ORIGINS OF *exo*-STEREOSELECTIVITY OF NORBORNENE IN HETERO DIELS-ALDER REACTIONS

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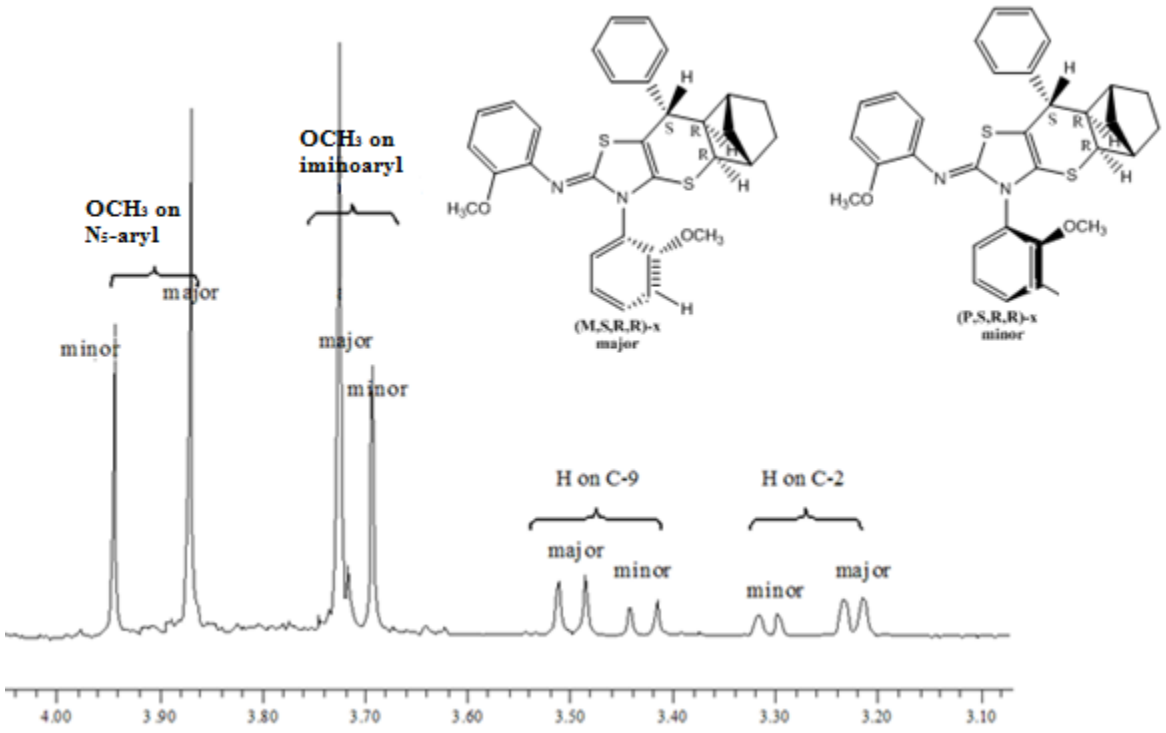

Figure S1. Partial ^{1}H NMR spectrum of **4b** in $CDCl_3$. **(M,S,R,R)-x** and its enantiomer is the major and **(P,S,R,R)-x** and its enantiomer is the minor product. (1H and 13C NMR spectra of all compounds were recorded on a Varian-Mercury VX-400 MHz-BB in $CDCl_3$ at room temperature.)

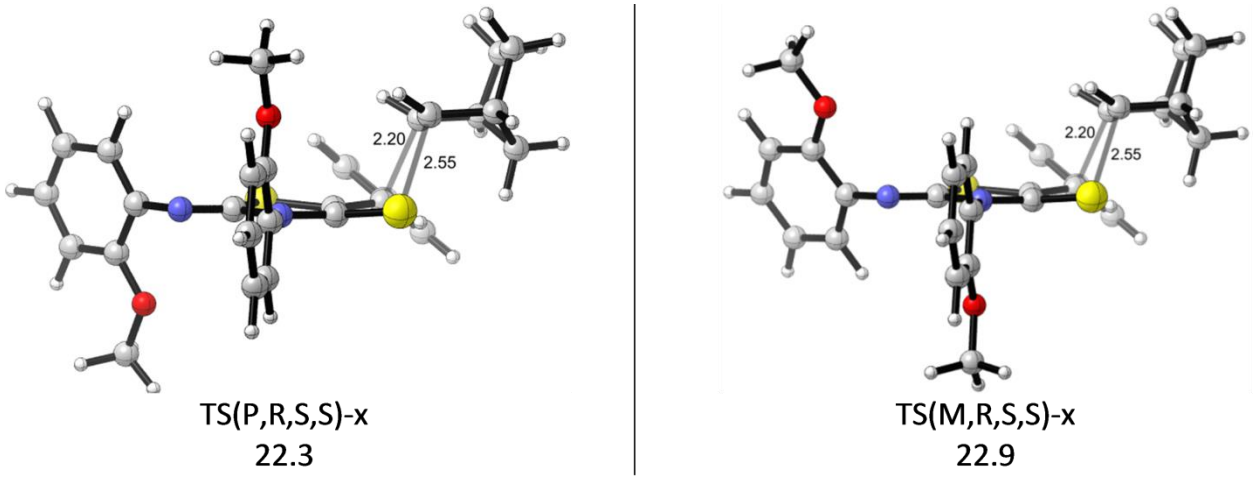

Figure S2. Transition structures for the reaction between **3b** and norbornene and their Gibbs free energies of activation in CH_2Cl_2 ($\Delta G^{\ddagger}$= G(TS) - G(3) – G(norbornene)) (M06-2X/6-31+G(d)// B3LYP/6-31+G(d)).

TS(P,R,S,S)-x and TS(M,S,R,R)-x as well as TS(P,S,R,R)-x and TS(M,R,S,S)-x are enantiomers and isoenergetic as expected.

CARTESIAN COORDINATES (Å) AND ABSOLUTE ENERGIES (au)

REACTANTS

1b

B3LYP/6-31+G*

N	0.69579500	-0.45836400	-0.12786400
C	2.04193600	-0.63697400	-0.50442800
C	2.37005400	-1.02587900	-1.80675300
C	3.69429300	-1.29110200	-2.16970300
C	4.70410900	-1.18155000	-1.21569900
C	4.39571700	-0.80745000	0.09820000
C	3.07254300	-0.53665500	0.46183600
H	1.56563300	-1.12254500	-2.53075100
H	3.92760400	-1.58509700	-3.18936400
H	5.73759600	-1.38827800	-1.48104900
H	5.19233000	-0.72907900	0.82996000
C	-2.01488000	-0.21876400	0.62109700
C	-2.79346400	-0.79845200	-0.39848500
C	-3.63408700	-1.87260300	-0.08280100
C	-3.68593600	-2.35398600	1.22954300
C	-2.91102900	-1.77832800	2.23594500
C	-2.07411100	-0.70437800	1.92187900

H	-4.24626300	-2.33730000	-0.84736900
H	-4.34277700	-3.18930600	1.45839900
H	-2.95526200	-2.15670800	3.25272500
H	-1.45567800	-0.23655500	2.68215800
C	-1.66085000	2.18634900	0.26056800
S	0.94152600	2.25449600	-0.52921900
C	0.16753300	0.69178400	-0.09650600
N	-1.16487200	0.89120800	0.29956300
O	-2.79741800	2.50426400	0.55261700
C	-0.59768700	3.18232900	-0.18491800
H	-0.44311600	3.91917000	0.60806400
H	-0.95110200	3.70172900	-1.07973600
O	-2.65910200	-0.25343300	-1.63820500
O	2.67454800	-0.16965900	1.71772700
C	-3.45272700	-0.77158600	-2.69972300
H	-3.21909200	-1.82668600	-2.89107000
H	-4.52277800	-0.66114400	-2.48344000
H	-3.19490600	-0.17678500	-3.57737000
C	3.66010100	-0.06213200	2.73415100
H	3.12226100	0.22750900	3.63882700
H	4.16693900	-1.02157700	2.90305200
H	4.40441500	0.70769500	2.49024600

Zero-point correction= 0.303218 (Hartree/Particle)
Thermal correction to Energy= 0.324144
Thermal correction to Enthalpy= 0.325088
Thermal correction to Gibbs Free Energy= 0.250104
Sum of electronic and zero-point Energies= -1390.524762
Sum of electronic and thermal Energies= -1390.503836
Sum of electronic and thermal Enthalpies= -1390.502891
Sum of electronic and thermal Free Energies= -1390.577875

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

N	-0.68928000	-0.40160100	0.16604300
C	-2.03715600	-0.48786600	0.57680500
C	-2.36856500	-0.51110100	1.93533700
C	-3.69267400	-0.68257200	2.35281400
C	-4.69769100	-0.84508200	1.40060100
C	-4.38554400	-0.83613800	0.03506500

C	-3.06245400	-0.66021500	-0.38480000
H	-1.56855000	-0.39862300	2.66210600
H	-3.92896100	-0.69237500	3.41328600
H	-5.73084800	-0.98294600	1.70845300
H	-5.17884900	-0.96567500	-0.69264900
C	2.03919800	-0.30554800	-0.56536200
C	2.74448200	-0.74131300	0.57318300
C	3.58126200	-1.85905800	0.46485000
C	3.70382000	-2.52119700	-0.76136400
C	3.00389200	-2.08500400	-1.88671900
C	2.16859000	-0.96961500	-1.78006300
H	4.13674800	-2.21696000	1.32407100
H	4.35696600	-3.38737300	-0.82851600
H	3.10369500	-2.60311300	-2.83563800
H	1.60770000	-0.60807900	-2.63692200
C	1.68625800	2.12621700	-0.64313700
S	-0.92028300	2.33850300	0.09242900
C	-0.14959500	0.72415200	-0.05167900
N	1.18969500	0.84678000	-0.45693700
O	2.83182200	2.38434400	-0.96954600
C	0.62412400	3.18786500	-0.40020700
H	0.47661800	3.76683200	-1.31577500
H	0.96622800	3.86188200	0.38942700
O	2.54997700	-0.02209000	1.71089400
O	-2.66207100	-0.63437600	-1.69123100
C	3.25417800	-0.40585700	2.89127000
H	2.97710700	-1.41989400	3.20359400
H	4.33853600	-0.34453900	2.74007100
H	2.95138800	0.30818900	3.65816400
C	-3.64567300	-0.81198200	-2.70536100
H	-3.10526500	-0.76432500	-3.65211300
H	-4.13872000	-1.78818600	-2.61508100
H	-4.39871300	-0.01427200	-2.67341100

Zero-point correction= 0.303173 (Hartree/Particle)
Thermal correction to Energy= 0.324102
Thermal correction to Enthalpy= 0.325046
Thermal correction to Gibbs Free Energy= 0.249970
Sum of electronic and zero-point Energies= -1390.532881
Sum of electronic and thermal Energies= -1390.511951

Sum of electronic and thermal Enthalpies= -1390.511007
Sum of electronic and thermal Free Energies= -1390.586083

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF= -1390.392069

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N	0.56658400	-0.49391100	0.22889800
C	1.92114600	-0.85128000	0.06200700
C	2.26933000	-1.92651500	-0.75031900
C	3.60185600	-2.31893600	-0.88684400
C	4.59117700	-1.63447800	-0.19064800
C	4.25951000	-0.56045400	0.63992600
C	2.92889600	-0.16405100	0.77183800
H	1.47320700	-2.44828500	-1.27441900
H	3.85816600	-3.15560900	-1.52912700
H	5.63199300	-1.93030300	-0.28284000
H	5.04431500	-0.04042000	1.17756800
C	-2.13553000	0.21045500	0.50587900
C	-2.60968700	-0.99448100	-0.03604900
C	-3.53370600	-1.74461500	0.69272400
C	-3.97870300	-1.27888900	1.93183000
C	-3.51528600	-0.07735200	2.45752500
C	-2.58242000	0.66642400	1.73515200
H	-3.91375700	-2.68246900	0.30469500
H	-4.70065100	-1.87125000	2.48640000
H	-3.86956200	0.27815300	3.41915500
H	-2.19231400	1.60500600	2.11741900
C	-1.56173000	2.07547200	-0.97781300
S	1.05270700	1.59142500	-1.47062600
C	0.13550400	0.53047000	-0.37140800
N	-1.18629300	0.96709500	-0.24555400
O	-2.67878700	2.54212600	-0.99538800
C	-0.39369000	2.65147700	-1.75912500
H	-0.20752200	3.67134900	-1.41574800
H	-0.65886700	2.67459500	-2.81775200
O	-2.12214400	-1.32943200	-1.25238300
O	2.50424800	0.86334000	1.55343000
C	-2.53212800	-2.56620200	-1.80856500
H	-2.24379700	-3.39994100	-1.15864200

H	-3.61502500	-2.58158400	-1.97566400
H	-2.01481800	-2.64970600	-2.76370700
C	3.48622400	1.60446000	2.25103700
H	2.94762400	2.38109800	2.79321100
H	4.02797700	0.96989500	2.96231400
H	4.19655600	2.06708100	1.55558300

Zero-point correction= 0.307695 (Hartree/Particle)
Thermal correction to Energy= 0.328213
Thermal correction to Enthalpy= 0.329157
Thermal correction to Gibbs Free Energy= 0.256127
Sum of electronic and zero-point Energies= -1390.086225
Sum of electronic and thermal Energies= -1390.065707
Sum of electronic and thermal Enthalpies= -1390.064763
Sum of electronic and thermal Free Energies= -1390.137794

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

N	0.56308200	-0.48989800	0.23738800
C	1.91555300	-0.85250700	0.07476300
C	2.26156600	-1.92919600	-0.73098100
C	3.59108100	-2.32202700	-0.86617100
C	4.57878100	-1.63567800	-0.17747800
C	4.24971200	-0.55794400	0.64456300
C	2.92274600	-0.15963000	0.77626900
H	1.46495300	-2.45181200	-1.24803600
H	3.84587900	-3.16036900	-1.50232200
H	5.61648400	-1.93237900	-0.26916700
H	5.03432500	-0.03591000	1.17554000
C	-2.13766000	0.21158200	0.49915800
C	-2.59923500	-0.99900500	-0.03604700
C	-3.52720300	-1.74301000	0.68890000
C	-3.99076100	-1.26563000	1.91340900
C	-3.54224800	-0.05861500	2.42921800
C	-2.60484900	0.67951800	1.71261800
H	-3.89703000	-2.68534800	0.30873500
H	-4.71538000	-1.85336600	2.46407700
H	-3.91058500	0.30556800	3.37936900
H	-2.22468400	1.62193900	2.08795600
C	-1.56143900	2.07317000	-0.98571600
S	1.05584800	1.58605400	-1.46701400

C	0.13520900	0.52826500	-0.36536200
N	-1.18488200	0.96556900	-0.24994400
O	-2.67053600	2.53477700	-1.00847400
C	-0.38775700	2.64533900	-1.75970200
H	-0.20267500	3.66125500	-1.41320400
H	-0.64821000	2.66633300	-2.81669200
O	-2.09558800	-1.34389000	-1.24016800
O	2.49900000	0.87387700	1.54569000
C	-2.48756100	-2.59257700	-1.78296200
H	-2.19953800	-3.41325500	-1.12010800
H	-3.56602100	-2.62210100	-1.96190200
H	-1.96071300	-2.68506400	-2.72927300
C	3.48299900	1.62385500	2.23031900
H	2.94774600	2.40409400	2.76592100
H	4.02900800	1.00040800	2.94489300
H	4.18885000	2.07987000	1.52918000

Zero-point correction= 0.306127 (Hartree/Particle)
Thermal correction to Energy= 0.326630
Thermal correction to Enthalpy= 0.327575
Thermal correction to Gibbs Free Energy= 0.254502
Sum of electronic and zero-point Energies= -1390.343178
Sum of electronic and thermal Energies= -1390.322674
Sum of electronic and thermal Enthalpies= -1390.321730
Sum of electronic and thermal Free Energies= -1390.394802

2b

B3LYP/6-31+G*

N	0.85303500	-0.54158300	-0.00020700
C	2.21905100	-0.74341300	-0.28146700
C	2.60233900	-1.56510100	-1.34573700
C	3.95007600	-1.83976600	-1.59677800
C	4.92840800	-1.30328800	-0.76169800
C	4.56499900	-0.49476100	0.32226100
C	3.21779700	-0.21252900	0.57127500
H	1.82222700	-1.98593700	-1.97399600
H	4.22649400	-2.47217600	-2.43587600
H	5.98005100	-1.51092000	-0.94086900
H	5.33755300	-0.09015400	0.96682700
C	-1.84228900	-0.30458500	0.64763700

C	-2.48967600	-1.24840900	-0.17035000
C	-3.22221000	-2.27675700	0.43428400
C	-3.29390400	-2.35391900	1.82897600
C	-2.64409200	-1.41878300	2.63412500
C	-1.91470300	-0.39050600	2.03221700
H	-3.73467200	-3.01711900	-0.16946800
H	-3.86603700	-3.15896400	2.28294000
H	-2.70201700	-1.48522500	3.71629200
H	-1.39675500	0.35273100	2.63096700
C	-1.66368300	1.94054600	-0.34080000
S	0.95060000	1.97397200	-1.11725100
C	0.27184900	0.54515900	-0.28938200
N	-1.09353900	0.75408800	0.02605100
C	-0.66192400	2.84873100	-1.02668900
H	-0.55915900	3.77802700	-0.46108500
H	-1.01785200	3.09426500	-2.03011800
O	-2.34383700	-1.07921800	-1.51180100
O	2.76659400	0.55565900	1.60853500
C	-3.01229700	-1.97874100	-2.38902700
H	-2.65575600	-3.00718100	-2.24913500
H	-4.09904700	-1.93875100	-2.24304000
H	-2.76734200	-1.64231500	-3.39759900
C	3.72011000	1.13383800	2.48788000
H	3.14197000	1.70025000	3.22024100
H	4.30712100	0.36297300	3.00472100
H	4.39674300	1.81305000	1.95240200
S	-3.23129700	2.39365900	-0.09327000

Zero-point correction= 0.300772 (Hartree/Particle)
Thermal correction to Energy= 0.322123
Thermal correction to Enthalpy= 0.323067
Thermal correction to Gibbs Free Energy= 0.247008
Sum of electronic and zero-point Energies= -1713.476429
Sum of electronic and thermal Energies= -1713.455077
Sum of electronic and thermal Enthalpies= -1713.454133
Sum of electronic and thermal Free Energies= -1713.530192

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

N 0.850020 -0.517945 0.003819

C	2.216436	-0.711977	-0.293516
C	2.593590	-1.483558	-1.396948
C	3.940176	-1.753917	-1.661458
C	4.921606	-1.261250	-0.802557
C	4.563524	-0.500416	0.317508
C	3.217533	-0.223134	0.581159
H	1.811756	-1.871264	-2.044273
H	4.212626	-2.348746	-2.528823
H	5.972079	-1.466104	-0.991472
H	5.338635	-0.128551	0.978305
C	-1.853861	-0.282432	0.641702
C	-2.486090	-1.251348	-0.159522
C	-3.215348	-2.270682	0.465479
C	-3.299346	-2.312524	1.861093
C	-2.664957	-1.351345	2.648999
C	-1.938051	-0.332592	2.027936
H	-3.715636	-3.030605	-0.123760
H	-3.868871	-3.110732	2.329898
H	-2.732440	-1.390752	3.731864
H	-1.432006	0.429775	2.612767
C	-1.673134	1.948686	-0.376939
S	0.934749	1.972769	-1.162231
C	0.261089	0.558674	-0.309439
N	-1.106675	0.767557	0.001498
C	-0.675742	2.850809	-1.073499
H	-0.567330	3.784187	-0.515926
H	-1.032333	3.088320	-2.078446
O	-2.331168	-1.114778	-1.502974
O	2.771602	0.502293	1.650087
C	-2.968245	-2.058336	-2.363724
H	-2.590970	-3.072176	-2.183950
H	-4.056838	-2.036077	-2.234405
H	-2.714085	-1.747737	-3.377859
C	3.730820	1.021230	2.565914
H	3.155815	1.554195	3.324781
H	4.303808	0.214882	3.040875
H	4.417156	1.718787	2.069388
S	-3.244965	2.403667	-0.129366

Zero-point correction= 0.300706 (Hartree/Particle)

Thermal correction to Energy= 0.322070
Thermal correction to Enthalpy= 0.323014
Thermal correction to Gibbs Free Energy= 0.246769
Sum of electronic and zero-point Energies= -1713.483635
Sum of electronic and thermal Energies= -1713.462271
Sum of electronic and thermal Enthalpies= -1713.461326
Sum of electronic and thermal Free Energies= -1713.537572

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF=-1713.3340227

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N	0.82364900	-0.64989800	0.09569800
C	2.18933300	-0.87034000	-0.18101900
C	2.56497800	-1.80311700	-1.14325300
C	3.91202000	-2.06202700	-1.40057100
C	4.88924500	-1.39325500	-0.67252000
C	4.53096800	-0.46884500	0.31198900
C	3.18515000	-0.20449000	0.56564300
H	1.78010400	-2.31793300	-1.68991800
H	4.18914000	-2.78368900	-2.16266400
H	5.94129900	-1.58664200	-0.85945100
H	5.30651600	0.03831500	0.87469300
C	-1.85765400	-0.26022300	0.67400200
C	-2.54474500	-1.16182100	-0.15038200
C	-3.34714200	-2.13691300	0.44343500
C	-3.44131900	-2.19862500	1.83527100
C	-2.74929200	-1.30448900	2.64584600
C	-1.95033200	-0.32715000	2.05315700
H	-3.89736300	-2.84619600	-0.16387600
H	-4.06910300	-2.96281300	2.28425100
H	-2.82845600	-1.36343400	3.72611700
H	-1.39406900	0.38958000	2.65036700
C	-1.55532400	1.91366600	-0.40406500
S	1.06169000	1.79987700	-1.10161300
C	0.30414200	0.45228200	-0.23674800
N	-1.04732200	0.73953800	0.04757700
C	-0.49960700	2.73879300	-1.10508000
H	-0.37468300	3.68930300	-0.58288200

H	-0.82225200	2.94001100	-2.12833800
O	-2.36475000	-1.00273700	-1.48140900
O	2.73464200	0.66576000	1.50716600
C	-3.07705800	-1.86795700	-2.34924400
H	-2.78830900	-2.91190600	-2.18376700
H	-4.15781500	-1.75333900	-2.21058600
H	-2.80315300	-1.56837700	-3.35993000
C	3.69637800	1.40895800	2.23099000
H	3.13074400	2.05991900	2.89706300
H	4.34054700	0.74990200	2.82458600
H	4.31105400	2.01752400	1.55730000
S	-3.10894500	2.42208700	-0.23505300

Zero-point correction= 0.304833 (Hartree/Particle)
Thermal correction to Energy= 0.325829
Thermal correction to Enthalpy= 0.326774
Thermal correction to Gibbs Free Energy= 0.251811
Sum of electronic and zero-point Energies= -1713.031160
Sum of electronic and thermal Energies= -1713.010164
Sum of electronic and thermal Enthalpies= -1713.009219
Sum of electronic and thermal Free Energies= -1713.084183

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

N	0.82200300	-0.64341700	0.09756500
C	2.18543900	-0.86671000	-0.18419200
C	2.55563300	-1.78317900	-1.15922900
C	3.89888700	-2.03956700	-1.42290000
C	4.87617200	-1.38359500	-0.69075300
C	4.52319000	-0.47287600	0.30435400
C	3.18168500	-0.20949900	0.56561900
H	1.76888300	-2.28821200	-1.70703600
H	4.17233600	-2.74905600	-2.19359800
H	5.92469600	-1.57602400	-0.88288800
H	5.29955200	0.02525600	0.86908500
C	-1.85405900	-0.26425300	0.67874500
C	-2.53547400	-1.15920700	-0.15355600
C	-3.33482100	-2.13809600	0.43152300
C	-3.42987300	-2.20994300	1.81985500
C	-2.74140500	-1.32397100	2.63611000
C	-1.94481200	-0.34260000	2.05378700

H	-3.88152600	-2.84264700	-0.17972400
H	-4.05522700	-2.97638400	2.26176400
H	-2.82069400	-1.39211800	3.71311000
H	-1.39026400	0.36801500	2.65469000
C	-1.55971000	1.90950000	-0.39473200
S	1.05833900	1.81171900	-1.08357800
C	0.30468600	0.45561600	-0.22752700
N	-1.04696600	0.74100500	0.05738000
C	-0.50770600	2.74049000	-1.09025900
H	-0.38940900	3.68685700	-0.56526200
H	-0.82710400	2.93661400	-2.11234600
O	-2.35176000	-0.98747400	-1.47959800
O	2.73301500	0.65114600	1.51304900
C	-3.05945000	-1.84817400	-2.35605400
H	-2.76791800	-2.89058300	-2.20006000
H	-4.13895500	-1.74020500	-2.21926900
H	-2.78636500	-1.53993600	-3.36175900
C	3.69768700	1.38595800	2.24149400
H	3.13692800	2.03102100	2.91349200
H	4.34117700	0.72253000	2.82703600
H	4.31175500	1.99859600	1.57450300
S	-3.11518800	2.40918200	-0.23252600

Zero-point correction= 0.303101 (Hartree/Particle)
Thermal correction to Energy= 0.324154
Thermal correction to Enthalpy= 0.325098
Thermal correction to Gibbs Free Energy= 0.249766
Sum of electronic and zero-point Energies= -1713.297410
Sum of electronic and thermal Energies= -1713.276358
Sum of electronic and thermal Enthalpies= -1713.275413
Sum of electronic and thermal Free Energies= -1713.350746

3b

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	-3.04860100	-1.12987500	-0.35723200
C	-1.73556100	-0.79173800	-0.26405300
C	-4.27256600	-0.35659000	-0.21180100
C	-0.64763700	-1.77199100	-0.45306400
S	-1.07695100	0.81612600	0.10897700
C	-5.49043800	-1.07338500	-0.29097900

C	-4.34256600	1.04003700	-0.00493200
S	-0.84069800	-3.39517500	-0.79267000
N	0.58155600	-1.16832400	-0.31323700
C	0.59787500	0.20495000	-0.01635600
C	1.82533700	-1.88679400	-0.39589800
C	-6.71910300	-0.43121500	-0.16090000
C	-5.57408200	1.68096700	0.12230100
C	-6.76621700	0.95175700	0.04755400
N	1.67667800	0.86304300	0.10425200
C	1.66677300	2.22542600	0.46751200
C	1.27649800	2.64054700	1.74684200
C	1.36469200	3.98414600	2.12692400
C	1.85289900	4.92390200	1.21983300
C	2.25662400	4.52805900	-0.06212700
C	2.17312400	3.18458300	-0.44441000
C	2.47983100	-2.01065300	-1.61664700
C	3.68869600	-2.70711800	-1.69567400
C	4.22824200	-3.26943000	-0.53718400
C	3.57939900	-3.14241700	0.69573500
C	2.36799900	-2.44347000	0.77807600
O	2.53719500	2.70588000	-1.66942400
C	3.08694000	3.61818000	-2.62056900
O	1.65435600	-2.25349600	1.91870200
C	2.15041500	-2.81056800	3.13943100
H	-3.20368800	-2.18456800	-0.57558400
H	-5.45993100	-2.14768400	-0.45434600
H	-3.44271300	1.64134700	0.04816400
H	-7.63849700	-1.00684500	-0.22342900
H	-5.60257400	2.75586000	0.27850600
H	-7.72253400	1.45773200	0.14818600
H	0.92119100	1.89293700	2.45084100
H	1.05962200	4.28459500	3.12535500
H	1.92839200	5.97123800	1.49969100
H	2.63451400	5.27211900	-0.75412300
H	2.03473400	-1.56212600	-2.49994600
H	4.19889600	-2.80680100	-2.64881300
H	5.16716300	-3.81471300	-0.58336300
H	4.02032500	-3.58562800	1.58106200
H	3.32300700	3.01811100	-3.50031200
H	2.36041600	4.39417100	-2.89006400

H	4.00232000	4.08483300	-2.23743300
H	1.42028700	-2.53832800	3.90212500
H	2.22252800	-3.90192600	3.07108300
H	3.12744500	-2.38551900	3.39586800

Zero-point correction= 0.386765 (Hartree/Particle)
Thermal correction to Energy= 0.413620
Thermal correction to Enthalpy= 0.414564
Thermal correction to Gibbs Free Energy= 0.325281
Sum of electronic and zero-point Energies= -1982.563116
Sum of electronic and thermal Energies= -1982.536261
Sum of electronic and thermal Enthalpies= -1982.535317
Sum of electronic and thermal Free Energies= -1982.624600

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -272.6050298

Norbornene

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.28079800	0.67217800	-0.50529500
C	0.08784300	1.12988000	0.32368400
C	1.28079400	-0.67218100	-0.50530000
C	0.08783700	-1.12988200	0.32367800
C	-1.19012700	0.78120400	-0.51911700
C	-1.19013400	-0.78119500	-0.51911700
H	1.92266500	-1.33027200	-1.08473000
H	1.92267300	1.33026800	-1.08472100
H	-2.08719400	1.17854200	-0.02961000
H	-1.14337000	1.20812400	-1.52604800
H	-2.08720000	-1.17852300	-0.02960100
H	-1.14339100	-1.20811700	-1.52604800
C	0.03656800	-0.00000400	1.38108500
H	-0.88684600	-0.00000400	1.97422700
H	0.90411400	-0.00000800	2.04998200
H	0.11854500	2.15944600	0.68942800
H	0.11853500	-2.15945100	0.68941400

Zero-point correction= 0.152929 (Hartree/Particle)
Thermal correction to Energy= 0.158158

Thermal correction to Enthalpy= 0.159103
Thermal correction to Gibbs Free Energy= 0.124399
Sum of electronic and zero-point Energies= -272.584021
Sum of electronic and thermal Energies= -272.578792
Sum of electronic and thermal Enthalpies= -272.577848
Sum of electronic and thermal Free Energies= -272.612551

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -1982.3767844

TRANSITION STATES

TS-rot-1b-O

B3LYP/6-31+G*

N	0.98936800	-0.35046700	-0.08940700
C	2.37490800	-0.35713300	-0.31836600
C	2.91909400	-0.30467300	-1.60721100
C	4.29833800	-0.41443400	-1.81519700
C	5.14592300	-0.58305900	-0.72303000
C	4.62228800	-0.64532400	0.57521700
C	3.24462500	-0.53900200	0.78662400
H	2.24516700	-0.19452900	-2.45264700
H	4.69791200	-0.37298000	-2.82461600
H	6.21950500	-0.67041900	-0.86771200
H	5.29609200	-0.77618700	1.41474000
C	-1.94993700	-0.52628600	-0.30148700
C	-3.31301700	-0.64701900	0.09554400
C	-3.97892900	-1.87265500	-0.06753200
C	-3.36406300	-2.97016800	-0.66358500
C	-2.05888500	-2.84014000	-1.12430500
C	-1.37740900	-1.63797600	-0.94299000
H	-5.00778100	-1.95664500	0.26116000
H	-3.91098100	-3.90240300	-0.77603000
H	-1.55306900	-3.66524600	-1.61717200
H	-0.35867200	-1.57958100	-1.29004400
C	-1.55200500	2.01508800	0.15428400
S	0.89854900	2.24745700	-0.92234100
C	0.26393200	0.65237800	-0.35866300
N	-1.14615000	0.68237300	-0.18060400
O	-2.38888500	2.35648900	0.95249700

C	-0.71329900	3.03166300	-0.60560100
H	-0.60425800	3.93301500	-0.00094400
H	-1.21702000	3.28295400	-1.54572600
O	-3.95466300	0.44295400	0.58004700
O	2.64325300	-0.58080500	2.00938900
C	-5.27591600	0.33343000	1.08446200
H	-5.98908400	0.06186300	0.29452500
H	-5.33395800	-0.39800400	1.90103500
H	-5.51731000	1.32639200	1.46769500
C	3.45270500	-0.79193800	3.15726000
H	2.76375800	-0.81221800	4.00346700
H	3.98816700	-1.74888600	3.09851800
H	4.17447000	0.02460900	3.29326000

Zero-point correction= 0.302672 (Hartree/Particle)
Thermal correction to Energy= 0.322707
Thermal correction to Enthalpy= 0.323652
Thermal correction to Gibbs Free Energy= 0.252121
Sum of electronic and zero-point Energies= -1390.487215
Sum of electronic and thermal Energies= -1390.467180
Sum of electronic and thermal Enthalpies= -1390.466236
Sum of electronic and thermal Free Energies= -1390.537766

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

N	0.95061700	-0.38125900	-0.07466600
C	2.34082200	-0.40404500	-0.28973000
C	2.89100200	-0.47792800	-1.57513200
C	4.27213000	-0.59989400	-1.76382100
C	5.11413700	-0.65322100	-0.65489500
C	4.58378300	-0.58807100	0.64058100
C	3.20389700	-0.46880800	0.83304400
H	2.22098100	-0.45804100	-2.43056400
H	4.67747200	-0.65763300	-2.77009600
H	6.18898500	-0.74828700	-0.78417400
H	5.25354000	-0.63021800	1.49213000
C	-1.99915300	-0.55120500	-0.32549500
C	-3.37294000	-0.62941600	0.02382600
C	-4.05739400	-1.84909900	-0.09662900
C	-3.44945500	-2.99949800	-0.58130400
C	-2.11636500	-2.91848600	-0.98309700

C	-1.41862100	-1.72142800	-0.86106000
H	-5.10964400	-1.84904500	0.17386900
H	-4.00993200	-3.92599800	-0.66940400
H	-1.60605900	-3.78301400	-1.39843900
H	-0.38833700	-1.70466300	-1.17708000
C	-1.59072400	1.99430900	-0.05939600
S	0.88107500	2.14454700	-1.10761800
C	0.23524900	0.60067200	-0.43588400
N	-1.17836400	0.64922400	-0.28117500
O	-2.47616400	2.37443400	0.66997200
C	-0.72132800	2.96668900	-0.83819100
H	-0.60157000	3.88821700	-0.26694500
H	-1.20863100	3.19292900	-1.79265600
O	-4.13474000	0.45601800	0.37656400
O	2.59652600	-0.39100500	2.05149600
C	-4.46846100	0.55914900	1.76581900
H	-5.02749900	-0.32435000	2.09973600
H	-3.56478700	0.68072700	2.37275000
H	-5.09258200	1.44900300	1.86253100
C	3.40430800	-0.48099400	3.22135400
H	2.71168400	-0.41873000	4.06203000
H	3.94276300	-1.43626400	3.26022700
H	4.12033600	0.34893100	3.27466900

Zero-point correction= 0.302337 (Hartree/Particle)
Thermal correction to Energy= 0.322412
Thermal correction to Enthalpy= 0.323356
Thermal correction to Gibbs Free Energy= 0.252162
Sum of electronic and zero-point Energies= -1390.493691
Sum of electronic and thermal Energies= -1390.473616
Sum of electronic and thermal Enthalpies= -1390.472672
Sum of electronic and thermal Free Energies= -1390.543866

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF=-1390.3543234

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N	-0.94760800	0.53815300	-0.00119300
C	-2.33715400	0.58060100	-0.22958900

C	-2.86262700	0.92839000	-1.47140500
C	-4.24234500	1.03276300	-1.66056100
C	-5.09804300	0.79014700	-0.59347300
C	-4.58799900	0.44233300	0.66101900
C	-3.21085700	0.33681500	0.85079900
H	-2.17286600	1.12514700	-2.28857800
H	-4.63644300	1.30593200	-2.63433600
H	-6.17323000	0.86907700	-0.72410400
H	-5.27164100	0.25269000	1.48074500
C	1.97982900	0.57079400	-0.19242300
C	3.33941500	0.52048100	0.20696500
C	4.08253600	1.70304300	0.29649800
C	3.54242900	2.93161800	-0.06387600
C	2.24288200	2.97891600	-0.54533100
C	1.48515300	1.81337400	-0.60838700
H	5.11062600	1.65396100	0.63364000
H	4.14584400	3.83089400	0.01332900
H	1.79936700	3.91485000	-0.86923600
H	0.47348400	1.88748300	-0.97446600
C	1.42816500	-1.97703300	-0.21779300
S	-1.01943900	-1.85433600	-1.26112300
C	-0.28187300	-0.43940200	-0.44588600
N	1.11503600	-0.58524800	-0.29738400
O	2.21457100	-2.51122900	0.51331300
C	0.54078900	-2.76412200	-1.16376200
H	0.39033600	-3.76571000	-0.76309500
H	1.02244600	-2.82117800	-2.14417600
O	3.89719000	-0.68336700	0.44462800
O	-2.61617100	-0.00769300	2.02020100
C	5.22500100	-0.75333300	0.92179800
H	5.93456600	-0.35840000	0.18539000
H	5.33425600	-0.21220700	1.86867700
H	5.41809300	-1.81357700	1.08399200
C	-3.45310000	-0.24751600	3.13527900
H	-2.78671000	-0.49120300	3.96207200
H	-4.03964600	0.64366300	3.38707100
H	-4.12738100	-1.09129000	2.94671400

Zero-point correction= 0.306809 (Hartree/Particle)
Thermal correction to Energy= 0.326536

Thermal correction to Enthalpy= 0.327480
Thermal correction to Gibbs Free Energy= 0.255686
Sum of electronic and zero-point Energies= -1390.048083
Sum of electronic and thermal Energies= -1390.028355
Sum of electronic and thermal Enthalpies= -1390.027411
Sum of electronic and thermal Free Energies= -1390.099206

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

N	-0.92364000	0.69551000	0.11397800
C	-2.32137600	0.78893000	-0.05180100
C	-2.87466800	1.58690600	-1.04403900
C	-4.25671700	1.71416800	-1.16842700
C	-5.08537900	1.04011900	-0.28628600
C	-4.54669500	0.23410600	0.71705100
C	-3.16714600	0.10066400	0.84037200
H	-2.20431800	2.11003900	-1.71668000
H	-4.67381200	2.33952800	-1.94751000
H	-6.16159800	1.13271200	-0.36808100
H	-5.20962600	-0.28738300	1.39399600
C	2.00483900	0.59986900	-0.09011300
C	3.36213300	0.40779500	0.26669300
C	4.17310600	1.51460000	0.52672100
C	3.70058700	2.81134600	0.39158800
C	2.39956700	3.00968900	-0.03316300
C	1.57672500	1.91739700	-0.27367600
H	5.19960200	1.35355000	0.82287500
H	4.35525800	3.64783700	0.60252700
H	2.00509400	4.00746100	-0.17663300
H	0.56487700	2.10441800	-0.58603400
C	1.32678600	-1.87364900	-0.56366600
S	-1.13273300	-1.47396400	-1.47055500
C	-0.31012100	-0.23978800	-0.46470500
N	1.07683300	-0.47363200	-0.37676700
O	2.07961800	-2.56614300	0.04373700
C	0.40073100	-2.41543400	-1.63347600
H	0.23239600	-3.47364300	-1.45568100
H	0.85071400	-2.25848600	-2.61474300
O	3.84660500	-0.84667900	0.30322700
O	-2.54239800	-0.66706000	1.76487400
C	5.16537800	-1.06946000	0.75722900

H	5.90095200	-0.61944300	0.08332300
H	5.30751800	-0.67990500	1.76949000
H	5.29009400	-2.14955500	0.76261400
C	-3.35413500	-1.41373700	2.65074900
H	-2.67009800	-1.96830300	3.28822000
H	-3.97545600	-0.75685600	3.26676600
H	-3.99251100	-2.11376000	2.10294300

Zero-point correction= 0.305223 (Hartree/Particle)
Thermal correction to Energy= 0.324921
Thermal correction to Enthalpy= 0.325866
Thermal correction to Gibbs Free Energy= 0.254736
Sum of electronic and zero-point Energies= -1390.306449
Sum of electronic and thermal Energies= -1390.286751
Sum of electronic and thermal Enthalpies= -1390.285807
Sum of electronic and thermal Free Energies= -1390.356936

TS-rot-1b-N

B3LYP/6-31+G*

N	0.74165300	-0.11835500	0.09341800
C	2.06326700	-0.24090900	-0.34211900
C	2.39528800	-0.33530000	-1.69945400
C	3.71577500	-0.55279000	-2.10704200
C	4.71822800	-0.67855900	-1.14852400
C	4.40737200	-0.59338500	0.21580800
C	3.08897700	-0.38218500	0.62746000
H	1.59751200	-0.26685200	-2.43439700
H	3.94984500	-0.62672700	-3.16537200
H	5.74903800	-0.84677200	-1.44887300
H	5.20061600	-0.69115900	0.94860100
C	-2.44555900	-0.05574600	0.04846600
C	-2.25678200	-1.46299800	-0.07233800
C	-3.37585700	-2.31260600	-0.09083200
C	-4.67673900	-1.82126500	-0.04289400
C	-4.87366900	-0.44581600	0.00686600
C	-3.77404900	0.40867200	0.04721600
H	-3.21831800	-3.38176100	-0.16441100
H	-5.51675700	-2.51041000	-0.06036600
H	-5.87344100	-0.02190900	0.02175300

H	-3.96532300	1.46821800	0.10693300
C	-1.67624400	2.27845800	0.47452600
S	0.55322500	2.35375800	-1.07636000
C	-0.00845300	0.83017500	-0.25735100
N	-1.39254400	0.95118800	0.10263000
O	-2.59417100	2.65206300	1.18018600
C	-0.69734600	3.27846800	-0.12592000
H	-0.23594800	3.86189100	0.67606300
H	-1.26439700	3.95806000	-0.76802100
O	-1.00368400	-1.95807500	-0.21464700
O	2.68992100	-0.27499500	1.92710400
C	-0.77735200	-3.35855200	-0.18047400
H	-1.16005500	-3.80349700	0.74715400
H	-1.22790500	-3.86283200	-1.04587100
H	0.30739900	-3.47287900	-0.21848200
C	3.66257500	-0.42990600	2.95083500
H	3.11854200	-0.32880300	3.89155400
H	4.13618200	-1.41977100	2.90682200
H	4.43452900	0.34874800	2.88982300

Zero-point correction= 0.302730 (Hartree/Particle)
Thermal correction to Energy= 0.322716
Thermal correction to Enthalpy= 0.323661
Thermal correction to Gibbs Free Energy= 0.252602
Sum of electronic and zero-point Energies= -1390.486146
Sum of electronic and thermal Energies= -1390.466159
Sum of electronic and thermal Enthalpies= -1390.465215
Sum of electronic and thermal Free Energies= -1390.536274

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

N	0.70674900	-0.14729100	0.01564200
C	2.03668900	-0.21140400	-0.41793500
C	2.37920000	-0.16502800	-1.77498100
C	3.70678900	-0.31870300	-2.18874900
C	4.70364300	-0.52219700	-1.23684800
C	4.38117800	-0.57943900	0.12621800
C	3.05519400	-0.43355300	0.54341200
H	1.58624100	-0.03949900	-2.50732200
H	3.95059300	-0.28495500	-3.24684600
H	5.73963700	-0.64200800	-1.54237900

H	5.17025400	-0.73653100	0.85290100
C	-2.44156200	-0.11785000	-0.01206000
C	-2.22473500	-1.49253900	-0.29048300
C	-3.32282100	-2.35717400	-0.43167500
C	-4.63592400	-1.91920300	-0.33051500
C	-4.86057500	-0.56093900	-0.10591500
C	-3.78767300	0.31136600	0.03964100
H	-3.10115800	-3.39580200	-0.66059000
H	-5.46148300	-2.61511400	-0.45097000
H	-5.87055900	-0.16475200	-0.04921500
H	-4.00847600	1.35257700	0.21239800
C	-1.72785600	2.18998400	0.62821100
S	0.51964000	2.44029600	-0.87284700
C	-0.03756500	0.83942400	-0.22911700
N	-1.42117500	0.90935500	0.13546600
O	-2.65133300	2.47467500	1.37002700
C	-0.77046900	3.25796300	0.12319800
H	-0.33562000	3.79081100	0.97312200
H	-1.34399900	3.96826300	-0.47857600
O	-0.99417000	-2.04394500	-0.54477900
O	2.64414800	-0.46593500	1.84441100
C	-0.45069200	-2.86138200	0.49942400
H	-0.23861500	-2.25789200	1.38792100
H	-1.13701100	-3.67979600	0.75143800
H	0.48210000	-3.27152100	0.10854200
C	3.61703200	-0.70026400	2.85853200
H	3.06580400	-0.70245700	3.80008700
H	4.11044500	-1.67059700	2.72030600
H	4.37030600	0.09734600	2.87756500

Zero-point correction= 0.302496 (Hartree/Particle)
Thermal correction to Energy= 0.322473
Thermal correction to Enthalpy= 0.323418
Thermal correction to Gibbs Free Energy= 0.252783
Sum of electronic and zero-point Energies= -1390.492909
Sum of electronic and thermal Energies= -1390.472931
Sum of electronic and thermal Enthalpies= -1390.471987
Sum of electronic and thermal Free Energies= -1390.542622

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF=-1390.3543793

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N	0.73144500	-0.18903300	0.16222300
C	2.04153400	-0.34468700	-0.30797500
C	2.31416700	-0.58250600	-1.65363000
C	3.62133100	-0.81272900	-2.08822100
C	4.65878800	-0.80491500	-1.16506500
C	4.40270900	-0.57081200	0.19037000
C	3.09888700	-0.34549000	0.62688900
H	1.48188900	-0.61216300	-2.35306500
H	3.81766700	-1.00122300	-3.13890200
H	5.68054500	-0.98287900	-1.48688100
H	5.22643800	-0.56465600	0.89506800
C	-2.45614100	-0.00498000	0.07105600
C	-2.32013400	-1.41554100	0.02695700
C	-3.46489600	-2.22204300	0.03493000
C	-4.74270100	-1.67665400	0.03156600
C	-4.88602400	-0.29746200	-0.00206400
C	-3.75654400	0.51445800	0.01170600
H	-3.34718700	-3.29871300	0.02475700
H	-5.60899900	-2.33091600	0.03655000
H	-5.86790800	0.16314700	-0.03680100
H	-3.90349900	1.58318700	-0.00791500
C	-1.58040300	2.29333800	0.38179100
S	0.60187900	2.16630100	-1.20676000
C	0.00830500	0.74384900	-0.26681800
N	-1.36028300	0.94198000	0.09554700
O	-2.47962000	2.74514900	1.05457200
C	-0.54384900	3.20168100	-0.25942900
H	-0.02103000	3.75695300	0.52267800
H	-1.07315500	3.90654400	-0.90336400
O	-1.08633700	-1.94945400	-0.06753700
O	2.74607600	-0.09582400	1.91231800
C	-0.92299000	-3.35012200	0.01370100
H	-1.33129500	-3.74257000	0.95202700
H	-1.39414900	-3.85708000	-0.83655800
H	0.15421600	-3.51609900	-0.01378500
C	3.77090100	-0.10964800	2.88763400
H	3.27984700	0.08685000	3.84016500

H	4.26612700	-1.08713900	2.92519000
H	4.51369300	0.67191900	2.68938800

Zero-point correction= 0.306755 (Hartree/Particle)
Thermal correction to Energy= 0.326418
Thermal correction to Enthalpy= 0.327362
Thermal correction to Gibbs Free Energy= 0.256849
Sum of electronic and zero-point Energies= -1390.046929
Sum of electronic and thermal Energies= -1390.027267
Sum of electronic and thermal Enthalpies= -1390.026323
Sum of electronic and thermal Free Energies= -1390.096836

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

N	0.71798400	-0.23412700	0.14408300
C	2.03364400	-0.40086900	-0.30822200
C	2.31720000	-0.69928100	-1.63546600
C	3.62867600	-0.92883800	-2.04879400
C	4.65669000	-0.85927000	-1.12358200
C	4.38846600	-0.56164300	0.21406500
C	3.08168300	-0.33524700	0.63132700
H	1.49131800	-0.77471700	-2.33445900
H	3.83493600	-1.16412900	-3.08533600
H	5.68056500	-1.03583900	-1.42967700
H	5.20564200	-0.50558100	0.92031900
C	-2.45595700	0.01562200	0.05773900
C	-2.34435000	-1.39650900	0.04915900
C	-3.50205900	-2.17916100	0.08318700
C	-4.76721200	-1.61330800	0.06895600
C	-4.88627000	-0.23718500	-0.00273800
C	-3.74545400	0.55336100	-0.01587600
H	-3.40489600	-3.25516400	0.10138300
H	-5.64261100	-2.25049400	0.09454600
H	-5.85756800	0.23815400	-0.04849500
H	-3.87530600	1.62055900	-0.06059700
C	-1.54466400	2.30614900	0.32548300
S	0.66593200	2.11835100	-1.21925100
C	0.02210400	0.71294200	-0.28328100
N	-1.34495800	0.94619000	0.05588400
O	-2.44239000	2.78188800	0.96755300
C	-0.47613800	3.18256500	-0.30415100

H	0.04316600	3.72621700	0.48427300
H	-0.97723100	3.89065800	-0.96205400
O	-1.12418000	-1.95447200	-0.03638500
O	2.71439300	-0.02473400	1.89660500
C	-0.98576100	-3.35488600	0.08212200
H	-1.39712700	-3.71626500	1.02918500
H	-1.46693200	-3.87624600	-0.75102100
H	0.08566300	-3.54095200	0.05687400
C	3.72977000	0.00878600	2.88135600
H	3.22998600	0.24157000	3.81828800
H	4.23000400	-0.96084900	2.96517900
H	4.46951200	0.78420100	2.65995300

Zero-point correction= 0.305283 (Hartree/Particle)
Thermal correction to Energy= 0.324934
Thermal correction to Enthalpy= 0.325879
Thermal correction to Gibbs Free Energy= 0.255406
Sum of electronic and zero-point Energies= -1390.304443
Sum of electronic and thermal Energies= -1390.284792
Sum of electronic and thermal Enthalpies= -1390.283848
Sum of electronic and thermal Free Energies= -1390.354320

TS-rot-2b-S

B3LYP/6-31+G*

N	-1.10724200	0.33669000	-0.00935300
C	-2.49325200	0.35337700	-0.22269900
C	-3.05911500	0.46297700	-1.49915600
C	-4.44294300	0.57747500	-1.67015300
C	-5.27426000	0.58343500	-0.55295100
C	-4.73003900	0.48076100	0.73423400
C	-3.34765900	0.37205000	0.90990300
H	-2.40027100	0.48118800	-2.36311900
H	-4.85872300	0.66585800	-2.66994500
H	-6.35134400	0.67044300	-0.66897200
H	-5.39189600	0.48609600	1.59306100
C	1.77641400	0.75634000	-0.34611900
C	3.10302800	0.97834700	0.11483800
C	3.65245200	2.26975000	0.06843100
C	2.95558500	3.34257200	-0.47988700

C	1.68914200	3.12100100	-1.01206300
C	1.12432800	1.85016800	-0.94449900
H	4.65455700	2.42731700	0.44899400
H	3.41124300	4.32864400	-0.50443700
H	1.12762200	3.92610300	-1.47671300
H	0.13615400	1.71666000	-1.35641400
C	1.53764600	-1.84738000	-0.22324700
S	-0.85658200	-1.99770100	-1.43200800
C	-0.34499500	-0.53516300	-0.51875500
N	1.07623300	-0.51385700	-0.33911700
C	0.82828500	-2.70046400	-1.25624800
H	0.77488600	-3.74023100	-0.93829900
H	1.35813800	-2.63441700	-2.21472300
O	3.82454300	-0.08307300	0.54673000
O	-2.72788600	0.26076100	2.11777700
C	5.10330300	0.10668900	1.13324800
H	5.82466300	0.49964200	0.40489100
H	5.04943300	0.77622500	2.00096900
H	5.41752500	-0.88646400	1.45945600
C	-3.52041600	0.30572400	3.29573500
H	-2.81699800	0.22520500	4.12624500
H	-4.06995000	1.25336100	3.37223300
H	-4.22795500	-0.53331900	3.33394600
S	2.51043800	-2.54665000	0.89403200

Zero-point correction= 0.300246 (Hartree/Particle)
Thermal correction to Energy= 0.320629
Thermal correction to Enthalpy= 0.321574
Thermal correction to Gibbs Free Energy= 0.249288
Sum of electronic and zero-point Energies= -1713.430262
Sum of electronic and thermal Energies= -1713.409878
Sum of electronic and thermal Enthalpies= -1713.408934
Sum of electronic and thermal Free Energies= -1713.481220

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

N	-1.10629500	0.33994200	0.01729700
C	-2.49162200	0.36698400	-0.20958800
C	-3.04216200	0.52260000	-1.48837300
C	-4.42415400	0.64266000	-1.67152900
C	-5.26859500	0.60818300	-0.56394700

C	-4.73962100	0.46031900	0.72532700
C	-3.35888400	0.34592900	0.91337800
H	-2.37351300	0.57437100	-2.34334800
H	-4.82812500	0.76735400	-2.67227500
H	-6.34432400	0.69885400	-0.68910500
H	-5.41152300	0.43523300	1.57573600
C	1.78358800	0.76126000	-0.32024800
C	3.11332200	0.96728500	0.14031800
C	3.66752300	2.25788700	0.11698100
C	2.97375500	3.34329200	-0.41050800
C	1.70527100	3.13721800	-0.94585600
C	1.13502400	1.86764100	-0.89980200
H	4.67037400	2.40500300	0.49936900
H	3.43360000	4.32761800	-0.41738400
H	1.14753500	3.95268000	-1.39671900
H	0.14733100	1.74513200	-1.31659000
C	1.52646600	-1.84201500	-0.24750400
S	-0.85327800	-1.94047400	-1.49230800
C	-0.34470200	-0.51476200	-0.52404200
N	1.07561300	-0.50525400	-0.33473400
C	0.81862400	-2.67083500	-1.30042600
H	0.74244500	-3.71422600	-0.99999600
H	1.36315100	-2.59929800	-2.24981900
O	3.83159000	-0.10490700	0.54845100
O	-2.75457300	0.19282400	2.12477600
C	5.12723600	0.06870700	1.11078800
H	5.83075400	0.47637900	0.37426000
H	5.09399000	0.71779600	1.99409100
H	5.44587700	-0.93228100	1.40621100
C	-3.56465300	0.19841000	3.29636500
H	-2.87209800	0.08886100	4.13218600
H	-4.11316100	1.14355300	3.39597500
H	-4.27181300	-0.64071600	3.29477100
S	2.49325600	-2.56684200	0.86236300

Zero-point correction= 0.300212 (Hartree/Particle)
Thermal correction to Energy= 0.320583
Thermal correction to Enthalpy= 0.321528
Thermal correction to Gibbs Free Energy= 0.249404
Sum of electronic and zero-point Energies= -1713.436268

Sum of electronic and thermal Energies= -1713.415897
Sum of electronic and thermal Enthalpies= -1713.414953
Sum of electronic and thermal Free Energies= -1713.487077

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF=-1713.2864719

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N	-1.02874200	0.74873100	0.27773500
C	-2.42882100	0.85062900	0.12118800
C	-2.99189100	1.86367500	-0.64840800
C	-4.37792100	1.99165500	-0.75769100
C	-5.20181500	1.09983600	-0.08221700
C	-4.65340900	0.07960800	0.70031600
C	-3.26916800	-0.05135000	0.80737800
H	-2.32731000	2.55348400	-1.16206900
H	-4.80278100	2.78427300	-1.36548200
H	-6.28170000	1.18812800	-0.15542200
H	-5.31183100	-0.60734700	1.21994200
C	1.88495000	0.81386000	-0.06835700
C	3.23705700	0.67427300	0.32552900
C	4.00360100	1.80966500	0.60988200
C	3.48519400	3.09035900	0.46190800
C	2.18521800	3.24153500	-0.00043400
C	1.41032300	2.11758800	-0.26407600
H	5.02882000	1.68438600	0.93619300
H	4.10319100	3.95295200	0.69089800
H	1.75830100	4.22663100	-0.15782800
H	0.40248500	2.26695300	-0.62003300
C	1.25581800	-1.62905000	-0.72905800
S	-1.15856700	-1.12005800	-1.68150600
C	-0.40207100	-0.05973000	-0.46242800
N	0.99747300	-0.28166100	-0.37895100
C	0.42902700	-1.96875700	-1.94719500
H	0.27706600	-3.04215600	-2.03442900
H	0.91692600	-1.57701500	-2.84631000
O	3.76047100	-0.56680600	0.37328700
O	-2.63578400	-1.00681900	1.53294900
C	5.08259700	-0.75201800	0.83607100

H	5.80672700	-0.27080400	0.16855800
H	5.20242100	-0.36742800	1.85504300
H	5.24123500	-1.83085900	0.83254300
C	-3.43581200	-1.95731800	2.20961300
H	-2.74018200	-2.62830400	2.71263900
H	-4.08036000	-1.47345800	2.95280300
H	-4.05036300	-2.52741500	1.50289300
S	2.08366000	-2.77364700	0.07254100

Zero-point correction= 0.303952 (Hartree/Particle)
Thermal correction to Energy= 0.324140
Thermal correction to Enthalpy= 0.325084
Thermal correction to Gibbs Free Energy= 0.252340
Sum of electronic and zero-point Energies= -1712.983707
Sum of electronic and thermal Energies= -1712.963519
Sum of electronic and thermal Enthalpies= -1712.962575
Sum of electronic and thermal Free Energies= -1713.035319

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

N	1.01758300	0.78414700	-0.27736200
C	2.41962900	0.88823000	-0.15012700
C	2.99770600	1.93702600	0.55164100
C	4.38299800	2.05728800	0.63961900
C	5.19010800	1.12267500	0.01128100
C	4.62654000	0.06641600	-0.70458000
C	3.24334300	-0.05845600	-0.79189800
H	2.34531900	2.66033500	1.02726700
H	4.82049900	2.87825900	1.19346000
H	6.26866200	1.20527900	0.06892200
H	5.27310600	-0.65267800	-1.18889300
C	-1.88868300	0.81534300	0.08320700
C	-3.23575400	0.66281400	-0.31575900
C	-4.00997500	1.79139000	-0.59327100
C	-3.50574900	3.07292800	-0.43344100
C	-2.21281500	3.23421900	0.03467200
C	-1.42936900	2.11912900	0.29339300
H	-5.03010800	1.65971900	-0.92434100
H	-4.12964400	3.92899700	-0.65839200
H	-1.79913000	4.22051700	0.20136800
H	-0.42652900	2.27366100	0.65318100

C	-1.23181200	-1.62374000	0.72692600
S	1.18348400	-1.11041800	1.65208200
C	0.40880900	-0.03970800	0.45204900
N	-0.98896300	-0.27144900	0.38608500
C	-0.40095900	-1.95686600	1.94091000
H	-0.24516200	-3.02626300	2.03138700
H	-0.87702800	-1.55335400	2.83747400
O	-3.74386600	-0.58092400	-0.37405800
O	2.59413600	-1.04405100	-1.45554300
C	-5.05545800	-0.77860100	-0.86116600
H	-5.79696300	-0.31520700	-0.20357200
H	-5.16451500	-0.38661800	-1.87622800
H	-5.20032600	-1.85686100	-0.87135300
C	3.37740300	-2.06562300	-2.04163700
H	2.67296300	-2.76289700	-2.48833200
H	4.03528100	-1.66410500	-2.81820800
H	3.97550200	-2.58351300	-1.28550700
S	-2.04474700	-2.76965300	-0.08166900

Zero-point correction= 0.302405 (Hartree/Particle)
Thermal correction to Energy= 0.322534
Thermal correction to Enthalpy= 0.323478
Thermal correction to Gibbs Free Energy= 0.251568
Sum of electronic and zero-point Energies= -1713.250220
Sum of electronic and thermal Energies= -1713.230091
Sum of electronic and thermal Enthalpies= -1713.229147
Sum of electronic and thermal Free Energies= -1713.301057

TS-rot-2b-N

B3LYP/6-31+G*

N	0.83451000	-0.12788400	0.05911600
C	2.17651200	-0.21718200	-0.32484700
C	2.56199800	-0.46250200	-1.64832000
C	3.90860500	-0.62930000	-1.98750400
C	4.88150600	-0.54939900	-0.99401100
C	4.51682400	-0.31224200	0.33836000
C	3.17189400	-0.15405500	0.68340800
H	1.78830300	-0.56085600	-2.40490000
H	4.18619500	-0.82554300	-3.01921800

H	5.93214500	-0.67452400	-1.24213200
H	5.28803700	-0.25140600	1.09816500
C	-2.27819600	-0.44257400	-0.08688200
C	-1.90010900	-1.80928900	-0.16983100
C	-2.88904100	-2.80621600	-0.14522300
C	-4.24317100	-2.51125300	-0.07454500
C	-4.62682200	-1.16991700	-0.06488800
C	-3.66279700	-0.17023800	-0.08318300
H	-2.55303700	-3.83579000	-0.22812100
H	-4.98142000	-3.30834300	-0.06334400
H	-5.67626600	-0.88943900	-0.05347300
H	-4.00001700	0.85397100	-0.08729300
C	-1.74139100	2.00835200	0.14058700
S	0.39076400	2.04794500	-1.57356900
C	0.01795900	0.65705800	-0.48996200
N	-1.38053900	0.69492000	-0.12605700
C	-0.92387600	2.98330700	-0.69576100
H	-0.48564900	3.75557100	-0.06062600
H	-1.59104300	3.46335200	-1.41755300
O	-0.61563300	-2.23090500	-0.39982300
O	2.71885300	0.08634300	1.94675000
C	0.02197500	-2.93131700	0.67524300
H	0.16214300	-2.26658300	1.53408500
H	-0.55868000	-3.81420700	0.97021600
H	0.99539200	-3.24481600	0.29379600
C	3.66412900	0.15094100	3.00623000
H	3.08059900	0.33200500	3.91047800
H	4.21521600	-0.79327900	3.10872700
H	4.37331200	0.97586200	2.85779700
S	-2.83543800	2.60619400	1.22502700

Zero-point correction= 0.300037 (Hartree/Particle)
Thermal correction to Energy= 0.320456
Thermal correction to Enthalpy= 0.321400
Thermal correction to Gibbs Free Energy= 0.249437
Sum of electronic and zero-point Energies= -1713.431963
Sum of electronic and thermal Energies= -1713.411544
Sum of electronic and thermal Enthalpies= -1713.410600
Sum of electronic and thermal Free Energies= -1713.482563

B3LYP/6-31+G* optimized with IEFPCM (toluene; ε=2.37)

N	0.83458000	-0.11626600	0.05517000
C	2.17904800	-0.19878400	-0.32373000
C	2.57311000	-0.40879100	-1.65123900
C	3.92192700	-0.56817400	-1.98596800
C	4.88831600	-0.51585400	-0.98347700
C	4.51530500	-0.31399500	0.35253800
C	3.16784500	-0.16359100	0.69311300
H	1.80586700	-0.48656200	-2.41675100
H	4.20603200	-0.73763400	-3.02062400
H	5.94046700	-0.63574500	-1.22760100
H	5.28153600	-0.27470400	1.11859100
C	-2.27855500	-0.44187600	-0.09325400
C	-1.89657500	-1.80654600	-0.19209600
C	-2.88178900	-2.80727800	-0.15913000
C	-4.23615300	-2.51600200	-0.07215000
C	-4.62489200	-1.17569000	-0.05647000
C	-3.66387800	-0.17286300	-0.07930600
H	-2.54665100	-3.83635800	-0.24919900
H	-4.97146200	-3.31556000	-0.05539800
H	-5.67517400	-0.89917200	-0.03707500
H	-4.00428600	0.85037800	-0.08160900
C	-1.74233600	2.00592400	0.15608000
S	0.37714300	2.06618100	-1.56910300
C	0.01617200	0.66705500	-0.49406500
N	-1.38364900	0.69814700	-0.12664100
C	-0.92840400	2.99260900	-0.66762200
H	-0.48086300	3.75261500	-0.02448500
H	-1.59753900	3.48580700	-1.37836700
O	-0.61306400	-2.21453900	-0.44896600
O	2.70834600	0.04416500	1.95937100
C	0.03683800	-2.96448300	0.58701500
H	0.16304900	-2.34648500	1.48180300
H	-0.52676100	-3.87271700	0.83106300
H	1.01580200	-3.23807400	0.19020600
C	3.65005600	0.07380900	3.02865200
H	3.06148700	0.22988100	3.93382300
H	4.19560700	-0.87521500	3.10427500
H	4.36127100	0.90031000	2.90720800
S	-2.83485300	2.58858400	1.25584300

Zero-point correction= 0.299932 (Hartree/Particle)
Thermal correction to Energy= 0.320363
Thermal correction to Enthalpy= 0.321307
Thermal correction to Gibbs Free Energy= 0.249607
Sum of electronic and zero-point Energies= -1713.437600
Sum of electronic and thermal Energies= -1713.417169
Sum of electronic and thermal Enthalpies= -1713.416225
Sum of electronic and thermal Free Energies= -1713.487925

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF=-1713.2892488

M062X/6-31+G(d) optimized with IEFPCM (toluene; ε=2.37)

N	0.81527900	-0.10195300	0.06921800
C	2.15382900	-0.15490900	-0.33277600
C	2.52494900	-0.22801600	-1.67449400
C	3.86767500	-0.33935100	-2.03918200
C	4.84167600	-0.38016200	-1.04976400
C	4.48725100	-0.32434700	0.30219800
C	3.14678800	-0.22328500	0.66950700
H	1.74391800	-0.23571900	-2.43139000
H	4.14102200	-0.39981000	-3.08767600
H	5.89080900	-0.46374000	-1.31721500
H	5.26337500	-0.36207500	1.05807200
C	-2.25728800	-0.45344600	-0.12142100
C	-1.84294000	-1.79786900	-0.26866200
C	-2.79981900	-2.81953400	-0.28649800
C	-4.15889600	-2.56513200	-0.21054400
C	-4.57804600	-1.23877200	-0.15640500
C	-3.64368300	-0.21549700	-0.12663600
H	-2.42828900	-3.83330500	-0.40598400
H	-4.87454700	-3.38100300	-0.23342900
H	-5.63392600	-0.98753500	-0.15004900
H	-4.00681200	0.80005500	-0.11322900
C	-1.76958400	1.97861600	0.24730200
S	0.36181300	2.14832900	-1.43889300
C	0.00401000	0.70197400	-0.44896000
N	-1.39178800	0.70113700	-0.09626700

C	-0.91728200	3.01319000	-0.47144500
H	-0.45937100	3.68725300	0.25428700
H	-1.56676600	3.59330900	-1.13055200
O	-0.55256200	-2.17910600	-0.50638300
O	2.70034900	-0.16201100	1.94760800
C	0.09641900	-2.81158800	0.59460600
H	0.10040300	-2.15163400	1.46674700
H	-0.39542300	-3.76112500	0.83606000
H	1.12377700	-2.99805200	0.27758700
C	3.66396100	-0.21518000	2.98326200
H	3.10287700	-0.16210700	3.91557500
H	4.22986600	-1.15339400	2.94800800
H	4.35394400	0.63423300	2.92100200
S	-2.90217100	2.48599200	1.32584300

Zero-point correction= 0.303961 (Hartree/Particle)
Thermal correction to Energy= 0.324022
Thermal correction to Enthalpy= 0.324966
Thermal correction to Gibbs Free Energy= 0.254113
Sum of electronic and zero-point Energies= -1712.987187
Sum of electronic and thermal Energies= -1712.967127
Sum of electronic and thermal Enthalpies= -1712.966182
Sum of electronic and thermal Free Energies= -1713.037036

M062X/6-311G(d,p) optimized with IEFPCM (toluene; ε=2.37)

N	0.81116400	-0.07558600	0.04198700
C	2.15279900	-0.11062800	-0.34479800
C	2.54296200	-0.11372300	-1.67970200
C	3.88824100	-0.21184600	-2.02712300
C	4.84318100	-0.31228000	-1.02854600
C	4.46890600	-0.32875000	0.31608100
C	3.12625000	-0.24060400	0.66790100
H	1.77569700	-0.07836700	-2.44550400
H	4.17835300	-0.21807100	-3.07007500
H	5.89320500	-0.38765600	-1.28354500
H	5.23120900	-0.41476200	1.07827500
C	-2.24037000	-0.46472800	-0.14650500
C	-1.80212300	-1.79673400	-0.31984900
C	-2.74252700	-2.82988700	-0.35049500
C	-4.10205700	-2.60003200	-0.27125400

C	-4.54320200	-1.28526900	-0.19768700
C	-3.62806900	-0.24997600	-0.15260300
H	-2.35467400	-3.83246900	-0.48826600
H	-4.80188700	-3.42545100	-0.30573800
H	-5.60073800	-1.05326000	-0.18988000
H	-4.00598800	0.75701900	-0.12550200
C	-1.79320700	1.96212000	0.29283700
S	0.33823000	2.22356500	-1.37982500
C	-0.00205400	0.73681200	-0.44500100
N	-1.39866100	0.70646800	-0.09859200
C	-0.94593500	3.03360800	-0.37342400
H	-0.48872900	3.66577100	0.38519100
H	-1.59529300	3.63982200	-1.00350800
O	-0.51014600	-2.15914300	-0.56444500
O	2.65652200	-0.25171500	1.93581200
C	0.14997200	-2.79406800	0.52932200
H	0.19469600	-2.12378300	1.38938500
H	-0.35779400	-3.72579100	0.79491300
H	1.16194100	-3.01044800	0.19011000
C	3.60057100	-0.37557900	2.98376300
H	3.02490500	-0.37051900	3.90574000
H	4.15731700	-1.31416600	2.90506900
H	4.29891200	0.46641500	2.98407900
S	-2.93883500	2.41304800	1.37901700

Zero-point correction= 0.302557 (Hartree/Particle)
Thermal correction to Energy= 0.322555
Thermal correction to Enthalpy= 0.323499
Thermal correction to Gibbs Free Energy= 0.252433
Sum of electronic and zero-point Energies= -1713.253812
Sum of electronic and thermal Energies= -1713.233814
Sum of electronic and thermal Enthalpies= -1713.232869
Sum of electronic and thermal Free Energies= -1713.303935

TS(M,S,R,R)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

N	-2.91244100	0.06145400	0.28886400
C	-3.55682300	-1.08077100	0.80633100
C	-3.75470200	-1.21732700	2.18561800

C	-4.46449200	-2.30099200	2.71477900
C	-4.99878800	-3.25855500	1.85297300
C	-4.82553200	-3.13694100	0.46789300
C	-4.11075700	-2.05634100	-0.06202400
H	-3.34292000	-0.45323700	2.83979800
H	-4.59890800	-2.38790100	3.78956500
H	-5.55661600	-4.10445400	2.24611000
H	-5.25084000	-3.88751800	-0.18901300
O	-3.89834600	-1.85471300	-1.39758800
C	-4.42449100	-2.80644600	-2.32111500
H	-4.13554200	-2.44803900	-3.31015900
H	-5.51810800	-2.85996100	-2.25589100
H	-3.99540000	-3.80162300	-2.15190600
C	-1.63652900	2.35880500	-0.76736500
C	-1.68451700	3.28138800	0.29695600
C	-2.32555800	4.51205500	0.10006500
C	-2.90599900	4.80707500	-1.13838100
C	-2.85927600	3.89011300	-2.18973500
C	-2.22160000	2.66169200	-1.99376900
H	-2.37572600	5.24149300	0.90023100
H	-3.39868100	5.76642100	-1.27335700
H	-3.31308700	4.12286300	-3.14837500
H	-2.17145400	1.92611400	-2.79160500
O	-1.08758000	2.89711800	1.45679000
C	-1.12130700	3.79038100	2.57246800
H	-0.59639100	3.27389000	3.37682800
H	-2.15302400	3.99690900	2.87977900
H	-0.60603700	4.72970500	2.34051600
C	3.21292100	0.23224800	0.77286600
C	4.69727900	0.01919400	0.47104200
C	2.99814400	1.61660700	0.63951300
C	4.32047200	2.23917700	0.23658100
C	5.47788900	0.63222500	1.67881100
C	4.94099000	1.10224100	-0.60438700
C	5.21181400	2.16410200	1.52519400
C	2.09224000	-0.88827500	-0.75467200
C	0.76084500	-0.45799900	-0.61925100
C	0.35921500	0.86466500	-0.89422500
S	1.45072700	2.07670500	-1.33689600
S	-0.57271400	-1.38586700	0.10678200

C	-1.67927000	0.01634000	-0.04136900
N	-0.98557900	1.09542700	-0.57704200
H	2.63359600	-0.32896100	-1.51096900
C	2.55340600	-2.28136700	-0.57664000
H	2.26433200	2.16132400	1.22323000
H	2.71353700	-0.33718500	1.55196700
H	4.98671900	-1.00493300	0.22415900
H	4.26670100	3.23225400	-0.21571800
H	5.13023200	0.23231600	2.63734000
H	6.54705200	0.40415300	1.59242400
H	6.00452900	1.26109700	-0.81596800
H	4.41148600	0.92647500	-1.54535200
H	4.71354600	2.60231300	2.39650600
H	6.14341600	2.71891700	1.36270600
C	3.44279700	-2.81881000	-1.52787400
C	3.90529000	-4.13158100	-1.42071800
C	3.50215100	-4.93194300	-0.34708100
C	2.63715100	-4.40523900	0.61824300
C	2.16798400	-3.09509200	0.50637000
H	3.76385400	-2.20223400	-2.36404300
H	4.58227600	-4.52693000	-2.17356800
H	3.86328900	-5.95313800	-0.25910100
H	2.32910200	-5.01393600	1.46437200
H	1.51873300	-2.70078000	1.28239400

Zero-point correction= 0.540897 (Hartree/Particle)
Thermal correction to Energy= 0.573587
Thermal correction to Enthalpy= 0.574531
Thermal correction to Gibbs Free Energy= 0.472963
Sum of electronic and zero-point Energies= -2255.114164
Sum of electronic and thermal Energies= -2255.081474
Sum of electronic and thermal Enthalpies= -2255.080530
Sum of electronic and thermal Free Energies= -2255.182098

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9665803

TS(P,S,R,R)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

N	2.83905000	0.28826400	0.10429900
C	3.42270600	1.56871900	0.10990100
C	3.59857500	2.30057300	-1.07240600
C	4.26651400	3.53018300	-1.07392300
C	4.77544800	4.03711600	0.12124200
C	4.61954600	3.32025000	1.31522400
C	3.95074100	2.09090000	1.31842100
H	3.21603000	1.88272700	-1.99994000
H	4.39061300	4.07749100	-2.00444100
H	5.29985700	4.98894100	0.13759500
H	5.02165100	3.72812500	2.23584200
O	3.74877000	1.32867200	2.43493900
C	4.28346900	1.78600000	3.67600600
H	4.02203000	1.02120100	4.40882000
H	3.83781000	2.74375000	3.97165700
H	5.37446300	1.88693800	3.62528400
C	1.75484100	-2.31319400	-0.13202800
C	2.27113400	-2.86591400	-1.32181300
C	3.03639900	-4.03789000	-1.25074000
C	3.28129000	-4.63690500	-0.01035200
C	2.77332900	-4.08425400	1.16665900
C	2.00809200	-2.91686400	1.09614000
H	3.44385900	-4.48509600	-2.15006600
H	3.87803300	-5.54454900	0.02699500
H	2.96765900	-4.55247700	2.12692300
H	1.60035600	-2.46264600	1.99451100
O	1.97623300	-2.20205900	-2.47141300
C	2.46324200	-2.72576700	-3.70961300
H	2.10142800	-2.04226900	-4.47840500
H	2.06630500	-3.73071400	-3.89402400
H	3.55905400	-2.74843800	-3.72326700
C	-3.20976300	-0.18664700	1.13760100
C	-4.72224100	-0.18852300	0.90677100
C	-2.87414800	-1.52313200	1.42405500
C	-4.15028700	-2.33648000	1.33730200
C	-5.37391100	-0.44803500	2.30398600
C	-4.91956100	-1.56893300	0.23957400
C	-4.97657600	-1.92799200	2.60633200
C	-2.28917700	0.46640900	-0.74785800
C	-0.91561600	0.20618100	-0.59707500

C	-0.39973600	-1.09872900	-0.47373000
S	-1.38842100	-2.46873300	-0.42589600
S	0.35718000	1.42040600	-0.32985700
C	1.59067400	0.13335300	-0.11634600
N	0.97452400	-1.11158500	-0.19878900
H	-2.81284700	-0.34519000	-1.24254300
C	-2.87256000	1.80430400	-0.98247600
H	-2.06528700	-1.80079000	2.09099100
H	-2.72554200	0.63393600	1.65996600
H	-5.12084700	0.68256600	0.38165800
H	-4.02592300	-3.41427900	1.20895600
H	-5.01135300	0.25458500	3.06188300
H	-6.46268000	-0.33369100	2.23997600
H	-5.97313900	-1.86351900	0.17347500
H	-4.46056300	-1.65861600	-0.74925900
H	-4.39617800	-2.03661600	3.52875200
H	-5.86025500	-2.57113400	2.69370000
C	-3.85095600	1.94066800	-1.98692100
C	-4.43087400	3.17985200	-2.26417900
C	-4.05758200	4.30908900	-1.52841100
C	-3.10379000	4.18540500	-0.51231900
C	-2.51756900	2.94763600	-0.24093900
H	-4.14816900	1.06673400	-2.56168000
H	-5.17530300	3.26184300	-3.05188700
H	-4.50982100	5.27449200	-1.73936300
H	-2.81704100	5.05409300	0.07462500
H	-1.79929800	2.87187600	0.57002000

Zero-point correction= 0.541043 (Hartree/Particle)
Thermal correction to Energy= 0.573681
Thermal correction to Enthalpy= 0.574625
Thermal correction to Gibbs Free Energy= 0.472983
Sum of electronic and zero-point Energies= -2255.114030
Sum of electronic and thermal Energies= -2255.081392
Sum of electronic and thermal Enthalpies= -2255.080448
Sum of electronic and thermal Free Energies= -2255.182090

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)

HF= -2254.9655992

TS(M,S,S,S)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.83847600	-2.02904100	-0.98950900
C	2.07284900	-2.99869400	0.00578400
C	2.94198900	-4.06208300	-0.27498900
C	3.55859400	-4.14993200	-1.52759700
C	3.32443000	-3.18784100	-2.51149700
C	2.46250200	-2.12415600	-2.23097900
H	3.14152800	-4.82166100	0.47207800
H	4.22850200	-4.98221600	-1.72713900
H	3.80710600	-3.25825800	-3.48161500
H	2.26558700	-1.35633900	-2.97388400
O	1.42133500	-2.82486000	1.18572600
C	1.64298800	-3.76897600	2.23573100
H	1.03409200	-3.42423800	3.07212200
H	2.69825400	-3.78707500	2.53176000
H	1.32218000	-4.77373400	1.93679600
C	-3.58305100	-0.82163900	0.06071500
C	-3.38566800	-0.63945100	1.56431100
C	-3.21210400	-2.15536100	-0.21346800
C	-2.77168900	-2.77065000	1.10284500
C	-4.51607000	-1.48041500	2.24424300
C	-4.09899700	-2.95073500	1.92007700
C	-2.36052800	0.58198600	-1.09953100
C	-0.99681700	0.34726300	-0.83949700
C	-0.37073300	-0.87588200	-1.15049800
S	-1.21845000	-2.20127900	-1.77308300
S	0.10968900	1.40914300	0.06360400
C	1.43325200	0.20744100	-0.06880400
N	0.96010300	-0.92810100	-0.71727300
H	-2.71113000	0.01338100	-1.95669500
C	-3.05549700	1.87331000	-0.91128400
H	-3.69737400	-2.74990700	-0.98047000
H	-4.44670900	-0.38508400	-0.43390800
H	-4.52348200	-1.29865400	3.32567400
H	-5.50818300	-1.22338900	1.85801600
H	-3.89280000	-3.52003000	2.83434500
H	-4.86112500	-3.49801100	1.35496600
C	-2.85774800	2.71971300	0.19687100

C	-3.55317000	3.92587600	0.30870300
C	-4.46434500	4.31238800	-0.67917900
C	-4.68255000	3.47598500	-1.77923100
C	-3.99147200	2.26889200	-1.88827300
H	-2.17450200	2.43458700	0.99023200
H	-3.38406600	4.56202000	1.17362800
H	-5.00220900	5.25250000	-0.59035200
H	-5.39104000	3.76267000	-2.55205200
H	-4.16782100	1.62432800	-2.74648500
C	-2.16320600	-1.54679600	1.82274700
H	-1.98743300	-1.72974700	2.88918200
H	-1.23816200	-1.18832900	1.36906900
H	-3.32821000	0.39376500	1.91491600
H	-2.15976300	-3.67191700	1.03267100
N	2.63240300	0.33408500	0.35206100
C	3.04849900	1.53109200	0.97016800
C	3.11400600	1.62375100	2.36555300
C	3.60098300	2.77458400	2.99554700
C	4.04376400	3.84647500	2.22095200
C	4.00151300	3.77197500	0.82238900
C	3.50987100	2.62346600	0.19134300
H	2.77741700	0.77256300	2.95171800
H	3.63552500	2.82493600	4.08047100
H	4.42874800	4.74640600	2.69337300
H	4.35377100	4.61215000	0.23436100
O	3.43782600	2.46032400	-1.16418200
C	3.88804400	3.52319700	-2.00276500
H	3.73900300	3.17443000	-3.02567600
H	4.95196900	3.73411700	-1.83921800
H	3.30098700	4.43487000	-1.83735200

Zero-point correction= 0.541368 (Hartree/Particle)
Thermal correction to Energy= 0.573893
Thermal correction to Enthalpy= 0.574837
Thermal correction to Gibbs Free Energy= 0.474713
Sum of electronic and zero-point Energies= -2255.110043
Sum of electronic and thermal Energies= -2255.077519
Sum of electronic and thermal Enthalpies= -2255.076574
Sum of electronic and thermal Free Energies= -2255.176699

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9643165

TS(P,S,S,S)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	2.13907100	-1.97582100	-0.10773300
C	2.82883000	-2.45408400	-1.24070500
C	3.83514900	-3.41410600	-1.06824900
C	4.14824200	-3.87435300	0.21530400
C	3.46981900	-3.39221900	1.33597400
C	2.46202700	-2.43900000	1.16429300
H	4.37879200	-3.80153800	-1.92219100
H	4.93348000	-4.61683300	0.33110400
H	3.71763300	-3.75161900	2.33021300
H	1.91601900	-2.04546600	2.01663800
O	2.45265600	-1.93300300	-2.43896400
C	3.10563100	-2.39637300	-3.62373600
H	2.64016200	-1.85165500	-4.44575300
H	2.95183200	-3.47290400	-3.76129400
H	4.17835900	-2.17301400	-3.59454000
C	-3.39311400	-1.19226200	0.53449700
C	-3.23803600	-0.39908200	1.83029400
C	-2.83932300	-2.46369300	0.79570700
C	-2.33778400	-2.43949100	2.22916000
C	-4.25253200	-1.03323500	2.83785600
C	-3.63951300	-2.44479500	3.10581700
C	-2.36658000	-0.22983300	-1.15217100
C	-0.98775900	-0.15152500	-0.87824500
C	-0.19522800	-1.29820700	-0.67639800
S	-0.83411600	-2.86395700	-0.68427700
S	-0.05522300	1.32601500	-0.54013600
C	1.41876900	0.36531400	-0.19945400
N	1.11149500	-0.98946700	-0.27540400
H	-2.62149900	-1.14287700	-1.68339000
C	-3.24149500	0.91784000	-1.47314000
H	-3.23027900	-3.37240800	0.34992600
H	-4.30380200	-1.10568800	-0.05212600
H	-4.29401700	-0.43683400	3.75722300
H	-5.26658600	-1.07856400	2.42656900

H	-3.37073500	-2.57139800	4.16135200
H	-4.31459800	-3.26428500	2.83678000
C	-3.18156200	2.16101900	-0.81370800
C	-4.04647200	3.19967000	-1.16556600
C	-4.99286800	3.02073500	-2.17940800
C	-5.07439900	1.78737700	-2.83475800
C	-4.21371300	0.74830900	-2.47964700
H	-2.47332800	2.32099900	-0.00722400
H	-3.98176200	4.14977500	-0.64166900
H	-5.66269800	3.83177900	-2.45237100
H	-5.80801600	1.63387200	-3.62191400
H	-4.28506900	-0.20761600	-2.99352900
C	-1.90777400	-0.96298800	2.37653900
H	-1.72220600	-0.67967700	3.41888100
H	-1.03518200	-0.69652400	1.77729200
H	-3.32200000	0.68637600	1.73745700
H	-1.61193600	-3.20877400	2.49949000
N	2.58687400	0.81217600	0.05929000
C	2.82582700	2.20007000	0.12508600
C	3.39960500	2.87111100	-0.96156100
C	3.72302900	4.23048200	-0.88832200
C	3.48232600	4.93113500	0.29325100
C	2.92120600	4.27848900	1.39882800
C	2.59305300	2.91980200	1.32502800
H	3.59260200	2.30492800	-1.86903700
H	4.16214300	4.72991700	-1.74768300
H	3.73103900	5.98641000	0.36923900
H	2.74464900	4.83613200	2.31181500
O	2.04921300	2.20217100	2.35478400
C	1.80303300	2.86872600	3.59185100
H	1.38356700	2.11193800	4.25630000
H	1.08221600	3.68597600	3.46569600
H	2.73231600	3.26029400	4.02347500

Zero-point correction= 0.541289 (Hartree/Particle)
Thermal correction to Energy= 0.573827
Thermal correction to Enthalpy= 0.574771
Thermal correction to Gibbs Free Energy= 0.474148
Sum of electronic and zero-point Energies= -2255.110551
Sum of electronic and thermal Energies= -2255.078013

Sum of electronic and thermal Enthalpies= -2255.077069
Sum of electronic and thermal Free Energies= -2255.177692

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9644569

TS(M,S,R,R)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.61756900	-2.36911000	-0.72962600
C	1.73289700	-3.26057100	0.35599100
C	2.38255800	-4.48696800	0.16103700
C	2.90446900	-4.80874800	-1.09664400
C	2.79037000	-3.92289500	-2.16928400
C	2.14466300	-2.69833600	-1.97534300
H	2.48446500	-5.19256700	0.97744700
H	3.40485900	-5.76434100	-1.22983400
H	3.19913400	-4.17626800	-3.14284200
H	2.04348300	-1.98635400	-2.78955700
O	1.18804600	-2.85265700	1.53345400
C	1.29546800	-3.71165400	2.67124700
H	0.80492700	-3.17954500	3.48705300
H	2.34528500	-3.89284100	2.92911200
H	0.78470000	-4.66527400	2.49424000
N	2.90881200	-0.03291800	0.21517000
C	3.55688700	1.12531300	0.69167800
C	3.80454100	1.28546700	2.06033500
C	4.51894600	2.38634400	2.54604700
C	5.00724100	3.33752600	1.65055500
C	4.78350800	3.19250200	0.27502800
C	4.06388400	2.09474600	-0.21132700
H	3.42896800	0.52590300	2.74107900
H	4.69283400	2.49133700	3.61353700
H	5.56801200	4.19647300	2.00975600
H	5.17343100	3.93826500	-0.40863100
O	3.80315500	1.87042000	-1.53453500
C	4.28368000	2.81284100	-2.49192400
H	3.96335700	2.43464800	-3.46378900
H	5.37820000	2.88012600	-2.46767300
H	3.84888300	3.80568900	-2.32349000

C	-3.18097400	-0.23806100	1.01583400
C	-4.70951100	-0.07845000	0.93910000
C	-2.94672800	-1.62252200	0.93892900
C	-4.30221800	-2.30444600	0.79999300
C	-5.24548000	-0.44814300	-0.47510800
C	-4.94715800	-1.97630800	-0.58025200
C	-2.15320600	0.82842900	-0.59311000
C	-0.81052000	0.41596100	-0.51804500
C	-0.40279400	-0.90472400	-0.79315200
S	-1.49355000	-2.13899900	-1.17479900
S	0.53905700	1.37437600	0.13360600
C	1.66003600	-0.01179900	-0.05209700
N	0.95868400	-1.10966800	-0.53954300
H	-2.71953200	0.25013400	-1.31614900
C	-2.60065800	2.23169600	-0.42887600
H	-2.10077100	-2.11599900	1.39976900
H	-2.60598400	0.38258300	1.69470600
H	-6.32256100	-0.24978300	-0.51688200
H	-4.78570300	0.13168700	-1.27821600
H	-5.86918900	-2.55641500	-0.70017700
H	-4.28365000	-2.22267400	-1.41174700
C	-2.22049000	3.03883800	0.66030100
C	-2.66490400	4.35856600	0.76213100
C	-3.49838500	4.90152300	-0.22145400
C	-3.89054100	4.10974200	-1.30536400
C	-3.45189700	2.78793800	-1.40279700
H	-1.59246100	2.63281800	1.44809200
H	-2.36206400	4.96159000	1.61418100
H	-3.84189000	5.92941300	-0.14118800
H	-4.53916800	4.51923500	-2.07542300
H	-3.75961100	2.18265300	-2.25184400
C	-5.13435800	-1.35803500	1.72079900
H	-6.21473700	-1.55872200	1.68889400
H	-4.79588800	-1.35948600	2.76256000
H	-5.08033300	0.87627900	1.31948600
H	-4.29856800	-3.36857600	1.04826100

Zero-point correction= 0.540839 (Hartree/Particle)
Thermal correction to Energy= 0.573544
Thermal correction to Enthalpy= 0.574488

Thermal correction to Gibbs Free Energy= 0.472371
Sum of electronic and zero-point Energies= -2255.100302
Sum of electronic and thermal Energies= -2255.067596
Sum of electronic and thermal Enthalpies= -2255.066652
Sum of electronic and thermal Free Energies= -2255.168769

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9523948

TS(P,S,R,R)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.79754700	-2.35564600	0.02598500
C	2.25094600	-2.99589500	-1.14550800
C	3.01124100	-4.16739600	-1.02909900
C	3.31532200	-4.67863100	0.23723900
C	2.87080600	-4.03872400	1.39560200
C	2.10923900	-2.87244300	1.28008700
H	3.37014400	-4.68096400	-1.91353300
H	3.90796200	-5.58682600	0.30969500
H	3.11090700	-4.43915100	2.37595200
H	1.74981600	-2.35147800	2.16280200
O	1.90502000	-2.41056900	-2.32306600
C	2.32523400	-3.02424100	-3.54433100
H	1.93249400	-2.39015800	-4.33981600
H	1.91006700	-4.03420000	-3.63981200
H	3.41873300	-3.06208400	-3.60993000
N	2.91322600	0.24597400	0.02933800
C	3.47830100	1.53775700	0.00737100
C	4.00387700	2.06460700	-1.17847600
C	4.64646500	3.30752300	-1.19931500
C	4.77734400	4.03300800	-0.01547400
C	4.26823600	3.52204000	1.18579500
C	3.62130700	2.28094400	1.20675000
H	3.90467400	1.47803800	-2.08813200
H	5.04197800	3.69722900	-2.13335700
H	5.27712900	4.99812800	-0.01250600
H	4.38052200	4.09717200	2.09816400
O	3.09627900	1.70504800	2.33091700
C	3.21821900	2.40050900	3.57068100

H	2.74318900	1.76046800	4.31563800
H	2.70191000	3.36769000	3.53535600
H	4.27087800	2.55409900	3.83781900
C	-3.12651200	-0.05989500	1.29303200
C	-4.66460700	-0.02628700	1.24109200
C	-2.79683500	-1.36766200	1.69228000
C	-4.10310600	-2.13327700	1.86143100
C	-5.20841300	-0.89614500	0.07015400
C	-4.80200200	-2.34472000	0.48453500
C	-2.23688200	0.43006700	-0.63756000
C	-0.86257200	0.16005100	-0.50604300
C	-0.35624200	-1.14195400	-0.32473000
S	-1.35435000	-2.49971500	-0.18748700
S	0.42453400	1.37439200	-0.33009400
C	1.65254200	0.08909800	-0.09964400
N	1.02419200	-1.15302700	-0.08644000
H	-2.77637300	-0.40255100	-1.07721900
C	-2.78634600	1.76958000	-0.95568300
H	-1.90747600	-1.61977600	2.25537000
H	-2.57983100	0.79124300	1.68504900
H	-6.29778900	-0.78891800	0.01563400
H	-4.81300300	-0.60508300	-0.90502200
H	-5.68179800	-2.98489000	0.61554600
H	-4.14143400	-2.82391100	-0.24109300
C	-2.44635200	2.93031400	-0.23555100
C	-2.98405300	4.17103200	-0.58363100
C	-3.87323700	4.27936500	-1.65803600
C	-4.22613400	3.13375000	-2.37828500
C	-3.69397500	1.89220300	-2.02513500
H	-1.77498700	2.86679400	0.61597800
H	-2.71032700	5.05340600	-0.01103800
H	-4.28971400	5.24613100	-1.92808800
H	-4.91678000	3.20485300	-3.21453100
H	-3.97112500	1.00874600	-2.59501800
C	-4.97757700	-0.97554500	2.43655400
H	-6.04127100	-1.23733300	2.52834200
H	-4.61409200	-0.59434100	3.39700200
H	-5.09270400	0.97791600	1.28409100
H	-4.01764600	-3.04186700	2.46233300

Zero-point correction= 0.541026 (Hartree/Particle)
Thermal correction to Energy= 0.573657
Thermal correction to Enthalpy= 0.574601
Thermal correction to Gibbs Free Energy= 0.472791
Sum of electronic and zero-point Energies= -2255.099964
Sum of electronic and thermal Energies= -2255.067333
Sum of electronic and thermal Enthalpies= -2255.066389
Sum of electronic and thermal Free Energies= -2255.168200

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9515176

TS(M,S,S,S)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.93354800	-1.91089900	-0.96991200
C	2.34001700	-2.83900600	0.00928600
C	3.29770900	-3.80604600	-0.32769400
C	3.83447800	-3.83989900	-1.61872600
C	3.43282800	-2.91690800	-2.58600400
C	2.48208800	-1.94968400	-2.24993300
H	3.62689200	-4.53209100	0.40653000
H	4.57468100	-4.59773700	-1.86172700
H	3.85434800	-2.94333100	-3.58637800
H	2.15550100	-1.21448700	-2.98004800
O	1.75729000	-2.72561400	1.23148500
C	2.15583900	-3.62543400	2.26779000
H	1.57217600	-3.33946900	3.14339100
H	3.22469800	-3.52204000	2.48779000
H	1.92935300	-4.66370600	1.99836900
C	-3.67950400	-1.11844300	0.08041200
C	-3.70905700	-1.01683000	1.61337600
C	-3.26253000	-2.43658200	-0.20119500
C	-3.01891700	-3.12496000	1.13693900
C	-2.27569000	-1.06033300	2.20998700
C	-4.18226700	-2.46515100	1.94547700
C	-1.79629400	-2.50825300	1.87517100
C	-2.47554800	0.33988200	-1.02328700
C	-1.09909600	0.19784200	-0.75333100
C	-0.38018200	-0.97514300	-1.05276600

S	-1.11610000	-2.37152500	-1.66604200
S	-0.06472700	1.37576000	0.09104300
C	1.34940200	0.28335600	-0.04111200
N	0.95893100	-0.90729600	-0.64726400
H	-2.77600900	-0.23792300	-1.89291800
C	-3.23027300	1.60136500	-0.84275800
H	-3.60194100	-2.98931900	-1.06814100
H	-4.49605000	-0.68393500	-0.48732900
H	-4.32684500	-0.19990600	1.99425900
H	-3.00315800	-4.21621700	1.08348700
H	-1.62007600	-0.29220400	1.79874200
H	-2.32771000	-0.89981800	3.29322600
H	-4.15502900	-2.70544000	3.01822700
H	-5.17588300	-2.69803300	1.54750500
H	-0.88821800	-2.53318500	1.27197500
H	-1.60198500	-3.08189800	2.78905900
C	-4.10723000	2.00929900	-1.86645400
C	-4.84561700	3.18871700	-1.75440300
C	-4.73364400	3.98042900	-0.60680200
C	-3.88194100	3.57768400	0.42717600
C	-3.14032500	2.39998600	0.31301000
H	-4.20142000	1.39887800	-2.76178800
H	-5.50821900	3.48797900	-2.56238200
H	-5.30898200	4.89789700	-0.51590600
H	-3.79780700	4.17785400	1.32947300
H	-2.50857900	2.09293800	1.14074000
N	2.54386400	0.52272000	0.34123700
C	2.87660800	1.77152500	0.90481700
C	2.99201900	1.91534200	2.29257200
C	3.39910800	3.12511800	2.86630300
C	3.71084500	4.20596500	2.04188700
C	3.61724300	4.08194600	0.64934100
C	3.20469000	2.87423800	0.07470300
H	2.75772100	1.05759100	2.91766400
H	3.47409800	3.21417600	3.94668400
H	4.03275800	5.15152000	2.47034700
H	3.86817500	4.92985300	0.02173600
O	3.09192600	2.66037800	-1.27081400
C	3.41402400	3.72873900	-2.15979800
H	3.25686700	3.33322400	-3.16433400

H	4.46080000	4.03656700	-2.04717400
H	2.75582500	4.59124000	-1.99871700

Zero-point correction= 0.541256 (Hartree/Particle)
Thermal correction to Energy= 0.573809
Thermal correction to Enthalpy= 0.574753
Thermal correction to Gibbs Free Energy= 0.474269
Sum of electronic and zero-point Energies= -2255.094986
Sum of electronic and thermal Energies= -2255.062433
Sum of electronic and thermal Enthalpies= -2255.061489
Sum of electronic and thermal Free Energies= -2255.161973

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9491486

TS(P,S,S,S)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	2.16583000	-1.90546400	-0.11212900
C	2.81257200	-2.37888800	-1.27254600
C	3.87437900	-3.28344200	-1.13799700
C	4.28604200	-3.69233700	0.13512700
C	3.65317400	-3.21140900	1.28247900
C	2.59001200	-2.31387900	1.14882700
H	4.38552100	-3.66647100	-2.01371600
H	5.11320500	-4.39206600	0.22140400
H	3.97904400	-3.52818900	2.26864100
H	2.08113900	-1.92069500	2.02377800
O	2.34363700	-1.90656600	-2.45816600
C	2.94831500	-2.36946800	-3.66851200
H	2.41267200	-1.86573000	-4.47374400
H	2.83559400	-3.45471700	-3.77353200
H	4.00982400	-2.09884000	-3.70663700
C	-3.45374700	-1.37705000	0.66476400
C	-3.46200300	-0.66375000	2.02514500
C	-2.87959100	-2.64303900	0.90625000
C	-2.53001500	-2.69962100	2.39051500
C	-2.02064500	-0.31333700	2.48964300
C	-3.74751800	-1.89144200	2.94327300
C	-1.37703800	-1.71446300	2.73495000

C	-2.45223600	-0.37736900	-1.02812400
C	-1.06976200	-0.24374400	-0.79235500
C	-0.22252800	-1.34974900	-0.58943200
S	-0.78895500	-2.94453700	-0.55526700
S	-0.18526800	1.28415300	-0.56068000
C	1.33366200	0.39579300	-0.22542000
N	1.08221200	-0.97405100	-0.24385100
H	-2.68588900	-1.29882800	-1.55376600
C	-3.35839000	0.74997900	-1.34358600
H	-3.17339100	-3.53290200	0.36329300
H	-4.32564700	-1.29485000	0.02398500
H	-4.16567800	0.16988600	2.08841100
H	-2.38275200	-3.71045400	2.77819400
H	-1.47223900	0.28449900	1.76123800
H	-2.06921500	0.26777600	3.41791100
H	-3.66953200	-1.66909500	4.01736700
H	-4.71298100	-2.36805900	2.74195500
H	-0.49053800	-1.89424100	2.12505800
H	-1.09084200	-1.84341200	3.78498400
C	-4.27959900	0.59382400	-2.39735600
C	-5.15874100	1.62154600	-2.74343200
C	-5.14630600	2.82504200	-2.03092800
C	-4.25204300	2.98658000	-0.96733000
C	-3.36906900	1.96059000	-0.62476700
H	-4.29658600	-0.33941600	-2.95573000
H	-5.85270200	1.48161000	-3.56820000
H	-5.83081500	3.62617400	-2.29670100
H	-4.24433000	3.91213900	-0.39749800
H	-2.70412800	2.09819500	0.22235700
N	2.48952100	0.89710700	-0.01926400
C	2.67382700	2.29477000	-0.00608700
C	3.18144500	2.95336900	-1.13236800
C	3.45299400	4.32594500	-1.11046000
C	3.22683400	5.05260800	0.05820600
C	2.73126300	4.41328600	1.20235800
C	2.45517100	3.04125800	1.18010000
H	3.36474200	2.36751200	-2.02933200
H	3.84127000	4.81550300	-1.99947000
H	3.43614600	6.11850800	0.09393100
H	2.56513900	4.99157600	2.10450600

O	1.97723000	2.33396600	2.24873200
C	1.74664700	3.02683500	3.47416100
H	1.37843400	2.27470900	4.17333900
H	0.99136700	3.81256400	3.34974400
H	2.67404100	3.46505700	3.86284100

Zero-point correction= 0.541206 (Hartree/Particle)
Thermal correction to Energy= 0.573790
Thermal correction to Enthalpy= 0.574734
Thermal correction to Gibbs Free Energy= 0.473690
Sum of electronic and zero-point Energies= -2255.095991
Sum of electronic and thermal Energies= -2255.063408
Sum of electronic and thermal Enthalpies= -2255.062463
Sum of electronic and thermal Free Energies= -2255.163508

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2254.9505211

TS-rot-4b-S

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

N	2.57044900	-0.04147300	-1.27292800
C	3.16684600	-1.30660100	-1.45088300
C	3.12720100	-1.90572300	-2.71593300
C	3.75525400	-3.13132200	-2.95689600
C	4.45530900	-3.75951800	-1.92633100
C	4.53232600	-3.16534200	-0.66082000
C	3.89817500	-1.94147600	-0.41543700
H	2.58784600	-1.39402600	-3.50859400
H	3.69888900	-3.58394200	-3.94295600
H	4.95278900	-4.71039000	-2.09766900
H	5.08934400	-3.66040000	0.12672700
O	3.94142000	-1.27736800	0.77863400
C	4.63891600	-1.87688100	1.87034900
H	4.52727100	-1.18493300	2.70611000
H	5.70339400	-2.00333200	1.63858300
H	4.19916400	-2.84605200	2.13448800
C	1.76532200	2.45904400	0.21163500
C	1.24399900	3.72821100	0.58103400
C	2.09423300	4.73464200	1.06012800

C	3.46489400	4.52123200	1.20015400
C	3.98731200	3.27578500	0.86565800
C	3.14709400	2.27064500	0.38361200
H	1.67637900	5.69743300	1.32815600
H	4.10246600	5.32006500	1.56855800
H	5.04824400	3.06810200	0.97364900
H	3.58679200	1.31805000	0.13310400
O	-0.09879900	3.92219500	0.46661800
C	-0.67607300	5.16978900	0.84735300
H	-1.74579100	5.05844900	0.66561800
H	-0.28241000	5.99019400	0.23630400
H	-0.50230900	5.37747000	1.90961300
C	-2.97192400	-0.49028500	-0.69464800
C	-4.51592600	-0.58558200	-0.54046800
C	-2.78689000	0.86315900	-1.45886800
C	-4.23835300	1.36629500	-1.65696700
C	-5.11671400	-0.89326300	-1.93373600
C	-4.92210300	0.89370200	-0.35571200
C	-4.90926000	0.44918000	-2.71207500
C	-2.19247300	-0.53561100	0.65528400
C	-0.77156900	-0.07834300	0.42507900
C	-0.45797100	1.17580500	0.02702300
S	-1.80112300	2.17980200	-0.56410900
S	0.59024000	-1.19761000	0.24734000
C	1.53365100	0.11999500	-0.55289500
N	0.93551500	1.37629100	-0.29219900
H	-2.64294500	0.22696000	1.30254300
C	-2.29600400	-1.86543100	1.39585100
H	-2.27685300	0.71488600	-2.41417900
H	-2.59789900	-1.30456100	-1.32469700
H	-4.83394800	-1.27975600	0.24268900
H	-4.31081000	2.43309200	-1.89150500
H	-4.62422900	-1.74442700	-2.41781400
H	-6.18183500	-1.13715100	-1.84631300
H	-6.00858200	1.04101500	-0.36777600
H	-4.51588800	1.36213000	0.54646700
H	-4.29018000	0.32998700	-3.60848800
H	-5.86711900	0.87650700	-3.02988600
C	-2.52969000	-1.86026800	2.78012700
C	-2.61560700	-3.05313900	3.50380800

C	-2.47065000	-4.28032800	2.84977500
C	-2.23942000	-4.30089900	1.47102700
C	-2.15294900	-3.10475000	0.75167400
H	-2.64525000	-0.90990200	3.29721800
H	-2.79861200	-3.02230400	4.57496500
H	-2.53929100	-5.21071200	3.40757600
H	-2.12634500	-5.24882700	0.95091300
H	-1.97259100	-3.14737500	-0.31863500

Zero-point correction= 0.545025 (Hartree/Particle)
Thermal correction to Energy= 0.576078
Thermal correction to Enthalpy= 0.577023
Thermal correction to Gibbs Free Energy= 0.480960
Sum of electronic and zero-point Energies= -2255.131046
Sum of electronic and thermal Energies= -2255.099992
Sum of electronic and thermal Enthalpies= -2255.099048
Sum of electronic and thermal Free Energies= -2255.195110

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2255.0133823

TS-rot-4b-N

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

N	-2.29458700	-0.24036700	1.12019000
C	-2.74676700	-1.53369800	1.41009900
C	-2.84197600	-1.89105700	2.76451600
C	-3.30917900	-3.14579200	3.15925000
C	-3.72932900	-4.05758400	2.18904700
C	-3.68282200	-3.71336100	0.83374600
C	-3.19855700	-2.46118200	0.43379500
H	-2.52853200	-1.15884000	3.50376700
H	-3.35280300	-3.40103900	4.21434400
H	-4.10341700	-5.03659700	2.47642600
H	-4.02450600	-4.42703100	0.09249400
O	-3.14892100	-2.04437900	-0.86590000
C	-3.60037800	-2.92872200	-1.89109000
H	-3.46816000	-2.38444100	-2.82696600
H	-4.65977100	-3.17904900	-1.75766500
H	-3.00225100	-3.84747900	-1.91307900

C	-1.74519200	2.48108600	-0.49898800
C	-3.17096100	2.53669400	-0.53587900
C	-3.81207500	3.70994800	-0.95933800
C	-3.09632800	4.81911400	-1.41262600
C	-1.70897700	4.74483700	-1.46910200
C	-1.06022300	3.58998100	-1.02788200
H	-4.89468800	3.74819900	-0.95607100
H	-3.62692700	5.70946600	-1.73816800
H	-1.11758200	5.56904900	-1.85752700
H	0.01663100	3.56160000	-1.12101300
O	-3.87081900	1.42147300	-0.19898700
C	-5.29504600	1.44969900	-0.21869200
H	-5.60746500	0.45420700	0.09991700
H	-5.67649200	1.64841700	-1.22787800
H	-5.68963400	2.19732600	0.48012400
C	3.10278600	0.12508900	0.74127400
C	4.65281700	0.24841300	0.69553300
C	2.67927800	1.45881100	1.44802300
C	4.02674400	2.16860400	1.72229200
C	5.19173000	0.06386700	2.13497600
C	4.85916800	1.76506700	0.48627200
C	4.74009100	1.38003800	2.85107300
C	2.44618600	-0.09006600	-0.66158600
C	0.95897000	0.15848700	-0.56549300
C	0.45256400	1.35252200	-0.19136200
S	1.56828700	2.58173500	0.44121400
S	-0.29004900	-1.10491500	-0.58973100
C	-1.40698100	0.05685500	0.26891700
N	-0.96747600	1.38399300	0.00558500
H	2.83697400	0.70205600	-1.31310400
C	2.81403800	-1.42121800	-1.30765500
H	2.12565200	1.26543000	2.36987600
H	2.80356700	-0.71418900	1.37814800
H	5.11897700	-0.41281200	-0.04014600
H	3.93192200	3.23975700	1.92567700
H	4.79324000	-0.83770200	2.61402600
H	6.28415200	-0.02489400	2.12613600
H	5.91035400	2.06658300	0.56477400
H	4.45505300	2.14730600	-0.45676000
H	4.08022900	1.19512300	3.70631400

H	5.60138200	1.94854400	3.21968300
C	3.26762400	-1.43965600	-2.63552000
C	3.60723200	-2.64014000	-3.26694800
C	3.49977800	-3.84972800	-2.57458000
C	3.05014700	-3.84632600	-1.25043800
C	2.71087200	-2.64353500	-0.62377500
H	3.35554500	-0.50313400	-3.18234700
H	3.95716300	-2.62799500	-4.29612900
H	3.76490800	-4.78521100	-3.06046200
H	2.96268900	-4.78069800	-0.70163200
H	2.36293800	-2.66548100	0.40504300

Zero-point correction= 0.544876 (Hartree/Particle)
Thermal correction to Energy= 0.575973
Thermal correction to Enthalpy= 0.576917
Thermal correction to Gibbs Free Energy= 0.480965
Sum of electronic and zero-point Energies= -2255.125168
Sum of electronic and thermal Energies= -2255.094072
Sum of electronic and thermal Enthalpies= -2255.093128
Sum of electronic and thermal Free Energies= -2255.189080

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF= -2255.0059644

PRODUCTS

(M,S,R,R)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

N	-2.92986000	0.27044200	0.17999600
C	-3.70670700	-0.85995500	0.49311500
C	-4.19044500	-1.04511200	1.79483900
C	-5.02764600	-2.11897700	2.11812700
C	-5.40327500	-3.02098200	1.12310800
C	-4.94791200	-2.84987900	-0.19102400
C	-4.10813900	-1.77774200	-0.51397900
H	-3.89673800	-0.32534700	2.55466500
H	-5.38179000	-2.24219300	3.13817100
H	-6.05455000	-3.85971400	1.35505500
H	-5.25470100	-3.55568500	-0.95509400

O	-3.63171400	-1.52828000	-1.77210300
C	-4.00117900	-2.41315800	-2.82752000
H	-3.51509200	-2.02347300	-3.72321700
H	-5.08810800	-2.42273400	-2.97594700
H	-3.64701200	-3.43298700	-2.63326500
C	-1.35547700	2.55672700	-0.49270900
C	-1.40006500	3.39438500	0.64207100
C	-1.90156900	4.69599600	0.50666800
C	-2.35122300	5.14535400	-0.73991900
C	-2.30833200	4.31528600	-1.86112300
C	-1.80887300	3.01644700	-1.72705000
H	-1.94475700	5.36199400	1.36084300
H	-2.73752900	6.15762600	-0.82577500
H	-2.66004500	4.66852000	-2.82578500
H	-1.76944100	2.34343800	-2.57900700
O	-0.93525300	2.86146500	1.80304700
C	-0.96664000	3.66403500	2.98610800
H	-0.55572300	3.03534300	3.77670800
H	-1.99394200	3.94976000	3.23972500
H	-0.34744200	4.56093900	2.86932800
C	3.24742600	-0.12013700	0.30237300
C	4.70356900	-0.35450600	-0.19223000
C	3.10052700	1.43962900	0.17228900
C	4.47516600	1.89095300	-0.37825900
C	5.67639300	0.18402400	0.88418800
C	4.85324500	0.71215200	-1.30004300
C	5.50554500	1.73514600	0.76926900
C	2.19020800	-0.98347600	-0.46268700
C	0.80480600	-0.41443800	-0.26669300
C	0.50996000	0.88195200	-0.49293200
S	1.74189400	2.05437000	-0.95206800
S	-0.65888900	-1.31877300	0.16342500
C	-1.66675600	0.16014700	-0.01339100
N	-0.84676100	1.22327300	-0.36687500
H	2.41920200	-0.89268500	-1.53454800
C	2.30354000	-2.46025200	-0.10300200
H	2.88490900	1.89175700	1.14321500
H	3.15807500	-0.37696100	1.36336200
H	4.89889800	-1.38998500	-0.48463100
H	4.46628900	2.88786800	-0.82990500

H	5.43818900	-0.19613300	1.88411100
H	6.70520400	-0.11719100	0.65570600
H	5.87632300	0.78528800	-1.68725700
H	4.16710900	0.58118000	-2.14286800
H	5.15935300	2.19631500	1.70131000
H	6.44920600	2.22031800	0.49549600
C	2.59502300	-3.40579500	-1.09682600
C	2.71032800	-4.76524200	-0.78770700
C	2.53336000	-5.20157600	0.52811100
C	2.23951500	-4.26927000	1.52888300
C	2.12651400	-2.91223000	1.21519700
H	2.73194900	-3.07546700	-2.12438600
H	2.93767900	-5.47966700	-1.57493700
H	2.62164700	-6.25701500	0.77245900
H	2.09670400	-4.59762400	2.55534900
H	1.89481000	-2.20356500	2.00651600

Zero-point correction= 0.545462 (Hartree/Particle)
Thermal correction to Energy= 0.577605
Thermal correction to Enthalpy= 0.578549
Thermal correction to Gibbs Free Energy= 0.478388
Sum of electronic and zero-point Energies= -2255.164151
Sum of electronic and thermal Energies= -2255.132008
Sum of electronic and thermal Enthalpies= -2255.131064
Sum of electronic and thermal Free Energies= -2255.231226

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0349223

(P,S,R,R)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

N	2.95315600	0.05954500	0.01463600
C	3.66639900	-1.14875900	0.11680900
C	4.32642200	-1.48066800	1.30722100
C	5.10897200	-2.63610600	1.41149600
C	5.24982500	-3.47297000	0.30487100
C	4.61315800	-3.15674900	-0.90279700
C	3.82754200	-2.00307000	-1.00603100
H	4.21476500	-0.81044100	2.15565800

H	5.60343200	-2.87278200	2.34989100
H	5.85622400	-4.37289600	0.36657700
H	4.73759800	-3.81364200	-1.75658900
O	3.18337000	-1.61275800	-2.14869100
C	3.30055400	-2.43245000	-3.30956400
H	2.71600000	-1.93294300	-4.08367800
H	2.89142900	-3.43455900	-3.13096000
H	4.34485000	-2.51376400	-3.63555200
C	1.50884900	2.50920000	-0.22896400
C	1.73590300	3.31004600	0.91023100
C	2.32806200	4.57062300	0.74999900
C	2.69400800	5.01209400	-0.52580300
C	2.47584900	4.21547400	-1.65158000
C	1.88043600	2.96117600	-1.49329400
H	2.50956500	5.20756400	1.60805800
H	3.15433400	5.99093500	-0.63183100
H	2.76322000	4.56302600	-2.63936200
H	1.69885900	2.31748300	-2.34920000
O	1.34828900	2.78296200	2.10282800
C	1.56261300	3.54588900	3.29330300
H	1.18378900	2.92783900	4.10791100
H	1.00887900	4.49126100	3.26044300
H	2.62998500	3.74276400	3.44590700
C	-3.20451600	-0.10105900	-0.57769700
C	-4.70899200	-0.09527800	-0.18134200
C	-2.96026000	1.39970400	-0.97477800
C	-4.34016300	2.06527900	-0.75203700
C	-5.55281500	0.07254400	-1.46720300
C	-4.87284900	1.29443900	0.47432900
C	-5.28163100	1.55887200	-1.87494400
C	-2.27727800	-0.67795500	0.54372700
C	-0.84262500	-0.27182100	0.30380400
C	-0.47446900	1.00867400	0.09533500
S	-1.65707600	2.31040600	0.00857600
S	0.57564700	-1.33636400	0.30324400
C	1.67154700	0.06866800	0.05631700
N	0.90508100	1.21934600	-0.07512200
H	-2.58281500	-0.19918200	1.48513900
C	-2.46947400	-2.17944800	0.72117000
H	-2.63481600	1.48055700	-2.01464400

H	-3.04587800	-0.71559500	-1.47032400
H	-4.99795100	-0.95701600	0.42700400
H	-4.29846900	3.15586000	-0.67024400
H	-5.26459800	-0.64088900	-2.24764300
H	-6.61516300	-0.08910200	-1.25122000
H	-5.91647300	1.53578900	0.70816400
H	-4.26869100	1.43827900	1.37573300
H	-4.82742500	1.65177100	-2.86799900
H	-6.20748900	2.14499700	-1.88296000
C	-2.89024200	-2.69224500	1.95679500
C	-3.07635700	-4.06617200	2.14217900
C	-2.84245600	-4.95304600	1.08771300
C	-2.42084300	-4.45527300	-0.14980100
C	-2.23682000	-3.08167100	-0.33001800
H	-3.07287800	-2.00967500	2.78404800
H	-3.40321100	-4.44023800	3.10917000
H	-2.98551100	-6.02138800	1.22782200
H	-2.23321900	-5.13604100	-0.97634800
H	-1.90651400	-2.71414300	-1.29847200

Zero-point correction= 0.545301 (Hartree/Particle)
Thermal correction to Energy= 0.577478
Thermal correction to Enthalpy= 0.578422
Thermal correction to Gibbs Free Energy= 0.477761
Sum of electronic and zero-point Energies= -2255.164032
Sum of electronic and thermal Energies= -2255.131855
Sum of electronic and thermal Enthalpies= -2255.130911
Sum of electronic and thermal Free Energies= -2255.231572

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0345436

(M,S,S,S)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.41290400	-2.41342300	-0.69078700
C	1.43675900	-3.28945300	0.41523800
C	2.01790200	-4.55602700	0.26675200
C	2.56364700	-4.93415200	-0.96503900
C	2.54143700	-4.06604900	-2.05762400

C	1.96498300	-2.80093300	-1.90973900
H	2.04821600	-5.24977300	1.09912300
H	3.00964100	-5.92057100	-1.06188100
H	2.96862000	-4.36360800	-3.01051000
H	1.93971800	-2.09970200	-2.73917600
O	0.87373100	-2.82653800	1.56202600
C	0.88245700	-3.66819700	2.71779500
H	0.38967100	-3.09279800	3.50211500
H	1.90812800	-3.90436800	3.02378400
H	0.32476000	-4.59391100	2.53448300
C	-3.43725900	-0.03308000	-0.42883200
C	-3.75464800	-0.11476200	1.09574700
C	-3.24163500	-1.55087500	-0.80231300
C	-3.56157200	-2.29310700	0.51864900
C	-5.20648600	-0.63764600	1.23473100
C	-5.08120200	-2.13182300	0.78814800
C	-2.29534200	0.93589300	-0.90342200
C	-0.92067400	0.43107800	-0.53894300
C	-0.52948700	-0.83095700	-0.80732600
S	-1.59016500	-2.03982700	-1.52776500
S	0.44682100	1.37894100	0.08343700
C	1.54292800	-0.03801700	-0.05635100
N	0.82159000	-1.11583900	-0.55035700
H	-2.35023600	0.88398000	-2.00245100
C	-2.59211500	2.38549900	-0.53835200
H	-3.92421600	-1.85103000	-1.60240300
H	-4.32849200	0.32786400	-0.95579600
H	-5.53842800	-0.56481200	2.27689000
H	-5.91566500	-0.06785600	0.62371700
H	-5.39710800	-2.81529300	1.58444900
H	-5.68502600	-2.36355100	-0.09728500
C	-2.32308700	2.92947900	0.72875100
C	-2.63840900	4.26014600	1.02198300
C	-3.23683200	5.07353700	0.05553700
C	-3.51344800	4.54546800	-1.20901300
C	-3.18997100	3.21700100	-1.49920300
H	-1.86069800	2.31911400	1.49869100
H	-2.41508000	4.65827100	2.00862200
H	-3.48148100	6.10762600	0.28411700
H	-3.97421800	5.16703500	-1.97270700

H	-3.40140100	2.81985100	-2.48999800
C	-2.95419000	-1.34645400	1.57378000
H	-3.20760600	-1.63930800	2.60008300
H	-1.87002500	-1.23746600	1.49632800
H	-3.57965900	0.81758500	1.63447200
H	-3.21752400	-3.33052100	0.52449500
N	2.78214300	-0.10031800	0.26606400
C	3.45915100	1.04446500	0.72612600
C	3.73054000	1.20701000	2.09073100
C	4.47441400	2.29414300	2.56350400
C	4.96965200	3.23307100	1.65904300
C	4.72406700	3.08748700	0.28705000
C	3.97623700	2.00276900	-0.18533300
H	3.34782100	0.45816100	2.77949600
H	4.66497700	2.39855900	3.62833700
H	5.55246600	4.08175600	2.00760600
H	5.12072700	3.82233300	-0.40465700
O	3.69875600	1.77889500	-1.50615900
C	4.18775000	2.70827400	-2.47101600
H	3.85014700	2.33390900	-3.43864500
H	5.28373900	2.75432600	-2.45876200
H	3.77487400	3.71043400	-2.30180700

Zero-point correction= 0.545569 (Hartree/Particle)
Thermal correction to Energy= 0.577636
Thermal correction to Enthalpy= 0.578580
Thermal correction to Gibbs Free Energy= 0.478323
Sum of electronic and zero-point Energies= -2255.157302
Sum of electronic and thermal Energies= -2255.125235
Sum of electronic and thermal Enthalpies= -2255.124291
Sum of electronic and thermal Free Energies= -2255.224548

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0293027

(P,S,S,S)-x

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.91518600	-2.17852500	0.02183700
C	2.41485600	-2.81523300	-1.13393800

C	3.28028800	-3.90850900	-0.98925200
C	3.64488700	-4.34494800	0.28871700
C	3.15711700	-3.70806700	1.43155000
C	2.28967500	-2.62202400	1.28806300
H	3.67458100	-4.41808700	-1.86091000
H	4.31851900	-5.19266200	0.38290300
H	3.44472600	-4.05027900	2.42111800
H	1.89381400	-2.10528900	2.15758500
O	2.00331200	-2.30626400	-2.32620000
C	2.47280000	-2.91558500	-3.53197100
H	2.01674500	-2.34677700	-4.34283100
H	2.15558100	-3.96304600	-3.59297200
H	3.56444300	-2.85090700	-3.60535800
C	-3.32355500	-0.81649500	0.04746500
C	-3.50241200	-0.31086500	1.51104000
C	-2.81193800	-2.28885400	0.27241300
C	-2.83667800	-2.45259900	1.81165700
C	-4.77246500	-0.99136800	2.08188100
C	-4.32485500	-2.48082600	2.25082900
C	-2.45539600	0.04313100	-0.94277000
C	-0.98670100	0.00138400	-0.60056100
C	-0.33980700	-1.16695900	-0.41226000
S	-1.15995500	-2.72331500	-0.49267000
S	0.13475600	1.36452700	-0.42115700
C	1.50791300	0.24342300	-0.12243700
N	1.03030500	-1.06005800	-0.11490500
H	-2.54715000	-0.49880000	-1.89661600
C	-3.05035800	1.42405200	-1.19000600
H	-3.46839800	-3.01473900	-0.21614400
H	-4.30745800	-0.86906900	-0.43384800
H	-5.03779500	-0.54804000	3.04860600
H	-5.63899200	-0.87841200	1.42053200
H	-4.40363700	-2.80587900	3.29445800
H	-4.92117200	-3.17559400	1.64767100
C	-2.90060200	2.50032700	-0.29906000
C	-3.48706700	3.74168900	-0.56545500
C	-4.24179800	3.93207300	-1.72638800
C	-4.40215000	2.87018000	-2.62130400
C	-3.80912300	1.63328800	-2.35329100
H	-2.32006700	2.38172800	0.61065500

H	-3.35143200	4.55963000	0.13767800
H	-4.69622900	4.89763300	-1.93281500
H	-4.98237300	3.00384700	-3.53086500
H	-3.93320100	0.81700600	-3.06199700
C	-2.39804500	-1.05481100	2.29549400
H	-2.50061300	-0.93341600	3.38074700
H	-1.37943800	-0.78352800	2.00803500
H	-3.51842200	0.77579200	1.60630200
H	-2.25317400	-3.30656400	2.16482300
N	2.74129500	0.55109900	0.04498500
C	3.14631700	1.89833600	0.06623700
C	3.81245700	2.45331700	-1.03417000
C	4.29537300	3.76655000	-1.00999800
C	4.12388200	4.54099900	0.13704900
C	3.47510700	4.00554200	1.25781200
C	2.98902200	2.69329500	1.23244700
H	3.94691200	1.83130400	-1.91543900
H	4.80203900	4.17358300	-1.88101600
H	4.49436300	5.56213600	0.17452500
H	3.35556600	4.61732200	2.14520600
O	2.35667200	2.08881800	2.28501500
C	2.17671300	2.83291600	3.48806600
H	1.66457800	2.16008600	4.17760000
H	1.55749500	3.72205000	3.31649700
H	3.14045100	3.13287000	3.91783300

Zero-point correction= 0.545525 (Hartree/Particle)
Thermal correction to Energy= 0.577555
Thermal correction to Enthalpy= 0.578499
Thermal correction to Gibbs Free Energy= 0.478733
Sum of electronic and zero-point Energies= -2255.157258
Sum of electronic and thermal Energies= -2255.125229
Sum of electronic and thermal Enthalpies= -2255.124284
Sum of electronic and thermal Free Energies= -2255.224050

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0289276

(M,S,R,R)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	-1.37625400	2.53742300	-0.42687900
C	-1.50965300	3.33572800	0.72911200
C	-2.03920300	4.62731700	0.60600700
C	-2.43058400	5.10487300	-0.64972200
C	-2.30169900	4.31302600	-1.79181500
C	-1.77363200	3.02420600	-1.67005400
H	-2.14980800	5.26357200	1.47666500
H	-2.83991400	6.10883400	-0.72605600
H	-2.60920700	4.68792600	-2.76336500
H	-1.66746900	2.38038300	-2.53870600
O	-1.09924400	2.77596300	1.89799700
C	-1.24296900	3.52802900	3.10565400
H	-0.86753600	2.88109700	3.89920100
H	-2.29534700	3.76930900	3.29438000
H	-0.64924700	4.44872200	3.06953600
N	-2.92130100	0.19603900	0.09691300
C	-3.68464000	-0.95918700	0.34593000
C	-4.22085400	-1.19030800	1.61940400
C	-5.04930100	-2.28867600	1.87579300
C	-5.36269500	-3.16906800	0.84065300
C	-4.85271700	-2.95298300	-0.44652700
C	-4.02084800	-1.85684600	-0.70217100
H	-3.97558900	-0.48645000	2.41066700
H	-5.44532500	-2.44738300	2.87531000
H	-6.00691200	-4.02593400	1.02011000
H	-5.11104400	-3.64267900	-1.24254900
O	-3.49220300	-1.56464900	-1.92984600
C	-3.79188400	-2.42987900	-3.02309600
H	-3.27082300	-2.00866500	-3.88420600
H	-4.86989100	-2.45647700	-3.22482100
H	-3.42697900	-3.44730400	-2.83610200
C	3.24995300	-0.02579500	0.53377200
C	4.76450300	-0.20928900	0.23144900
C	3.07105900	1.53483700	0.40686900
C	4.48710700	2.03889300	0.03368500
C	5.08572100	0.05919000	-1.25889600
C	4.88078200	1.60245100	-1.39806200

C	2.25778600	-0.91407200	-0.27330400
C	0.85216700	-0.37560900	-0.12557600
C	0.53422600	0.91591700	-0.35013900
S	1.74328400	2.13783800	-0.74854500
S	-0.60991100	-1.33063500	0.18453200
C	-1.64705500	0.12244500	-0.02709100
N	-0.83800100	1.21442800	-0.31224600
H	2.51274800	-0.81756600	-1.33719000
C	2.39877300	-2.38731900	0.09119400
H	2.78912800	1.94438600	1.38002100
H	3.09009600	-0.26833900	1.59032400
H	6.12503600	-0.22079200	-1.46605900
H	4.46144200	-0.51333600	-1.95148800
H	5.81081400	2.10142900	-1.69304900
H	4.12173300	1.86123300	-2.14219000
C	2.16908900	-2.84564700	1.39914800
C	2.31208200	-4.19803400	1.72034600
C	2.68927300	-5.11942400	0.73746400
C	2.91922900	-4.67675500	-0.56800300
C	2.77301600	-3.32205900	-0.88485700
H	1.87175100	-2.14514600	2.17582800
H	2.12666900	-4.53164700	2.73829200
H	2.80056400	-6.17136700	0.98745900
H	3.21066600	-5.38280100	-1.34157400
H	2.95066000	-2.98808000	-1.90492300
C	5.33988800	1.06824000	0.88744600
H	6.41594500	1.19353700	0.71783600
H	5.14040900	1.13752800	1.96341600
H	5.15940200	-1.15892400	0.60383900
H	4.62673300	3.10617600	0.22931800

Zero-point correction= 0.545642 (Hartree/Particle)
Thermal correction to Energy= 0.577696
Thermal correction to Enthalpy= 0.578640
Thermal correction to Gibbs Free Energy= 0.478940
Sum of electronic and zero-point Energies= -2255.160527
Sum of electronic and thermal Energies= -2255.128473
Sum of electronic and thermal Enthalpies= -2255.127529
Sum of electronic and thermal Free Energies= -2255.227229

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0321409

(P,S,R,R)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.41367100	2.53186300	-0.27318500
C	1.58350700	3.32855300	0.87903200
C	2.14399900	4.60669700	0.74710000
C	2.53353500	5.07042700	-0.51376500
C	2.37131300	4.27864800	-1.65230400
C	1.80917700	3.00583600	-1.52208100
H	2.28179100	5.24087300	1.61538000
H	2.96792000	6.06317100	-0.59786500
H	2.67704500	4.64367400	-2.62818600
H	1.67199200	2.36479800	-2.38821100
O	1.17580200	2.77990900	2.05482700
C	1.33852100	3.53524200	3.25816900
H	0.95273800	2.89975300	4.05593200
H	0.76294400	4.46720500	3.21923100
H	2.39617800	3.75630900	3.44206900
N	2.91885300	0.13271500	0.08406700
C	3.65425000	-1.05225700	0.27434500
C	4.14996400	-1.38546700	1.54146200
C	4.95191300	-2.51537100	1.73814400
C	5.27680900	-3.32486400	0.65001400
C	4.80418900	-3.00749900	-0.63051300
C	3.99876100	-1.87969900	-0.82641800
H	3.89672000	-0.73576000	2.37538100
H	5.31875600	-2.75319200	2.73309500
H	5.90104600	-4.20464100	0.78318400
H	5.06926300	-3.64410800	-1.46735000
O	3.50097800	-1.49319800	-2.04128500
C	3.82607800	-2.27526100	-3.18853800
H	3.33421200	-1.78407200	-4.02955600
H	3.44798200	-3.30048000	-3.09128600
H	4.90937400	-2.29707700	-3.36034700
C	-3.19836600	-0.22209000	-0.81987800
C	-4.73749300	-0.29031200	-0.60816200
C	-2.98291200	1.28715000	-1.21743500

C	-4.40951000	1.88829400	-1.17022100
C	-5.17325600	0.47547300	0.66465700
C	-4.93568900	1.97231600	0.28263100
C	-2.30403900	-0.77795800	0.32756500
C	-0.87462800	-0.32366300	0.13240100
C	-0.53716600	0.96654600	-0.06969200
S	-1.74255100	2.24649500	-0.21328400
S	0.57667800	-1.33676700	0.24909200
C	1.63765800	0.10220300	0.05260500
N	0.84327400	1.22367300	-0.14650400
H	-2.64281700	-0.31877400	1.26597400
C	-2.45824000	-2.28632600	0.48528500
H	-2.60402900	1.33988700	-2.24115300
H	-2.95907100	-0.81207700	-1.71171100
H	-6.23410400	0.28331100	0.86266100
H	-4.62613500	0.17706000	1.56396100
H	-5.87264400	2.54038200	0.30349100
H	-4.23520700	2.47365100	0.95684800
C	-2.15618100	-3.17091700	-0.56348400
C	-2.30916600	-4.55080200	-0.40430200
C	-2.76858700	-5.07315200	0.80944200
C	-3.07100100	-4.20423000	1.86137200
C	-2.91529200	-2.82379800	1.69724200
H	-1.79403100	-2.78433500	-1.51308200
H	-2.06704300	-5.21742400	-1.22824600
H	-2.88722800	-6.14649000	0.93331900
H	-3.42687300	-4.59744400	2.81036900
H	-3.15070700	-2.15605900	2.52323900
C	-5.21694400	0.68274600	-1.71135900
H	-6.29911200	0.85881000	-1.69171900
H	-4.92629900	0.37678100	-2.72349900
H	-5.12816000	-1.31035600	-0.66464500
H	-4.49889000	2.82258900	-1.73225000

Zero-point correction= 0.545313 (Hartree/Particle)
Thermal correction to Energy= 0.577508
Thermal correction to Enthalpy= 0.578453
Thermal correction to Gibbs Free Energy= 0.477389
Sum of electronic and zero-point Energies= -2255.160469
Sum of electronic and thermal Energies= -2255.128274

Sum of electronic and thermal Enthalpies= -2255.127330
Sum of electronic and thermal Free Energies= -2255.228394

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0313833

(M,S,S,S)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	1.67204700	-2.19170600	-0.74432900
C	1.94683300	-3.07831600	0.31848400
C	2.74384200	-4.20517400	0.07390800
C	3.25183700	-4.43867500	-1.20850400
C	2.97882000	-3.56174800	-2.25935500
C	2.18970400	-2.43404400	-2.01557100
H	2.97091900	-4.90226900	0.87214100
H	3.86753200	-5.31811700	-1.37823500
H	3.37733100	-3.74538100	-3.25257400
H	1.97049700	-1.72622700	-2.81022600
O	1.40049400	-2.76729800	1.52280700
C	1.66775600	-3.62109400	2.63814300
H	1.14232000	-3.17259200	3.48182700
H	2.74179400	-3.66177900	2.85271900
H	1.28383700	-4.63250600	2.46109700
C	-3.50889800	-0.55606500	-0.45596400
C	-3.96005900	-0.66074700	1.02841600
C	-3.07536700	-2.04111200	-0.77169500
C	-3.37677900	-2.80186600	0.54707000
C	-2.78401200	-0.93898000	1.99777900
C	-4.64766100	-2.04728100	1.00316000
C	-2.38203100	-2.41117800	1.66135000
C	-2.51056600	0.55553900	-0.91367200
C	-1.08351300	0.24321400	-0.52999600
C	-0.50939200	-0.95011200	-0.78484900
S	-1.38037000	-2.31330200	-1.49022700
S	0.11709300	1.38479800	0.10661200
C	1.41737800	0.15033400	-0.02840700
N	0.86748800	-1.02856000	-0.51231200
H	-2.53653300	0.49378000	-2.01315400
C	-2.99606700	1.95898000	-0.56833600

H	-3.70808200	-2.44377100	-1.56806400
H	-4.41737700	-0.36114000	-1.04032300
H	-4.59641900	0.17444000	1.33261800
H	-3.47596500	-3.88059900	0.39438800
H	-1.94786500	-0.24619700	1.88202100
H	-3.13763500	-0.85147100	3.03231300
H	-4.99955400	-2.36999100	1.99056700
H	-5.48058900	-2.11176700	0.29258000
H	-1.33837200	-2.50610700	1.35142800
H	-2.52409500	-3.06843300	2.52732800
C	-3.53743200	2.76088200	-1.58568600
C	-4.01797800	4.04631400	-1.31818800
C	-3.96114400	4.55805400	-0.01884500
C	-3.42242400	3.77263900	1.00492400
C	-2.94769800	2.48620200	0.73299600
H	-3.57881400	2.37582000	-2.60253000
H	-4.42998500	4.64664800	-2.12547200
H	-4.32929200	5.55841200	0.19383300
H	-3.37057700	4.15956500	2.01957100
H	-2.53777300	1.89509700	1.54562900
N	2.65406300	0.28467300	0.28214500
C	3.14472900	1.52540100	0.72985000
C	3.40096900	1.73679200	2.09078900
C	3.96076100	2.93384800	2.55168900
C	4.28449000	3.93713300	1.63879600
C	4.05247500	3.74597900	0.27000800
C	3.48946600	2.55018100	-0.19066400
H	3.15320900	0.93894300	2.78630700
H	4.14261600	3.07349700	3.61401000
H	4.72224700	4.87232000	1.97824700
H	4.31473200	4.53322100	-0.42821800
O	3.24022000	2.27630600	-1.50768900
C	3.56152400	3.26783800	-2.48102900
H	3.28329500	2.83695200	-3.44402500
H	4.63486000	3.49456300	-2.47827600
H	2.98991800	4.18890400	-2.31309800

Zero-point correction= 0.545862 (Hartree/Particle)
Thermal correction to Energy= 0.577785
Thermal correction to Enthalpy= 0.578729

Thermal correction to Gibbs Free Energy= 0.479574
Sum of electronic and zero-point Energies= -2255.155086
Sum of electronic and thermal Energies= -2255.123163
Sum of electronic and thermal Enthalpies= -2255.122219
Sum of electronic and thermal Free Energies= -2255.221374

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.0307723

(P,S,S,S)-n

B3LYP/6-31+G* optimized with IEFPCM (dichloromethane; ε=8.93)

C	2.01603100	-2.04163800	0.05077300
C	2.56482000	-2.64241800	-1.10218900
C	3.51847900	-3.65897600	-0.95279700
C	3.92051800	-4.05580000	0.32680000
C	3.38430100	-3.45401500	1.46683900
C	2.42954400	-2.44443100	1.31881200
H	3.95209700	-4.13954500	-1.82220100
H	4.66253200	-4.84392600	0.42445200
H	3.70213400	-3.76401500	2.45776500
H	1.99674400	-1.95512000	2.18652600
O	2.11072900	-2.17770800	-2.29676600
C	2.63003400	-2.75196800	-3.49935900
H	2.12670700	-2.22908400	-4.31316300
H	2.40366700	-3.82309900	-3.55390900
H	3.71219100	-2.59470500	-3.57389400
C	-3.34323400	-1.16536700	-0.03211100
C	-3.76217800	-0.76269600	1.41002900
C	-2.69586800	-2.58572400	0.20029600
C	-2.88199800	-2.83273300	1.72118700
C	-2.55194400	-0.50285500	2.34213700
C	-4.24569000	-2.13514500	1.93955600
C	-1.94981900	-1.92877700	2.55579000
C	-2.52761000	-0.18289800	-0.93473100
C	-1.06834400	-0.12364100	-0.55117400
C	-0.32383600	-1.23084600	-0.35765100
S	-0.97940800	-2.86532300	-0.46007900
S	-0.05998900	1.33174000	-0.43258100
C	1.40739000	0.33528100	-0.14095900

N	1.03894300	-1.00290500	-0.09179300
H	-2.55009200	-0.65854300	-1.92783300
C	-3.22192600	1.16387300	-1.10531900
H	-3.26118700	-3.34010200	-0.35452000
H	-4.27551300	-1.33000900	-0.58754700
H	-4.50830200	0.03593900	1.42244500
H	-2.82729300	-3.89343600	1.98311400
H	-1.82232800	0.19602200	1.92764400
H	-2.90730400	-0.07830900	3.28885800
H	-4.54302300	-2.10925200	2.99497300
H	-5.06419600	-2.56794300	1.35182300
H	-0.90412600	-2.00200600	2.24468300
H	-1.99419300	-2.22550700	3.61002800
C	-3.88787200	1.43880000	-2.31034100
C	-4.56250300	2.64758700	-2.50728600
C	-4.57911500	3.61238000	-1.49625900
C	-3.91822900	3.35469100	-0.29125400
C	-3.24981000	2.14221400	-0.09731300
H	-3.87489800	0.69820200	-3.10739500
H	-5.06843300	2.83494100	-3.45110500
H	-5.09858800	4.55539000	-1.64571300
H	-3.92218800	4.09723400	0.50279900
H	-2.74922200	1.96441900	0.84917900
N	2.61409100	0.74633400	-0.00517800
C	2.91055800	2.12147200	-0.03760000
C	3.50042900	2.68933600	-1.17447400
C	3.87800400	4.03639300	-1.20650400
C	3.67677800	4.83347300	-0.07993700
C	3.10247700	4.28736700	1.07574300
C	2.72103000	2.94101000	1.10640200
H	3.66026000	2.04999200	-2.03896400
H	4.32709500	4.45208100	-2.10461600
H	3.96651800	5.88105200	-0.08573400
H	2.95811500	4.91786000	1.94618100
O	2.16492000	2.32590800	2.19513000
C	1.95548900	3.09564700	3.37711600
H	1.51253400	2.41015700	4.10119000
H	1.26597700	3.92848900	3.19183700
H	2.90277200	3.48297000	3.77221300

Zero-point correction= 0.545941 (Hartree/Particle)
Thermal correction to Energy= 0.577833
Thermal correction to Enthalpy= 0.578778
Thermal correction to Gibbs Free Energy= 0.479604
Sum of electronic and zero-point Energies= -2255.155153
Sum of electronic and thermal Energies= -2255.123261
Sum of electronic and thermal Enthalpies= -2255.122317
Sum of electronic and thermal Free Energies= -2255.221490

M06-2X/6-31+G(d)// B3LYP/6-31+G(d) (IEFPCM)
HF=-2255.030698