Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

AMIDINOQUINOXALINE *N*-OXIDES: SPIN TRAPPING OF O- AND C-CENTERED RADICALS

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Scheme 1 SI: Synthesis of nitrones **1-5**

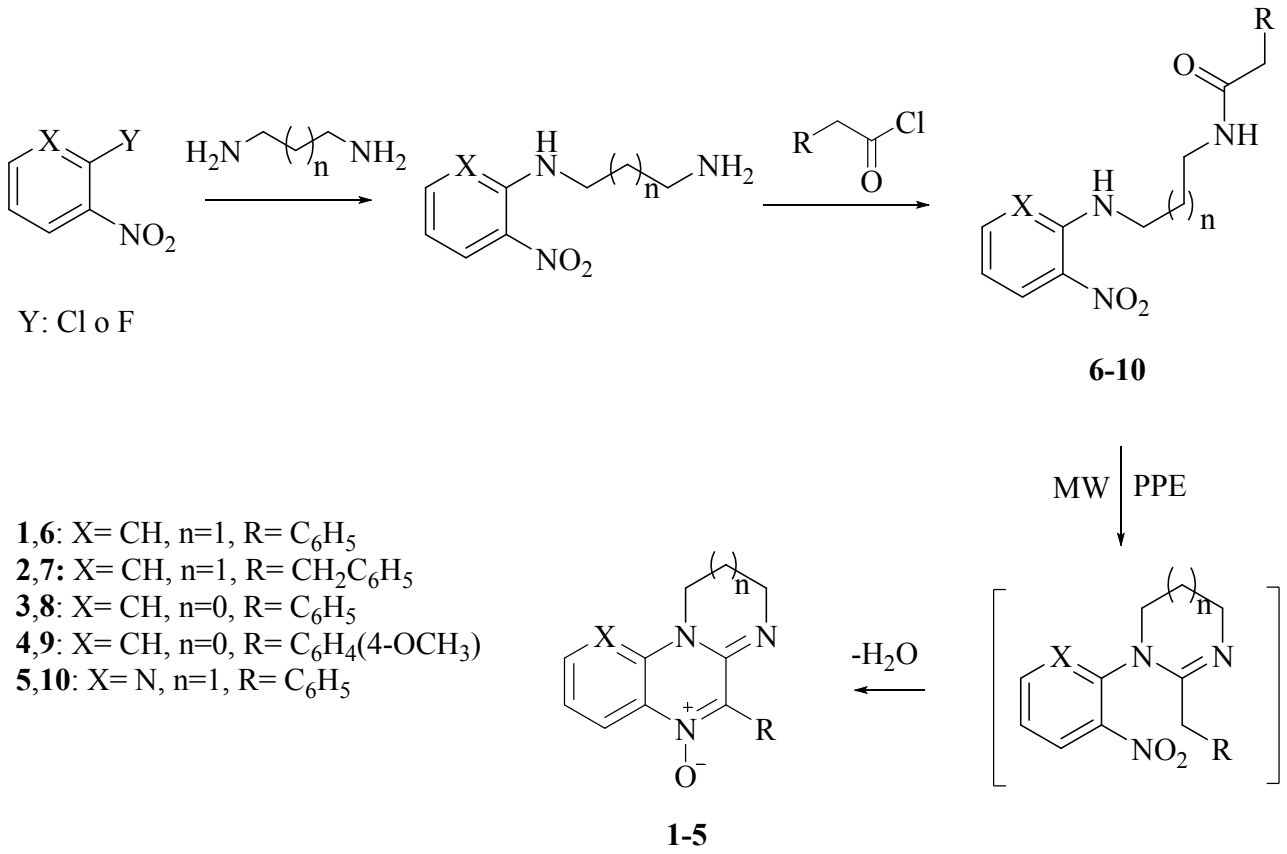


Table 1 SI: Selected bond distances (Å), dihedral angles (°) for nitrones **1-5** computed at the B3LYP/6-31+G(d,p)// B3LYP/6-31G(d) level.

Nitrone	N(19)-C(8)	N(19)-O(22)	C(8)-N(19)-C(3)-C(4)
1	1.33966	1.2748	4.075
2	1.33021	1.27925	4.278
3	1.34890	1.27286	0.151
4	1.35041	1.27511	0.590
5	1.34027	1.27563	1.280

^{1}H and ^{13}C NMR spectra of compounds 4, 8, 9

Figure 1 SI. ^{1}H NMR spectrum of compound **4** (600 MHz, $CDCl_3$).

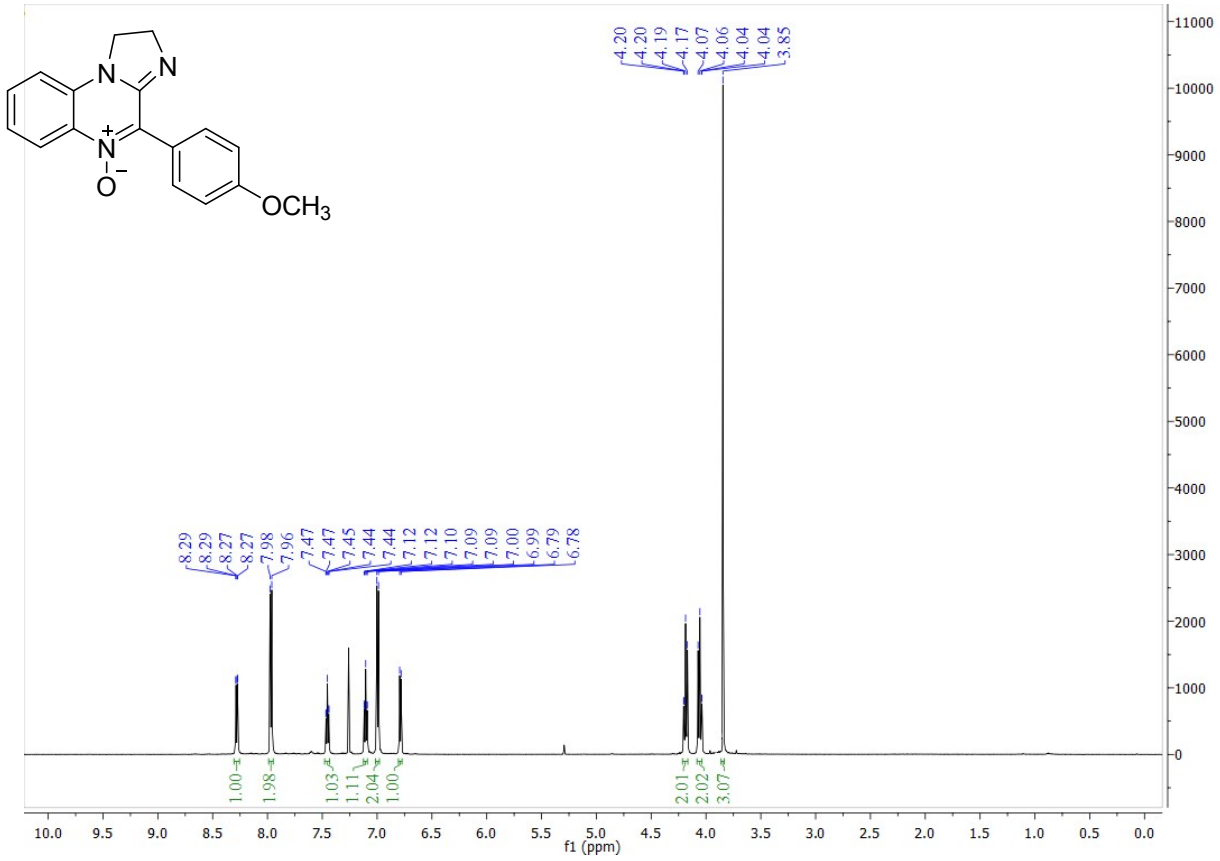


Figure 2 SI. ^{13}C NMR spectrum of compound **4** (125 MHz, $CDCl_3$).

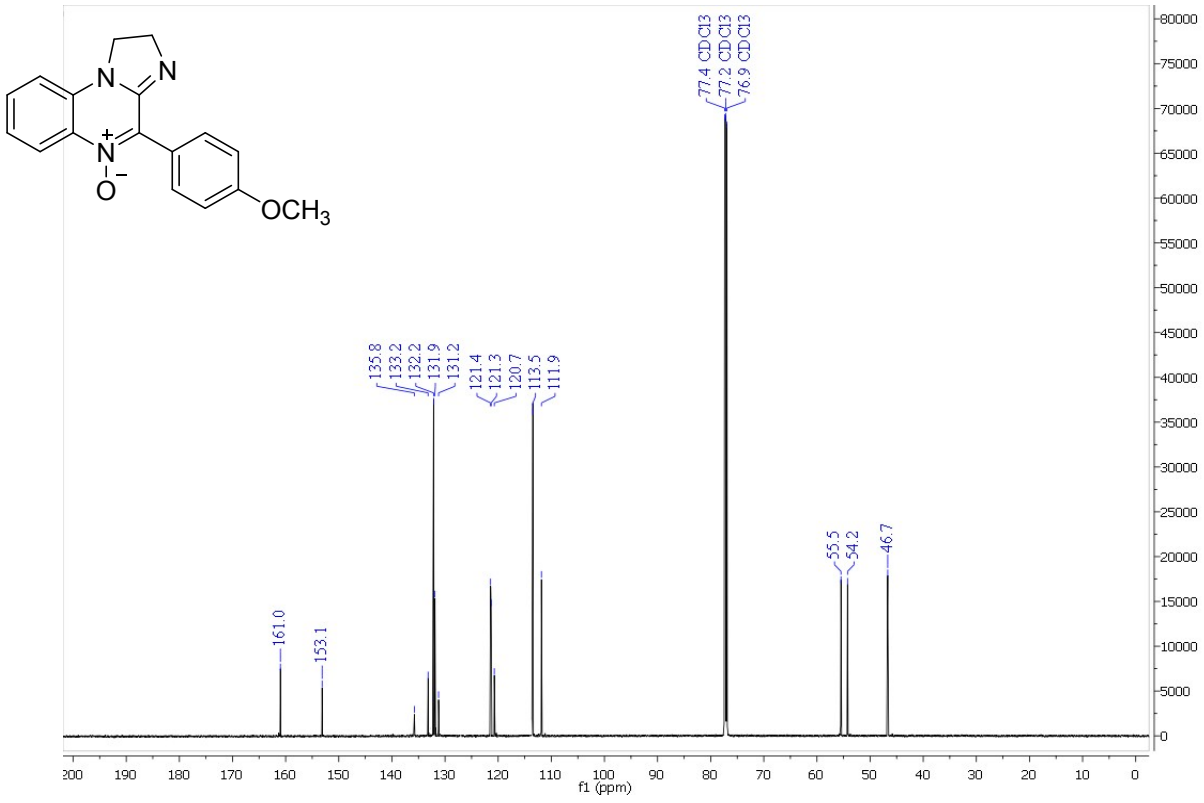


Figure 3 SI. ^{1}H NMR spectrum of compound **8** (500 MHz, $CDCl_3$).

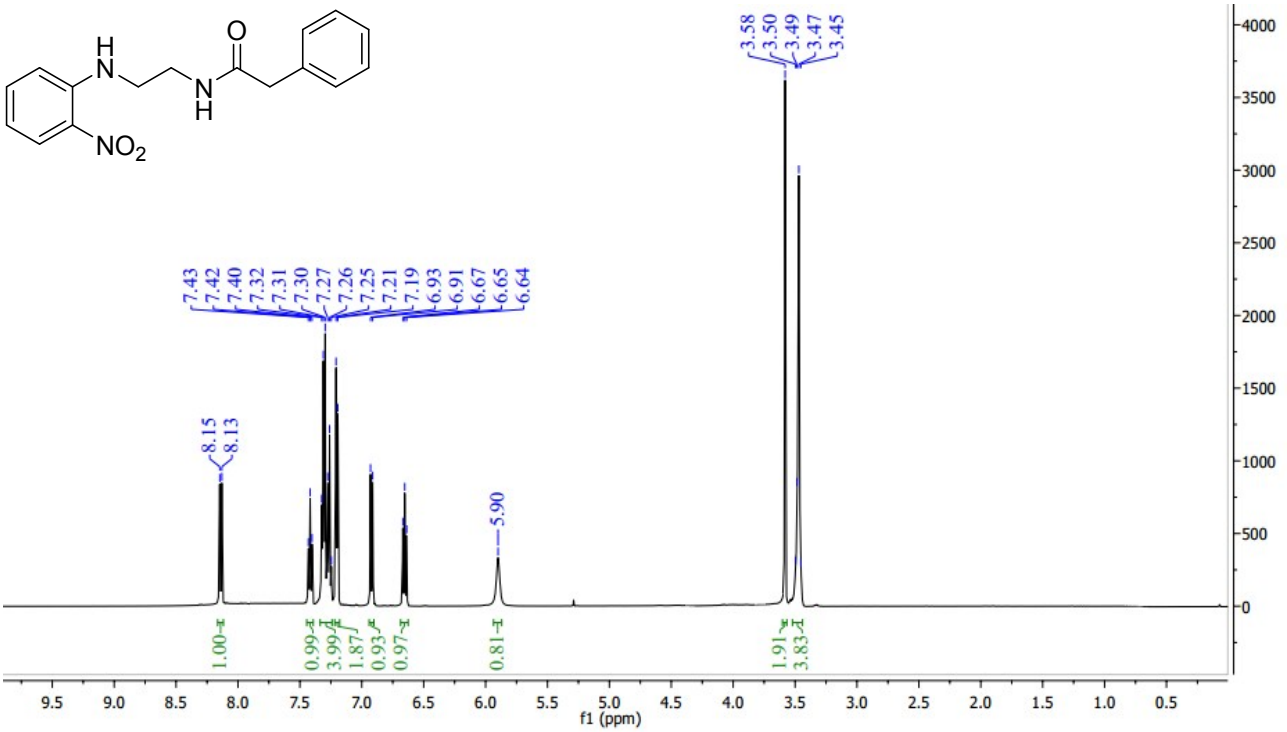


Figure 4 SI. ^{13}C NMR spectrum of compound **8** (125 MHz, $CDCl_3$).

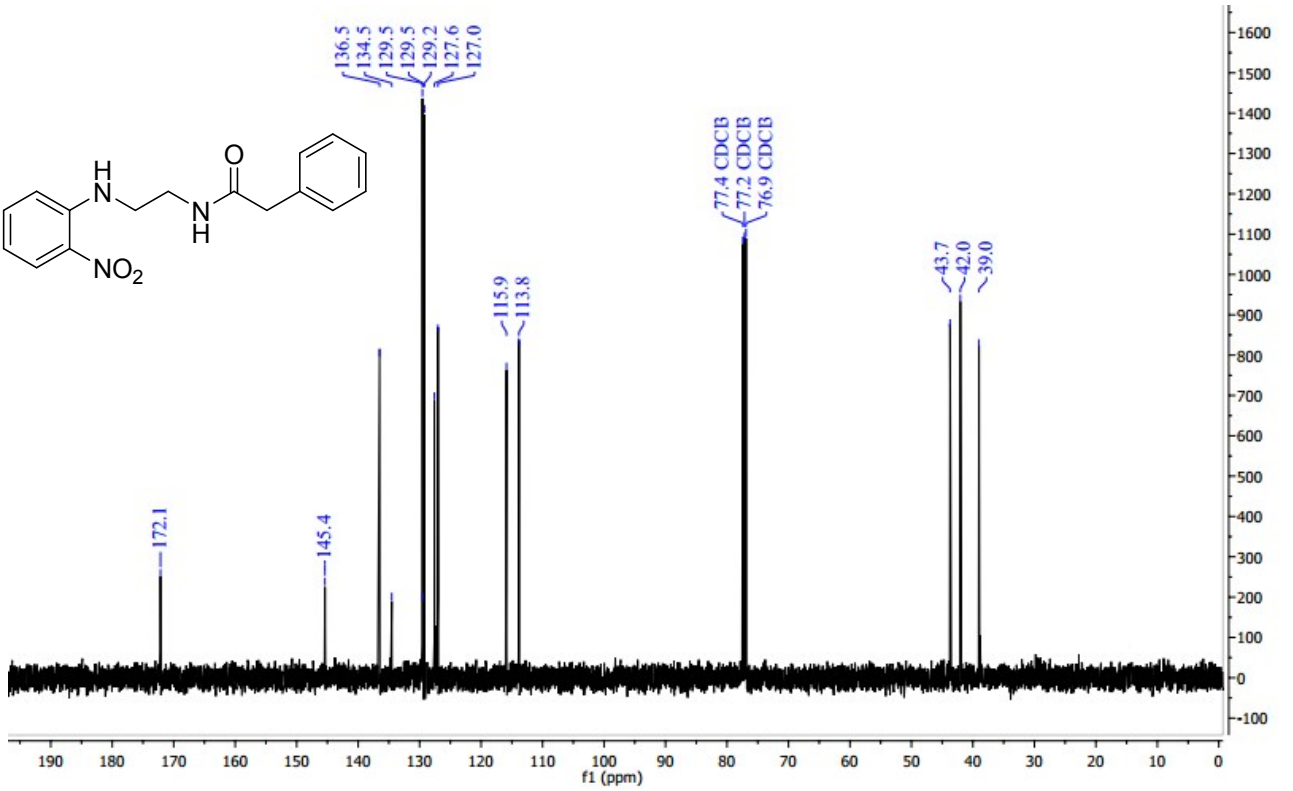


Figure 5 SI. ^{1}H NMR spectrum of compound **9** (300 MHz, $CDCl_3$).

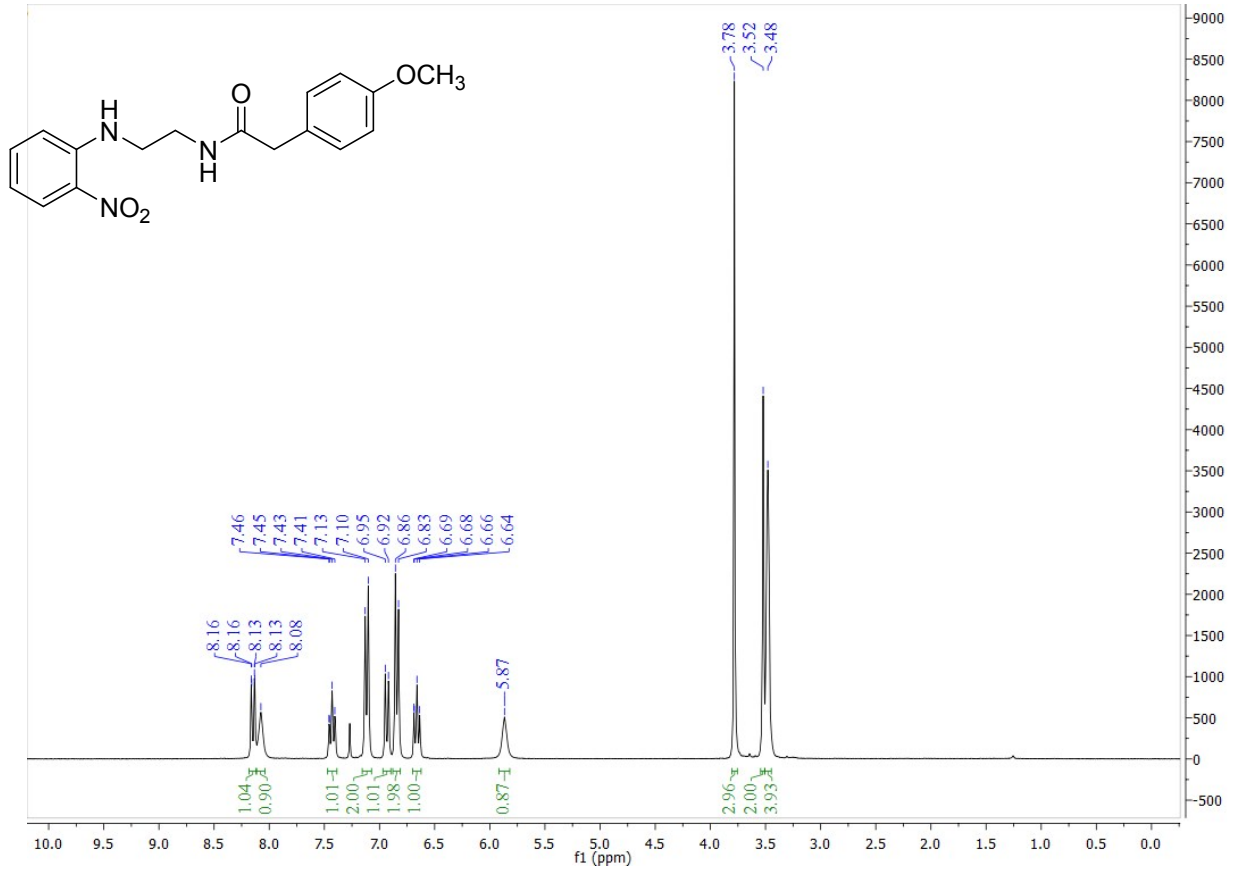
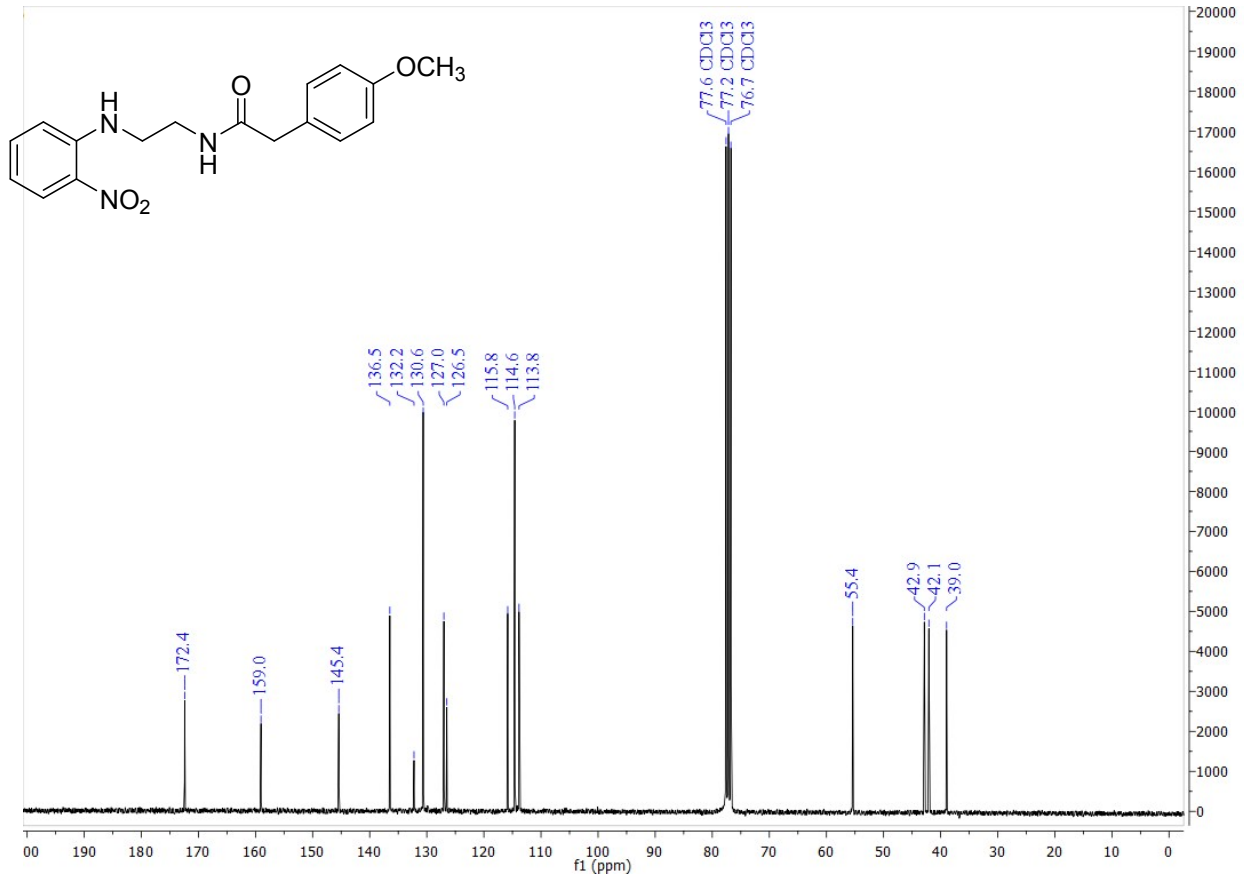


Figure 6 SI. ^{13}C NMR spectrum of compound **9** (75 MHz, $CDCl_3$).



M062X/6-31+G(d,p)//B3LYP/6-31G(d) cartesian coordinates and thermochemical parameters from frequency calculations of nitrones 1-5.

Nitrone 1

C	-3.67429700	-2.45247300	-0.08653400
C	-2.28515500	-2.49154600	-0.10050900
C	-1.55697900	-1.30359700	-0.06203600
C	-2.19092400	-0.04895600	-0.01589000
C	-3.59871200	-0.02827600	0.00500400
C	-4.32318100	-1.21617100	-0.03119500
C	-0.02234600	1.04563800	0.17692900
C	0.61798300	-0.27065800	0.00925000
C	0.11973600	3.36314700	0.59821700
C	-1.09957800	3.53349600	-0.30629600
C	-2.09429200	2.41357700	-0.02302700
H	-4.24495400	-3.37521700	-0.11537300
H	-1.72764800	-3.41808900	-0.14470500
H	-4.13048100	0.91275800	0.06450500
H	-5.40852300	-1.17023800	-0.01084200
H	-0.17102800	3.51182400	1.65130000
H	-0.78031300	3.48968100	-1.35469800
H	-2.85803800	2.38038200	-0.80713400
N	-0.12292800	-1.38233700	-0.09023000
N	-1.42233600	1.10585800	0.01584500
N	0.73069700	2.05557900	0.44505300
O	0.37719500	-2.54807800	-0.21690300
C	2.09362000	-0.39219600	-0.01934900
C	2.86281900	0.47330300	-0.81452900
C	2.75317200	-1.37429200	0.73874200
C	4.25005400	0.35611000	-0.85497200
H	2.36928300	1.24266200	-1.39586400
C	4.14232100	-1.47380400	0.71322800
H	2.17380300	-2.06455000	1.33901700
C	4.89644400	-0.61398500	-0.08716300
H	4.82695900	1.02873200	-1.48419800
H	4.63533200	-2.23373900	1.31366500
H	5.97961600	-0.70096300	-0.11423900
H	-2.60792000	2.58771800	0.93298600
H	-1.59286700	4.49963800	-0.15170900
H	0.87707500	4.12443700	0.37860700

Zero-point correction= 0.292532 (Hartree/Particle)
Thermal correction to Energy= 0.308018
Thermal correction to Enthalpy= 0.308962
Thermal correction to Gibbs Free Energy= 0.250009
Sum of electronic and zero-point Energies= -895.638929
Sum of electronic and thermal Energies= -895.623442
Sum of electronic and thermal Enthalpies= -895.622498
Sum of electronic and thermal Free Energies= -895.681452

Nitrone 2

C	-3.79181500	-2.43398000	-0.48070900
C	-2.50439900	-2.45518000	0.04212300
C	-1.79267600	-1.26509700	0.17811500
C	-2.33640300	-0.02573500	-0.21008800
C	-3.64481500	-0.02347700	-0.72990900
C	-4.35528000	-1.21304600	-0.86143300
C	-0.34627200	1.11633600	0.60309800
C	0.21020800	-0.19398000	0.94224100
C	-0.18294100	3.46963100	0.58652400
C	-0.99357500	3.44309700	-0.70815600
C	-2.10603600	2.40572100	-0.59024100
H	-4.35146700	-3.35773600	-0.58729800
H	-2.01465100	-3.36864000	0.35425400
H	-4.11647900	0.90774000	-1.01703600
H	-5.36433300	-1.18014200	-1.26284200
H	-0.80932300	3.84231600	1.41395100
H	-0.33202700	3.18092400	-1.54244000
H	-2.54607600	2.21395700	-1.57401700
N	-0.46718800	-1.31791100	0.72460000
N	-1.58448900	1.13391700	-0.06601400
N	0.34197300	2.15912400	0.92710500
O	0.00324900	-2.47460900	1.00248100
H	-2.90718300	2.77068000	0.06759300
H	-1.43661300	4.42002500	-0.93137800
H	0.65887300	4.16617500	0.50114700
C	1.58010300	-0.30269300	1.55090300
H	1.74588600	0.59350900	2.15072600
H	1.58386400	-1.18329400	2.19888700
C	2.68208100	-0.42698400	0.50270600
C	3.39561300	0.70497800	0.08850300
C	2.99235600	-1.67018800	-0.06698000
C	4.40610000	0.59708200	-0.86853400
H	3.14700100	1.67150300	0.51753200
C	4.00157500	-1.77641400	-1.02505900
H	2.43063200	-2.54641200	0.24149400
C	4.71313800	-0.64447600	-1.42794100
H	4.95559700	1.48395300	-1.17503200
H	4.23427200	-2.74746200	-1.45529500
H	5.50218000	-0.72971400	-2.17090500

Zero-point correction= 0.321208 (Hartree/Particle)
Thermal correction to Energy= 0.337976
Thermal correction to Enthalpy= 0.338920
Thermal correction to Gibbs Free Energy= 0.276233
Sum of electronic and zero-point Energies= -934.915517
Sum of electronic and thermal Energies= -934.898749
Sum of electronic and thermal Enthalpies= -934.897805
Sum of electronic and thermal Free Energies= -934.960492

Nitrone 3

C	-3.81617800	-2.08728200	-0.13149200
C	-2.42971200	-2.19620500	-0.14159700
C	-1.64584600	-1.04506700	-0.07669200
C	-2.23614100	0.23150700	-0.00316700
C	-3.63830300	0.32995200	0.00843000
C	-4.41319000	-0.82328800	-0.05517100
C	-0.00925000	1.22167000	0.06630200
C	0.59918700	-0.10245300	-0.02376600
C	-0.38868000	3.40715800	0.23381900
C	-1.78904500	2.72291600	0.19290200
H	-4.42918200	-2.98144300	-0.18174000
H	-1.92279800	-3.15074300	-0.19798200
H	-4.10726600	1.30637900	0.06576700
H	-5.49592000	-0.73377400	-0.04536600
H	-0.25088700	3.99316800	1.14997200
H	-2.40275000	3.04430100	-0.65672700
N	-0.21015300	-1.17973700	-0.08670100
N	-1.40544700	1.31838600	0.05101800
N	0.61976900	2.34312500	0.16921900
O	0.23375700	-2.36994400	-0.16740700
C	2.06639800	-0.27143300	-0.02424100
C	2.88225200	0.66077700	-0.69289000
C	2.68561300	-1.34072800	0.65251900
C	4.26814300	0.52176600	-0.69101000
H	2.42620900	1.50048600	-1.20042200
C	4.07242700	-1.46026200	0.66737500
H	2.07649500	-2.07735900	1.15823700
C	4.87069700	-0.53578800	-0.00893900
H	4.87791100	1.24762000	-1.22234600
H	4.53007900	-2.28740700	1.20354100
H	5.95263100	-0.64014300	-0.00524100
H	-2.36997600	2.87058700	1.11166900
H	-0.25402200	4.09602700	-0.60913300

Zero-point correction= 0.262522 (Hartree/Particle)
Thermal correction to Energy= 0.277350
Thermal correction to Enthalpy= 0.278294
Thermal correction to Gibbs Free Energy= 0.219901
Sum of electronic and zero-point Energies= -856.372445
Sum of electronic and thermal Energies= -856.357617
Sum of electronic and thermal Enthalpies= -856.356672
Sum of electronic and thermal Free Energies= -856.415066

Nitrone 4

C	-4.49404900	-2.11982300	-0.18265400
C	-3.10627000	-2.21242100	-0.17020900
C	-2.33665200	-1.05227800	-0.09214300
C	-2.94434400	0.21626100	-0.02814300
C	-4.34724300	0.29873100	-0.03920300
C	-5.10776800	-0.86349000	-0.11568500
C	-0.73028200	1.23301800	0.08466600
C	-0.10160600	-0.08406000	0.00309300
C	-1.14279200	3.41401100	0.24790600
C	-2.53196000	2.71037300	0.18487700
H	-5.09528800	-3.02139200	-0.24308500
H	-2.58701400	-3.16068800	-0.21866400
H	-4.82842000	1.26965300	0.01076500
H	-6.19151400	-0.78685500	-0.12335700
H	-1.02925800	4.00561100	1.16379800
H	-3.14001400	3.02896600	-0.66976900
N	-0.90108900	-1.16916600	-0.08038600
N	-2.12657700	1.31275100	0.03867300
N	-0.11943300	2.36361800	0.20446100
O	-0.44237100	-2.35620100	-0.16059700
C	1.36251800	-0.23678900	0.03268200
C	2.19029600	0.73362300	-0.55845400
C	1.99060800	-1.33375800	0.66614700
C	3.57902900	0.62385600	-0.53353900
H	1.74331500	1.59732400	-1.03186300
C	3.37031000	-1.43795800	0.71352500
H	1.38561900	-2.10689000	1.11817600
C	4.17997200	-0.46502800	0.10796200
H	4.17569800	1.39258600	-1.01117700
H	3.84930000	-2.27679400	1.20880000
H	-3.12621600	2.84337900	1.09753600
H	-1.00310600	4.10156200	-0.59555200
O	5.52396600	-0.66953000	0.19833100
C	6.39095600	0.27984700	-0.40259500
H	7.40438900	-0.07836700	-0.21256700
H	6.22676100	0.34675200	-1.48607600
H	6.26835200	1.27587900	0.04252500

Zero-point correction= 0.295633 (Hartree/Particle)
Thermal correction to Energy= 0.312887
Thermal correction to Enthalpy= 0.313831
Thermal correction to Gibbs Free Energy= 0.250283
Sum of electronic and zero-point Energies= -970.823398
Sum of electronic and thermal Energies= -970.806144
Sum of electronic and thermal Enthalpies= -970.805200
Sum of electronic and thermal Free Energies= -970.868748

Nitrone 5

C	3.65741700	-2.41797400	0.13886900
C	2.26762000	-2.51253500	0.13347900
C	1.52637300	-1.34067100	0.06290300
C	2.18866600	-0.10107300	0.00150400
C	4.22859500	-1.14706900	0.07387000
C	0.04658000	1.03776900	-0.15301800
C	-0.62119800	-0.27222500	-0.01022600
C	-0.07691000	3.38447600	-0.46019600
C	1.25553600	3.48610900	0.28231800
C	2.16789300	2.35133100	-0.16514700
H	4.28080100	-3.30399400	0.19142300
H	1.73466000	-3.45370800	0.18457100
H	5.31030800	-1.02685900	0.07563300
H	0.06862700	3.61561300	-1.52758000
H	1.08036400	3.41604200	1.36317100
H	3.06655200	2.27612100	0.44782700
N	0.09640500	-1.40143800	0.06888100
N	1.45486900	1.06361100	-0.06935900
N	-0.69221900	2.07362100	-0.34380800
O	-0.41603200	-2.56545300	0.16742600
C	-2.09784300	-0.36771900	0.01724200
C	-2.85260200	0.48954000	0.83524600
C	-2.77234100	-1.31986000	-0.76584000
C	-4.24155400	0.39324800	0.87202800
H	-2.34682600	1.23418900	1.43737100
C	-4.16283200	-1.39709400	-0.74352900
H	-2.20388400	-2.00364200	-1.38382300
C	-4.90296900	-0.54558800	0.07862500
H	-4.80794400	1.05821100	1.51859500
H	-4.66789000	-2.13300600	-1.36345300
H	-5.98741600	-0.61522500	0.10291200
H	2.49606500	2.49975700	-1.20229600
H	1.74904700	4.44552100	0.09089500
H	-0.79050500	4.12744700	-0.08432300
N	3.52433300	-0.01248200	0.00441400

Zero-point correction= 0.280505 (Hartree/Particle)
Thermal correction to Energy= 0.295916
Thermal correction to Enthalpy= 0.296861
Thermal correction to Gibbs Free Energy= 0.237865
Sum of electronic and zero-point Energies= -911.694511
Sum of electronic and thermal Energies= -911.679099
Sum of electronic and thermal Enthalpies= -911.678155
Sum of electronic and thermal Free Energies= -911.737151

M062X/6-31+G(d,p)//B3LYP/6-31G(d) cartesian coordinates and thermochemical parameters from frequency calculations of all aminoxyls.

1a,*syn*

C	4.64646600	-1.47047200	-0.76268200
C	3.37706100	-1.52955000	-1.32488800
C	2.38732100	-0.62133400	-0.92813600
C	2.66878800	0.38379100	0.02764900
C	3.95310000	0.41781900	0.59051400
C	4.92854700	-0.50079900	0.20174700
C	0.43662200	1.30863500	-0.27917600
C	-0.04783400	-0.08324600	-0.72067900
C	0.13250100	3.60836100	0.05153400
C	0.90706400	3.45304700	1.36007900
C	2.08648000	2.51155800	1.13821700
H	5.40763000	-2.18156600	-1.06904500
H	3.11278300	-2.26874500	-2.07081800
H	4.20585100	1.17044400	1.32660300
H	5.91451400	-0.44751800	0.65434600
H	0.77216200	4.07449100	-0.71431200
H	0.23566900	3.04358800	2.12431000
H	2.46896900	2.15506900	2.10197200
N	1.10189300	-0.69784200	-1.48418200
N	1.69515900	1.34613900	0.32907600
N	-0.33739800	2.31565100	-0.43176500
O	0.87253900	-1.53122700	-2.42792600
C	-0.33800800	-0.96810100	0.50872700
C	-0.90919000	-0.41596000	1.66264000
C	-0.08619100	-2.34575500	0.47429400
C	-1.20922400	-1.21995100	2.76195400
H	-1.14129100	0.64380700	1.69380000
C	-0.38805800	-3.14914100	1.57501000
H	0.34317100	-2.79446800	-0.41565800
C	-0.94633200	-2.58977700	2.72450200
H	-1.65402700	-0.77292500	3.64717600
H	-0.18240600	-4.21544600	1.53066400
H	-1.17795800	-3.21588600	3.58203800
H	2.90787600	3.03587700	0.63089300
H	1.27851900	4.41425400	1.73202600
H	-0.73475100	4.26421400	0.18137400
C	-1.26403800	-0.00128900	-1.69660900
H	-1.09847300	0.85802600	-2.35100500
H	-1.18908200	-0.89945600	-2.31212900
C	-2.65789600	0.06207100	-1.09893300
C	-3.31348300	1.28144300	-0.87948200
C	-3.35597800	-1.12339100	-0.82475700
C	-4.61974700	1.31391000	-0.38858600
H	-2.78219000	2.20346300	-1.08728400
C	-4.65913700	-1.09504400	-0.32808000

H	-2.87055200	-2.07997700	-1.00113800
C	-5.29726700	0.12643200	-0.10732100
H	-5.11073200	2.27117900	-0.22976500
H	-5.17781200	-2.02788500	-0.12139400
H	-6.31516300	0.15210600	0.27363900

Zero-point correction= 0.413106 (Hartree/Particle)
Thermal correction to Energy= 0.434876
Thermal correction to Enthalpy= 0.435820
Thermal correction to Gibbs Free Energy= 0.361863
Sum of electronic and zero-point Energies= -1166.379664
Sum of electronic and thermal Energies= -1166.357894
Sum of electronic and thermal Enthalpies= -1166.356949
Sum of electronic and thermal Free Energies= -1166.430907

1a,*anti*

C	-2.80636100	-3.02980300	1.77756100
C	-1.57149100	-2.39716400	1.71075000
C	-1.41224000	-1.23046700	0.94861800
C	-2.50335800	-0.68166700	0.23473900
C	-3.74283300	-1.33377800	0.32348100
C	-3.89265600	-2.49469000	1.08328000
C	-1.13818500	1.22284600	-0.49101800
C	0.14945900	0.47626000	-0.06027800
C	-2.14922000	3.11919800	-1.44954200
C	-3.08976700	2.16246100	-2.17881700
C	-3.49565000	1.03781300	-1.23330900
H	-2.91920800	-3.93380200	2.36839000
H	-0.70232400	-2.77478800	2.23412100
H	-4.60800600	-0.93322400	-0.18883700
H	-4.86665300	-2.97298600	1.13068600
H	-2.67968500	3.62092100	-0.62532800
H	-2.57176200	1.74660600	-3.05171600
H	-3.95687800	0.22227200	-1.80069900
N	-0.16244800	-0.60223200	0.91573500
N	-2.33184600	0.49399600	-0.51323200
N	-0.99039200	2.41864600	-0.91701100
O	0.81730300	-1.10883000	1.56669000
C	1.12010700	1.47649100	0.58830000
C	1.10584600	1.68490700	1.97423400
C	1.96708400	2.27579900	-0.18789300
C	1.93046500	2.64173000	2.56445900
H	0.46102300	1.08710100	2.60702500
C	2.79750800	3.23049600	0.40059700
H	1.97036300	2.18262500	-1.26729000
C	2.78653100	3.41639100	1.78192200
H	1.90383800	2.77579200	3.64271700
H	3.44609000	3.83449200	-0.22860700

H	3.43329800	4.15840500	2.24269600
H	-4.23802900	1.39446900	-0.50561700
H	-3.99034000	2.66967500	-2.54241200
H	-1.79448800	3.91042000	-2.11911600
C	0.69147700	-0.22104700	-1.36966700
H	-0.17131700	-0.71828900	-1.82787800
H	0.98287400	0.57546500	-2.05934600
C	1.80447600	-1.23625500	-1.21329300
C	1.49676000	-2.60331800	-1.16743500
C	3.15346900	-0.85785000	-1.16381100
C	2.50121500	-3.56498200	-1.06349900
H	0.45648300	-2.91786600	-1.21348700
C	4.16073300	-1.81657200	-1.05936000
H	3.41983600	0.19380700	-1.19937700
C	3.83930400	-3.17399800	-1.00805300
H	2.23748700	-4.61893700	-1.02920000
H	5.20018100	-1.50090200	-1.02090200
H	4.62555200	-3.92028300	-0.92958600

Zero-point correction= 0.412801 (Hartree/Particle)
Thermal correction to Energy= 0.434578
Thermal correction to Enthalpy= 0.435522
Thermal correction to Gibbs Free Energy= 0.361556
Sum of electronic and zero-point Energies= -1166.370982
Sum of electronic and thermal Energies= -1166.349205
Sum of electronic and thermal Enthalpies= -1166.348261
Sum of electronic and thermal Free Energies= -1166.422227

1b,*syn*

C	4.13705300	-1.22693100	-0.81552600
C	2.84851900	-1.37508400	-1.31356100
C	1.82169500	-0.53003500	-0.87364900
C	2.08209000	0.49869100	0.06069100
C	3.38783500	0.62460900	0.55847200
C	4.40123000	-0.23088800	0.12730900
C	-0.21346300	1.27385000	-0.16012000
C	-0.62937800	-0.15876700	-0.57103200
C	-0.67888700	3.54623000	0.20780300
C	0.16646400	3.43532000	1.47658900
C	1.40283100	2.58875800	1.18919100
H	4.92763000	-1.88897500	-1.15507100
H	2.59951400	-2.13670600	-2.04182400
H	3.62540400	1.40043300	1.27528800
H	5.40273000	-0.10788400	0.52923600
H	-0.12019400	4.07878700	-0.57746400
H	-0.43479900	2.96776000	2.26517500
H	1.86369000	2.26644500	2.13012400
N	0.51804800	-0.69909100	-1.37373000

N	1.06130600	1.39113300	0.40378000
N	-1.05279100	2.22627100	-0.27956200
O	0.32227300	-1.54716400	-2.31331400
C	-0.79094300	-1.02005800	0.70406400
C	-1.42862200	-0.49253700	1.83572600
C	-0.33713900	-2.34546800	0.74088600
C	-1.60371200	-1.27322900	2.97859400
H	-1.80717200	0.52372200	1.81915000
C	-0.51118800	-3.12251600	1.88649100
H	0.14404300	-2.77824400	-0.12972300
C	-1.14219900	-2.58931500	3.01060900
H	-2.10536500	-0.84814600	3.84365900
H	-0.15157200	-4.14790300	1.89584000
H	-1.27620300	-3.19523000	3.90260000
H	2.15120500	3.17378400	0.63719000
H	0.48113500	4.41812400	1.84394500
H	-1.59622200	4.11522800	0.38838400
C	-1.96762800	-0.16321500	-1.44341100
C	-1.79189200	0.57087300	-2.79741600
C	-2.52082300	-1.59596300	-1.70386100
H	-1.05923200	0.04200900	-3.40922200
H	-2.74954800	0.57440100	-3.32701600
H	-1.47958000	1.60487300	-2.64918400
H	-3.46681600	-1.50298700	-2.24576500
H	-1.81808700	-2.17201600	-2.30235200
H	-2.72191300	-2.12417200	-0.76948100
C	-3.05458500	0.50006400	-0.68437800
N	-4.01947300	0.88564100	-0.16446200

Zero-point correction= 0.386104 (Hartree/Particle)
Thermal correction to Energy= 0.407827
Thermal correction to Enthalpy= 0.408771
Thermal correction to Gibbs Free Energy= 0.336897
Sum of electronic and zero-point Energies= -1106.240977
Sum of electronic and thermal Energies= -1106.219254
Sum of electronic and thermal Enthalpies= -1106.218310
Sum of electronic and thermal Free Energies= -1106.290184

1b,*anti*

C	3.96454900	-2.28677800	-0.08706900
C	2.62379800	-2.35043400	0.26881500
C	1.79662100	-1.22689900	0.11785800
C	2.31476600	-0.01534600	-0.39363400
C	3.67113600	0.02484700	-0.75049900
C	4.48667300	-1.09634800	-0.59728700
C	0.08036200	0.97293600	-0.45203800
C	-0.52267000	-0.20359200	0.36426100
C	-0.29474700	3.02563600	-1.55894600

C	1.03637500	3.48819900	-0.97129600
C	2.04442000	2.34809900	-1.05567100
H	4.59702600	-3.16107100	0.03220200
H	2.18051800	-3.25205000	0.67147600
H	4.09924700	0.93059600	-1.16008600
H	5.53218800	-1.03258500	-0.88428000
H	-0.20090100	2.84828000	-2.64118600
H	0.88281800	3.77654800	0.07529500
H	2.93686400	2.58447800	-0.46632600
N	0.45315300	-1.31853300	0.50029200
N	1.47361000	1.09528300	-0.53129500
N	-0.76191000	1.80736300	-0.91811000
O	0.03598700	-2.39746800	1.05554000
C	-1.76692200	-0.73160100	-0.38404900
C	-2.99072100	-0.04915600	-0.33283700
C	-1.67415400	-1.86509600	-1.20266900
C	-4.09295400	-0.50363300	-1.05632300
H	-3.08953700	0.85484800	0.25399600
C	-2.77541800	-2.31316000	-1.93363400
H	-0.74673200	-2.42070100	-1.26858200
C	-3.99261600	-1.63866300	-1.86061300
H	-5.03066800	0.04190400	-0.99291800
H	-2.67535500	-3.19780000	-2.55694100
H	-4.85204100	-1.99117000	-2.42473400
H	2.36452200	2.19598300	-2.09628100
H	1.43482600	4.36088300	-1.50030100
H	-1.06776600	3.79048600	-1.43100500
C	-0.82679000	0.30757800	1.87720800
C	-1.44740000	1.64820600	1.88192100
N	-1.91697000	2.70163600	2.02301500
C	-1.77227800	-0.64529100	2.65419000
H	-1.91045400	-0.25777200	3.66883400
H	-2.75029800	-0.72410700	2.17815600
H	-1.32844500	-1.63959100	2.70184400
C	0.49729100	0.44830700	2.67630400
H	0.94882900	-0.53490400	2.82825400
H	1.21495000	1.09906300	2.16989400
H	0.28138800	0.88134500	3.65712000

Zero-point correction= 0.386326 (Hartree/Particle)
Thermal correction to Energy= 0.407953
Thermal correction to Enthalpy= 0.408897
Thermal correction to Gibbs Free Energy= 0.336905
Sum of electronic and zero-point Energies= -1106.235813
Sum of electronic and thermal Energies= -1106.214185
Sum of electronic and thermal Enthalpies= -1106.213241
Sum of electronic and thermal Free Energies= -1106.285233

1c,*anti*(N-O)

C	2.97191000	-2.77879300	-0.27875400
C	1.93652000	-2.47336100	0.59518100
C	1.32288700	-1.21416500	0.54142000
C	1.76613400	-0.21964300	-0.36442500
C	2.78619200	-0.56762100	-1.26287900
C	3.38252900	-1.82840700	-1.21757400
C	0.05393600	1.36720900	0.41309500
C	-0.70148500	0.18391200	1.04504800
C	0.14592300	3.68142500	-0.05664600
C	1.64149800	3.49436800	-0.29741000
C	1.88510600	2.17049300	-1.01937200
H	3.44394300	-3.75564000	-0.23977700
H	1.57104900	-3.18322000	1.32753800
H	3.11805200	0.14265500	-2.01017100
H	4.17234300	-2.06354600	-1.92501300
H	-0.37159400	3.89969100	-1.00330600
H	2.16897400	3.48154400	0.66402900
H	2.95580800	1.95557800	-1.04157200
N	0.25678600	-0.91322700	1.38237300
N	1.21092700	1.06656400	-0.31728000
N	-0.48056800	2.51701300	0.54878700
O	-0.12794500	-1.72166000	2.30143000
C	-1.79006400	-0.34080600	0.08284200
C	-2.84286500	0.52992000	-0.23588500
C	-1.79662600	-1.63895400	-0.43580500
C	-3.87477500	0.10961800	-1.07131400
H	-2.83645300	1.53189500	0.17978100
C	-2.83445400	-2.05710500	-1.27359200
H	-1.00813300	-2.33887800	-0.18284200
C	-3.87287700	-1.18578000	-1.59643900
H	-4.68507200	0.79362500	-1.31014200
H	-2.82807400	-3.07004200	-1.66738100
H	-4.67892100	-1.51327800	-2.24783800
H	1.53052700	2.22185700	-2.05838800
H	2.05917900	4.31502200	-0.89161200
H	-0.03691600	4.54207200	0.59714600
O	-1.26368800	0.61755300	2.24489800
H	-1.42858900	-0.21277600	2.73682300

Zero-point correction= 0.307643 (Hartree/Particle)
Thermal correction to Energy= 0.324449
Thermal correction to Enthalpy= 0.325393
Thermal correction to Gibbs Free Energy= 0.263083
Sum of electronic and zero-point Energies= -971.418524
Sum of electronic and thermal Energies= -971.401717
Sum of electronic and thermal Enthalpies= -971.400773
Sum of electronic and thermal Free Energies= -971.463083

1c,*syn*(amid)

C	-3.16806700	-2.48892200	-0.37082500
C	-2.14868000	-2.28463600	0.55159000
C	-1.40031100	-1.10087600	0.52620900
C	-1.68643000	-0.09023600	-0.42437800
C	-2.71197300	-0.31964300	-1.34985300
C	-3.44292100	-1.50874000	-1.32631100
C	-0.01229900	1.33902900	0.58060700
C	0.70314400	0.09457200	1.14215200
C	-0.22820700	3.67369300	0.50514200
C	-0.58101800	3.49786100	-0.97360100
C	-1.48445800	2.27913000	-1.15470200
H	-3.74017300	-3.41151700	-0.34799200
H	-1.89929700	-3.01923000	1.30766500
H	-2.95844100	0.43331700	-2.08836700
H	-4.23335700	-1.65851900	-2.05582400
H	-1.13314700	3.89770400	1.09047100
H	0.34447300	3.36203200	-1.54574300
H	-1.51232100	1.99198000	-2.21156000
N	-0.36393200	-0.91095700	1.45203300
N	-0.99124700	1.13416300	-0.37118400
N	0.39996400	2.46707200	1.02960200
O	-0.13945600	-1.76845100	2.36884000
C	1.69721400	-0.48682800	0.11785800
C	2.62057100	0.37917900	-0.48366900
C	1.75400400	-1.85237100	-0.17415300
C	3.57052300	-0.11022200	-1.37755100
H	2.59863300	1.43702800	-0.23840600
C	2.70977900	-2.34181400	-1.06773100
H	1.06951600	-2.54122900	0.30807800
C	3.61571800	-1.47426400	-1.67604400
H	4.27971400	0.57316900	-1.83751300
H	2.74489200	-3.40651200	-1.28261700
H	4.35675500	-1.85700400	-2.37281900
H	-2.51381800	2.50505600	-0.84521300
H	-1.08822300	4.38173500	-1.37517600
H	0.45835400	4.51410900	0.64872200
O	1.36742100	0.43447800	2.30838900
H	1.24969400	1.40825300	2.38687100

Zero-point correction= 0.308062 (Hartree/Particle)
Thermal correction to Energy= 0.324799
Thermal correction to Enthalpy= 0.325744
Thermal correction to Gibbs Free Energy= 0.263533
Sum of electronic and zero-point Energies= -971.421657
Sum of electronic and thermal Energies= -971.404920
Sum of electronic and thermal Enthalpies= -971.403976
Sum of electronic and thermal Free Energies= -971.466186

1c,*syn*(N-O)

C	0.01205935	-0.03223104	0.04033062
C	0.01287627	0.01225506	1.42808789
C	1.22631563	0.01255049	2.13157924
C	2.46935942	-0.01548626	1.44847334
C	2.43891555	-0.06496476	0.04643971
C	1.22780047	-0.07601208	-0.64684560
C	3.69295318	0.23767603	3.55578229
C	2.45128848	-0.24184595	4.32109878
C	5.89933085	1.01464520	3.53036827
C	6.13684180	0.06250819	2.35812344
C	4.93639831	0.10740116	1.41799257
H	-0.92878308	-0.03630378	-0.50129858
H	-0.90373718	0.04500728	2.00433438
H	3.36257861	-0.08102290	-0.51755760
H	1.24275106	-0.11246497	-1.73223156
H	5.83013206	2.05324714	3.17163312
H	6.26816791	-0.95412690	2.74756735
H	4.96866282	-0.74129508	0.72525193
N	1.22150774	0.04277166	3.52123302
N	3.67047548	0.04646080	2.16746275
N	4.67681419	0.66695924	4.24314772
O	0.13186215	0.11538704	4.19439246
C	2.56412544	-1.75552124	4.60060667
C	3.56095779	-2.17036324	5.49550425
C	1.71541518	-2.70778289	4.03003345
C	3.70873387	-3.52003848	5.80575026
H	4.20858819	-1.42230076	5.94113359
C	1.86616753	-4.06137458	4.34443019
H	0.92407268	-2.40486933	3.35292714
C	2.86228110	-4.47130888	5.22880759
H	4.48298360	-3.83039801	6.50264489
H	1.19678594	-4.79213181	3.89829677
H	2.97695217	-5.52421258	5.47269802
H	4.95347463	1.02708231	0.81674788
H	7.04176432	0.32050283	1.79694359
H	6.73226403	0.98192248	4.24049868
O	2.34667175	0.48156308	5.50617822
H	1.40645430	0.37687269	5.75875346

Zero-point correction= 0.307582 (Hartree/Particle)
Thermal correction to Energy= 0.324433
Thermal correction to Enthalpy= 0.325377
Thermal correction to Gibbs Free Energy= 0.262570
Sum of electronic and zero-point Energies= -971.420226
Sum of electronic and thermal Energies= -971.403375
Sum of electronic and thermal Enthalpies= -971.402431
Sum of electronic and thermal Free Energies= -971.465238

1c,*anti*(amid)

C	-0.16701391	-0.03648581	0.95291416
C	0.24092148	-0.80063725	2.04013689
C	1.54166187	-0.67134937	2.54048359
C	2.46243831	0.21220081	1.93050166
C	2.02216091	0.99917434	0.85983416
C	0.72031214	0.87290279	0.37243248
C	4.15973877	-0.33884276	3.58509745
C	3.04145068	-0.84421095	4.51774932
C	6.48796484	-0.08672000	3.23416764
C	6.16008885	-0.00605474	1.74269002
C	4.86657435	0.78276166	1.52982311
H	-1.17878599	-0.13647127	0.57168326
H	-0.42009320	-1.50271170	2.53387298
H	2.69163482	1.71929351	0.40315948
H	0.40432131	1.49252406	-0.46162577
H	6.82886139	0.89049907	3.60721105
H	6.03156881	-1.01816584	1.34054316
H	4.54247549	0.69438947	0.49091395
N	1.95184553	-1.41875662	3.65332356
N	3.79603891	0.25161193	2.39051171
N	5.34789672	-0.51305700	4.03319215
O	1.20716486	-2.32918058	4.14279453
C	2.42586773	0.25655404	5.39521495
C	1.62168913	-0.15025754	6.46960981
C	2.62178699	1.62135947	5.16664340
C	1.02393322	0.79736287	7.29660352
H	1.47604673	-1.21031479	6.64565561
C	2.02667730	2.57012960	6.00247811
H	3.24360793	1.95729583	4.34246827
C	1.22560410	2.16156638	7.06717705
H	0.40243192	0.47081028	8.12627847
H	2.19333084	3.62822343	5.81796979
H	0.76203338	2.89946784	7.71664259
H	5.02089893	1.84904357	1.74430999
H	6.97338805	0.46977712	1.18374674
H	7.31143740	-0.78745814	3.41139966
O	3.54230342	-1.87550638	5.30030319
H	4.51747028	-1.74880634	5.25698278

Zero-point correction= 0.307613 (Hartree/Particle)
Thermal correction to Energy= 0.324463
Thermal correction to Enthalpy= 0.325407
Thermal correction to Gibbs Free Energy= 0.262868
Sum of electronic and zero-point Energies= -971.421004
Sum of electronic and thermal Energies= -971.404153
Sum of electronic and thermal Enthalpies= -971.403209
Sum of electronic and thermal Free Energies= -971.465748

1d,*syn*

C	3.54283300	-3.02752400	-0.19496500
C	2.17469300	-2.80928900	-0.29955100
C	1.67281600	-1.50415600	-0.38944500
C	2.54618100	-0.39104000	-0.39678800
C	3.92307200	-0.63498000	-0.28400400
C	4.41457100	-1.93698200	-0.18062300
C	0.66399900	1.13099900	-0.76140500
C	-0.28954700	0.05468400	-0.18698000
C	1.05051500	3.22325700	-1.72883700
C	2.23958700	3.35935100	-0.77792600
C	2.97224000	2.02430900	-0.69501800
H	3.92512500	-4.04100600	-0.11980800
H	1.46093600	-3.62373900	-0.31249900
H	4.62560900	0.18844800	-0.29053400
H	5.48638800	-2.09132600	-0.09642400
H	1.40169000	2.98778300	-2.74561500
H	1.86995700	3.64624800	0.21380400
H	3.63980300	2.01580500	0.17420300
N	0.29067200	-1.29860300	-0.48140400
N	2.02843000	0.90133500	-0.56591400
N	0.14267800	2.17754100	-1.27462000
O	-0.50586200	-2.29383200	-0.55642500
C	-0.46080900	0.26051100	1.32733000
C	-0.85482200	1.52338100	1.78936800
C	-0.25362100	-0.77257700	2.24465100
C	-1.02403200	1.75051400	3.15331000
H	-1.03595700	2.31596500	1.07033400
C	-0.41998200	-0.53980300	3.61174500
H	0.01668500	-1.76376400	1.89911100
C	-0.80087000	0.72040700	4.07050700
H	-1.33304500	2.73308400	3.50051700
H	-0.25571500	-1.35099700	4.31598100
H	-0.92920300	0.89903600	5.13489100
H	3.59101700	1.86864100	-1.58943500
H	2.94107500	4.13459900	-1.10532200
H	0.48871600	4.16058000	-1.79787000
O	-1.47832900	0.21403600	-0.90302900
O	-2.58467900	-0.36529200	-0.12069500
C	-3.69525500	-0.53090800	-1.03085500
C	-4.14905300	0.83581200	-1.56042700
C	-3.33624800	-1.49628400	-2.16614900
C	-4.74916300	-1.14305200	-0.09782400
H	-4.41025000	1.49927300	-0.72909700
H	-3.35286000	1.30966400	-2.14044700
H	-5.02877900	0.72174600	-2.20433100
H	-2.94518800	-2.43179200	-1.75852600
H	-4.22546400	-1.71048500	-2.77042800
H	-2.57258400	-1.06453100	-2.81766200
H	-5.67864700	-1.30733000	-0.65305500

H	-4.40375500	-2.10309100	0.29783700
H	-4.95968100	-0.47378700	0.74245600

Zero-point correction= 0.422356 (Hartree/Particle)
Thermal correction to Energy= 0.446208
Thermal correction to Enthalpy= 0.447152
Thermal correction to Gibbs Free Energy= 0.369406
Sum of electronic and zero-point Energies= -1203.585085
Sum of electronic and thermal Energies= -1203.561233
Sum of electronic and thermal Enthalpies= -1203.560289
Sum of electronic and thermal Free Energies= -1203.638035

1d,*anti*

C	-3.66983400	-2.25223900	-1.72603100
C	-2.28004100	-2.27003600	-1.74604100
C	-1.55364500	-1.54354600	-0.79701900
C	-2.21102800	-0.79366200	0.20732400
C	-3.61487300	-0.78322900	0.20254100
C	-4.33327600	-1.50180400	-0.75337900
C	-0.06722800	-0.20919600	1.21826600
C	0.59212600	-0.47267200	-0.14599900
C	0.01721400	0.31328800	3.49192800
C	-1.19764000	1.20990200	3.24991700
C	-2.17286800	0.50060400	2.31482400
H	-4.22960700	-2.81393100	-2.46758300
H	-1.72192600	-2.83204100	-2.48490300
H	-4.15805800	-0.22664700	0.95576300
H	-5.41889600	-1.47528100	-0.72704700
H	-0.29109100	-0.61685000	3.99529700
H	-0.85521600	2.14584600	2.79313600
H	-2.89268700	1.21988000	1.90604000
N	-0.14798100	-1.56812600	-0.82841600
N	-1.46423900	-0.14104600	1.19640000
N	0.67840500	-0.00983900	2.23486300
O	0.47398900	-2.34543100	-1.62740000
C	2.06805200	-0.82418500	-0.06095000
C	3.01033100	-0.10084100	-0.79122000
C	2.48811300	-1.91126300	0.71506900
C	4.36176600	-0.44956600	-0.73619900
H	2.68802500	0.73610500	-1.39725300
C	3.83362000	-2.26303700	0.76358900
H	1.76142300	-2.48443100	1.28159900
C	4.77751900	-1.52978100	0.03950700
H	5.08711800	0.12492500	-1.30648900
H	4.14656200	-3.11040000	1.36786900
H	5.82885000	-1.80297400	0.07986000
H	-2.74477000	-0.26284900	2.86031000
H	-1.71308900	1.46410600	4.18266800

H	0.74521900	0.80155200	4.14802600
O	0.31885300	0.62547500	-1.03335100
O	0.67115300	1.88073400	-0.33441200
C	0.09162800	2.96928800	-1.09266300
C	0.66956200	3.00124700	-2.51314800
C	-1.43783400	2.86582400	-1.10550900
C	0.55996900	4.18427800	-0.28053400
H	1.76220900	3.06631300	-2.47922300
H	0.39251200	2.10181400	-3.06887200
H	0.28957200	3.87322200	-3.05721700
H	-1.82669500	2.83769200	-0.08203100
H	-1.87210100	3.73326700	-1.61493300
H	-1.76451100	1.96158100	-1.62449600
H	0.19988900	5.10401600	-0.75339900
H	0.16966200	4.14434800	0.74159700
H	1.65255700	4.22135500	-0.23299200

Zero-point correction= 0.422390 (Hartree/Particle)
Thermal correction to Energy= 0.446126
Thermal correction to Enthalpy= 0.447070
Thermal correction to Gibbs Free Energy= 0.370001
Sum of electronic and zero-point Energies= -1203.587900
Sum of electronic and thermal Energies= -1203.564164
Sum of electronic and thermal Enthalpies= -1203.563220
Sum of electronic and thermal Free Energies= -1203.640289

1e,*syn*(N-O)

C	-3.65967400	-2.12108500	-0.40818400
C	-2.47067200	-2.18689600	0.30512400
C	-1.61613100	-1.07538800	0.35413600
C	-1.95244900	0.13349400	-0.30354000
C	-3.15808600	0.17220300	-1.02120900
C	-3.99747500	-0.94054200	-1.07487600
C	0.01809900	1.25041900	0.63005900
C	0.65680200	-0.12657100	0.91517200
C	0.09654000	3.58839400	0.71850700
C	-0.46068800	3.58261100	-0.70461700
C	-1.54136700	2.51270800	-0.81980200
H	-4.31614500	-2.98474700	-0.44776100
H	-2.16723300	-3.08111700	0.83513200
H	-3.45914700	1.07721100	-1.53266700
H	-4.92381600	-0.87496500	-1.63800800
H	-0.68868000	3.86974800	1.43689800
H	0.35509000	3.36769300	-1.40503800
H	-1.76240100	2.31313800	-1.87432300
N	-0.41840100	-1.15641800	1.06238100
N	-1.11582900	1.25007000	-0.19119500
N	0.62675000	2.27869100	1.07341900

O	-0.12246800	-2.22419800	1.71654400
C	1.62743300	-0.49844700	-0.21400800
C	2.73937500	0.32929100	-0.42001000
C	1.43490300	-1.61162900	-1.03527400
C	3.64262400	0.04536000	-1.44067100
H	2.88592700	1.18418800	0.23162300
C	2.34151000	-1.88999500	-2.06165800
H	0.59343000	-2.27617200	-0.87344800
C	3.44411500	-1.06327300	-2.26872800
H	4.50630200	0.68839100	-1.58788000
H	2.18357300	-2.75978700	-2.69362800
H	4.14912600	-1.28251900	-3.06623800
H	-2.47143700	2.85287500	-0.34403000
H	-0.88640500	4.55318900	-0.98176100
H	0.90018800	4.32403800	0.82628700
O	1.29074000	0.01562700	2.16570000
O	2.21060100	-1.08732400	2.38327600
H	1.55384600	-1.81433600	2.47592200

Zero-point correction= 0.311007 (Hartree/Particle)
Thermal correction to Energy= 0.328917
Thermal correction to Enthalpy= 0.329861
Thermal correction to Gibbs Free Energy= 0.264455
Sum of electronic and zero-point Energies= -1046.514995
Sum of electronic and thermal Energies= -1046.497085
Sum of electronic and thermal Enthalpies= -1046.496141
Sum of electronic and thermal Free Energies= -1046.561547

1e,*syn*(amid)

C	-3.64330600	-2.05324800	-0.25731700
C	-2.52724600	-2.00850700	0.56910900
C	-1.60748200	-0.95748000	0.45728600
C	-1.80971400	0.08037700	-0.48339500
C	-2.93822200	0.01150100	-1.31143700
C	-3.84333800	-1.04542400	-1.20223700
C	0.13541000	1.27006900	0.36798800
C	0.67554400	-0.05541800	0.94366900
C	0.30589400	3.59573800	0.08821800
C	-0.13983700	3.36610300	-1.35520700
C	-1.25167300	2.32145600	-1.38384500
H	-4.34934600	-2.87319000	-0.16762600
H	-2.33043100	-2.77076300	1.31287100
H	-3.12971600	0.78891400	-2.04026600
H	-4.70922200	-1.06940300	-1.85726100
H	-0.52029100	4.02114800	0.67903300
H	0.71741000	3.01501100	-1.94188300
H	-1.39718500	1.95822800	-2.40716100
N	-0.47531900	-0.94152800	1.28258300

N	-0.92064100	1.17102200	-0.52678200
N	0.74893000	2.34755100	0.70081300
O	-0.28094900	-1.86160500	2.14343300
C	1.62706800	-0.73285000	-0.05605600
C	2.70093000	0.00833300	-0.56808200
C	1.46921800	-2.06966000	-0.43419400
C	3.59393200	-0.57763000	-1.46286500
H	2.83317100	1.03780800	-0.25213000
C	2.36445100	-2.65082700	-1.33425400
H	0.66545600	-2.66473900	-0.01669700
C	3.42444500	-1.90795100	-1.85334500
H	4.42525500	0.00425800	-1.85183900
H	2.23294500	-3.69008400	-1.62265300
H	4.11971100	-2.36429100	-2.55293400
H	-2.20264700	2.75637800	-1.04759800
H	-0.50189000	4.28921200	-1.82045700
H	1.13136100	4.31326200	0.13764000
O	1.46960500	0.15158600	2.07651900
O	0.73869400	0.93718600	3.05977600
H	0.90938500	1.82410700	2.67061400

Zero-point correction= 0.311907 (Hartree/Particle)
Thermal correction to Energy= 0.329618
Thermal correction to Enthalpy= 0.330562
Thermal correction to Gibbs Free Energy= 0.266246
Sum of electronic and zero-point Energies= -1046.517638
Sum of electronic and thermal Energies= -1046.499926
Sum of electronic and thermal Enthalpies= -1046.498982
Sum of electronic and thermal Free Energies= -1046.563298

1e,*anti*(N-O)

C	2.46239000	-3.25758000	-0.23623900
C	1.50747700	-2.72431700	0.62051800
C	1.11431000	-1.38713000	0.48374800
C	1.70722800	-0.54526300	-0.48637400
C	2.64382100	-1.11489300	-1.36199900
C	3.01609600	-2.45343900	-1.23635400
C	0.27364000	1.33786700	0.16265700
C	-0.67161400	0.31956300	0.83960300
C	0.74724700	3.57426500	-0.43116600
C	2.20008000	3.13749200	-0.60392900
C	2.24778300	1.75330400	-1.24788400
H	2.76149400	-4.29626700	-0.13536700
H	1.04244600	-3.31220600	1.40290400
H	3.08569500	-0.51604700	-2.14932200
H	3.74546700	-2.86530900	-1.92776100
H	0.30088200	3.81828200	-1.40739900
H	2.68846000	3.09461300	0.37694500

H	3.26884300	1.36483200	-1.22130600
N	0.13225000	-0.84888300	1.31716400
N	1.38327200	0.81665800	-0.51286200
N	-0.07816000	2.56241400	0.21120400
O	-0.26857900	-1.47492600	2.36213100
C	-1.80016400	-0.13650300	-0.10008600
C	-2.48748900	0.81702000	-0.86224600
C	-2.19814900	-1.47748600	-0.15223200
C	-3.54328400	0.42654400	-1.68501100
H	-2.19654900	1.85921100	-0.79183900
C	-3.25094300	-1.86345500	-0.98211900
H	-1.70016000	-2.21926900	0.46179100
C	-3.92310000	-0.91492300	-1.75365400
H	-4.07132500	1.17413200	-2.27090900
H	-3.54778400	-2.90804000	-1.01928200
H	-4.74308700	-1.21832400	-2.39920100
H	1.93434700	1.80201800	-2.30024600
H	2.76164100	3.84701800	-1.22206100
H	0.68625300	4.48873700	0.16986600
O	-1.34860800	0.87053200	1.93376000
O	-0.38349900	1.21524200	2.96765400
H	-0.34464900	0.34212300	3.41286700

Zero-point correction= 0.311462 (Hartree/Particle)
Thermal correction to Energy= 0.329298
Thermal correction to Enthalpy= 0.330243
Thermal correction to Gibbs Free Energy= 0.265482
Sum of electronic and zero-point Energies= -1046.515525
Sum of electronic and thermal Energies= -1046.497689
Sum of electronic and thermal Enthalpies= -1046.496744
Sum of electronic and thermal Free Energies= -1046.561505

1e,*anti*(amid)

C	-2.47660000	-3.33176500	-0.12978200
C	-1.41158000	-2.77389200	-0.82697000
C	-1.09425800	-1.42109200	-0.65727100
C	-1.85841500	-0.60405000	0.20251400
C	-2.91032600	-1.19037300	0.91774900
C	-3.21883200	-2.54089600	0.75001500
C	-0.37287100	1.29751500	-0.16826100
C	0.67286700	0.34238000	-0.79226200
C	-0.94437000	3.52689200	0.41792900
C	-2.40223400	3.08980400	0.29966000
C	-2.56700800	1.68430100	0.87300800
H	-2.71679200	-4.38231200	-0.26159900
H	-0.80024100	-3.35368700	-1.50732700
H	-3.49092900	-0.59829200	1.61534900
H	-4.04062300	-2.97055400	1.31512500

H	-0.68065500	3.71144100	1.47022200
H	-2.69841500	3.08741600	-0.75603200
H	-3.55737800	1.29296500	0.62767900
N	-0.01170600	-0.86508200	-1.35559200
N	-1.56464700	0.77022000	0.29867100
N	-0.02664400	2.53454500	-0.12543400
O	0.61616600	-1.55541500	-2.22440400
C	1.75055600	-0.11222400	0.18971200
C	2.91479200	-0.70024400	-0.32265400
C	1.57210300	-0.02943000	1.57302300
C	3.88658300	-1.19129300	0.54495100
H	3.04676300	-0.75970100	-1.39646500
C	2.54834400	-0.52472900	2.44075400
H	0.67683600	0.42666300	1.98525200
C	3.70700700	-1.10618500	1.92877200
H	4.79016400	-1.63888800	0.13989900
H	2.40040400	-0.45191300	3.51492100
H	4.46863800	-1.48966600	2.60259300
H	-2.47357200	1.69682400	1.96770200
H	-3.06986600	3.77858500	0.82861000
H	-0.77712500	4.47040400	-0.11264200
O	1.20362100	0.95681200	-1.96129000
O	2.15953000	1.97603000	-1.57524000
H	1.53468700	2.59519700	-1.11465000

Zero-point correction= 0.311330 (Hartree/Particle)
Thermal correction to Energy= 0.329164
Thermal correction to Enthalpy= 0.330108
Thermal correction to Gibbs Free Energy= 0.265595
Sum of electronic and zero-point Energies= -1046.513615
Sum of electronic and thermal Energies= -1046.495781
Sum of electronic and thermal Enthalpies= -1046.494837
Sum of electronic and thermal Free Energies= -1046.559350

2a,*anti*

C	0.00690506	0.04461879	0.01484711
C	0.00548491	0.04117959	1.40402214
C	1.21578309	0.01417460	2.11066053
C	2.45244655	-0.03017266	1.42695150
C	2.43058474	-0.00012187	0.02443755
C	1.22252266	0.03311441	-0.67304096
C	3.71142387	0.10909592	3.53068016
C	2.41413460	0.43467574	4.28229950
C	6.06327323	-0.13025322	3.60140716
C	5.92853043	-1.03968241	2.38344953
C	4.88623069	-0.46025423	1.43229684
H	-0.93358637	0.06813550	-0.52718332
H	-0.91155359	0.06228126	1.97934982

H	3.35883084	0.00602798	-0.53350271
H	1.23964296	0.05344265	-1.75886304
H	6.52021786	0.83019056	3.31702911
H	5.60919968	-2.03593967	2.71182854
H	4.63593420	-1.19355092	0.66014026
N	1.20773573	0.01878504	3.50829613
N	3.64894275	-0.11949380	2.15234749
N	4.77964974	0.12587765	4.23503581
O	0.08803328	0.00758318	4.13426388
H	5.27918248	0.43358390	0.92670468
H	6.88037578	-1.15310562	1.85243095
H	6.72883656	-0.57715470	4.34885855
C	2.38855298	-0.28196019	5.65891074
H	3.20518571	0.14426168	6.24176337
H	1.44457558	-0.00402866	6.13521314
C	2.52219803	-1.79423506	5.62674494
C	3.74311955	-2.40421551	5.95110474
C	1.43066713	-2.61830833	5.31203654
C	3.87542957	-3.79362997	5.95110298
H	4.59311809	-1.77737210	6.20392828
C	1.56214971	-4.00798050	5.30865348
H	0.47487912	-2.16374482	5.07050062
C	2.78471505	-4.60186963	5.62627465
H	4.83015571	-4.24449440	6.21145850
H	0.70310837	-4.62759631	5.06303641
H	2.88457364	-5.68442326	5.62779418
C	2.24518798	1.99609417	4.44935372
H	2.23612808	2.42618824	3.44019745
H	1.23772411	2.12665311	4.85850841
C	3.24832972	2.73673770	5.30205208
C	4.38318643	3.32876837	4.73017739
C	3.04093483	2.89714194	6.67939969
C	5.29182010	4.04331794	5.50945956
H	4.55112557	3.23280542	3.65997504
C	3.94952004	3.60748822	7.46520923
H	2.15384964	2.46805558	7.13907908
C	5.08012350	4.18156208	6.88273919
H	6.16301934	4.49719518	5.04390692
H	3.76786535	3.71959773	8.53096899
H	5.78586164	4.74025740	7.49176424

Zero-point correction= 0.442097 (Hartree/Particle)
Thermal correction to Energy= 0.465054
Thermal correction to Enthalpy= 0.465998
Thermal correction to Gibbs Free Energy= 0.388925
Sum of electronic and zero-point Energies= -1205.651279
Sum of electronic and thermal Energies= -1205.628322
Sum of electronic and thermal Enthalpies= -1205.627378
Sum of electronic and thermal Free Energies= -1205.704451

2a,*syn*

C	-0.00844714	-0.03575835	0.03228179
C	-0.00326380	-0.01261218	1.42063808
C	1.20984388	-0.00412219	2.12593249
C	2.44560025	-0.02016518	1.43596563
C	2.41452296	-0.03127303	0.03331076
C	1.20358203	-0.04299016	-0.66035219
C	3.69023566	0.15724638	3.54131456
C	2.40992581	-0.13169536	4.34413646
C	6.00884251	0.58222627	3.54540627
C	6.10351968	-0.31267302	2.31265494
C	4.91471990	-0.03934195	1.39800043
H	-0.95189974	-0.04427896	-0.50512733
H	-0.91831238	0.00208481	1.99886927
H	3.33604846	-0.01498773	-0.53414182
H	1.21733939	-0.05081505	-1.74634837
H	6.12008909	1.63931930	3.25844664
H	6.09475666	-1.36283632	2.62937732
H	4.83668029	-0.83091132	0.64548935
N	1.18806606	0.03927419	3.52053302
N	3.65214838	-0.00195093	2.15418795
N	4.73917976	0.40372441	4.23324418
O	0.06426512	0.08353992	4.13703468
H	5.04685654	0.91238955	0.86472660
H	7.03195705	-0.14533525	1.75538825
H	6.81704043	0.36315536	4.25203775
C	2.30520806	0.79798289	5.58402605
H	1.39757897	0.50412330	6.11462201
H	3.16188120	0.56324746	6.21812541
C	2.28070096	2.29112342	5.30460213
C	1.10325305	2.93829431	4.89851065
C	3.43328526	3.06847423	5.49282845
C	1.08566946	4.31571873	4.67371435
H	0.19835680	2.35498979	4.76002490
C	3.41607826	4.44647103	5.27314625
H	4.34963200	2.58097724	5.81125767
C	2.24140193	5.07604471	4.85863235
H	0.16202725	4.79621378	4.36025513
H	4.32100637	5.02860604	5.43052951
H	2.22491659	6.14964677	4.68825399
C	2.52659602	-1.64607312	4.77609371
H	2.62960256	-2.23181371	3.85403307
H	3.47972019	-1.72094266	5.30860528
C	1.41669522	-2.22882283	5.62152633
C	0.29823705	-2.83256850	5.02954674
C	1.50733588	-2.22444431	7.02062422
C	-0.70546777	-3.40242362	5.81107304
H	0.21281393	-2.85349013	3.94620690
C	0.50352217	-2.79116478	7.80704700

H	2.37728026	-1.77958533	7.49830314
C	-0.60763878	-3.38155343	7.20379449
H	-1.56438649	-3.86489226	5.33179322
H	0.59456983	-2.77780119	8.89009234
H	-1.38857436	-3.82801187	7.81368709

Zero-point correction= 0.442362 (Hartree/Particle)
Thermal correction to Energy= 0.465290
Thermal correction to Enthalpy= 0.466234
Thermal correction to Gibbs Free Energy= 0.389133
Sum of electronic and zero-point Energies= -1205.650359
Sum of electronic and thermal Energies= -1205.627430
Sum of electronic and thermal Enthalpies= -1205.626486
Sum of electronic and thermal Free Energies= -1205.703588

2b,*syn*

C	3.65304700	-2.41658000	-0.80453200
C	2.74141200	-1.56925000	-1.42169900
C	1.76983600	-0.90460300	-0.66000000
C	1.68288800	-1.10463500	0.73570300
C	2.62571700	-1.94890100	1.34093600
C	3.59755500	-2.59834500	0.57927200
C	-0.10304200	0.56469500	0.94091400
C	0.04570500	0.94587000	-0.54703600
C	-1.16499000	1.00453300	3.00754400
C	-0.94447600	-0.46853300	3.34053000
C	0.43866900	-0.89340200	2.85914200
H	4.40627500	-2.92519700	-1.39829100
H	2.74984000	-1.39808100	-2.49079600
H	2.61035900	-2.10153200	2.41281400
H	4.31254300	-3.24693900	1.07689700
H	-0.49489200	1.64180300	3.60443300
H	-1.70887700	-1.07007100	2.83493300
H	0.53534200	-1.98225000	2.90464700
N	0.85436800	-0.05630600	-1.29103800
N	0.66400000	-0.47860600	1.46393200
N	-0.94062900	1.27298700	1.59578600
O	0.79196400	-0.04262400	-2.57326400
H	1.21975500	-0.46238600	3.50155600
H	-1.02636100	-0.65956500	4.41628700
H	-2.18590900	1.31525500	3.25507800
C	-1.36650500	1.01011800	-1.20666300
H	-1.88452200	1.85774900	-0.75662700
H	-1.21488400	1.22168100	-2.26647800
C	-2.21529800	-0.23927400	-1.05275200
C	-3.25227600	-0.27393700	-0.10848000
C	-2.01312800	-1.36773100	-1.86192400
C	-4.05612400	-1.40601600	0.03484300

H	-3.42556900	0.59854200	0.51498400
C	-2.81396000	-2.50184400	-1.71720500
H	-1.22624600	-1.35303200	-2.60997400
C	-3.83634300	-2.52720700	-0.76733100
H	-4.85911900	-1.40806400	0.76789400
H	-2.64190200	-3.36515300	-2.35517600
H	-4.46255500	-3.40919400	-0.65975900
C	0.79651900	2.36774100	-0.64927300
C	2.11934500	2.36052200	0.15634400
C	1.11050200	2.78338600	-2.11098700
H	2.80958500	1.61711000	-0.25258300
H	2.59702600	3.34214400	0.08569400
H	1.94995900	2.14566300	1.21461600
H	1.57294200	3.77535500	-2.09998900
H	1.80003100	2.07583100	-2.57380000
H	0.20988200	2.83760900	-2.72572300
C	-0.05983200	3.43808100	-0.09487300
N	-0.65055800	4.37129500	0.26426900

Zero-point correction= 0.414974 (Hartree/Particle)
Thermal correction to Energy= 0.437893
Thermal correction to Enthalpy= 0.438837
Thermal correction to Gibbs Free Energy= 0.363172
Sum of electronic and zero-point Energies= -1145.515961
Sum of electronic and thermal Energies= -1145.493043
Sum of electronic and thermal Enthalpies= -1145.492098
Sum of electronic and thermal Free Energies= -1145.567763

2b,*anti*

C	-1.82191200	-3.36236800	-1.91199600
C	-1.24151800	-2.12258500	-2.14360500
C	-0.99723200	-1.24557800	-1.07575400
C	-1.34195300	-1.60453000	0.24675800
C	-1.92019000	-2.86480200	0.45768000
C	-2.15927900	-3.73261800	-0.60866900
C	-0.32972000	0.44801200	1.12730600
C	-0.15516000	1.02234300	-0.29308700
C	0.05236000	0.67989100	3.44632100
C	-1.29623600	-0.00007200	3.66505400
C	-1.44911500	-1.13873900	2.66443600
H	-2.00779700	-4.03561900	-2.74314900
H	-0.96419800	-1.79454100	-3.13718000
H	-2.17953700	-3.18734200	1.45753600
H	-2.60745100	-4.70175200	-0.41034800
H	0.87273500	-0.01146500	3.69298000
H	-2.09979000	0.73358000	3.52437400
H	-2.48694300	-1.48768300	2.64869600
N	-0.41554300	-0.00422000	-1.33563800

N	-1.09110400	-0.71136400	1.30111600
N	0.20896300	1.12644100	2.07037000
O	-0.15186100	0.33223200	-2.54357700
H	-0.81780900	-1.99032700	2.95360000
H	-1.39263300	-0.39884800	4.68089300
H	0.16715300	1.54854300	4.10400100
C	1.31022000	1.52785500	-0.48328800
H	1.36746800	1.95340800	-1.48707700
H	1.46806600	2.32895000	0.23874200
C	2.39247000	0.47676700	-0.31363400
C	2.71914000	-0.39862600	-1.36091600
C	3.12439200	0.38906600	0.87969500
C	3.73472900	-1.34396700	-1.21072200
H	2.17501900	-0.33261700	-2.29837500
C	4.14292700	-0.55309700	1.02988600
H	2.88993000	1.06985200	1.69247400
C	4.44939400	-1.42666800	-0.01459600
H	3.97314800	-2.01122400	-2.03515500
H	4.70187600	-0.59910600	1.96140900
H	5.24446800	-2.15917100	0.09911400
C	-1.21022200	2.21568800	-0.54134900
C	-2.65441000	1.66671000	-0.65129100
C	-1.17466500	3.31033000	0.55686500
H	-2.93020100	1.14040500	0.26799500
H	-3.35172400	2.49809100	-0.79035900
H	-2.76753800	0.98648400	-1.49811200
H	-1.83391500	4.12941600	0.25301200
H	-1.52494400	2.91306200	1.51048100
H	-0.17221000	3.71579600	0.70402700
C	-0.89790800	2.91289500	-1.80853200
N	-0.72588200	3.57468800	-2.74732500

Zero-point correction= 0.415296 (Hartree/Particle)
Thermal correction to Energy= 0.438180
Thermal correction to Enthalpy= 0.439124
Thermal correction to Gibbs Free Energy= 0.363791
Sum of electronic and zero-point Energies= -1145.513718
Sum of electronic and thermal Energies= -1145.490834
Sum of electronic and thermal Enthalpies= -1145.489890
Sum of electronic and thermal Free Energies= -1145.565223

2c,*syn(N-O)*

C	-3.77285100	-1.66446300	-0.95883900
C	-2.77010300	-1.86165900	-0.01966200
C	-1.81109600	-0.86352100	0.20860900
C	-1.84056100	0.35355100	-0.51317400
C	-2.87443300	0.53559400	-1.44423100
C	-3.82510900	-0.46096600	-1.66656800

C	0.03035600	1.27812400	0.78274900
C	0.09250500	0.00438100	1.63855200
C	0.84896600	3.45248700	0.39733500
C	0.51359200	3.23169800	-1.07571500
C	-0.81857500	2.49719400	-1.18741800
H	-4.51319700	-2.43940500	-1.13223900
H	-2.69568700	-2.77257600	0.56098900
H	-2.95486200	1.46421800	-1.99476200
H	-4.61185100	-0.28625600	-2.39468500
H	0.12994000	4.14888600	0.85543100
H	1.30428200	2.62895600	-1.53812500
H	-0.96322200	2.14056000	-2.21186500
N	-0.81089000	-1.07389800	1.15159100
N	-0.86072900	1.33065600	-0.29006400
N	0.83808300	2.20173500	1.14094200
O	-0.77567200	-2.15667600	1.84440000
H	-1.65232700	3.17202000	-0.94813500
H	0.45059600	4.17693800	-1.62630500
H	1.83820800	3.90995900	0.50992500
C	1.54040000	-0.54623600	1.70582400
H	2.12035900	0.24147000	2.18958600
H	1.50784500	-1.41480000	2.37058600
C	2.15810000	-0.92725800	0.37671000
C	3.04349600	-0.05541600	-0.27307300
C	1.86798700	-2.15902300	-0.22871200
C	3.62054500	-0.40054700	-1.49642000
H	3.28172800	0.89752500	0.19181800
C	2.44210800	-2.50508600	-1.45265700
H	1.18960500	-2.84804900	0.26711900
C	3.31942600	-1.62679600	-2.09169500
H	4.31131200	0.28559400	-1.98044500
H	2.20735400	-3.46540500	-1.90477100
H	3.77044700	-1.89905100	-3.04246200
O	-0.35666900	0.36144700	2.92869200
H	-0.41557000	-0.48055300	3.41664100

Zero-point correction= 0.336646 (Hartree/Particle)
Thermal correction to Energy= 0.354741
Thermal correction to Enthalpy= 0.355685
Thermal correction to Gibbs Free Energy= 0.289620
Sum of electronic and zero-point Energies= -1010.692828
Sum of electronic and thermal Energies= -1010.674732
Sum of electronic and thermal Enthalpies= -1010.673788
Sum of electronic and thermal Free Energies= -1010.739854

2c,*anti(N-O)*

C	1.89326300	-3.49024100	-0.61375700
C	1.12050100	-2.90877300	0.38174400

C	0.99574900	-1.51300500	0.45289500
C	1.66559300	-0.67355500	-0.47011700
C	2.43029400	-1.28641700	-1.47393800
C	2.54335100	-2.67540200	-1.54412300
C	0.60921100	1.33789500	0.45310100
C	-0.06203200	0.51297400	1.56065000
C	0.93165700	3.45374500	-0.53040900
C	2.36740200	3.01239800	-0.80426600
C	2.37137900	1.55706400	-1.25993900
H	1.98508900	-4.57070700	-0.66698200
H	0.59997500	-3.49926700	1.12544600
H	2.93917300	-0.68411200	-2.21551000
H	3.14332300	-3.11621600	-2.33488800
H	0.35316200	3.47826700	-1.46705600
H	2.95622200	3.11275600	0.11522100
H	3.39338300	1.16444100	-1.25704100
N	0.22292000	-0.94293700	1.45550600
N	1.56172400	0.72011800	-0.35995900
N	0.26755100	2.56869900	0.41488300
O	-0.25159400	-1.65126700	2.41779700
H	1.98573300	1.47310700	-2.28581700
H	2.84434900	3.63171000	-1.57200200
H	0.90540700	4.47004800	-0.12189200
C	-1.59817200	0.72289200	1.58089200
H	-1.96557900	0.17901200	2.45649200
H	-1.73919300	1.79136400	1.75189000
C	-2.33810200	0.27159200	0.33914500
C	-2.71512900	-1.06988800	0.17690600
C	-2.66899800	1.18573800	-0.67101700
C	-3.40011000	-1.48604400	-0.96521300
H	-2.46805100	-1.78843800	0.95418100
C	-3.35612800	0.77195900	-1.81325400
H	-2.38480400	2.22770700	-0.55276200
C	-3.72263300	-0.56638000	-1.96493000
H	-3.68661500	-2.52930700	-1.07141300
H	-3.61006300	1.49707100	-2.58259500
H	-4.26069600	-0.88936900	-2.85245200
O	0.50479200	0.95141700	2.77761500
H	0.21566900	0.29025500	3.43464800

Zero-point correction= 0.336511 (Hartree/Particle)
Thermal correction to Energy= 0.354568
Thermal correction to Enthalpy= 0.355513
Thermal correction to Gibbs Free Energy= 0.289805
Sum of electronic and zero-point Energies= -1010.693130
Sum of electronic and thermal Energies= -1010.675073
Sum of electronic and thermal Enthalpies= -1010.674129
Sum of electronic and thermal Free Energies= -1010.739837

2c,*syn*(amid)

C	3.22242900	-2.14458100	-0.70902400
C	2.60952000	-1.70052600	0.45570100
C	1.27001400	-1.28656400	0.43816300
C	0.52529000	-1.31918800	-0.76546200
C	1.16317800	-1.76967400	-1.92799500
C	2.49831300	-2.17616300	-1.90200700
C	-1.49321500	-0.66752500	0.41436600
C	-0.68568500	-0.26650600	1.65988600
C	-3.62040500	-0.96575000	-0.54381900
C	-3.00069200	-0.44746000	-1.84255000
C	-1.60101400	-1.03092100	-2.01599600
H	4.26033500	-2.46272300	-0.68547400
H	3.13517400	-1.65550000	1.40128400
H	0.62128400	-1.81439900	-2.86422000
H	2.96435500	-2.52098900	-2.82033500
H	-3.77948400	-2.05343400	-0.60374300
H	-2.94036600	0.64631600	-1.79857400
H	-1.05911800	-0.48340500	-2.79445500
N	0.68283000	-0.82874800	1.62170300
N	-0.82900300	-0.93430400	-0.76587300
N	-2.76385300	-0.66372100	0.59508600
O	1.37747100	-0.70203700	2.68767400
H	-1.65545800	-2.08378600	-2.32506800
H	-3.60934200	-0.70989600	-2.71466800
H	-4.60221700	-0.51336500	-0.36847800
C	-0.59716700	1.28446300	1.81714600
H	-1.62751400	1.62272600	1.96160300
H	-0.06105200	1.42814300	2.76013400
C	0.06218700	2.05441800	0.69644900
C	-0.70926600	2.68964900	-0.28708300
C	1.45889000	2.16150700	0.62136300
C	-0.10590800	3.40481800	-1.32276900
H	-1.79443800	2.63504600	-0.22837100
C	2.06531800	2.87400700	-0.41358600
H	2.06970100	1.68272200	1.38262000
C	1.28538600	3.49692800	-1.38996500
H	-0.72211400	3.89798000	-2.07054100
H	3.14899600	2.94734800	-0.45363800
H	1.75822400	4.05738800	-2.19219700
O	-1.32271600	-0.78569500	2.79338600
H	-2.25787500	-0.87648400	2.51231600

Zero-point correction= 0.336613 (Hartree/Particle)
Thermal correction to Energy= 0.354704
Thermal correction to Enthalpy= 0.355648
Thermal correction to Gibbs Free Energy= 0.289409
Sum of electronic and zero-point Energies= -1010.695847
Sum of electronic and thermal Energies= -1010.677756
Sum of electronic and thermal Enthalpies= -1010.676812

Sum of electronic and thermal Free Energies= -1010.743051

2c,*anti*(amid)

C	2.25200100	3.04424300	-0.26490300
C	1.74046800	2.34609400	0.82142900
C	0.61928700	1.51904200	0.66666400
C	-0.02463200	1.41006000	-0.58835700
C	0.53156900	2.09125100	-1.67828800
C	1.65498700	2.90375500	-1.51920500
C	-1.65913500	-0.15219000	0.32033300
C	-0.80273400	-0.33110000	1.58847000
C	-3.66858600	-0.75907700	-0.78006900
C	-3.50543400	0.52642800	-1.58881700
C	-2.03063900	0.75441100	-1.92058800
H	3.12181400	3.68141100	-0.13648900
H	2.18529500	2.40689900	1.80683600
H	0.10038700	1.98283400	-2.66597400
H	2.06018600	3.42179300	-2.38338700
H	-3.49276600	-1.63829700	-1.41811900
H	-3.87686100	1.37590600	-1.00300000
H	-1.90045100	1.75738500	-2.33178600
N	0.14701100	0.79025300	1.76372800
N	-1.20113500	0.64383600	-0.70888800
N	-2.75828800	-0.81598400	0.35376100
O	0.73332400	0.86896100	2.89732100
H	-1.67921200	0.03415000	-2.67159300
H	-4.08416000	0.48989600	-2.51841300
H	-4.69335200	-0.85307600	-0.40346900
C	-0.01662100	-1.67991600	1.57206000
H	0.49027200	-1.71111500	2.54125800
H	-0.78330700	-2.46059400	1.56811900
C	0.96187500	-1.89515200	0.44064000
C	2.28909500	-1.45476500	0.54537700
C	0.56571300	-2.54675000	-0.73622200
C	3.19215000	-1.65262600	-0.49931500
H	2.61099800	-0.95246200	1.45437500
C	1.46644500	-2.74688700	-1.78317400
H	-0.45586400	-2.91039100	-0.82411400
C	2.78350200	-2.29861300	-1.66773200
H	4.21721400	-1.30567000	-0.39859300
H	1.14252800	-3.26138600	-2.68454000
H	3.48838400	-2.45800800	-2.47953200
O	-1.65373100	-0.33331100	2.69998500
H	-2.49684500	-0.68046000	2.33994000

Zero-point correction= 0.336467 (Hartree/Particle)
Thermal correction to Energy= 0.354550
Thermal correction to Enthalpy= 0.355494

Thermal correction to Gibbs Free Energy= 0.289850
Sum of electronic and zero-point Energies= -1010.694557
Sum of electronic and thermal Energies= -1010.676475
Sum of electronic and thermal Enthalpies= -1010.675531
Sum of electronic and thermal Free Energies= -1010.741175

2d,*syn*

C	-1.93486500	3.53984300	-2.12568800
C	-1.50454400	2.22095600	-2.21403300
C	-0.79833200	1.64191200	-1.15471900
C	-0.49087700	2.38553100	0.00495500
C	-0.95224300	3.70728200	0.08451300
C	-1.66439300	4.27759800	-0.97109800
C	0.47333700	0.42495900	1.11412100
C	-0.14147500	-0.45414100	0.00897800
C	1.63594000	0.56171200	3.16250700
C	2.03666500	1.97411600	2.74197900
C	0.85180500	2.66109900	2.06857200
H	-2.48706500	3.98531600	-2.94759900
H	-1.69881900	1.60801500	-3.08560200
H	-0.76519000	4.29726000	0.97362600
H	-2.00873500	5.30398100	-0.88279300
H	0.90951300	0.59738500	3.98879400
H	2.87434900	1.91775100	2.03674200
H	1.17279600	3.59679800	1.60173400
N	-0.35089700	0.31569900	-1.24213100
N	0.28416900	1.80209300	1.01889600
N	1.05660000	-0.19943500	2.06567000
O	-0.45556600	-0.31967700	-2.34983500
H	0.07615700	2.90573200	2.80826400
H	2.36428700	2.57250900	3.59936100
H	2.50390000	0.00808800	3.53868400
C	0.67624400	-1.73140400	-0.27177200
H	0.62046300	-2.31177700	0.64995600
H	0.14174500	-2.27294700	-1.05288800
C	2.13195500	-1.53321400	-0.66104500
C	3.14759400	-1.79748600	0.27032400
C	2.50522500	-1.13793700	-1.95435300
C	4.49314900	-1.66342800	-0.07351200
H	2.87276000	-2.10628100	1.27429600
C	3.85103400	-0.99800600	-2.29837300
H	1.73417400	-0.94051200	-2.69149500
C	4.85100600	-1.25863500	-1.36055700
H	5.26207900	-1.87906400	0.66458700
H	4.11689100	-0.69050500	-3.30684100
H	5.89864600	-1.15387000	-1.63149900
O	-1.41780100	-0.73909000	0.58729400
O	-2.16563600	-1.60152500	-0.34450400

C	-3.13927700	-2.33719100	0.43435900
C	-2.44327500	-3.26168100	1.43906800
C	-4.10461500	-1.36545500	1.12498900
C	-3.85398800	-3.14013300	-0.66064100
H	-1.77262100	-3.95520300	0.92072700
H	-1.85631300	-2.68169000	2.15596900
H	-3.18485300	-3.84875400	1.99258700
H	-4.54782000	-0.68516200	0.39050000
H	-4.91141900	-1.91803100	1.61940500
H	-3.58514400	-0.76807300	1.87905500
H	-4.64057500	-3.75574100	-0.21175700
H	-4.31165600	-2.47057200	-1.39543500
H	-3.15105900	-3.79859000	-1.18050500

Zero-point correction= 0.451764 (Hartree/Particle)
Thermal correction to Energy= 0.476648
Thermal correction to Enthalpy= 0.477592
Thermal correction to Gibbs Free Energy= 0.397269
Sum of electronic and zero-point Energies= -1242.864162
Sum of electronic and thermal Energies= -1242.839279
Sum of electronic and thermal Enthalpies= -1242.838335
Sum of electronic and thermal Free Energies= -1242.918658

2d,*anti*

C	0.36448000	4.40176900	-1.66886400
C	0.04388700	3.08662700	-1.97857800
C	0.08801500	2.09623700	-0.98898900
C	0.45191500	2.41364900	0.34123700
C	0.77135300	3.75043300	0.63006400
C	0.73037900	4.72960300	-0.36161100
C	0.00567600	0.12446600	1.06321300
C	0.05432500	-0.33315700	-0.39891300
C	-0.23785900	-0.37175500	3.34171700
C	0.94976000	0.55715000	3.58893800
C	0.81755300	1.79226400	2.70415200
H	0.33179200	5.16364300	-2.44158000
H	-0.23924600	2.78534300	-2.97921300
H	1.04199500	4.03945800	1.63742700
H	0.98196500	5.75396100	-0.10229800
H	-1.17701000	0.11696300	3.64467100
H	1.87423000	0.02112700	3.34386000
H	1.76867000	2.33553200	2.67409200
N	-0.24133900	0.77556900	-1.32676300
N	0.45435000	1.42163800	1.32747100
N	-0.32259700	-0.74691300	1.93782200
O	-0.54666000	0.47964800	-2.53536400
H	0.05772200	2.47629000	3.10746900
H	1.01376700	0.87008500	4.63693200

H	-0.15279200	-1.28698500	3.93739300
C	-0.83162900	-1.55668900	-0.69733500
H	-0.64550400	-1.80018800	-1.74577500
H	-0.43362100	-2.36331200	-0.08272100
C	-2.32513800	-1.40975900	-0.45131800
C	-3.15431400	-0.71825600	-1.34734400
C	-2.91973600	-2.02910600	0.65785600
C	-4.53120000	-0.63666500	-1.13046100
H	-2.71672200	-0.24492900	-2.22025100
C	-4.29583100	-1.95388800	0.87285800
H	-2.28989300	-2.56516300	1.36053000
C	-5.10855200	-1.25310600	-0.01995700
H	-5.15391000	-0.09509500	-1.83841800
H	-4.73331400	-2.44568000	1.73842100
H	-6.18144200	-1.19334800	0.14521900
O	1.43675900	-0.57964700	-0.74948600
O	1.94136700	-1.68975400	0.07713200
C	3.00985400	-2.32563600	-0.66687400
C	2.48359500	-2.91805100	-1.97862800
C	4.14743600	-1.32570100	-0.90938600
C	3.44292600	-3.42862000	0.30807800
H	1.66960100	-3.62355500	-1.78191800
H	2.10813900	-2.13025400	-2.63647600
H	3.28473500	-3.45300000	-2.50091800
H	4.48272900	-0.89449100	0.03979200
H	4.99939800	-1.82516100	-1.38408600
H	3.81852700	-0.51225600	-1.56121300
H	4.27173800	-3.99818200	-0.12520000
H	3.77638400	-2.99859300	1.25792500
H	2.61607000	-4.11709900	0.50922000

Zero-point correction=	0.451856 (Hartree/Particle)
Thermal correction to Energy=	0.476694
Thermal correction to Enthalpy=	0.477638
Thermal correction to Gibbs Free Energy=	0.397677
Sum of electronic and zero-point Energies=	-1242.861745
Sum of electronic and thermal Energies=	-1242.836907
Sum of electronic and thermal Enthalpies=	-1242.835963
Sum of electronic and thermal Free Energies=	-1242.915924

2e,*anti*(N-O)

C	-2.02692400	3.43999800	-0.81625000
C	-1.26507200	2.88075500	0.20040000
C	-1.04926500	1.49541800	0.24304900
C	-1.60723700	0.64364300	-0.73976500
C	-2.36412900	1.23426000	-1.76376200
C	-2.57322400	2.61258500	-1.80030700
C	-0.46992800	-1.30896400	0.19390500

C	0.05263300	-0.47686800	1.37793100
C	-0.56578400	-3.41114700	-0.86186800
C	-2.00926900	-3.06802800	-1.22221100
C	-2.09152500	-1.60457900	-1.64301900
H	-2.18931000	4.51308600	-0.84389500
H	-0.82160400	3.48272800	0.98354200
H	-2.78874900	0.62172300	-2.54878000
H	-3.16352500	3.03556300	-2.60794100
H	0.07506900	-3.35717900	-1.75583900
H	-2.64735400	-3.23565900	-0.34659500
H	-3.13785800	-1.28621700	-1.69011700
N	-0.28487600	0.95816800	1.27921200
N	-1.39695000	-0.73823100	-0.67674800
N	-0.04073000	-2.51282700	0.15511100
O	0.10676000	1.69848000	2.25168900
H	-1.65495400	-1.46374600	-2.64186800
H	-2.38718600	-3.69849300	-2.03464400
H	-0.48890500	-4.43669800	-0.48417400
C	1.57485300	-0.65140700	1.59726900
H	1.80631100	-0.10750800	2.51595000
H	1.73375300	-1.71693000	1.76732500
C	2.43524900	-0.15539400	0.45252900
C	2.77218500	1.20211000	0.34674800
C	2.92931800	-1.04619400	-0.51055200
C	3.57576300	1.65713900	-0.69921400
H	2.40045200	1.90136900	1.09079700
C	3.73570500	-0.59261200	-1.55552300
H	2.67646000	-2.09978300	-0.43379500
C	4.05992700	0.76145400	-1.65443500
H	3.82863200	2.71238200	-0.76391400
H	4.11484200	-1.29905700	-2.28984300
H	4.69009200	1.11531200	-2.46635500
O	-0.50205600	-0.97589700	2.59397400
O	-1.93900200	-0.76751700	2.56556600
H	-1.99354500	0.05578600	3.08772900

Zero-point correction= 0.340063 (Hartree/Particle)
Thermal correction to Energy= 0.359322
Thermal correction to Enthalpy= 0.360266
Thermal correction to Gibbs Free Energy= 0.291992
Sum of electronic and zero-point Energies= -1085.791302
Sum of electronic and thermal Energies= -1085.772043
Sum of electronic and thermal Enthalpies= -1085.771099
Sum of electronic and thermal Free Energies= -1085.839373

2e,*syn*(N-O)

C	-3.79116400	-1.32230100	-1.52886800
C	-2.76682700	-1.74631100	-0.69473900

C	-1.81100900	-0.83022600	-0.22974200
C	-1.86601400	0.53246100	-0.60636200
C	-2.92135500	0.94012900	-1.43668200
C	-3.86818800	0.02462300	-1.89438700
C	0.01414900	1.10923100	0.85990600
C	0.08008500	-0.34056000	1.37193300
C	0.83462500	3.31139900	1.02632900
C	0.47459800	3.46891200	-0.44895400
C	-0.86217900	2.78726700	-0.72084700
H	-4.52926800	-2.03397800	-1.88540400
H	-2.67208700	-2.77730200	-0.37833200
H	-3.01947200	1.97993900	-1.72093500
H	-4.67230400	0.37355200	-2.53558300
H	0.13025000	3.87319100	1.65839700
H	1.25534100	3.00295900	-1.06171100
H	-1.02867600	2.70580600	-1.79916300
N	-0.77985600	-1.27023300	0.59638400
N	-0.88898500	1.42722100	-0.15454100
N	0.82186200	1.91518600	1.43501400
O	-0.72446300	-2.51121800	0.95234100
H	-1.68893000	3.37451900	-0.29777700
H	0.40689100	4.52264000	-0.74106000
H	1.83008100	3.71911900	1.23354100
C	1.53379400	-0.86110800	1.40454900
H	2.05958200	-0.19592100	2.09092000
H	1.51093400	-1.85707500	1.84583400
C	2.21689800	-0.89016100	0.05189400
C	3.10141900	0.13182400	-0.32219500
C	1.99611200	-1.94452200	-0.84693700
C	3.74249000	0.10699100	-1.56196500
H	3.28869600	0.94727700	0.37100200
C	2.63378100	-1.96942000	-2.08804600
H	1.32121300	-2.74866400	-0.56730100
C	3.50797200	-0.94319000	-2.45111600
H	4.43145500	0.90447100	-1.82943900
H	2.45157900	-2.79639200	-2.76970500
H	4.00854000	-0.96608600	-3.41567400
O	-0.50366400	-0.24836400	2.67647100
O	-0.26804600	-1.46369300	3.43566200
H	-0.68070100	-2.13729100	2.84596600

Zero-point correction= 0.340112 (Hartree/Particle)
Thermal correction to Energy= 0.359131
Thermal correction to Enthalpy= 0.360075
Thermal correction to Gibbs Free Energy= 0.292486
Sum of electronic and zero-point Energies= -1085.788521
Sum of electronic and thermal Energies= -1085.769503
Sum of electronic and thermal Enthalpies= -1085.768558
Sum of electronic and thermal Free Energies= -1085.836147

2e,*anti*(amid)

C	-0.21100200	4.11023900	0.17056600
C	0.11046800	3.05911800	1.01887400
C	-0.30682500	1.75508700	0.71714000
C	-1.07055800	1.49417400	-0.44150300
C	-1.36430100	2.56590200	-1.29562500
C	-0.94269500	3.86035600	-0.99213900
C	-1.06033300	-0.90574200	-0.00169500
C	-0.22725200	-0.70359800	1.27736300
C	-2.21629500	-2.45563000	-1.37340600
C	-3.22999100	-1.34420100	-1.62843000
C	-2.49711300	-0.01658400	-1.79350400
H	0.11511700	5.11735300	0.41136300
H	0.68451100	3.20692100	1.92466500
H	-1.91396100	2.39695500	-2.21307200
H	-1.18697200	4.66974800	-1.67362200
H	-1.59692500	-2.62052300	-2.26793500
H	-3.92081700	-1.28037800	-0.77931100
H	-3.21199200	0.81007800	-1.75876200
N	0.05487100	0.71039700	1.57355200
N	-1.51905600	0.18760500	-0.70964300
N	-1.34425400	-2.14044700	-0.24747700
O	0.74935800	0.94593300	2.62184300
H	-1.98180400	0.02626800	-2.76252200
H	-3.82684600	-1.54003200	-2.52582600
H	-2.71825600	-3.40545400	-1.16205200
C	1.09552300	-1.50343500	1.27078500
H	1.54390000	-1.33163200	2.25210600
H	0.83486300	-2.55804700	1.19936500
C	2.04570900	-1.11056000	0.15868800
C	2.92246900	-0.02564200	0.30830500
C	2.07706200	-1.83429500	-1.04209000
C	3.80072900	0.32841900	-0.71637200
H	2.91318000	0.54024000	1.23605100
C	2.95548600	-1.48233500	-2.06793000
H	1.41000600	-2.68365100	-1.16550900
C	3.81979300	-0.39795100	-1.90861300
H	4.47503400	1.17006500	-0.58027500
H	2.97013800	-2.06059300	-2.98851900
H	4.50781500	-0.12504100	-2.70456400
O	-1.08757500	-1.07955800	2.37467700
O	-1.18112100	-2.52337200	2.46975600
H	-1.48846100	-2.73912200	1.55070100

Zero-point correction= 0.340189 (Hartree/Particle)
Thermal correction to Energy= 0.359206
Thermal correction to Enthalpy= 0.360150
Thermal correction to Gibbs Free Energy= 0.292398
Sum of electronic and zero-point Energies= -1085.788083
Sum of electronic and thermal Energies= -1085.769066

Sum of electronic and thermal Enthalpies= -1085.768122
Sum of electronic and thermal Free Energies= -1085.835874

2e,*syn*(amid)

C	-4.00392900	-1.52648700	-0.30506600
C	-3.00080900	-1.44547700	0.65191300
C	-1.91311700	-0.58271000	0.46217400
C	-1.81423300	0.20774200	-0.70383400
C	-2.84105200	0.11619000	-1.65381400
C	-3.92274800	-0.74256800	-1.45756200
C	0.17662300	1.33148800	0.14196100
C	0.17973200	0.46017600	1.40950300
C	1.11038600	3.19022200	-0.98312400
C	0.78719500	2.44715400	-2.27716000
C	-0.58620700	1.79587000	-2.15451200
H	-4.84559300	-2.19444800	-0.15024300
H	-3.02341800	-2.03565400	1.55924000
H	-2.81034100	0.72104200	-2.55110700
H	-4.70307900	-0.79007800	-2.21130100
H	0.41206300	4.02876600	-0.83817300
H	1.54710800	1.67595100	-2.44886900
H	-0.73992200	1.08132300	-2.96935600
N	-0.89939500	-0.54047100	1.42574300
N	-0.71331000	1.06455100	-0.88178000
N	1.03675200	2.29095200	0.16226000
O	-0.90770900	-1.36344500	2.40555200
H	-1.37996700	2.55255800	-2.21809200
H	0.79078200	3.11885200	-3.14225600
H	2.11683400	3.62056500	-1.01583700
C	1.53969500	-0.24208700	1.63271500
H	2.27356700	0.54003600	1.82076500
H	1.42121300	-0.82245500	2.55061800
C	1.97592600	-1.12041900	0.47874000
C	2.91362600	-0.65432000	-0.45432300
C	1.46385100	-2.41700600	0.31990800
C	3.32341700	-1.45527500	-1.52174800
H	3.32901200	0.34304600	-0.33391800
C	1.87128100	-3.21899800	-0.74706100
H	0.74592300	-2.79721000	1.04149800
C	2.80028100	-2.74060100	-1.67300300
H	4.05837200	-1.07870300	-2.22900100
H	1.46601500	-4.22226600	-0.85094900
H	3.12092700	-3.36802800	-2.50059600
O	-0.18089700	1.31448700	2.51615900
O	0.93654100	2.16048300	2.89362000
H	1.10919700	2.61191400	2.02713000

Zero-point correction= 0.340761 (Hartree/Particle)
Thermal correction to Energy= 0.359714

Thermal correction to Enthalpy= 0.360659
Thermal correction to Gibbs Free Energy= 0.293374
Sum of electronic and zero-point Energies= -1085.789082
Sum of electronic and thermal Energies= -1085.770129
Sum of electronic and thermal Enthalpies= -1085.769184
Sum of electronic and thermal Free Energies= -1085.836469

3a

C	-0.86793000	4.15230400	-1.11925000
C	-0.65488400	2.85723600	-1.57891900
C	-0.46791700	1.80906900	-0.66732100
C	-0.48710200	2.06853300	0.72397000
C	-0.70534400	3.37664600	1.17122900
C	-0.89452600	4.41098300	0.25464500
C	-0.02584000	-0.28991200	1.18960300
C	-0.30886600	-0.69728600	-0.24741000
C	0.41021600	-0.34825900	3.36409900
C	0.02979100	1.12317900	3.02467900
H	-1.01441900	4.95828100	-1.83182400
H	-0.62126000	2.62285200	-2.63553000
H	-0.72440800	3.58143900	2.23647100
H	-1.06130000	5.42052400	0.61879900
H	-0.28631900	-0.79092400	4.08510000
H	0.85124300	1.83128800	3.18912500
N	-0.22597700	0.50794000	-1.13094700
N	-0.26763900	1.01347600	1.59350600
N	0.35193400	-1.10582900	2.10283500
O	-0.14162800	0.29423100	-2.39328200
C	-1.73750400	-1.30011600	-0.33368300
C	-2.64853100	-0.90034400	-1.31935900
C	-2.11957800	-2.30044800	0.57290500
C	-3.91568700	-1.48327100	-1.38910600
H	-2.36983600	-0.14804800	-2.04730500
C	-3.38390600	-2.88336700	0.49585100
H	-1.42612000	-2.61079200	1.34784700
C	-4.28999900	-2.47520000	-0.48417300
H	-4.60872400	-1.15746800	-2.16028900
H	-3.66021600	-3.65651800	1.20812400
H	-5.27669000	-2.92703200	-0.54194300
H	-0.84647800	1.47811600	3.57900900
H	1.41516900	-0.42526000	3.79312700
C	0.73347400	-1.75221000	-0.73874300
H	0.57098400	-2.64226900	-0.12718600
H	0.45203100	-1.99783600	-1.76506300
C	2.19578200	-1.34870500	-0.67195000
C	2.78426800	-0.56856100	-1.67872100
C	3.00392800	-1.79176300	0.38574000
C	4.13836200	-0.23483800	-1.62291500

H	2.17368200	-0.22190200	-2.50652300
C	4.35867900	-1.46210100	0.44033400
H	2.55882300	-2.39240600	1.17313400
C	4.93124300	-0.67981100	-0.56392200
H	4.57522800	0.36926500	-2.41426200
H	4.96756400	-1.82094200	1.26664300
H	5.98706300	-0.42386600	-0.52445100

Zero-point correction= 0.383550 (Hartree/Particle)
Thermal correction to Energy= 0.404435
Thermal correction to Enthalpy= 0.405379
Thermal correction to Gibbs Free Energy= 0.332909
Sum of electronic and zero-point Energies= -1127.114621
Sum of electronic and thermal Energies= -1127.093736
Sum of electronic and thermal Enthalpies= -1127.092792
Sum of electronic and thermal Free Energies= -1127.165262

3b

C	-4.11026100	1.10888500	0.93487900
C	-2.82589800	1.03541000	1.46349000
C	-1.84285500	0.27997700	0.81225800
C	-2.15490300	-0.41985700	-0.37485300
C	-3.45029000	-0.33311400	-0.89817200
C	-4.42034900	0.42701600	-0.24611300
C	0.10930500	-1.32469200	-0.41428200
C	0.61600800	-0.18981200	0.47572600
C	-0.04832400	-3.10799200	-1.72388500
C	-1.41669600	-2.37012000	-1.81285400
H	-4.86693400	1.70037600	1.44106800
H	-2.55466000	1.54443100	2.38004200
H	-3.69384100	-0.86407300	-1.81258900
H	-5.42132600	0.48388700	-0.66370100
H	0.45753100	-3.14675700	-2.69451600
H	-2.25246300	-2.95926700	-1.41583600
N	-0.54773800	0.17645600	1.36251700
N	-1.16863400	-1.20441300	-0.95362800
N	0.78533000	-2.34459300	-0.78156100
O	-0.33449000	0.67777600	2.52179600
C	0.96167200	1.02699000	-0.41602200
C	1.62382200	0.84049600	-1.63755900
C	0.64448200	2.32974000	-0.00771300
C	1.96179700	1.93639200	-2.43200500
H	1.88838900	-0.15962700	-1.96327700
C	0.98123100	3.42214100	-0.80743700
H	0.14275300	2.49468200	0.93970700
C	1.63928100	3.23032900	-2.02258700
H	2.47932800	1.77307800	-3.37326600
H	0.72651500	4.42503300	-0.47562400

H	1.89978600	4.08243800	-2.64447900
H	-1.66835700	-2.05953700	-2.83257400
H	-0.15158300	-4.13977200	-1.37142500
C	1.86545500	-0.65343700	1.35602900
C	2.52829900	0.50795300	2.15275200
C	1.48787800	-1.80280500	2.32283000
H	2.82526700	1.32414600	1.49070100
H	1.84684400	0.88825400	2.91038800
H	3.43077500	0.12025400	2.63482500
H	1.09974700	-2.66592500	1.77932300
H	2.38007800	-2.11840600	2.87201600
H	0.74544800	-1.44962700	3.04113600
C	2.94559100	-1.12628100	0.45807000
N	3.90120600	-1.42732200	-0.12898500

Zero-point correction= 0.356976 (Hartree/Particle)
Thermal correction to Energy= 0.377817
Thermal correction to Enthalpy= 0.378761
Thermal correction to Gibbs Free Energy= 0.308332
Sum of electronic and zero-point Energies= -1066.971189
Sum of electronic and thermal Energies= -1066.950347
Sum of electronic and thermal Enthalpies= -1066.949403
Sum of electronic and thermal Free Energies= -1067.019832

3c,(N-O)

C	-3.50754000	-2.05229400	-0.36331800
C	-2.37136600	-2.01182600	0.43678600
C	-1.54332100	-0.88086500	0.41899500
C	-1.86212200	0.23041300	-0.40229600
C	-3.00821800	0.16880400	-1.20395900
C	-3.82279000	-0.96361200	-1.18346800
C	0.07397100	1.46617000	0.46153200
C	0.67675600	0.20019600	1.04491400
C	-0.25622500	3.54376700	-0.21391700
C	-1.39408900	2.68626700	-0.84605800
H	-4.14494300	-2.93100500	-0.34963400
H	-2.09899800	-2.83188300	1.09027800
H	-3.26094000	1.01024800	-1.84048800
H	-4.70834900	-0.99164700	-1.81160600
H	-0.64759600	4.34798800	0.41841500
H	-1.39882900	2.71965000	-1.94129400
N	-0.41151100	-0.81810600	1.23313500
N	-1.04028100	1.34566700	-0.36363000
N	0.57059400	2.63402500	0.59796200
O	-0.13142200	-1.75043500	2.06908300
C	1.76281400	-0.35783000	0.10201300
C	1.68000600	-1.61839400	-0.49603800
C	2.89334600	0.44050200	-0.12405800

C	2.71507800	-2.07369700	-1.31723400
H	0.82334500	-2.25807500	-0.31528200
C	3.92248600	-0.01750800	-0.94298600
H	2.95121200	1.41751500	0.34506200
C	3.83551300	-1.27641900	-1.54428700
H	2.64203400	-3.05681600	-1.77446200
H	4.79485500	0.60844400	-1.11121400
H	4.63896800	-1.63289500	-2.18344900
H	-2.39310000	2.96481100	-0.48876700
H	0.37270400	4.01016400	-0.98035700
O	1.19746500	0.49658400	2.30381300
H	1.30388100	-0.37884500	2.72763700

Zero-point correction= 0.278110 (Hartree/Particle)
Thermal correction to Energy= 0.294183
Thermal correction to Enthalpy= 0.295127
Thermal correction to Gibbs Free Energy= 0.233846
Sum of electronic and zero-point Energies= -932.150976
Sum of electronic and thermal Energies= -932.134904
Sum of electronic and thermal Enthalpies= -932.133959
Sum of electronic and thermal Free Energies= -932.195241

3c,(amid*)*

C	-2.99341900	-2.65953100	-0.19391800
C	-1.85571600	-2.36161000	0.54841100
C	-1.28286000	-1.08488100	0.47698600
C	-1.86367200	-0.09828400	-0.35631200
C	-3.00369900	-0.41376700	-1.10014100
C	-3.56856800	-1.68720800	-1.01728400
C	-0.19718400	1.50389500	0.38324100
C	0.70072200	0.42561700	0.96069700
C	-1.02472400	3.49065500	-0.11870800
C	-1.99851000	2.42453500	-0.71062400
H	-3.42961300	-3.65198400	-0.13227700
H	-1.38772600	-3.08903900	1.20036400
H	-3.44661800	0.34018300	-1.74333900
H	-4.45633100	-1.91589200	-1.59942700
H	-1.53013500	4.18363600	0.56167500
H	-2.14737000	2.53610900	-1.78905100
N	-0.15817800	-0.77694200	1.26247500
N	-1.28395600	1.17398600	-0.39808400
N	0.02199000	2.74537400	0.60305400
O	0.32209200	-1.63130700	2.07584300
C	1.82186100	-0.01303500	0.00977900
C	1.69756100	0.06591100	-1.38132800
C	2.98586900	-0.55481700	0.56862200
C	2.73186900	-0.38097400	-2.20594200
H	0.79930300	0.47976500	-1.82981100

C	4.01296600	-1.00635400	-0.25816100
H	3.07409900	-0.61246400	1.64713300
C	3.89101500	-0.91874400	-1.64704700
H	2.62884600	-0.30642800	-3.28529100
H	4.91314700	-1.42491200	0.18412500
H	4.69564300	-1.26704700	-2.28922700
H	-2.98181600	2.42164000	-0.22409700
H	-0.55684300	4.09033000	-0.90769300
O	1.21565000	0.87854500	2.17914400
H	1.14341000	1.85282100	2.14528300

Zero-point correction= 0.278277 (Hartree/Particle)
Thermal correction to Energy= 0.294320
Thermal correction to Enthalpy= 0.295264
Thermal correction to Gibbs Free Energy= 0.234037
Sum of electronic and zero-point Energies= -932.148607
Sum of electronic and thermal Energies= -932.132564
Sum of electronic and thermal Enthalpies= -932.131620
Sum of electronic and thermal Free Energies= -932.192848

3d

C	-3.99530100	0.56631100	-1.87364200
C	-2.60840900	0.65224300	-1.94096400
C	-1.81486200	-0.00190000	-0.99072800
C	-2.42329400	-0.76070600	0.03636700
C	-3.82072900	-0.83555700	0.09389700
C	-4.60046600	-0.17615600	-0.85537300
C	-0.22351000	-1.40293800	0.89387900
C	0.47277200	-0.33923100	0.04556900
C	-0.63735400	-3.00246800	2.35950700
C	-2.02154800	-2.49798000	1.84956000
H	-4.60205700	1.07851300	-2.61414800
H	-2.10700600	1.21029100	-2.72185300
H	-4.29229700	-1.41307700	0.88218500
H	-5.68276000	-0.24620000	-0.79702800
H	-0.49447800	-4.07372300	2.18125700
H	-2.65868400	-2.11016000	2.65220600
N	-0.40902100	0.05821400	-1.08752200
N	-1.60969900	-1.42244500	0.94098500
N	0.39422100	-2.23901900	1.63741500
O	0.12734000	0.69255000	-2.06299700
C	1.82594100	-0.83472900	-0.45108800
C	1.93635400	-1.55868600	-1.64277700
C	2.95543200	-0.65411100	0.35092900
C	3.16798200	-2.08231200	-2.03356400
H	1.06834900	-1.70365200	-2.27662100
C	4.18695600	-1.17505600	-0.04452800

H	2.86623500	-0.10280100	1.27880400
C	4.29793600	-1.89002000	-1.23736200
H	3.24321700	-2.63689200	-2.96510700
H	5.06001100	-1.02277800	0.58446900
H	5.25837200	-2.29544000	-1.54496500
H	-2.58629500	-3.26264300	1.30141900
H	-0.51595200	-2.83410100	3.43544600
O	0.56553000	0.73701400	0.98350400
O	1.31948500	1.83103800	0.35444800
C	0.74416800	3.09287300	0.77452200
C	-0.69408000	3.23658600	0.26957100
C	0.83462100	3.23343300	2.29854500
C	1.67992300	4.08285800	0.06700300
H	-0.73213000	3.07600400	-0.81180800
H	-1.35367600	2.51062200	0.75226500
H	-1.07279500	4.24088100	0.49054500
H	1.87001200	3.11056900	2.63307900
H	0.48416800	4.22369900	2.61057000
H	0.21814700	2.47974300	2.79641100
H	1.37278600	5.10816600	0.29864200
H	2.71344300	3.94518200	0.39970700
H	1.64085200	3.94099900	-1.01718800

Zero-point correction= 0.392267 (Hartree/Particle)
Thermal correction to Energy= 0.415366
Thermal correction to Enthalpy= 0.416310
Thermal correction to Gibbs Free Energy= 0.339918
Sum of electronic and zero-point Energies= -1164.320876
Sum of electronic and thermal Energies= -1164.297777
Sum of electronic and thermal Enthalpies= -1164.296833
Sum of electronic and thermal Free Energies= -1164.373225

3e,(N-O)

C	-3.42402100	-2.23894000	-0.37653900
C	-2.29789700	-2.08724900	0.42443600
C	-1.52031500	-0.92598100	0.32608600
C	-1.88492600	0.10651000	-0.57289000
C	-3.02136200	-0.06367000	-1.37334100
C	-3.78202400	-1.22832900	-1.27552500
C	0.01495400	1.46112800	0.17785100
C	0.67132000	0.25088600	0.83094800
C	-0.39259600	3.47920500	-0.62598100
C	-1.50952800	2.54655400	-1.18604600
H	-4.02033500	-3.14298600	-0.30187200
H	-1.99604400	-2.84296900	1.13958100
H	-3.30928000	0.72022000	-2.06594900
H	-4.66044200	-1.34285700	-1.90387400
H	-0.80237600	4.29432300	-0.01972200

H	-1.51213400	2.49092700	-2.28080500
N	-0.40103400	-0.75248300	1.15065400
N	-1.12091100	1.25967800	-0.59827300
N	0.49021500	2.64567200	0.20920700
O	-0.17766400	-1.55007300	2.12993500
C	1.75795900	-0.35914000	-0.06694300
C	2.69855100	0.48844200	-0.66669100
C	1.85930000	-1.74352000	-0.24356300
C	3.72066700	-0.04690900	-1.44910600
H	2.62459500	1.55961000	-0.51081400
C	2.87984500	-2.27193400	-1.03463300
H	1.15659500	-2.40908600	0.24435700
C	3.81016300	-1.42693700	-1.64073100
H	4.44779200	0.61676800	-1.90905600
H	2.94839600	-3.34764200	-1.17116100
H	4.60414900	-1.84204800	-2.25581200
H	-2.51556900	2.82830000	-0.85305200
H	0.19636500	3.93556200	-1.42886800
O	1.34909000	0.58023300	2.01328300
O	0.38311200	1.04458100	2.99727000
H	0.14355500	0.17319200	3.37804200

Zero-point correction= 0.281438 (Hartree/Particle)
Thermal correction to Energy= 0.298534
Thermal correction to Enthalpy= 0.299478
Thermal correction to Gibbs Free Energy= 0.236031
Sum of electronic and zero-point Energies= -1007.247117
Sum of electronic and thermal Energies= -1007.230021
Sum of electronic and thermal Enthalpies= -1007.229077
Sum of electronic and thermal Free Energies= -1007.292524

3e,(amid)

C	3.51187300	-2.40218800	0.03418500
C	2.25522600	-2.26645900	-0.54586500
C	1.54577500	-1.06586000	-0.41278200
C	2.10708400	0.00707900	0.31647900
C	3.36995600	-0.14410000	0.89715500
C	4.07011300	-1.34211200	0.75421300
C	0.15546400	1.38305400	-0.17266000
C	-0.63587000	0.21286000	-0.74569400
C	0.75388300	3.44873200	0.38352600
C	1.92807900	2.50697700	0.78723200
H	4.05435200	-3.33631500	-0.07436300
H	1.79532200	-3.06666900	-1.11207800
H	3.80107500	0.67675900	1.46093300
H	5.05085900	-1.44370500	1.20917900
H	1.06819500	4.22147900	-0.32558200
H	2.16320700	2.55069000	1.85569100

N	0.28511700	-0.93479000	-1.02407500
N	1.38087100	1.19068500	0.42403700
N	-0.27322400	2.59246400	-0.23442600
O	-0.20441400	-1.90028700	-1.69819500
C	-1.77751800	-0.25828100	0.14823200
C	-1.73926100	-0.06508900	1.53195400
C	-2.83697700	-0.97270900	-0.42347600
C	-2.75629800	-0.57439600	2.34148400
H	-0.91979800	0.48354800	1.98795200
C	-3.85062300	-1.47786800	0.38736400
H	-2.85844600	-1.11862000	-1.49638600
C	-3.81398000	-1.28117000	1.77035800
H	-2.71976000	-0.41575300	3.41586500
H	-4.67428000	-2.02517800	-0.06292300
H	-4.60785200	-1.67624300	2.39868400
H	2.84856200	2.69796200	0.22264500
H	0.32424600	3.95786400	1.25318400
O	-1.06057100	0.58817700	-2.06123400
O	-2.13018200	1.56017700	-1.94704000
H	-1.63524700	2.32032700	-1.55002500

Zero-point correction= 0.281840 (Hartree/Particle)
Thermal correction to Energy= 0.298834
Thermal correction to Enthalpy= 0.299779
Thermal correction to Gibbs Free Energy= 0.236752
Sum of electronic and zero-point Energies= -1007.243132
Sum of electronic and thermal Energies= -1007.226137
Sum of electronic and thermal Enthalpies= -1007.225193
Sum of electronic and thermal Free Energies= -1007.288220

4a

C	-3.93630400	-0.21571000	-2.79932400
C	-2.73651700	-0.80710400	-2.41590300
C	-2.27724000	-0.66902900	-1.10090200
C	-3.03851900	0.05576200	-0.15437400
C	-4.24164100	0.64762500	-0.55418300
C	-4.68540300	0.51260500	-1.87009400
C	-1.36976800	-0.43473500	1.56605700
C	-0.32915700	-0.78529100	0.50765200
C	-2.40859900	0.00350200	3.47698500
C	-3.36925500	0.45288600	2.33530100
H	-4.28482100	-0.32043500	-3.82229200
H	-2.13643600	-1.38706800	-3.10648100
H	-4.82977100	1.20576400	0.16705200
H	-5.62180200	0.97669400	-2.16586900
H	-2.85275500	-0.77600700	4.10638700
H	-3.59003200	1.52659200	2.36133700
N	-1.08916900	-1.29558300	-0.68577200

N	-2.57596700	0.11042400	1.15152100
N	-1.19134900	-0.52125000	2.83262300
O	-0.51401800	-2.13432800	-1.46309800
C	0.43894200	0.49012700	0.10493400
C	0.73738000	1.47930100	1.04484700
C	0.90167400	0.66263800	-1.20997900
C	1.46772500	2.61899100	0.69655700
H	0.40749000	1.36266200	2.07252000
C	1.62393200	1.79150300	-1.56910700
H	0.70316000	-0.09906400	-1.95611200
C	1.91179300	2.78204200	-0.61933400
H	1.67792900	3.36386800	1.45565500
H	1.98089200	1.92683500	-2.58522000
H	-4.32079300	-0.09223000	2.32791500
H	-2.14178400	0.83674700	4.13597800
C	0.59807300	-1.91911300	1.06205700
H	0.05546500	-2.86202700	0.94465300
H	0.66612000	-1.72408700	2.13521200
C	2.00191100	-2.04971600	0.50141700
C	2.30047300	-2.92660900	-0.55017300
C	3.05591400	-1.33487400	1.08856900
C	3.61084200	-3.07567900	-1.00629700
H	1.49618500	-3.48525600	-1.01568800
C	4.36609100	-1.47558900	0.63054500
H	2.84665500	-0.65999500	1.91481000
C	4.64864500	-2.34846600	-0.42089500
H	3.82061100	-3.76385100	-1.82149100
H	5.16602500	-0.90891300	1.10060300
H	5.66901600	-2.46495000	-0.77732600
O	2.62243000	3.85454100	-1.07483500
C	2.94533800	4.88442700	-0.15492800
H	3.56940300	4.51062600	0.66772200
H	3.50634300	5.62875500	-0.72309300
H	2.04301700	5.35153700	0.26202300

Zero-point correction= 0.416073 (Hartree/Particle)
Thermal correction to Energy= 0.439657
Thermal correction to Enthalpy= 0.440601
Thermal correction to Gibbs Free Energy= 0.362031
Sum of electronic and zero-point Energies= -1241.560989
Sum of electronic and thermal Energies= -1241.537405
Sum of electronic and thermal Enthalpies= -1241.536461
Sum of electronic and thermal Free Energies= -1241.615032

4b

C	-2.19213500	-3.29535100	-1.87279400
C	-1.64913800	-2.03710300	-2.11443500
C	-1.54342000	-1.11280000	-1.06963300

C	-1.99949300	-1.44283100	0.22441700
C	-2.54128900	-2.71214900	0.45531500
C	-2.63434500	-3.63181600	-0.58962500
C	-1.36187400	0.78947500	1.02320100
C	-0.41094200	0.96042400	-0.16404000
C	-2.50238900	1.01337600	2.91919000
C	-2.71274900	-0.45351100	2.44678100
H	-2.26698600	-4.01343200	-2.68362400
H	-1.30549800	-1.73936800	-3.09761800
H	-2.89271700	-2.97430900	1.44785200
H	-3.05711100	-4.61359800	-0.39739900
H	-2.03323400	1.06125900	3.90749300
H	-3.76119800	-0.69693000	2.23814700
N	-1.03653900	0.17974900	-1.30074000
N	-1.93216800	-0.46521200	1.20584200
N	-1.62004900	1.65747600	1.93099800
O	-0.83509800	0.56344000	-2.50406400
C	0.94686000	0.30818600	0.17682200
C	1.43543200	0.27826900	1.49356400
C	1.73949100	-0.24577200	-0.83407100
C	2.67101000	-0.28262300	1.78660800
H	0.84930200	0.70944700	2.29877200
C	2.98310700	-0.81250600	-0.55178300
H	1.39388100	-0.23265700	-1.86197100
C	3.45724500	-0.83348000	0.76456600
H	3.05001700	-0.30383600	2.80352700
H	3.56720000	-1.22760700	-1.36473300
H	-2.32448400	-1.19076200	3.15917000
H	-3.44531900	1.56819700	2.98198700
C	-0.25176800	2.47821900	-0.61503600
C	-1.60970500	3.10392500	-1.01883800
C	0.41152500	3.34764000	0.49051100
H	-2.07074500	2.55703300	-1.84261600
H	-2.28043200	3.11445200	-0.15650100
H	-1.44804000	4.13669700	-1.34205500
H	1.39231600	2.95520700	0.76863400
H	0.55366200	4.35699600	0.09289600
H	-0.22681400	3.38931600	1.37199600
C	0.67758400	2.57411400	-1.76452500
N	1.45752600	2.79861400	-2.59528800
O	4.65155600	-1.36095800	1.15337300
C	5.50113200	-1.91009300	0.15631700
H	6.39343000	-2.25470000	0.68187300
H	5.02864900	-2.76067700	-0.35213000
H	5.78623900	-1.15651900	-0.58892800

Zero-point correction= 0.389666 (Hartree/Particle)
Thermal correction to Energy= 0.413020
Thermal correction to Enthalpy= 0.413964
Thermal correction to Gibbs Free Energy= 0.338092
Sum of electronic and zero-point Energies= -1181.423029

Sum of electronic and thermal Energies= -1181.399676
Sum of electronic and thermal Enthalpies= -1181.398731
Sum of electronic and thermal Free Energies= -1181.474603

4c,(N-O)

C	-3.61560200	-2.55751900	-0.65811100
C	-2.69103200	-2.25775600	0.33609300
C	-2.04942300	-1.01148300	0.34214700
C	-2.34630600	-0.04615100	-0.65314400
C	-3.27686200	-0.36821500	-1.64837800
C	-3.90490300	-1.61405700	-1.64967400
C	-0.82889800	1.56466900	0.40974200
C	-0.18628900	0.47309500	1.24758400
C	-1.30247400	3.48920000	-0.56789500
C	-2.14855800	2.40209100	-1.29721900
H	-4.10793700	-3.52511200	-0.66160600
H	-2.44699900	-2.95953300	1.12457800
H	-3.50880700	0.35973100	-2.41867600
H	-4.62471700	-1.84469700	-2.42957000
H	-1.92889700	4.27045800	-0.12380300
H	-1.92362200	2.33012100	-2.36733100
N	-1.13522300	-0.68904100	1.34603900
N	-1.72201600	1.18934600	-0.58961500
N	-0.54017600	2.80578000	0.49122600
O	-0.90540200	-1.48433800	2.32639100
C	1.13518800	0.01320400	0.60616900
C	1.37596000	-1.30326600	0.19126600
C	2.15886800	0.95725700	0.47194500
C	2.60510800	-1.66166500	-0.35056600
H	0.61172400	-2.06432100	0.30295300
C	3.39584100	0.60904800	-0.06840300
H	1.98001500	1.97864700	0.79318800
C	3.62364600	-0.70932600	-0.48609700
H	2.79994300	-2.68014800	-0.67127800
H	4.16745500	1.36534700	-0.15628800
H	-3.22961300	2.54730900	-1.18150500
H	-0.60299900	3.98346900	-1.25131800
O	0.00800100	0.96656200	2.53782200
H	0.16250700	0.16501500	3.07654700
O	4.78987500	-1.16044100	-1.03086400
C	5.86162900	-0.24284900	-1.18269300
H	6.18490100	0.16459000	-0.21577700
H	6.68104100	-0.81142800	-1.62622500
H	5.59275700	0.58602800	-1.85083200

Zero-point correction= 0.311075 (Hartree/Particle)
Thermal correction to Energy= 0.329574
Thermal correction to Enthalpy= 0.330518

Thermal correction to Gibbs Free Energy= 0.264043
Sum of electronic and zero-point Energies= -1046.601127
Sum of electronic and thermal Energies= -1046.582628
Sum of electronic and thermal Enthalpies= -1046.581683
Sum of electronic and thermal Free Energies= -1046.648158

4c,(amid)

C	-3.30636900	-2.78863200	-0.55908900
C	-2.51305400	-2.30977400	0.47876500
C	-1.94543200	-1.03168300	0.39791100
C	-2.18592800	-0.22371500	-0.73967100
C	-2.97910900	-0.72095900	-1.77719000
C	-3.53806900	-1.99665700	-1.68718800
C	-0.92558900	1.57086200	0.28791400
C	-0.22174900	0.62238300	1.24340100
C	-1.63707700	3.41388300	-0.70549500
C	-2.24785400	2.20783800	-1.48518300
H	-3.74014200	-3.78160100	-0.48889400
H	-2.31962900	-2.89403600	1.37029500
H	-3.15788600	-0.10572400	-2.65337900
H	-4.15371500	-2.36783200	-2.50117300
H	-2.40468600	4.09574300	-0.32423800
H	-1.96779800	2.20151100	-2.54343700
N	-1.16310700	-0.53799100	1.45933000
N	-1.64995200	1.06637400	-0.77170600
N	-0.86768000	2.84432600	0.41619600
O	-1.00952500	-1.22337300	2.52430500
C	1.10569100	0.12239300	0.65716900
C	1.43059800	-1.23573200	0.55105600
C	2.04994300	1.07098000	0.25382100
C	2.66192400	-1.63109000	0.04190800
H	0.73195700	-1.99365500	0.88638400
C	3.28797700	0.68749500	-0.26014700
H	1.81689000	2.12769300	0.34725800
C	3.59850700	-0.67435500	-0.37072500
H	2.92287100	-2.68159300	-0.03818500
H	3.99634300	1.44995000	-0.56341800
H	-3.34149100	2.15881300	-1.41680600
H	-0.96422200	4.00250700	-1.33874400
O	0.01356300	1.26917600	2.45273500
H	-0.42745100	2.13816600	2.39795900
O	4.77364300	-1.16501300	-0.85982700
C	5.76984900	-0.24166800	-1.26949200
H	6.09303100	0.39894600	-0.43845000
H	6.61411800	-0.84411500	-1.60969200
H	5.41997700	0.39053300	-2.09652100

Zero-point correction= 0.311127 (Hartree/Particle)

Thermal correction to Energy= 0.329613
Thermal correction to Enthalpy= 0.330557
Thermal correction to Gibbs Free Energy= 0.264331
Sum of electronic and zero-point Energies= -1046.598639
Sum of electronic and thermal Energies= -1046.580153
Sum of electronic and thermal Enthalpies= -1046.579209
Sum of electronic and thermal Free Energies= -1046.645435

4d

C	-4.34742200	-0.45207200	-2.16425700
C	-3.02164500	-0.03182700	-2.12944600
C	-2.18185800	-0.43389700	-1.08363400
C	-2.67883000	-1.27849700	-0.06375800
C	-4.01642700	-1.69157000	-0.10989300
C	-4.84433300	-1.28032000	-1.15372400
C	-0.47691600	-1.32048300	1.00452700
C	0.01559000	-0.15267000	0.14922000
C	-0.62541900	-2.90988000	2.53127800
C	-2.03779900	-2.78385600	1.88317400
H	-4.99107400	-0.13324800	-2.97847000
H	-2.60192700	0.60092500	-2.90155900
H	-4.40309200	-2.33648900	0.67236000
H	-5.87857700	-1.61139100	-1.17502700
H	-0.21036300	-3.91839900	2.42799000
H	-2.81936700	-2.52437100	2.60619300
N	-0.82910800	-0.03542000	-1.07440700
N	-1.81359200	-1.68571500	0.93771400
N	0.25181800	-1.94296700	1.85059100
O	-0.37440400	0.66523400	-2.04564300
C	1.48522800	-0.30643600	-0.20723200
C	1.89073300	-1.03603500	-1.33365800
C	2.45965900	0.18865100	0.65682100
C	3.23688500	-1.24913900	-1.59263400
H	1.15351100	-1.43060200	-2.02435200
C	3.81789300	-0.01327700	0.40466300
H	2.15835600	0.74436200	1.53633900
C	4.21236800	-0.73660300	-0.72535100
H	3.55893300	-1.80597300	-2.46688500
H	4.54926300	0.39264100	1.09394800
H	-2.35182500	-3.68875800	1.34796500
H	-0.64859300	-2.67759000	3.60188700
O	-0.25095900	0.94892000	1.02398100
O	0.25247600	2.17498800	0.38728700
C	-0.65426700	3.26189400	0.69434600
C	-2.03684400	3.01456400	0.08464300
C	-0.72562100	3.47865000	2.21056600
C	0.05471600	4.43171600	-0.00242700
H	-1.94504200	2.80552600	-0.98518000
H	-2.53129500	2.16513400	0.56309400

H	-2.67169300	3.89780500	0.21800900
H	0.27671100	3.63934600	2.62121000
H	-1.34023200	4.35619600	2.44098300
H	-1.16788700	2.61088300	2.70779300
H	-0.51864200	5.35219300	0.15021700
H	1.05967400	4.57524400	0.40657600
H	0.13931900	4.24476000	-1.07713200
O	5.50800900	-0.99632300	-1.07080900
C	6.53716600	-0.50078800	-0.23093900
H	6.46983500	-0.91948500	0.78212300
H	7.47635600	-0.81674000	-0.68927200
H	6.51571300	0.59543300	-0.16833100

Zero-point correction= 0.426345 (Hartree/Particle)
Thermal correction to Energy= 0.451612
Thermal correction to Enthalpy= 0.452556
Thermal correction to Gibbs Free Energy= 0.372018
Sum of electronic and zero-point Energies= -1278.770075
Sum of electronic and thermal Energies= -1278.744809
Sum of electronic and thermal Enthalpies= -1278.743864
Sum of electronic and thermal Free Energies= -1278.824402

4e,(N-O)

C	-2.863696	3.268463	-0.229180
C	-2.083452	2.558329	0.676376
C	-1.729608	1.230415	0.404793
C	-2.179673	0.596829	-0.780061
C	-2.963365	1.327462	-1.681961
C	-3.299347	2.652838	-1.407670
C	-1.067867	-1.484761	-0.115551
C	-0.227861	-0.749342	0.921199
C	-1.914296	-3.017408	-1.464868
C	-2.486945	-1.646959	-1.939185
H	-3.130414	4.299446	-0.018239
H	-1.737749	2.997766	1.604343
H	-3.312926	0.852383	-2.592604
H	-3.908307	3.203951	-2.118364
H	-1.342420	-3.515290	-2.255250
H	-3.579043	-1.584661	-1.863944
N	-0.969611	0.497060	1.324838
N	-1.857595	-0.733492	-0.979527
N	-1.027524	-2.744461	-0.319888
O	-0.754076	0.948977	2.505828
C	1.167794	-0.413886	0.388668
C	1.888008	-1.379801	-0.333255
C	1.776397	0.811397	0.669336
C	3.173717	-1.113621	-0.778894
H	1.432953	-2.344154	-0.533274

C	3.067564	1.091168	0.219208
H	1.252284	1.557480	1.255989
C	3.772634	0.127278	-0.511421
H	3.739352	-1.853569	-1.336262
H	3.509333	2.053752	0.449118
H	-2.197643	-1.394484	-2.966128
H	-2.705648	-3.707678	-1.152680
O	0.009529	-1.521549	2.067073
O	-1.259239	-1.784562	2.732382
H	-1.296403	-0.973536	3.282408
O	5.032205	0.293452	-1.001327
C	5.697960	1.522257	-0.750192
H	5.830224	1.696222	0.325528
H	6.676844	1.433383	-1.224512
H	5.157541	2.370765	-1.189789

Zero-point correction= 0.314862 (Hartree/Particle)
Thermal correction to Energy= 0.334329
Thermal correction to Enthalpy= 0.335273
Thermal correction to Gibbs Free Energy= 0.266849
Sum of electronic and zero-point Energies= -1121.697444
Sum of electronic and thermal Energies= -1121.677978
Sum of electronic and thermal Enthalpies= -1121.677033
Sum of electronic and thermal Free Energies= -1121.745457

4e,(amid)

C	-3.42925800	-2.88688700	-0.31513000
C	-2.56586700	-2.33095500	0.62341100
C	-1.96004900	-1.09291500	0.37404300
C	-2.23270000	-0.40320500	-0.83074500
C	-3.09749300	-0.97695300	-1.76728500
C	-3.69363600	-2.21226400	-1.51035100
C	-0.85039100	1.45700200	-0.08593000
C	-0.17938200	0.60429400	0.98236200
C	-1.42772700	3.15083900	-1.39137900
C	-2.16944500	1.89001200	-1.92784600
H	-3.89300400	-3.84791800	-0.11445800
H	-2.34509900	-2.82299800	1.56273600
H	-3.30309900	-0.45388200	-2.69562200
H	-4.36464500	-2.64375700	-2.24714500
H	-2.11867300	3.96049000	-1.13413500
H	-1.92853500	1.66625600	-2.97213400
N	-1.10176300	-0.52514400	1.33242000
N	-1.64917900	0.84704200	-1.03119500
N	-0.68151000	2.72533800	-0.19190000
O	-0.89874900	-1.11016200	2.44760400

C	1.18159000	0.08373300	0.51123100
C	1.54410200	-1.26652700	0.62076900
C	2.11037100	0.99241700	-0.00576500
C	2.79698600	-1.69462400	0.20377700
H	0.85540100	-1.98442300	1.05037500
C	3.37318700	0.57330500	-0.42216100
H	1.84323800	2.04167600	-0.08027700
C	3.72133300	-0.78015300	-0.32163300
H	3.08687500	-2.73736500	0.28418400
H	4.07058400	1.30372100	-0.81574400
H	-3.26018200	1.95608500	-1.83129000
H	-0.72221700	3.54774300	-2.12999300
O	0.11131600	1.36689200	2.12461100
O	-1.08102900	2.08782000	2.55089500
H	-1.00097300	2.86678200	1.95915700
O	4.92013900	-1.30236300	-0.70230400
C	5.90620900	-0.42188400	-1.22012300
H	6.19107900	0.34125700	-0.48435500
H	6.77267800	-1.04520900	-1.44768700
H	5.56333100	0.07198300	-2.13880800

Zero-point correction= 0.315210 (Hartree/Particle)
Thermal correction to Energy= 0.334646
Thermal correction to Enthalpy= 0.335590
Thermal correction to Gibbs Free Energy= 0.267297
Sum of electronic and zero-point Energies= -1121.697417
Sum of electronic and thermal Energies= -1121.677981
Sum of electronic and thermal Enthalpies= -1121.677037
Sum of electronic and thermal Free Energies= -1121.745331

5a,*syn*

C	4.64198600	-1.44692600	-0.72096700
C	3.38257600	-1.57697700	-1.30120700
C	2.37819300	-0.68028800	-0.93325500
C	2.69170700	0.34478200	-0.00734900
C	4.84451200	-0.42194900	0.20144200
C	0.47018500	1.28739800	-0.27552800
C	-0.04270100	-0.09863000	-0.71414000
C	0.16651400	3.58126700	0.12313000
C	1.01395200	3.40425400	1.38457500
C	2.19290200	2.48919300	1.07844700
H	5.44675000	-2.12874600	-0.97560700
H	3.14879800	-2.34842500	-2.02488300
H	5.81067400	-0.28927600	0.68362000
H	0.75387600	4.08561900	-0.65970000
H	0.39145500	2.96903500	2.17593900
H	2.67397700	2.12448700	1.98906700
N	1.09050700	-0.75883000	-1.46853600

N	1.74456900	1.31668100	0.29975100
N	-0.30539000	2.29736000	-0.38601500
O	0.84462200	-1.62013700	-2.38240700
C	-0.35854000	-0.96395800	0.52436200
C	-0.93128200	-0.38631100	1.66526200
C	-0.12681900	-2.34573000	0.51301500
C	-1.25173600	-1.16940300	2.77365600
H	-1.14702800	0.67692600	1.67909700
C	-0.44938800	-3.12790900	1.62323900
H	0.30099400	-2.81599200	-0.36639200
C	-1.00852100	-2.54329300	2.75940800
H	-1.69639400	-0.70222300	3.64837100
H	-0.25938900	-4.19767100	1.59619300
H	-1.25584400	-3.15272000	3.62448000
H	2.96243200	3.01807100	0.50321900
H	1.38893600	4.36451500	1.75532000
H	-0.70712900	4.21250100	0.31726900
C	-1.25068200	0.00819500	-1.69903300
H	-1.06617500	0.86882300	-2.34669900
H	-1.18525800	-0.88813400	-2.31864700
C	-2.64882900	0.08984900	-1.11412400
C	-3.29257700	1.31793700	-0.90979000
C	-3.36232300	-1.08608500	-0.83895200
C	-4.60330500	1.36840100	-0.43259300
H	-2.74934000	2.23288300	-1.11812200
C	-4.66996400	-1.03965500	-0.35557700
H	-2.88605700	-2.04929200	-1.00400900
C	-5.29658500	0.19039400	-0.14992300
H	-5.08505300	2.33210600	-0.28528700
H	-5.20110300	-1.96512800	-0.14757200
H	-6.31783500	0.22996600	0.22062700
N	3.89690000	0.46142500	0.54742700

Zero-point correction= 0.401358 (Hartree/Particle)
Thermal correction to Energy= 0.423003
Thermal correction to Enthalpy= 0.423947
Thermal correction to Gibbs Free Energy= 0.350125
Sum of electronic and zero-point Energies= -1182.435319
Sum of electronic and thermal Energies= -1182.413674
Sum of electronic and thermal Enthalpies= -1182.412730
Sum of electronic and thermal Free Energies= -1182.486553

5a,*anti*

C	-3.19485600	-3.28408800	-0.25686700
C	-1.94688100	-2.85646700	-0.70291100
C	-1.63169400	-1.50029000	-0.61203300
C	-2.60621000	-0.60636100	-0.10715100
C	-4.07460700	-2.33301200	0.25742900

C	-1.11040000	1.28545100	-0.50030200
C	0.08791000	0.30082200	-0.47589200
C	-1.97474600	3.49009400	-0.75591400
C	-3.37476300	2.87380800	-0.78417300
C	-3.42591200	1.71375100	0.20586800
H	-3.47562100	-4.33124100	-0.30021400
H	-1.20919200	-3.53348100	-1.11684700
H	-5.05572200	-2.62398100	0.62656400
H	-1.85340600	4.11705700	0.13953200
H	-3.60399200	2.49922200	-1.78934300
H	-4.36704100	1.16776700	0.16734800
N	-0.40145900	-0.99851200	-1.03965300
N	-2.34817400	0.76247300	-0.11091700
N	-0.88838700	2.51708700	-0.76191100
O	0.40132500	-1.75912600	-1.68273600
C	0.52686600	0.07380400	0.98701400
C	1.02301500	-1.17085100	1.39637900
C	0.48370500	1.12120800	1.91665200
C	1.45300100	-1.36541400	2.70870700
H	1.08789200	-1.98657400	0.68423000
C	0.91710100	0.92496200	3.22868800
H	0.12132700	2.09769200	1.61143100
C	1.39917000	-0.32037200	3.63157800
H	1.83480300	-2.33816200	3.00691300
H	0.87469200	1.74953200	3.93562700
H	1.73307300	-0.47423100	4.65418200
H	-3.28985100	2.07312000	1.23472300
H	-4.13581000	3.62039000	-0.53001300
H	-1.82343500	4.15769700	-1.61277100
C	1.24165800	0.84487400	-1.37912200
H	0.97410500	0.60942700	-2.41355400
H	1.18387200	1.92993400	-1.27802900
C	2.66459700	0.39882000	-1.09507100
C	3.25632700	-0.67210900	-1.77884500
C	3.45164900	1.11764700	-0.18330500
C	4.58870100	-1.01882700	-1.54993100
H	2.66219500	-1.23878300	-2.48704700
C	4.78132200	0.76922400	0.05445600
H	3.01590700	1.96052500	0.34721400
C	5.35596700	-0.30282500	-0.62965700
H	5.02811000	-1.85081600	-2.09487000
H	5.36951600	1.34084300	0.76806300
H	6.39362900	-0.57378100	-0.45178700
N	-3.79357700	-1.02422600	0.32776200

Zero-point correction= 0.400971 (Hartree/Particle)
Thermal correction to Energy= 0.422701
Thermal correction to Enthalpy= 0.423645
Thermal correction to Gibbs Free Energy= 0.349551
Sum of electronic and zero-point Energies= -1182.434776
Sum of electronic and thermal Energies= -1182.413046

Sum of electronic and thermal Enthalpies= -1182.412102
Sum of electronic and thermal Free Energies= -1182.486196

5b,*syn*

C	4.09558300	-1.30647600	-0.74516400
C	2.82225900	-1.47879200	-1.28193900
C	1.80044500	-0.62057200	-0.87316700
C	2.10920700	0.40973000	0.04644000
C	4.29348700	-0.27878400	0.17588500
C	-0.14889700	1.27028500	-0.15550300
C	-0.62765700	-0.14365300	-0.57560500
C	-0.54932500	3.54779500	0.28280100
C	0.35418500	3.39261000	1.50779000
C	1.56215700	2.53694400	1.14600900
H	4.91467700	-1.95759700	-1.03194000
H	2.59269800	-2.25415000	-2.00270500
H	5.27064200	-0.11403700	0.62474100
H	-0.02613000	4.10393700	-0.51000500
H	-0.21618000	2.91877200	2.31585800
H	2.10151200	2.19667400	2.03283200
N	0.49712400	-0.74615300	-1.37131900
N	1.13781200	1.34093900	0.38865400
N	-0.95884000	2.25014500	-0.23907200
O	0.27568800	-1.59967400	-2.29995400
C	-0.83844500	-0.99743200	0.69811900
C	-1.45671300	-0.44015500	1.82645600
C	-0.44910000	-2.34336000	0.73701600
C	-1.67438300	-1.21170800	2.96806400
H	-1.78524100	0.59312200	1.80888700
C	-0.66590300	-3.11116200	1.88161900
H	0.01324600	-2.80029000	-0.13150300
C	-1.27612300	-2.54820500	3.00253800
H	-2.15896700	-0.76275200	3.83068700
H	-0.35611300	-4.15265100	1.89244400
H	-1.44290600	-3.14664700	3.89397500
H	2.27688000	3.10241500	0.53576800
H	0.69856600	4.36441800	1.87767300
H	-1.45487400	4.11433400	0.52219900
C	-1.95629100	-0.08102500	-1.45945600
C	-1.72636200	0.65123100	-2.80556000
C	-2.57432300	-1.48454500	-1.73353900
H	-1.01484400	0.08908400	-3.41313800
H	-2.67526900	0.70914400	-3.34741000
H	-1.36168800	1.66647800	-2.64624500
H	-3.51187800	-1.34303800	-2.27949300
H	-1.89698800	-2.09026000	-2.33178800
H	-2.80495100	-2.00772500	-0.80324900

C	-3.02042500	0.62717000	-0.70872300
N	-3.97707600	1.04803500	-0.20110700
N	3.32841500	0.56828900	0.55964000

Zero-point correction= 0.374441 (Hartree/Particle)
Thermal correction to Energy= 0.396009
Thermal correction to Enthalpy= 0.396953
Thermal correction to Gibbs Free Energy= 0.325345
Sum of electronic and zero-point Energies= -1122.296135
Sum of electronic and thermal Energies= -1122.274567
Sum of electronic and thermal Enthalpies= -1122.273622
Sum of electronic and thermal Free Energies= -1122.345231

5b,*anti*

C	3.40589700	-2.66071100	-1.05838500
C	2.04906500	-2.63231700	-0.75073600
C	1.45614000	-1.40585100	-0.43345000
C	2.25934000	-0.24390900	-0.44644500
C	4.11508700	-1.46128700	-1.04080800
C	0.33665600	1.18085700	0.10335300
C	-0.58053000	-0.05888200	0.30185900
C	0.53285700	3.54400300	0.12829600
C	1.99188000	3.35133300	0.53444200
C	2.58101300	2.18271000	-0.24325700
H	3.90120400	-3.59333700	-1.30755000
H	1.43069400	-3.52129400	-0.74474500
H	5.17672500	-1.43515400	-1.27581000
H	0.46976500	3.90888500	-0.90819300
H	2.04994600	3.14990600	1.61165900
H	3.55963900	1.88929500	0.13663400
N	0.10135800	-1.32758800	-0.12642000
N	1.69790000	0.99988300	-0.15230200
N	-0.24078300	2.31468900	0.23373400
O	-0.61928500	-2.37985200	-0.18874200
C	-1.82910200	0.06330000	-0.60108900
C	-3.05026300	-0.54060000	-0.27907500
C	-1.71157400	0.68482700	-1.85333300
C	-4.13072400	-0.48657400	-1.16201800
H	-3.17295400	-1.08130800	0.65016400
C	-2.78492600	0.72999800	-2.74020900
H	-0.77476500	1.14635900	-2.14669200
C	-4.00628500	0.15098300	-2.39428900
H	-5.06799700	-0.95915600	-0.88152100
H	-2.66369400	1.22110200	-3.70204400
H	-4.84721800	0.18995000	-3.08142600
H	2.71567000	2.44288000	-1.30111400
H	2.58497400	4.25185800	0.34022900
H	0.04511900	4.30346100	0.74984900

C	-0.87207500	-0.18840300	1.88338500
C	0.45793800	-0.14105000	2.68415200
C	-1.81687000	0.91952900	2.41635100
H	0.92423900	0.84330700	2.59312800
H	0.24818700	-0.32050500	3.74217800
H	1.16512600	-0.90507500	2.34985700
H	-1.97412800	0.76390300	3.48835200
H	-1.37153900	1.89994200	2.24921100
H	-2.78658800	0.89965800	1.91720600
C	-1.49612600	-1.48321800	2.23896800
N	-1.98585200	-2.43452900	2.69149000
N	3.55559100	-0.27878200	-0.74588800

Zero-point correction= 0.374315 (Hartree/Particle)
Thermal correction to Energy= 0.395914
Thermal correction to Enthalpy= 0.396858
Thermal correction to Gibbs Free Energy= 0.324650
Sum of electronic and zero-point Energies= -1122.286888
Sum of electronic and thermal Energies= -1122.265289
Sum of electronic and thermal Enthalpies= -1122.264345
Sum of electronic and thermal Free Energies= -1122.336552

5c,*syn*(N-O)

C	-3.54491100	-2.05287700	-0.46388100
C	-2.44744200	-2.14667600	0.38688600
C	-1.55481400	-1.07331800	0.44931000
C	-1.81368500	0.08060700	-0.33669500
C	-3.70275100	-0.88862200	-1.21531000
C	0.08475300	1.25428700	0.65483200
C	0.66417500	-0.09478000	1.11611600
C	0.22177100	3.59047300	0.51376300
C	-0.28183200	3.45666700	-0.92468800
C	-1.38894600	2.41089800	-0.98405800
H	-4.25971100	-2.86498000	-0.54536200
H	-2.25447400	-3.01837800	1.00098000
H	-4.54220800	-0.77690700	-1.89810800
H	-0.57658300	3.97874500	1.16435500
H	0.55346400	3.15604000	-1.56906200
H	-1.61902000	2.11852100	-2.01076500
N	-0.43410400	-1.10210300	1.26287300
N	-0.98656700	1.19505800	-0.24683100
N	0.68302600	2.31080000	1.04026300
O	-0.18218800	-2.09689000	2.03119400
H	-2.31854800	2.79589600	-0.54713600
H	-0.66578700	4.40877500	-1.30729400
H	1.05122000	4.30277700	0.57796800
O	1.23562200	0.07447200	2.37425600
H	1.31217800	-0.83595900	2.72400900

N	-2.86465200	0.15623700	-1.15155100
C	1.70360800	-0.59848300	0.09259300
C	2.86932300	0.16459900	-0.06825900
C	1.55099600	-1.77935000	-0.63938700
C	3.85955700	-0.24503200	-0.95762900
H	2.98379400	1.07418400	0.51237200
C	2.54713000	-2.18716900	-1.53103100
H	0.67017400	-2.39866400	-0.50970800
C	3.70018200	-1.42189400	-1.69504500
H	4.75951900	0.35324500	-1.07339000
H	2.41834400	-3.10887500	-2.09212800
H	4.47355200	-1.74099100	-2.38871800

Zero-point correction= 0.295525 (Hartree/Particle)
Thermal correction to Energy= 0.312287
Thermal correction to Enthalpy= 0.313231
Thermal correction to Gibbs Free Energy= 0.250633
Sum of electronic and zero-point Energies= -987.475797
Sum of electronic and thermal Energies= -987.459035
Sum of electronic and thermal Enthalpies= -987.458090
Sum of electronic and thermal Free Energies= -987.520689

5c,*anti*(N-O)

C	3.73326800	-2.31336500	-0.26781400
C	2.36402900	-2.46649700	-0.06946500
C	1.56447600	-1.32543200	0.01830600
C	2.17845100	-0.05383700	-0.09607500
C	4.24569000	-1.02076000	-0.36608200
C	0.02331100	1.07477600	0.07841200
C	-0.60810200	-0.22523000	0.61603200
C	-0.19751600	3.34105400	-0.49984900
C	1.18361500	3.55280100	0.12145400
C	2.09943900	2.39744900	-0.26335900
H	4.38742800	-3.17583800	-0.34146900
H	1.89058700	-3.43637600	0.02444500
H	5.30965600	-0.85332800	-0.51971400
H	-0.13639100	3.39815700	-1.59749900
H	1.08244200	3.60147900	1.21252500
H	3.01919500	2.39212000	0.32421500
N	0.18631900	-1.42313700	0.21098900
N	1.41546800	1.10730500	-0.03850000
N	-0.76920500	2.05294700	-0.12845900
O	-0.35693300	-2.56877100	0.40895900
H	2.39539600	2.46233400	-1.31801900
H	1.63303400	4.49542700	-0.20996800
H	-0.89687900	4.12371000	-0.18630900
O	-0.50787000	-0.12409100	2.02697300
H	-0.88194800	-0.95209100	2.37970700

N	3.49090800	0.08350000	-0.28514200
C	-2.04708000	-0.39241900	0.13548800
C	-3.09860600	0.00800200	0.96142300
C	-2.32954400	-0.90326700	-1.13598100
C	-4.42029900	-0.11278500	0.52875900
H	-2.87744700	0.42868200	1.93623100
C	-3.64822300	-1.01970500	-1.56934700
H	-1.52038400	-1.22222100	-1.78606600
C	-4.69909100	-0.62744000	-0.73657500
H	-5.23010000	0.20229100	1.18148700
H	-3.85585200	-1.42369300	-2.55660800
H	-5.72765900	-0.72215300	-1.07459300

Zero-point correction= 0.295912 (Hartree/Particle)
Thermal correction to Energy= 0.312658
Thermal correction to Enthalpy= 0.313603
Thermal correction to Gibbs Free Energy= 0.251273
Sum of electronic and zero-point Energies= -987.472346
Sum of electronic and thermal Energies= -987.455600
Sum of electronic and thermal Enthalpies= -987.454656
Sum of electronic and thermal Free Energies= -987.516985

5c,*anti*(amid)

C	-1.89313100	3.49438600	-0.12173600
C	-0.94511300	2.88854800	0.69784200
C	-0.76142700	1.50702600	0.60850000
C	-1.56340200	0.77902200	-0.30556600
C	-2.62044500	2.69359500	-1.00062000
C	-0.51179800	-1.29680900	0.38087800
C	0.67103700	-0.50662600	0.97818400
C	-1.56097200	-3.40992000	0.12037700
C	-2.82458900	-2.63909300	-0.27503300
C	-2.44649500	-1.41559800	-1.10994900
H	-2.05969800	4.56594800	-0.08446800
H	-0.34006900	3.44301800	1.40524700
H	-3.36765700	3.12522600	-1.66259200
H	-1.16651800	-3.96833800	-0.74068000
H	-3.35663900	-2.30819600	0.62523500
H	-3.29755500	-0.76738800	-1.31377900
N	0.16666000	0.84314600	1.41310100
N	-1.44792000	-0.61682100	-0.37645800
N	-0.49357100	-2.55327900	0.62365300
O	0.81814600	1.46939800	2.30983000
H	-2.02002700	-1.71790400	-2.07530100
H	-3.50804200	-3.27968000	-0.84334600
H	-1.78557200	-4.15592400	0.89117000
O	1.11822200	-1.16526200	2.11557100
H	0.78114100	-2.08279900	2.00129100

N	-2.46054400	1.36488800	-1.09169800
C	1.81914400	-0.28227600	-0.01928100
C	3.08995100	-0.01280000	0.50703800
C	1.64328600	-0.30189900	-1.40680400
C	4.16479900	0.23174500	-0.34482500
H	3.22128500	-0.00362000	1.58289000
C	2.72504400	-0.06409800	-2.25822200
H	0.66827000	-0.50879700	-1.83682300
C	3.98702100	0.20501500	-1.73058300
H	5.14580300	0.43907800	0.07452700
H	2.57654100	-0.09150200	-3.33451700
H	4.82794400	0.39095200	-2.39346200

Zero-point correction= 0.295959 (Hartree/Particle)
Thermal correction to Energy= 0.312606
Thermal correction to Enthalpy= 0.313550
Thermal correction to Gibbs Free Energy= 0.251343
Sum of electronic and zero-point Energies= -987.477110
Sum of electronic and thermal Energies= -987.460464
Sum of electronic and thermal Enthalpies= -987.459520
Sum of electronic and thermal Free Energies= -987.521726

5c,*syn*(amid)

C	-3.01539200	-2.60540900	-0.46914900
C	-2.01151800	-2.43088000	0.48042100
C	-1.31928600	-1.21872700	0.51174000
C	-1.69166400	-0.20875100	-0.41076100
C	-3.29049500	-1.55895200	-1.34749700
C	-0.11328300	1.31219200	0.59637800
C	0.68749900	0.11286700	1.14841300
C	-0.44562300	3.63513000	0.49550000
C	-0.83637900	3.41940300	-0.97017000
C	-1.69461100	2.16453100	-1.10592400
H	-3.57091400	-3.53568600	-0.52793400
H	-1.74336900	-3.19716900	1.19815100
H	-4.06300000	-1.65555000	-2.10697800
H	-1.33936400	3.84067300	1.10371500
H	0.07553900	3.31508300	-1.57067800
H	-1.78853700	1.84647100	-2.14639700
N	-0.29801500	-0.98204600	1.43542500
N	-1.09086600	1.05308100	-0.34362400
N	0.23977000	2.46349700	1.03317800
O	-0.01182300	-1.84781900	2.32645200
H	-2.71080300	2.33612700	-0.73067100
H	-1.39080900	4.27815400	-1.36363500
H	0.21619300	4.50038500	0.60430900
O	1.31281800	0.48312300	2.32674400
H	1.15029600	1.45081600	2.40061400

N	-2.64949000	-0.38050200	-1.31586100
C	1.72811300	-0.37875300	0.12170400
C	2.57885800	0.56233500	-0.47432300
C	1.89629300	-1.73386800	-0.17787900
C	3.56548300	0.15612200	-1.37014700
H	2.47123300	1.61366000	-0.22484000
C	2.88865600	-2.13931100	-1.07346000
H	1.27195300	-2.47999300	0.30088100
C	3.72116600	-1.19783900	-1.67658600
H	4.21647300	0.89754300	-1.82604800
H	3.01000300	-3.19646700	-1.29397600
H	4.49045300	-1.51522200	-2.37546900

Zero-point correction= 0.295904 (Hartree/Particle)
Thermal correction to Energy= 0.312556
Thermal correction to Enthalpy= 0.313500
Thermal correction to Gibbs Free Energy= 0.251237
Sum of electronic and zero-point Energies= -987.477731
Sum of electronic and thermal Energies= -987.461079
Sum of electronic and thermal Enthalpies= -987.460135
Sum of electronic and thermal Free Energies= -987.522398

5d,*syn*

C	3.57224400	-2.96693600	-0.15012900
C	2.19055500	-2.82167500	-0.24573800
C	1.65617700	-1.53622700	-0.35433000
C	2.54418700	-0.43402900	-0.39114900
C	4.36211900	-1.81896000	-0.17023600
C	0.68854800	1.10973000	-0.75076800
C	-0.28569000	0.04478700	-0.17854200
C	1.09598900	3.22479300	-1.67331100
C	2.33331100	3.29534800	-0.77679300
C	3.03381500	1.94238000	-0.77201900
H	4.02531300	-3.94863300	-0.05841000
H	1.51053300	-3.66504500	-0.23716300
H	5.44507400	-1.88563100	-0.09163400
H	1.39174300	3.03441600	-2.71638900
H	2.02267900	3.56222600	0.24084500
H	3.77363900	1.86815000	0.02770800
N	0.28059900	-1.32482300	-0.44374200
N	2.05178000	0.85459300	-0.58026200
N	0.18174400	2.17496700	-1.23688400
O	-0.51885900	-2.31882300	-0.49464800
C	-0.47740600	0.26635000	1.33150800
C	-0.86072400	1.53826300	1.77760600
C	-0.29985600	-0.76211400	2.26055400
C	-1.04746000	1.77837300	3.13696400
H	-1.01839400	2.32785400	1.05016600

C	-0.48321800	-0.51603400	3.62305900
H	-0.04231200	-1.76108700	1.92804600
C	-0.85266400	0.75311200	4.06585700
H	-1.34720700	2.76814300	3.47137300
H	-0.34150900	-1.32389000	4.33592600
H	-0.99399000	0.94245100	5.12668100
H	3.56690000	1.77126000	-1.71523500
H	3.03576800	4.06372200	-1.11802200
H	0.54918100	4.17365200	-1.67069000
O	-1.45881700	0.20664600	-0.91731000
O	-2.58664300	-0.34499000	-0.14503500
C	-3.68520800	-0.50717100	-1.07068000
C	-4.11002700	0.85803400	-1.62714700
C	-3.32200400	-1.49482400	-2.18531100
C	-4.76268500	-1.08972700	-0.14568800
H	-4.37340600	1.53768300	-0.80974800
H	-3.29850000	1.31152000	-2.20217300
H	-4.98173900	0.74746500	-2.28238700
H	-2.94891300	-2.42859200	-1.75696500
H	-4.20488300	-1.70827300	-2.79895600
H	-2.54418400	-1.08297300	-2.83308600
H	-5.68596300	-1.24678400	-0.71315500
H	-4.43914100	-2.04955200	0.26850000
H	-4.97527100	-0.40532400	0.68172200
N	3.86432100	-0.57991700	-0.29529100

Zero-point correction= 0.410654 (Hartree/Particle)
Thermal correction to Energy= 0.434387
Thermal correction to Enthalpy= 0.435331
Thermal correction to Gibbs Free Energy= 0.357684
Sum of electronic and zero-point Energies= -1219.640686
Sum of electronic and thermal Energies= -1219.616953
Sum of electronic and thermal Enthalpies= -1219.616009
Sum of electronic and thermal Free Energies= -1219.693656

5d,*anti*

C	-3.66289200	-2.18487300	-1.73555600
C	-2.27251800	-2.23436900	-1.81327400
C	-1.52413400	-1.54158300	-0.86387600
C	-2.20376600	-0.83285900	0.15738300
C	-4.24150700	-1.44224900	-0.70822300
C	-0.08933800	-0.23450500	1.20311400
C	0.59594700	-0.46856700	-0.15705900
C	-0.03761600	0.31138000	3.47761600
C	-1.30534600	1.13185000	3.22989100
C	-2.24201900	0.36001600	2.30750600
H	-4.28172800	-2.70663300	-2.45808300
H	-1.74784000	-2.78676000	-2.58381900

H	-5.32314100	-1.37118000	-0.61425700
H	-0.28550500	-0.62178500	4.00721700
H	-1.02226000	2.08460800	2.76625900
H	-3.03549700	0.99498400	1.90629400
N	-0.12359300	-1.55299700	-0.88523500
N	-1.48789400	-0.20190500	1.16893600
N	0.63809100	-0.01237600	2.22682800
O	0.50846300	-2.29608800	-1.70799700
C	2.07125600	-0.81439300	-0.05358200
C	3.01960400	-0.08567200	-0.77069200
C	2.48463700	-1.90327500	0.72325100
C	4.37103600	-0.43107900	-0.70117600
H	2.70165300	0.75277700	-1.37705500
C	3.83051800	-2.25185500	0.78583400
H	1.75329900	-2.47943300	1.28093300
C	4.78045900	-1.51330000	0.07533600
H	5.10159900	0.14753600	-1.26042700
H	4.13891000	-3.10011500	1.39110500
H	5.83199300	-1.78358700	0.12713200
H	-2.73445100	-0.46120200	2.84272000
H	-1.82752600	1.36119900	4.16533600
H	0.66858800	0.85520000	4.11383900
O	0.32924200	0.64478600	-1.02656800
O	0.66951100	1.88730100	-0.30082500
C	0.08674100	2.98883300	-1.03879600
C	0.68613400	3.06500500	-2.44836700
C	-1.44079700	2.86879900	-1.07679600
C	0.52910400	4.18574100	-0.18607500
H	1.77707800	3.14452400	-2.39564900
H	0.43049400	2.17600500	-3.03079000
H	0.30183100	3.94471900	-2.97664700
H	-1.84364500	2.78745200	-0.06197400
H	-1.87791700	3.75423900	-1.55150100
H	-1.75156900	1.98732400	-1.64288200
H	0.16802000	5.11431400	-0.64049300
H	0.12172600	4.11411400	0.82746500
H	1.62034600	4.23188900	-0.11899000
N	-3.53449000	-0.78507300	0.22213400

Zero-point correction= 0.410845 (Hartree/Particle)
Thermal correction to Energy= 0.434374
Thermal correction to Enthalpy= 0.435319
Thermal correction to Gibbs Free Energy= 0.358697
Sum of electronic and zero-point Energies= -1219.643435
Sum of electronic and thermal Energies= -1219.619905
Sum of electronic and thermal Enthalpies= -1219.618961
Sum of electronic and thermal Free Energies= -1219.695582

5e,*syn*(N-O)

C	-3.39342600	-2.30090200	-0.57607900
C	-2.29581300	-2.29224800	0.27936400
C	-1.48435000	-1.15609100	0.31746000
C	-1.82827400	-0.04203100	-0.49060600
C	-3.63574100	-1.16796400	-1.35254400
C	-0.00214000	1.26957600	0.45528200
C	0.67417800	-0.04097400	0.91842700
C	-0.00951300	3.60879800	0.28791900
C	-0.56852900	3.43466600	-1.12543500
C	-1.60681400	2.31909100	-1.13376200
H	-4.04467400	-3.16613400	-0.64126400
H	-2.04340600	-3.13129100	0.91684000
H	-4.47902000	-1.13433900	-2.03900500
H	-0.79874500	3.95400100	0.97258500
H	0.25333900	3.18651300	-1.80844100
H	-1.86065700	2.00587200	-2.14824400
N	-0.37229600	-1.08566400	1.14850600
N	-1.09534800	1.13587000	-0.41042000
N	0.54864700	2.36394600	0.80332500
O	-0.13650400	-2.00017600	2.01461800
C	1.71898500	-0.52200900	-0.10066800
C	2.66592300	0.39088000	-0.58365400
C	1.77967600	-1.85959500	-0.50653300
C	3.64818800	-0.02873300	-1.47917900
H	2.62925500	1.42020200	-0.24354400
C	2.76033900	-2.27215900	-1.40952300
H	1.07752400	-2.58438100	-0.11032000
C	3.69357900	-1.35910900	-1.90080300
H	4.38018300	0.68563700	-1.84616700
H	2.79568100	-3.31192000	-1.72291500
H	4.45652100	-1.68348700	-2.60344000
H	-2.53973300	2.64515300	-0.65739400
H	-1.03049500	4.35821600	-1.49142000
H	0.77803400	4.36943500	0.31062200
O	1.40399800	0.12212200	2.10099300
N	-2.88083500	-0.06150400	-1.30774900
O	0.48875400	0.44132900	3.18644400
H	0.27741700	-0.47537900	3.46203700

Zero-point correction= 0.299614 (Hartree/Particle)
Thermal correction to Energy= 0.317376
Thermal correction to Enthalpy= 0.318320
Thermal correction to Gibbs Free Energy= 0.253717
Sum of electronic and zero-point Energies= -1062.571854
Sum of electronic and thermal Energies= -1062.554092
Sum of electronic and thermal Enthalpies= -1062.553148
Sum of electronic and thermal Free Energies= -1062.617751

5e,*anti*(N-O)

C	2.93637000	-2.85721300	-0.36377000
C	1.88002600	-2.57095600	0.49553800
C	1.26435600	-1.32041900	0.40903200
C	1.76272300	-0.37327400	-0.52272000
C	3.33269100	-1.87561900	-1.27185500
C	0.15482200	1.29879600	0.25150000
C	-0.69658800	0.16578600	0.86760900
C	0.48363400	3.61151400	-0.14689900
C	1.89492600	3.26026500	-0.62396600
C	1.85172000	1.94665100	-1.40112500
H	3.43553100	-3.81999800	-0.33585600
H	1.51308400	-3.27965400	1.22853700
H	4.14582300	-2.06024600	-1.97057600
H	-0.11611000	4.00200500	-0.98220700
H	2.56519100	3.14630600	0.23665900
H	2.84181800	1.59135900	-1.68193300
N	0.19638000	-0.97847700	1.23232300
N	1.22932500	0.90948100	-0.56002100
N	-0.24764700	2.49280300	0.43426700
O	-0.15393900	-1.73467700	2.20574000
C	-1.81042000	-0.28541500	-0.08980500
C	-2.06538000	-1.64065600	-0.32644900
C	-2.62358000	0.68619900	-0.68833900
C	-3.10572400	-2.01796200	-1.17645200
H	-1.46822800	-2.40347700	0.16023000
C	-3.66646800	0.30297400	-1.52999200
H	-2.43655300	1.73386700	-0.47884500
C	-3.90587000	-1.04925400	-1.78261400
H	-3.29237900	-3.07282300	-1.35811600
H	-4.29372700	1.06332700	-1.98739100
H	-4.71591400	-1.34627400	-2.44337400
H	1.26163200	2.05641300	-2.32068400
H	2.30415100	4.05602300	-1.25680200
H	0.51230300	4.41022900	0.60361700
O	-1.38343600	0.57464800	2.01620700
N	2.76697400	-0.66366900	-1.34934200
O	-0.42040800	0.89876900	3.05807100
H	-0.33301700	0.00357400	3.44785300

Zero-point correction= 0.299316 (Hartree/Particle)
Thermal correction to Energy= 0.317107
Thermal correction to Enthalpy= 0.318051
Thermal correction to Gibbs Free Energy= 0.253308
Sum of electronic and zero-point Energies= -1062.571326
Sum of electronic and thermal Energies= -1062.553535
Sum of electronic and thermal Enthalpies= -1062.552590
Sum of electronic and thermal Free Energies= -1062.617334

5e,*anti*(amid)

C	-2.76866900	-3.12929800	-0.05385800
C	-1.62335000	-2.73966600	-0.74171200
C	-1.16485800	-1.42834100	-0.59727500
C	-1.89315600	-0.54662000	0.23421100
C	-3.40914100	-2.19055100	0.75298000
C	-0.32913200	1.26090200	-0.23031100
C	0.68778800	0.24631400	-0.80826200
C	-0.86812900	3.54626400	0.17951300
C	-2.31942700	3.09153100	0.33707400
C	-2.35655000	1.75106400	1.06603300
H	-3.15217600	-4.14076900	-0.13717900
H	-1.06922000	-3.41178600	-1.38554600
H	-4.30432500	-2.45161600	1.31268100
H	-0.46995100	3.90408900	1.14011200
H	-2.78508000	2.97978500	-0.64957500
H	-3.35657000	1.32196500	1.10378700
N	-0.02285200	-0.98936400	-1.27180000
N	-1.48890800	0.78740600	0.36250500
N	0.01635900	2.49431900	-0.30959400
O	0.59261700	-1.77194000	-2.06705400
C	1.77537300	-0.15753800	0.18649200
C	2.94085600	-0.76006700	-0.30554000
C	1.60312400	-0.01456800	1.56609300
C	3.92128700	-1.20374000	0.57788800
H	3.06829300	-0.86652700	-1.37606700
C	2.58834500	-0.46220900	2.44928300
H	0.70575100	0.44950400	1.96437200
C	3.74894800	-1.05701900	1.95732500
H	4.82603400	-1.66226900	0.18807400
H	2.44525900	-0.34234100	3.51981900
H	4.51736700	-1.40343200	2.64333700
H	-2.00416800	1.85778900	2.10032500
H	-2.90259700	3.83300200	0.89415000
H	-0.79656400	4.39067900	-0.51523100
O	1.20640200	0.76345800	-2.02793600
N	-2.98196700	-0.92783800	0.89544200
O	2.18204800	1.79490700	-1.73448400
H	1.57113500	2.46012900	-1.32275100

Zero-point correction= 0.299414 (Hartree/Particle)
Thermal correction to Energy= 0.317120
Thermal correction to Enthalpy= 0.318064
Thermal correction to Gibbs Free Energy= 0.253600
Sum of electronic and zero-point Energies= -1062.569577
Sum of electronic and thermal Energies= -1062.551871
Sum of electronic and thermal Enthalpies= -1062.550927
Sum of electronic and thermal Free Energies= -1062.615391

5e,*syn*(amid)

C	-3.48301700	-2.22926800	-0.34813700
C	-2.39025800	-2.18661400	0.51388500
C	-1.52753300	-1.09032200	0.45122200
C	-1.81714000	-0.05651200	-0.47213100
C	-3.66952900	-1.17304100	-1.23786600
C	0.03390400	1.26488200	0.37265000
C	0.67445200	-0.02082200	0.94404900
C	0.05530400	3.59711800	0.07099500
C	-0.43806400	3.33079500	-1.35202000
C	-1.49268200	2.23044700	-1.33111700
H	-4.17286800	-3.06663100	-0.33214200
H	-2.17868800	-2.97039200	1.23139300
H	-4.50579800	-1.16912300	-1.93322700
H	-0.76377500	3.99417500	0.69010600
H	0.41133300	3.02536400	-1.97520000
H	-1.70456200	1.84855700	-2.33190800
N	-0.40570500	-1.00092400	1.27640500
N	-1.02810700	1.09710300	-0.50471300
N	0.57870100	2.38174800	0.69046200
O	-0.15036900	-1.91332900	2.12878700
C	1.67612700	-0.62225200	-0.05536300
C	2.67089600	0.20715700	-0.59161200
C	1.64554500	-1.97605500	-0.40478700
C	3.60883400	-0.30933600	-1.48306500
H	2.70729900	1.25069000	-0.29739400
C	2.58545900	-2.48761400	-1.30134700
H	0.90787500	-2.63801100	0.03364200
C	3.56487000	-1.65741700	-1.84560400
H	4.37713500	0.34144900	-1.89176800
H	2.55233500	-3.54055600	-1.56713300
H	4.29508400	-2.05917300	-2.54297700
H	-2.44169200	2.59831500	-0.92275200
H	-0.86705400	4.23291000	-1.80129900
H	0.84966500	4.35068400	0.08041200
O	1.44466300	0.24013800	2.08055600
N	-2.85960200	-0.10506500	-1.29612800
O	0.65350600	0.97246300	3.05860400
H	0.77129600	1.87064000	2.67598200

Zero-point correction= 0.299909 (Hartree/Particle)
Thermal correction to Energy= 0.317536
Thermal correction to Enthalpy= 0.318480
Thermal correction to Gibbs Free Energy= 0.254346
Sum of electronic and zero-point Energies= -1062.573540
Sum of electronic and thermal Energies= -1062.555913
Sum of electronic and thermal Enthalpies= -1062.554969
Sum of electronic and thermal Free Energies= -1062.619103

Table 2 SI: Experimental (*exp* - in italic)[a] and computed [b] hyperfine coupling constants (hfccs in Gauss) and *g*-factors of isomeric **1b** spin adducts from a simultaneous relaxed PES scan of both C(7)-C(8)-C(23)-C(25) and N(19)-C(8)-C(37)-C(46) dihedral angles, according to the arbitrary atom labelling of manuscript Figure 2.

Aminoxyl	*N-19*	*H-12*	*H-14*	*H-13*	*H-15*	*N-21*	*H-16*	*H-36*	*g*	E (M062X)[c]	H (M062X)[c]	G (M062X)[c]	ΔG (Kcal)[d]
1b-*syn*-1	11.66	1.12	0.95	-2.83	-2.83	0.76	1.52	0.21	2.00563	-1106.2193	-1106.2183	-1106.2902	0.00
1b-*syn*-13	11.03	1.17	1.00	-2.62	-2.62	0.80	1.74	0.11	2.00568	-1106.2155	-1106.2145	-1106.2847	3.47
1b-*syn*-25	11.66	1.12	0.95	-2.83	-2.83	0.76	1.52	0.21	2.00565	-1106.2177	-1106.2167	-1106.2885	1.07
1b-*anti*-1	11.33	1.21	1.02	-2.58	-2.55	0.74	0.91	0.40	2.00571	-1106.2167	-1106.2157	-1106.2875	1.66
1b-*anti*-13	9.58	1.15	1.03	-3.14	-3.15	0.18	0.77	0.14	2.00569	-1106.2087	-1106.2078	-1106.2800	6.37
1b-*anti*-25	11.33	1.21	1.02	-2.58	-2.55	0.74	0.91	0.40	2.00571	-1106.2167	-1106.2157	-1106.2875	1.66
exp	*10.17*	*1.07*	*0.85*	*-3.02*	*-2.73*	*0.37*	*0.54*	*0.23*	*2.00569*				

[a]: in benzene solution; [b]: manuscript ref. 20; [c]: in Hartrees from frequency computations at the M062X/6-31+G(d,p) level; [d]: Differences in Gibbs Free Energy (in Kcal/mol) from **1b-syn-1** assumed as the lowest Energy isomer.

Figure 7 SI: B3LYP/6-31G(d) optimised geometries of isomeric **1b** spin adducts from a simultaneous relaxed PES scan of both C(7)-C(8)-C(23)-C(25) and N(19)-C(8)-C(37)-C(46) dihedral angles, according to the arbitrary atom labelling of manuscript Figure 2.

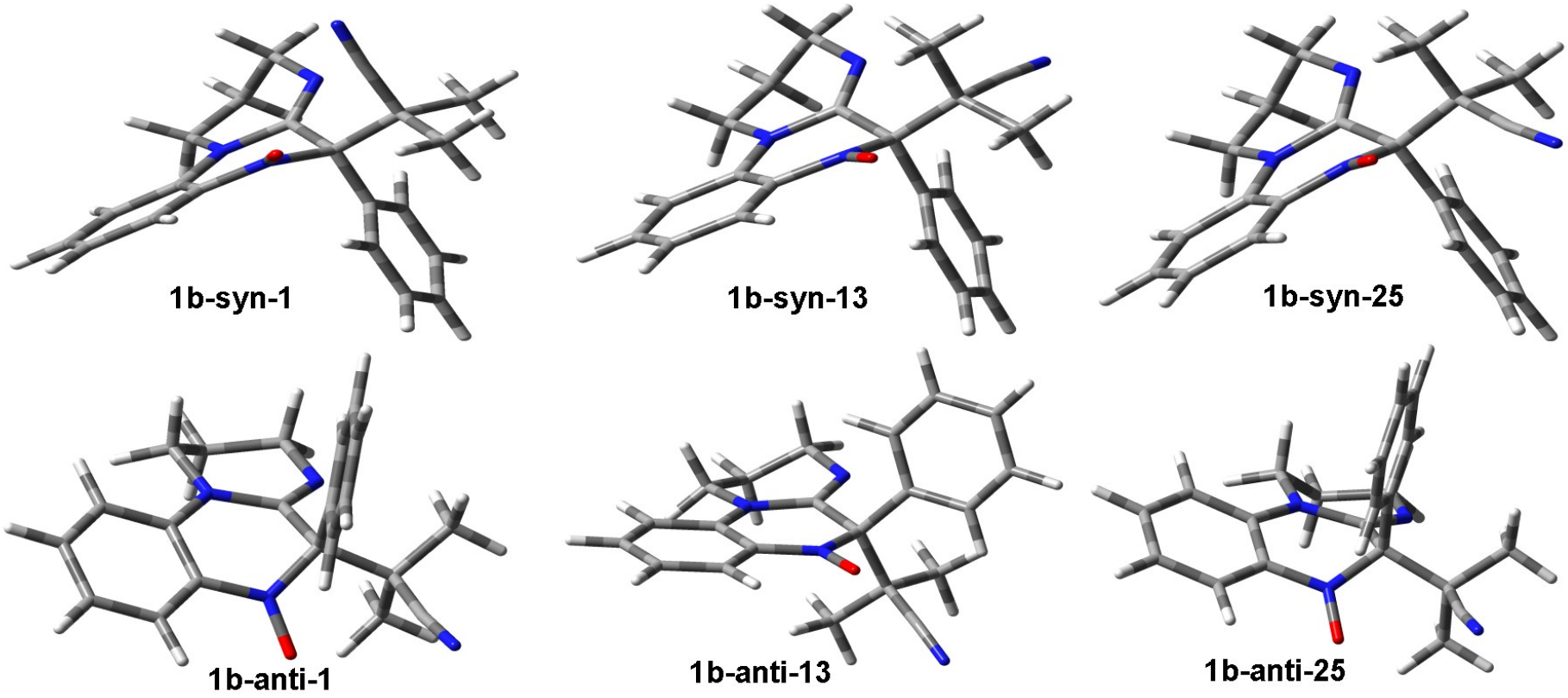


Table 3 SI: relative energies (Kcal/mol) and IHB distances (Å) and angles (º) for OH· and OOH· adducts

Nitroxide	Geometry	IHB distance	IHB angle	Relative energy
1c	**1c,*syn*(N-O)**	2.04	115	0.59
	1c,*anti*(N-O)	2.03	114	1.95
	1c,*syn*(amid)	1.92	123	0.00
	1c,*anti*(amid)	1.93	123	0.27
1e	**1e,*syn*(N-O)**	1.89	136	1.10
	1e,*anti*(N-O)	2.10	123	1.13
	1e,*syn*(amid)	2.04	127	0.00
	1e,*anti*(amid)	1.85	139	2.48
2c	**2c,*syn*(N-O)**	2.33	107	2.01
	2c,*anti*(N-O)	2.24	110	2.02
	2c,*syn*(amid)	1.99	121	0.00
	2c,*anti*(amid)	2.01	120	1.18
2e	**2e,*syn*(N-O)**	1.93	137	2.02
	2e,*anti*(N-O)	2.79	107	0.00
	2e,*syn*(amid)	1.89	141	1.82
	2e,*anti*(amid)	1.90	142	2.20
3c	**3c,(N-O)**	2.09	112	0.00
	3c,(amid)	2.11	119	1.50
3e	**3e,(N-O)**	2.15	122	0.00
	3e,(amid)	1.91	138	2.70
4c	**4c,(N-O)**	2.10	111	0.00
	4c,(amid)	2.11	119	1.23
4e	**4e,(N-O)**	2.14	122	0.00
	4e,(amid)	2.18	124	0.08
5c	**5c,*syn*(N-O)**	2.07	113	1.07
	5c,*anti*(N-O)	2.60	100	3.40
	5c,*syn*(amid)	1.93	123	0.00
	5c,*anti*(amid)	1.93	122	0.42
5e	**5e,*syn*(N-O)**	2.14	121	0.85
	5e,*anti*(N-O)	2.14	121	1.11
	5e,*syn*(amid)	2.06	126	0.00
	5e,*anti*(amid)	1.86	139	2.33

Figure 8 SI: IHB distances and angles in **3c** and **3e** adducts

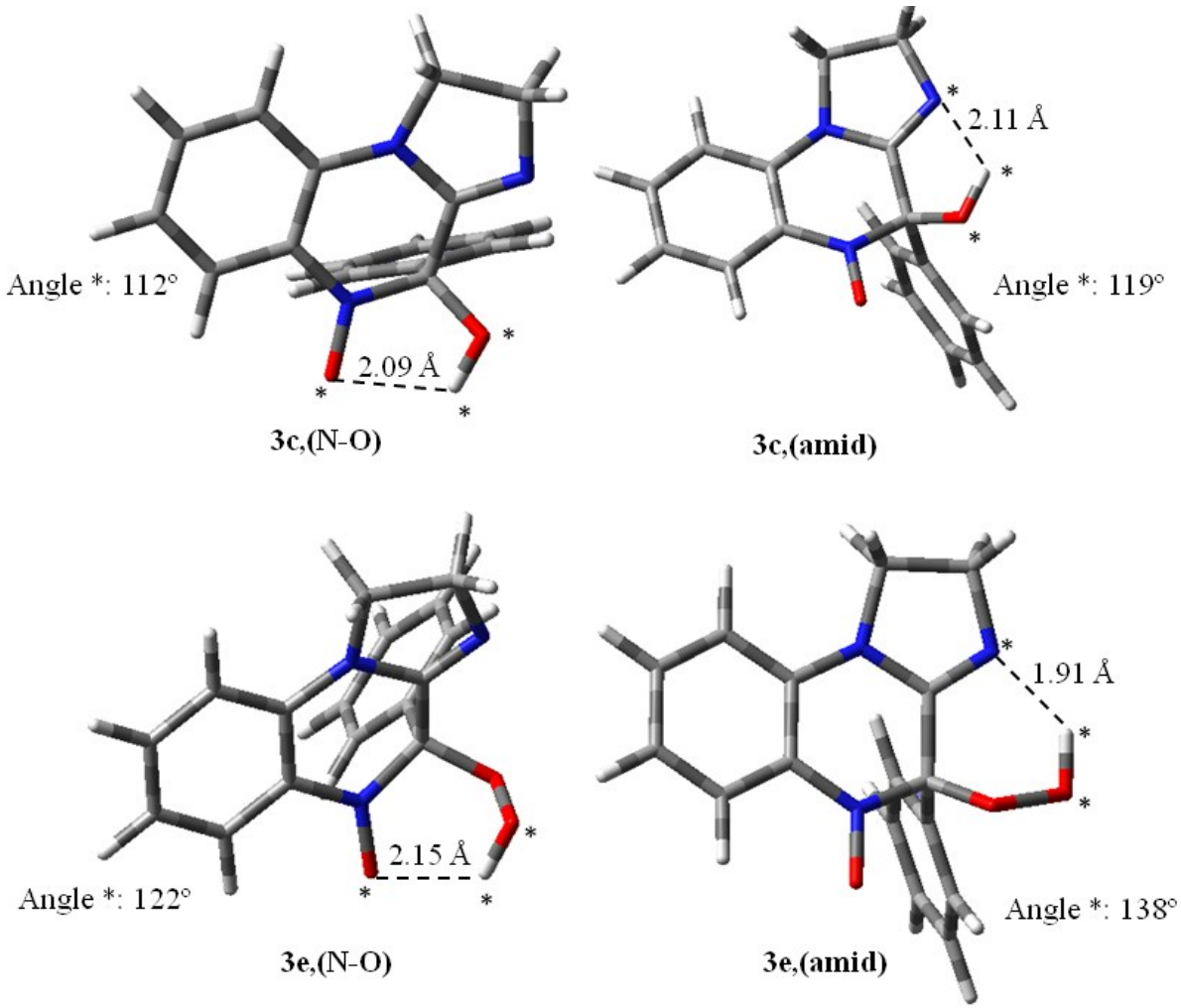


Table 4 SI: N(19) Pyramidalization degree

Geometry	N(19) Pyramidalization (º)
1a,*syn*	2.09
1a,*anti*	1.15
1b,*syn*	1.89
1b,*anti*	0.07
1c,*anti*(N-O)	1.74
1c,*syn*(amid)	2.05
1c,*syn*(N-O)	0.80
1c,anti(amid)	2.96
1d,*syn*	1.39
1d,*anti*	1.38
1e,*syn*(N-O)	0.75
1e,*syn*(amid)	1.71
1e,*anti*(N-O)	1.31

1e,*anti*(amid)	0.82
2a,*anti*	2.42
2a,*syn*	0.43
2b,*syn*	0.34
2b,*anti*	0.13
2c,*syn*(N-O)	1.25
2c,*anti*(N-O)	0.09
2c,*syn*(amid)	0.72
2c,*anti(*amid)	1.74
2d,*syn*	2.43
2d,*anti*	1.49
2e,*anti*(N-O)	0.10
2e,*syn(*N-O)	1.73
2e,anti(amid)	0.20
2e,*syn(*amid)	0.05
3a	0.97
3b	1.81
3c,(N-O)	0.77
3c,(amid)	1.41
3d	1.25
3e,(N-O)	0.44
3e,(amid)	0.75
4a	1.33
4b	1.83
4c,(N-O)	0.81
4c,(amid)	1.73
4d	1.25
4e,(N-O)	0.48
4e,(amid)	1.28
5a,*anti*	1.49
5a,*syn*	2.03
5b,*syn*	1.84
5b,*anti*	0.01
5c,*syn*(N-O)	0.84
5c,*anti*(N-O)	2.73
5c,*syn*(amid)	2.09
5c,*anti(*amid)	1.97
5d,*syn*	1.34
5d,*anti*	1.43
5e,*anti*(N-O)	0.69
5e,*syn(*N-O)	0.54
5e,anti(amid)	1.92
5e,*syn(*amid)	1.65