1.198272\C,-1.899876,1.514679,2.55491\
 C,0.348232,3.813748,0.004288\C,-0.583621,1.742931,2.956838\C,1.639957,
 0.87042,-2.939477\C,-0.289387,-2.702307,-2.30502\C,-2.477475,-2.302316
 ,1.152009\C,-2.444833,0.169021,2.569888\C,-0.319071,3.429572,1.181178\
 C,1.672602,2.139277,-2.204867\C,0.577706,-1.77335,-3.016741\C,-1.96148
 5,-2.989423,-0.018499\C,-0.667431,-3.513972,-0.006363\C,3.228634,-1.35
 2003,0.730653\C,3.266079,-0.101066,1.451289\C,2.379533,-0.212163,2.600
 397\C,1.833591,-1.559483,2.612633\C,2.352183,-2.262723,1.450881\C,3.24
 3747,-1.353762,-0.671678\C,3.35296,1.100726,0.757739\C,1.583039,0.8685
 41,2.970702\C,0.520508,-1.774024,3.026002\C,1.530978,-3.138926,0.74304
 9\C,3.296891,-0.102065,-1.392538\C,2.582936,2.262325,1.199973\C,0.2268
 14,0.639371,3.416977\C,-0.332514,-2.702633,2.297914\C,1.544856,-3.1399
 44,-0.71372\C,2.379661,-2.267126,-1.404822\C,3.367965,1.100068,-0.6955
 67\C,1.628011,2.13622,2.23703\C,-0.295916,-0.653676,3.450085\C,0.16287
 2,-3.37002,1.176488\C,2.431947,-0.211643,-2.55747\C,2.486625,3.064539,
 0.025043\C,-1.677763,-2.160202,2.286314\C,0.184708,-3.370218,-1.17372\
 C,1.884028,-1.559847,-2.579481\C,2.610346,2.263148,-1.152626\C,0.27194
 9,2.67456,2.228253\C,-1.656043,-0.894184,3.003599\N,-0.032457,0.124898

,0.04797\H,0.631906,-0.566997,-0.359396\H,1.338224,3.296439,-0.025106\
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 al=0.4130592\ZPE=243.1053378\Dipole=0.3397889,0.7478355,-0.0313326\Dip
 0014076,0.1033602,0.0336633,0.0012397,0.0008154,0.0030399,-0.0084394\P
 2\PG=C01 [X(C60H2N1)]\NImag=1\0.24608708,0.11465623,0.48791276,-0.090
 102,0.00284081,0.00249028,0.00905232\|-0.00007001,-0.00003769,0.000075
 46128,-0.00035258,-0.00057714,-0.00034641\\@

Vibrational Normal Modes

63

C	-3.266196	1.273864	-0.729892
C	-2.423188	2.208153	-1.438910
C	-1.851816	1.517068	-2.587876
C	-2.395937	0.170519	-2.613642
C	-3.262326	0.015828	-1.457109
C	-3.278229	1.273170	0.669938
C	-1.665543	3.139714	-0.742160
C	-0.527417	1.745492	-2.964038
C	-1.599640	-0.892643	-3.034442
C	-3.280754	-1.187948	-0.758310
C	-2.447891	2.206399	1.394728
C	-0.300042	3.434656	-1.187342
C	0.291768	0.641519	-3.410003
C	-1.634759	-2.159521	-2.318332
C	-3.294634	-1.188582	0.697417
C	-3.288314	0.014912	1.396576
C	-1.677931	3.138794	0.712575
C	0.314039	2.678830	-2.219904
C	-0.230841	-0.651715	-3.454423
C	-2.454772	-2.301179	-1.198272
C	-1.899875	1.514680	2.554910
C	0.348234	3.813748	0.004288
C	-0.583620	1.742931	2.956838
C	1.639957	0.870419	-2.939477
C	-0.289388	-2.702307	-2.305020
C	-2.477476	-2.302315	1.152009
C	-2.444833	0.169022	2.569888
C	-0.319069	3.429572	1.181178
C	1.672603	2.139276	-2.204867
C	0.577705	-1.773350	-3.016741
C	-1.961486	-2.989422	-0.018499
C	-0.667433	-3.513972	-0.006363
C	3.228633	-1.352005	0.730653
C	3.266079	-0.101068	1.451289
C	2.379533	-0.212164	2.600397
C	1.833590	-1.559484	2.612633

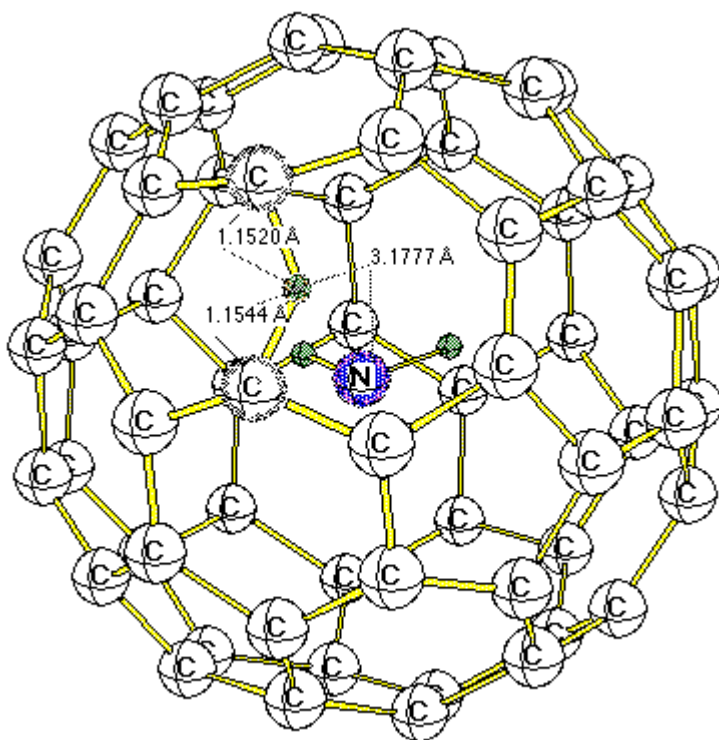
TS3a⁺ (TS of NH₂·@C₆₀H⁺ → NH₃⁺@C₆₀ by breaking [5,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN088\SP\ROMP2-FC\6-31G(d)\C60H3N1(1+,2)\DRAL\14-Aug-201
0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Na
me=Dral\TS of NH2@C60H(+) -> NH3(+@C60\1,2\C,0,1.1121380937,0.96664
24494,3.2246753185\C,0,-0.3230021661,0.7989412417,3.4078947628\C,0,-0.
6132567864,-0.6170314456,3.4050027353\C,0,0.6391189706,-1.3349746207,3
.2210799992\C,0,1.7046381434,-0.3542651656,3.1022529293\C,0,1.59587739
01,2.0231643476,2.4519973807\C,0,-1.2186207495,1.6965250848,2.82369434
24\C,0,-1.7893523441,-1.0879841569,2.8179163679\C,0,0.667249803,-2.490
4603584,2.4434706877\C,0,2.7501592411,-0.5667553222,2.2002962729\C,0,0
.6648537107,2.9648436838,1.8513302131\C,0,-2.4490773255,1.2182593817,2
.2088731483\C,0,-1.759132456,-2.3172627625,2.0433388406\C,0,1.75318738
01,-2.7136896599,1.506083586\C,0,3.2469126843,0.5333108826,1.389078336
9\C,0,2.6826255986,1.80392992,1.5145848887\C,0,-0.7047626939,2.8187244
362,2.0517030187\C,0,-2.7309180865,-0.1610548374,2.2059580595\C,0,-0.5
575695926,-2.987085997,1.8406963468\C,0,2.7749306563,-1.7709512524,1.3
855736013\C,0,1.1756719395,3.3237918171,0.5338951205\C,0,-2.7155186921
,2.1490960437,1.0792546181\C,0,0.2975783039,3.522602274,-0.534375593\C
,0,-2.6980573177,-2.1891053821,0.947291978\C,0,1.1974781368,-3.3419733
607,0.319830425\C,0,3.5740362913,0.0098897469,0.0730907576\C,0,2.41995
05053,2.6041692052,0.3291673359\C,0,-1.618294879,3.0742388934,0.954806
4183\C,0,-3.3423854184,-0.907498103,1.0749443144\C,0,-0.2291080494,-3.
5137997647,0.5235171989\C,0,3.2820341481,-1.4147020032,0.071373058\C,0
,2.7466985416,-2.015336791,-1.0685671929\C,0,-1.0800590551,-0.97084830
47,-3.1975595962\C,0,-1.6702889899,0.347103616,-3.0345665905\C,0,-0.60
86383169,1.3272351875,-3.1942924989\C,0,0.6387469037,0.6139109716,-3.4
24067827\C,0,0.3470838369,-0.8063431786,-3.4260276646\C,0,-1.543980732
2,-2.0454284114,-2.4440475493\C,0,-2.7264621117,0.5622368597,-2.136861
8869\C,0,-0.6129558038,2.4982691459,-2.4404832578\C,0,1.8235696906,1.0
837106814,-2.8543345752\C,0,1.2493426369,-1.7048477864,-2.856380614\C,
0,-2.6358075277,-1.8522504775,-1.51819432\C,0,-2.7475800685,1.81827254
73,-1.3905711688\C,0,0.6189614499,2.9899975284,-1.8463527548\C,0,2.761
2368416,0.148978747,-2.2536660331\C,0,0.7625370997,-2.8109710344,-2.04
826368\C,0,-0.6058996556,-2.9842834183,-1.8523063844\C,0,-3.2417359773
,-0.5853668581,-1.3945424106\C,0,-1.6932008488,2.7468351943,-1.5132827
176\C,0,1.808971458,2.2924625981,-2.0437152597\C,0,2.479084174,-1.2161
919526,-2.2543254747\C,0,-2.3689393628,-2.6528652375,-0.3351858972\C,0
,-3.3336504688,1.7802510864,-0.1004264185\C,0,3.3209358615,0.776034116
6,-1.0658145367\C,0,1.6844865282,-2.9972698996,-0.9425010075\C,0,-1.11
33966153,-3.3511708613,-0.5430830816\C,0,-3.7677375789,-0.3251151232,-
0.1041564337\C,0,-1.1323967121,3.3750744527,-0.3272247125\C,0,2.731457
9539,2.0978174865,-0.9359961954\N,0,-0.2490508369,-0.0365897557,0.0123
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049537\H,0,0.2971195721,0.2749189315,0.8258363764\H,0,0.3253912304,0.2
 755907276,-0.7835731599\H,0,-3.3346766221,0.6837099379,0.2525980623\\V
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UB3LYP/6-31G(d)



1 2

C	1.112138094	0.966642449	3.224675318
C	-0.323002166	0.798941242	3.407894763
C	-0.613256786	-0.617031446	3.405002735
C	0.639118971	-1.334974621	3.221079999
C	1.704638143	-0.354265166	3.102252929
C	1.595877390	2.023164348	2.451997381
C	-1.218620750	1.696525085	2.823694342
C	-1.789352344	-1.087984157	2.817916368
C	0.667249803	-2.490460358	2.443470688
C	2.750159241	-0.566755322	2.200296273
C	0.664853711	2.964843684	1.851330213
C	-2.449077326	1.218259382	2.208873148
C	-1.759132456	-2.317262762	2.043338841
C	1.753187380	-2.713689660	1.506083586
C	3.246912684	0.533310883	1.389078337
C	2.682625599	1.803929920	1.514584889
C	-0.704762694	2.818724436	2.051703019
C	-2.730918086	-0.161054837	2.205958060
C	-0.557569593	-2.987085997	1.840696347
C	2.774930656	-1.770951252	1.385573601

C	1.175671940	3.323791817	0.533895120
C	-2.715518692	2.149096044	1.079254618
C	0.297578304	3.522602274	-0.534375593
C	-2.698057318	-2.189105382	0.947291978
C	1.197478137	-3.341973361	0.319830425
C	3.574036291	0.009889747	0.073090758
C	2.419950505	2.604169205	0.329167336
C	-1.618294879	3.074238893	0.954806418
C	-3.342385418	-0.907498103	1.074944314
C	-0.229108049	-3.513799765	0.523517199
C	3.282034148	-1.414702003	0.071373058
C	2.746698542	-2.015336791	-1.068567193
C	-1.080059055	-0.970848305	-3.197559596
C	-1.670288990	0.347103616	-3.034566590
C	-0.608638317	1.327235188	-3.194292499
C	0.638746904	0.613910972	-3.424067827
C	0.347083837	-0.806343179	-3.426027665
C	-1.543980732	-2.045428411	-2.444047549
C	-2.726462112	0.562236860	-2.136861887
C	-0.612955804	2.498269146	-2.440483258
C	1.823569691	1.083710681	-2.854334575
C	1.249342637	-1.704847786	-2.856380614
C	-2.635807528	-1.852250478	-1.518194320
C	-2.747580068	1.818272547	-1.390571169
C	0.618961450	2.989997528	-1.846352755
C	2.761236842	0.148978747	-2.253666033
C	0.762537100	-2.810971034	-2.048263680
C	-0.605899656	-2.984283418	-1.852306384
C	-3.241735977	-0.585366858	-1.394542411
C	-1.693200849	2.746835194	-1.513282718
C	1.808971458	2.292462598	-2.043715260
C	2.479084174	-1.216191953	-2.254325475
C	-2.368939363	-2.652865238	-0.335185897
C	-3.333650469	1.780251086	-0.100426418
C	3.320935862	0.776034117	-1.065814537
C	1.684486528	-2.997269900	-0.942501008
C	-1.113396615	-3.351170861	-0.543083082
C	-3.767737579	-0.325115123	-0.104156434
C	-1.132396712	3.375074453	-0.327224712
C	2.731457954	2.097817486	-0.935996195
N	-0.249050837	-0.036589756	0.012304954
H	0.297119572	0.274918932	0.825836376
H	0.325391230	0.275590728	-0.783573160
H	-3.334676622	0.683709938	0.252598062

Zero-point correction=	0.404205 (Hartree/Particle)
Thermal correction to Energy=	0.429007
Thermal correction to Enthalpy=	0.429952
Thermal correction to Gibbs Free Energy=	0.356770
Sum of electronic and zero-point Energies=	-2341.843783

Sum of electronic and thermal Energies= -2341.818980
 Sum of electronic and thermal Enthalpies= -2341.818036
 Sum of electronic and thermal Free Energies= -2341.891218

1\1\FAU-CCC-CCDH156\Freq\UB3LYP\6-31G(d)\C60H3N1(1+,2)\DRAL\09-Jun-200
 9\0\#P B3LYP/6-31G* Freq=NoRaman Geom=AllCheck Pop=None NAME=DRAL\TS
 of NH2@C60H(+)-> NH3(+)\C60\1,2\C,1.1121380937,0.9666424494,3.22467
 53185\C,-0.3230021661,0.7989412417,3.4078947628\C,-0.6132567864,-0.617
 0314456,3.4050027353\C,0.6391189706,-1.3349746207,3.2210799992\C,1.704
 6381434,-0.3542651656,3.1022529293\C,1.5958773901,2.0231643476,2.45199
 73807\C,-1.2186207495,1.6965250848,2.8236943424\C,-1.7893523441,-1.087
 9841569,2.8179163679\C,0.667249803,-2.4904603584,2.4434706877\C,2.7501
 592411,-0.5667553222,2.2002962729\C,0.6648537107,2.9648436838,1.851330
 2131\C,-2.4490773255,1.2182593817,2.2088731483\C,-1.759132456,-2.31726
 27625,2.0433388406\C,1.7531873801,-2.7136896599,1.506083586\C,3.246912
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 66985416,-2.015336791,-1.0685671929\C,-1.0800590551,-0.9708483047,-3.1
 975595962\C,-1.6702889899,0.347103616,-3.0345665905\C,-0.6086383169,1.
 3272351875,-3.1942924989\C,0.6387469037,0.6139109716,-3.424067827\C,0.
 3470838369,-0.8063431786,-3.4260276646\C,-1.5439807322,-2.0454284114,-
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 8,2.4982691459,-2.4404832578\C,1.8235696906,1.0837106814,-2.8543345752
 \C,1.2493426369,-1.7048477864,-2.856380614\C,-2.6358075277,-1.85225047
 75,-1.51819432\C,-2.7475800685,1.8182725473,-1.3905711688\C,0.61896144
 99,2.9899975284,-1.8463527548\C,2.7612368416,0.148978747,-2.2536660331
 \C,0.7625370997,-2.8109710344,-2.04826368\C,-0.6058996556,-2.984283418
 3,-1.8523063844\C,-3.2417359773,-0.5853668581,-1.3945424106\C,-1.69320
 08488,2.7468351943,-1.5132827176\C,1.808971458,2.2924625981,-2.0437152
 597\C,2.479084174,-1.2161919526,-2.2543254747\C,-2.3689393628,-2.65286
 52375,-0.3351858972\C,-3.3336504688,1.7802510864,-0.1004264185\C,3.320
 9358615,0.7760341166,-1.0658145367\C,1.6844865282,-2.9972698996,-0.942
 5010075\C,-1.1133966153,-3.3511708613,-0.5430830816\C,-3.7677375789,-0
 .3251151232,-0.1041564337\C,-1.1323967121,3.3750744527,-0.3272247125\C
 ,2.7314579539,2.0978174865,-0.9359961954\N,-0.2490508369,-0.0365897557
 ,0.0123049537\H,0.2971195721,0.2749189315,0.8258363764\H,0.3253912304,
 0.2755907276,-0.7835731599\H,-3.3346766221,0.6837099379,0.2525980623\\
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 al=0.4290073\ZPE=253.642309\Dipole=-0.8888652,0.2745117,0.0468129\Dipo
 -0.0011761,-0.0025379\Polar=483.7980368,-2.1318382,473.5021832,-0.0892
 288,0.0455268,466.8518143\PG=C01 [X(C60H3N1)]\NImag=1\0.51572442,0.02

990\\0.00009492,-0.00070976,0.00024789,0.00011957,-0.00016224,0.000115
6222,-0.00012281,0.00005731,-0.00000790\\\\@

Vibrational Normal Modes

64

C	1.241471	0.791507	3.224491
C	-0.202638	0.838037	3.408081
C	-0.699222	-0.519398	3.405497
C	0.433083	-1.414779	3.221396
C	1.631959	-0.602549	3.102150
C	1.876019	1.764717	2.451519
C	-0.955732	1.858190	2.823943
C	-1.932212	-0.811214	2.818771
C	0.289721	-2.561809	2.443975
C	2.634292	-0.967526	2.199979
C	1.094430	2.833717	1.850916
C	-2.243574	1.567182	2.209496
C	-2.084426	-2.031534	2.044393
C	1.330428	-2.943393	1.506366
C	3.288145	0.046818	1.388457
C	2.918119	1.386965	1.513885
C	-0.281678	2.891898	2.051640
C	-2.726413	0.244756	2.206881
C	-0.995259	-2.871808	1.841577
C	2.480391	-2.162238	1.385454
C	1.652396	3.112954	0.533298
C	-2.369639	2.527049	1.079785
C	0.813108	3.439369	-0.534796
C	-2.994337	-1.765996	0.948549
C	0.687558	-3.482686	0.320352
C	3.533872	-0.519419	0.072480
C	2.776439	2.217107	0.328395
C	-1.147631	3.279633	0.954919
C	-3.441897	-0.403138	1.076139
C	-0.748696	-3.441499	0.524408
C	3.034284	-1.885120	0.071072
C	2.415667	-2.400078	-1.068639
C	-1.214964	-0.801113	-3.196894
C	-1.603634	0.589689	-3.033982
C	-0.408680	1.401915	-3.194127
C	0.719361	0.511835	-3.424080
C	0.220751	-0.849627	-3.425731
C	-1.832590	-1.795118	-2.443090
C	-2.616112	0.958856	-2.136062
C	-0.239473	2.560795	-2.440514
C	1.960807	0.801217	-2.854708
C	0.980272	-1.871675	-2.856148

C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00

```

C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.01 -0.01  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.05  0.06 -0.01
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C  0.00  0.00  0.00
C -0.01 -0.08 -0.01
C  0.00  0.00  0.00
C  0.00  0.00  0.00
N  0.00  0.00  0.00
H  0.00  0.01  0.00
H  0.00  0.01  0.00
H -0.92  0.34  0.17
-1082.9705

```

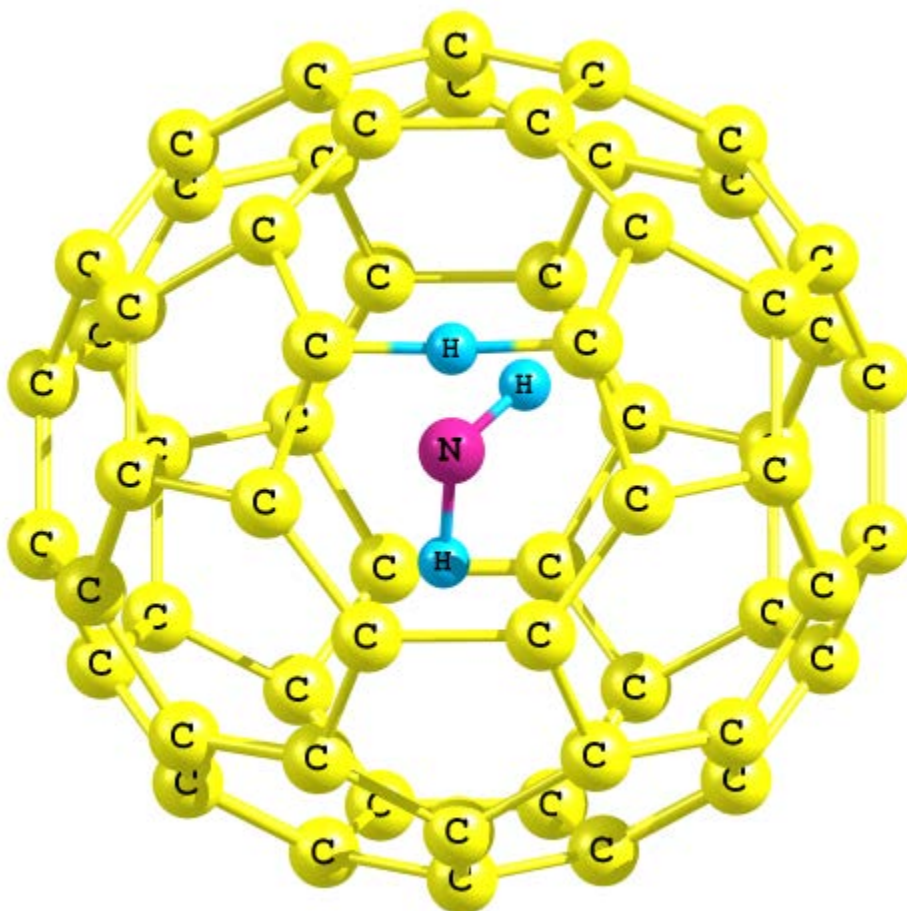
TS3b⁺ (TS of NH₂•@C₆₀H⁺ → NH₃^{•+}@C₆₀ by breaking [6,6]-bond)

ROMP2/6-31G(d)//UB3LYP/6-31G(d)

1\1\FAU-CCC-CCDN089\SP\ROMP2-FC\6-31G(d)\C60H3N1(1+,2)\DRAL\14-Aug-201
 0\0\#P ROMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Na
 me=Dral\TS of NH2@C60H(+) -> NH3(+)@C60 via breaking 6,6-bond\1,2\C,

-1.595916748,3.169158936,-0.726333618\C,-0.341812134,3.22845459,-1.440
 490723\C,-0.434234619,2.339096069,-2.591567993\C,-1.773834229,1.775482
 178,-2.611251831\C,-2.489227295,2.280227661,-1.450576782\C,-1.60102844
 2,3.178710938,0.67401123\C,0.854904175,3.343551636,-0.746444702\C,0.65
 9103394,1.559631348,-2.968063354\C,-1.969497681,0.461486816,-3.0312652
 59\C,-3.355743408,1.445785522,-0.748977661\C,-0.352264404,3.24822998,1
 .395812988\C,2.025100708,2.582595825,-1.19329834\C,0.451370239,0.20190
 4297,-3.415802002\C,-2.890380859,-0.406326294,-2.311035156\C,-3.361022
 949,1.455612183,0.70753479\C,-2.499893188,2.299697876,1.403991699\C,0.
 849487305,3.35256958,0.707824707\C,1.920501709,1.619400024,-2.22946167
 \C,-0.8359375,-0.339172363,-3.456787109\C,-3.565414429,0.075668335,-1.
 188171387\C,-0.452453613,2.374588013,2.558242798\C,2.767562866,2.41589
 3555,-0.006759644\C,0.638961792,1.600891113,2.953720093\C,1.565689087,
 -0.593154907,-2.949081421\C,-2.327850342,-1.743972778,-2.299819946\C,-
 3.573226929,0.091110229,1.163192749\C,-1.792312622,1.810516357,2.57627
 8687\C,2.016174316,2.597717285,1.172912598\C,2.490020752,0.278121948,-
 2.217590332\C,-1.059997559,-1.703918457,-3.016601562\C,-3.702163696,-0
 .759185791,-0.007339478\C,-3.161453247,-2.046859741,0.002929688\C,1.12
 0635986,-3.286987305,0.726776123\C,2.038024902,-2.432540894,1.44404602
 1\C,1.3387146,-1.88053894,2.595855713\C,-0.001968384,-2.442779541,2.61
 3021851\C,-0.14024353,-3.305480957,1.450332642\C,1.125274658,-3.296691
 895,-0.675231934\C,2.949768066,-1.648071289,0.747650146\C,1.545623779,
 -0.553466797,2.967193604\C,-1.076416016,-1.663818359,3.03326416\C,-1.3
 4262085,-3.341751099,0.746490479\C,2.048202515,-2.452453613,-1.3978881
 84\C,3.231521606,-0.283126831,1.191436768\C,0.429031372,0.247894287,3.
 417831421\C,-2.342590332,-1.713348389,2.307846069\C,-1.338272095,-3.35
 256958,-0.711181641\C,-0.131103516,-3.326339722,-1.407592773\C,2.95524
 5972,-1.658477783,-0.705429077\C,2.47416687,0.308242798,2.230636597\C,
 -0.858184814,-0.293991089,3.456787109\C,-2.469436646,-2.533859253,1.18
 4127808\C,1.356811523,-1.915893555,-2.562515259\C,3.702178955,0.352661
 133,0.009994507\C,-2.90625,-0.376251221,2.297424316\C,-2.462921143,-2.
 550765991,-1.16734314\C,0.015792847,-2.478790283,-2.580749512\C,3.2407
 68433,-0.300140381,-1.166259766\C,1.904129028,1.650665283,2.221740723\
 C,-1.990814209,0.501281738,3.013275146\N,-0.044241211,0.090832275,-0.0
 28963867\H,-0.243496948,-0.656740112,-0.722299927\H,-0.744113281,-0.10
 8449829,0.745077026\H,3.090530396,1.335968018,-0.007095337\\Version=AM
 64L-G03RevD.02\\State=2-A\\HF=-2327.4741045\\MP2=-2335.4914844\\RMSD=4.183
 e-10\\Thermal=0.\\PG=C01 [X(C60H3N1)]\\@

UB3LYP/6-31G(d)



1 2

C	-1.595916748	3.169158936	-0.726333618
C	-0.341812134	3.228454590	-1.440490723
C	-0.434234619	2.339096069	-2.591567993
C	-1.773834229	1.775482178	-2.611251831
C	-2.489227295	2.280227661	-1.450576782
C	-1.601028442	3.178710938	0.674011230
C	0.854904175	3.343551636	-0.746444702
C	0.659103394	1.559631348	-2.968063354
C	-1.969497681	0.461486816	-3.031265259
C	-3.355743408	1.445785522	-0.748977661
C	-0.352264404	3.248229980	1.395812988
C	2.025100708	2.582595825	-1.193298340
C	0.451370239	0.201904297	-3.415802002
C	-2.890380859	-0.406326294	-2.311035156
C	-3.361022949	1.455612183	0.707534790
C	-2.499893188	2.299697876	1.403991699
C	0.849487305	3.352569580	0.707824707
C	1.920501709	1.619400024	-2.229461670
C	-0.835937500	-0.339172363	-3.456787109
C	-3.565414429	0.075668335	-1.188171387
C	-0.452453613	2.374588013	2.558242798

C	2.767562866	2.415893555	-0.006759644
C	0.638961792	1.600891113	2.953720093
C	1.565689087	-0.593154907	-2.949081421
C	-2.327850342	-1.743972778	-2.299819946
C	-3.573226929	0.091110229	1.163192749
C	-1.792312622	1.810516357	2.576278687
C	2.016174316	2.597717285	1.172912598
C	2.490020752	0.278121948	-2.217590332
C	-1.059997559	-1.703918457	-3.016601562
C	-3.702163696	-0.759185791	-0.007339478
C	-3.161453247	-2.046859741	0.002929688
C	1.120635986	-3.286987305	0.726776123
C	2.038024902	-2.432540894	1.444046021
C	1.338714600	-1.880538940	2.595855713
C	-0.001968384	-2.442779541	2.613021851
C	-0.140243530	-3.305480957	1.450332642
C	1.125274658	-3.296691895	-0.675231934
C	2.949768066	-1.648071289	0.747650146
C	1.545623779	-0.553466797	2.967193604
C	-1.076416016	-1.663818359	3.033264160
C	-1.342620850	-3.341751099	0.746490479
C	2.048202515	-2.452453613	-1.397888184
C	3.231521606	-0.283126831	1.191436768
C	0.429031372	0.247894287	3.417831421
C	-2.342590332	-1.713348389	2.307846069
C	-1.338272095	-3.352569580	-0.711181641
C	-0.131103516	-3.326339722	-1.407592773
C	2.955245972	-1.658477783	-0.705429077
C	2.474166870	0.308242798	2.230636597
C	-0.858184814	-0.293991089	3.456787109
C	-2.469436646	-2.533859253	1.184127808
C	1.356811523	-1.915893555	-2.562515259
C	3.702178955	0.352661133	0.009994507
C	-2.906250000	-0.376251221	2.297424316
C	-2.462921143	-2.550765991	-1.167343140
C	0.015792847	-2.478790283	-2.580749512
C	3.240768433	-0.300140381	-1.166259766
C	1.904129028	1.650665283	2.221740723
C	-1.990814209	0.501281738	3.013275146
N	-0.044241211	0.090832275	-0.028963867
H	-0.243496948	-0.656740112	-0.722299927
H	-0.744113281	-0.108449829	0.745077026
H	3.090530396	1.335968018	-0.007095337

Zero-point correction=	0.400895 (Hartree/Particle)
Thermal correction to Energy=	0.425741
Thermal correction to Enthalpy=	0.426685
Thermal correction to Gibbs Free Energy=	0.353417
Sum of electronic and zero-point Energies=	-2341.806732
Sum of electronic and thermal Energies=	-2341.781886

Sum of electronic and thermal Enthalpies= -2341.780942
 Sum of electronic and thermal Free Energies= -2341.854210

1\1\FAU-CCC-CCDH159\Freq\UB3LYP\6-31G(d)\C60H3N1(1+,2)\DRAL\15-Jul-2009\0\#P B3LYP/6-31G* Freq=NoRaman scf=qc scfcyc=1200 NAME=DRAL\TS of NH2@C60H(+)->NH3(+@C60 via breaking 6,6-bond\1,2\C,-1.595916748,3.169158936,-0.726333618\C,-0.341812134,3.22845459,-1.440490723\C,-0.434234619,2.339096069,-2.591567993\C,-1.773834229,1.775482178,-2.611251831\C,-2.489227295,2.280227661,-1.450576782\C,-1.601028442,3.178710938,0.67401123\C,0.854904175,3.343551636,-0.746444702\C,0.659103394,1.559631348,-2.968063354\C,-1.969497681,0.461486816,-3.031265259\C,-3.355743408,1.445785522,-0.748977661\C,-0.352264404,3.24822998,1.395812988\C,2.025100708,2.582595825,-1.19329834\C,0.451370239,0.201904297,-3.41580202\C,-2.890380859,-0.406326294,-2.311035156\C,-3.361022949,1.455612183,0.70753479\C,-2.499893188,2.299697876,1.403991699\C,0.849487305,3.35256958,0.707824707\C,1.920501709,1.619400024,-2.22946167\C,-0.8359375,-0.339172363,-3.456787109\C,-3.565414429,0.075668335,-1.188171387\C,-0.452453613,2.374588013,2.558242798\C,2.767562866,2.415893555,-0.006759644\C,0.638961792,1.600891113,2.953720093\C,1.565689087,-0.593154907,-2.949081421\C,-2.327850342,-1.743972778,-2.299819946\C,-3.573226929,0.091110229,1.163192749\C,-1.792312622,1.810516357,2.576278687\C,2.016174316,2.597717285,1.172912598\C,2.490020752,0.278121948,-2.217590332\C,-1.059997559,-1.703918457,-3.016601562\C,-3.702163696,-0.759185791,-0.007339478\C,-3.161453247,-2.046859741,0.002929688\C,1.120635986,-3.286987305,0.726776123\C,2.038024902,-2.432540894,1.444046021\C,1.3387146,-1.88053894,2.595855713\C,-0.001968384,-2.442779541,2.613021851\C,-0.14024353,-3.305480957,1.450332642\C,1.125274658,-3.296691895,-0.675231934\C,2.949768066,-1.648071289,0.747650146\C,1.545623779,-0.553466797,2.967193604\C,-1.076416016,-1.663818359,3.03326416\C,-1.34262085,-3.341751099,0.746490479\C,2.048202515,-2.452453613,-1.397888184\C,3.231521606,-0.283126831,1.191436768\C,0.429031372,0.247894287,3.417831421\C,-2.342590332,-1.713348389,2.307846069\C,-1.338272095,-3.35256958,-0.711181641\C,-0.131103516,-3.326339722,-1.407592773\C,2.955245972,-1.658477783,-0.705429077\C,2.47416687,0.308242798,2.230636597\C,-0.858184814,-0.293991089,3.456787109\C,-2.469436646,-2.533859253,1.184127808\C,1.356811523,-1.915893555,-2.562515259\C,3.702178955,0.352661133,0.009994507\C,-2.90625,-0.376251221,2.297424316\C,-2.462921143,-2.550765991,-1.16734314\C,0.015792847,-2.478790283,-2.580749512\C,3.240768433,-0.300140381,-1.166259766\C,1.904129028,1.650665283,2.221740723\C,-1.990814209,0.501281738,3.013275146\C,-0.044241211,0.090832275,-0.028963867\C,-0.243496948,-0.656740112,-0.722299927\C,-0.744113281,-0.108449829,0.745077026\C,3.090530396,1.335968018,-0.007095337\Version=AM64L-G03RevD.02\State=2-AHF=-2342.2076271\S2=0.794316\S2-1=0.\S2A=0.750502\RMSD=0.000e+00\RMSF=2.412e-03\ZeroPoint=0.4008951\Thermal=0.4257408\ZPE=251.5654544\Dipole=0.7168627,0.2775485,0.0043314\DipoleDeriv=0.0028739,0.02545244\Polar=496.7858691,3.418937,486.6033795,-0.1375803,0.1455426,471.5756196\PG=C01 [X(C60H3N1)]\NImag=1\0.48054312,0.11939847,0.25213618,-0.6444,-0.00180824,0.00764594\0.00014178,0.00011598,-0.00001763,-0.000499106,-0.00354501,0.01853165,-0.00066074,-0.00034808,-0.00010181\@

Vibrational Normal Modes

64

C	-1.617409	3.105046	-0.735323
C	-0.368320	3.250890	-1.445830
C	-0.394718	2.355533	-2.595664
C	-1.691531	1.699533	-2.618391
C	-2.444082	2.154707	-1.460719
C	-1.627517	3.116300	0.664982
C	0.815253	3.450478	-0.748408
C	0.751641	1.653927	-2.967564
C	-1.793471	0.374444	-3.036752
C	-3.252258	1.262720	-0.760294
C	-0.388921	3.274105	1.390392
C	2.037205	2.772609	-1.190468
C	0.640807	0.284327	-3.413612
C	-2.653603	-0.554609	-2.317802
C	-3.262727	1.274320	0.696177
C	-2.464932	2.177630	1.393768
C	0.804711	3.461258	0.705821
C	2.003470	1.802915	-2.225300
C	-0.605353	-0.345564	-3.457523
C	-3.364185	-0.119362	-1.197781
C	-0.431338	2.397324	2.554002
C	2.785831	2.660035	-0.001435
C	0.710307	1.702485	2.954054
C	1.806574	-0.430113	-2.942212
C	-1.998893	-1.849595	-2.302631
C	-3.380347	-0.101007	1.153519
C	-1.728494	1.740905	2.568994
C	2.019909	2.790589	1.175676
C	2.665404	0.504796	-2.209446
C	-0.734735	-1.721987	-3.015688
C	-3.445843	-0.959981	-0.015945
C	-2.816393	-2.206646	-0.001870
C	1.539709	-3.143014	0.736875
C	2.392836	-2.225401	1.455429
C	1.653049	-1.721974	2.604203
C	0.354945	-2.376625	2.618320
C	0.280977	-3.248616	1.456692
C	1.549361	-3.154456	-0.665094
C	3.249609	-1.380092	0.760427
C	1.765443	-0.383126	2.973900
C	-0.772671	-1.674134	3.034025
C	-0.913728	-3.369982	0.749323
C	2.413191	-2.248780	-1.386424
C	3.433789	0.001882	1.202731
C	0.594124	0.338807	3.419836
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C	-0.904114	-3.382638	-0.708309

[illegible]

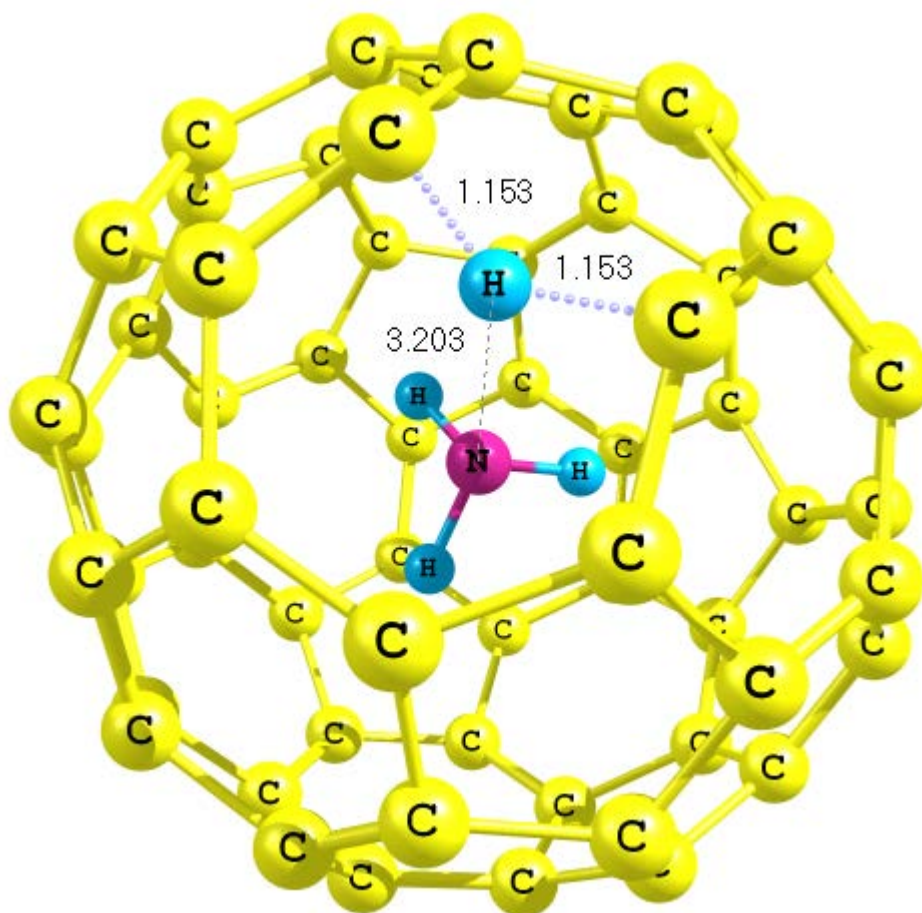
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 C 0.01 -0.01 -0.03
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 N -0.06 0.06 -0.03
 H 0.01 0.01 0.01
 H -0.05 0.05 -0.03
 H -0.02 -0.12 0.04
 92.7318

TS4a⁺ (TS of NH₃@C₆₀H⁺ → NH₄⁺@C₆₀ by breaking [5,6]-bond)

MP2/6-31G(d)//B3LYP/6-31G(d)

```
1\1\FAU-CCC-CCDN090\SP\RMP2-FC\6-31G(d)\C60H4N1(1+)\DRAL\14-Aug-2010\0
\#P RMP2/6-31G* Guess=Read Geom=AllCheck SCF=Tight SCFCyc=1200 Name=D
ral\TS NH3@C60H(+) -> NH4(+ )@C60 via breaking 5,6-bond\1,1\C,0,1.392
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,3.095895\C,0,2.547031,-0.44092,2.441404\C,0,0.918675,1.874224,2.82635
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49,2.72864,2.218216\C,0,-2.867347,0.435779,2.056856\C,0,-1.544538,-2.8
39523,1.506111\C,0,2.021818,-2.599629,1.373638\C,0,2.869196,-1.498116,
1.499293\C,0,2.145731,1.959763,2.048917\C,0,-1.436927,2.31931,2.220614
\C,0,-2.88639,-0.940026,1.851712\C,0,-0.228197,-3.284292,1.377289\C,0,
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.313399\C,0,1.930604,2.887301,0.955799\C,0,-2.38891,2.501512,1.091988\
C,0,-3.199196,-1.476762,0.533273\C,0,0.32168,-3.555915,0.059746\C,0,-0
.465844,-3.37006,-1.077283\C,0,-1.382041,0.497913,-3.189908\C,0,-0.504
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.442239\C,0,1.809871,-1.072995,-2.86416\C,0,-0.914596,-1.901243,-2.8598
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0,3.141313,-1.394121,-0.951708\N,0,-0.066555,0.208108,0.011863\H,0,0.2
12106,-0.193663,0.903652\H,0,-0.801336,-0.401504,-0.340361\H,0,0.72631
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B3LYP/6-31G(d)



Zero-point correction=	0.419981 (Hartree/Particle)
Thermal correction to Energy=	0.444635
Thermal correction to Enthalpy=	0.445579
Thermal correction to Gibbs Free Energy=	0.373541
Sum of electronic and zero-point Energies=	-2342.502144
Sum of electronic and thermal Energies=	-2342.477490
Sum of electronic and thermal Enthalpies=	-2342.476546
Sum of electronic and thermal Free Energies=	-2342.548584

1\1\GINC-A02\Freq\RB3LYP\6-31G(d)\C60H4N1(1+)\DRAL\31-Dec-2008\0\#P B
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 \C,2.547031,-0.44092,2.441404\C,0.918675,1.874224,2.826357\C,-1.79776,
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 2.189244\C,2.926921,0.827301,1.842484\C,-0.090649,2.72864,2.218216\C,-
 2.867347,0.435779,2.056856\C,-1.544538,-2.839523,1.506111\C,2.021818,-
 2.599629,1.373638\C,2.869196,-1.498116,1.499293\C,2.145731,1.959763,2.
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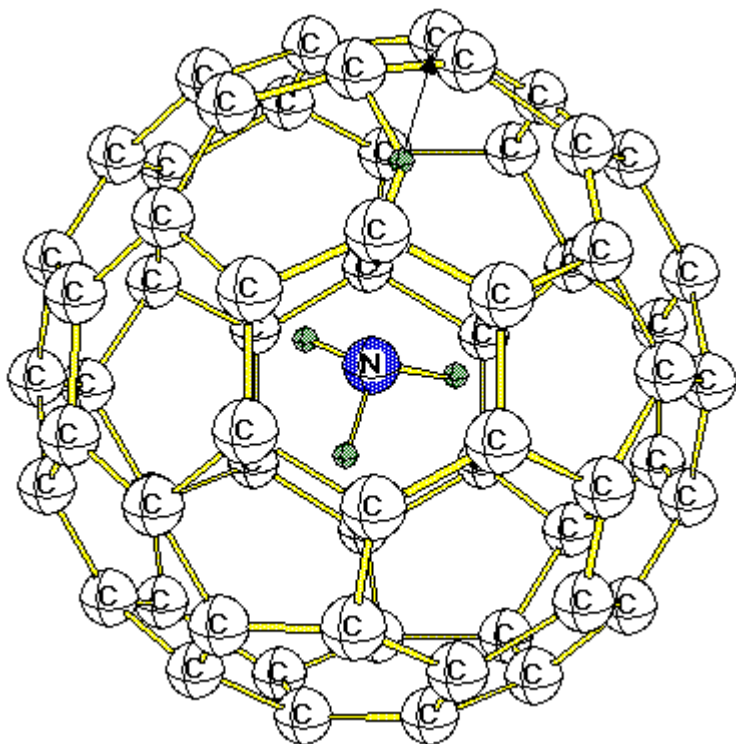
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 435103\C,-0.815774,2.672824,-2.125074\C,1.891666,1.740698,-2.442239\C,
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VIBRATIONAL NORMAL MODES



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C	-1.797642	1.048375	2.830332
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C	0.821291	-2.690725	2.189244
C	2.927014	0.826972	1.842484
C	-0.090343	2.728650	2.218216
C	-2.867298	0.436101	2.056856
C	-1.544857	-2.839350	1.506111
C	2.021526	-2.599856	1.373638
C	2.869028	-1.498438	1.499293
C	2.145951	1.959522	2.048917
C	-1.436667	2.319471	2.220614
C	-2.886496	-0.939702	1.851712
C	-0.228566	-3.284266	1.377289

C	3.481309	0.553762	0.522543
C	0.595931	3.408920	1.087196
C	3.234253	1.423896	-0.541595
C	-3.207941	1.325156	0.963866
C	-2.367699	-2.648292	0.322692
C	1.712129	-3.132520	0.057529
C	3.442123	-0.882550	0.313399
C	1.930928	2.887084	0.955799
C	-2.388629	2.501780	1.091988
C	-3.199362	-1.476403	0.533273
C	0.321281	-3.555951	0.059746
C	-0.466222	-3.370008	-1.077283
C	-1.381985	0.498068	-3.189908
C	-0.504587	1.645025	-3.026433
C	0.862093	1.179967	-3.193808
C	0.829594	-0.255327	-3.428005
C	-0.557496	-0.676929	-3.425445
C	-2.547486	0.391506	-2.435103
C	-0.815474	2.672916	-2.125074
C	1.891861	1.740486	-2.442239
C	1.809750	-1.073198	-2.864160
C	-0.914809	-1.901140	-2.859823
C	-2.894097	1.440118	-1.503685
C	0.281072	3.289374	-1.382327
C	2.914914	0.890408	-1.854010
C	1.438148	-2.345459	-2.265924
C	-2.117101	-2.003892	-2.047500
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C	-2.066793	2.574730	-1.378177
C	1.599243	2.806028	-1.511030
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C	-0.024539	3.782009	-0.089563
C	2.260505	-2.542221	-1.081838
C	-1.836855	-2.907516	-0.944057
C	-3.481932	-0.617137	-0.531293
C	-2.083432	3.155263	-0.086153
C	2.422538	2.609352	-0.328574
C	3.141156	-1.394474	-0.951708
N	-0.066532	0.208115	0.011863
H	0.212084	-0.193687	0.903652
H	-0.801381	-0.401414	-0.340361
H	0.726318	0.063472	-0.609629
H	-0.991220	3.264282	0.267599

NORMALMODES 189

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[illegible]

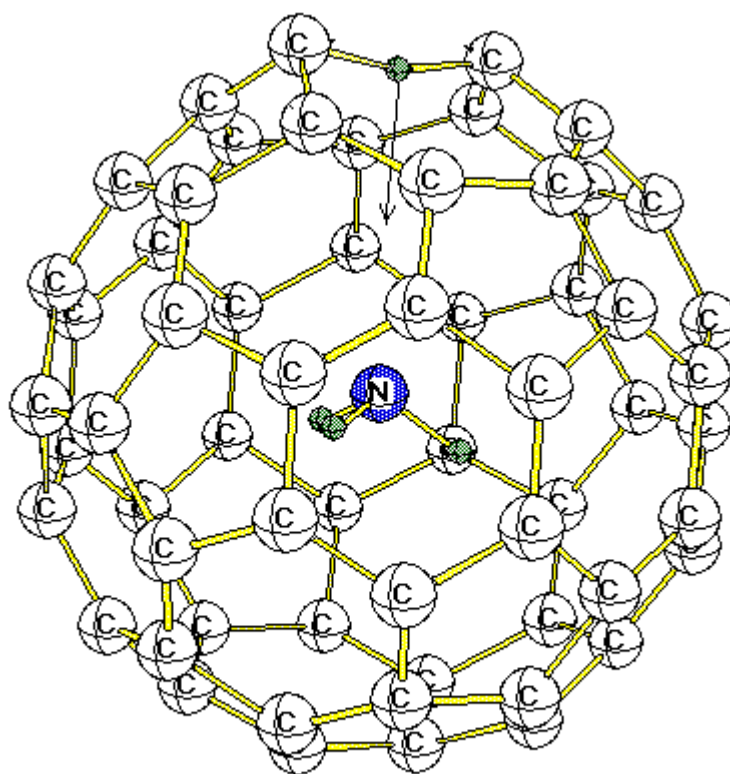
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MP2/6-31G(d)//B3LYP/6-31G(d)

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8959\C,0,-0.404230454,-2.56600471,2.387222434\C,0,0.756077109,-1.87267
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\C,0,-0.310135586,-3.259447296,1.180434774\C,0,1.970299051,-1.91845179
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B3LYP/6-31G(d)



Vib 1 = -1241.10 cm⁻¹

1 1

C	-1.145198915	-0.554167586	3.348380134
C	-1.583543217	-1.761602313	2.685968959
C	-0.404230454	-2.566004710	2.387222434
C	0.756077109	-1.872672756	2.922397974
C	0.299399788	-0.621165302	3.506958059
C	-1.759922526	0.667270879	3.045536798
C	-2.643964112	-1.725269279	1.789980952
C	-0.310135586	-3.259447296	1.180434774
C	1.970299051	-1.918451793	2.238635190
C	1.067489711	0.533952866	3.368159522
C	-2.828817193	0.711453766	2.074157299
C	-2.573170204	-2.518162128	0.558043430
C	0.953759953	-3.316491393	0.481453105
C	2.783665523	-0.717137488	2.111150590
C	0.427055015	1.804580396	3.054589617
C	-0.955307082	1.868964674	2.891420742
C	-3.283074550	-0.456425164	1.476358486
C	-1.385381506	-3.201404344	0.192275425
C	2.076759745	-2.667616130	0.999446716
C	2.337734640	0.486309835	2.660530605
C	-2.665524638	1.922652721	1.278437194
C	-3.372697881	-1.782473945	-0.335146929
C	-2.913781354	1.904946898	-0.094011754

C	0.677580678	-3.281037591	-0.937754637
C	3.397460481	-0.731778100	0.796318921
C	1.303753008	2.537326310	2.154285949
C	-1.523606392	2.651353888	1.805051300
C	-3.614036201	-0.451435331	0.047056496
C	-0.774510556	-3.219482901	-1.132383727
C	2.967277500	-1.943774176	0.112147828
C	2.483859858	1.724632602	1.914146942
C	3.075004142	1.710108683	0.648758062
C	1.210763070	0.596710195	-3.311468458
C	-0.218660761	0.653384046	-3.509321630
C	-0.713861205	1.881906913	-2.903672292
C	0.430500133	2.608242627	-2.374718366
C	1.620382504	1.808056834	-2.618943395
C	1.828133319	-0.626744877	-3.011563324
C	-0.978253218	-0.508746413	-3.437568934
C	-1.922469760	1.877812716	-2.210361770
C	0.309804585	3.331104116	-1.189057118
C	2.630749484	1.751149678	-1.661029147
C	1.031976906	-1.827345908	-2.900362474
C	-2.287052717	-0.490377062	-2.785613445
C	-2.049758735	2.641972226	-0.988703923
C	1.373393075	3.285521658	-0.194214027
C	3.271634040	0.480717778	-1.347890655
C	2.877737006	-0.683820199	-2.005641987
C	-0.339468940	-1.775999709	-3.125356346
C	-2.728712074	0.658926033	-2.088566940
C	-0.960502464	3.359825205	-0.487056464
C	2.509941294	2.507981833	-0.425463618
C	1.555059994	-2.619764731	-1.795549569
C	-2.490730202	-1.852751677	-2.421672079
C	0.758859135	3.300736413	1.120312757
C	3.543029653	0.457680172	0.080123174
C	2.714165658	-1.921840111	-1.258462146
C	-1.251964593	-2.544061554	-2.280013031
C	-3.340425110	0.678572743	-0.765553729
C	-0.685315549	3.351681000	0.939172094
N	-0.145647401	-0.084861385	-0.057807142
H	0.111190413	-0.130762447	0.924999257
H	0.653466498	-0.460835112	-0.560623925
H	-0.163592956	0.905393655	-0.285688633
H	-2.816902338	-1.748268842	-1.304774394

Zero-point correction=	0.415679 (Hartree/Particle)
Thermal correction to Energy=	0.441494
Thermal correction to Enthalpy=	0.442438
Thermal correction to Gibbs Free Energy=	0.367517
Sum of electronic and zero-point Energies=	-2342.465712
Sum of electronic and thermal Energies=	-2342.439897
Sum of electronic and thermal Enthalpies=	-2342.438953

Sum of electronic and thermal Free Energies= -2342.513874

```

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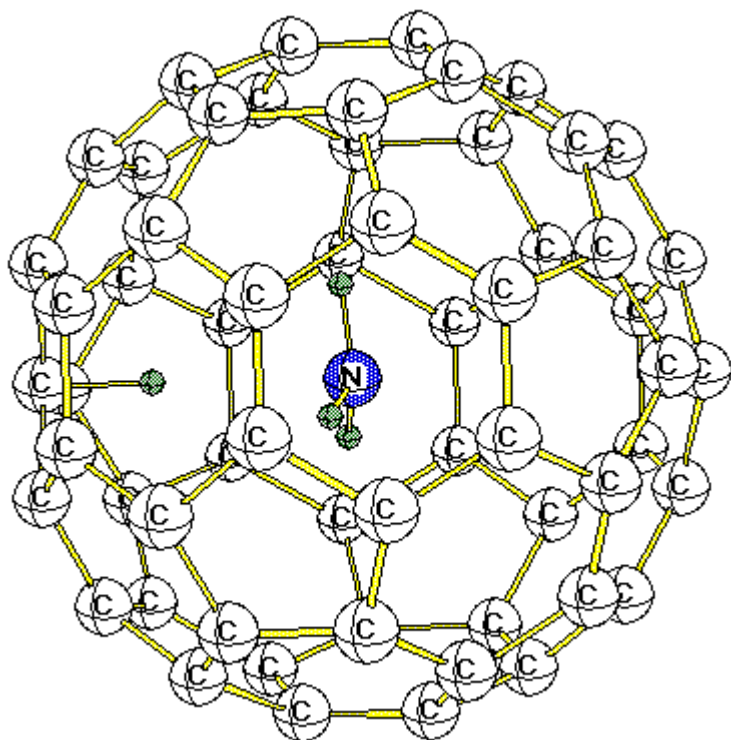
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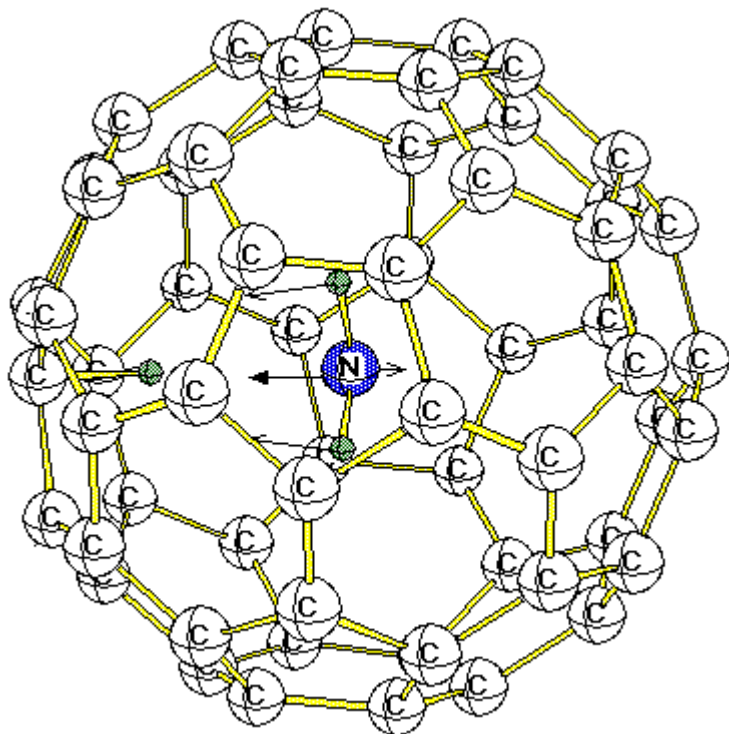
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 -0.00000687,0.00001930\\@

Vibrational Normal Modes



65

C	-2.099302	0.797684	-2.782383
C	-0.805959	1.292603	-3.200488
C	0.051299	0.092584	-3.322686
C	-0.790954	-1.123003	-3.267010
C	-2.090201	-0.667804	-2.823135
C	-2.753775	1.468443	-1.734107
C	-0.201422	2.409543	-2.626906
C	1.519585	0.101105	-3.304887
C	-0.172743	-2.261569	-2.754182
C	-2.737255	-1.404408	-1.814426
C	-2.141438	2.626985	-1.117060
C	1.249517	2.372180	-2.318791
C	2.080323	-1.091011	-2.701974
C	-0.844932	-3.010294	-1.723859
C	-3.420118	-0.700180	-0.736683
C	-3.427181	0.697975	-0.697853
C	-0.883073	3.091444	-1.556193

C	2.065110	1.264188	-2.636281
C	1.277984	-2.224154	-2.444618
C	-2.109992	-2.587913	-1.261520
C	-2.433132	2.579761	0.303775
C	1.431175	3.057567	-1.062234
C	-1.472273	2.987323	1.234318
C	3.065840	-0.662264	-1.716268
C	0.165650	-3.452627	-0.775100
C	-3.215581	-1.460284	0.486616
C	-3.231366	1.391000	0.565113
C	0.122825	3.493825	-0.584073
C	3.056074	0.794380	-1.675642
C	1.467949	-2.975669	-1.228021
C	-2.401814	-2.622712	0.160141
C	-1.434189	-3.067702	1.066721
C	2.063959	-0.791012	2.784272
C	2.054384	0.661258	2.823607
C	0.748022	1.087331	3.298303
C	-0.046994	-0.098358	3.554662
C	0.763057	-1.258313	3.233406
C	2.733671	-1.458207	1.758271
C	2.714637	1.391743	1.836034
C	0.152023	2.228254	2.757454
C	-1.413741	-0.098684	3.262092
C	0.180885	-2.374703	2.630249
C	3.422007	-0.697177	0.728361
C	2.091831	2.577770	1.269943
C	-1.271441	2.228822	2.453729
C	-2.021775	-1.259438	2.638492
C	0.870913	-3.066309	1.559846
C	2.125232	-2.619103	1.127630
C	3.412005	0.697809	0.766093
C	0.833451	2.986628	1.727145
C	-2.035952	1.086897	2.703218
C	-1.242798	-2.375773	2.326135
C	3.238698	-1.392966	-0.537515
C	2.402155	2.618241	-0.144058
C	-3.025120	-0.792748	1.697355
C	-0.124555	-3.488631	0.588422
C	2.435353	-2.577599	-0.287162
C	3.219379	1.459797	-0.458867
C	-0.167735	3.450570	0.780514
C	-3.033906	0.660585	1.737148
N	0.013051	-0.003804	-0.082276
H	0.105513	0.991696	-0.172728
H	0.828089	-0.572033	-0.223639
H	-0.886396	-0.417632	-0.247545
H	0.075799	0.062522	-2.170687

NORMALMODES 189

[illegible]

C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	0.00	-0.01	0.18
H	0.01	-0.06	-0.57
H	-0.05	0.06	-0.53
H	0.08	0.06	-0.58
H	0.01	0.01	-0.09
	-697.2666		
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	-0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.00

C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.00
C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.00	0.01	-0.01
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.01	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.00	0.01	0.00
C	0.00	0.01	0.00
C	0.01	0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
N	-0.10	-0.16	0.06
H	-0.62	-0.10	0.21
H	0.20	0.28	-0.01
H	0.11	-0.62	0.03
H	-0.01	0.00	0.01

128.4477