Supplementary Material

Electron spin, kinetic energy, and stereodynamics control of the reaction between 9-methyl-8-oxoguanine radical cation and nitric oxide

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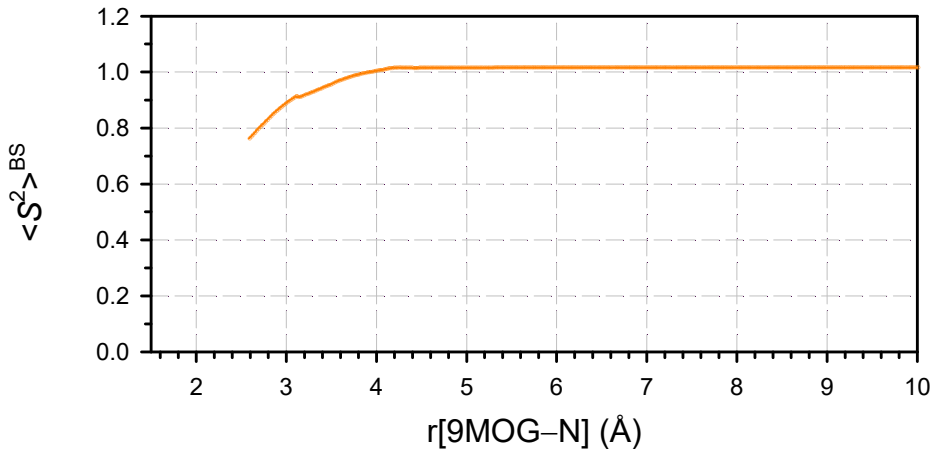

Figure S1. The change of $\langle \hat{S}^2 \rangle^{BS}$ in the open-shell singlet collision of 9MOG$^{\bullet+}$ + $^{\bullet}$NO along r[9MOG−N], the distance between the center-of-mass of 9MOG$^{\bullet+}$ and the N-terminal of $^{\bullet}$NO, calculated at ωB97XD/6-31+G(d,p).

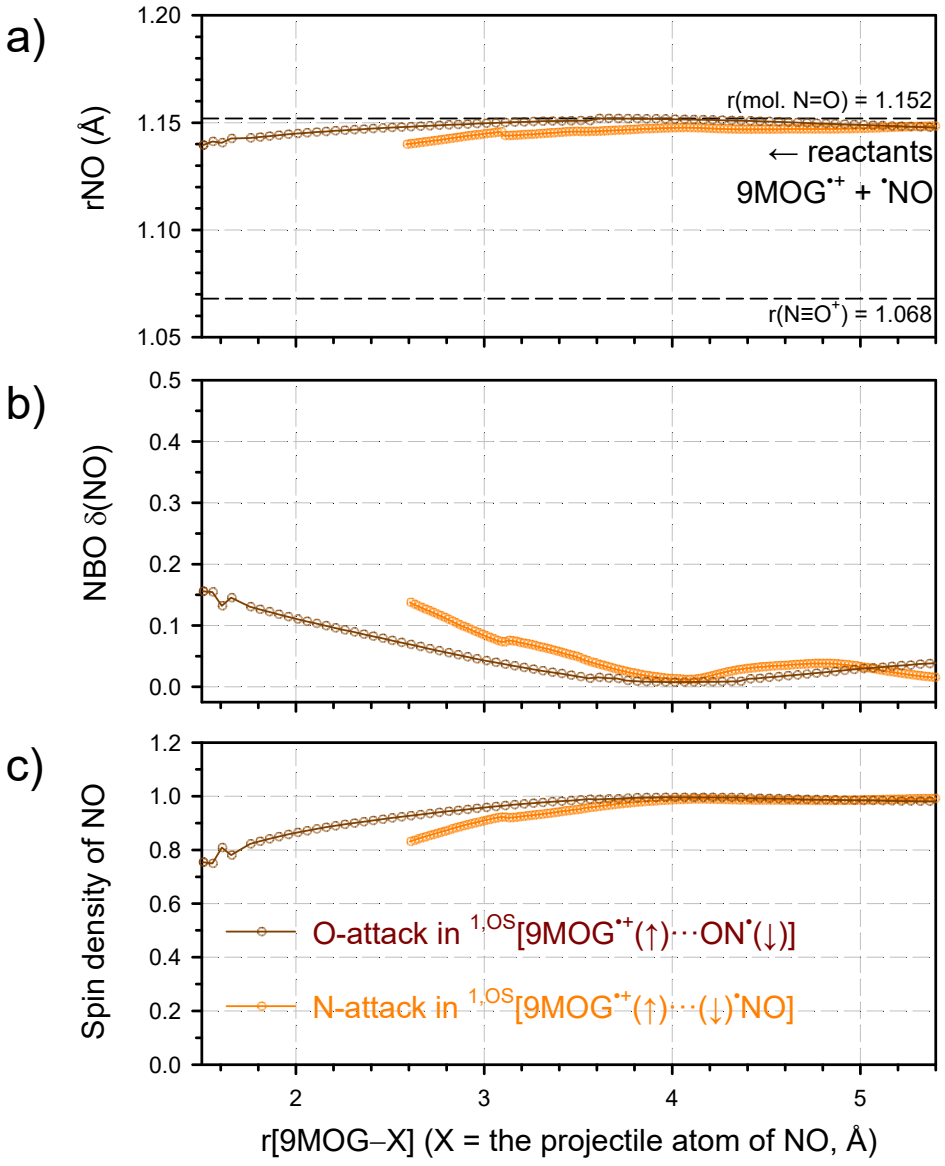

Figure S2. Comparison of the •NO collision with 9MOG•+ at different orientations in the open-shell singlet state. The changes of a) bond length, b) charge, and c) spin density of NO were calculated at ωB97XD/6-31+G(d,p).

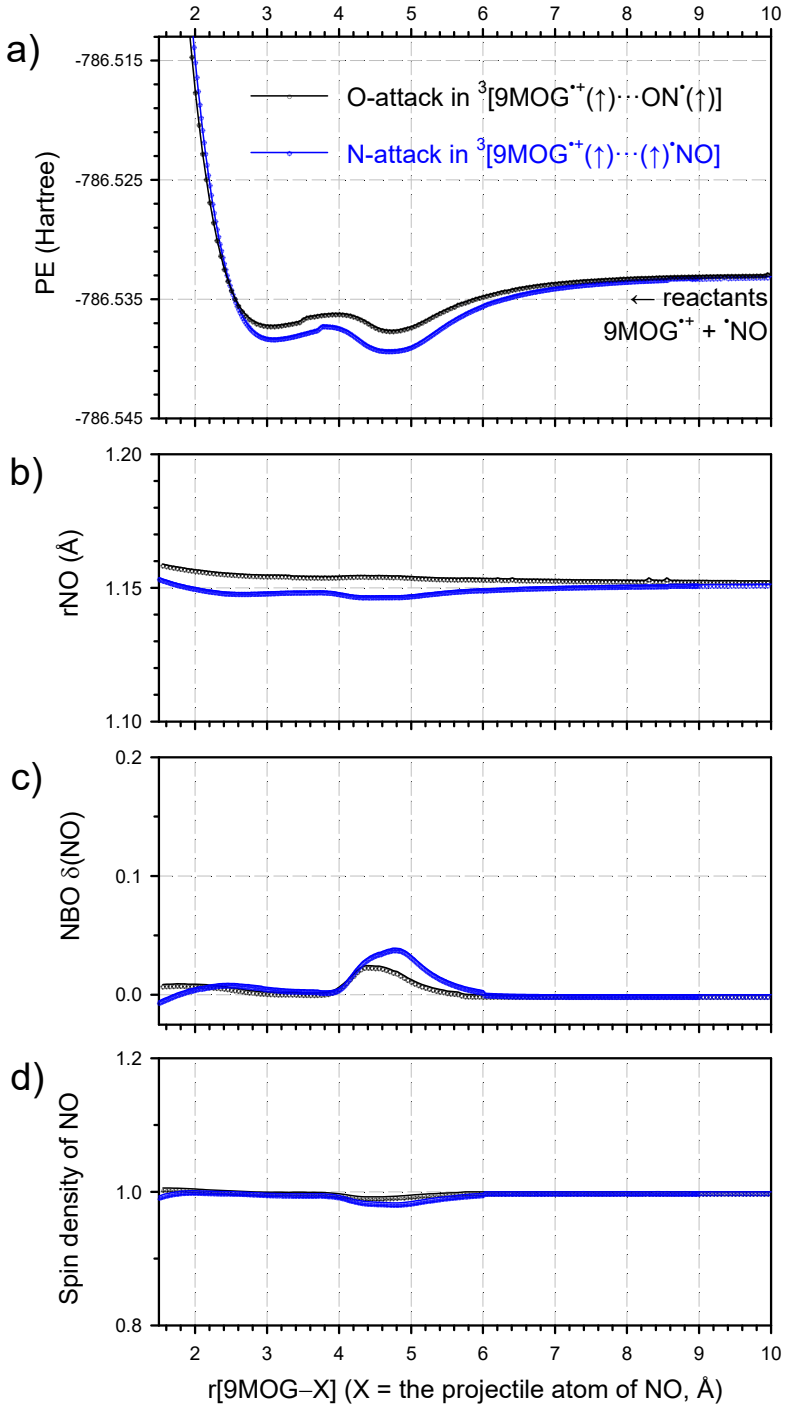

Figure S3. Comparison of the $^{\bullet}$NO collision with 9MOG$^{\bullet+}$ at different orientations in the triplet state. The changes of a) reaction potential energy, and b–d) the bond length, charge, and spin of NO were calculated at ωB97XD/6-31+G(d,p).

Table S1. $<\hat{S}^2>$ and *T*1 diagnostics for reaction structures and energy differences at different levels of theory [a,b]

Species	$<\hat{S}^2>$	T_1	$\Delta_{\omega B97XD-CASPT2}$	$\Delta_{CCSD(T)-CASPT2}$
^{1,CS}[2-NHNO-3H-9MOG]$^+$	—	0.016 (0.016)	-0.28 (0.04)	0.25 (0.34)
^{1,CS}[3-NO-9MOG]$^+$	—	0.016 (0.017)	-0.22 (-0.08)	0.23 (0.22)
^{1,CS}[5-NO-9MOG]$^+$	—	0.016 (anti), 0.016 (syn) (0.016)[c]	-0.24 (anti), -0.22 (syn) (-0.26)[c]	0.13 (anti), 0.13 (syn) (0.12)[c]
^{1,OS}precursor	0.664	—	—	—
^{1,OS}[2,4-ṄO-9MOĠ]$^+$	0.917 (0.658)	—	—	—
^{3}precursor	2.016	0.018	-0.44	0.02
^{3}[2NHNO-3H-9MOG]$^+$	2.010 (2.011)	0.022 (0.0228)	-0.48 (-0.38)	0.32 (0.30)
^{3}[3-NO-9MOG]$^+$	2.014 (2.032)	0.021 (0.0208)	-0.46 (-0.44)	0.35 (0.61)
^{3}[5-NO-9MOG]$^+$	2.009 (2.014)	0.020 (0.019)	-0.41 (-0.41)	0.23 (0.17)
^{3}[8-NO-9MOG]$^+$	2.014 (2.019)	0.019 (0.020)	-0.44 (-0.38)	0.10 (0.23)
^{3}[3-ON-9MOG]$^+$	2.009 (2.032)	0.017 (0.018)	-0.38 (-0.34)	0.23 (0.22)
^{3}[5-ON-9MOG]$^+$	2.009 (2.023)	0.017 (0.019)	-0.45 (-0.47)	0.08 (0.10)
^{3}[8-ON-9MOG]$^+$	2.009 (2.024)	0.018 (0.022)	-0.44 (-0.34)	-0.05 (0.10)
^{3}[2,4-NO-9MOG]$^+$	2.010 (2.039)	0.018 (0.021)	-0.48 (-0.43)	-0.01 (0.08)
^{3}[7,8-NO-9MOG]$^+$	2.013 (2.023 from precursor, 2.052 from [8-ON-9MOG]$^+$)	0.020 (0.020 from precursor, 0.021 from [8-ON-9MOG]$^+$)	-0.64 (-0.27 from precursor, -0.46 from [8-ON-9MOG]$^+$)	0.07 (0.32 from precursor, 0.10 from [8-ON-9MOG]$^+$)
^{3}[7,8-ON-9MOG]$^+$	2.016 (2.037 from [8-NO-9MOG]$^+$)	0.020 (0.023 from [8-NO-9MOG]$^+$)	-0.62 (-0.54 from [8-NO-9MOG]$^+$)	0.11 (0.11 from [8-NO-9MOG]$^+$)

[a] $<\hat{S}^2>$ was evaluated at ωB97XD/6-31+G(d,p). T1 diagnostics were conducted at DLPNO-CCSD(T)/aug-cc-pVTZ.

[b] Numbers in parentheses are for activation barriers.

[c] The value refers to the barrier between *syn*- and *anti*-^{1,CS}[5-NO-9MOG]$^+$.

Cartesian coordinates for representative points in Figure 3

① ^{1,OS}encounter

N 1.32536100 -2.04102700 0.01284000
C 2.39693100 -1.19270400 -0.01627400
N 2.28751000 0.14498700 -0.02775300
C 1.05227500 0.60207100 -0.00716100
C -0.12978600 -0.20017000 0.02674100
C -0.03090700 -1.63946800 0.03570800
N -1.18889700 0.61678800 0.04051300
C -0.75046100 1.96113000 0.01675000
N 0.66193600 1.89140300 -0.01243100
H 1.46267900 -3.04624000 0.01877000
N 3.62035600 -1.70840800 -0.03477500
H 3.80804600 -2.69934000 -0.02764300
H 4.40191000 -1.06818400 -0.05615200
O -0.94138600 -2.43541200 0.05788200
H -2.17175800 0.33549000 0.06984100
O -1.43323700 2.94362500 0.02047400
C 1.52602400 3.06680100 -0.04320700
H 0.88209800 3.94549800 -0.03871500
H 2.16990600 3.07085600 0.83705000
H 2.13198000 3.05215600 -0.94988800
N -3.92974000 -0.78054000 0.35287600
O -4.68850400 -1.26304000 -0.35929200

① ^{3}encounter

N -1.34333500 -2.03254900 0.01140300
C -2.40719400 -1.17448000 -0.01386900
N -2.28563700 0.16218300 -0.02448600
C -1.04623200 0.60794700 -0.00722100
C 0.12856700 -0.20505000 0.02157800
C 0.01663400 -1.64338700 0.02996700
N 1.19515300 0.60212700 0.03142700
C 0.76879300 1.95051200 0.01269400
N -0.64419700 1.89372500 -0.01241100
H -1.48979600 -3.03647300 0.01717900
N -3.63532000 -1.67899000 -0.02922100
H -3.83201500 -2.66817400 -0.02254500
H -4.41105800 -1.03164600 -0.04779200
O 0.91982500 -2.44765300 0.04920400
H 2.17581800 0.31169100 0.06390800
O 1.46057200 2.92669100 0.01670700
C -1.49763600 3.07698800 -0.03820500
H -0.84571500 3.94977300 -0.03449000
H -2.10681500 3.06939200 -0.94280800
H -2.13842300 3.08545000 0.84427700
N 3.92650600 -0.79595500 0.37130300
O 4.66688100 -1.28015900 -0.35884900

② ^{1,OS}divergence point

N 0.76934900 -2.17743600 -0.20533200
C 1.95841200 -1.59951300 0.14024800
N 2.13502500 -0.27402000 0.25656500
C 1.06401200 0.45318700 0.01540600
C -0.22264600 -0.05491100 -0.34521600
C -0.42628000 -1.47694400 -0.48765300
N -1.04565600 0.98681800 -0.51339300
C -0.35219300 2.19109700 -0.24992600
N 0.96790100 1.79631400 0.06395400
H 0.68970100 -3.18549300 -0.28804800
N 3.00487100 -2.38130200 0.37709700
H 2.97415800 -3.38765000 0.31696400
H 3.87708900 -1.93828600 0.63048700
O -1.44597600 -2.04620800 -0.80267700
H -2.04618400 0.94111500 -0.68421900
O -0.79607700 3.30134400 -0.28581800
C 2.03241300 2.73745900 0.39618500
H 1.60870800 3.73989700 0.34780400
H 2.39879100 2.53479000 1.40323400
H 2.84522400 2.63994700 -0.32439200
N -3.41512200 -0.44544800 0.69278200
O -4.45599400 -0.92776800 0.72376900

② ^{3}divergence point

N -0.74445900 -2.18530000 0.18462100
C -1.94859200 -1.61855600 -0.12541000
N -2.14311100 -0.29444500 -0.22733700
C -1.07446700 0.44338400 -0.00902000
C 0.22673700 -0.05254100 0.31447400
C 0.45023500 -1.47329400 0.43892600
N 1.04351700 0.99691800 0.46245200
C 0.33073300 2.19476400 0.22458600
N -0.99357700 1.78762600 -0.05415700
H -0.65095200 -3.19298500 0.25668000
N -2.99172700 -2.41084800 -0.34094400
H -2.94782300 -3.41717100 -0.28918100
H -3.87535100 -1.97634200 -0.56820400
O 1.48466500 -2.03419700 0.71988900
H 2.04978000 0.95856100 0.60316700
O 0.76437300 3.30932700 0.25246900
C -2.07559700 2.71927500 -0.35471200
H -1.65984600 3.72548900 -0.31657200
H -2.86699600 2.61342300 0.38816100
H -2.46815800 2.51466900 -1.35144800
N 3.43296300 -0.40037300 -0.63710800
O 4.46843800 -0.89499000 -0.64340400

③ ^{3}precursor

N 2.05736000 0.57855300 0.74757700
C 1.81621000 -0.76071900 0.85900100
N 0.59493600 -1.30949600 0.75473000
C -0.37934500 -0.45615600 0.52148200
C -0.22940800 0.95834500 0.38507000
C 1.07699000 1.56246000 0.48283800
N -1.43776200 1.47958600 0.13679000
C -2.40628400 0.44716700 0.10644300
N -1.68597600 -0.74143000 0.35733000
H 3.00154800 0.94157400 0.82386600
N 2.83702500 -1.57848700 1.08738000
H 3.79087000 -1.26542500 1.18421800
H 2.64024900 -2.56563700 1.17583900
O 1.34988600 2.73467600 0.36621500
H -1.66423800 2.45601700 -0.01321300
O -3.57987200 0.56636500 -0.09072100
C -2.30375600 -2.06246000 0.40478400
H -3.36981000 -1.93152800 0.22282400
H -2.14422600 -2.50607600 1.38819000
H -1.86792500 -2.69757300 -0.36736700
N 0.89392500 -0.27559200 -2.39960600
O 1.14880100 -0.50543000 -3.49567700

④ ^{1,OS}precursor

N -2.10329500 0.43173600 -0.61335500
C -1.86019700 -0.91149000 -0.53022300
N -0.63503400 -1.43502900 -0.38184200
C 0.34432000 -0.55237400 -0.32816800
C 0.19126600 0.86561500 -0.38285600
C -1.11642000 1.44618000 -0.57000500
N 1.41628200 1.41610900 -0.33437400
C 2.38933500 0.40435800 -0.20010900
N 1.66093800 -0.81023700 -0.20287900
H -3.04770100 0.77749000 -0.74667300
N -2.88686000 -1.75237200 -0.60273000
H -3.84332000 -1.45501900 -0.71883500
H -2.69061400 -2.74204700 -0.55106400
O -1.39292100 2.61919500 -0.66574100
H 1.64289400 2.40289300 -0.35109500
O 3.57403300 0.54168500 -0.10245700
C 2.29008800 -2.12296800 -0.10965000
H 3.35837000 -1.96279100 0.03193600
H 1.87744600 -2.66738800 0.74041000
H 2.11573400 -2.68183900 -1.03003800
N -0.35131600 0.56423300 2.27598400
O -1.24963300 -0.07941700 2.56392200

⑤ IC

N -2.13570600 0.46203500 -0.53316600
C -1.89677300 -0.88472500 -0.49760100
N -0.67039000 -1.41735300 -0.40971500
C 0.31518500 -0.53966800 -0.36590400
C 0.16809400 0.87941700 -0.38508300
C -1.14334600 1.47116900 -0.49824100
N 1.39662800 1.42472400 -0.33936600
C 2.36559900 0.40786000 -0.22773600
N 1.63194000 -0.80470100 -0.25699400
H -3.08341300 0.81528500 -0.61252600
N -2.93170900 -1.71754300 -0.54927100
H -3.88950100 -1.41162700 -0.62450700
H -2.74031300 -2.70936000 -0.53468300
O -1.41823300 2.64792100 -0.53375700
H 1.62568200 2.41078300 -0.32429200
O 3.55059600 0.53682300 -0.12246500
C 2.25621600 -2.12049300 -0.17663100
H 3.32279000 -1.96534800 -0.01744800
H 1.83006400 -2.67775800 0.65839600
H 2.09404800 -2.66432900 -1.10811700
N -0.16098800 0.43652300 2.16168600
O -1.06456700 -0.15534400 2.52598800

Cartesian coordinates for representative structures in Figure 4

***syn*-[5-NO-9MG]$^+$**

N -2.26764400 -0.35022300 0.44315900
C -2.09320900 0.93817900 0.00951500
N -0.89047300 1.51217700 -0.15166100
C 0.13685700 0.71024800 0.02549500
C 0.04934100 -0.75155800 0.10335300
C -1.21511700 -1.25734700 0.68179900
N 1.31269100 -1.16084800 0.49572500
C 2.21307400 -0.10899800 0.44393600
N 1.41745700 1.05154100 0.11781100
H -3.18788700 -0.68385100 0.71057100
N -3.16500100 1.68010400 -0.22038700
H -4.10913500 1.33257900 -0.14388100
H -3.02370300 2.64108800 -0.50091200
O -1.38812200 -2.32723900 1.19979800
H 1.59417300 -2.10614700 0.71460000
O 3.39131800 -0.10337300 0.63525300
C 1.97521500 2.39776900 0.05253200
H 3.06016800 2.29865600 0.06474400
H 1.64510400 2.97857300 0.91536000
H 1.64894900 2.88011000 -0.86903800
N -0.19066500 -1.16165600 -1.66216400
O 0.80440400 -1.55794300 -2.07862700

TS

N -2.24911500 -0.46068300 0.40109400
C -2.24005000 0.79455400 -0.13698300
N -1.11623900 1.45320100 -0.43897000
C -0.00187000 0.78666500 -0.19981800
C 0.10397500 -0.60213900 0.17193800
C -1.08913100 -1.21471500 0.71752900
N 1.40516000 -0.77940900 0.59660700
C 2.12519700 0.41937300 0.46611000
N 1.22056800 1.34201300 -0.12501700
H -3.11535500 -0.87667100 0.72552800
N -3.39780200 1.41789100 -0.33727600
H -4.29446400 1.00357800 -0.13603500
H -3.36940100 2.35635900 -0.70963000
O -1.16291400 -2.24930300 1.34130600
H 1.71416000 -1.49746700 1.23925400
O 3.25443600 0.64331900 0.79329700
C 1.53907700 2.75383200 -0.31444500
H 2.61330200 2.86691500 -0.17333100
H 1.00172500 3.35698800 0.41968600
H 1.25751500 3.05898700 -1.32211100
N 0.34455500 -2.26724000 -1.56079400
O 1.42341000 -2.49833100 -1.38695900

^{1,CS}CT

N 1.35342500 1.49471900 -0.24463900
C 0.26800400 2.28262500 -0.00466500
N -0.95359400 1.77687700 0.15084000
C -1.04609400 0.46353400 0.02394900
C 0.03566900 -0.42736900 -0.24837900
C 1.27840500 0.10864800 -0.37961100
N -0.49671400 -1.69751900 -0.29901000
C -1.87292800 -1.64409700 -0.10271500
N -2.16755100 -0.26891000 0.12057300
H 2.26925800 1.90107500 -0.39410800
N 0.43118800 3.60767400 0.08287900
H 1.31909900 4.06952600 -0.02650500
H -0.38885200 4.17030800 0.25320400
O 2.40435400 -0.52028400 -0.63070800
H -0.03733700 -2.54344900 -0.59876000
O -2.66219800 -2.54741400 -0.11224600
C -3.51300700 0.22468100 0.37875200
H -4.17801400 -0.63847300 0.37851000
H -3.54520300 0.72097300 1.34959700
H -3.80817500 0.92315300 -0.40554500
N 2.98938800 -1.34694800 0.73519000
O 3.92983500 -1.88386400 0.44530200

Cartesian coordinates for 9MOG$^{\bullet+}$·H_2O in Scheme 2, optimized at ωB97XD/6-31+G(d,p)

H_2O

O1 0.000000 0.000000 0.115783
H2 0.000000 0.765980 -0.463132
H3 0.000000 -0.765980 -0.463132

Zero-point correction= 0.021754 (Hartree/Particle)
Thermal correction to Energy= 0.024589
Thermal correction to Enthalpy= 0.025533
Thermal correction to Gibbs Free Energy= 0.004120
Sum of electronic and zero-point Energies= -76.387785
Sum of electronic and thermal Energies= -76.384949
Sum of electronic and thermal Enthalpies= -76.384005
Sum of electronic and thermal Free Energies= -76.405418

9MOG$^{\bullet+}$·W12

C1 -0.827406 1.403529 -0.000066
C2 0.519863 0.879862 -0.000075
H3 -2.754649 0.618757 0.000046
C4 -1.452336 -0.974799 0.000107
C5 2.745691 0.516548 -0.000119
N6 -1.764055 0.354814 0.000031
N7 1.714830 1.486884 -0.000151
N8 2.080805 -0.727044 -0.000018
N9 -0.191845 -1.453936 0.000098
C10 0.744070 -0.531674 0.000009
N11 -2.450404 -1.845073 0.000195
H12 -2.224135 -2.828984 0.000251
H13 -3.417929 -1.533575 0.000207
O14 -1.146871 2.571889 -0.000132
O15 -4.623470 0.102978 0.000145
H16 -5.160044 0.324992 0.769322
H17 -5.160100 0.324894 -0.769021
O18 3.925218 0.719979 -0.000167
C19 2.772797 -2.010903 0.000042
H20 2.500303 -2.574127 0.893398
H21 2.500382 -2.574175 -0.893308
H22 3.842703 -1.805717 0.000082
H23 1.893055 2.484270 -0.000220

Zero-point correction= 0.177169 (Hartree/Particle)
Thermal correction to Energy= 0.191210
Thermal correction to Enthalpy= 0.192154
Thermal correction to Gibbs Free Energy= 0.135691
Sum of electronic and zero-point Energies= -732.946404
Sum of electronic and thermal Energies= -732.932364
Sum of electronic and thermal Enthalpies= -732.931419
Sum of electronic and thermal Free Energies= -732.987883

9MOG$^{\bullet+}$· W67

O1 -2.788759 -2.648731 0.000017
H2 -2.115212 -3.338401 -0.000017
H3 -3.655094 -3.064448 -0.000001
N4 1.966548 -1.276102 -0.000001
C5 2.457215 0.001932 0.000001
N6 1.684023 1.095207 0.000002
C7 0.386372 0.856103 -0.000001
C8 -0.223180 -0.436333 -0.000004
C9 0.597589 -1.621918 -0.000004
N10 -1.549039 -0.283158 -0.000006
C11 -1.857545 1.092400 -0.000004
N12 -0.607797 1.762371 -0.000002
H13 2.597674 -2.070126 0.000000
N14 3.774947 0.176633 0.000003
H15 4.124235 1.124620 0.000005
H16 4.438339 -0.582619 0.000003
O17 0.229452 -2.777765 -0.000005
O18 -2.945315 1.594018 -0.000005
C19 -0.470569 3.214017 0.000007
H20 -1.474865 3.636211 -0.000047
H21 0.068109 3.531852 0.893550
H22 0.068205 3.531851 -0.893478
H23 -2.234483 -1.070974 -0.000004

Zero-point correction= 0.175627 (Hartree/Particle)
Thermal correction to Energy= 0.190167
Thermal correction to Enthalpy= 0.191111
Thermal correction to Gibbs Free Energy= 0.133071
Sum of electronic and zero-point Energies= -732.943979
Sum of electronic and thermal Energies= -732.929439
Sum of electronic and thermal Enthalpies= -732.928495
Sum of electronic and thermal Free Energies= -732.986536

9MOG$^{\bullet+}$· W16

C1 1.092334 -1.054340 -0.000050
C2 -0.328017 -0.793889 -0.000079
H3 2.850489 0.006445 0.000082
C4 1.272060 1.386930 0.000143
C5 -2.582638 -0.843384 -0.000150
N6 1.823207 0.144275 0.000061
N7 -1.391136 -1.609279 -0.000174
N8 -2.156558 0.501026 -0.000034
N9 -0.054223 1.629694 0.000119
C10 -0.807138 0.552958 0.000010
N11 2.082233 2.438979 0.000254
H12 1.668255 3.360180 0.000314
H13 3.087140 2.353127 0.000289
O14 1.625149 -2.145510 -0.000111
O15 4.394120 -0.780800 0.000112
H16 5.344579 -0.637481 0.000040
H17 4.244702 -1.733451 0.000056
O18 -3.704499 -1.259783 -0.000215
C19 -3.072052 1.636753 0.000035
H20 -2.907075 2.240034 0.893550
H21 -2.907101 2.240129 -0.893420
H22 -4.086321 1.239207 0.000028
H23 -1.384791 -2.622460 -0.000251

Zero-point correction= 0.175938 (Hartree/Particle)
Thermal correction to Energy= 0.190575

Thermal correction to Enthalpy= 0.191519
Thermal correction to Gibbs Free Energy= 0.132944
Sum of electronic and zero-point Energies= -732.943110
Sum of electronic and thermal Energies= -732.928473
Sum of electronic and thermal Enthalpies= -732.927529
Sum of electronic and thermal Free Energies= -732.986103

9MOG$^{\bullet+}$·W2

C1 0.344879 2.132934 -0.000003
C2 1.067223 0.883885 0.000000
H3 -1.611176 2.738725 -0.000007
C4 -1.645400 0.662143 -0.000003
C5 2.574516 -0.793334 0.000005
N6 -1.046526 1.896217 -0.000005
N7 2.379066 0.609156 0.000002
N8 1.277487 -1.345714 0.000004
N9 -0.948618 -0.493489 0.000000
C10 0.356562 -0.356381 0.000001
N11 -2.962372 0.590460 -0.000005
H12 -3.432640 -0.327213 -0.000004
H13 -3.542736 1.415998 -0.000007
O14 0.815820 3.247476 -0.000005
O15 -4.538906 -1.708756 -0.000001
H16 -4.882321 -2.168007 -0.771823
H17 -4.882260 -2.168049 0.771822
O18 3.621444 -1.373218 0.000007
C19 1.012234 -2.779494 0.000005
H20 0.446591 -3.047347 0.893223
H21 0.446631 -3.047357 -0.893235
H22 1.974502 -3.290264 0.000030
H23 3.143197 1.274568 0.000001

Zero-point correction= 0.175641 (Hartree/Particle)
Thermal correction to Energy= 0.190504
Thermal correction to Enthalpy= 0.191448
Thermal correction to Gibbs Free Energy= 0.132054
Sum of electronic and zero-point Energies= -732.938929
Sum of electronic and thermal Energies= -732.924066
Sum of electronic and thermal Enthalpies= -732.923122
Sum of electronic and thermal Free Energies= -732.982516

9MOG$^{\bullet+}$·W9

C1 2.428862 -0.694862 0.000008
C2 1.007826 -0.944548 0.000001
H3 3.670411 0.938184 0.000011
C4 1.727883 1.672190 -0.000001
C5 -1.084400 -1.782239 -0.000007
N6 2.685249 0.696224 0.000006
N7 0.301448 -2.081854 0.000000
N8 -1.158449 -0.372595 -0.000010
N9 0.410108 1.423135 -0.000007
C10 0.083191 0.146489 -0.000006
N11 2.111857 2.943711 -0.000003
H12 1.391829 3.652706 -0.000008
H13 3.077342 3.234882 0.000001
O14 3.315615 -1.517053 0.000015
O15 -5.104869 1.504941 0.000023
H16 -5.666049 1.663405 -0.764261
H17 -5.666110 1.663172 0.764310
O18 -1.985866 -2.568300 -0.000008
C19 -2.418628 0.371654 -0.000017
H20 -2.477302 0.996461 -0.890522
H21 -3.235715 -0.346210 -0.000036
H22 -2.477326 0.996443 0.890498
H23 0.663983 -3.028211 0.000004

Zero-point correction= 0.174877 (Hartree/Particle)
Thermal correction to Energy= 0.190259
Thermal correction to Enthalpy= 0.191203
Thermal correction to Gibbs Free Energy= 0.129128
Sum of electronic and zero-point Energies= -732.928124
Sum of electronic and thermal Energies= -732.912742
Sum of electronic and thermal Enthalpies= -732.911798
Sum of electronic and thermal Free Energies= -732.973873

Cartesian coordinates for singlet structures in Scheme 3, optimized at ωB97XD/6-31+G(d,p)

9MOG$^{\bullet+}$

N1 1.540775 -0.777861 -0.000001
C2 0.057997 0.900169 0.000000
C3 -1.262653 1.482720 0.000000
O4 -1.542217 2.658545 0.000001
N5 -2.249380 0.468297 0.000000
H6 -3.202828 0.815382 0.000001
C7 -1.997533 -0.874589 0.000000
N8 -3.021448 -1.718903 0.000000
H9 -3.986507 -1.425359 0.000000
H10 -2.817161 -2.708704 0.000000
N11 -0.761285 -1.400025 0.000000
C12 0.217881 -0.520343 -0.000001
C13 2.175177 -2.092463 0.000001
H14 1.877687 -2.641974 0.893817
H15 1.877663 -2.641987 -0.893798
H16 3.253080 -1.934825 -0.000015
C17 2.263665 0.435771 0.000000
O18 3.450183 0.583531 0.000000
N19 1.277786 1.453012 0.000000
H20 1.501993 2.441634 0.000000

Zero-point correction= 0.151576 (Hartree/Particle)
Thermal correction to Energy= 0.162634
Thermal correction to Enthalpy= 0.163579
Thermal correction to Gibbs Free Energy= 0.114025
Sum of electronic and zero-point Energies= -656.531429
Sum of electronic and thermal Energies= -656.520371
Sum of electronic and thermal Enthalpies= -656.519427
Sum of electronic and thermal Free Energies= -656.568981

$^{\bullet}$NO

O1 0.000000 0.000000 0.537659
N2 0.000000 0.000000 -0.614468

Zero-point correction= 0.004648 (Hartree/Particle)
Thermal correction to Energy= 0.007009
Thermal correction to Enthalpy= 0.007953
Thermal correction to Gibbs Free Energy= -0.015347
Sum of electronic and zero-point Energies= -129.845214
Sum of electronic and thermal Energies= -129.842853
Sum of electronic and thermal Enthalpies= -129.841909
Sum of electronic and thermal Free Energies= -129.865209

NO^{+}

O1 0.000000 0.000000 0.498521
N2 0.000000 0.000000 -0.569739

Zero-point correction= 0.005768 (Hartree/Particle)
Thermal correction to Energy= 0.008129
Thermal correction to Enthalpy= 0.009073
Thermal correction to Gibbs Free Energy= -0.013429
Sum of electronic and zero-point Energies= -129.486980
Sum of electronic and thermal Energies= -129.484620
Sum of electronic and thermal Enthalpies= -129.483675
Sum of electronic and thermal Free Energies= -129.506178

^{1,OS}precursor

N1 1.395546 -1.077468 -0.154740
C2 2.184641 0.029777 -0.556609
N3 1.266200 1.079539 -0.755828
C4 0.014518 0.650688 -0.489981
C5 -1.272142 1.274050 -0.683997
O6 -1.494306 2.406912 -1.043143
N7 -2.310382 0.367948 -0.359415
H8 -3.243531 0.752545 -0.460999
C9 -2.132573 -0.933639 0.019023
N10 -3.204893 -1.671146 0.290528
H11 -4.149402 -1.323413 0.231139
H12 -3.059682 -2.635141 0.555206
N13 -0.931409 -1.516842 0.130515
C14 0.092656 -0.731984 -0.146762
C15 1.950540 -2.397321 0.124250
H16 1.650235 -2.717124 1.122554
H17 1.593692 -3.112491 -0.618203
H18 3.035295 -2.313183 0.067957
O19 1.106111 1.632064 2.073888
N20 0.032020 1.275715 1.978776
O21 3.373018 0.061141 -0.694447
H22 1.539407 1.994221 -1.092447

Zero-point correction= 0.157450 (Hartree/Particle)
Thermal correction to Energy= 0.172141
Thermal correction to Enthalpy= 0.173085
Thermal correction to Gibbs Free Energy= 0.114755
Sum of electronic and zero-point Energies= -786.385274
Sum of electronic and thermal Energies= -786.370583
Sum of electronic and thermal Enthalpies= -786.369639
Sum of electronic and thermal Free Energies= -786.427969

Spin projection
E^{BS} = -786.542724 $<S^2>^{BS}$ = 0.6637
E^{HS} = -786.530051 $<S^2>^{HS}$ = 2.0155
E^{AP} = -786.548946

TS-^{1,CS}[2-NHNO-3H-9MOG]$^{+}$

C1 0.827884 0.973699 0.001742
C2 -0.199361 1.970635 -0.075533
O3 -0.127348 3.164839 0.077826
N4 -1.477474 1.352202 -0.386251
C5 -1.612905 0.044588 -0.587803
N6 -2.740852 -0.759209 -0.840861
H7 -3.347968 -0.556553 -1.636560
N8 -0.642787 -0.842419 -0.505067
C9 0.603751 -0.372237 -0.209051
N10 2.165521 1.112432 0.264493
C11 2.801339 -0.126123 0.225101
N12 1.768152 -1.050064 -0.081103
C13 1.999529 -2.478336 -0.224561
H14 3.065150 -2.642824 -0.062614

H15 1.430663 -3.034239 0.523497
H16 1.731314 -2.808505 -1.230124
H17 -2.258544 1.995557 -0.470483
N18 -3.774234 -1.065948 0.509139
O19 -3.233804 -0.858563 1.485963
H20 -1.689873 -1.596448 -0.836873
O21 3.962029 -0.385706 0.405462
H22 2.652530 1.976134 0.457327

Zero-point correction= 0.153831 (Hartree/Particle)
Thermal correction to Energy= 0.167234
Thermal correction to Enthalpy= 0.168178
Thermal correction to Gibbs Free Energy= 0.112992
Sum of electronic and zero-point Energies= -786.288205
Sum of electronic and thermal Energies= -786.274802
Sum of electronic and thermal Enthalpies= -786.273857
Sum of electronic and thermal Free Energies= -786.329043

^{1,CS}[2-NHNO-3H-9MOG]$^{+}$

C1 1.096106 0.952905 -0.000014
C2 0.245338 2.093918 -0.000023
O3 0.495201 3.269984 -0.000092
N4 -1.158187 1.668660 0.000077
C5 -1.616627 0.421284 0.000160
N6 -2.953049 0.161713 0.000327
H7 -3.664122 0.892389 -0.000171
N8 -0.749840 -0.599440 0.000180
C9 0.603224 -0.323086 0.000074
N10 2.471216 0.843983 -0.000101
C11 2.851544 -0.486947 -0.000071
N12 1.618770 -1.211939 0.000048
C13 1.561735 -2.664868 0.000093
H14 2.594184 -3.017054 0.000151
H15 1.063700 -3.032931 0.900657
H16 1.063781 -3.032994 -0.900490
H17 -1.807663 2.450275 0.000134
N18 -3.364847 -1.180071 -0.000071
O19 -4.542098 -1.302738 -0.000381
H20 -1.106905 -1.549830 0.000159
O21 3.950420 -0.974298 -0.000127
H22 3.132472 1.606974 -0.000180

Zero-point correction= 0.159628 (Hartree/Particle)
Thermal correction to Energy= 0.172972
Thermal correction to Enthalpy= 0.173916
Thermal correction to Gibbs Free Energy= 0.119537
Sum of electronic and zero-point Energies= -786.367607
Sum of electronic and thermal Energies= -786.354264
Sum of electronic and thermal Enthalpies= -786.353319
Sum of electronic and thermal Free Energies= -786.407698

TS-^{1,CS}[3-NO-9MOG]$^{+}$

C1 -0.825559 1.822044 -0.036244
C2 0.370300 1.032851 0.071123
H3 -2.789289 1.525357 -0.607519
C4 -1.864619 -0.320772 -0.725304
C5 2.515981 0.315714 0.065350
N6 -1.926679 1.007707 -0.472813
N7 1.668645 1.403819 0.283450
N8 1.655900 -0.739191 -0.318623
N9 -0.731194 -1.034358 -0.613646
C10 0.375526 -0.291620 -0.328050
N11 -2.988557 -1.002825 -0.967790
H12 -2.898786 -1.952830 -1.301343
H13 -3.887174 -0.552938 -1.063067
O14 -0.986184 2.997689 0.180697
C15 2.158842 -2.059983 -0.668542
H16 1.347359 -2.633333 -1.115548
H17 2.974280 -1.949986 -1.384242
H18 2.533883 -2.567334 0.222012
O19 -1.887649 -1.321211 1.956581
N20 -0.874911 -1.444731 1.510383
O21 3.712884 0.259322 0.174362
H22 2.002067 2.322315 0.539854

Zero-point correction= 0.158010 (Hartree/Particle)
Thermal correction to Energy= 0.171431
Thermal correction to Enthalpy= 0.172375
Thermal correction to Gibbs Free Energy= 0.117727
Sum of electronic and zero-point Energies= -786.349187
Sum of electronic and thermal Energies= -786.335765
Sum of electronic and thermal Enthalpies= -786.334821
Sum of electronic and thermal Free Energies= -786.389469

^{1,CS}[3-NO-9MOG]$^{+}$

N1 1.482145 -0.910855 -0.028991
C2 2.582464 0.006372 0.004832
N3 1.999800 1.255542 0.053561
C4 0.627541 1.141936 0.049997
C5 -0.368786 2.156996 0.030760
O6 -0.267979 3.355195 0.052868
N7 -1.694561 1.563614 -0.044310
H8 -2.433473 2.259926 -0.088913
C9 -2.018822 0.269742 -0.073674
N10 -3.286382 -0.109665 -0.133609
H11 -4.024108 0.581035 -0.114738
H12 -3.541104 -1.086834 -0.165192
N13 -0.991472 -0.657362 -0.031150
C14 0.332536 -0.190110 0.001771
C15 1.741503 -2.344950 -0.132042
H16 1.422590 -2.864139 0.771372
H17 1.242702 -2.763877 -1.007028
H18 2.821402 -2.441806 -0.247470
O19 -2.235107 -2.493608 0.144483
N20 -1.129642 -2.077097 0.186702
O21 3.746241 -0.297649 -0.013559
H22 2.528908 2.115036 0.076347

Zero-point correction= 0.159576 (Hartree/Particle)
Thermal correction to Energy= 0.172784
Thermal correction to Enthalpy= 0.173728
Thermal correction to Gibbs Free Energy= 0.119860
Sum of electronic and zero-point Energies= -786.356914

Sum of electronic and thermal Energies= -786.343705
Sum of electronic and thermal Enthalpies= -786.342761
Sum of electronic and thermal Free Energies= -786.396630

***anti*-^{1,CS}[5-NO-9MOG]$^{+}$**

C1	-1.099343	1.284575	-0.671762
C2	0.116681	0.823934	0.070378
H3	-3.001024	0.593440	-1.025914
C4	-1.890673	-1.002637	-0.282202
C5	2.345340	0.355376	-0.184855
N6	-2.102884	0.301189	-0.654717
N7	1.385258	1.345429	-0.207749
N8	1.608691	-0.887183	-0.057243
N9	-0.673080	-1.512363	-0.038657
C10	0.308053	-0.640737	-0.026422
N11	-2.926431	-1.821705	-0.225403
H12	-2.751741	-2.791053	0.003929
H13	-3.879545	-1.523700	-0.371228
O14	-1.262301	2.376565	-1.141312
O15	-1.144937	0.586489	2.129800
C16	2.253207	-2.193695	-0.127658
H17	3.326470	-2.028424	-0.038645
H18	1.895593	-2.816934	0.692089
H19	2.027281	-2.667777	-1.084404
N20	-0.212533	1.141613	1.704775
O21	3.532894	0.434164	-0.272885
H22	1.625003	2.326931	-0.212558

Zero-point correction= 0.159292 (Hartree/Particle)
Thermal correction to Energy= 0.172847
Thermal correction to Enthalpy= 0.173791
Thermal correction to Gibbs Free Energy= 0.119227
Sum of electronic and zero-point Energies= -786.383482
Sum of electronic and thermal Energies= -786.369927
Sum of electronic and thermal Enthalpies= -786.368983
Sum of electronic and thermal Free Energies= -786.423547

***syn*-^{1,CS}[5-NO-9MOG]$^{+}$**

C1	1.215172	-1.257453	-0.681591
C2	-0.049348	-0.751619	-0.103251
H3	3.187934	-0.683931	-0.710363
C4	2.093153	0.938195	-0.009664
C5	-2.213144	-0.109330	-0.443751
N6	2.267667	-0.350285	-0.443054
N7	-1.312698	-1.161073	-0.495519
N8	-1.417541	1.051397	-0.118019
N9	0.890366	1.512189	0.151312
C10	-0.136932	0.710233	-0.025767
N11	3.164883	1.680213	0.220206
H12	3.023494	2.641242	0.500531
H13	4.109046	1.332745	0.143771
O14	1.388215	-2.327460	-1.199366
O15	-0.803968	-1.557116	2.078735
C16	-1.975441	2.397565	-0.052863
H17	-1.645935	2.978109	-0.916099
H18	-3.060390	2.298314	-0.064397
H19	-1.648675	2.880272	0.868339
N20	0.190953	-1.160823	1.661831
O21	-3.391426	-0.103817	-0.634857
H22	-1.594210	-2.106478	-0.713856

Zero-point correction= 0.159194 (Hartree/Particle)
Thermal correction to Energy= 0.172952
Thermal correction to Enthalpy= 0.173896
Thermal correction to Gibbs Free Energy= 0.118656
Sum of electronic and zero-point Energies= -786.386424
Sum of electronic and thermal Energies= -786.372666
Sum of electronic and thermal Enthalpies= -786.371722
Sum of electronic and thermal Free Energies= -786.426962

TS-*rot*-^{1,CS}[5-NO-9MOG]$^{+}$

C1	1.221201	-1.326443	-0.586924
C2	-0.045675	-0.820182	0.001791
H3	3.177059	-0.701286	-0.708882
C4	2.043199	0.947237	-0.142639
C5	-2.232549	-0.273004	-0.409405
N6	2.253313	-0.372828	-0.446426
N7	-1.308726	-1.298207	-0.384623
N8	-1.463902	0.936820	-0.192783
N9	0.824245	1.491698	-0.008230
C10	-0.177917	0.643518	-0.082641
N11	3.092142	1.743791	-0.012308
H12	2.921966	2.723112	0.173265
H13	4.046527	1.424430	-0.086092
O14	1.413732	-2.427696	-1.021155
O15	-0.357728	-0.514828	2.407604
C16	-2.059469	2.266431	-0.256057
H17	-1.758486	2.763070	-1.180104
H18	-3.141160	2.137674	-0.238356
H19	-1.730950	2.848183	0.605227
N20	0.089565	-1.293745	1.674396
O21	-3.411978	-0.307912	-0.590176
H22	-1.566355	-2.269750	-0.490168

Zero-point correction= 0.158685 (Hartree/Particle)
Thermal correction to Energy= 0.171733
Thermal correction to Enthalpy= 0.172677
Thermal correction to Gibbs Free Energy= 0.119172
Sum of electronic and zero-point Energies= -786.379767
Sum of electronic and thermal Energies= -786.366719
Sum of electronic and thermal Enthalpies= -786.365775
Sum of electronic and thermal Free Energies= -786.419280

TS-^{1,OS}[2,4-ṄO-9MOĠ]$^{+}$

C1	0.313761	-0.479450	-0.008094
C2	0.217993	1.008323	-0.013477
C3	-1.121367	1.685264	-0.016748
C4	-1.870560	-0.686616	-0.206822
C5	2.417867	0.418473	-0.098232
O6	-1.226379	2.881946	0.082282
N7	1.400528	1.506279	-0.060237

N8 1.680017 -0.740071 -0.095772
N9 -0.631067 -0.934099 -0.923477
N10 -3.036927 -1.334243 -0.625944
H11 -3.039455 -2.323826 -0.406772
H12 -3.240872 -1.181253 -1.607422
C13 2.268041 -2.078604 -0.187241
H14 2.152920 -2.604170 0.761676
H15 3.327100 -1.958590 -0.413100
H16 1.779418 -2.625743 -0.994691
N17 -2.117339 0.751592 -0.126733
H18 -3.082174 1.058230 -0.030459
N19 -1.526865 -1.104528 1.201381
O20 -0.268608 -0.882592 1.365814
O21 3.586338 0.615618 -0.148004
H22 1.639412 2.496728 -0.110818

Zero-point correction= 0.156204 (Hartree/Particle)
Thermal correction to Energy= 0.168609
Thermal correction to Enthalpy= 0.169553
Thermal correction to Gibbs Free Energy= 0.117746
Sum of electronic and zero-point Energies= -786.246711
Sum of electronic and thermal Energies= -786.234306
Sum of electronic and thermal Enthalpies= -786.233362
Sum of electronic and thermal Free Energies= -786.285169

Spin projection
E^{BS} = -786.402915 $\langle S^2 \rangle^{BS}$ = 0.6583
E^{HS} = -786.3939329 $\langle S^2 \rangle^{HS}$ = 2.0100
E^{AP} = -786.407289

^{1,OS}[2,4-ṄO-9MOĠ]$^{+}$
C1 0.304447 -0.482389 0.018687
C2 0.223984 1.021037 0.001858
C3 -1.120220 1.700253 0.005314
C4 -1.887540 -0.684790 -0.181088
C5 2.422155 0.405333 -0.110099
O6 -1.216969 2.897847 0.106548
N7 1.401469 1.508565 -0.040403
N8 1.678873 -0.741070 -0.114061
N9 -0.646002 -0.898724 -0.949516
N10 -3.053109 -1.316875 -0.621412
H11 -3.137829 -2.271890 -0.294535
H12 -3.205909 -1.245120 -1.620433
C13 2.260367 -2.084918 -0.171945
H14 2.089258 -2.604530 0.771862
H15 3.330833 -1.973882 -0.341380
H16 1.813028 -2.632668 -1.002557
N17 -2.108017 0.769049 -0.135481
H18 -3.075114 1.080303 -0.093560
N19 -1.534723 -1.164603 1.178524
O20 -0.227051 -0.908270 1.316540
O21 3.587858 0.611191 -0.168690
H22 1.646432 2.500091 -0.054503

Zero-point correction= 0.157900 (Hartree/Particle)
Thermal correction to Energy= 0.170449
Thermal correction to Enthalpy= 0.171393
Thermal correction to Gibbs Free Energy= 0.119385
Sum of electronic and zero-point Energies= -786.246723
Sum of electronic and thermal Energies= -786.234174
Sum of electronic and thermal Enthalpies= -786.233230
Sum of electronic and thermal Free Energies= -786.285237

Spin projection
E^{BS} = -786.404623 $\langle S^2 \rangle^{BS}$ = 0.9166
E^{HS} = -786.4009081 $\langle S^2 \rangle^{HS}$ = 2.0100
E^{AP} = -786.407737

Cartesian coordinates for triplet structures in Scheme 4, optimized at ωB97XD/6-31+G(d,p)

^{3}precursor

C1 -1.223068 1.442924 -0.541188
C2 0.098376 0.865692 -0.492402
H3 -3.160647 0.770240 -0.558583
C4 -1.951672 -0.912705 -0.449747
C5 2.302691 0.411962 -0.379275
N6 -2.206532 0.426685 -0.528603
N7 1.315432 1.423426 -0.467945
N8 1.584163 -0.803634 -0.359248
N9 -0.714972 -1.434009 -0.395096
C10 0.261989 -0.551980 -0.415928
N11 -2.974032 -1.759130 -0.426954
H12 -2.767844 -2.747033 -0.375022
H13 -3.939152 -1.468529 -0.464809
O14 -1.505090 2.617685 -0.588005
O15 -0.800559 0.213807 2.657284
C16 2.220785 -2.112245 -0.254139
H17 3.298417 -1.953767 -0.271191
H18 1.928993 -2.588455 0.682899
H19 1.919878 -2.732608 -1.098879
N20 0.349019 0.185891 2.735476
O21 3.487807 0.564979 -0.334197
H22 1.536948 2.411876 -0.502418

Zero-point correction= 0.156889 (Hartree/Particle)
Thermal correction to Energy= 0.172066
Thermal correction to Enthalpy= 0.173010
Thermal correction to Gibbs Free Energy= 0.110713
Sum of electronic and zero-point Energies= -786.380923
Sum of electronic and thermal Energies= -786.365746
Sum of electronic and thermal Enthalpies= -786.364802
Sum of electronic and thermal Free Energies= -786.427098

TS-^{3}[2-NHNO-3H-9MOG]$^+$

C1 0.880631 0.970661 0.005312
C2 -0.127414 1.993264 -0.029370
O3 -0.023361 3.182566 0.125111
N4 -1.430606 1.401303 -0.304668
C5 -1.582252 0.097161 -0.477840
N6 -2.752274 -0.708278 -0.758156
H7 -3.219572 -0.533961 -1.652896
N8 -0.651417 -0.818981 -0.413985
C9 0.618856 -0.373548 -0.181574
N10 2.224249 1.080380 0.231238
C11 2.831518 -0.175448 0.188503
N12 1.769117 -1.077864 -0.079039
C13 1.959724 -2.515933 -0.190990
H14 3.023689 -2.704796 -0.045944
H15 1.391321 -3.036476 0.582276
H16 1.663209 -2.862981 -1.182716
H17 -2.210923 2.051583 -0.344212
N18 -3.795728 -0.709448 0.249271
O19 -3.548316 -1.153156 1.354184
H20 -1.755045 -1.568989 -0.696586
O21 3.989541 -0.457429 0.341715
H22 2.734648 1.933035 0.415128

Zero-point correction= 0.153864 (Hartree/Particle)
Thermal correction to Energy= 0.166953
Thermal correction to Enthalpy= 0.167897
Thermal correction to Gibbs Free Energy= 0.112336
Sum of electronic and zero-point Energies= -786.225255
Sum of electronic and thermal Energies= -786.212167
Sum of electronic and thermal Enthalpies= -786.211222
Sum of electronic and thermal Free Energies= -786.266783

^{3}[2-NHNO-3H-9MOG]$^+$

C1 1.092448 0.949909 -0.021146
C2 0.274797 2.115639 -0.018948
O3 0.560919 3.283207 -0.043883
N4 -1.138966 1.734296 0.024804
C5 -1.633503 0.498563 0.043566
N6 -2.976945 0.284370 0.018444
H7 -3.611185 1.043819 0.256609
N8 -0.797217 -0.546446 0.045201
C9 0.564191 -0.310437 0.013708
N10 2.464194 0.801403 -0.040605
C11 2.806399 -0.539291 -0.020135
N12 1.553737 -1.228429 0.016058
C13 1.455760 -2.678760 0.042128
H14 2.477811 -3.059973 0.029133
H15 0.965267 -3.017869 0.958136
H16 0.930830 -3.047657 -0.842737
H17 -1.764334 2.535006 0.007933
N18 -3.427457 -0.987776 0.339247
O19 -4.210398 -1.615624 -0.361844
H20 -1.177328 -1.486559 0.086172
O21 3.890765 -1.058493 -0.029605
H22 3.146669 1.544852 -0.069669

Zero-point correction= 0.158921 (Hartree/Particle)
Thermal correction to Energy= 0.172514
Thermal correction to Enthalpy= 0.173458
Thermal correction to Gibbs Free Energy= 0.117164
Sum of electronic and zero-point Energies= -786.300959
Sum of electronic and thermal Energies= -786.287367
Sum of electronic and thermal Enthalpies= -786.286422
Sum of electronic and thermal Free Energies= -786.342717

TS-^{3}[3-NO-9MOG]$^+$

N1 1.494854 -0.758276 -0.007160
C2 2.510936 0.239882 0.025122
N3 1.821198 1.449994 0.061723
C4 0.475406 1.224050 0.069947
C5 -0.617363 2.147700 -0.011358
O6 -0.600277 3.350204 -0.026931
N7 -1.877355 1.446246 -0.098268
H8 -2.682129 2.063602 -0.152691

C9 -2.059052 0.120835 -0.047465
N10 -3.264663 -0.416915 -0.003303
H11 -4.096795 0.153680 0.042666
H12 -3.373617 -1.421143 0.063926
N13 -0.959670 -0.705696 -0.064619
C14 0.292003 -0.139860 0.017823
C15 1.827516 -2.176395 -0.118549
H16 1.564432 -2.707991 0.795935
H17 1.314961 -2.616861 -0.975517
H18 2.905870 -2.225708 -0.270288
O19 -1.178513 -3.018417 -0.222291
N20 -1.189489 -2.036132 0.507172
O21 3.695776 0.049773 0.009289
H22 2.280578 2.350121 0.033504

Zero-point correction= 0.156774 (Hartree/Particle)
Thermal correction to Energy= 0.170008
Thermal correction to Enthalpy= 0.170952
Thermal correction to Gibbs Free Energy= 0.115960
Sum of electronic and zero-point Energies= -786.299983
Sum of electronic and thermal Energies= -786.286749
Sum of electronic and thermal Enthalpies= -786.285805
Sum of electronic and thermal Free Energies= -786.340797

^{3}[3-NO-9MOG]$^+$
N1 1.498349 -0.769285 0.030385
C2 2.525945 0.226247 0.014666
N3 1.847659 1.432132 0.004546
C4 0.488550 1.217312 0.023212
C5 -0.592633 2.145247 -0.037157
O6 -0.586016 3.346737 -0.082514
N7 -1.868244 1.444382 -0.051107
H8 -2.666272 2.071730 -0.089900
C9 -2.070541 0.128372 0.020931
N10 -3.281935 -0.401601 0.093653
H11 -4.105771 0.181032 0.136461
H12 -3.411991 -1.402616 0.155630
N13 -0.972915 -0.699035 -0.003564
C14 0.302721 -0.137007 0.037440
C15 1.828655 -2.190951 0.015246
H16 1.490947 -2.678337 0.930626
H17 1.398281 -2.676518 -0.862159
H18 2.916466 -2.244463 -0.040134
O19 -1.268373 -2.955578 -0.406992
N20 -1.174966 -2.027101 0.385834
O21 3.708766 0.012472 0.006984
H22 2.311504 2.328371 -0.034605

Zero-point correction= 0.158718 (Hartree/Particle)
Thermal correction to Energy= 0.172183
Thermal correction to Enthalpy= 0.173128
Thermal correction to Gibbs Free Energy= 0.117627
Sum of electronic and zero-point Energies= -786.298795
Sum of electronic and thermal Energies= -786.285329
Sum of electronic and thermal Enthalpies= -786.284385
Sum of electronic and thermal Free Energies= -786.339886

TS-^{3}[3-ON-9MOG]$^+$
N1 -1.556455 -0.705491 -0.225276
C2 -2.499670 0.333317 0.015170
N3 -1.725028 1.470978 0.214403
C4 -0.390691 1.159457 0.135477
C5 0.758291 2.012848 0.094903
O6 0.844452 3.201868 0.240409
N7 1.963964 1.247303 -0.194157
H8 2.802067 1.819143 -0.252863
C9 2.049089 -0.076322 -0.331788
N10 3.204456 -0.711686 -0.414513
H11 4.082778 -0.234086 -0.270307
H12 3.225721 -1.711241 -0.568529
N13 0.883307 -0.805189 -0.429429
C14 -0.312152 -0.178269 -0.140207
C15 -1.964589 -2.076631 -0.502858
H16 -1.437741 -2.452848 -1.381048
H17 -1.776760 -2.718609 0.359622
H18 -3.036018 -2.047182 -0.702056
O19 1.054753 -2.219144 0.206194
N20 1.057127 -2.166888 1.488759
O21 -3.695831 0.217727 0.024515
H22 -2.120306 2.391629 0.343544

Zero-point correction= 0.155686 (Hartree/Particle)
Thermal correction to Energy= 0.169087
Thermal correction to Enthalpy= 0.170031
Thermal correction to Gibbs Free Energy= 0.114757
Sum of electronic and zero-point Energies= -786.251816
Sum of electronic and thermal Energies= -786.238416
Sum of electronic and thermal Enthalpies= -786.237472
Sum of electronic and thermal Free Energies= -786.292746

^{3}[3-ON-9MOG]$^+$
N1 -1.524407 -0.735111 -0.064915
C2 -2.514500 0.302338 -0.013577
N3 -1.791662 1.476226 0.042739
C4 -0.437272 1.210564 0.022786
C5 0.678530 2.095158 0.069405
O6 0.720094 3.295282 0.141598
N7 1.928296 1.346923 0.013977
H8 2.749532 1.944413 0.017189
C9 2.082274 0.024370 -0.085130
N10 3.267596 -0.558271 -0.213335
H11 4.113849 -0.009966 -0.260594
H12 3.347535 -1.558654 -0.327383
N13 0.954750 -0.733807 -0.033545
C14 -0.307921 -0.147642 -0.050469
C15 -1.914312 -2.138799 -0.146651
H16 -1.531105 -2.594374 -1.060312
H17 -1.573491 -2.687224 0.733569
H18 -3.004605 -2.143734 -0.169580
O19 1.097344 -2.085056 -0.328753
N20 1.121338 -2.813361 0.809248
O21 -3.704195 0.128031 -0.022784

H22 -2.219828 2.389365 0.089247

Zero-point correction= 0.157686 (Hartree/Particle)
Thermal correction to Energy= 0.171283
Thermal correction to Enthalpy= 0.172227
Thermal correction to Gibbs Free Energy= 0.116563
Sum of electronic and zero-point Energies= -786.255162
Sum of electronic and thermal Energies= -786.241566
Sum of electronic and thermal Enthalpies= -786.240621
Sum of electronic and thermal Free Energies= -786.296285

TS-^{3}[5-NO-9MOG]$^+$

C1 1.268865 -1.324855 -0.574879
C2 -0.037003 -0.805918 -0.067681
H3 3.221621 -0.697595 -0.614423
C4 2.064453 0.947561 -0.090658
C5 -2.204059 -0.242623 -0.452802
N6 2.284746 -0.367450 -0.406430
N7 -1.257545 -1.269693 -0.480438
N8 -1.452419 0.960744 -0.219550
N9 0.842023 1.505639 -0.019495
C10 -0.162234 0.671268 -0.106834
N11 3.105999 1.735544 0.106995
H12 2.929867 2.711636 0.305617
H13 4.061449 1.409858 0.095309
O14 1.465499 -2.418976 -1.019113
O15 -0.744790 -0.844173 2.374598
C16 -2.059110 2.288736 -0.218538
H17 -1.726584 2.846698 -1.095101
H18 -3.139367 2.151707 -0.250182
H19 -1.771758 2.813031 0.693025
N20 0.192831 -1.081815 1.676309
O21 -3.381892 -0.308964 -0.619311
H22 -1.520676 -2.244230 -0.557014

Zero-point correction= 0.157758 (Hartree/Particle)
Thermal correction to Energy= 0.171113
Thermal correction to Enthalpy= 0.172057
Thermal correction to Gibbs Free Energy= 0.116500
Sum of electronic and zero-point Energies= -786.347970
Sum of electronic and thermal Energies= -786.334616
Sum of electronic and thermal Enthalpies= -786.333672
Sum of electronic and thermal Free Energies= -786.389229

^{3}[5-NO-9MOG]$^+$

C1 1.210459 -1.310751 -0.613995
C2 -0.050885 -0.839480 0.104461
H3 3.157572 -0.687094 -0.818390
C4 2.062520 0.926447 -0.093443
C5 -2.214003 -0.230729 -0.409900
N6 2.248678 -0.371159 -0.495737
N7 -1.303287 -1.267836 -0.387029
N8 -1.438450 0.975450 -0.179071
N9 0.850424 1.489743 0.046440
C10 -0.167228 0.671585 -0.016931
N11 3.122017 1.690167 0.097437
H12 2.970285 2.659578 0.343947
H13 4.070648 1.350142 0.035334
O14 1.341683 -2.366829 -1.156471
O15 -0.553537 -0.815755 2.427635
C16 -2.015738 2.312114 -0.282339
H17 -1.664431 2.796573 -1.194915
H18 -3.098309 2.194368 -0.314275
H19 -1.722562 2.896240 0.590068
N20 0.197111 -1.188705 1.544337
O21 -3.387218 -0.248143 -0.616871
H22 -1.606826 -2.232720 -0.387871

Zero-point correction= 0.159550 (Hartree/Particle)
Thermal correction to Energy= 0.172842
Thermal correction to Enthalpy= 0.173786
Thermal correction to Gibbs Free Energy= 0.118603
Sum of electronic and zero-point Energies= -786.351301
Sum of electronic and thermal Energies= -786.338009
Sum of electronic and thermal Enthalpies= -786.337065
Sum of electronic and thermal Free Energies= -786.392247

TS-^{3}[5-ON-9MOG]$^+$

C1 1.260158 -1.310054 -0.576587
C2 -0.044550 -0.792810 -0.054004
H3 3.211779 -0.680062 -0.628018
C4 2.055525 0.958453 -0.078972
C5 -2.214344 -0.234942 -0.418226
N6 2.275611 -0.353357 -0.411207
N7 -1.264240 -1.259080 -0.453708
N8 -1.461875 0.974423 -0.191013
N9 0.833435 1.518290 0.001161
C10 -0.172699 0.688705 -0.090367
N11 3.097249 1.743470 0.123741
H12 2.921917 2.717593 0.333374
H13 4.052614 1.417143 0.108823
O14 1.449497 -2.400787 -1.031399
C15 -2.074938 2.299232 -0.179002
H16 -1.741248 2.867079 -1.048756
H17 -3.154362 2.157132 -0.216030
H18 -1.793562 2.815525 0.739063
O19 0.236829 -1.059194 1.600396
N20 -0.792931 -1.000321 2.318957
O21 -3.391129 -0.299485 -0.580208
H22 -1.524377 -2.234159 -0.531333

Zero-point correction= 0.156980 (Hartree/Particle)
Thermal correction to Energy= 0.170302
Thermal correction to Enthalpy= 0.171246
Thermal correction to Gibbs Free Energy= 0.115719
Sum of electronic and zero-point Energies= -786.325049
Sum of electronic and thermal Energies= -786.311726
Sum of electronic and thermal Enthalpies= -786.310782
Sum of electronic and thermal Free Energies= -786.366309

^{3}[5-ON-9MOG]$^+$

C1 1.205150 -1.311182 -0.594251
C2 -0.050240 -0.833318 0.134316

H3 3.146449 -0.677090 -0.825980
C4 2.045947 0.935420 -0.104988
C5 -2.222299 -0.258197 -0.366156
N6 2.237287 -0.363216 -0.502151
N7 -1.302177 -1.286531 -0.303384
N8 -1.455757 0.963359 -0.182298
N9 0.831247 1.496442 0.031886
C10 -0.182739 0.673760 -0.013646
N11 3.101832 1.705152 0.078334
H12 2.945995 2.675515 0.318909
H13 4.051960 1.368527 0.019151
O14 1.333527 -2.374132 -1.123797
C15 -2.047152 2.290930 -0.312896
H16 -1.660598 2.779674 -1.208667
H17 -3.125356 2.157521 -0.393471
H18 -1.803487 2.879900 0.571692
O19 0.272106 -1.163610 1.521321
N20 -0.577095 -0.696107 2.417995
O21 -3.394118 -0.292913 -0.573248
H22 -1.586446 -2.256982 -0.312792

Zero-point correction= 0.158716 (Hartree/Particle)
Thermal correction to Energy= 0.172024
Thermal correction to Enthalpy= 0.172968
Thermal correction to Gibbs Free Energy= 0.117713
Sum of electronic and zero-point Energies= -786.328587
Sum of electronic and thermal Energies= -786.315279
Sum of electronic and thermal Enthalpies= -786.314335
Sum of electronic and thermal Free Energies= -786.369591

TS-^{3}[8-NO-9MOG]$^+$

C1 1.559109 -1.459618 -0.196956
C2 0.212200 -0.879066 -0.411882
H3 3.475749 -0.817777 0.135769
C4 2.270848 0.876270 0.041992
C5 -2.230864 -0.106410 -0.313319
N6 2.531759 -0.468615 0.005493
N7 -0.879286 -1.474350 -0.703389
N8 -1.227817 0.937904 -0.313606
N9 1.046336 1.407560 -0.054955
C10 0.045349 0.569188 -0.244154
N11 3.287822 1.708732 0.204613
H12 3.086312 2.698539 0.245833
H13 4.247443 1.408349 0.289255
O14 1.816527 -2.633434 -0.216141
C15 -1.702466 2.321216 -0.209999
H16 -2.033114 2.523092 0.811805
H17 -0.878455 2.982765 -0.470549
H18 -2.531213 2.448766 -0.906089
N19 -2.242597 -0.819750 1.152055
O20 -1.460508 -0.479944 1.984195
O21 -3.230353 -0.101532 -0.940373
H22 -0.910619 -2.494297 -0.753039

Zero-point correction= 0.155407 (Hartree/Particle)
Thermal correction to Energy= 0.168950
Thermal correction to Enthalpy= 0.169894
Thermal correction to Gibbs Free Energy= 0.114203
Sum of electronic and zero-point Energies= -786.289575
Sum of electronic and thermal Energies= -786.276033
Sum of electronic and thermal Enthalpies= -786.275089
Sum of electronic and thermal Free Energies= -786.330780

^{3}[8-NO-9MOG]$^+$

C1 -1.886477 1.403483 -0.001064
C2 -0.416876 1.055997 0.042951
H3 -3.733877 0.516392 0.009446
C4 -2.291060 -0.987136 0.071542
C5 2.268532 0.147554 -0.562546
N6 -2.741784 0.302155 0.015018
N7 0.484040 1.921880 0.219858
N8 1.191512 -0.772367 -0.190783
N9 -1.003915 -1.334258 0.014343
C10 -0.071027 -0.395680 -0.064031
N11 -3.182986 -1.960606 0.165519
H12 -2.843651 -2.912601 0.186429
H13 -4.178399 -1.802044 0.216170
O14 -2.288716 2.534564 -0.019745
C15 1.551891 -2.202085 -0.220059
H16 2.637203 -2.283504 -0.171216
H17 1.104779 -2.703732 0.637397
H18 1.190078 -2.652279 -1.146638
N19 3.164979 0.395048 0.480537
O20 3.046241 0.050520 1.632089
O21 2.419432 0.536562 -1.681592
H22 0.095393 2.868857 0.290200

Zero-point correction= 0.157911 (Hartree/Particle)
Thermal correction to Energy= 0.171867
Thermal correction to Enthalpy= 0.172811
Thermal correction to Gibbs Free Energy= 0.115128
Sum of electronic and zero-point Energies= -786.309488
Sum of electronic and thermal Energies= -786.295533
Sum of electronic and thermal Enthalpies= -786.294588
Sum of electronic and thermal Free Energies= -786.352272

TS-^{3}[8-ON-9MOG]$^+$

C1 -1.593231 1.411996 -0.217811
C2 -0.205334 0.930968 -0.490435
H3 -3.450752 0.656334 0.213258
C4 -2.152930 -0.955867 0.034756
C5 2.318347 0.079580 -0.182427
N6 -2.494591 0.365064 0.035838
N7 0.785145 1.626667 -0.874063
N8 1.340371 -0.874740 -0.418717
N9 -0.896218 -1.405245 -0.116800
C10 0.045592 -0.508356 -0.296685
N11 -3.100854 -1.860243 0.216951
H12 -2.828663 -2.833698 0.240420
H13 -4.075220 -1.628904 0.343409
O14 -1.931932 2.562793 -0.238414
C15 1.764363 -2.289432 -0.343585

H16 1.750432 -2.628931 0.694090
H17 1.067987 -2.875809 -0.939988
H18 2.767413 -2.361702 -0.760802
O19 1.957031 0.775896 1.388329
N20 0.878661 0.484691 1.892603
O21 3.413430 0.245426 -0.528228
H22 0.612147 2.633115 -0.937453

Zero-point correction= 0.154876 (Hartree/Particle)
Thermal correction to Energy= 0.168679
Thermal correction to Enthalpy= 0.169623
Thermal correction to Gibbs Free Energy= 0.113586
Sum of electronic and zero-point Energies= -786.270326
Sum of electronic and thermal Energies= -786.256524
Sum of electronic and thermal Enthalpies= -786.255580
Sum of electronic and thermal Free Energies= -786.311617

^{3}[8-ON-9MOG]$^+$

C1 -1.862076 1.411546 -0.013603
C2 -0.396560 1.051471 0.019112
H3 -3.715267 0.536419 0.002899
C4 -2.284637 -0.978322 0.049617
C5 2.284774 0.129658 -0.515110
N6 -2.724666 0.314904 0.003904
N7 0.521969 1.904206 0.163164
N8 1.204189 -0.779258 -0.157390
N9 -0.998628 -1.336161 -0.001938
C10 -0.062233 -0.402812 -0.066265
N11 -3.183370 -1.945899 0.129593
H12 -2.850530 -2.900407 0.146530
H13 -4.178244 -1.781257 0.173403
O14 -2.256442 2.545131 -0.029459
C15 1.570975 -2.209274 -0.172181
H16 2.653885 -2.286428 -0.081335
H17 1.094187 -2.707293 0.671039
H18 1.244027 -2.661163 -1.110609
O19 3.135595 0.392560 0.521917
N20 2.756533 0.071941 1.751595
O21 2.503273 0.476882 -1.624301
H22 0.158888 2.861811 0.220892

Zero-point correction= 0.157015 (Hartree/Particle)
Thermal correction to Energy= 0.171021
Thermal correction to Enthalpy= 0.171965
Thermal correction to Gibbs Free Energy= 0.114285
Sum of electronic and zero-point Energies= -786.285850
Sum of electronic and thermal Energies= -786.271845
Sum of electronic and thermal Enthalpies= -786.270901
Sum of electronic and thermal Free Energies= -786.328581

TS-^{3}[2,4-NO-9MOG]$^+$

C1 0.338884 -0.465925 -0.193350
C2 0.241099 0.992150 -0.060519
C3 -1.088618 1.677614 -0.148510
C4 -1.914955 -0.684189 -0.098167
C5 2.431146 0.384831 -0.024983
O6 -1.190837 2.878363 -0.118455
N7 1.428926 1.470752 0.072828
N8 1.681199 -0.752689 -0.263896
N9 -0.679282 -1.051579 -0.881002
N10 -3.094629 -1.354579 -0.407764
H11 -3.185505 -2.244735 0.066599
H12 -3.284812 -1.428074 -1.399940
C13 2.261518 -2.093941 -0.370413
H14 2.106413 -2.641528 0.560630
H15 3.328256 -1.977258 -0.557525
H16 1.795911 -2.614295 -1.207569
N17 -2.082630 0.747434 -0.308986
H18 -3.042639 1.083441 -0.317454
N19 -1.536220 -0.965839 1.319436
O20 -0.289677 -0.692339 1.455093
O21 3.601892 0.545869 0.075737
H22 1.675358 2.449571 0.217608

Zero-point correction= 0.156313 (Hartree/Particle)
Thermal correction to Energy= 0.168762
Thermal correction to Enthalpy= 0.169707
Thermal correction to Gibbs Free Energy= 0.116917
Sum of electronic and zero-point Energies= -786.239161
Sum of electronic and thermal Energies= -786.226712
Sum of electronic and thermal Enthalpies= -786.225768
Sum of electronic and thermal Free Energies= -786.278558

^{3}[2,4-NO-9MOG]$^+$

C1 0.300516 -0.480183 0.004740
C2 0.232548 1.026686 0.014818
C3 -1.109803 1.712989 -0.011760
C4 -1.896082 -0.681938 -0.158969
C5 2.427037 0.392903 -0.093391
O6 -1.202731 2.912581 0.071882
N7 1.411806 1.504971 0.001176
N8 1.674116 -0.744228 -0.143551
N9 -0.662045 -0.905652 -0.952818
N10 -3.064548 -1.319782 -0.580875
H11 -3.206459 -2.225412 -0.150544
H12 -3.185449 -1.347401 -1.586081
C13 2.247161 -2.091188 -0.217637
H14 2.063107 -2.624458 0.716149
H15 3.319860 -1.985067 -0.375540
H16 1.804185 -2.622528 -1.060971
N17 -2.093499 0.784912 -0.180932
H18 -3.060522 1.098977 -0.189809
N19 -1.550611 -1.124429 1.211316
O20 -0.218215 -0.936676 1.301573
O21 3.594102 0.594698 -0.133164
H22 1.665237 2.494909 0.017440

Zero-point correction= 0.157851 (Hartree/Particle)
Thermal correction to Energy= 0.170443
Thermal correction to Enthalpy= 0.171387
Thermal correction to Gibbs Free Energy= 0.118249
Sum of electronic and zero-point Energies= -786.244048
Sum of electronic and thermal Energies= -786.231455

Sum of electronic and thermal Enthalpies= -786.230511
Sum of electronic and thermal Free Energies= -786.283649

TS-7,8-NO-addition (concerted from precursor)

C1 1.433101 -1.491785 -0.236732
C2 0.173416 -0.778400 -0.207974
H3 3.432934 -1.059303 -0.071544
C4 2.402718 0.740432 0.096697
C5 -2.112503 0.123126 -0.360339
N6 2.522137 -0.612104 -0.074154
N7 -1.098134 -1.287899 -0.251874
N8 -1.093575 1.121797 -0.141538
N9 1.232875 1.392280 0.092691
C10 0.152523 0.647656 -0.058781
N11 3.504661 1.456821 0.267892
H12 3.405906 2.455289 0.389597
H13 4.431350 1.058489 0.286944
O14 1.570511 -2.683449 -0.380869
O15 -2.478008 -0.431598 1.206548
C16 -1.489875 2.524212 -0.046782
H17 -1.969195 2.701227 0.918928
H18 -0.594168 3.136356 -0.137917
H19 -2.190336 2.738262 -0.855156
N20 -1.807312 -1.522446 1.170702
O21 -3.022032 0.197699 -1.109423
H22 -1.261090 -2.122122 -0.823474

Zero-point correction= 0.155994 (Hartree/Particle)
Thermal correction to Energy= 0.169028
Thermal correction to Enthalpy= 0.169973
Thermal correction to Gibbs Free Energy= 0.115405
Sum of electronic and zero-point Energies= -786.257155
Sum of electronic and thermal Energies= -786.244120
Sum of electronic and thermal Enthalpies= -786.243176
Sum of electronic and thermal Free Energies= -786.297744

TS-7,8-NO-addition (from 8-ON)

C1 -1.708787 1.418720 -0.187615
C2 -0.304289 0.941758 -0.249490
H3 -3.620149 0.689656 -0.017721
C4 -2.300734 -0.917067 0.088479
C5 2.421990 -0.219355 -0.209325
N6 -2.649888 0.393242 -0.041552
N7 0.698616 1.735675 -0.440621
N8 1.210879 -0.954718 0.020752
N9 -1.036255 -1.352062 0.107999
C10 -0.048677 -0.480764 -0.029851
N11 -3.258908 -1.823616 0.211489
H12 -2.985097 -2.791289 0.311931
H13 -4.242573 -1.598564 0.203879
O14 -2.026855 2.577009 -0.274556
C15 1.410138 -2.425028 0.056866
H16 2.469418 -2.623590 0.196488
H17 0.836020 -2.830367 0.888116
H18 1.071596 -2.866725 -0.881432
O19 2.739147 0.783709 0.717049
N20 1.827773 1.582295 1.185012
O21 3.248789 -0.569861 -0.979111
H22 0.418787 2.718726 -0.524258

Zero-point correction= 0.156603 (Hartree/Particle)
Thermal correction to Energy= 0.169530
Thermal correction to Enthalpy= 0.170474
Thermal correction to Gibbs Free Energy= 0.115894
Sum of electronic and zero-point Energies= -786.269270
Sum of electronic and thermal Energies= -786.256343
Sum of electronic and thermal Enthalpies= -786.255399
Sum of electronic and thermal Free Energies= -786.309979

7-member macrocycle 1

C1 1.604192 -1.401041 -0.233421
C2 0.237591 -0.894866 -0.095504
H3 3.548937 -0.759912 -0.155237
C4 2.303174 0.883264 0.145577
C5 -2.397505 0.316374 -0.042171
N6 2.593317 -0.426514 -0.083528
N7 -0.773852 -1.781953 -0.295516
N8 -1.202463 1.063374 -0.071820
N9 1.055885 1.354696 0.177888
C10 0.034747 0.515984 0.050981
N11 3.296741 1.742621 0.331563
H12 3.061299 2.712531 0.489508
H13 4.269128 1.473980 0.343213
O14 1.864200 -2.562067 -0.458944
O15 -2.389360 -0.725043 0.894094
C16 -1.322648 2.513531 -0.327407
H17 -0.973842 3.060791 0.548702
H18 -0.717610 2.780325 -1.194092
H19 -2.369329 2.729643 -0.524037
N20 -1.782834 -1.909520 0.686291
O21 -3.403295 0.639666 -0.579163
H22 -0.455812 -2.716211 -0.558433

Zero-point correction= 0.159350 (Hartree/Particle)
Thermal correction to Energy= 0.172276
Thermal correction to Enthalpy= 0.173220
Thermal correction to Gibbs Free Energy= 0.118389
Sum of electronic and zero-point Energies= -786.302366
Sum of electronic and thermal Energies= -786.289440
Sum of electronic and thermal Enthalpies= -786.288496
Sum of electronic and thermal Free Energies= -786.343327

TS-7,8-ON-addition (from 8-NO)

C1 1.696752 -1.391406 -0.177155
C2 0.300537 -0.916193 -0.217935
H3 3.608127 -0.666794 -0.025699
C4 2.284829 0.940149 0.094137
C5 -2.476093 0.245792 -0.105585
N6 2.637916 -0.370206 -0.041147
N7 -0.685037 -1.763843 -0.453391
N8 -1.228858 0.982131 -0.020688

N9 1.021381 1.366584 0.108903
C10 0.027156 0.494322 -0.024298
N11 3.242400 1.848083 0.222749
H12 2.966869 2.815154 0.323856
H13 4.226166 1.623910 0.223527
O14 2.005961 -2.555159 -0.269105
C15 -1.391650 2.455362 -0.022741
H16 -2.454084 2.678761 -0.027957
H17 -0.913967 2.864363 0.867144
H18 -0.923779 2.871521 -0.915530
N19 -2.659077 -0.888909 0.711029
O20 -1.727486 -1.736401 0.844350
O21 -3.412009 0.713102 -0.689302
H22 -0.391332 -2.744295 -0.503614

Zero-point correction= 0.157107 (Hartree/Particle)
Thermal correction to Energy= 0.169774
Thermal correction to Enthalpy= 0.170718
Thermal correction to Gibbs Free Energy= 0.116904
Sum of electronic and zero-point Energies= -786.263252
Sum of electronic and thermal Energies= -786.250586
Sum of electronic and thermal Enthalpies= -786.249641
Sum of electronic and thermal Free Energies= -786.303455

7-member macrocycle 2

C1 1.630516 -1.403022 -0.234235
C2 0.269173 -0.904784 -0.043765
H3 3.563481 -0.727765 -0.276019
C4 2.306525 0.897081 0.089031
C5 -2.425382 0.287142 -0.194771
N6 2.606972 -0.409631 -0.162010
N7 -0.731527 -1.802876 -0.133619
N8 -1.206246 1.024664 0.048583
N9 1.059626 1.352222 0.188187
C10 0.038241 0.504643 0.086748
N11 3.299900 1.767282 0.222907
H12 3.062434 2.735017 0.390176
H13 4.274282 1.511052 0.173496
O14 1.892943 -2.570348 -0.423264
C15 -1.352818 2.495307 0.004491
H16 -2.410004 2.732258 0.086153
H17 -0.797053 2.925244 0.836095
H18 -0.963752 2.879839 -0.939840
N19 -2.722839 -0.827329 0.616157
O20 -1.762344 -1.712260 0.846654
O21 -3.281267 0.750153 -0.893563
H22 -0.462771 -2.784544 -0.215109

Zero-point correction= 0.159000 (Hartree/Particle)
Thermal correction to Energy= 0.171807
Thermal correction to Enthalpy= 0.172751
Thermal correction to Gibbs Free Energy= 0.118831
Sum of electronic and zero-point Energies= -786.267029
Sum of electronic and thermal Energies= -786.254222
Sum of electronic and thermal Enthalpies= -786.253278
Sum of electronic and thermal Free Energies= -786.307197