In Silico Characterization and Prediction of Thiourea-like Neutral Bidentate Halogen Bond Catalysts

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Supporting Information

Contents

Huber's Bidentate Halogen Bond Catalyst

Structure of Huber's bidentate halogen bond catalyst, which uses the steric factor as a preorganization strategy, was optimized by the authors at M06-2X/def2-TZVPP level. The chloride-binding complex was reported as well. **Figure S1** showed the overlaid structures of the catalyst (red), together with chloride complex (red), all taken from the supporting information of the origin reference.[1] As can be clearly seen from **Figure S1**, there are some large structural distortions, particularly around the two C-C bonds connecting the benzene spacer group to the iodobenzimidazolium moieties.

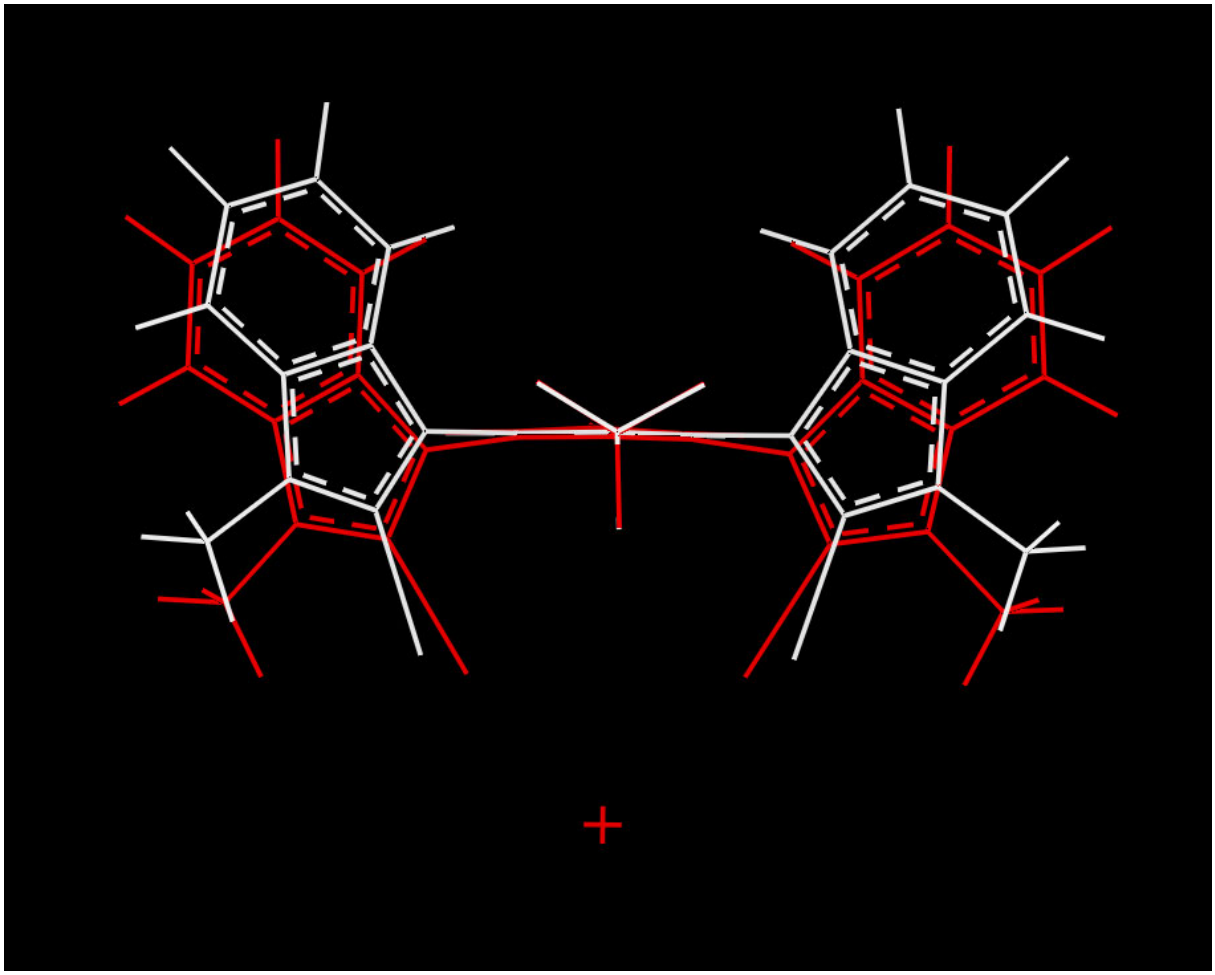

Figure S1. Overlay of Huber's bidentate halogen bond catalyst (white) and its structure when it binds to a chloride (red)

Bidentate Halogen Bond Donors

Structures of the three other bidentate halogen bond donors presented in **Table 1**, reported by Huber et al, Schubert et al, and Berryman et al, were taken from the original references and re-optimized at the same level as **2a**. For Schubert's donor, the N-methyl group on the carbazole spacer group caused the optimized ground state geometry to have a C_1 symmetry, resulting in the two C-I bonds' not intersecting at a focal point. This deviation from C_s symmetry is slight, and we have used the C_s symmetric structure of Schubert's donor in **Table 1** and **Figure 2** instead. It should be noted that there is a small negative frequency of 12.7 cm^{-1} after this treatment, which corresponds to torsional rotations around C-C single bonds. Energy calculations indicated that the C_s structure is only slightly higher than the ground state structure. The same treatment of the trifluoromethyl group of Huber's donor was applied.

Uncatalyzed Diels-Alder Reaction

We have performed a conformational analysis on the uncatalyzed and **2a**-catalyzed Diels-Alder reaction between vinylmethylketone **4** and cyclopentadiene **5**. Both results indicated that the endo-cis conformation of the C-C bond-formation transition state is lowest in energy.

Thiourea-catalyzed Diels-Alder Reaction

In the experimental report by Huber et al. of the Diels-Alder reaction between cyclopentadiene **5** and methyl vinyl ketone **4**,[2] background reaction was found to be substantial, yielding 24% product in 6 hours in dichloromethane at room temperature. Use of 20 mol% of thiourea catalyst **1** increased the yield to 38% over the same period of time. The increase of reaction rate was estimated to be by a factor of 2, which corresponds to a lowering of reaction free energy barrier by approximately 1.7 kJ/mol by catalyst **1**. The calculated barrier of **1**-catalyzed reaction is 103.8 kJ/mol, and that of the uncatalyzed reaction is 95.1 kJ/mol. The discrepancy of calculated results warrants a careful investigation to determine the source of it.

We believe it originates from the difficulty in calculating accurate free energy values when there are many low-frequency vibrations present in the thiourea catalyst, but not in the uncatalyzed reaction or the rigid designed XB catalysts. The trifluoromethyl groups are notorious for having very low rotational frequencies, as illustrated in **Figure S2** of an 8 cm^{-1} rotation.

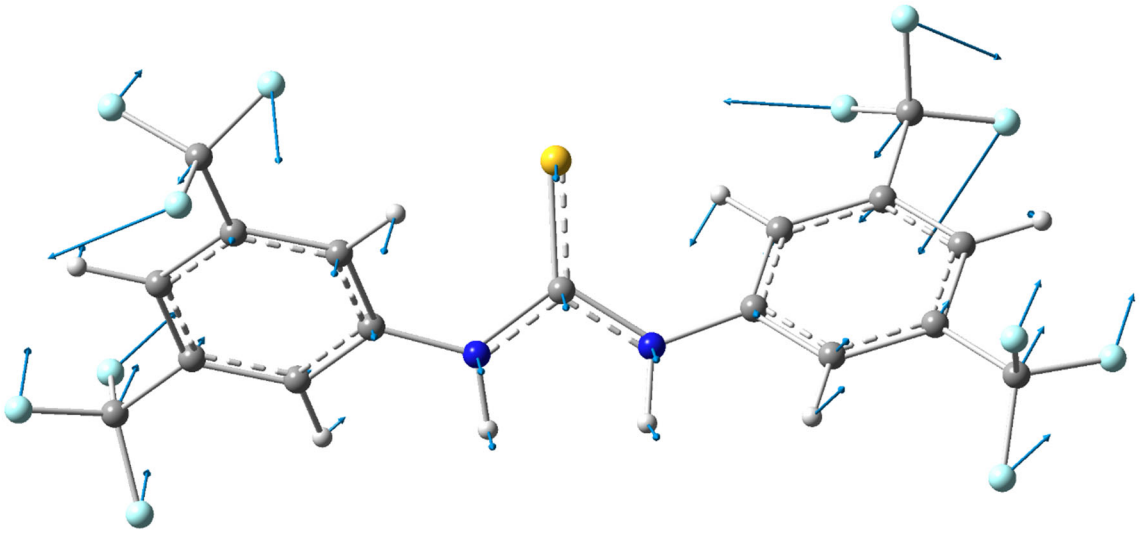

Figure S2. Displacement vectors of an extremely low frequency vibration of thiourea **1**.

The calculated activation enthalpies of thiourea **1**-catalyzed and XB **2a**-catalyzed DA reactions are very close to each other, at 6.3 and 6.6 kJ/mol, respectively. However, their activation free energies are 103.8 and 95.1 kJ/mol, respectively. This is a clear indication that quantitative comparison between thiourea, XB-catalyzed, and the uncatalyzed reactions require an accurate treatment of entropy and thus the low-frequency vibrations, which is extremely difficult to do. In addition, we do not think such a treatment will change the current conclusions. We based our judgement on two reasons. First, our designed XB catalyst **2b** was calculated to promote the reaction with both a lower enthalpy barrier of -1.7 kJ/mol and a lower free energy barrier of 91.2 kJ/mol, compared to thiourea **1**. Second, although our current calculations may overestimate the entropy cost of restricting the low-frequency vibrations of thiourea in transition state, it should be pointed out that the entropy cost of reaction should still be higher for thiourea than our designed XB catalysts, owning to their more flexible nature.

Calculation of Anion-binding Free Energies

All the anion-binding complexes and ammonium salts were optimized at the same level as stated in the computational methods part of the main text. However, in the cases of binding to halides, for the purpose of comparability, the halide anions were treated using Def2 series of basis sets as for iodine atoms of the halogen bond donors. For fluorine atoms of thiourea catalyst **1**, the Pople-type basis sets were used.

Optimized Structures

Bidentate Donors

Berryman-donor

C	-0.16633600	-1.36455900	-6.11199800
N	-0.20154500	-0.61123100	-7.23322800
C	-0.16941600	-0.77524600	-4.86166900
N	-0.19633300	-0.60463900	7.23437300
C	-0.20573700	0.63477500	-4.74768400
C	-0.24251000	1.38086100	-5.94396700
C	-0.24023300	0.73904200	-7.16227800
C	-0.19808700	1.29761100	-3.49822600
C	-0.16478200	1.92563700	-2.45314100
C	-0.10706700	2.62377400	-1.21900400
C	0.09928400	4.01274200	-1.20882900
C	0.19495900	4.68546500	-0.00209400
C	0.09995100	4.01409100	1.20547300
C	-0.23155500	1.89624700	-0.00041600
C	-0.10629800	2.62515400	1.21730000
C	-0.16312000	1.92824900	2.45218200
C	-0.19572600	1.30092400	3.49770500
C	-0.20270100	0.63913500	4.74773300
C	-0.23879000	1.38629500	5.94336200
C	-0.23544300	0.74555900	7.16224000

C	-0.16621500	-0.77079100	4.86293500
C	-0.16197300	-1.35897400	6.11379000
I	-0.10423600	-2.00867000	-3.17614900
I	-0.10248700	-2.00564600	3.17840400
H	-0.13269900	-2.43984000	-6.25823100
H	-0.27604600	2.46391200	-5.90886700
H	-0.26827800	1.27158300	-8.10616500
H	0.18935200	4.55746900	-2.14382200
H	0.19051200	4.55988700	2.13979400
H	-0.27255700	2.46930500	5.90730800
H	-0.26288900	1.27893100	8.10566900
H	-0.12791800	-2.43410900	6.26095200
N	-0.42848000	0.55050800	0.00049800
H	-0.74061500	0.10785900	0.86095400
H	-0.73982400	0.10664700	-0.85962500
F	0.39515800	6.01216700	-0.00287800
C	-0.14899100	-1.26580400	8.55307100
H	-0.70989100	-2.19968600	8.50066600
H	0.89319100	-1.46433200	8.81390600
H	-0.60127500	-0.60192000	9.28958100
C	-0.15567700	-1.27374600	-8.55129400
H	0.88614800	-1.47358600	-8.81257800
H	-0.71747500	-2.20703200	-8.49758400
H	-0.60774300	-0.61011600	-9.28816700

Zero-point correction= 0.331651 (Hartree/Particle)

Thermal correction to Energy= 0.358200

Thermal correction to Enthalpy= 0.359144

Thermal correction to Gibbs Free Energy= 0.270516

Sum of electronic and zero-point Energies= -1703.912787

Sum of electronic and thermal Energies= -1703.886238

Sum of electronic and thermal Enthalpies= -1703.885294

Sum of electronic and thermal Free Energies= -1703.973922

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -1704.62343336

Huber-donor

C	-0.49883100	0.43942000	0.00000000
C	-3.29480500	0.00731900	0.00000000
C	-1.22789300	0.34648900	1.19466100
C	-1.22789300	0.34648900	-1.19466100
C	-2.60451400	0.12873300	-1.20261000
C	-2.60451400	0.12873300	1.20261000
H	-3.12005100	0.06100200	-2.15685600
H	-3.12005100	0.06100200	2.15685600
C	-0.18094400	-0.50643100	3.27456900
N	0.41742500	-0.01260800	4.35949700
C	-0.18094400	-0.50643100	-3.27456900
N	0.41742500	-0.01260800	-4.35949700
I	-0.40073800	-2.50373200	2.83873900
I	-0.40073800	-2.50373200	-2.83873900
H	-4.36588400	-0.16541100	0.00000000
C	-0.19570500	1.70669400	3.04926100
C	0.42788000	1.38249300	4.25864800
C	-0.19570500	1.70669400	-3.04926100
C	0.42788000	1.38249300	-4.25864800
N	-0.57426200	0.49492000	2.46337700
N	-0.57426200	0.49492000	-2.46337700
C	0.92252300	2.37262800	5.11193100
C	0.76359200	3.68516500	4.68814400
H	1.13490500	4.49004100	5.31567100
C	0.13772200	4.00633800	3.46428500
H	0.04274800	5.04995500	3.17916100
C	-0.35818600	3.02409600	2.61828500

C	-0.35818600	3.02409600	-2.61828500
C	0.13772200	4.00633800	-3.46428500
H	0.04274800	5.04995500	-3.17916100
C	0.76359200	3.68516500	-4.68814400
H	1.13490500	4.49004100	-5.31567100
C	0.92252300	2.37262800	-5.11193100
H	1.40757600	2.13013200	6.05247400
H	-0.83852900	3.25381500	1.67124300
H	-0.83852900	3.25381500	-1.67124300
H	1.40757600	2.13013200	-6.05247400
C	1.00087300	0.68299600	0.00000000
F	1.59458100	0.14613500	1.07184100
F	1.26854800	1.99303400	0.00000000
F	1.59458100	0.14613500	-1.07184100
C	0.98179000	-0.80244700	-5.45629100
H	1.81857400	-1.40131300	-5.08792500
H	0.20738200	-1.44577200	-5.88103200
H	1.33875000	-0.11469600	-6.22216000
C	0.98179000	-0.80244700	5.45629100
H	0.20738200	-1.44577200	5.88103200
H	1.81857400	-1.40131300	5.08792500
H	1.33875000	-0.11469600	6.22216000

Zero-point correction= 0.366028 (Hartree/Particle)

Thermal correction to Energy= 0.392879

Thermal correction to Enthalpy= 0.393823

Thermal correction to Gibbs Free Energy= 0.306847

Sum of electronic and zero-point Energies= -1996.900704

Sum of electronic and thermal Energies= -1996.873852

Sum of electronic and thermal Enthalpies= -1996.872908

Sum of electronic and thermal Free Energies= -1996.959884

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -1997.74012550

Schubert-donor

I	-1.16666000	-0.60031800	2.63067600
I	-1.16666000	-0.60031800	-2.63067600
0	4.32854800	0.05678800	4.72542700
0	4.32854800	0.05678800	-4.72542700
H	3.58210800	0.32703800	-5.30942100
N	5.37506700	-0.10882900	0.00000000
N	1.81727500	0.71320500	5.36629100
N	0.74929700	0.71192100	6.11035100
N	-0.27315900	0.35475500	5.33036600
N	1.81727500	0.71320500	-5.36629100
N	0.74929700	0.71192100	-6.11035100
N	-0.27315900	0.35475500	-5.33036600
C	3.22973800	0.19479600	-0.72462500
C	4.57404500	-0.00541400	-1.12595200
C	4.57404500	-0.00541400	1.12595200
C	3.22973800	0.19479600	0.72462500
C	2.24330200	0.33630200	1.69282000
H	1.21575700	0.51804600	1.38827400
C	2.56585800	0.26711200	3.05453900
C	3.93118100	0.09567800	3.43398900
C	4.93269800	-0.05362000	2.47112500
H	5.95799500	-0.19514100	2.80154900
C	1.51999700	0.35262800	4.08146100
C	0.15186500	0.10861000	4.05855700
C	-1.60540300	0.27231200	5.86653200
C	-2.00201600	-0.92413900	6.47895600
C	-3.29587000	-0.97724900	6.99747200
H	-3.63190800	-1.89399500	7.48078900
C	-4.16793400	0.11691700	6.91167500

C	-3.72361600	1.28820300	6.29044300
H	-4.39235600	2.14513200	6.22126500
C	-2.43596800	1.39157800	5.75519100
C	-1.05916900	-2.09461800	6.55978100
H	-1.52172100	-2.92493300	7.10169000
H	-0.12896200	-1.81961100	7.07173100
H	-0.78407500	-2.45229500	5.55798200
C	-5.55835700	0.02431800	7.48526600
H	-6.12056900	-0.79593900	7.02261200
H	-6.11600400	0.95295400	7.32629100
H	-5.52589600	-0.17412300	8.56353700
C	-1.95222200	2.64629500	5.07901300
H	-1.78817100	2.48056900	4.00513000
H	-0.99961500	2.98437500	5.50490900
H	-2.68674200	3.44988600	5.18754600
C	6.80579600	-0.33088600	0.00000000
H	7.05151500	-1.39961100	0.00000000
C	4.93269800	-0.05362000	-2.47112500
H	5.95799500	-0.19514100	-2.80154900
C	3.93118100	0.09567800	-3.43398900
C	2.56585800	0.26711200	-3.05453900
C	2.24330200	0.33630200	-1.69282000
H	1.21575700	0.51804600	-1.38827400
C	1.51999700	0.35262800	-4.08146100
C	0.15186500	0.10861000	-4.05855700
C	-1.60540300	0.27231200	-5.86653200
C	-2.00201600	-0.92413900	-6.47895600
C	-3.29587000	-0.97724900	-6.99747200
H	-3.63190800	-1.89399500	-7.48078900
C	-4.16793400	0.11691700	-6.91167500
C	-3.72361600	1.28820300	-6.29044300

H	-4.39235600	2.14513200	-6.22126500
C	-2.43596800	1.39157800	-5.75519100
C	-1.05916900	-2.09461800	-6.55978100
H	-1.52172100	-2.92493300	-7.10169000
H	-0.78407500	-2.45229500	-5.55798200
H	-0.12896200	-1.81961100	-7.07173100
C	-5.55835700	0.02431800	-7.48526600
H	-6.12056900	-0.79593900	-7.02261200
H	-5.52589600	-0.17412300	-8.56353700
H	-6.11600400	0.95295400	-7.32629100
C	-1.95222200	2.64629500	-5.07901300
H	-1.78817100	2.48056900	-4.00513000
H	-2.68674200	3.44988600	-5.18754600
H	-0.99961500	2.98437500	-5.50490900
H	3.58210800	0.32703800	5.30942100
H	7.24621300	0.13654200	0.88536200
H	7.24621300	0.13654200	-0.88536200

Zero-point correction= 0.601352 (Hartree/Particle)

Thermal correction to Energy= 0.644391

Thermal correction to Enthalpy= 0.645335

Thermal correction to Gibbs Free Energy= 0.518409

Sum of electronic and zero-point Energies= -2477.158977

Sum of electronic and thermal Energies= -2477.115939

Sum of electronic and thermal Enthalpies= -2477.114994

Sum of electronic and thermal Free Energies= -2477.241920

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2478.39161952

Uncatalyzed Diels-Alder Reaction

4-cis

C	2.00452600	-0.10283200	0.00019100

H 2.92177800 -0.68580500 -0.00036000
C 0.79708400 -0.67351600 0.00038400
H 0.67273100 -1.75517400 0.00009500
C -0.44147400 0.16063900 0.00086800
H 2.09302500 0.98205200 0.00019700
0 -0.39189700 1.38353900 0.00035600
C -1.74799100 -0.58921500 0.00004900
H -2.58852100 0.10784800 -0.00020300
H -1.80321800 -1.24099200 0.88111000
H -1.80239400 -1.24062200 -0.88134000
Zero-point correction= 0.090161 (Hartree/Particle)
Thermal correction to Energy= 0.095999
Thermal correction to Enthalpy= 0.096943
Thermal correction to Gibbs Free Energy= 0.061194
Sum of electronic and zero-point Energies= -230.870892
Sum of electronic and thermal Energies= -230.865054
Sum of electronic and thermal Enthalpies= -230.864110
Sum of electronic and thermal Free Energies= -230.899858
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -231.032487222

Zero-point correction= 0.089203 (Hartree/Particle)
Thermal correction to Energy= 0.094811
Thermal correction to Enthalpy= 0.095755
Thermal correction to Gibbs Free Energy= 0.060755
Sum of electronic and zero-point Energies= -230.943285
Sum of electronic and thermal Energies= -230.937677
Sum of electronic and thermal Enthalpies= -230.936732
Sum of electronic and thermal Free Energies= -230.971732
4-trans
C 0.46539100 -1.87503100 0.00000000
H 1.16164100 -2.71039700 0.00000000

C 0.89655000 -0.60975000 0.00000000
H 1.95910400 -0.37138500 0.00000000
C 0.00017400 0.57627100 0.00000000
H -0.59395000 -2.12475700 0.00000000
0 0.48604500 1.70066800 0.00000000
C -1.49469100 0.36163100 0.00000000
H -1.99593700 1.33191900 0.00000000
H -1.80082600 -0.20977500 0.88395100
H -1.80082600 -0.20977500 -0.88395100
Zero-point correction= 0.090320 (Hartree/Particle)
Thermal correction to Energy= 0.096065
Thermal correction to Enthalpy= 0.097009
Thermal correction to Gibbs Free Energy= 0.061622
Sum of electronic and zero-point Energies= -230.871114
Sum of electronic and thermal Energies= -230.865369
Sum of electronic and thermal Enthalpies= -230.864425
Sum of electronic and thermal Free Energies= -230.899812
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -231.033864110

Zero-point correction= 0.089382 (Hartree/Particle)
Thermal correction to Energy= 0.094917
Thermal correction to Enthalpy= 0.095861
Thermal correction to Gibbs Free Energy= 0.061079
Sum of electronic and zero-point Energies= -230.944482
Sum of electronic and thermal Energies= -230.938947
Sum of electronic and thermal Enthalpies= -230.938003
Sum of electronic and thermal Free Energies= -230.972785
5
H 0.87770700 0.00000000 1.87828300
C 0.00000000 0.00000000 1.21423400
H -0.87770700 0.00000000 1.87828300

C 0.00000000 1.17715600 0.28264400
H 0.00000000 2.21058900 0.61459400
C 0.00000000 0.73532200 -0.99147200
H 0.00000000 1.34929000 -1.88767100
C -0.00000000 -0.73532200 -0.99147200
H -0.00000000 -1.34929000 -1.88767100
C -0.00000000 -1.17715600 0.28264400
H -0.00000000 -2.21058900 0.61459400
Zero-point correction= 0.093351 (Hartree/Particle)
Thermal correction to Energy= 0.097513
Thermal correction to Enthalpy= 0.098457
Thermal correction to Gibbs Free Energy= 0.067398
Sum of electronic and zero-point Energies= -193.766222
Sum of electronic and thermal Energies= -193.762060
Sum of electronic and thermal Enthalpies= -193.761116
Sum of electronic and thermal Free Energies= -193.792175
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -193.911150666

Zero-point correction= 0.092288 (Hartree/Particle)
Thermal correction to Energy= 0.096410
Thermal correction to Enthalpy= 0.097355
Thermal correction to Gibbs Free Energy= 0.066370
Sum of electronic and zero-point Energies= -193.818862
Sum of electronic and thermal Energies= -193.814740
Sum of electronic and thermal Enthalpies= -193.813796
Sum of electronic and thermal Free Energies= -193.844781
6-cis
C -8.79049600 0.04337400 1.99533700
0 -7.57297500 -0.02963600 2.05030300
C -9.65739000 -0.37469600 3.16050700
H -9.07600400 -0.97065400 3.86821500

H -10.53531800 -0.93518900 2.82012100
H -10.02367300 0.52486000 3.67363300
C -9.52479800 0.57699800 0.77990200
C -8.61642200 1.13922000 -0.33491800
H -7.56082900 1.07229400 -0.05548900
H -8.76053100 0.59333400 -1.27405100
H -10.16471200 -0.23660800 0.40945300
C -10.44346800 1.80170100 1.14070600
H -11.34670200 1.53239100 1.69381300
C -9.10795500 2.61062700 -0.47631200
H -8.79450000 3.10255400 -1.40009400
C -10.61817800 2.41566600 -0.25675100
H -11.07322700 1.72457700 -0.97803800
H -11.17480700 3.35919900 -0.23447500
C -9.52792600 2.82826100 1.78254900
H -9.46451000 3.02551300 2.84965200
C -8.72913200 3.30481600 0.81705500
H -7.87948700 3.97161600 0.93655800

Zero-point correction= 0.191414 (Hartree/Particle)
Thermal correction to Energy= 0.200127
Thermal correction to Enthalpy= 0.201071
Thermal correction to Gibbs Free Energy= 0.157657
Sum of electronic and zero-point Energies= -424.679714
Sum of electronic and thermal Energies= -424.671001
Sum of electronic and thermal Enthalpies= -424.670057
Sum of electronic and thermal Free Energies= -424.713472
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -424.988379154

Zero-point correction= 0.189430 (Hartree/Particle)
Thermal correction to Energy= 0.197885
Thermal correction to Enthalpy= 0.198829

Thermal correction to Gibbs Free Energy= 0.156396

Sum of electronic and zero-point Energies= -424.798949

Sum of electronic and thermal Energies= -424.790495

Sum of electronic and thermal Enthalpies= -424.789550

Sum of electronic and thermal Free Energies= -424.831983

6-trans

C	-8.61357000	0.43008100	2.22035300
0	-9.07727800	0.74247400	3.30689500
C	-7.33400000	-0.36564500	2.10835600
H	-7.13393700	-0.88942100	3.04654800
H	-6.50230200	0.32269000	1.90922400
H	-7.37652800	-1.07518400	1.27464600
C	-9.30179300	0.80090200	0.92447900
C	-8.39820900	1.50297300	-0.13701300
H	-7.40419300	1.75604200	0.24804900
H	-8.26519800	0.87131400	-1.02222000
H	-9.66780200	-0.14718900	0.50109900
C	-10.49055800	1.78885000	1.09126100
H	-11.35886700	1.35466500	1.59119300
C	-9.21949500	2.78306800	-0.47426800
H	-8.92977600	3.26269900	-1.41238800
C	-10.65442900	2.23822400	-0.37094700
H	-10.85137900	1.40655400	-1.06044600
H	-11.41533500	3.01677200	-0.49329600
C	-9.91882400	3.05362100	1.70621000
H	-10.02559100	3.33633100	2.74834300
C	-9.16520800	3.64771800	0.77067500
H	-8.52293900	4.51577700	0.89372700

Zero-point correction= 0.191319 (Hartree/Particle)

Thermal correction to Energy= 0.200132

Thermal correction to Enthalpy= 0.201076

Thermal correction to Gibbs Free Energy= 0.157146
Sum of electronic and zero-point Energies= -424.678328
Sum of electronic and thermal Energies= -424.669515
Sum of electronic and thermal Enthalpies= -424.668571
Sum of electronic and thermal Free Energies= -424.712501
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -424.986831833

Zero-point correction= 0.189394 (Hartree/Particle)
Thermal correction to Energy= 0.197899
Thermal correction to Enthalpy= 0.198844
Thermal correction to Gibbs Free Energy= 0.156267
Sum of electronic and zero-point Energies= -424.797438
Sum of electronic and thermal Energies= -424.788932
Sum of electronic and thermal Enthalpies= -424.787988
Sum of electronic and thermal Free Energies= -424.830565
DA-un-endo-cis

C	0.32899100	-1.65712000	-0.43223800
H	0.90391100	-2.23197900	-1.15583300
C	-0.62890500	-0.75339200	-0.88668100
H	-0.70047300	-0.46248100	-1.93196000
C	-1.63063200	-0.27218400	0.05210900
H	0.12244000	-2.16619700	0.50550600
0	-1.60263700	-0.59695200	1.24550400
C	-2.70867000	0.65107500	-0.47733900
H	-3.45138800	0.06843400	-1.03768900
H	-2.29034900	1.39654100	-1.16323300
H	-3.21261800	1.15059200	0.35424800
C	0.80293000	1.33944600	-0.54169600
H	0.37183300	2.10677300	-1.17786700
C	0.70450100	1.27971300	0.83385400
H	0.09696900	1.93098000	1.45429300

C 1.40006800 0.14114000 1.29271800
H 1.43457500 -0.19825600 2.32313900
C 1.90967500 -0.56107300 0.19062000
H 2.66569200 -1.33681000 0.28438900
C 1.88147500 0.39688800 -0.97906000
H 1.74414900 -0.05878400 -1.96287100
H 2.83672500 0.94866100 -0.99314200
Zero-point correction= 0.186331 (Hartree/Particle)
Thermal correction to Energy= 0.196018
Thermal correction to Enthalpy= 0.196962
Thermal correction to Gibbs Free Energy= 0.151113
Sum of electronic and zero-point Energies= -424.619253
Sum of electronic and thermal Energies= -424.609566
Sum of electronic and thermal Enthalpies= -424.608621
Sum of electronic and thermal Free Energies= -424.654470
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -424.926878910

Zero-point correction= 0.184371 (Hartree/Particle)
Thermal correction to Energy= 0.193717
Thermal correction to Enthalpy= 0.194661
Thermal correction to Gibbs Free Energy= 0.150334
Sum of electronic and zero-point Energies= -424.742507
Sum of electronic and thermal Energies= -424.733162
Sum of electronic and thermal Enthalpies= -424.732218
Sum of electronic and thermal Free Energies= -424.776545
DA-un-endo-trans
C 0.19410700 0.09514700 1.63452700
H 0.71570200 -0.37645700 2.46523100
C -0.62535100 -0.69917500 0.82983300
H -0.58273900 -1.78374000 0.90912100
C -1.78300700 -0.19754500 0.08295400

H	-0.07381800	1.13306900	1.81650900
0	-2.57343100	-0.96522200	-0.46884200
C	-2.01489400	1.29963000	0.04467400
H	-2.75040300	1.53025500	-0.73021300
H	-1.08858000	1.85571400	-0.14152600
H	-2.40535800	1.63403700	1.01472000
C	0.85207900	-0.84033600	-1.06615700
H	0.41837900	-1.65189800	-1.64198200
C	0.84036400	0.50084400	-1.42545500
H	0.29121800	0.92477300	-2.26099600
C	1.53108000	1.23829200	-0.44555700
H	1.61308300	2.32112500	-0.41568700
C	1.93853300	0.36745000	0.57653200
H	2.64255200	0.65130900	1.35449600
C	1.90408000	-1.02159300	-0.01409800
H	1.74258400	-1.83969700	0.69139500
H	2.86737300	-1.19394600	-0.52400800

Zero-point correction= 0.186560 (Hartree/Particle)
Thermal correction to Energy= 0.195990
Thermal correction to Enthalpy= 0.196934
Thermal correction to Gibbs Free Energy= 0.152239
Sum of electronic and zero-point Energies= -424.615695
Sum of electronic and thermal Energies= -424.606266
Sum of electronic and thermal Enthalpies= -424.605321
Sum of electronic and thermal Free Energies= -424.650016
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -424.924214651

Zero-point correction= 0.184471 (Hartree/Particle)
Thermal correction to Energy= 0.193677
Thermal correction to Enthalpy= 0.194621
Thermal correction to Gibbs Free Energy= 0.150666

Sum of electronic and zero-point Energies= -424.739744

Sum of electronic and thermal Energies= -424.730538

Sum of electronic and thermal Enthalpies= -424.729594

Sum of electronic and thermal Free Energies= -424.773548

DA-un-exo-cis

C	0.22915500	-1.27891300	-1.01752000
H	0.79273800	-1.47545700	-1.92473900
C	-0.62484100	-0.17878500	-0.95665500
H	-0.55831400	0.61623900	-1.69490700
C	-1.79306500	-0.16855100	-0.07793300
H	-0.06887600	-2.16530400	-0.45863900
0	-2.01696700	-1.05620000	0.75213900
C	-2.75831400	0.98699700	-0.24891600
H	-3.42828000	1.04459400	0.61271400
H	-3.36099900	0.82762800	-1.15251800
H	-2.22397400	1.93526700	-0.37524100
C	0.69022100	1.10306600	0.71499400
H	-0.00151500	1.81771400	1.15203300
C	1.69576800	1.40204700	-0.19465600
H	1.84226900	2.36206200	-0.68048100
C	2.41640500	0.22764100	-0.47799200
H	3.21072600	0.14067100	-1.21360000
C	1.82464900	-0.84609000	0.20524600
H	2.29170700	-1.82262800	0.30375700
C	0.96707400	-0.24771900	1.29011800
H	1.59386600	-0.11710100	2.18886400
H	0.08311000	-0.82589100	1.57059500

Zero-point correction= 0.186405 (Hartree/Particle)

Thermal correction to Energy= 0.196033

Thermal correction to Enthalpy= 0.196977

Thermal correction to Gibbs Free Energy= 0.151506

Sum of electronic and zero-point Energies= -424.617914

Sum of electronic and thermal Energies= -424.608287

Sum of electronic and thermal Enthalpies= -424.607342

Sum of electronic and thermal Free Energies= -424.652814

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -424.924806196

Zero-point correction= 0.184344 (Hartree/Particle)

Thermal correction to Energy= 0.193672

Thermal correction to Enthalpy= 0.194616

Thermal correction to Gibbs Free Energy= 0.150350

Sum of electronic and zero-point Energies= -424.740462

Sum of electronic and thermal Energies= -424.731134

Sum of electronic and thermal Enthalpies= -424.730190

Sum of electronic and thermal Free Energies= -424.774456

DA-un-exo-trans

C	0.10174000	-1.17158300	-1.04650700
H	0.66141500	-1.38054800	-1.95355200
C	-0.59669700	0.03389900	-0.94248100
H	-0.37938800	0.84472400	-1.63294000
C	-1.84729800	0.23186000	-0.20015500
H	-0.30250200	-2.06264100	-0.56790300
0	-2.43665300	1.31447900	-0.23431400
C	-2.48554700	-0.93287400	0.53623600
H	-3.16455600	-0.54159200	1.29824700
H	-1.77161900	-1.62170700	0.99689000
H	-3.07535700	-1.51445100	-0.18454900
C	0.82420400	1.06035100	0.73899000
H	0.19540900	1.83868900	1.15969000
C	1.88258600	1.25532000	-0.13889100
H	2.14749600	2.19815200	-0.60766200
C	2.46174800	0.00814900	-0.43307500

H 3.25619300 -0.16025300 -1.15426400
C 1.72685000 -1.00058500 0.21065600
H 2.07113500 -2.02842400 0.29311300
C 0.95536200 -0.31597900 1.31078800
H 1.61842600 -0.25738900 2.19095800
H 0.02782200 -0.79687000 1.62381900
Zero-point correction= 0.186547 (Hartree/Particle)
Thermal correction to Energy= 0.196150
Thermal correction to Enthalpy= 0.197094
Thermal correction to Gibbs Free Energy= 0.151384
Sum of electronic and zero-point Energies= -424.611584
Sum of electronic and thermal Energies= -424.601981
Sum of electronic and thermal Enthalpies= -424.601037
Sum of electronic and thermal Free Energies= -424.646747
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -424.919946725

Zero-point correction= 0.184582 (Hartree/Particle)
Thermal correction to Energy= 0.193864
Thermal correction to Enthalpy= 0.194809
Thermal correction to Gibbs Free Energy= 0.150475
Sum of electronic and zero-point Energies= -424.735365
Sum of electronic and thermal Energies= -424.726082
Sum of electronic and thermal Enthalpies= -424.725138
Sum of electronic and thermal Free Energies= -424.769472

2a-catalyzed Diels-Alder Reaction

2a-c2
H -2.53874700 -0.09630200 1.93382400
C -1.45570800 -0.05592800 1.96886600
C 1.45570800 0.05592800 1.96886600

C	-0.64980100	-1.18860900	1.96854300
C	-0.73756000	1.13349600	1.97247900
C	0.64980100	1.18860900	1.96854300
C	0.73756000	-1.13349600	1.97247900
H	2.53874700	0.09630200	1.93382400
0	-1.23986100	2.40623700	1.89307200
0	1.05092700	2.49587700	1.89491100
0	-1.05092700	-2.49587700	1.89491100
0	1.23986100	-2.40623700	1.89307200
C	-0.13408700	3.30341900	1.87435400
C	0.13408700	-3.30341900	1.87435400
C	-0.10484800	4.21484300	0.65739300
C	0.14441000	6.23795900	-1.21049000
C	0.22803400	5.50438600	1.07372300
C	-0.28471900	3.90745100	-0.69107200
C	-0.16778600	4.93955700	-1.61619600
C	0.35219700	6.51694100	0.13441400
C	0.10484800	-4.21484300	0.65739300
C	-0.14441000	-6.23795900	-1.21049000
C	-0.22803400	-5.50438600	1.07372300
C	0.28471900	-3.90745100	-0.69107200
C	0.16778600	-4.93955700	-1.61619600
C	-0.35219700	-6.51694100	0.13441400
C	-0.18591200	4.27570600	3.05842600
H	0.30206900	3.84029500	3.93451300
H	-1.24519400	4.43568500	3.28722600
C	0.18591200	-4.27570600	3.05842600
H	-0.30206900	-3.84029500	3.93451300
H	1.24519400	-4.43568500	3.28722600
C	-0.44715000	-5.58415200	2.56244700
H	-1.52178800	-5.62212100	2.77922700

H	0.01083600	-6.47296200	3.00669900
C	0.44715000	5.58415200	2.56244700
H	1.52178800	5.62212100	2.77922700
H	-0.01083600	6.47296200	3.00669900
I	0.69168500	-1.98064500	-1.41517100
I	-0.69168500	1.98064500	-1.41517100
F	0.66716900	7.76229700	0.49434100
F	0.24594400	7.20142100	-2.12258100
F	-0.34330200	4.72997000	-2.91980900
F	-0.66716900	-7.76229700	0.49434100
F	-0.24594400	-7.20142100	-2.12258100
F	0.34330200	-4.72997000	-2.91980900

Zero-point correction= 0.295392 (Hartree/Particle)

Thermal correction to Energy= 0.324979

Thermal correction to Enthalpy= 0.325923

Thermal correction to Gibbs Free Energy= 0.232026

Sum of electronic and zero-point Energies= -2412.209273

Sum of electronic and thermal Energies= -2412.179685

Sum of electronic and thermal Enthalpies= -2412.178741

Sum of electronic and thermal Free Energies= -2412.272639

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2413.16299780

2a-cs

H	-2.00524600	-2.34457800	-0.00000000
C	-1.91160600	-1.26431300	0.00000000
C	-1.59440100	1.63241400	0.00000000
C	-1.82897700	-0.50648000	1.16254900
C	-1.82897700	-0.50648000	-1.16254900
C	-1.68273500	0.87471200	-1.16152600
C	-1.68273500	0.87471200	1.16152600
H	-1.45167000	2.70731600	0.00000000

0	-1.81941900	-0.96054300	-2.45460800
0	-1.57690700	1.31798000	-2.45393000
0	-1.81941900	-0.96054300	2.45460800
0	-1.57690700	1.31798000	2.45393000
C	-1.77801600	0.19287100	-3.30511200
C	-1.77801600	0.19287100	3.30511200
C	-0.68342400	0.01895200	-4.34012300
C	0.92538400	-0.44555800	-6.53535500
C	-1.26722500	-0.27182100	-5.57285800
C	0.69990000	0.04703300	-4.17198700
C	1.49597500	-0.17633600	-5.29011200
C	-0.45584100	-0.50419400	-6.67347200
C	-0.68342400	0.01895200	4.34012300
C	0.92538400	-0.44555800	6.53535500
C	-1.26722500	-0.27182100	5.57285800
C	0.69990000	0.04703300	4.17198700
C	1.49597500	-0.17633600	5.29011200
C	-0.45584100	-0.50419400	6.67347200
C	-3.05659300	0.34573000	-4.14080500
H	-3.20897200	1.42037800	-4.28798100
H	-3.91823300	-0.06137500	-3.60464300
C	-3.05659300	0.34573000	4.14080500
H	-3.91823300	-0.06137500	3.60464300
H	-3.20897200	1.42037800	4.28798100
C	-2.77071700	-0.33286600	5.48963000
H	-3.10038800	-1.37897200	5.49589600
H	-3.25828100	0.17114700	6.32950100
C	-2.77071700	-0.33286600	-5.48963000
H	-3.25828100	0.17114700	-6.32950100
H	-3.10038800	-1.37897200	-5.49589600
I	1.64613900	0.35359600	2.32660100

I 1.64613900 0.35359600 -2.32660100
F -0.97278700 -0.78496500 -7.87083400
F 1.71610200 -0.65440500 -7.58495400
F 2.82549300 -0.14946500 -5.21618400
F -0.97278700 -0.78496500 7.87083400
F 1.71610200 -0.65440500 7.58495400
F 2.82549300 -0.14946500 5.21618400
Zero-point correction= 0.295365 (Hartree/Particle)
Thermal correction to Energy= 0.324057
Thermal correction to Enthalpy= 0.325001
Thermal correction to Gibbs Free Energy= 0.233882
Sum of electronic and zero-point Energies= -2412.208857
Sum of electronic and thermal Energies= -2412.180164
Sum of electronic and thermal Enthalpies= -2412.179220
Sum of electronic and thermal Free Energies= -2412.270339
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2413.16278560

DA-2a-Binary-C2-cis-2
H -0.11759400 -2.14059600 2.52590700
C -0.09219700 -2.14285900 1.44181100
C -0.01906800 -2.09667600 -1.47056000
C -1.23607600 -2.12344500 0.65205200
C 1.08797100 -2.14315600 0.70758000
C 1.12450100 -2.13328700 -0.68110100
C -1.19911700 -2.08981300 -0.73639400
H 0.00690000 -2.06025000 -2.55402900
0 2.36920300 -2.10657300 1.19078600
0 2.42929300 -2.11015100 -1.09793100
0 -2.54003400 -2.07876500 1.06952200
0 -2.47843400 -2.00454600 -1.21791900
C 3.24189600 -2.26689700 0.07201500

C	-3.35558600	-2.17981300	-0.10477900
C	4.36546600	-1.25383900	0.05744900
C	6.69608300	0.21085600	-0.07414600
C	5.57680400	-1.91017400	-0.15338500
C	4.27938200	0.13542900	0.15965100
C	5.46889000	0.85302700	0.10385300
C	6.74808400	-1.16969300	-0.21643900
C	-4.45616000	-1.14284800	-0.05804500
C	-6.75327500	0.36755600	0.12017900
C	-5.68105600	-1.77876300	0.13743300
C	-4.33837800	0.24659100	-0.12190400
C	-5.51246900	0.98705100	-0.04303300
C	-6.83564500	-1.01498200	0.22408900
C	3.95536000	-3.62976100	0.12523500
H	3.40973600	-4.37190600	-0.46404600
H	3.95018200	-3.94482900	1.17373600
C	-4.09965300	-3.52358400	-0.20117200
H	-3.56799200	-4.29877100	0.35758600
H	-4.10813500	-3.80061400	-1.26041100
C	-5.53578200	-3.27053100	0.28771700
H	-5.66420100	-3.55085700	1.34028400
H	-6.28143500	-3.82446400	-0.29105000
C	5.40012100	-3.39351200	-0.34676400
H	5.53045800	-3.64669900	-1.40593500
H	6.12960600	-3.97940100	0.22102300
I	-2.50349100	1.26822100	-0.21658100
I	2.46945100	1.19285800	0.28069900
F	7.93099100	-1.75554700	-0.41720500
F	7.81253100	0.93500200	-0.12454100
F	5.48599100	2.18304600	0.20296700
F	-8.03116400	-1.57994300	0.41085500

F	-7.85363000	1.11434300	0.19374200
F	-5.50110700	2.31980800	-0.10513600
C	1.00612000	4.97387400	0.23203300
H	1.17672900	5.91345900	-0.29024200
C	1.58118900	4.70790800	1.41006400
H	2.26107600	5.40824100	1.88868100
H	1.36772100	3.77799400	1.93446000
C	0.05880300	4.01446100	-0.39058900
0	-0.03003300	2.84996600	0.00617600
C	-0.79101200	4.54210400	-1.51078200
H	-0.15148100	5.00232900	-2.27415800
H	-1.44947600	5.33230700	-1.12675700
H	-1.39157600	3.74565200	-1.95692800

Zero-point correction= 0.386321 (Hartree/Particle)
Thermal correction to Energy= 0.423826
Thermal correction to Enthalpy= 0.424770
Thermal correction to Gibbs Free Energy= 0.310844
Sum of electronic and zero-point Energies= -2643.080706
Sum of electronic and thermal Energies= -2643.043200
Sum of electronic and thermal Enthalpies= -2643.042256
Sum of electronic and thermal Free Energies= -2643.156182
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2644.20778423

DA-2a-Binary-C2-cis

H	0.10852400	-2.35300300	-2.39172700
C	0.07775800	-2.21285900	-1.31693900
C	-0.00935900	-1.79019200	1.56505200
C	1.21767400	-2.09969500	-0.52977000
C	-1.10580800	-2.11069600	-0.59585700
C	-1.15028600	-1.92001800	0.77957700
C	1.17528000	-1.88747000	0.84277900

H	-0.04019700	-1.61982700	2.63581800
0	-2.38353000	-2.13340800	-1.08780800
0	-2.45784500	-1.83858500	1.18078700
0	2.52299300	-2.12270500	-0.94251300
0	2.45378500	-1.75782400	1.31660600
C	-3.26278000	-2.15316800	0.03720300
C	3.33287700	-2.08463900	0.23917500
C	-4.39193600	-1.15537100	-0.09480900
C	-6.73146900	0.29637000	-0.21180800
C	-5.60442900	-1.78712500	0.17502700
C	-4.31137200	0.20819700	-0.37929200
C	-5.50379800	0.91950400	-0.44583800
C	-6.78023500	-1.05343600	0.11265300
C	4.44875500	-1.07838100	0.06278200
C	6.76683600	0.36270000	-0.31167000
C	5.66295600	-1.75261600	-0.05641500
C	4.35304400	0.30944600	-0.04801700
C	5.53656300	1.01754100	-0.22265200
C	6.82813200	-1.02324000	-0.24203000
C	-3.96816400	-3.51645400	0.15829800
H	-3.43072000	-4.16626300	0.85445200
H	-3.94053500	-3.97265000	-0.83651800
C	4.05779200	-3.41495000	0.50762100
H	3.51080000	-4.24880500	0.05896600
H	4.07122100	-3.55052800	1.59408100
C	5.49320700	-3.24906900	-0.01900500
H	5.60693300	-3.65951400	-1.02970600
H	6.23519200	-3.73953300	0.61864000
C	-5.42366300	-3.23058100	0.56592200
H	-5.57546100	-3.34301100	1.64629000
H	-6.13796800	-3.89179000	0.06564900

I 2.53158900 1.35323700 -0.05934200
I -2.50094200 1.24562100 -0.58690600
F -7.96490200 -1.61571700 0.36281300
F -7.85194900 1.01168600 -0.28488900
F -5.52275500 2.22398300 -0.72095400
F 8.01435400 -1.62484600 -0.36017600
F 7.87769800 1.07723100 -0.48109800
F 5.54390000 2.34733700 -0.32537900
C -0.23610600 3.41882700 2.08776600
H -0.32160100 4.23177700 2.80659500
C -0.21441000 2.13765000 2.47419000
H -0.26830400 1.85415300 3.52248200
H -0.15064400 1.33393900 1.74127400
C -0.18338000 3.78852100 0.65003200
0 0.02751600 2.94944200 -0.22942400
C -0.41402500 5.23453000 0.31552000
H 0.33620500 5.85365900 0.82405700
H -1.39575300 5.54785000 0.69353600
H -0.36040800 5.39170900 -0.76377000

Zero-point correction= 0.386415 (Hartree/Particle)
Thermal correction to Energy= 0.423803
Thermal correction to Enthalpy= 0.424748
Thermal correction to Gibbs Free Energy= 0.311772
Sum of electronic and zero-point Energies= -2643.080125
Sum of electronic and thermal Energies= -2643.042736
Sum of electronic and thermal Enthalpies= -2643.041792
Sum of electronic and thermal Free Energies= -2643.154767
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2644.20850466

DA-2a-Binary-C2-trans
H 0.04445000 -2.26334700 -2.47493200

C	0.01742300	-2.22920900	-1.39143500
C	-0.05894000	-2.08348700	1.51781800
C	1.16013700	-2.20501300	-0.60026100
C	-1.16346300	-2.18245100	-0.65995500
C	-1.20184100	-2.12597600	0.72761800
C	1.12198000	-2.12316700	0.78608800
H	-0.08574500	-2.00899400	2.59928600
0	-2.44289200	-2.13625800	-1.14685400
0	-2.50662500	-2.06428100	1.14053700
0	2.46513000	-2.19837400	-1.01669400
0	2.40206400	-2.04310300	1.26670000
C	-3.32020000	-2.24502600	-0.02530900
C	3.27745100	-2.27109700	0.16174100
C	-4.42510100	-1.21214700	-0.04858000
C	-6.72891700	0.29752000	0.01523200
C	-5.64958100	-1.83954500	0.17424300
C	-4.31174100	0.17115800	-0.19565900
C	-5.48868400	0.91097400	-0.17315200
C	-6.80744200	-1.07637300	0.20301300
C	4.39311600	-1.25289300	0.07991800
C	6.71176600	0.21691400	-0.14919600
C	5.60910700	-1.91304700	-0.08908000
C	4.29498500	0.13936200	0.09141100
C	5.47968100	0.85969200	-0.01207300
C	6.77466500	-1.16956200	-0.20134500
C	-4.05750300	-3.59633100	-0.03545800
H	-3.52910300	-4.32654900	0.58363900
H	-4.05101900	-3.94854600	-1.07204400
C	4.00099100	-3.62168400	0.30677900
H	3.45975900	-4.40744700	-0.22745000
H	4.00169600	-3.86261400	1.37480400

C	5.44249500	-3.40712700	-0.18495700
H	5.57079200	-3.72775400	-1.22595300
H	6.17788600	-3.95007000	0.41689700
C	-5.50106300	-3.31860800	0.41756900
H	-5.64347400	-3.53443200	1.48344100
H	-6.23700000	-3.90984700	-0.13618600
I	2.47615000	1.19223000	0.14501300
I	-2.48123200	1.19403900	-0.33251900
F	-8.00275600	-1.63348800	0.41270800
F	-7.83247200	1.04284700	0.03135400
F	-5.48100200	2.23737200	-0.31628300
F	7.96236500	-1.75791300	-0.36414800
F	7.82268700	0.94480100	-0.24809600
F	5.48752500	2.19379300	0.00061100
C	1.00960700	4.75927100	0.75012800
H	1.79786400	4.12267200	1.14966000
C	1.01168500	6.08089000	0.95959700
H	1.80291600	6.55749700	1.53336200
H	0.22954800	6.73184200	0.57367500
C	-0.04830000	4.04960300	-0.00279800
0	0.00994000	2.82204200	-0.12053500
C	-1.18825000	4.83262700	-0.59737500
H	-0.81303700	5.66960500	-1.19645000
H	-1.81156800	5.24945500	0.20338000
H	-1.79705800	4.17771800	-1.22501300

Zero-point correction= 0.386713 (Hartree/Particle)

Thermal correction to Energy= 0.424054

Thermal correction to Enthalpy= 0.424998

Thermal correction to Gibbs Free Energy= 0.311582

Sum of electronic and zero-point Energies= -2643.081163

Sum of electronic and thermal Energies= -2643.043823

Sum of electronic and thermal Enthalpies= -2643.042878

Sum of electronic and thermal Free Energies= -2643.156294

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2644.20866749

DA-2a-Binary-Cs-cis

H	0.00003900	-2.81577600	-2.03538100
C	0.00003500	-2.48728200	-1.00204300
C	0.00001900	-1.55662900	1.75926000
C	1.16267000	-2.24316200	-0.28026700
C	-1.16260900	-2.24320100	-0.28025700
C	-1.16252000	-1.80262000	1.03715900
C	1.16256200	-1.80257800	1.03715500
H	0.00003200	-1.19848800	2.78316100
0	-2.45464300	-2.34347800	-0.72215000
0	-2.45532300	-1.61857900	1.45118800
0	2.45472000	-2.34338500	-0.72214200
0	2.45534700	-1.61848200	1.45119400
C	-3.30284500	-2.09200900	0.40631300
C	3.30289000	-2.09193200	0.40636300
C	-4.38481600	-1.10698500	0.01453000
C	-6.64549600	0.26701100	-0.76036700
C	-5.59126600	-1.79257700	-0.12548500
C	-4.26786600	0.25539200	-0.26248500
C	-5.42371000	0.93149400	-0.63839800
C	-6.72656600	-1.09781300	-0.51447000
C	4.38486400	-1.10693200	0.01456500
C	6.64551100	0.26704200	-0.76038500
C	5.59127300	-1.79255700	-0.12556200
C	4.26789900	0.25545300	-0.26238800
C	5.42374300	0.93154500	-0.63830800
C	6.72656900	-1.09780300	-0.51459000

C	-4.07812700	-3.34365700	0.84295900
H	-4.21257900	-3.26743400	1.92738700
H	-3.50630900	-4.24936400	0.62253500
C	4.07814800	-3.34358300	0.84299400
H	3.50626200	-4.24928400	0.62272300
H	4.21277900	-3.26728200	1.92739700
C	5.44260100	-3.26860500	0.13946100
H	5.44070600	-3.81844800	-0.80965600
H	6.25683200	-3.67005000	0.75044600
C	-5.44266600	-3.26861300	0.13961500
H	-6.25684100	-3.66994200	0.75075100
H	-5.44097200	-3.81853300	-0.80945800
I	2.45861200	1.31837400	-0.19453200
I	-2.45861400	1.31839600	-0.19464000
F	-7.90272100	-1.71251800	-0.66029600
F	-7.72914200	0.95062100	-1.12296000
F	-5.41055100	2.23796400	-0.90565100
F	7.90269500	-1.71253100	-0.66052700
F	7.72914500	0.95066900	-1.12298000
F	5.41061300	2.23803700	-0.90547300
C	0.00010300	3.49654300	2.31206400
H	0.00021500	4.30177100	3.04453000
C	0.00009700	2.21019700	2.68070800
H	0.00023100	1.91309000	3.72664700
H	-0.00003500	1.41608700	1.93487000
C	-0.00008500	3.88619400	0.87838800
0	-0.00006100	3.04547500	-0.02444900
C	-0.00035500	5.35775900	0.57872600
H	-0.00052700	5.52959700	-0.49959300
H	0.88128100	5.82617500	1.03492300
H	-0.88200200	5.82591100	1.03517100

Zero-point correction= 0.386523 (Hartree/Particle)
Thermal correction to Energy= 0.423863
Thermal correction to Enthalpy= 0.424808
Thermal correction to Gibbs Free Energy= 0.311468
Sum of electronic and zero-point Energies= -2643.081095
Sum of electronic and thermal Energies= -2643.043755
Sum of electronic and thermal Enthalpies= -2643.042810
Sum of electronic and thermal Free Energies= -2643.156150
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2644.20936483

DA-2a-Binary-Cs-trans

H	-0.04827800	-2.82943300	-2.09801900
C	-0.04301200	-2.56765500	-1.04578300
C	-0.02811500	-1.80888200	1.76734700
C	1.12326900	-2.38659500	-0.31145200
C	-1.20158700	-2.35255500	-0.30833800
C	-1.19383700	-1.99410800	1.03374300
C	1.12952200	-2.03024800	1.03112000
H	-0.02215200	-1.50686800	2.80871300
0	-2.49506000	-2.40384800	-0.75436600
0	-2.48367100	-1.81307300	1.45952300
0	2.41330300	-2.47423000	-0.76153700
0	2.42516100	-1.88881300	1.45422900
C	-3.33830500	-2.20656300	0.38908200
C	3.26678400	-2.28957700	0.37654300
C	-4.40233800	-1.18153600	0.05608900
C	-6.63582300	0.26847200	-0.65332600
C	-5.61563200	-1.84109400	-0.14162000
C	-4.26297000	0.19449000	-0.12880800
C	-5.40740900	0.90662400	-0.47323800
C	-6.73743200	-1.10818700	-0.49759100

C	4.34137300	-1.27669600	0.03790900
C	6.58755500	0.14521600	-0.68926300
C	5.54253400	-1.95247200	-0.17860800
C	4.22073800	0.10253800	-0.13537600
C	5.37118400	0.80019600	-0.48954300
C	6.67059400	-1.23383100	-0.54362000
C	-4.13538800	-3.46898100	0.74620900
H	-4.28377600	-3.45069500	1.83138900
H	-3.57330100	-4.36940300	0.48303100
C	4.05132900	-3.56237300	0.72249600
H	3.47358500	-4.45491800	0.46659600
H	4.21516900	-3.54665500	1.80552800
C	5.39572400	-3.44330900	-0.01236300
H	5.36333800	-3.92609000	-0.99685000
H	6.22530200	-3.88834500	0.54539200
C	-5.48847500	-3.33301700	0.03042300
H	-6.31623700	-3.76261400	0.60284100
H	-5.47839200	-3.82114800	-0.95188300
I	2.42476500	1.17925800	0.06043000
I	-2.44722500	1.24388300	0.03194200
F	-7.91964300	-1.69647700	-0.69611800
F	-7.70638600	0.98897100	-0.98284300
F	-5.37719400	2.22823300	-0.65438100
F	7.84162500	-1.83795700	-0.75974900
F	7.66458700	0.85207300	-1.02707200
F	5.35837800	2.12334200	-0.66070000
C	1.28329800	4.85613100	0.67295000
H	2.16045900	4.21375100	0.73208000
C	1.38102500	6.18069800	0.83532400
H	2.34057900	6.65354600	1.03082800
H	0.51569500	6.83854000	0.78119500

C 0.00603900 4.15621100 0.40824100

0 0.00085100 2.92924600 0.27272200

C -1.26274600 4.96033700 0.31149700

H -2.10712400 4.30209900 0.09544100

H -1.17349800 5.71186700 -0.48150700

H -1.44538200 5.49257600 1.25240400

Zero-point correction= 0.386849 (Hartree/Particle)

Thermal correction to Energy= 0.424074

Thermal correction to Enthalpy= 0.425018

Thermal correction to Gibbs Free Energy= 0.312440

Sum of electronic and zero-point Energies= -2643.082032

Sum of electronic and thermal Energies= -2643.044807

Sum of electronic and thermal Enthalpies= -2643.043863

Sum of electronic and thermal Free Energies= -2643.156441

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2644.20920516

DA-2a-endo-cis-2

H -0.06431800 -1.75496300 2.81408100

C -0.07673700 -2.13082000 1.79674800

C -0.10850700 -3.09603100 -0.95185200

C -1.24720600 -2.35507000 1.08070300

C 1.07684100 -2.42363900 1.07810600

C 1.06192100 -2.87584700 -0.23524500

C -1.26237000 -2.81260100 -0.23055300

H -0.11979800 -3.43407700 -1.98205700

0 2.37531900 -2.27392600 1.48880700

0 2.34831900 -3.01436600 -0.68089400

0 -2.53393800 -2.12573300 1.49286100

0 -2.55683700 -2.88229800 -0.67047700

C 3.21140800 -2.73944000 0.43244200

C -3.39730800 -2.56914100 0.44882200

C	4.27447800	-1.74512800	0.00881000
C	6.50010100	-0.37085800	-0.85501100
C	5.47207500	-2.43305900	-0.19144700
C	4.14417800	-0.37834700	-0.24436900
C	5.28716400	0.29337300	-0.66627400
C	6.59000200	-1.73814700	-0.62600500
C	-4.42561700	-1.53840000	0.02835600
C	-6.60590800	-0.07890800	-0.81568700
C	-5.65820800	-2.17262400	-0.12903000
C	-4.24088900	-0.18590400	-0.26239300
C	-5.35898600	0.53233000	-0.67350700
C	-6.75306100	-1.43492600	-0.55254300
C	4.01058900	-3.97860600	0.85511900
H	3.43154400	-4.89036500	0.68395300
H	4.20317200	-3.87879400	1.92903600
C	-4.23806800	-3.77286800	0.89602500
H	-4.39146800	-3.66514400	1.97533200
H	-3.70421400	-4.70861700	0.70822800
C	-5.58172200	-3.64965800	0.16064600
H	-6.42658800	-4.00541200	0.75826700
H	-5.58234900	-4.21419800	-0.77989100
C	5.33373800	-3.90980900	0.07678600
H	5.27338000	-4.45778800	-0.87168000
H	6.17955700	-4.31695400	0.63918800
I	-2.39381600	0.81250400	-0.14254700
I	2.35033300	0.71540800	-0.04652000
F	7.75829200	-2.35358500	-0.82967000
F	7.56850600	0.31465300	-1.26034700
F	5.27088500	1.60579800	-0.91424700
F	-7.95222700	-1.99962100	-0.71610000
F	-7.65009500	0.64652200	-1.21275200

F	-5.28503500	1.83439400	-0.95581300
C	-0.91885900	4.19917900	1.22859600
H	-1.11535300	4.73249500	2.15473500
C	-1.38441900	4.65521600	-0.00395800
H	-2.12825200	5.44933700	-0.03027000
H	-1.44266900	3.93742500	-0.81832200
C	-0.14575100	2.99138200	1.26538300
0	0.08687500	2.35051000	0.20817100
C	0.41478600	2.49556000	2.57545300
H	1.50874500	2.58697100	2.56071700
H	0.17834500	1.42975000	2.68894800
H	0.02370300	3.05300800	3.43211500
C	1.11963600	4.87990300	-1.03561500
H	1.25441300	4.30355700	-1.94578300
C	0.09574600	5.80577900	-0.80470700
H	-0.47012600	6.27319600	-1.60652300
C	1.88600200	4.72422300	0.14661500
H	2.66806100	3.98367900	0.28721400
C	1.39312700	5.57083000	1.11144100
H	1.75977300	5.66119900	2.12970500
C	0.44814000	6.53759800	0.47111800
H	1.01716800	7.44316200	0.19933500
H	-0.39685400	6.85299900	1.08898400

Zero-point correction= 0.482946 (Hartree/Particle)

Thermal correction to Energy= 0.523940

Thermal correction to Enthalpy= 0.524884

Thermal correction to Gibbs Free Energy= 0.405003

Sum of electronic and zero-point Energies= -2836.823256

Sum of electronic and thermal Energies= -2836.782262

Sum of electronic and thermal Enthalpies= -2836.781318

Sum of electronic and thermal Free Energies= -2836.901199

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.10933968

DA-2a-endo-cis

H	0.14331900	-3.46859400	-1.87962000
C	0.13115400	-3.10500500	-0.85812800
C	0.09788000	-2.07213400	1.86570000
C	1.28490400	-2.80861200	-0.14133800
C	-1.04006000	-2.86106900	-0.15014300
C	-1.05492400	-2.37145400	1.14975700
C	1.26841300	-2.32245400	1.15950700
H	0.08508200	-1.66794000	2.87178700
0	-2.32738200	-3.00274100	-0.59394400
0	-2.35264300	-2.19404200	1.55021500
0	2.58053700	-2.89143400	-0.57650800
0	2.55483500	-2.09182200	1.57148900
C	-3.18770000	-2.71194700	0.51681000
C	3.41944300	-2.55341000	0.53703300
C	-4.27123700	-1.74826500	0.08010900
C	-6.53390300	-0.41732500	-0.75114000
C	-5.47223300	-2.44742200	-0.04353800
C	-4.15468500	-0.39417400	-0.23952100
C	-5.31622800	0.25665500	-0.64261900
C	-6.60941000	-1.77385900	-0.46200200
C	4.44590000	-1.52686300	0.10120600
C	6.62641300	-0.07490700	-0.75483700
C	5.67934300	-2.16179300	-0.04746400
C	4.26048700	-0.17733800	-0.20279500
C	5.37916100	0.53705500	-0.61965500
C	6.77411300	-1.42816000	-0.47789300
C	-3.95833100	-3.95157800	0.99379600
H	-4.10331500	-3.83518600	2.07333200

H	-3.37880900	-4.86125500	0.81333900
C	4.26331200	-3.74656700	1.00549000
H	3.73049100	-4.68671100	0.83779400
H	4.42063000	-3.61724100	2.08188200
C	5.60390700	-3.63476500	0.26272100
H	5.59972700	-4.21250200	-0.66980400
H	6.45133100	-3.98252700	0.86138300
C	-5.31678300	-3.91200700	0.27584200
H	-6.13389400	-4.29691800	0.89373400
H	-5.30227700	-4.49670300	-0.65220200
I	2.41031900	0.82017100	-0.11466700
I	-2.35202400	0.70314400	-0.19726400
F	-7.78214600	-2.40018900	-0.59418900
F	-7.62009800	0.24820100	-1.14217000
F	-5.31457800	1.55622300	-0.95140800
F	7.97397600	-1.99359600	-0.63400800
F	7.67055400	0.64695600	-1.15867700
F	5.30509100	1.83607500	-0.91590200
C	0.85482900	4.47210600	-0.36614500
H	1.01017800	5.31167600	-1.03827200
C	1.36159500	4.45793000	0.93288100
H	2.09930200	5.20357500	1.22334600
H	1.45535900	3.49546600	1.42903400
C	0.08592500	3.34695100	-0.81657000
0	-0.08608600	2.35119800	-0.06779000
C	-0.55404200	3.37103300	-2.18259800
H	-0.24710300	4.24203200	-2.76978700
H	-1.64595900	3.38484900	-2.06956300
H	-0.29440600	2.45293900	-2.72345800
C	-1.11201600	4.23834200	2.04167900
H	-1.21540200	3.36459600	2.67796300

C	-0.09968100	5.20078300	2.14043700
H	0.48687500	5.35025600	3.04339500
C	-1.91152300	4.51537800	0.90513000
H	-2.69233800	3.86605900	0.51971600
C	-1.45137600	5.66490000	0.30627700
H	-1.84781900	6.11598400	-0.59861400
C	-0.49626500	6.34534300	1.23454400
H	-1.06502600	7.07554600	1.83538400
H	0.32683500	6.88241900	0.75582300

Zero-point correction= 0.482807 (Hartree/Particle)
Thermal correction to Energy= 0.523894
Thermal correction to Enthalpy= 0.524838
Thermal correction to Gibbs Free Energy= 0.404245
Sum of electronic and zero-point Energies= -2836.823074
Sum of electronic and thermal Energies= -2836.781987
Sum of electronic and thermal Enthalpies= -2836.781043
Sum of electronic and thermal Free Energies= -2836.901636
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.10896431

DA-2a-endo-trans

H	0.08005400	-3.81761300	-1.15298300
C	0.07112900	-3.15510700	-0.29453100
C	0.04668800	-1.33174200	1.97720800
C	1.22726200	-2.66240000	0.29932400
C	-1.09780300	-2.69291200	0.29866600
C	-1.10922200	-1.82399600	1.38196200
C	1.21570500	-1.79716300	1.38591500
H	0.03666400	-0.64134400	2.81387100
0	-2.38544700	-2.95414400	-0.08506700
0	-2.40561600	-1.51625100	1.69998900
0	2.52100700	-2.89070800	-0.08317300

0	2.50384800	-1.46419200	1.71163800
C	-3.24586500	-2.30879900	0.86384400
C	3.36430300	-2.22828800	0.87041500
C	-4.29556100	-1.50539200	0.12339000
C	-6.50670200	-0.46463600	-1.15073400
C	-5.51296700	-2.18308200	0.19469000
C	-4.14020100	-0.32589800	-0.60636900
C	-5.27418900	0.18591200	-1.22932100
C	-6.62353300	-1.65612500	-0.44647400
C	4.39528700	-1.39767700	0.13300800
C	6.58032300	-0.31996700	-1.15359800
C	5.61862100	-2.06811700	0.17561300
C	4.21963300	-0.20492600	-0.57103500
C	5.34273600	0.32364200	-1.20028300
C	6.71590900	-1.52298300	-0.47260100
C	-4.05893600	-3.31598900	1.68885400
H	-4.21609200	-2.86100700	2.67285900
H	-3.50272200	-4.24859600	1.81779600
C	4.20085800	-3.22389900	1.68392500
H	3.65590700	-4.16103500	1.82785200
H	4.37537900	-2.76308600	2.66242800
C	5.53073800	-3.37077700	0.92866300
H	5.50385900	-4.20939200	0.22187400
H	6.38318100	-3.52987300	1.59611100
C	-5.40425000	-3.47470100	0.96337000
H	-6.24154700	-3.62626500	1.65146100
H	-5.39214900	-4.32232200	0.26714500
I	2.39380000	0.83579700	-0.76193300
I	-2.32276200	0.70859700	-0.85311800
F	-7.80893200	-2.26964200	-0.40352100
F	-7.56608500	0.06217500	-1.76243800

F	-5.23066500	1.31866300	-1.93336100
F	7.90653000	-2.12848400	-0.45722000
F	7.62743300	0.22514800	-1.77110100
F	5.28355700	1.47030700	-1.88142000
C	0.81952500	4.07587600	0.37583600
H	1.73680500	3.50229900	0.48778700
C	0.69765300	5.31886700	1.00141900
H	1.60203800	5.79318400	1.37815500
H	-0.06018900	6.02233300	0.66500700
C	-0.13440800	3.53510000	-0.57235700
0	0.03852000	2.42521800	-1.11936600
C	-1.34433900	4.36633800	-0.92904000
H	-1.02126900	5.26572400	-1.46896100
H	-1.87670000	4.70259700	-0.02989300
H	-2.02045400	3.79022800	-1.56571600
C	-1.33531200	4.62230100	2.64392600
H	-2.15729100	5.33214600	2.67436800
C	0.01000800	4.93233100	2.89424300
H	0.32255100	5.82149600	3.43585400
C	-1.42431300	3.29163900	2.18666300
H	-2.31773400	2.82225100	1.78525100
C	-0.15677600	2.73094300	2.19983900
H	0.09191100	1.72020300	1.88384600
C	0.73071900	3.61056100	3.02595600
H	1.79069200	3.60990600	2.76268600
H	0.64074400	3.28879900	4.07791900

Zero-point correction= 0.483162 (Hartree/Particle)

Thermal correction to Energy= 0.523968

Thermal correction to Enthalpy= 0.524912

Thermal correction to Gibbs Free Energy= 0.405807

Sum of electronic and zero-point Energies= -2836.820251

Sum of electronic and thermal Energies= -2836.779446

Sum of electronic and thermal Enthalpies= -2836.778501

Sum of electronic and thermal Free Energies= -2836.897606

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.10591569

DA-2a-exo-cis

H	0.18686000	-3.59026200	-1.68312200
C	0.16968800	-3.13153400	-0.70071800
C	0.12213300	-1.84397600	1.91160100
C	1.31981700	-2.75837000	-0.01431900
C	-1.00537700	-2.83197400	-0.02050300
C	-1.02688200	-2.22017400	1.22639600
C	1.29630700	-2.15102600	1.23468000
H	0.10384500	-1.34653700	2.87491900
0	-2.29124200	-3.02522800	-0.45041500
0	-2.32694300	-2.01550400	1.60608700
0	2.61737500	-2.86970000	-0.43758900
0	2.57949700	-1.87321100	1.62584800
C	-3.15441000	-2.64729600	0.63101000
C	3.44994700	-2.43705000	0.64766900
C	-4.25916700	-1.75042900	0.11231300
C	-6.55400900	-0.54000000	-0.81360700
C	-5.45153600	-2.47362800	0.08014300
C	-4.16939400	-0.43483700	-0.34656900
C	-5.34465000	0.15710500	-0.79660800
C	-6.60477200	-1.86058100	-0.38558500
C	4.49008900	-1.46280900	0.13280700
C	6.69443300	-0.10362200	-0.80726600
C	5.72268500	-2.11325600	0.06965400
C	4.31664300	-0.14669300	-0.29918000
C	5.44748300	0.52172100	-0.75690400

C	6.82975100	-1.42606500	-0.40400500
C	-3.89788600	-3.84989900	1.23214900
H	-4.02452000	-3.63822900	2.29935600
H	-3.30702900	-4.76371300	1.12361000
C	4.27722500	-3.58867800	1.23623600
H	3.74161600	-4.53747300	1.14225700
H	4.41444700	-3.36539300	2.29985000
C	5.63319100	-3.55063300	0.51391600
H	5.64519000	-4.21271000	-0.36068300
H	6.46641400	-3.84395800	1.15982500
C	-5.26999300	-3.89687900	0.54087000
H	-6.07010600	-4.22754100	1.21026200
H	-5.26596700	-4.57071100	-0.32472900
I	2.46432200	0.85150700	-0.34711500
I	-2.37498100	0.66543500	-0.45402300
F	-7.76979800	-2.51236500	-0.43361400
F	-7.65528200	0.06714600	-1.25352800
F	-5.36410800	1.41645500	-1.23982200
F	8.03009500	-2.00692600	-0.48194900
F	7.75064600	0.57452600	-1.25367100
F	5.38594200	1.78784100	-1.17463400
C	0.46854000	4.55107500	-0.24200600
H	0.37346300	5.52527700	-0.71361800
C	1.20870700	4.41142300	0.93429300
H	1.93045200	5.17805400	1.20193100
H	1.47834700	3.40217300	1.24417900
C	-0.12119600	3.43406900	-0.93133000
0	-0.02326700	2.25074200	-0.52053600
C	-0.89596900	3.70137700	-2.20100300
H	-0.83237000	4.74618200	-2.51850800
H	-1.95089600	3.44130600	-2.04476000

H	-0.51839900	3.05050800	-2.99796200
C	-0.47734100	6.02067200	2.30656200
H	0.01328800	6.88879000	2.73703700
C	-0.07834100	4.68966900	2.49691200
H	0.55099600	4.36751700	3.32245500
C	-1.50907800	6.06186700	1.34556500
H	-1.92789500	6.96455400	0.91162400
C	-1.82775900	4.76595700	0.97641500
H	-2.59737100	4.47378300	0.26665800
C	-1.17277100	3.82306800	1.92760500
H	-0.85266700	2.86976300	1.49762100
H	-1.89026000	3.60222700	2.73672100

Zero-point correction= 0.482864 (Hartree/Particle)

Thermal correction to Energy= 0.524007

Thermal correction to Enthalpy= 0.524951

Thermal correction to Gibbs Free Energy= 0.403895

Sum of electronic and zero-point Energies= -2836.820120

Sum of electronic and thermal Energies= -2836.778976

Sum of electronic and thermal Enthalpies= -2836.778032

Sum of electronic and thermal Free Energies= -2836.899088

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.10573217

DA-2a-exo-trans

H	-0.63586900	-3.09778900	-2.25129100
C	-0.61469200	-2.92340000	-1.18124500
C	-0.55076000	-2.40057400	1.68432000
C	0.55552700	-2.93204300	-0.43085600
C	-1.75137500	-2.64049100	-0.43285300
C	-1.72013700	-2.39228800	0.93353200
C	0.58433600	-2.69049700	0.93669200
H	-0.52417400	-2.18450400	2.74656000

0	-3.03628900	-2.51069600	-0.88672600
0	-2.98546700	-2.09627800	1.36706600
0	1.83365800	-3.12450500	-0.88260900
0	1.88168500	-2.73373000	1.37533600
C	-3.86599100	-2.28519600	0.26191200
C	2.68539600	-3.14133100	0.27169700
C	-4.77390800	-1.10075400	0.00116200
C	-6.77688800	0.69107200	-0.60291900
C	-6.06413400	-1.57038100	-0.24684900
C	-4.44070700	0.25264500	-0.08075700
C	-5.47401200	1.13682100	-0.37429700
C	-7.07001400	-0.66553200	-0.54937000
C	3.88110900	-2.24324900	0.02858000
C	6.29943200	-1.05760900	-0.54644300
C	4.99167600	-3.04333500	-0.24311300
C	3.93249300	-0.84849900	-0.01403100
C	5.17055600	-0.27750800	-0.29075500
C	6.20721200	-2.44340400	-0.53279100
C	-4.83334200	-3.45003400	0.51575700
H	-4.98915900	-3.49830000	1.59894500
H	-4.39695500	-4.39530200	0.18122500
C	3.30217800	-4.52626500	0.51000600
H	2.62112400	-5.31591900	0.18048300
H	3.45622700	-4.62103700	1.59048800
C	4.65780600	-4.51277100	-0.21310300
H	4.57395500	-4.89692700	-1.23725800
H	5.41961000	-5.10730100	0.30033000
C	-6.14752200	-3.07391000	-0.18640400
H	-7.03221900	-3.42475800	0.35381400
H	-6.19719600	-3.48540800	-1.20207600
I	2.27310000	0.42311700	0.27101600

I	-2.49777500	1.03444100	0.16857300
F	-8.32009300	-1.06856600	-0.79347000
F	-7.73344900	1.57561400	-0.88220000
F	-5.26190600	2.45252700	-0.45781800
F	7.29721500	-3.16805400	-0.79891800
F	7.46228400	-0.46270000	-0.80839200
F	5.33738100	1.04853400	-0.33054700
C	1.47678300	4.01597200	1.18032300
H	2.20925500	3.25718800	1.44689700
C	1.75790000	5.35532900	1.46914300
H	2.52946100	5.57020800	2.20339500
H	0.95626900	6.09191300	1.45278700
C	0.21554400	3.47421800	0.72663000
0	0.06760700	2.24013500	0.57209900
C	-0.98133200	4.36386600	0.47505100
H	-0.78010500	5.43170000	0.58509600
H	-1.77044600	4.08558700	1.18466200
H	-1.36782100	4.16934600	-0.53222200
C	3.90211200	5.35591600	-0.16633200
H	4.83212000	5.62670600	0.32523300
C	2.72931400	6.12695300	-0.15541800
H	2.71956300	7.19089100	0.06801000
C	3.63027300	4.10692800	-0.76055800
H	4.29868800	3.25225000	-0.77314400
C	2.31840400	4.10293400	-1.20400600
H	1.81714900	3.27688500	-1.70035600
C	1.81017800	5.50779600	-1.17910100
H	0.73923100	5.63100700	-1.00703200
H	2.04614200	5.96908900	-2.15360000

Zero-point correction= 0.483381 (Hartree/Particle)

Thermal correction to Energy= 0.524227

Thermal correction to Enthalpy= 0.525171

Thermal correction to Gibbs Free Energy= 0.405654

Sum of electronic and zero-point Energies= -2836.818204

Sum of electronic and thermal Energies= -2836.777357

Sum of electronic and thermal Enthalpies= -2836.776413

Sum of electronic and thermal Free Energies= -2836.895931

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.10241388

DA-2a-product-complex

H	0.14152000	-3.72852100	-1.25023700
C	0.11984500	-3.08156000	-0.38025500
C	0.06093500	-1.30277400	1.92600200
C	-1.05783900	-2.63797200	0.20969100
C	1.26673400	-2.59346600	0.23497800
C	1.23910100	-1.74739700	1.33618900
C	-1.08623000	-1.79249500	1.31142000
H	0.03878600	-0.62799600	2.77531600
0	-2.33961000	-2.90175400	-0.19119500
0	-2.38921300	-1.50686900	1.62681800
0	2.52319400	-1.41150900	1.67900800
0	2.56602400	-2.80802300	-0.13815700
C	3.39515100	-2.16561300	0.84040900
C	-3.21316300	-2.29476600	0.77117600
C	-4.00749900	-3.33813100	1.56796200
H	-3.42434700	-4.25454200	1.69436000
H	-4.19758200	-2.90204000	2.55477600
C	-5.33273700	-3.52703100	0.81376800
H	-5.27585000	-4.35484400	0.09619600
H	-6.17649900	-3.72710300	1.48114500
C	4.21601700	-3.17532400	1.65335000
H	4.37091200	-2.73067100	2.64250400

H	3.66767800	-4.11408500	1.77117800
C	5.56104400	-3.31243500	0.92320000
H	6.39990700	-3.47806600	1.60600300
H	5.54978500	-4.14272600	0.20631700
C	4.44249700	-1.32991900	0.13088100
C	6.65002300	-0.24382500	-1.11527600
C	4.28545200	-0.13274300	-0.56812600
C	5.66390200	-2.00182000	0.18608500
C	6.77182700	-1.45233000	-0.44088100
C	5.41493700	0.40336300	-1.17775800
C	-4.27949700	-1.50053200	0.04300100
C	-6.50705400	-0.50013300	-1.23866600
C	-5.47427600	-2.22017600	0.07647400
C	-4.15758700	-0.29653300	-0.65164000
C	-5.29762500	0.19540000	-1.27920300
C	-6.59253700	-1.71372800	-0.56802200
I	2.45998900	0.88573300	-0.76241600
I	-2.37539900	0.80009300	-0.81505900
F	-7.57480100	0.00611200	-1.85253900
F	-7.75629300	-2.36816200	-0.56022900
F	-5.28011800	1.34849700	-1.94924800
F	5.36273000	1.55392600	-1.85029000
F	7.70714100	0.30291500	-1.71247800
F	7.96021400	-2.06018800	-0.41261900
C	0.17337400	3.70374100	-0.36204600
0	0.00766600	2.64925000	-0.97139700
C	0.04568500	5.02794300	-1.06927000
H	0.04283700	4.87762600	-2.15150800
H	0.85802300	5.70344800	-0.77703200
H	-0.89763600	5.50577000	-0.77282300
C	0.53839400	3.74960400	1.10569800

H	1.58844100	4.08062400	1.13884100
C	0.34446800	2.42851300	1.88674700
H	-0.08232200	1.64168800	1.25539000
H	1.29785100	2.05908800	2.28324900
C	-0.61336000	2.84721300	3.04140800
H	-0.65074100	2.13726400	3.87174600
C	-1.93602900	3.18231100	2.38171600
H	-2.80442000	2.52916400	2.36785100
C	-1.77520400	4.33347100	1.71212800
H	-2.48638800	4.81335600	1.04443500
C	-0.33533500	4.77320100	1.91534500
H	-0.10462000	5.82057900	1.70521300
C	-0.08232600	4.25969800	3.34121400
H	0.97894800	4.27135700	3.62249500
H	-0.67843300	4.79265800	4.09054000

Zero-point correction= 0.487352 (Hartree/Particle)

Thermal correction to Energy= 0.527758

Thermal correction to Enthalpy= 0.528702

Thermal correction to Gibbs Free Energy= 0.408526

Sum of electronic and zero-point Energies= -2836.879128

Sum of electronic and thermal Energies= -2836.838723

Sum of electronic and thermal Enthalpies= -2836.837778

Sum of electronic and thermal Free Energies= -2836.957954

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.16678822

2b-catalyzed Diels-Alder Reaction

2b-C2

H	2.54032700	-0.09692800	-1.54341500
C	1.45695600	-0.05613800	-1.56318900
C	-1.45695600	0.05613800	-1.56318900
C	0.65002500	-1.18797300	-1.56407300

C	0.73815000	1.13306200	-1.56756000
C	-0.65002500	1.18797300	-1.56407300
C	-0.73815000	-1.13306200	-1.56756000
H	-2.54032700	0.09692800	-1.54341500
0	1.23875000	2.40889700	-1.51724300
0	-1.04869800	2.49821200	-1.50853000
0	1.04869800	-2.49821200	-1.50853000
0	-1.23875000	-2.40889700	-1.51724300
C	0.13241600	3.29388300	-1.65547500
C	-0.13241600	-3.29388300	-1.65547500
C	0.11726800	4.40659700	-0.62295600
C	-0.05976700	6.74655700	0.87972000
C	-0.17948700	5.61552400	-1.25300000
C	0.27951700	4.33206000	0.75576500
C	0.20583800	5.52190700	1.50875600
C	-0.26671400	6.79563100	-0.50115000
C	-0.11726800	-4.40659700	-0.62295600
C	0.05976700	-6.74655700	0.87972000
C	0.17948700	-5.61552400	-1.25300000
C	-0.27951700	-4.33206000	0.75576500
C	-0.20583800	-5.52190700	1.50875600
C	0.26671400	-6.79563100	-0.50115000
C	0.17768000	4.03746100	-2.99778200
H	-0.34303600	3.46911400	-3.77296100
H	1.23387900	4.12632600	-3.27346100
C	-0.17768000	-4.03746100	-2.99778200
H	0.34303600	-3.46911400	-3.77296100
H	-1.23387900	-4.12632600	-3.27346100
C	0.41214100	-5.42899000	-2.72758700
H	1.49147500	-5.45990500	-2.92569700
H	-0.05253600	-6.21896000	-3.32640300

C	-0.41214100	5.42899000	-2.72758700
H	-1.49147500	5.45990500	-2.92569700
H	0.05253600	6.21896000	-3.32640300
I	-0.57403500	-2.49540500	1.72329700
I	0.57403500	2.49540500	1.72329700
H	-0.11209800	7.65273100	1.47541000
H	0.11209800	-7.65273100	1.47541000
C	-0.56608200	8.03978200	-1.15329200
N	-0.80879900	9.03672700	-1.70013500
C	0.39266600	5.51681800	2.93338900
N	0.54077800	5.54356400	4.08628800
C	-0.39266600	-5.51681800	2.93338900
N	-0.54077800	-5.54356400	4.08628800
C	0.56608200	-8.03978200	-1.15329200
N	0.80879900	-9.03672700	-1.70013500

Zero-point correction= 0.337758 (Hartree/Particle)

Thermal correction to Energy= 0.369250

Thermal correction to Enthalpy= 0.370194

Thermal correction to Gibbs Free Energy= 0.271089

Sum of electronic and zero-point Energies= -2185.790065

Sum of electronic and thermal Energies= -2185.758573

Sum of electronic and thermal Enthalpies= -2185.757629

Sum of electronic and thermal Free Energies= -2185.856734

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2186.66039942

2b-Cs

H	0.37125200	-2.07883500	2.80040100
C	0.41339500	-2.28997900	1.73772600
C	0.51786200	-2.78517000	-1.13240400
C	1.59381300	-2.29135800	1.00658200
C	-0.71124400	-2.55633600	0.96784000

C	-0.66499400	-2.79044100	-0.40028500
C	1.64648400	-2.52598500	-0.36151500
H	0.55456100	-2.94662300	-2.20414000
0	2.85168000	-2.00798900	1.46592800
0	2.94254300	-2.39783300	-0.78932000
0	-2.01515600	-2.56410800	1.38403600
0	-1.94246300	-2.95241600	-0.87205000
C	3.75076800	-2.22108700	0.38009900
C	-2.80980600	-2.96089300	0.26732900
C	4.70925100	-1.06208700	0.18602200
C	6.82180000	0.71134200	-0.16274100
C	6.00715600	-1.55187700	0.05092600
C	4.41702600	0.29863700	0.09513700
C	5.50542700	1.18438000	-0.06295100
C	7.07726900	-0.66151400	-0.12279800
H	7.63807700	1.41744400	-0.28262300
C	-3.98648200	-2.02922600	0.05204600
C	-6.41941200	-0.72667200	-0.28590600
C	-5.15455000	-2.77553000	-0.09015400
C	-3.97916600	-0.63727700	-0.02945000
C	-5.22824200	0.00533600	-0.17596500
C	-6.38508100	-2.12333000	-0.26314500
H	-7.36459900	-0.20397800	-0.39851200
C	6.04221000	-3.05585700	0.07679800
H	6.87574300	-3.44443000	0.67119800
H	6.17091800	-3.42923800	-0.94743800
C	-3.45595700	-4.33581200	0.51017400
H	-2.84348300	-5.13183300	0.07871600
H	-3.50085400	-4.47667400	1.59503300
C	-4.87796600	-4.25400800	-0.06717700
H	-4.92626100	-4.64435300	-1.09197100

H -5.61474300 -4.80665100 0.52525100
C 4.66638700 -3.42598900 0.65113700
H 4.23640100 -4.34009000 0.23325100
H 4.73264300 -3.53371100 1.73883100
I -2.18720100 0.49630000 -0.07587000
I 2.43446300 1.03111700 0.05611500
C 8.41602100 -1.16297200 -0.25375500
N 9.49355600 -1.58855800 -0.35651300
C 5.30148300 2.60623400 -0.13665500
N 5.18131400 3.76152300 -0.19648400
C -7.59080800 -2.88925600 -0.40659300
N -8.55715800 -3.52649100 -0.52002100
C -5.31525400 1.44077100 -0.21174300
N -5.42117200 2.59941500 -0.22979300
Zero-point correction= 0.337935 (Hartree/Particle)
Thermal correction to Energy= 0.369382
Thermal correction to Enthalpy= 0.370326
Thermal correction to Gibbs Free Energy= 0.270734
Sum of electronic and zero-point Energies= -2185.789887
Sum of electronic and thermal Energies= -2185.758440
Sum of electronic and thermal Enthalpies= -2185.757496
Sum of electronic and thermal Free Energies= -2185.857088
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2186.66027776

DA-2b-Binary-1
H 0.00005100 -2.73506900 -2.07455900
C 0.00003300 -2.42957500 -1.03426300
C 0.00002000 -1.55404300 1.74680200
C 1.16183600 -2.20014300 -0.30679600
C -1.16178900 -2.20014400 -0.30681200
C -1.16168900 -1.78581300 1.01910800

C	1.16174200	-1.78581300	1.01913100
H	0.00000800	-1.21513000	2.77712900
0	-2.45458300	-2.28349700	-0.75254600
0	-2.45526100	-1.60298200	1.43412000
0	2.45463500	-2.28351800	-0.75252100
0	2.45531000	-1.60302900	1.43415100
C	-3.29868300	-2.06547200	0.38351600
C	3.29873300	-2.06551000	0.38353500
C	-4.39481300	-1.08436000	0.01019200
C	-6.70132400	0.29316100	-0.72008800
C	-5.59705400	-1.77559300	-0.13961400
C	-4.30066900	0.28073400	-0.24646700
C	-5.48043500	0.97125800	-0.59695300
C	-6.76184000	-1.08601100	-0.50563800
C	4.39483700	-1.08437100	0.01022800
C	6.70129400	0.29323500	-0.72005200
C	5.59710100	-1.77556100	-0.13957400
C	4.30064500	0.28071800	-0.24641900
C	5.48038100	0.97128900	-0.59690700
C	6.76186100	-1.08593500	-0.50560200
C	-4.06092400	-3.33188100	0.79792700
H	-4.19998600	-3.27677600	1.88291000
H	-3.48115200	-4.22802700	0.56137800
C	4.06100500	-3.33190700	0.79793900
H	3.48126300	-4.22806000	0.56134100
H	4.20002100	-3.27683100	1.88292900
C	5.42174300	-3.25207900	0.09111100
H	5.40794500	-3.76682000	-0.87838900
H	6.23938300	-3.68330700	0.67798600
C	-5.42163400	-3.25210800	0.09104500
H	-6.23927800	-3.68340500	0.67786400

H	-5.40775100	-3.76681600	-0.87847200
I	2.46572000	1.29950400	-0.17953900
I	-2.46579200	1.29961900	-0.17965900
C	-0.00028500	3.51399400	2.26248500
H	-0.00050100	4.34805800	2.96171400
C	-0.00026500	2.24327700	2.68217100
H	-0.00049000	1.98804300	3.73899600
H	-0.00001700	1.41986400	1.96842300
C	0.00005500	3.84479900	0.81450300
0	0.00018500	2.96496500	-0.05208000
C	0.00038200	5.30080400	0.45225100
H	0.00066200	5.42691500	-0.63226700
H	0.88203300	5.78744400	0.88893400
H	-0.88131600	5.78773300	0.88851400
H	-7.59571600	0.84601400	-0.99148900
H	7.59566600	0.84612200	-0.99145300
C	8.00021400	-1.79749000	-0.65541500
N	8.99330900	-2.39143800	-0.77018400
C	5.46830300	2.38714300	-0.84470200
N	5.49334700	3.53185300	-1.04773200
C	-5.46840600	2.38711000	-0.84476300
N	-5.49349300	3.53181300	-1.04782000
C	-8.00016600	-1.79761100	-0.65545200
N	-8.99324100	-2.39159700	-0.77020500

Zero-point correction= 0.428825 (Hartree/Particle)
Thermal correction to Energy= 0.468064
Thermal correction to Enthalpy= 0.469009
Thermal correction to Gibbs Free Energy= 0.350871
Sum of electronic and zero-point Energies= -2416.663509
Sum of electronic and thermal Energies= -2416.624270
Sum of electronic and thermal Enthalpies= -2416.623326

Sum of electronic and thermal Free Energies= -2416.741464

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2417.70783868

DA-2b-Bindary-2

H	-0.04779000	-2.63741100	-2.25045300
C	-0.04530200	-2.47605800	-1.17825500
C	-0.03762600	-1.97455600	1.69347500
C	1.11847300	-2.36185300	-0.42682900
C	-1.20514800	-2.32852800	-0.42645900
C	-1.20034400	-2.09390000	0.94256000
C	1.12078100	-2.12771300	0.94218900
H	-0.03429400	-1.76272000	2.75684600
0	-2.49835700	-2.32494200	-0.87974900
0	-2.49064000	-1.93872000	1.37822900
0	2.41099600	-2.39439300	-0.88091400
0	2.41502700	-2.00841200	1.37731600
C	-3.34224400	-2.22313300	0.27311000
C	3.25897800	-2.30737800	0.27004300
C	-4.39237900	-1.15390500	0.03589500
C	-6.63420700	0.41386000	-0.48529600
C	-5.62431000	-1.76332800	-0.20120600
C	-4.23519500	0.22735000	-0.02869000
C	-5.38355800	1.01123200	-0.27615400
C	-6.75650700	-0.97807400	-0.46265500
C	4.32680400	-1.25554200	0.03284800
C	6.59558600	0.27616400	-0.48028500
C	5.54926300	-1.88455300	-0.20163900
C	4.19270800	0.12809300	-0.03060100
C	5.35422100	0.89366500	-0.27406200
C	6.69493900	-1.11762700	-0.45855800
C	-4.16111400	-3.49921500	0.51217300

H	-4.30159300	-3.58693300	1.59479500
H	-3.62036600	-4.37930200	0.15417400
C	4.05670400	-3.59722700	0.50727900
H	3.50218000	-4.46743400	0.14630900
H	4.19368200	-3.68986700	1.58991500
C	5.41523800	-3.38312400	-0.17614000
H	5.41639600	-3.76040700	-1.20703700
H	6.24419700	-3.86809500	0.34943800
C	-5.51450700	-3.26395900	-0.17423600
H	-6.35207300	-3.73532500	0.35006400
H	-5.51954800	-3.64202600	-1.20484200
I	2.34195600	1.10691400	0.15820400
I	-2.36875700	1.17617900	0.16288700
C	1.31141500	4.82400200	0.07942900
H	2.19941800	4.19381300	0.11044100
C	1.41571400	6.15382200	-0.02949300
H	2.38887900	6.63535500	-0.08830700
H	0.54553900	6.80643800	-0.06406700
C	0.01638500	4.11182100	0.16165800
0	0.00384300	2.88061400	0.26891300
C	-1.26162700	4.90586800	0.11149000
H	-2.12798000	4.24247400	0.17140700
H	-1.30950600	5.48184000	-0.81994500
H	-1.29188200	5.62069800	0.94216000
H	-7.50281200	1.03767900	-0.67354700
H	7.47485300	0.88583700	-0.66523700
C	7.95394200	-1.76692500	-0.69336000
N	8.96415200	-2.31192300	-0.87976000
C	5.28816000	2.32926900	-0.32386600
N	5.24856500	3.49107300	-0.36482100
C	-5.29510100	2.44552000	-0.32771400

N -5.23904900 3.60653500 -0.37053500

C -8.02534800 -1.60631500 -0.70183100

N -9.04403100 -2.13400600 -0.89191200

Zero-point correction= 0.429398 (Hartree/Particle)

Thermal correction to Energy= 0.468366

Thermal correction to Enthalpy= 0.469310

Thermal correction to Gibbs Free Energy= 0.353227

Sum of electronic and zero-point Energies= -2416.666157

Sum of electronic and thermal Energies= -2416.627189

Sum of electronic and thermal Enthalpies= -2416.626245

Sum of electronic and thermal Free Energies= -2416.742328

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2417.70917379

DA-2b-endo-cis

H 0.10078400 -3.34453200 -2.00317900

C 0.09660400 -3.05419600 -0.95850800

C 0.08223000 -2.20508500 1.82962700

C 1.25429700 -2.78610300 -0.23689500

C -1.06832900 -2.87836900 -0.22087300

C -1.07388500 -2.47532700 1.10821800

C 1.24657500 -2.38755000 1.09351100

H 0.07576600 -1.86335300 2.85857000

0 -2.35987000 -2.99883400 -0.66147600

0 -2.36935300 -2.32838400 1.52986600

0 2.54620600 -2.80449000 -0.69435000

0 2.53388500 -2.15171900 1.50134600

C -3.21307000 -2.75363600 0.46373500

C 3.38938700 -2.55157700 0.43554100

C -4.26641100 -1.72804400 0.08454500

C -6.50778700 -0.25279200 -0.66224800

C -5.49421200 -2.36849800 -0.08023800

C	-4.10950600	-0.36603500	-0.15997300
C	-5.26010900	0.36977000	-0.52242300
C	-6.62676400	-1.62967500	-0.45355200
C	4.42444400	-1.50269700	0.07153100
C	6.64827700	0.02213400	-0.62294900
C	5.66380900	-2.12036200	-0.09565700
C	4.24983900	-0.13885300	-0.14992700
C	5.39060000	0.62490600	-0.48056500
C	6.78679500	-1.35696800	-0.44564900
C	-4.02904200	-3.99225700	0.85866800
H	-4.17234700	-3.94310500	1.94338100
H	-3.48424500	-4.90847500	0.61643800
C	4.22741900	-3.77804500	0.82328600
H	3.69768600	-4.70254600	0.57866800
H	4.37439100	-3.73086700	1.90760300
C	5.57407500	-3.60897100	0.10522800
H	5.57790800	-4.10418900	-0.87453400
H	6.42068600	-4.00593600	0.67486800
C	-5.38174300	-3.85210900	0.14475900
H	-6.21967400	-4.25161700	0.72551500
H	-5.38445800	-4.36376600	-0.82650700
I	2.36473400	0.79103700	-0.06923800
I	-2.25145100	0.62842700	-0.09060100
C	0.76842600	4.44044900	-0.57769600
H	0.83404900	5.25581400	-1.29291100
C	1.38587300	4.50016700	0.67165300
H	2.12113800	5.27938100	0.86305700
H	1.55290500	3.56720800	1.20294900
C	-0.00871300	3.28368000	-0.90897000
0	-0.07011100	2.30728300	-0.11367600
C	-0.79657300	3.25071700	-2.19517800

H	-0.56636100	4.10480200	-2.83947200
H	-1.87064600	3.26065100	-1.96317400
H	-0.58779300	2.31779600	-2.73243000
C	-0.98341600	4.26347300	1.99794700
H	-1.00588400	3.41876300	2.67991800
C	0.00571000	5.25447100	1.96553900
H	0.66277100	5.45944800	2.80693300
C	-1.88896000	4.46943100	0.92708900
H	-2.68759200	3.79077900	0.63926700
C	-1.51766400	5.60378900	0.24362300
H	-2.00483400	6.00245200	-0.64135700
C	-0.50229900	6.34707600	1.05085800
H	-1.03579200	7.08898300	1.66950000
H	0.25869700	6.88297400	0.47745500
H	7.50993100	0.63143200	-0.87884700
H	-7.37589300	0.33661100	-0.94203800
C	-5.16701700	1.78380900	-0.77043200
N	-5.09560900	2.92737600	-0.97328300
C	-7.89114000	-2.28951500	-0.61888900
N	-8.90631800	-2.84238900	-0.74663300
C	5.29601300	2.04555200	-0.68336100
N	5.25254000	3.19623100	-0.84669400
C	8.06245900	-1.99395500	-0.61389300
N	9.08676000	-2.52892500	-0.74435800

Zero-point correction= 0.525496 (Hartree/Particle)

Thermal correction to Energy= 0.568287

Thermal correction to Enthalpy= 0.569231

Thermal correction to Gibbs Free Energy= 0.444627

Sum of electronic and zero-point Energies= -2610.407663

Sum of electronic and thermal Energies= -2610.364872

Sum of electronic and thermal Enthalpies= -2610.363928

Sum of electronic and thermal Free Energies= -2610.488531

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2611.60939070

DA-2b-product-complex

H	0.24452400	-3.40005600	-1.92191500
C	0.21944800	-3.04789100	-0.89673000
C	0.14865800	-2.03700300	1.83653300
C	-0.95826300	-2.86952400	-0.18006200
C	1.36020800	-2.69783600	-0.18281100
C	1.32563400	-2.22050200	1.12140500
C	-0.98972700	-2.39061900	1.12321100
H	0.11981800	-1.63883200	2.84460700
0	-2.24227400	-3.05580900	-0.62294000
0	-2.29316200	-2.26405100	1.52576500
0	2.60096400	-1.92282400	1.52676800
0	2.65824900	-2.70526800	-0.62404700
C	3.47709200	-2.39777700	0.51020400
C	-3.11098500	-2.79203900	0.48435400
C	-3.86914000	-4.04390900	0.95289700
H	-3.30098800	-4.94850700	0.72126600
H	-3.97226700	-3.96173000	2.03995100
C	-5.25369200	-3.98191900	0.28937600
H	-5.28147800	-4.54706500	-0.65125300
H	-6.05404900	-4.37177500	0.92691700
C	4.28549600	-3.61086600	0.99221800
H	4.40792300	-3.49946600	2.07489600
H	3.74714500	-4.54096700	0.79130100
C	5.65079100	-3.50505800	0.29780700
H	6.47774500	-3.87838000	0.91067900
H	5.66981400	-4.05886900	-0.64987400
C	4.53598600	-1.38787300	0.11060800

C	6.79769400	0.05695200	-0.62906300
C	4.38913100	-0.03817700	-0.19907300
C	5.76866500	-2.03297500	0.00941300
C	6.91063300	-1.30974400	-0.36280800
C	5.54745100	0.68675200	-0.55354200
C	-4.21131900	-1.83376900	0.06506100
C	-6.53037700	-0.46410000	-0.64783300
C	-5.42368800	-2.51777500	-0.01147600
C	-4.11400300	-0.48452400	-0.26093300
C	-5.29917700	0.20388900	-0.59923300
C	-6.59397200	-1.83247800	-0.37061300
I	2.51394700	0.90802600	-0.22701500
I	-2.27831800	0.52757800	-0.34326800
C	-0.40733500	3.46670000	-0.94124800
0	-0.01850000	2.33897100	-0.63824200
C	-1.32343800	3.67326800	-2.11884600
H	-1.22875300	2.84163300	-2.82254800
H	-1.12088300	4.62689600	-2.61818400
H	-2.36214800	3.70236700	-1.75619900
C	-0.05179400	4.68909700	-0.13196300
H	0.50198600	5.36958400	-0.79410100
C	0.70890800	4.41082700	1.18261400
H	0.90202200	3.34208500	1.32051200
H	1.66903800	4.93846900	1.19932000
C	-0.25260700	4.98359100	2.26609700
H	0.21424000	5.13764200	3.24186700
C	-1.48763800	4.10356800	2.24246200
H	-1.70650400	3.32264500	2.96603900
C	-2.15726400	4.37033600	1.11099300
H	-3.03360500	3.85647100	0.72048000
C	-1.35995100	5.42139500	0.35899000

H	-1.88287700	5.96855700	-0.42905800
C	-0.77971400	6.22767300	1.53032700
H	0.01696300	6.91954900	1.22714700
H	-1.55374800	6.76353100	2.09118600
H	-7.42969600	0.08484300	-0.91050700
C	-7.84265700	-2.53745400	-0.44684100
C	-5.26162100	1.60922900	-0.90153300
C	5.48251800	2.09013200	-0.85825000
C	8.17884400	-1.97484100	-0.46752000
N	-8.84418400	-3.12575900	-0.50271400
N	-5.23350300	2.74792500	-1.13871200
N	5.46653500	3.22556900	-1.10890800
N	9.19665100	-2.53173600	-0.54617900
H	7.67394200	0.63569800	-0.90551300

Zero-point correction= 0.530160 (Hartree/Particle)

Thermal correction to Energy= 0.572226

Thermal correction to Enthalpy= 0.573170

Thermal correction to Gibbs Free Energy= 0.449143

Sum of electronic and zero-point Energies= -2610.462523

Sum of electronic and thermal Energies= -2610.420457

Sum of electronic and thermal Enthalpies= -2610.419513

Sum of electronic and thermal Free Energies= -2610.543540

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2611.66561396

3-catalyzed Diels-Alder Reaction

3-Cs

C	-1.52824500	1.07595200	1.16911700
C	-1.52388900	1.06838500	-1.17871100
C	-2.09820300	-1.08808000	-0.00005800
C	-1.37158800	-0.44526300	-1.17671800
C	-1.37708100	-0.43776500	1.17574700

C	-0.81090800	1.72678900	-0.00562300
H	-2.60136300	1.30551900	-1.11852000
H	-3.16488200	-0.83080700	-0.00350000
H	-0.29852700	-0.68481600	-1.09343600
H	-0.30369700	-0.67765300	1.09838400
H	0.25853400	1.47697700	-0.00285500
H	-2.60521200	1.31434600	1.10483800
H	-1.98746500	-2.17693600	0.00386900
H	-0.92966500	2.81453200	-0.00942100
0	-1.06421300	1.39555900	2.47143600
0	-1.83598800	-0.75709100	2.47853100
0	-1.05733500	1.38164800	-2.48155600
0	-1.82498700	-0.77227800	-2.47957800
C	-1.60080900	0.39325400	3.29741100
C	-1.59423000	0.37589800	-3.30295700
C	-2.90739700	0.79788300	3.99394500
H	-2.81464500	1.85031300	4.28507800
H	-3.76220200	0.68026900	3.32282300
C	-2.96320800	-0.08728500	5.24416800
H	-3.52254500	0.35546500	6.07454100
H	-3.41378200	-1.06406000	5.02279900
C	-2.90317600	0.77695000	-3.99760300
H	-3.75661700	0.65744200	-3.32508500
H	-2.81346800	1.82957900	-4.28897500
C	-2.95948200	-0.10825700	-5.24780000
H	-3.40944400	-1.08531500	-5.02648900
H	-3.51978400	0.33445200	-6.07756800
C	-0.69332200	0.02248200	4.46850300
C	0.44716700	-0.80223900	6.88897200
C	-1.50557100	-0.27506600	5.56907400
C	0.68907300	-0.10286900	4.55668500

C	1.25756900	-0.50815000	5.78565900
C	-0.94150200	-0.69212700	6.78053300
C	-0.68883300	0.00338100	-4.47479100
C	0.44960300	-0.82305600	-6.89543100
C	-1.50210800	-0.29525700	-5.57418700
C	0.69345600	-0.12241800	-4.56381600
C	1.26097500	-0.52841900	-5.79292300
C	-0.93897000	-0.71308700	-6.78588700
I	1.98376900	0.25904600	-2.94924600
I	1.97916700	0.27926500	2.94198000
C	-1.78847200	-1.01098600	-7.90520300
N	-2.49235500	-1.24626600	-8.80028900
C	2.68311400	-0.65519200	-5.95801600
N	3.82710900	-0.76913400	-6.13270100
C	2.67983900	-0.63466200	5.94982800
N	3.82394700	-0.74856100	6.12383100
C	-1.78994500	-0.98905800	7.90090800
N	-2.49287300	-1.22361900	8.79693000
H	0.90657500	-1.13258700	-7.83037600
H	0.90492400	-1.11118800	7.82373000

Zero-point correction= 0.409462 (Hartree/Particle)
Thermal correction to Energy= 0.441718
Thermal correction to Enthalpy= 0.442662
Thermal correction to Gibbs Free Energy= 0.341219
Sum of electronic and zero-point Energies= -2189.317449
Sum of electronic and thermal Energies= -2189.285193
Sum of electronic and thermal Enthalpies= -2189.284249
Sum of electronic and thermal Free Energies= -2189.385692
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2190.26733920

DA-3-Binary

C	1.18227500	-2.05984800	1.40655600
C	-1.18233500	-2.06030100	1.40704800
C	-0.00012200	-3.08136700	-0.58146900
C	-1.17007400	-2.22894200	-0.10460600
C	1.16951000	-2.22817400	-0.10512100
C	-0.00005900	-1.24883200	1.91365800
H	-1.15884700	-3.06563300	1.86390700
H	0.00031600	-4.06718800	-0.09990600
H	-1.07555100	-1.23133600	-0.56427700
H	1.07399500	-1.23055500	-0.56456400
H	1.15933300	-3.06526600	1.86326000
H	-0.00033000	-3.20621400	-1.66869600
0	2.46433900	-1.48245500	1.60122400
0	2.47957800	-2.71957200	-0.32455000
0	-2.47994600	-2.72127200	-0.32313700
0	-2.46455100	-1.48334500	1.60209000
C	-3.30933500	-2.07225200	0.64289000
C	3.30906700	-2.07156500	0.64218700
C	-4.28396800	-3.10434000	1.21437800
H	-4.66731500	-2.71376800	2.16376200
H	-3.78083000	-4.05900500	1.38926800
C	4.28283700	-3.10449300	1.21373200
H	3.77920300	-4.05909600	1.38752600
H	4.66548700	-2.71472100	2.16372900
C	-4.24276700	-1.07052800	-0.04602200
C	-6.32082400	0.23198300	-1.39853400
C	-5.43501900	-1.74652800	-0.33943200
C	-4.07150600	0.26238200	-0.41655200
C	-5.13416100	0.90772100	-1.09393200
C	-6.47423000	-1.10467800	-1.02191900
H	-7.11935600	0.75375600	-1.91697100

C	4.24330300	-1.07011400	-0.04587600
C	6.32238600	0.23225000	-1.39681500
C	4.07236500	0.26281300	-0.41653400
C	5.43560500	-1.74629500	-0.33855400
C	6.47536700	-1.10447100	-1.02025000
C	5.13557200	0.90811200	-1.09303100
H	7.12134200	0.75397600	-1.91464800
C	-5.40983000	-3.16132600	0.17591000
H	-6.37620500	-3.47384600	0.58459600
H	-5.15764900	-3.84534300	-0.64541700
C	5.40966200	-3.16125300	0.17629500
H	6.37557800	-3.47413000	0.58579800
H	5.15817700	-3.84490000	-0.64555600
I	2.33823100	1.40116100	-0.02632300
I	-2.33785100	1.40100100	-0.02489700
C	-5.04461200	2.28643000	-1.49317000
C	-7.68967000	-1.81254000	-1.31256100
C	5.04637800	2.28685600	-1.49221100
C	7.69091500	-1.81242300	-1.31021400
N	-8.66717100	-2.40062200	-1.53830900
N	-5.02233400	3.39780400	-1.83521900
N	5.02446700	3.39830000	-1.83405700
N	8.66850000	-2.40057700	-1.53541200
C	-0.00176600	4.15244900	1.10977400
0	0.00040200	3.21392400	0.30854000
C	-0.00510100	3.92664700	2.57830900
H	0.00013600	-1.15375800	3.00420100
H	-0.00030100	-0.24972300	1.46290600
H	-0.00900100	4.80839500	3.21629600
C	-0.00275600	2.68957500	3.08645500
H	0.00166600	1.82044500	2.42993000

H	-0.00488500	2.50643100	4.15787700
C	-0.00118600	5.57899100	0.64408900
H	-0.88426600	6.09534300	1.04201200
H	0.87896400	6.09641700	1.04705100
H	0.00185500	5.62690400	-0.44664700

Zero-point correction= 0.501074 (Hartree/Particle)
Thermal correction to Energy= 0.541018
Thermal correction to Enthalpy= 0.541962
Thermal correction to Gibbs Free Energy= 0.421991
Sum of electronic and zero-point Energies= -2420.189226
Sum of electronic and thermal Energies= -2420.149282
Sum of electronic and thermal Enthalpies= -2420.148338
Sum of electronic and thermal Free Energies= -2420.268309
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2421.31369539

DA-3-endo-cis

C	1.27477400	-2.34490800	1.63189400
C	-1.08883800	-2.42289300	1.63726200
C	0.13284500	-3.64973000	-0.20728700
C	-1.06661900	-2.78563900	0.16001800
C	1.27065200	-2.70237400	0.15334700
C	0.06585600	-1.51626100	2.04046000
H	-1.03356800	-3.36085200	2.21843100
H	0.16783900	-4.56551800	0.39617000
H	-1.00804400	-1.85308900	-0.42461400
H	1.14237500	-1.77418700	-0.42815200
H	0.03421900	-0.57270700	1.48318000
H	1.28164100	-3.28641300	2.20952200
H	0.13896500	-3.91201500	-1.26981900
H	0.06093800	-1.29944300	3.11337500
0	2.53954400	-1.71033600	1.75158300

0	2.59579600	-3.17608700	-0.00534300
0	-2.35736600	-3.34874600	0.01174700
0	-2.39095900	-1.86945200	1.75776300
C	-3.21221100	-2.58336200	0.86321900
C	3.40314100	-2.38231400	0.86674700
C	-4.19695200	-3.53906200	1.53998700
H	-4.60568100	-3.03144300	2.42100200
H	-3.69493800	-4.45943400	1.84997000
C	4.41596700	-3.30068300	1.55442000
H	3.94696900	-4.24204400	1.85286700
H	4.79081200	-2.78117000	2.44352600
C	-4.13133000	-1.68636500	0.02601000
C	-6.17634200	-0.58537800	-1.53906100
C	-5.31214600	-2.40325800	-0.20711800
C	-3.95048200	-0.40974600	-0.50704000
C	-5.00001500	0.13021900	-1.29130000
C	-6.33531400	-1.86278400	-0.99473200
H	-6.96229300	-0.14160600	-2.14268800
C	4.29761600	-1.44398600	0.04840700
C	6.31832400	-0.25767800	-1.48486300
C	4.07548800	-0.17482500	-0.48601900
C	5.50946600	-2.11223100	-0.17048500
C	6.52097600	-1.52879400	-0.94165200
C	5.11116100	0.41112900	-1.25367600
H	7.09390200	0.21947000	-2.07623500
C	-5.29633200	-3.73817800	0.48998100
H	-6.27154100	-4.00166700	0.91221800
H	-5.02093000	-4.52309000	-0.22716600
C	5.53744900	-3.45009400	0.52026400
H	6.51653500	-3.67544300	0.95535500
H	5.30484700	-4.24149100	-0.20482500

I	2.30770800	0.94742600	-0.20276900
I	-2.23853000	0.80545900	-0.21928100
C	-4.89292200	1.44814300	-1.85958200
C	-7.53950600	-2.61147700	-1.22119900
C	4.96992600	1.72323900	-1.82584400
C	7.75722300	-2.22816200	-1.15282700
N	-8.50837100	-3.23164000	-1.39264900
N	-4.83662900	2.51034300	-2.33103000
N	4.90542900	2.77941100	-2.30873000
N	8.75218600	-2.80894700	-1.31169500
C	-0.01205500	3.59525500	-0.57860900
0	-0.10313000	2.52180800	0.07642000
C	0.77747500	4.68163200	-0.07900000
H	0.85932800	5.59095000	-0.66799700
C	1.39031900	4.54882700	1.16650000
H	1.54256500	3.54528400	1.55535400
H	2.13335600	5.28238800	1.47330900
C	-0.97678100	4.14257800	2.44556500
H	-1.00191400	3.20925700	2.99971800
C	0.01286000	5.12638800	2.55773300
H	0.67088800	5.20698800	3.41916400
C	-1.87861300	4.50068100	1.41250100
H	-2.67146000	3.86523400	1.02805300
C	-1.50420900	5.71965500	0.89756600
H	-1.98811700	6.24162400	0.07736500
C	-0.48955000	6.33848200	1.80544600
H	0.27466600	6.94778400	1.31587700
H	-1.02266700	6.98717500	2.52148100
C	-0.76566200	3.74520100	-1.87669700
H	-0.54780300	4.69646900	-2.37162900
H	-0.50463200	2.91678400	-2.54684500

H -1.84590900 3.68013400 -1.68798100

Zero-point correction= 0.597479 (Hartree/Particle)

Thermal correction to Energy= 0.640968

Thermal correction to Enthalpy= 0.641912

Thermal correction to Gibbs Free Energy= 0.515259

Sum of electronic and zero-point Energies= -2613.934012

Sum of electronic and thermal Energies= -2613.890524

Sum of electronic and thermal Enthalpies= -2613.889580

Sum of electronic and thermal Free Energies= -2614.016232

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2615.21532885

DA-3-product-complex

C 1.34069900 -1.59857600 1.75129400

C -1.01859300 -1.67876400 1.72309300

C 0.24302100 -3.33906300 0.28999800

C -0.96522600 -2.41867700 0.39538000

C 1.37660500 -2.32985700 0.41816000

C 0.12628900 -0.68827700 1.88741000

H -0.97066300 -2.42821400 2.53295500

H 0.26411800 -4.06690100 1.11090300

H -0.90109200 -1.67334300 -0.41462200

H 1.27567400 -1.58700100 -0.39104700

H 1.31015200 -2.35663000 2.55397300

H 0.27126200 -3.86859100 -0.66733300

0 2.61425700 -0.97024300 1.75355900

0 2.69809100 -2.83681500 0.43214500

0 -2.24682900 -3.02105900 0.38147700

0 -2.32897500 -1.13099400 1.66982000

C -3.12675000 -2.08967900 1.01400100

C 3.49216400 -1.84855000 1.09058100

C -4.06363500 -2.86315200 1.94356400

H	-4.49611700	-2.14924500	2.65361100
H	-3.51705400	-3.63589100	2.49064000
C	4.48297700	-2.56730800	2.00806800
H	3.99602700	-3.39120500	2.53645400
H	4.86064400	-1.83865600	2.73423400
C	-4.08924900	-1.50394000	-0.02623000
C	-6.17036300	-1.00996400	-1.83607500
C	-5.22956100	-2.31826100	-0.03912200
C	-3.97356800	-0.43123000	-0.90920400
C	-5.03632700	-0.19059500	-1.81242400
C	-6.26948600	-2.08182700	-0.94535400
H	-6.97042400	-0.80189600	-2.53986000
C	4.41328700	-1.15935200	0.07628900
C	6.46530600	-0.43974300	-1.68847000
C	4.22486600	-0.06078600	-0.76089700
C	5.61214400	-1.88370400	0.04726900
C	6.63841100	-1.53527700	-0.83819800
C	5.27363600	0.29211100	-1.64334100
H	7.25274400	-0.14424400	-2.37500200
C	-5.15107600	-3.39935400	1.00630600
H	-6.11343100	-3.57609100	1.49738500
H	-4.83926400	-4.34087300	0.53457600
C	5.60770200	-2.99901700	1.05935600
H	6.57930900	-3.12352100	1.54824400
H	5.36108800	-3.94553200	0.55985600
I	2.48882700	1.13305800	-0.74148300
I	-2.32815300	0.88369600	-0.93475300
C	-4.99776200	0.90980100	-2.73735000
C	-7.42980200	-2.92818700	-0.94432300
C	5.15974300	1.42268400	-2.52438800
C	7.86064600	-2.28934700	-0.85458500

N	-8.36198000	-3.62326700	-0.92844900
N	-5.01089200	1.78766300	-3.50015900
N	5.11295700	2.32765800	-3.25345000
N	8.84388100	-2.91036100	-0.85283300
C	-0.36158300	3.80531300	-0.10956200
0	0.00865600	2.72956200	-0.57779900
C	0.01239300	4.26086600	1.28275100
C	-1.58343700	2.47153700	2.78441900
H	-1.89262100	1.43087700	2.85375500
C	-0.30261100	3.04753500	3.35917600
C	-2.16982500	3.43433900	2.05725100
H	-3.05161400	3.33928500	1.42849000
C	-1.26756200	4.65329200	2.11469300
C	-0.70998100	4.52056900	3.53988100
H	0.14418300	5.18208600	3.73507900
H	-1.48243500	4.66395800	4.30381700
H	0.10051000	-0.18420400	2.85984900
H	0.10086100	0.06719500	1.09146800
H	0.11586600	2.53156200	4.22721900
H	-1.70867300	5.61070600	1.82689700
H	0.64525400	5.15267000	1.16625800
C	0.68683200	3.18736400	2.16533800
H	0.82446300	2.24492100	1.62782200
H	1.66839700	3.52635900	2.51567700
C	-1.25319600	4.71731000	-0.91055100
H	-1.22169100	4.44015600	-1.96757600
H	-2.28591400	4.61059700	-0.55025900
H	-0.96736300	5.76682500	-0.77754500

Zero-point correction= 0.602088 (Hartree/Particle)

Thermal correction to Energy= 0.644768

Thermal correction to Enthalpy= 0.645712

Thermal correction to Gibbs Free Energy= 0.521790

Sum of electronic and zero-point Energies= -2613.990136

Sum of electronic and thermal Energies= -2613.947456

Sum of electronic and thermal Enthalpies= -2613.946512

Sum of electronic and thermal Free Energies= -2614.070435

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2615.27308433

1-catalyzed Diels-Alder Reaction

1-A

N	0.45089600	-0.70965000	-0.50087700
H	-0.21226000	0.06381500	-0.55255400
C	-0.03454000	-1.95087700	-0.78536800
S	0.89309900	-3.27210600	-1.22457000
N	-1.39515500	-2.06746700	-0.73857800
H	-1.74745800	-2.93455500	-1.13915900
C	-2.36683800	-1.14725300	-0.27929400
C	-4.38433200	0.59956700	0.59432400
C	-2.19023800	-0.40130900	0.89103800
C	-3.56131900	-1.03395400	-0.99972100
C	-4.55788100	-0.17256700	-0.55313000
C	-3.19539100	0.47035800	1.30585100
H	-1.28436400	-0.50608800	1.48096300
H	-3.69877700	-1.61462200	-1.90770900
H	-5.15806100	1.28533400	0.92508100
C	1.80281300	-0.31222100	-0.39275800
C	4.42980200	0.63443300	-0.11442500
C	2.16582700	0.92224600	-0.93458200
C	2.74688900	-1.06951800	0.30720900
C	4.04906900	-0.59270700	0.42637300
C	3.47175200	1.38542800	-0.78878600
H	1.42634800	1.51812300	-1.46368300
H	2.46312000	-2.00987200	0.76539000

H	5.44504300	1.00152500	-0.00021400
C	-3.01393000	1.23595000	2.58889300
C	-5.86065800	-0.09092300	-1.30274600
F	-5.71640200	-0.42782000	-2.59207900
F	-6.37590200	1.14639300	-1.26011800
F	-6.78353700	-0.91614900	-0.78178800
F	-3.68875000	2.39393900	2.57281700
F	-1.72304300	1.51941900	2.81769500
F	-3.45467500	0.53944400	3.64914800
C	3.86288400	2.69471600	-1.41680600
C	5.07561900	-1.43146000	1.13767800
F	4.51670000	-2.23195000	2.05694100
F	5.98723900	-0.67098100	1.76317700
F	5.74896100	-2.22356600	0.28669400
F	2.82701100	3.54542500	-1.47881600
F	4.30844300	2.53221700	-2.67398000
F	4.84417500	3.29932700	-0.73137900

Zero-point correction= 0.244281 (Hartree/Particle)
Thermal correction to Energy= 0.272499
Thermal correction to Enthalpy= 0.273443
Thermal correction to Gibbs Free Energy= 0.177556
Sum of electronic and zero-point Energies= -2356.277784
Sum of electronic and thermal Energies= -2356.249566
Sum of electronic and thermal Enthalpies= -2356.248622
Sum of electronic and thermal Free Energies= -2356.344509
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2357.22671417

1-B2

N	-0.00464300	1.13077200	1.03314000
H	-0.24803400	1.01362300	2.01632300
C	-0.00000000	0.00000000	0.26261100

S	-0.00000000	0.00000000	-1.40617800
N	0.00464300	-1.13077200	1.03314000
H	0.24803400	-1.01362300	2.01632300
C	-0.05211500	-2.47607800	0.60246300
C	-0.15680500	-5.19170800	-0.10347600
C	-0.97139900	-2.91385500	-0.35659500
C	0.79599200	-3.39681500	1.21916100
C	0.73406600	-4.74401800	0.86577000
C	-1.00503700	-4.26107800	-0.70322900
H	-1.65565700	-2.21082200	-0.81751700
H	1.50489200	-3.05707200	1.97049300
H	-0.19572500	-6.23953800	-0.38306000
C	0.05211500	2.47607800	0.60246300
C	0.15680500	5.19170800	-0.10347600
C	-0.79599200	3.39681500	1.21916100
C	0.97139900	2.91385500	-0.35659500
C	1.00503700	4.26107800	-0.70322900
C	-0.73406600	4.74401800	0.86577000
H	-1.50489200	3.05707200	1.97049300
H	1.65565700	2.21082200	-0.81751700
H	0.19572500	6.23953800	-0.38306000
C	-2.03431200	-4.73781100	-1.69134000
C	1.69700300	-5.70256700	1.50949300
F	1.28574900	-6.97345800	1.40415600
F	1.85742200	-5.43378700	2.81547700
F	2.91717900	-5.63529100	0.95053500
F	-1.60396900	-5.80803400	-2.37609500
F	-2.35231000	-3.78659100	-2.58042500
F	-3.17754900	-5.10020900	-1.08282100
C	-1.69700300	5.70256700	1.50949300
C	2.03431200	4.73781100	-1.69134000

F 1.60396900 5.80803400 -2.37609500
F 2.35231000 3.78659100 -2.58042500
F 3.17754900 5.10020900 -1.08282100
F -1.85742200 5.43378700 2.81547700
F -2.91717900 5.63529100 0.95053500
F -1.28574900 6.97345800 1.40415600
Zero-point correction= 0.244309 (Hartree/Particle)
Thermal correction to Energy= 0.272538
Thermal correction to Enthalpy= 0.273482
Thermal correction to Gibbs Free Energy= 0.179683
Sum of electronic and zero-point Energies= -2356.276291
Sum of electronic and thermal Energies= -2356.248062
Sum of electronic and thermal Enthalpies= -2356.247118
Sum of electronic and thermal Free Energies= -2356.340917
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2357.22606463

1-B3
N -0.00430400 1.13090300 1.03951200
H -0.25250800 1.01311600 2.02139700
C -0.00000000 0.00000000 0.26849100
S -0.00000000 0.00000000 -1.40006600
N 0.00430400 -1.13090300 1.03951200
H 0.25250800 -1.01311600 2.02139700
C -0.05311900 -2.47627900 0.61079800
C -0.16850600 -5.19550500 -0.07830100
C -0.96851400 -2.91497800 -0.35102700
C 0.78492700 -3.39826200 1.24076700
C 0.71869600 -4.74649000 0.89485100
C -1.00494300 -4.26420900 -0.69163600
H -1.65340600 -2.21415400 -0.81391200
H 1.48503400 -3.05959300 2.00053400

H	-0.21804000	-6.24680900	-0.34355300
C	0.05311900	2.47627900	0.61079800
C	0.16850600	5.19550500	-0.07830100
C	-0.78492700	3.39826200	1.24076700
C	0.96851400	2.91497800	-0.35102700
C	1.00494300	4.26420900	-0.69163600
C	-0.71869600	4.74649000	0.89485100
H	-1.48503400	3.05959300	2.00053400
H	1.65340600	2.21415400	-0.81391200
H	0.21804000	6.24680900	-0.34355300
C	-1.95629300	-4.72374900	-1.76232600
C	1.66322000	-5.71557100	1.55036500
F	1.92350900	-5.36904800	2.82082000
F	2.84532400	-5.76972900	0.91381300
F	1.16879900	-6.96160800	1.56290300
F	-3.05128500	-3.95145000	-1.82103700
F	-2.36135400	-5.98609800	-1.55459400
F	-1.39063400	-4.69252000	-2.98041400
C	-1.66322000	5.71557100	1.55036500
C	1.95629300	4.72374900	-1.76232600
F	3.05128500	3.95145000	-1.82103700
F	2.36135400	5.98609800	-1.55459400
F	1.39063400	4.69252000	-2.98041400
F	-1.92350900	5.36904800	2.82082000
F	-2.84532400	5.76972900	0.91381300
F	-1.16879900	6.96160800	1.56290300

Zero-point correction= 0.244191 (Hartree/Particle)

Thermal correction to Energy= 0.272527

Thermal correction to Enthalpy= 0.273471

Thermal correction to Gibbs Free Energy= 0.177480

Sum of electronic and zero-point Energies= -2356.276556

Sum of electronic and thermal Energies= -2356.248220

Sum of electronic and thermal Enthalpies= -2356.247276

Sum of electronic and thermal Free Energies= -2356.343267

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2357.22613969

1-B

N	1.12884700	-0.03825200	-1.02708400
H	1.00410900	-0.33869000	-1.99340900
C	0.00306900	0.01028800	-0.25030100
S	0.01476700	0.10382800	1.41536500
N	-1.13150500	-0.02688700	-1.01511900
H	-1.01696400	0.17175500	-2.00894300
C	-2.47648800	-0.07021700	-0.58501200
C	-5.19529200	-0.15081400	0.11539700
C	-2.90744300	-0.90829900	0.44926800
C	-3.40687700	0.70393300	-1.28029200
C	-4.75501500	0.65423700	-0.92919600
C	-4.25594200	-0.92890500	0.79151200
H	-2.19908800	-1.54007000	0.97214300
H	-3.07384200	1.34609700	-2.09245300
H	-6.24374200	-0.17934200	0.39400700
C	2.47731300	0.03964400	-0.61155100
C	5.20278400	0.18529800	0.05036300
C	3.39304100	-0.83206400	-1.20207300
C	2.92536700	1.00372900	0.29794700
C	4.27661300	1.05440500	0.62661300
C	4.74480700	-0.74973300	-0.87111400
H	3.04671600	-1.57220100	-1.91986200
H	2.22910900	1.71299300	0.73009100
H	6.25580800	0.24581400	0.30528000
C	-4.72771700	-1.86946200	1.86639100

C	-5.72277500	1.53832400	-1.66556400
F	-6.99005500	1.13037700	-1.51502800
F	-5.45824000	1.56530300	-2.98217200
F	-5.66318900	2.81011500	-1.23589900
F	-5.78739700	-1.37485700	2.52395100
F	-3.76929700	-2.12025300	2.76887900
F	-5.10594400	-3.05583700	1.35850800
C	5.69708000	-1.72849400	-1.50004300
C	4.74387800	2.05571900	1.64721900
F	3.98293300	3.16015900	1.64628800
F	6.01096000	2.43610700	1.42275300
F	4.70336500	1.55495200	2.89321100
F	5.44092000	-1.88968700	-2.80882000
F	5.60286200	-2.94558300	-0.93833300
F	6.97243400	-1.33633900	-1.38194300

Zero-point correction= 0.244162 (Hartree/Particle)

Thermal correction to Energy= 0.272549

Thermal correction to Enthalpy= 0.273494

Thermal correction to Gibbs Free Energy= 0.176342

Sum of electronic and zero-point Energies= -2356.276486

Sum of electronic and thermal Energies= -2356.248099

Sum of electronic and thermal Enthalpies= -2356.247155

Sum of electronic and thermal Free Energies= -2356.344306

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2357.22607639

1-C

N	1.13362900	-0.68236900	-0.82646000
H	1.01383400	-1.48834700	-1.43902000
C	0.00422200	-0.15244900	-0.26850100
S	0.00880300	1.03534600	0.90572100
N	-1.12928900	-0.74000400	-0.75952800

H	-1.01016200	-1.59179500	-1.30689400
C	-2.47279200	-0.43413600	-0.44371200
C	-5.18614100	0.06106400	0.08012700
C	-2.94904100	0.88023900	-0.40810300
C	-3.35480900	-1.49621900	-0.23746100
C	-4.70165700	-1.24132500	0.01440800
C	-4.29394200	1.11086200	-0.13317800
H	-2.27845200	1.70923600	-0.60261100
H	-2.98583900	-2.51817800	-0.26877400
H	-6.23385500	0.25527300	0.28652700
C	2.47986400	-0.40074900	-0.49225600
C	5.19384000	0.04783900	0.06175900
C	3.35046300	-1.47843300	-0.32564000
C	2.96720400	0.90684600	-0.40496100
C	4.31319100	1.11399400	-0.11622100
C	4.69795900	-1.24652200	-0.05399000
H	2.97294300	-2.49475500	-0.40750100
H	2.30511500	1.74786900	-0.57507200
H	6.24363600	0.22444500	0.27267100
C	-4.78584400	2.52868400	-0.02990600
C	-5.64482700	-2.40127100	0.17342400
F	-6.72464200	-2.07137200	0.89523300
F	-5.05193000	-3.44155500	0.77997300
F	-6.08853000	-2.84897900	-1.01428200
F	-6.07981000	2.63015600	-0.37001300
F	-4.09156900	3.35516500	-0.82647700
F	-4.67333900	3.00643300	1.22059000
C	5.60448300	-2.42483800	0.16994900
C	4.82123600	2.52213500	0.03145100
F	4.13815600	3.38114600	-0.73975600
F	6.11688200	2.61858600	-0.30368400

F 4.71233700 2.96190900 1.29613100

F 5.30780200 -3.43894600 -0.65881400

F 5.49739200 -2.90527200 1.42031800

F 6.89284700 -2.10905900 -0.02027100

Zero-point correction= 0.244064 (Hartree/Particle)

Thermal correction to Energy= 0.272400

Thermal correction to Enthalpy= 0.273344

Thermal correction to Gibbs Free Energy= 0.177331

Sum of electronic and zero-point Energies= -2356.276331

Sum of electronic and thermal Energies= -2356.247994

Sum of electronic and thermal Enthalpies= -2356.247050

Sum of electronic and thermal Free Energies= -2356.343064

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2357.22594735

DA-1-Binary-cis

C 2.72984300 3.35128600 1.84502500

H 2.40944900 2.32287500 2.00711200

H 3.75854800 3.59524100 2.09524000

C 1.87871300 4.27246800 1.37922800

H 2.17539800 5.31153100 1.25245700

C 0.47077000 3.93265200 1.05717500

0 0.09343000 2.76171000 0.97001400

C -0.47488100 5.07491800 0.84142300

H -1.48555900 4.70882900 0.65031300

H -0.12681200 5.67571100 -0.00830000

H -0.46982000 5.73266700 1.71902500

N 1.02049200 0.10109000 0.32365000

H 0.91352300 1.07094000 0.64656700

C -0.13246300 -0.55458500 -0.00481500

S -0.18615700 -2.03559200 -0.77761800

N -1.23047500 0.18633300 0.34188200

H	-1.04613200	1.15364700	0.62285600
C	-2.59689000	-0.09183900	0.14174500
C	-5.36693000	-0.45507300	-0.19261000
C	-3.16067200	-1.36264300	0.29554900
C	-3.42574200	0.99612200	-0.15417500
C	-4.79508500	0.80851800	-0.31580500
C	-4.53285700	-1.52642100	0.11691200
H	-2.53939600	-2.21012700	0.55822900
H	-2.99035300	1.98751400	-0.25728500
H	-6.43405800	-0.59966600	-0.32670200
C	2.35614000	-0.27080600	0.06827300
C	5.09344300	-0.80571900	-0.30414300
C	3.23013600	0.74316400	-0.32969100
C	2.85339100	-1.56228800	0.28324200
C	4.20715000	-1.81340200	0.07982000
C	4.58698400	0.47343700	-0.49727000
H	2.84750000	1.74752700	-0.50105200
H	2.19378400	-2.35197100	0.62194900
H	6.14983700	-1.01403600	-0.43864400
C	-5.13147000	-2.88779200	0.34243400
C	-5.65335000	1.98304800	-0.69518400
F	-5.20703000	3.12207900	-0.14203300
F	-6.92619200	1.81589800	-0.30816700
F	-5.67210800	2.18068900	-2.02454000
F	-6.28005700	-3.04523600	-0.33231900
F	-5.41047500	-3.10017500	1.64088100
F	-4.29894500	-3.86731900	-0.03897600
C	5.48483800	1.62110300	-0.86127200
C	4.73204100	-3.21155500	0.25882700
F	3.97993900	-3.92561500	1.10861800
F	5.98787600	-3.20941700	0.73395200

F 4.75973900 -3.88698000 -0.90243700

F 5.51874300 2.54188600 0.12078100

F 5.05100900 2.25815700 -1.96121700

F 6.74487600 1.23221100 -1.08863600

Zero-point correction= 0.335946 (Hartree/Particle)

Thermal correction to Energy= 0.371756

Thermal correction to Enthalpy= 0.372701

Thermal correction to Gibbs Free Energy= 0.258759

Sum of electronic and zero-point Energies= -2587.162665

Sum of electronic and thermal Energies= -2587.126855

Sum of electronic and thermal Enthalpies= -2587.125910

Sum of electronic and thermal Free Energies= -2587.239852

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2588.27049951

DA-1-Binary-trans

C 0.74159000 6.16437500 1.14174300

H -0.22472400 6.66089400 1.20035300

H 1.62052000 6.80350900 1.16647200

C 0.85485500 4.83509400 1.04349900

H 1.82638300 4.34762300 0.98602300

C -0.30269100 3.91938000 1.00165300

0 -0.09869100 2.70574200 0.90207700

C -1.70152400 4.46414900 1.07689200

H -2.42254000 3.64413800 1.04027900

H -1.88367000 5.15129000 0.24278500

H -1.83803000 5.03082700 2.00483600

N 1.14699700 0.08738900 0.33395700

H 0.99033300 1.06263800 0.60633700

C 0.02939600 -0.63410500 0.00842600

S 0.05077900 -2.12989500 -0.73736400

N -1.10522400 0.05487600 0.33178300

H	-0.97037600	1.02968500	0.62575700
C	-2.45531800	-0.27955600	0.11042800
C	-5.21169700	-0.72760700	-0.23433600
C	-2.98165100	-1.56533100	0.27908100
C	-3.31317900	0.77589900	-0.21472400
C	-4.67669900	0.54910800	-0.37527400
C	-4.34671800	-1.77048000	0.09384500
H	-2.33696200	-2.38875900	0.56032100
H	-2.90491800	1.77580600	-0.34385600
H	-6.27411400	-0.90641500	-0.36759400
C	2.50322600	-0.23535600	0.12858400
C	5.25597400	-0.69752600	-0.21595600
C	3.35749800	0.80957000	-0.23728400
C	3.03223900	-1.51248700	0.34699400
C	4.39524900	-1.72712800	0.16036300
C	4.72003200	0.57319400	-0.40094900
H	2.94885100	1.80486400	-0.39699600
H	2.39029700	-2.32262800	0.66999600
H	6.31699500	-0.88053100	-0.35351900
C	-4.92375700	-3.13901800	0.33216500
C	-5.56045100	1.70167500	-0.76222600
F	-5.14418000	2.85001500	-0.20120000
F	-6.83168700	1.50431700	-0.38621300
F	-5.57118700	1.90399000	-2.09054000
F	-5.94840900	-3.39320900	-0.49684200
F	-5.39994900	-3.26653700	1.58360000
F	-4.01308300	-4.10672700	0.16069300
C	5.62569400	1.72515300	-0.73560300
C	4.95076900	-3.11366300	0.33692500
F	4.21664100	-3.84304700	1.18968000
F	6.20791300	-3.08560700	0.80727200

F 4.98748600 -3.78895700 -0.82421100

F 6.01949400 2.38633700 0.36724400

F 5.01589600 2.62317700 -1.52528400

F 6.73768600 1.31975200 -1.36482400

Zero-point correction= 0.336069 (Hartree/Particle)

Thermal correction to Energy= 0.371897

Thermal correction to Enthalpy= 0.372841

Thermal correction to Gibbs Free Energy= 0.257851

Sum of electronic and zero-point Energies= -2587.161853

Sum of electronic and thermal Energies= -2587.126024

Sum of electronic and thermal Enthalpies= -2587.125080

Sum of electronic and thermal Free Energies= -2587.240071

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2588.27016082

DA-1-endo-cis-2

C 2.25699100 2.51993000 1.33615800

H 2.35146600 1.43849500 1.34434500

C 3.08446800 3.40090000 0.63022800

H 4.06546600 3.11553500 0.25987300

C 1.22096300 3.25047600 1.96815900

H 0.37200800 2.81025400 2.48146500

C 1.40957800 4.59006300 1.72313200

H 0.76780800 5.39793900 2.06111400

C 2.77387500 4.78956200 1.14387500

H 2.86552000 5.60095800 0.41764900

H 3.46695700 5.00699400 1.97400600

C 2.13253600 3.62662000 -1.15666700

H 2.10414900 2.57611200 -1.42914000

H 2.94337200 4.19564200 -1.60631200

C 0.91746200 4.25849100 -0.89723500

H 0.80840600 5.33824700 -0.93708900

C	-0.22364500	3.45934300	-0.56108100
0	-0.13803500	2.20841500	-0.49507700
C	-1.54124400	4.11834500	-0.23753800
H	-1.80663300	3.89884400	0.80416000
H	-2.32984700	3.69819400	-0.87266900
H	-1.50692000	5.20283200	-0.37399800
N	-1.39093300	-0.30138700	-0.22669100
H	-1.12648900	0.69635800	-0.24199700
C	-0.34224000	-1.17375700	-0.17814300
S	-0.46497000	-2.83473100	-0.02613900
N	0.84276500	-0.49285700	-0.27704300
H	0.76703100	0.51220100	-0.48381600
C	2.16999300	-0.95623300	-0.22060300
C	4.91701300	-1.58344400	-0.08867200
C	2.61309300	-2.00635000	0.59204900
C	3.10944000	-0.22682500	-0.95988900
C	4.46421300	-0.52980100	-0.87744500
C	3.97306800	-2.31057200	0.63320300
H	1.91055400	-2.56969100	1.19395000
H	2.76928600	0.58091600	-1.60390200
H	5.97274700	-1.82634400	-0.03064300
C	-2.78027100	-0.49180000	-0.17542700
C	-5.60083200	-0.56525800	-0.10071700
C	-3.52189500	0.64292400	0.18956100
C	-3.46227000	-1.66479400	-0.51682800
C	-4.85683300	-1.68329300	-0.46333400
C	-4.90843300	0.60169900	0.22002600
H	-2.99843900	1.56270300	0.44164800
H	-2.91860100	-2.54524500	-0.83371700
H	-6.68564000	-0.59544100	-0.07994400
C	4.43439900	-3.40399500	1.55803300

C	5.42469900	0.28982200	-1.69218000
F	6.68511800	0.17002900	-1.25674700
F	5.10389900	1.59799300	-1.65073400
F	5.41628100	-0.06179800	-2.98791900
F	5.61008200	-3.92087300	1.17159500
F	3.54925800	-4.40920000	1.62031000
F	4.59970700	-2.95519700	2.81514800
C	-5.66863600	1.82544700	0.64910500
C	-5.57011500	-2.96902000	-0.78246500
F	-4.90725800	-3.69531000	-1.69485500
F	-6.80387100	-2.74742800	-1.26138400
F	-5.70905000	-3.74563400	0.30588600
F	-4.98166600	2.95244100	0.39900700
F	-5.93241000	1.81612700	1.96681800
F	-6.84825400	1.92126200	0.01822700

Zero-point correction= 0.432620 (Hartree/Particle)

Thermal correction to Energy= 0.472092

Thermal correction to Enthalpy= 0.473037

Thermal correction to Gibbs Free Energy= 0.351948

Sum of electronic and zero-point Energies= -2780.918819

Sum of electronic and thermal Energies= -2780.879347

Sum of electronic and thermal Enthalpies= -2780.878402

Sum of electronic and thermal Free Energies= -2780.999491

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2782.17131833

DA-1-endo-cis

C	0.06345500	-1.71664600	2.44275100
H	-0.19866100	-0.68389800	2.23289100
C	-0.81593700	-2.68691600	2.93848300
H	-1.74552500	-2.43770100	3.44292700
C	1.31451400	-2.31718100	2.16105600

H	2.14402000	-1.82812000	1.65631600
C	1.26116500	-3.64469600	2.52133100
H	2.06247400	-4.36872300	2.40913200
C	0.02952700	-3.87403700	3.33773200
H	-0.43789100	-4.85525300	3.22782100
H	0.29906200	-3.75114800	4.40046200
C	-1.57859800	-3.50801900	1.23025800
H	-1.92788100	-2.58532700	0.77100200
H	-2.34650500	-4.06898900	1.75862300
C	-0.53199300	-4.20236800	0.62445400
H	-0.34203500	-5.24883800	0.84490400
C	0.33980400	-3.52522200	-0.28874400
0	0.14761400	-2.32614200	-0.61167400
C	1.53537500	-4.24407300	-0.86170400
H	2.45010900	-3.69859200	-0.59627500
H	1.46695600	-4.24988000	-1.95568400
H	1.61441300	-5.27288000	-0.49930200
N	-1.16059200	0.21432000	-0.22362200
H	-0.94948400	-0.79256100	-0.28125500
C	-0.07134800	1.04379000	-0.29888700
S	-0.14345800	2.70308300	-0.47548600
N	1.07694900	0.30367600	-0.24429100
H	0.93198500	-0.71348200	-0.31407100
C	2.43358100	0.65163600	-0.31751600
C	5.22430200	1.04052600	-0.43460000
C	2.98368900	1.89092600	0.02898000
C	3.28933500	-0.38840400	-0.71273200
C	4.66308500	-0.19189000	-0.76293100
C	4.36599300	2.06361300	-0.04157000
H	2.34795100	2.70484100	0.35353700
H	2.86063200	-1.35232100	-0.98343700

H	6.29730000	1.19654400	-0.47814400
C	-2.53335100	0.51151300	-0.29668500
C	-5.32203700	0.87712400	-0.43388500
C	-3.34960700	-0.45101800	-0.90598800
C	-3.12031300	1.65089000	0.26464300
C	-4.50068500	1.82207400	0.17516100
C	-4.72725900	-0.26581200	-0.96262300
H	-2.89626700	-1.34022900	-1.33896600
H	-2.51173600	2.38857200	0.77297200
H	-6.39571100	1.02383900	-0.48896000
C	4.94995700	3.37836300	0.39927600
C	5.53882800	-1.32041400	-1.23139900
F	5.05490100	-2.51394900	-0.84522100
F	6.78557000	-1.21610200	-0.75055000
F	5.63644900	-1.35919400	-2.57047300
F	6.11123200	3.63910400	-0.21999000
F	5.20302200	3.39105400	1.72020900
F	4.12050000	4.40245200	0.15369000
C	-5.58616200	-1.34485300	-1.56076200
C	-5.10618000	3.08483500	0.72377600
F	-4.45638900	3.51305800	1.81709600
F	-6.39401900	2.91502800	1.05962700
F	-5.06494700	4.08750500	-0.16959700
F	-5.91303600	-2.28082900	-0.65172200
F	-4.96031900	-1.98191600	-2.56208400
F	-6.73608700	-0.85559600	-2.04600600

Zero-point correction= 0.432769 (Hartree/Particle)

Thermal correction to Energy= 0.472111

Thermal correction to Enthalpy= 0.473055

Thermal correction to Gibbs Free Energy= 0.352647

Sum of electronic and zero-point Energies= -2780.919323

Sum of electronic and thermal Energies= -2780.879981

Sum of electronic and thermal Enthalpies= -2780.879037

Sum of electronic and thermal Free Energies= -2780.999445

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2782.17278230

DA-1-product-complex

C	0.06833700	-1.75551700	2.56419800
H	-0.13285100	-0.68848100	2.62005900
C	-0.96335200	-2.84394200	2.78274000
H	-1.81704500	-2.58234900	3.41120700
C	1.20690300	-2.34667600	2.16874900
H	2.12223000	-1.86162100	1.83297700
C	0.93572300	-3.83661600	2.09856900
H	1.80419800	-4.49833500	2.07404800
C	-0.06041400	-3.99587000	3.25671800
H	-0.56743400	-4.96885400	3.25977200
H	0.40189600	-3.80644100	4.23133400
C	-1.35063000	-3.37083800	1.36908600
H	-1.69223900	-2.57158700	0.70306600
H	-2.15531800	-4.10984500	1.44539000
C	-0.04974000	-4.03914100	0.87513900
H	-0.17573700	-5.11639600	0.71332100
C	0.57577800	-3.44708000	-0.36096700
0	0.19718200	-2.38305900	-0.85168400
C	1.78357700	-4.15086000	-0.91752700
H	2.65051000	-3.87962300	-0.29731300
H	1.97565600	-3.82466100	-1.94274200
H	1.67546700	-5.23888600	-0.87023700
N	-1.17347200	0.20079200	-0.18800700
H	-0.95557400	-0.79692000	-0.29050900
C	-0.08858600	1.03918600	-0.23319700

S	-0.14903900	2.67499800	-0.55183700
N	1.05504700	0.32425300	-0.01346400
H	0.91085000	-0.67875000	0.11674700
C	2.41224300	0.66048700	-0.17023400
C	5.18418700	1.06033700	-0.42303800
C	2.96763900	1.90418300	0.14331000
C	3.24608500	-0.37901400	-0.60385600
C	4.61581600	-0.17707500	-0.71932200
C	4.34371500	2.08501400	0.00335400
H	2.34085500	2.71196400	0.50066600
H	2.80479200	-1.33960300	-0.86351900
H	6.25365600	1.21996500	-0.51787900
C	-2.54537500	0.49342200	-0.27718900
C	-5.33030700	0.86670600	-0.43800300
C	-3.36018300	-0.47864800	-0.87177400
C	-3.13051500	1.64536100	0.25895100
C	-4.50924400	1.81989600	0.15883500
C	-4.73662800	-0.28822700	-0.94116400
H	-2.90771600	-1.37831600	-1.28397600
H	-2.52178200	2.39126300	0.75550000
H	-6.40294500	1.01648900	-0.50339900
C	4.94329900	3.40415800	0.40880000
C	5.48199900	-1.29378400	-1.23232400
F	4.97403700	-2.49883900	-0.92245400
F	6.72041600	-1.23377800	-0.72235200
F	5.60774000	-1.25868000	-2.56894000
F	6.07940000	3.65924100	-0.25713100
F	5.24595700	3.42922700	1.71878600
F	4.10312300	4.42429200	0.18516400
C	-5.59681700	-1.37429100	-1.52478600
C	-5.11198300	3.09525600	0.68084400

F	-4.47090400	3.53550100	1.77455800
F	-6.40445300	2.93998300	1.00482500
F	-5.05298200	4.08359800	-0.22737600
F	-5.94197200	-2.28679300	-0.59908400
F	-4.96409000	-2.03864100	-2.50396800
F	-6.73676700	-0.88715100	-2.03500800

Zero-point correction= 0.437253 (Hartree/Particle)

Thermal correction to Energy= 0.476009

Thermal correction to Enthalpy= 0.476953

Thermal correction to Gibbs Free Energy= 0.356545

Sum of electronic and zero-point Energies= -2780.973271

Sum of electronic and thermal Energies= -2780.934515

Sum of electronic and thermal Enthalpies= -2780.933571

Sum of electronic and thermal Free Energies= -2781.053978

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2782.22811075

Anion Binding of 2b

2b-AcO-complex

H	0.38306700	-1.49655200	-2.87773100
C	0.46808900	-1.92413000	-1.88494400
C	0.69312700	-3.01020900	0.80945700
C	-0.62691800	-2.33469000	-1.13448800
C	1.68058400	-2.08760000	-1.22721100
C	1.78928500	-2.60498200	0.05702700
C	-0.52107900	-2.84641500	0.15252200
H	0.77446400	-3.38878100	1.82228100
0	-1.95022600	-2.25555700	-1.48156200
0	-1.77625600	-3.09266000	0.64388600
0	2.92185200	-1.71675300	-1.67156700
0	3.10265200	-2.57731700	0.44516400
C	-2.68918700	-2.88776600	-0.44046700
C	3.86320700	-2.11073500	-0.67608300

C	-3.87357400	-2.06890100	0.03578300
C	-6.30310500	-1.02056300	0.88835300
C	-4.98028000	-2.90704400	0.16974200
C	-3.91893100	-0.71495100	0.36982300
C	-5.17174700	-0.20002400	0.77442000
C	-6.20764600	-2.38502100	0.60363800
H	-7.24885600	-0.59152600	1.20605400
C	4.77747400	-0.98056200	-0.23957600
C	6.82260800	0.74291200	0.52703900
C	6.09273900	-1.44128200	-0.20239100
C	4.43352000	0.31413500	0.14820000
C	5.48978900	1.17737900	0.51789600
C	7.12872000	-0.57559100	0.17942200
H	7.61211900	1.43069000	0.81472400
C	-4.64125200	-4.33568600	-0.16099700
H	-5.42763900	-4.83068500	-0.74029800
H	-4.51735000	-4.90098200	0.77198200
C	4.82333200	-3.17996200	-1.21730500
H	4.43105000	-4.18309600	-1.03046300
H	4.89092100	-3.02423400	-2.29923200
C	6.18361600	-2.89978100	-0.56176800
H	6.32259400	-3.48739300	0.35507800
H	7.03188600	-3.11774000	-1.21910900
C	-3.31586100	-4.20318700	-0.92434800
H	-2.62517300	-5.03856200	-0.78089400
H	-3.51217500	-4.08670100	-1.99566800
I	2.43538400	1.00584000	0.28550200
I	-2.20112600	0.53325000	0.38463900
C	-7.34711100	-3.24657400	0.74379000
N	-8.25968000	-3.96001100	0.84934200
C	-5.33366800	1.19732200	1.07631400

N	-5.51361700	2.32329700	1.30841300
C	8.48449300	-1.04648800	0.20959300
N	9.57666800	-1.44627100	0.22598100
C	5.21876800	2.53552500	0.90917100
N	5.02359100	3.63737700	1.22757300
N	-2.82286200	4.61789400	-1.74530000
C	-3.77985400	3.99578500	-0.77748200
H	-3.20523900	3.68876400	0.10096800
H	-4.24439500	3.13388100	-1.26353900
H	-4.53852800	4.73803000	-0.51568000
C	-2.16819600	5.79460700	-1.09755000
H	-1.46070900	6.23000300	-1.80771700
H	-1.65776000	5.43865500	-0.19844600
H	-2.94431400	6.52004800	-0.84106600
C	-1.78160100	3.61207500	-2.11337000
H	-1.07376200	4.08397900	-2.79985300
H	-2.27643800	2.76807200	-2.60156700
H	-1.27907300	3.28055700	-1.19998800
C	-3.55081900	5.05796200	-2.96784600
H	-2.83342100	5.50488600	-3.66059900
H	-4.30669600	5.79173600	-2.67742600
H	-4.02490900	4.18525600	-3.42340100
C	-0.19394700	3.17588000	1.19398800
0	0.00390100	2.06942200	0.57180000
0	-1.28210900	3.78736700	1.21563700
C	0.99421100	3.76635400	1.94486000
H	1.38640800	3.03624200	2.66263500
H	0.69766200	4.67672200	2.47212400
H	1.81069700	3.99814700	1.24919500

Zero-point correction= 0.555770 (Hartree/Particle)

Thermal correction to Energy= 0.600867

Thermal correction to Enthalpy= 0.601811

Thermal correction to Gibbs Free Energy= 0.473611

Sum of electronic and zero-point Energies= -2627.924906

Sum of electronic and thermal Energies= -2627.879809

Sum of electronic and thermal Enthalpies= -2627.878865

Sum of electronic and thermal Free Energies= -2628.007065

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2629.17613780

2b-Br-complex

H	-0.61614400	-1.96442800	2.72183700
C	-0.64157900	-2.15491700	1.65473900
C	-0.70393500	-2.62868900	-1.22040700
C	0.48822100	-2.46741700	0.90850300
C	-1.80581400	-2.10030900	0.89793600
C	-1.83584800	-2.32284800	-0.47356700
C	0.46028400	-2.68789200	-0.46288400
H	-0.72471000	-2.78995800	-2.29248100
0	1.78121100	-2.56880300	1.35468700
0	1.73619000	-2.92292800	-0.90644900
0	-3.06970900	-1.79501800	1.33214100
0	-3.11767400	-2.15461500	-0.92804400
C	2.55398600	-3.05431600	0.26217100
C	-3.94618600	-2.02805700	0.23416900
C	3.85205900	-2.29780900	0.05526700
C	6.43359300	-1.37808600	-0.42191100
C	4.87967100	-3.21091500	-0.18037000
C	4.06075500	-0.92065900	0.01140800
C	5.38145500	-0.47411200	-0.21542300
C	6.18397100	-2.75271100	-0.41873900
H	7.43877800	-1.00413200	-0.59240800
C	-4.95431700	-0.91741000	0.01495500

C	-7.13386100	0.73527300	-0.48570100
C	-6.20764900	-1.47990700	-0.22470300
C	-4.73792500	0.45867800	-0.03760900
C	-5.86006100	1.28228900	-0.27491500
C	-7.31093200	-0.65070400	-0.47579700
H	-7.97817000	1.39399200	-0.66587400
C	4.37568000	-4.62889800	-0.17845400
H	5.05359600	-5.31403000	0.34108800
H	4.28814800	-4.97939900	-1.21522600
C	-4.81099300	-3.27516100	0.46929600
H	-4.30423300	-4.17401000	0.10739300
H	-4.95476300	-3.36182500	1.55165100
C	-6.15421600	-2.98419600	-0.21500100
H	-6.17115500	-3.35034900	-1.24986100
H	-7.00894100	-3.43156800	0.30293600
C	3.00258300	-4.50412800	0.49753600
H	2.25186700	-5.20851000	0.12907700
H	3.10651200	-4.63221700	1.58033400
I	-2.80572800	1.30652200	0.15857400
I	2.46811200	0.46846600	0.20266200
C	7.24422200	-3.69139000	-0.65563000
N	8.09055000	-4.46631700	-0.84486200
C	5.69166900	0.92934000	-0.25434000
N	5.98039100	2.05633900	-0.29375400
C	-8.60375100	-1.22624000	-0.71760100
N	-9.64330200	-1.71095900	-0.91040200
C	-5.73338500	2.71432800	-0.31837200
N	-5.67388700	3.87513400	-0.35971700
N	3.45761600	4.97192800	-0.26149400
C	4.76521100	5.65010700	-0.49325500
H	5.54368300	4.88330000	-0.53114200

H	4.95026600	6.34198500	0.33206600
H	4.71449000	6.19171300	-1.44091000
C	3.19327200	4.01414200	-1.37873800
H	2.22871100	3.53066100	-1.19430700
H	3.99871400	3.27607400	-1.39660600
H	3.17010000	4.57993000	-2.31354500
C	3.50884300	4.23529800	1.03890800
H	2.54092100	3.74900600	1.19616300
H	3.71188400	4.95915500	1.83247000
H	4.30950900	3.49382000	0.98217900
C	2.35576700	5.97796200	-0.21318400
H	1.41707500	5.44253100	-0.04067200
H	2.32729500	6.50760900	-1.16868700
H	2.55642200	6.67537500	0.60382100
Br	0.11369600	2.70271600	0.42224000

Zero-point correction= 0.504887 (Hartree/Particle)

Thermal correction to Energy= 0.546885

Thermal correction to Enthalpy= 0.547829

Thermal correction to Gibbs Free Energy= 0.424832

Sum of electronic and zero-point Energies= -4973.932923

Sum of electronic and thermal Energies= -4973.890925

Sum of electronic and thermal Enthalpies= -4973.889981

Sum of electronic and thermal Free Energies= -4974.012978

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I, Br)) = -4975.38712257

2b-Cl-complex

H	0.50201500	-1.92287200	2.73826300
C	0.52748400	-2.11711100	1.67184400
C	0.58831300	-2.58894900	-1.20337600
C	1.69404600	-2.07946900	0.91742500
C	-0.60566800	-2.41000400	0.92263800

C	-0.57829000	-2.63042700	-0.44851200
C	1.72333800	-2.30113000	-0.45402500
H	0.60830800	-2.74600000	-2.27609900
0	2.96000700	-1.78664600	1.35355100
0	3.00689500	-2.14559100	-0.90756300
0	-1.90175800	-2.47888500	1.36439200
0	-1.85689500	-2.83623300	-0.89754700
C	3.83615700	-2.01183400	0.25354800
C	-2.69409100	-2.91054700	0.26260500
C	4.83508000	-0.89251200	0.03283400
C	7.00147100	0.77587600	-0.47090600
C	6.09167300	-1.44581500	-0.21092600
C	4.60668500	0.48244500	-0.01703300
C	5.72414000	1.31274000	-0.25554200
C	7.18857700	-0.60876700	-0.46416400
H	7.84055200	1.44096000	-0.65218700
C	-3.93542700	-2.06551400	0.04439200
C	-6.44426000	-0.96709400	-0.44543500
C	-5.02380000	-2.90430000	-0.19322500
C	-4.04518600	-0.67678800	-0.00443600
C	-5.33099800	-0.13979500	-0.23757300
C	-6.29201600	-2.35594200	-0.43746300
H	-7.42001600	-0.52349300	-0.62064200
C	6.04981700	-2.95050700	-0.20251600
H	6.90983700	-3.39194000	0.31181700
H	6.06552100	-3.31585700	-1.23770400
C	-3.24440600	-4.32547700	0.49335700
H	-2.54342700	-5.07949400	0.12540800
H	-3.35939000	-4.44804600	1.57568000
C	-4.62123300	-4.35431000	-0.18595200
H	-4.55622800	-4.71344300	-1.22141200

H	-5.34723200	-4.98824500	0.33375100
C	4.71130400	-3.25188300	0.48633800
H	4.21029400	-4.15471600	0.12641000
H	4.85929400	-3.33705100	1.56826000
I	-2.36680300	0.60707900	0.19080500
I	2.66822500	1.32081400	0.18064900
C	8.48448800	-1.17484800	-0.71125500
N	9.52676300	-1.65191000	-0.90865200
C	5.58812600	2.74422500	-0.29541300
N	5.52152700	3.90482300	-0.33341100
C	-7.41524200	-3.21811600	-0.67449700
N	-8.31372700	-3.93205800	-0.86346500
C	-5.53696300	1.28305900	-0.27824800
N	-5.73805700	2.42900700	-0.31627200
N	-2.89720600	5.16750000	-0.12300700
C	-4.07287800	6.05875300	-0.33236500
H	-3.91962500	6.62766100	-1.25273400
H	-4.15585500	6.73357300	0.52311700
H	-4.96670600	5.43458200	-0.41414900
C	-2.76254400	4.23934700	-1.28747200
H	-1.88232400	3.61165800	-1.11653600
H	-2.64191200	4.84225400	-2.19132300
H	-3.66816800	3.63064400	-1.34968800
C	-1.64826800	5.97688500	-0.00280500
H	-0.81602700	5.28237600	0.14772500
H	-1.75144800	6.65031600	0.85171500
H	-1.51452100	6.54853000	-0.92461000
C	-3.08664400	4.38021500	1.13416900
H	-2.20061000	3.75350000	1.27567200
H	-3.98375600	3.76572300	1.02431900
H	-3.20240600	5.08476900	1.96218300

Cl -0.07525600 2.60936200 0.41650900

Zero-point correction= 0.505146 (Hartree/Particle)

Thermal correction to Energy= 0.546878

Thermal correction to Enthalpy= 0.547822

Thermal correction to Gibbs Free Energy= 0.426075

Sum of electronic and zero-point Energies= -2859.704569

Sum of electronic and thermal Energies= -2859.662837

Sum of electronic and thermal Enthalpies= -2859.661893

Sum of electronic and thermal Free Energies= -2859.783640

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I, Cl)) = -2861.00938707

2b-F-complex

H -0.16949200 -2.02556300 2.78706300

C -0.18333100 -2.25330000 1.72703000

C -0.21259600 -2.77385200 -1.13873000

C 0.96733000 -2.47521800 0.98052300

C -1.35009200 -2.30691100 0.97425500

C -1.36446900 -2.55172900 -0.39283400

C 0.95467800 -2.71992000 -0.38591800

H -0.22151200 -2.93939600 -2.21033000

0 2.26545500 -2.41077200 1.41571900

0 2.24279900 -2.82303000 -0.83987300

0 -2.62912500 -2.06802500 1.40384400

0 -2.65185800 -2.47307800 -0.85257100

C 3.10471200 -2.68078900 0.29764800

C -3.49391200 -2.28049400 0.29264000

C 4.12936800 -1.59175300 0.01901900

C 6.32607900 -0.00528100 -0.62178800

C 5.35676200 -2.18919400 -0.26663100

C 3.94227100 -0.21012500 -0.04619800

C 5.07724700 0.57416500 -0.35849000

C	6.46807800	-1.39504900	-0.58821100
H	7.17672900	0.62704600	-0.85865400
C	-4.44956900	-1.13042700	0.02236800
C	-6.54801300	0.58391500	-0.60482500
C	-5.71162100	-1.65340200	-0.25844500
C	-4.17650400	0.23804800	-0.04380800
C	-5.26510500	1.08770900	-0.34775200
C	-6.77472600	-0.79420400	-0.57402600
H	-7.35954900	1.26760400	-0.83571500
C	5.27268500	-3.69116100	-0.21651700
H	6.14008200	-4.14356900	0.27550700
H	5.23600300	-4.08457700	-1.24088200
C	-4.41720200	-3.48160000	0.53315000
H	-3.93419500	-4.41126400	0.22032200
H	-4.60512300	-3.52600600	1.61143200
C	-5.71892500	-3.15778700	-0.21241500
H	-5.70768600	-3.55008000	-1.23782400
H	-6.61138400	-3.55814200	0.27995800
C	3.95498700	-3.93502000	0.53242800
H	3.41550200	-4.83272100	0.21913500
H	4.14243100	-3.99339100	1.61010900
I	-2.23058900	1.05249800	0.23529800
I	2.06907400	0.74836700	0.24418600
C	7.73170200	-2.01090100	-0.87799400
N	8.74772600	-2.52799900	-1.10910400
C	4.97229000	2.00831200	-0.42590300
N	4.91099200	3.16919500	-0.48667200
C	-8.07434100	-1.33181900	-0.86055600
N	-9.12076800	-1.78556700	-1.08924700
C	-5.08900700	2.51432300	-0.41667200
N	-4.98996500	3.67158500	-0.48258600

N	1.12010700	5.11142400	0.04062500
C	1.72692200	6.44857600	-0.19963100
H	1.23024500	6.90905200	-1.05730000
H	2.79196400	6.31250600	-0.40479800
H	1.58750500	7.06161000	0.69434100
C	-0.34136200	5.23977200	0.32227500
H	-0.72148300	4.22754600	0.48773500
H	-0.82448100	5.70509600	-0.54042100
H	-0.47140800	5.85968000	1.21292200
C	1.29489100	4.24285200	-1.16395400
H	0.79588700	3.29602900	-0.93811500
H	2.36554100	4.09413600	-1.33172500
H	0.83660800	4.74594100	-2.01965800
C	1.77258400	4.45661800	1.21556500
H	1.26019200	3.50248100	1.36570800
H	1.65954000	5.11432800	2.08153800
H	2.83056800	4.30355600	0.98403100
F	-0.00754000	2.07498700	0.53458200

Zero-point correction= 0.506191 (Hartree/Particle)

Thermal correction to Energy= 0.547270

Thermal correction to Enthalpy= 0.548214

Thermal correction to Gibbs Free Energy= 0.429621

Sum of electronic and zero-point Energies= -2499.423460

Sum of electronic and thermal Energies= -2499.382381

Sum of electronic and thermal Enthalpies= -2499.381437

Sum of electronic and thermal Free Energies= -2499.500030

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I, F)) = -2500.67226195

2b-I-complex

H	0.69799100	-1.87194900	2.73370100
C	0.73507300	-2.11124600	1.67682200

C	0.83050900	-2.73127100	-1.17012200
C	1.90521100	-2.07688800	0.92750400
C	-0.38248600	-2.48534100	0.93950000
C	-0.33837500	-2.77486600	-0.41891000
C	1.94996500	-2.36675000	-0.43132800
H	0.86389900	-2.94937800	-2.23175300
0	3.16374800	-1.74026200	1.35658300
0	3.23364100	-2.20594600	-0.88277900
0	-1.67665500	-2.60259500	1.38170100
0	-1.60438100	-3.06707200	-0.85724000
C	4.05016400	-2.03295700	0.28201000
C	-2.41329000	-3.19429100	0.31767100
C	5.07359600	-0.94781200	0.01212400
C	7.27310600	0.64253000	-0.59745200
C	6.31452200	-1.54181900	-0.21713500
C	4.88236200	0.42757900	-0.10022300
C	6.01231900	1.22134400	-0.39303600
C	7.42697100	-0.74428700	-0.52285800
H	8.12545300	1.27692900	-0.82174700
C	-3.75922600	-2.54363000	0.06433300
C	-6.39080500	-1.83972900	-0.50405600
C	-4.71332300	-3.53979200	-0.14414000
C	-4.06854900	-1.19050300	-0.05118500
C	-5.41178600	-0.85170000	-0.32417500
C	-6.04215200	-3.19032900	-0.42662700
H	-7.41667900	-1.54947000	-0.71047300
C	6.23745700	-3.04269200	-0.13275200
H	7.09242700	-3.47743000	0.39538800
H	6.23329100	-3.45965200	-1.14837200
C	-2.76160300	-4.65746500	0.62640600
H	-1.95474100	-5.32476100	0.31110400

H	-2.87981100	-4.73331000	1.71267300
C	-4.10726100	-4.91515500	-0.06580400
H	-3.97301500	-5.30486000	-1.08343100
H	-4.74407900	-5.62389400	0.47376800
C	4.89938000	-3.27599300	0.58272200
H	4.37646500	-4.18767900	0.28063400
H	5.05495300	-3.29946300	1.66672300
I	-2.58040900	0.31079300	0.12445500
I	2.96885300	1.31305400	0.10347000
C	8.70596000	-1.35405800	-0.75389700
N	9.73369800	-1.86684200	-0.93691900
C	5.90678800	2.65144800	-0.50145500
N	5.86294600	3.80974500	-0.59634500
C	-7.02701200	-4.21451100	-0.63262600
N	-7.81108600	-5.05788400	-0.79510800
C	-5.82239600	0.52107000	-0.43729200
N	-6.19430100	1.61951900	-0.53669800
I	-0.15727200	2.82815800	0.47880400
N	-4.03686800	4.76552500	-0.29282500
C	-5.41717300	5.26512700	-0.55979700
H	-6.08414200	4.40220600	-0.63336100
H	-5.40789600	5.82543900	-1.49792900
H	-5.71818500	5.91251300	0.26744100
C	-4.03058900	3.99774900	0.98957800
H	-3.01344600	3.63770000	1.17349600
H	-4.72400800	3.15897900	0.89292700
H	-4.34993000	4.66909000	1.79074100
C	-3.60878500	3.88105700	-1.41943700
H	-2.59450400	3.52429200	-1.21444000
H	-3.62879800	4.46883300	-2.34065600
H	-4.30629800	3.04236800	-1.48330500

C	-3.09153100	5.91548200	-0.18164100
H	-2.08974100	5.51870000	0.01046700
H	-3.41656300	6.55196300	0.64479300
H	-3.10854200	6.47129700	-1.12221500

Zero-point correction= 0.504667 (Hartree/Particle)
Thermal correction to Energy= 0.546799
Thermal correction to Enthalpy= 0.547743
Thermal correction to Gibbs Free Energy= 0.424034
Sum of electronic and zero-point Energies= -2696.759546
Sum of electronic and thermal Energies= -2696.717414
Sum of electronic and thermal Enthalpies= -2696.716470
Sum of electronic and thermal Free Energies= -2696.840179
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2697.88742655

2b-NO3-complex

H	0.41614000	-2.19469900	2.71597200
C	0.43176400	-2.38284900	1.64824800
C	0.46270500	-2.82732200	-1.23129400
C	1.59007700	-2.33018600	0.88123800
C	-0.70774500	-2.67800300	0.90964800
C	-0.69477200	-2.88257100	-0.46383100
C	1.60435700	-2.53895200	-0.49228200
H	0.47104400	-2.97202800	-2.30590000
0	2.85969700	-2.02962200	1.30414900
0	2.88043700	-2.36857000	-0.96060500
0	-1.99987400	-2.74967800	1.36387600
0	-1.97631100	-3.08399100	-0.90357300
C	3.72277500	-2.23795800	0.19195700
C	-2.82112600	-3.09829500	0.25525100
C	4.71307300	-1.11314900	-0.04718200
C	6.85795700	0.55431100	-0.64818100

C	5.95791400	-1.66595800	-0.34806400
C	4.48783500	0.26290300	-0.08257000
C	5.59316000	1.09300300	-0.37312800
C	7.04308500	-0.83034400	-0.64961200
H	7.68802100	1.21857700	-0.86919300
C	-3.98944300	-2.15281000	0.02630300
C	-6.38251200	-0.85828000	-0.56888400
C	-5.12662000	-2.90183800	-0.27455500
C	-3.99814400	-0.75927700	0.00313400
C	-5.22359500	-0.12015400	-0.29138500
C	-6.33617400	-2.25506900	-0.56970100
H	-7.31078200	-0.33988900	-0.79027200
C	5.91726800	-3.17057200	-0.34219000
H	6.79835100	-3.61190400	0.13522000
H	5.89013600	-3.53318400	-1.37813100
C	-3.49029400	-4.46223300	0.46188300
H	-2.83798300	-5.27018000	0.12013600
H	-3.65728400	-4.57320600	1.53877500
C	-4.83650600	-4.37878100	-0.27183800
H	-4.75600000	-4.73126400	-1.30853300
H	-5.62901400	-4.96064900	0.21005400
C	4.60859600	-3.47356200	0.39996200
H	4.09633300	-4.37978500	0.06518400
H	4.79840400	-3.55081400	1.47600900
I	-2.27504700	0.39948300	0.35763600
I	2.57717300	1.09768800	0.22985300
C	8.32413200	-1.39948200	-0.95951600
N	9.35407100	-1.87917700	-1.20818400
C	5.45643300	2.52402500	-0.41286700
N	5.38881600	3.68419900	-0.45844200
C	-7.50776300	-3.02763500	-0.87254600

N	-8.44622100	-3.67054900	-1.11478300
C	-5.30727000	1.31583500	-0.33469800
N	-5.39682200	2.47505800	-0.38466300
N	-2.32563300	5.41402700	-0.74937600
C	-2.06907000	6.08052400	-2.05792500
H	-1.06783500	5.80510300	-2.39733500
H	-2.13918500	7.16157800	-1.91749800
H	-2.82046200	5.73917500	-2.77382400
C	-2.22970500	3.93103700	-0.90892000
H	-2.45218700	3.47482900	0.05789400
H	-1.21227000	3.67812200	-1.21889300
H	-2.95532900	3.61348600	-1.66168700
C	-1.30939900	5.86464600	0.25004100
H	-1.48767000	5.33733600	1.19051100
H	-1.40746700	6.94508400	0.38015400
H	-0.31723700	5.61085800	-0.13028100
C	-3.69432900	5.76314900	-0.26716300
H	-3.86200400	5.26009900	0.68827400
H	-4.42188900	5.41776000	-1.00556700
H	-3.75489300	6.84732900	-0.14616100
N	-0.14242900	2.95801000	1.42628000
0	-0.03213800	1.96955100	0.62460200
0	0.80882300	3.74118900	1.55638200
0	-1.21364000	3.11141400	2.04721100

Zero-point correction= 0.520337 (Hartree/Particle)

Thermal correction to Energy= 0.564850

Thermal correction to Enthalpy= 0.565794

Thermal correction to Gibbs Free Energy= 0.437059

Sum of electronic and zero-point Energies= -2679.745861

Sum of electronic and thermal Energies= -2679.701348

Sum of electronic and thermal Enthalpies= -2679.700404

Sum of electronic and thermal Free Energies= -2679.829139

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2680.98453089

2b-SMe-complex

H	0.45918300	-1.90399500	2.80643600
C	0.50000300	-2.15836400	1.75316900
C	0.60158100	-2.79477900	-1.08812600
C	1.67598200	-2.15098900	1.01213300
C	-0.62079400	-2.50988300	1.01007100
C	-0.57377200	-2.80741400	-0.34594000
C	1.72401400	-2.45002400	-0.34392900
H	0.63656700	-3.01288800	-2.14975600
0	2.93382500	-1.82031300	1.44529500
0	3.01061100	-2.30694500	-0.79147400
0	-1.92102400	-2.57302700	1.44050400
0	-1.84253800	-3.05689000	-0.79779200
C	3.82507900	-2.09556900	0.36943300
C	-2.69806500	-3.06387800	0.35295300
C	4.81431500	-0.98111900	0.08742100
C	6.96448500	0.66666100	-0.53457900
C	6.07181700	-1.54124500	-0.13609000
C	4.57364900	0.38747900	-0.03532400
C	5.68506400	1.20585900	-0.33470300
C	7.16094000	-0.71415300	-0.44870900
H	7.79766600	1.32452700	-0.76379100
C	-3.93509700	-2.23534300	0.05846300
C	-6.42206900	-1.18031300	-0.60022400
C	-5.00752100	-3.09352800	-0.18308700
C	-4.04627400	-0.85050000	-0.05970900
C	-5.32185100	-0.33785600	-0.38300600
C	-6.26607100	-2.56621000	-0.51065900

H	-7.39005900	-0.75306900	-0.84557500
C	6.04154700	-3.04309300	-0.03775300
H	6.90921800	-3.44664900	0.49471200
H	6.05066800	-3.47073500	-1.04895500
C	-3.25221300	-4.46394200	0.64939600
H	-2.53492400	-5.23647900	0.35931200
H	-3.41323000	-4.51898600	1.73153600
C	-4.59886900	-4.53899500	-0.08499200
H	-4.48646100	-4.95043400	-1.09673300
H	-5.34264400	-5.15162000	0.43531400
C	4.71077100	-3.31035900	0.67954500
H	4.21509700	-4.23953700	0.38491900
H	4.86659700	-3.32085300	1.76375600
I	-2.37135100	0.48465900	0.16969600
I	2.60807500	1.24103800	0.15261800
C	8.45739800	-1.28739000	-0.67461000
N	9.50039500	-1.77040800	-0.85347100
C	5.54058000	2.63269800	-0.45581500
N	5.46874900	3.78892000	-0.56159800
C	-7.37526600	-3.44558500	-0.74984000
N	-8.26297300	-4.17318200	-0.93865100
C	-5.52868100	1.08027300	-0.51518700
N	-5.73068700	2.22011800	-0.63316600
N	-2.70752200	5.72409700	0.27645200
C	-3.66375700	6.86095300	0.15425800
H	-3.15352200	7.77797200	0.45855500
H	-4.51984200	6.66738400	0.80499400
H	-3.98669400	6.93230100	-0.88715300
C	-1.53502500	5.95641000	-0.61957800
H	-0.82497600	5.13828700	-0.46555600
H	-1.08033600	6.91328000	-0.35146100

H	-1.88793400	5.97767600	-1.65360500
C	-2.22955600	5.61414600	1.68731400
H	-1.53921600	4.76725500	1.74419200
H	-3.09485200	5.45231000	2.33451600
H	-1.72099400	6.54383900	1.95405300
C	-3.38993100	4.45091700	-0.11132400
H	-2.66533400	3.63541300	-0.01619400
H	-3.74119600	4.54376200	-1.14172500
H	-4.23473800	4.29129400	0.56232900
C	-0.23462800	2.69575800	-1.56381600
H	-0.05655500	1.73472900	-2.06251800
H	0.51563400	3.40805800	-1.92935000
H	-1.22525400	3.05440200	-1.87924400
S	-0.14422900	2.52047800	0.24951000

Zero-point correction= 0.542649 (Hartree/Particle)

Thermal correction to Energy= 0.586844

Thermal correction to Enthalpy= 0.587788

Thermal correction to Gibbs Free Energy= 0.461126

Sum of electronic and zero-point Energies= -2837.586223

Sum of electronic and thermal Energies= -2837.542028

Sum of electronic and thermal Enthalpies= -2837.541084

Sum of electronic and thermal Free Energies= -2837.667746

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2838.82709582

NMe4AcO

N	-2.25842800	5.27251100	0.80827800
C	-2.89088100	6.38747800	1.56349200
H	-2.42617800	7.32619800	1.25244400
H	-2.73165700	6.22073200	2.63129300
H	-3.95960900	6.39956000	1.33642600
C	-2.46052800	5.47370800	-0.65876600

H -1.98818800 4.64304100 -1.20589500
H -2.00578800 6.42884300 -0.93524700
H -3.53643400 5.50323300 -0.85127000
C -0.79336300 5.22394800 1.09669900
H -0.38799300 4.36173700 0.55568900
H -0.66120200 5.10641000 2.17544200
H -0.34461400 6.16199300 0.76046500
C -2.86880400 3.96959200 1.21053900
H -2.33778000 3.18336200 0.66256500
H -3.93165300 3.99413600 0.95734600
H -2.73940100 3.85025000 2.28942000
C -0.62900600 2.35131600 -1.67019000
0 -0.60343800 2.42479000 -0.40553700
0 -1.16331600 3.16390600 -2.46444100
C 0.07679400 1.12684800 -2.27310800
H 1.12999500 1.11777100 -1.96733600
H 0.01800700 1.12270700 -3.36555400
H -0.37647600 0.20765400 -1.88270500
Zero-point correction= 0.215961 (Hartree/Particle)
Thermal correction to Energy= 0.228367
Thermal correction to Enthalpy= 0.229311
Thermal correction to Gibbs Free Energy= 0.175918
Sum of electronic and zero-point Energies= -442.121486
Sum of electronic and thermal Energies= -442.109080
Sum of electronic and thermal Enthalpies= -442.108135
Sum of electronic and thermal Free Energies= -442.161528
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -442.484699779

NMe4Br
N -1.77207500 0.00078000 0.00048400
C -3.26152100 0.00398400 0.00528100

H	-3.60683800	0.80510800	0.66309100
H	-3.60998300	-0.96444300	0.37220800
H	-3.61356200	0.17220800	-1.01525500
C	-1.26313900	1.31543900	-0.49619200
H	-0.16785700	1.27254100	-0.49100100
H	-1.62640000	2.09950400	0.17267300
H	-1.64400600	1.47255500	-1.50817500
C	-1.25990200	-0.22970200	1.38607600
H	-0.16459500	-0.22381100	1.34061200
H	-1.63353400	-1.19634000	1.73301100
H	-1.63183800	0.57305500	2.02799900
C	-1.27000000	-1.08768300	-0.89173800
H	-0.17448700	-1.05865800	-0.86940900
H	-1.64675800	-0.90749300	-1.90129000
H	-1.64328700	-2.04218000	-0.51215700
Br	2.19753800	-0.00583000	-0.01046000

Zero-point correction= 0.165636 (Hartree/Particle)

Thermal correction to Energy= 0.174401

Thermal correction to Enthalpy= 0.175345

Thermal correction to Gibbs Free Energy= 0.131076

Sum of electronic and zero-point Energies= -2788.107617

Sum of electronic and thermal Energies= -2788.098852

Sum of electronic and thermal Enthalpies= -2788.097908

Sum of electronic and thermal Free Energies= -2788.142177

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2788.70016388

NMe4Cl

N	1.09653700	0.00043100	0.00027300
C	2.58440900	0.00253900	-0.00317100
H	2.93669300	-0.88605700	0.52677800
H	2.93444700	0.90751300	0.49961200

H	2.93030200	-0.01285300	-1.04010200
C	0.58327400	-1.22677500	-0.68173100
H	-0.51327000	-1.17545200	-0.65102600
H	0.95686500	-2.10125100	-0.14260200
H	0.95373600	-1.22868200	-1.71029700
C	0.58449000	0.02101100	1.40445700
H	-0.51221400	0.01886600	1.34702900
H	0.95654500	0.92627600	1.89184200
H	0.95849800	-0.86808900	1.91931900
C	0.57937200	1.20379300	-0.72059600
H	-0.51706700	1.15273200	-0.68452100
H	0.94651200	1.17162100	-1.74994700
H	0.95491800	2.09578100	-0.21193100
Cl	-2.59835200	-0.00251700	0.00856400

Zero-point correction= 0.166188 (Hartree/Particle)
Thermal correction to Energy= 0.174556
Thermal correction to Enthalpy= 0.175501
Thermal correction to Gibbs Free Energy= 0.133613
Sum of electronic and zero-point Energies= -673.872303
Sum of electronic and thermal Energies= -673.863935
Sum of electronic and thermal Enthalpies= -673.862990
Sum of electronic and thermal Free Energies= -673.904878
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -674.321262226

NMe4F

N	0.55221300	-0.00000400	0.00014300
C	2.03549000	-0.00068200	0.00026700
H	2.38641300	-1.02756300	-0.13256600
H	2.38731500	0.39759100	0.95566000
H	2.38701100	0.62743300	-0.82267900
C	0.01158800	-0.53855800	-1.28610900

H	-1.08290900	-0.48628100	-1.16353200
H	0.37193900	-1.56393500	-1.40943100
H	0.37333500	0.09137300	-2.10376600
C	0.01044800	-0.84530700	1.10875000
H	-1.08389700	-0.76393900	1.00211000
H	0.37081600	-0.44150900	2.05919900
H	0.37088700	-1.86876100	0.97039900
C	0.01173400	1.38326600	0.17741400
H	-1.08278800	1.25139000	0.15950600
H	0.37330700	2.00376300	-0.64773400
H	0.37237300	1.77495300	1.13296900
F	-2.50484100	0.00217700	-0.00154900

Zero-point correction= 0.166789 (Hartree/Particle)

Thermal correction to Energy= 0.174637

Thermal correction to Enthalpy= 0.175581

Thermal correction to Gibbs Free Energy= 0.135843

Sum of electronic and zero-point Energies= -313.580771

Sum of electronic and thermal Energies= -313.572923

Sum of electronic and thermal Enthalpies= -313.571979

Sum of electronic and thermal Free Energies= -313.611717

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -313.977304826

NMe4I

I	-0.01545800	3.33486700	0.49302500
N	-3.93775100	4.74681800	-0.68840800
C	-5.28768300	5.23151600	-1.09470500
H	-5.98747400	4.39391400	-1.04672200
H	-5.22485400	5.61655600	-2.11556700
H	-5.59468800	6.02371100	-0.40793400
C	-3.99111900	4.21342400	0.70610000
H	-2.98821700	3.86486900	0.97648000

H	-4.70665100	3.38790500	0.73201000
H	-4.31210200	5.01809500	1.37188000
C	-3.49583900	3.66063300	-1.61437200
H	-2.50294800	3.32381000	-1.29705800
H	-3.46040600	4.06513500	-2.62881800
H	-4.21888700	2.84327100	-1.55475100
C	-2.96006600	5.87510600	-0.74661900
H	-1.97923900	5.49283100	-0.44340900
H	-3.29724100	6.65814800	-0.06288700
H	-2.92760400	6.25129200	-1.77204600

Zero-point correction= 0.165651 (Hartree/Particle)
Thermal correction to Energy= 0.174530
Thermal correction to Enthalpy= 0.175474
Thermal correction to Gibbs Free Energy= 0.129948
Sum of electronic and zero-point Energies= -510.939409
Sum of electronic and thermal Energies= -510.930530
Sum of electronic and thermal Enthalpies= -510.929586
Sum of electronic and thermal Free Energies= -510.975111
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -511.201134660

NMe4MeS

N	-3.55905200	4.99450200	0.64294600
C	-4.06163800	6.33124100	1.06361400
H	-3.32859000	7.08605700	0.76955500
H	-4.19043600	6.32920300	2.14852700
H	-5.01719100	6.51670300	0.56790900
C	-3.37871600	4.96080900	-0.84057700
H	-3.03871700	3.95111900	-1.10846600
H	-2.64064600	5.71901200	-1.11369600
H	-4.34133500	5.18372600	-1.30766400
C	-2.24815700	4.71298800	1.30341600

H	-1.93864200	3.70443000	1.00183400
H	-2.39047800	4.77145400	2.38534600
H	-1.52834500	5.46571400	0.97293400
C	-4.53496400	3.93483800	1.03753400
H	-4.12303800	2.97380700	0.71250800
H	-5.48737300	4.14017800	0.54321800
H	-4.65423700	3.96325100	2.12311900
C	-0.51129300	2.58850600	-1.08798900
H	-0.10860200	2.31224900	-2.07226200
H	0.31190600	2.48091300	-0.36756200
H	-0.74440300	3.66507500	-1.13892700
S	-1.96243200	1.57500500	-0.63705800

Zero-point correction= 0.203291 (Hartree/Particle)
Thermal correction to Energy= 0.214443
Thermal correction to Enthalpy= 0.215387
Thermal correction to Gibbs Free Energy= 0.164509
Sum of electronic and zero-point Energies= -651.783630
Sum of electronic and thermal Energies= -651.772478
Sum of electronic and thermal Enthalpies= -651.771534
Sum of electronic and thermal Free Energies= -651.822413
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -652.129038577

NMe4NO3

N	1.67223100	-0.00094300	-0.07591000
C	3.09557600	0.07608100	-0.50500000
H	3.56911500	-0.89073800	-0.31957200
H	3.59253000	0.85922900	0.07212900
H	3.12471400	0.31428600	-1.57064000
C	0.96477300	-1.06687600	-0.84846500
H	-0.08488900	-1.05298900	-0.54674800
H	1.43963500	-2.02501400	-0.62434100

H	1.05702800	-0.83558900	-1.91230300
C	1.60098000	-0.32308900	1.38068100
H	0.54614900	-0.37309800	1.65720600
H	2.11344200	0.46740400	1.93422600
H	2.09501200	-1.28348800	1.54629900
C	0.99524200	1.30860900	-0.32079300
H	-0.05431500	1.19612600	-0.04016200
H	1.08119000	1.54404900	-1.38419700
H	1.49680100	2.07104000	0.27995700
N	-2.47345700	0.00203200	0.17415200
0	-2.05139000	0.24414700	-0.98475400
0	-1.64742200	-0.21341300	1.10553400
0	-3.69612700	-0.02651200	0.40902800

Zero-point correction= 0.181094 (Hartree/Particle)

Thermal correction to Energy= 0.192655

Thermal correction to Enthalpy= 0.193599

Thermal correction to Gibbs Free Energy= 0.141853

Sum of electronic and zero-point Energies= -493.951540

Sum of electronic and thermal Energies= -493.939979

Sum of electronic and thermal Enthalpies= -493.939035

Sum of electronic and thermal Free Energies= -493.990782

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -494.302582571

Anion Binding of 1

1-AcO-complex

C	-4.32317400	2.02298000	-0.08732100
C	-3.18831000	-0.48648100	-0.40016700
C	-3.01395200	1.91897100	-0.54726100
C	-5.08298500	0.89387000	0.22472700
C	-4.50065400	-0.35612400	0.05475000
C	-2.43246700	0.65260700	-0.68763300
H	-2.44839800	2.80642400	-0.80663900

H	-6.10359500	0.99110300	0.57989000
H	-2.74521600	-1.47002900	-0.54794900
N	-1.11917400	0.45843400	-1.16292200
H	-1.00804300	-0.45004200	-1.67521300
C	0.01000500	1.02415000	-0.64434100
S	0.00963300	2.21375200	0.54192000
N	1.13894700	0.44192900	-1.14626300
H	1.02291700	-0.47515100	-1.64089000
C	2.45084000	0.63255300	-0.66661400
C	5.09868600	0.86559400	0.25233300
C	3.03791500	1.89631200	-0.53327900
C	3.19837100	-0.50948600	-0.36537600
C	4.51018200	-0.38380500	0.09030100
C	4.34627800	1.99631900	-0.06873300
H	2.47784700	2.78521100	-0.79963500
H	2.74607700	-1.48982300	-0.50142900
H	6.11801200	0.96049900	0.61225700
C	5.28779800	-1.63625600	0.37751800
C	4.95124300	3.35785400	0.13289900
C	-5.25395700	-1.61284600	0.38154300
C	-4.92415000	3.38582800	0.11709900
F	-4.39524400	4.29723500	-0.71226500
F	-4.72729800	3.83716700	1.36843800
F	-6.25152700	3.37725700	-0.08478600
F	-5.31588600	-2.44487700	-0.67040900
F	-6.50832900	-1.37076700	0.78011600
F	-4.64881300	-2.30222200	1.37168900
F	4.53625800	-2.54355900	1.03172300
F	6.37053900	-1.39830100	1.12999100
F	5.71083400	-2.23625100	-0.74727800
F	4.74337500	3.81856400	1.37900200

F	6.28048700	3.34266500	-0.05553600
F	4.43443300	4.26580300	-0.70794900
N	-0.07728800	-3.13365300	1.52460300
C	-0.03997700	-1.68429700	1.16925300
H	0.85738400	-1.23736400	1.60647400
H	-0.93740900	-1.20019600	1.56436800
H	-0.01215200	-1.62032100	0.07949300
C	1.14445900	-3.79566600	0.97354300
H	1.09738900	-4.86254100	1.20334700
H	2.02251900	-3.34296700	1.44076500
H	1.16992600	-3.62678100	-0.10689300
C	-0.11146500	-3.29402600	3.00697100
H	-0.13994500	-4.36044500	3.24101400
H	-1.00515500	-2.79572500	3.38875000
H	0.78722400	-2.83577200	3.42556700
C	-1.30038200	-3.74640500	0.92277000
H	-1.30782000	-4.81317600	1.15700700
H	-1.27232000	-3.58361700	-0.15839700
H	-2.17918700	-3.25714700	1.34976600
C	-0.00335700	-2.68445100	-2.39388700
0	-1.12093700	-2.11816000	-2.21868500
0	1.12067500	-2.16572300	-2.12957600
C	-0.01208200	-4.11932200	-2.89921100
H	0.89501100	-4.33790500	-3.46883800
H	-0.90013700	-4.31554500	-3.50554500
H	-0.03700600	-4.79630600	-2.03376100

Zero-point correction= 0.461738 (Hartree/Particle)

Thermal correction to Energy= 0.503757

Thermal correction to Enthalpy= 0.504701

Thermal correction to Gibbs Free Energy= 0.377571

Sum of electronic and zero-point Energies= -2798.441007

Sum of electronic and thermal Energies= -2798.398987

Sum of electronic and thermal Enthalpies= -2798.398043

Sum of electronic and thermal Free Energies= -2798.525173

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2799.74712205

1-Br-complex

C	0.20167800	1.85539900	-4.38297400
C	0.74339000	-0.62221500	-3.26842800
C	0.55668900	1.77797500	-3.03829400
C	0.10135300	0.71900800	-5.18419600
C	0.38523000	-0.51599300	-4.60974200
C	0.80584400	0.52441800	-2.46802500
H	0.65123600	2.67860900	-2.44418800
H	-0.17754800	0.79700300	-6.22979400
H	0.98032200	-1.59189200	-2.82988300
N	1.18239000	0.33720300	-1.12434700
H	1.64229100	-0.57158700	-0.95914700
C	0.66979300	0.92469300	0.00000000
S	-0.47901100	2.14344400	0.00000000
N	1.18239000	0.33720300	1.12434700
H	1.64229100	-0.57158700	0.95914700
C	0.80584400	0.52441800	2.46802500
C	0.10135300	0.71900800	5.18419600
C	0.55668900	1.77797500	3.03829400
C	0.74339000	-0.62221500	3.26842800
C	0.38523000	-0.51599300	4.60974200
C	0.20167800	1.85539900	4.38297400
H	0.65123600	2.67860900	2.44418800
H	0.98032200	-1.59189200	2.82988300
H	-0.17754800	0.79700300	6.22979400
C	0.24802900	-1.78156600	5.40792000

C	-0.12313800	3.20077600	4.97184800
C	0.24802900	-1.78156600	-5.40792000
C	-0.12313800	3.20077600	-4.97184800
F	0.57566700	4.18468400	-4.38694200
F	-1.42395400	3.50784700	-4.82515500
F	0.13902000	3.24364500	-6.28701400
F	1.27636700	-2.61621500	-5.19344200
F	0.18180900	-1.54695600	-6.72481600
F	-0.86824000	-2.45414500	-5.06846200
F	-0.86824000	-2.45414500	5.06846200
F	0.18180900	-1.54695600	6.72481600
F	1.27636700	-2.61621500	5.19344200
F	-1.42395400	3.50784700	4.82515500
F	0.13902000	3.24364500	6.28701400
F	0.57566700	4.18468400	4.38694200
N	-2.46548400	-2.07493900	0.00000000
C	-1.80376600	-1.50655400	-1.21410500
H	-1.92784700	-0.41972300	-1.20302900
H	-2.26624300	-1.93964100	-2.10468500
H	-0.74584400	-1.77818100	-1.15406700
C	-1.80376600	-1.50655400	1.21410500
H	-2.26624300	-1.93964100	2.10468500
H	-1.92784700	-0.41972300	1.20302900
H	-0.74584400	-1.77818100	1.15406700
C	-3.91479900	-1.73401500	0.00000000
H	-4.37234300	-2.15703000	0.89711200
H	-4.37234300	-2.15703000	-0.89711200
H	-4.01333000	-0.64604000	0.00000000
C	-2.28402300	-3.55840000	0.00000000
H	-2.75613200	-3.96496900	0.89739400
H	-1.20908500	-3.76455900	0.00000000

H -2.75613200 -3.96496900 -0.89739400

Br 1.52783300 -2.78668800 0.00000000

Zero-point correction= 0.411629 (Hartree/Particle)

Thermal correction to Energy= 0.450079

Thermal correction to Enthalpy= 0.451023

Thermal correction to Gibbs Free Energy= 0.332207

Sum of electronic and zero-point Energies= -5144.341251

Sum of electronic and thermal Energies= -5144.302801

Sum of electronic and thermal Enthalpies= -5144.301857

Sum of electronic and thermal Free Energies= -5144.420673

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I, Br)) = -5145.95081079

1-Cl-complex

C -4.37566200 1.73019500 -0.15903500

C -3.30257900 -0.73183000 -0.83252400

C -3.01657100 1.63810900 -0.44967500

C -5.21385100 0.61573200 -0.18879700

C -4.65858100 -0.61128500 -0.53740300

C -2.46571900 0.38968100 -0.76881900

H -2.39554800 2.52555900 -0.44483800

H -6.27110800 0.70628900 0.03864700

H -2.88091700 -1.69546700 -1.11911600

N -1.11659400 0.18877800 -1.10629400

H -0.94487600 -0.70237800 -1.60864100

C 0.00646900 0.74279300 -0.55671100

S 0.00871900 1.89251500 0.66244600

N 1.12716600 0.16891300 -1.09093000

H 0.95036600 -0.72588300 -1.58532200

C 2.47596700 0.37196500 -0.75479400

C 5.22157100 0.60728600 -0.16591100

C 3.02711800 1.62633000 -0.45928900

C	3.31135200	-0.75140300	-0.78973400
C	4.66652700	-0.62598100	-0.49058700
C	4.38432300	1.72326000	-0.16365700
H	2.40653300	2.51403600	-0.47403700
H	2.88975300	-1.72107000	-1.05515600
H	6.27686000	0.70104000	0.06900900
C	5.51256400	-1.86722700	-0.53178300
C	4.95609400	3.06346800	0.20931600
C	-5.49842100	-1.85699900	-0.55953700
C	-4.94894400	3.06446900	0.23284600
F	-4.27554700	4.08204000	-0.32175900
F	-4.91055800	3.25065700	1.56339300
F	-6.23360400	3.17901200	-0.13637800
F	-5.29774800	-2.56920200	-1.67856900
F	-6.80741900	-1.58814900	-0.47793900
F	-5.19431500	-2.66916600	0.46921700
F	4.97396800	-2.84765200	0.21445800
F	6.75314000	-1.65132400	-0.07662200
F	5.62092500	-2.35374700	-1.77811600
F	4.91616100	3.26867600	1.53703900
F	6.24115900	3.17351800	-0.15994900
F	4.28268800	4.07242000	-0.36071200
N	-0.02390800	-2.54819800	2.19049300
C	-1.21771500	-1.86102500	1.61000900
H	-1.16407600	-0.79586500	1.85695400
H	-2.12130600	-2.31068600	2.02987000
H	-1.17188100	-2.01261600	0.52736200
C	1.20869900	-1.94051500	1.60300800
H	2.08293100	-2.44917400	2.01790200
H	1.22677500	-0.87475600	1.85186600
H	1.14744600	-2.08740500	0.52037200

C	-0.01400400	-2.40169600	3.67234500
H	0.86852500	-2.91182000	4.06612200
H	-0.92467400	-2.85343200	4.07330800
H	0.02154800	-1.33707000	3.91577900
C	-0.07290000	-3.99335200	1.81540600
H	0.80842600	-4.48973000	2.22868400
H	-0.07550900	-4.05469800	0.72251500
H	-0.98585700	-4.42794200	2.22986500
Cl	-0.01903800	-2.68583500	-1.76281000

Zero-point correction= 0.412022 (Hartree/Particle)
Thermal correction to Energy= 0.450343
Thermal correction to Enthalpy= 0.451287
Thermal correction to Gibbs Free Energy= 0.332441
Sum of electronic and zero-point Energies= -3030.113039
Sum of electronic and thermal Energies= -3030.074718
Sum of electronic and thermal Enthalpies= -3030.073774
Sum of electronic and thermal Free Energies= -3030.192619
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I, Cl)) = -3031.57383333

1-F-complex

C	4.41162300	-1.82966900	-0.04046600
C	3.21438500	0.62928400	-0.45269700
C	3.06720700	-1.78059100	-0.40649100
C	5.17461800	-0.67427900	0.12334700
C	4.55742700	0.55488100	-0.09614200
C	2.45202000	-0.53694300	-0.59840800
H	2.50412800	-2.69491100	-0.55145900
H	6.22021400	-0.73154900	0.40884700
H	2.73885200	1.59523100	-0.61160300
N	1.11645300	-0.36638200	-0.98726600
H	0.89788400	0.54533400	-1.46423500

C	0.00005400	-1.00006800	-0.51493800
S	-0.00000800	-2.29763200	0.54632100
N	-1.11634900	-0.36653700	-0.98745100
H	-0.89782300	0.54516900	-1.46445000
C	-2.45189600	-0.53713000	-0.59855100
C	-5.17444900	-0.67460600	0.12332800
C	-3.06692200	-1.78080300	-0.40629600
C	-3.21438400	0.62904600	-0.45308900
C	-4.55741000	0.55457000	-0.09648100
C	-4.41131700	-1.82994900	-0.04020900
H	-2.50372200	-2.69508900	-0.55102000
H	-2.73897000	1.59501300	-0.61225100
H	-6.22002800	-0.73193100	0.40887600
C	-5.34611500	1.82882200	0.01070700
C	-5.04101700	-3.16954000	0.22666500
C	5.34603900	1.82916800	0.01131900
C	5.04149000	-3.16925900	0.22602400
F	4.51061200	-4.13283300	-0.54056100
F	4.87427200	-3.55279500	1.50308700
F	6.36346500	-3.15236000	-0.00290800
F	5.78434900	2.25040000	-1.18621100
F	6.42266600	1.68989800	0.79618400
F	4.60344300	2.82994600	0.51946300
F	-4.60370600	2.82963400	0.51907400
F	-6.42298400	1.68953600	0.79523100
F	-5.78404000	2.25002900	-1.18697200
F	-4.87379400	-3.55266500	1.50385100
F	-6.36298800	-3.15287800	-0.00231500
F	-4.50999100	-4.13327800	-0.53961100
F	-0.00005300	1.81463700	-1.90776900
N	-0.00047900	3.89595700	0.59405100

C	-0.00065900	2.47561200	1.06064400
H	-0.89881600	2.30557000	1.66077400
H	0.89716600	2.30550100	1.66124700
H	-0.00044800	1.86365100	0.15511800
C	-1.21282900	4.12161300	-0.25144600
H	-1.21337300	5.16181200	-0.58710500
H	-2.10203700	3.91525600	0.35067500
H	-1.13568700	3.43104800	-1.09689200
C	-0.00075400	4.82098500	1.75983800
H	-0.00059100	5.84894600	1.38926300
H	0.89639900	4.63130000	2.35460200
H	-0.89826300	4.63139700	2.35409800
C	1.21233400	4.12150900	-0.25080200
H	1.21316400	5.16171200	-0.58644700
H	1.13557300	3.43097400	-1.09630700
H	2.10121000	3.91504800	0.35177200

Zero-point correction= 0.412857 (Hartree/Particle)

Thermal correction to Energy= 0.450550

Thermal correction to Enthalpy= 0.451494

Thermal correction to Gibbs Free Energy= 0.334175

Sum of electronic and zero-point Energies= -2669.836860

Sum of electronic and thermal Energies= -2669.799167

Sum of electronic and thermal Enthalpies= -2669.798223

Sum of electronic and thermal Free Energies= -2669.915543

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I, F)) = -2671.27516923

1-I-complex

C	2.08168800	-0.27144100	-4.32852200
C	-0.49013400	-0.48355800	-3.31563700
C	1.90197400	-0.60295500	-2.98855500
C	0.99946000	-0.03530100	-5.17769300

C	-0.28301300	-0.15489300	-4.65516100
C	0.60369600	-0.68720300	-2.47010000
H	2.75713400	-0.80728800	-2.35482700
H	1.15572300	0.22300100	-6.22001300
H	-1.50228900	-0.58300100	-2.92285900
N	0.33809200	-1.03254200	-1.12831700
H	-0.56602500	-1.50642900	-0.98771800
C	0.93285000	-0.54309400	-0.00000000
S	2.17949500	0.57914600	-0.00000000
N	0.33809200	-1.03254200	1.12831700
H	-0.56602500	-1.50642900	0.98771800
C	0.60369600	-0.68720300	2.47010000
C	0.99946000	-0.03530100	5.17769300
C	1.90197400	-0.60295500	2.98855500
C	-0.49013400	-0.48355800	3.31563700
C	-0.28301300	-0.15489300	4.65516100
C	2.08168800	-0.27144100	4.32852200
H	2.75713400	-0.80728800	2.35482700
H	-1.50228900	-0.58300100	2.92285900
H	1.15572300	0.22300100	6.22001300
C	-1.49527300	0.10084000	5.50522100
C	3.47968500	-0.12368100	4.86354900
C	-1.49527300	0.10084000	-5.50522100
C	3.47968500	-0.12368100	-4.86354900
F	4.34860300	-0.91265800	-4.21630900
F	3.92847700	1.13670000	-4.73735000
F	3.54622000	-0.42962000	-6.16773800
F	-2.32360500	-0.95432300	-5.51625400
F	-1.17780600	0.38008000	-6.77496100
F	-2.20726300	1.13951600	-5.03088100
F	-2.20726300	1.13951600	5.03088100

F	-1.17780600	0.38008000	6.77496100
F	-2.32360500	-0.95432300	5.51625400
F	3.92847700	1.13670000	4.73735000
F	3.54622000	-0.42962000	6.16773800
F	4.34860300	-0.91265800	4.21630900
N	-1.77880900	2.76524500	0.00000000
C	-1.34969700	2.00942900	-1.21613600
H	-0.25800400	1.93191100	-1.20707800
H	-1.69002600	2.54787300	-2.10466700
H	-1.80757800	1.01583100	-1.16889300
C	-1.34969700	2.00942900	1.21613600
H	-1.69002600	2.54787300	2.10466700
H	-0.25800400	1.93191100	1.20707800
H	-1.80757800	1.01583100	1.16889300
C	-1.15040000	4.11713500	0.00000000
H	-1.47107600	4.65122400	0.89768400
H	-1.47107600	4.65122400	-0.89768400
H	-0.06481100	3.99146000	0.00000000
C	-3.26623700	2.89472400	0.00000000
H	-3.56632200	3.43989200	0.89812700
H	-3.69697200	1.88881200	0.00000000
H	-3.56632200	3.43989200	-0.89812700
I	-3.09501900	-1.58822100	0.00000000

Zero-point correction= 0.410640 (Hartree/Particle)

Thermal correction to Energy= 0.449638

Thermal correction to Enthalpy= 0.450582

Thermal correction to Gibbs Free Energy= 0.329208

Sum of electronic and zero-point Energies= -2867.167384

Sum of electronic and thermal Energies= -2867.128386

Sum of electronic and thermal Enthalpies= -2867.127442

Sum of electronic and thermal Free Energies= -2867.248817

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2868.45016488

1-NO3-complex

C	-4.33614000	1.85893300	-0.13361900
C	-3.34029600	-0.65115700	-0.76319000
C	-2.98725800	1.72137400	-0.45053700
C	-5.20224600	0.76652800	-0.12519300
C	-4.68788400	-0.48454200	-0.45078000
C	-2.48037400	0.45165600	-0.74881800
H	-2.34095300	2.59018400	-0.48331600
H	-6.25338900	0.89195300	0.11425400
H	-2.94323300	-1.63054900	-1.02580300
N	-1.13879200	0.22401300	-1.12355800
H	-1.00602900	-0.54066900	-1.80300700
C	-0.00229800	0.74919100	-0.57956100
S	0.02143000	1.81083000	0.72077500
N	1.11978600	0.25547100	-1.18389200
H	0.97415700	-0.50579000	-1.86366400
C	2.46584400	0.47364700	-0.81515300
C	5.17740600	0.77686100	-0.14437900
C	2.98289200	1.74729200	-0.55049900
C	3.31166900	-0.63711700	-0.78060600
C	4.65424400	-0.47648900	-0.43927600
C	4.32615900	1.88043000	-0.21215800
H	2.34530200	2.62047200	-0.62146200
H	2.91118900	-1.62199000	-1.01993300
H	6.22284300	0.89646400	0.12036900
C	5.50723200	-1.70935700	-0.34418200
C	4.86694700	3.24217200	0.12575500
C	-5.57677100	-1.69584000	-0.41191800
C	-4.86874800	3.21612200	0.23455100

F	-4.16710700	4.20321900	-0.34093500
F	-4.82292100	3.42723100	1.56171700
F	-6.15072900	3.36109500	-0.13527900
F	-5.25560800	-2.57853000	-1.36935900
F	-6.86869000	-1.37474900	-0.57112500
F	-5.47733400	-2.34651900	0.76175100
F	5.14713900	-2.47074900	0.70658200
F	6.80649500	-1.42001800	-0.19646800
F	5.38349700	-2.48196600	-1.43439200
F	4.79371100	3.49525700	1.44426900
F	6.15862200	3.36083400	-0.21883700
F	4.19022600	4.21836900	-0.49615200
N	0.08453800	-2.34938800	2.43836500
C	0.03096300	-3.80909800	2.12230300
H	0.94197400	-4.27817100	2.50077300
H	-0.03817500	-3.92018700	1.03648600
H	-0.84849300	-4.23498600	2.61107600
C	0.19221800	-2.14750100	3.91117100
H	0.22991500	-1.07423500	4.11163800
H	1.10577500	-2.63254200	4.26199900
H	-0.68290400	-2.59326000	4.38882300
C	1.27233800	-1.74849800	1.76003700
H	1.29256900	-0.67574600	1.96936900
H	1.17080200	-1.93417400	0.68860200
H	2.17542500	-2.23479400	2.13804200
C	-1.15881300	-1.69566500	1.92681400
H	-1.09839500	-0.62193900	2.12327000
H	-2.01706900	-2.13543000	2.44052500
H	-1.22011000	-1.89134100	0.85322100
N	-0.00680800	-2.77961500	-1.64458800
0	-1.08253600	-3.13597500	-1.12054000

0 1.08495800 -3.21717600 -1.23148500

0 -0.02659200 -1.94870100 -2.60653100

Zero-point correction= 0.427742 (Hartree/Particle)

Thermal correction to Energy= 0.468557

Thermal correction to Enthalpy= 0.469501

Thermal correction to Gibbs Free Energy= 0.345879

Sum of electronic and zero-point Energies= -2850.261791

Sum of electronic and thermal Energies= -2850.220976

Sum of electronic and thermal Enthalpies= -2850.220032

Sum of electronic and thermal Free Energies= -2850.343654

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2851.55405246

1-SMe-complex

C -4.33490200 1.83764500 -0.21530400

C -3.33534000 -0.71193600 -0.62831000

C -2.98347600 1.67501900 -0.50468800

C -5.20381500 0.75012400 -0.12211700

C -4.68579700 -0.52090500 -0.34120100

C -2.46894500 0.38470300 -0.69066600

H -2.33686300 2.53912600 -0.59853500

H -6.25537000 0.89443100 0.10223500

H -2.94607100 -1.71292100 -0.81196600

N -1.12458300 0.12863900 -1.01314200

H -0.96125000 -0.78243100 -1.49635000

C -0.00069200 0.70436400 -0.49238200

S -0.00134400 1.88257000 0.70530200

N 1.12366000 0.12962800 -1.01310500

H 0.96098100 -0.78163900 -1.49637000

C 2.46790600 0.38610700 -0.69062900

C 5.20290000 0.75140900 -0.12235000

C 2.98202400 1.67623900 -0.50229300

C	3.33483100	-0.71033100	-0.63079000
C	4.68525300	-0.51941100	-0.34369300
C	4.33354800	1.83874800	-0.21317100
H	2.33511300	2.54032800	-0.59413900
H	2.94574400	-1.71104700	-0.81639500
H	6.25450100	0.89566100	0.10183400
C	5.55818000	-1.73781000	-0.24088800
C	4.86368700	3.22158100	0.04772000
C	-5.55837800	-1.73944200	-0.23699000
C	-4.86539700	3.22079300	0.04318100
F	-4.17134300	4.15637100	-0.62090400
F	-4.80421200	3.54306500	1.34738700
F	-6.15176100	3.33465100	-0.32247100
F	-5.45375100	-2.51704000	-1.32647200
F	-6.85214600	-1.42938200	-0.08380500
F	-5.20449700	-2.50509500	0.81230600
F	5.20840300	-2.50171900	0.81106300
F	6.85252500	-1.42748500	-0.09313800
F	5.44934500	-2.51719200	-1.32866200
F	4.80334300	3.54117600	1.35262800
F	6.14974500	3.33667700	-0.31863000
F	4.16879900	4.15824400	-0.61395500
N	0.00134700	-2.36768500	2.46838500
C	0.00005400	-1.91542000	3.88893600
H	0.89711600	-2.30087000	4.37816700
H	-0.89643100	-2.30315600	4.37739200
H	-0.00131900	-0.82286200	3.90128500
C	1.21789400	-1.84489600	1.77543500
H	1.18833400	-2.19589200	0.73895600
H	2.10441600	-2.23049000	2.28516400
H	1.19575300	-0.75169500	1.81756900

C	0.00359300	-3.85991900	2.40657300
H	0.00453300	-4.15687500	1.35395700
H	-0.89349100	-4.22945400	2.90843900
H	0.90132500	-4.22673900	2.90928400
C	-1.21597200	-1.84850100	1.77404500
H	-1.18386700	-2.19928800	0.73755300
H	-1.19726100	-0.75525500	1.81644700
H	-2.10193100	-2.23695100	2.28256300
C	0.00341700	-3.53645000	-3.37534300
H	-0.88640100	-4.15362700	-3.54559800
H	0.88191200	-4.17194000	-3.53680800
H	0.01537800	-2.75339900	-4.14194900
S	0.00251300	-2.83180700	-1.69381900

Zero-point correction= 0.448795 (Hartree/Particle)

Thermal correction to Energy= 0.489915

Thermal correction to Enthalpy= 0.490859

Thermal correction to Gibbs Free Energy= 0.364156

Sum of electronic and zero-point Energies= -3008.091692

Sum of electronic and thermal Energies= -3008.050571

Sum of electronic and thermal Enthalpies= -3008.049627

Sum of electronic and thermal Free Energies= -3008.176331

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3009.38403815

Uncatalyzed and 2b-catalyzed Sulfa-Michael Addition Reaction

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H	-1.07866700	-1.65319800	-0.08152400
C	-0.79229700	-1.04327600	0.78392300
C	-1.84017700	-1.25023100	1.86678700
C	-3.73451000	-1.68433600	3.88670600
C	-2.72252000	-2.33258600	1.78936400
C	-1.90905400	-0.38947400	2.96898800
C	-2.85059200	-0.60629800	3.97424100

C	-3.66872500	-2.54759800	2.79207600
H	-2.66612200	-3.00578000	0.93542000
H	-1.22449500	0.45460700	3.03573600
H	-2.89667000	0.06909300	4.82494700
H	-4.35462800	-3.38779700	2.71689100
H	-4.47180700	-1.84949700	4.66836700
C	-0.66713600	0.38676300	0.32170700
H	-1.35488400	0.65799400	-0.47521200
C	0.13303000	1.36498900	0.79396300
0	1.00878500	1.22439000	1.82868500
H	1.01684200	0.28387900	2.12218400
S	0.75323400	-1.78912200	1.45164200
C	1.90650600	-1.54143600	0.05899700
H	1.77096600	-0.51836000	-0.31090900
H	1.65137700	-2.24028200	-0.74436500
C	3.31598300	-1.75707600	0.54381500
C	5.92400400	-2.14962400	1.49340600
C	3.98181200	-0.73389000	1.23148600
C	3.96523100	-2.97939300	0.34368200
C	5.26483500	-3.17512200	0.81450300
C	5.27916600	-0.92751600	1.70206000
H	3.47130400	0.21505200	1.39258100
H	3.44839800	-3.77712400	-0.18706900
H	5.76177600	-4.12798100	0.64944100
H	5.78904800	-0.12488300	2.22923400
H	6.93686900	-2.30044700	1.85865400
C	0.13617700	2.74685200	0.25215200
C	0.57535000	3.80313100	1.06347400
C	-0.28192200	3.02857500	-1.05713000
C	0.57234500	5.11275800	0.58494700
H	0.91170900	3.59107200	2.07391400

C -0.28604400 4.33774800 -1.53246800
H -0.58354200 2.21762100 -1.71546900
C 0.13888800 5.38602800 -0.71284800
H 0.90942800 5.92112500 1.22922300
H -0.60932200 4.53806900 -2.55093700
H 0.13935100 6.40678000 -1.08686300
Zero-point correction= 0.361154 (Hartree/Particle)
Thermal correction to Energy= 0.382135
Thermal correction to Enthalpy= 0.383079
Thermal correction to Gibbs Free Energy= 0.307599
Sum of electronic and zero-point Energies= -1322.185885
Sum of electronic and thermal Energies= -1322.164903
Sum of electronic and thermal Enthalpies= -1322.163959
Sum of electronic and thermal Free Energies= -1322.239440
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -1322.84353309

11
H -1.61446500 3.33192900 -0.23887700
C -0.53441800 3.36072400 -0.04848600
H -0.27982000 4.38665400 0.23171500
C -0.22523600 2.39033700 1.10118600
H -0.41036900 1.37300700 0.73350000
C 0.14220300 2.89325800 -1.33028200
0 -0.14023800 1.78238700 -1.76308500
C 1.11588800 3.76233400 -2.05638900
C 2.96636500 5.27528700 -3.51160200
C 1.67085900 4.92352700 -1.50082000
C 1.50211400 3.36420000 -3.34583700
C 2.41601300 4.11851700 -4.07273400
C 2.59790500 5.67244300 -2.22600700
H 1.40197400 5.24448700 -0.49827800

H	1.06836400	2.45781700	-3.75903700
H	2.70379200	3.80809000	-5.07381800
H	3.03094200	6.56667900	-1.78579200
H	3.68357500	5.86503000	-4.07706500
C	-1.07731200	2.63915800	2.32460700
C	-2.68557400	3.07665200	4.58317100
C	-1.89124700	1.61854100	2.82593800
C	-1.06802900	3.88128500	2.97378800
C	-1.86940800	4.10028500	4.09221400
C	-2.69292500	1.83456100	3.94955300
H	-1.89541900	0.64971300	2.32855900
H	-0.42010200	4.67415400	2.60254500
H	-1.85608300	5.06940900	4.58512400
H	-3.31996500	1.03106300	4.32826600
H	-3.30811400	3.24794500	5.45783600
S	1.56311500	2.53053000	1.45785600
C	1.73031000	1.20895400	2.70003400
H	1.09497400	1.45199700	3.55912700
H	1.37519600	0.27020600	2.25852000
C	3.17366100	1.09775100	3.11673600
C	5.87231300	0.93364000	3.86480400
C	3.65899600	1.84982200	4.19281300
C	4.05589700	0.26897800	2.41365700
C	5.39729900	0.18424400	2.78641500
C	5.00034400	1.76769500	4.56723300
H	2.97567700	2.49832300	4.73886800
H	3.68256800	-0.31313100	1.57260400
H	6.07147000	-0.46753700	2.23605800
H	5.36421200	2.35295100	5.40827200
H	6.91736500	0.86669700	4.15716400

Zero-point correction= 0.361088 (Hartree/Particle)

Thermal correction to Energy= 0.382369

Thermal correction to Enthalpy= 0.383313

Thermal correction to Gibbs Free Energy= 0.305434

Sum of electronic and zero-point Energies= -1322.202979

Sum of electronic and thermal Energies= -1322.181698

Sum of electronic and thermal Enthalpies= -1322.180753

Sum of electronic and thermal Free Energies= -1322.258633

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -1322.85681800

8

S	-0.86481200	0.86772800	0.59598900
H	0.05530800	1.77036200	0.97157300
C	0.24384300	-0.21998100	-0.37586200
H	1.03738500	-0.59506300	0.27651100
H	0.69525300	0.36163200	-1.18452800
C	-0.57118700	-1.35911500	-0.93091700
C	-2.13277900	-3.45864900	-1.94002400
C	-1.20179200	-1.23981800	-2.17475000
C	-0.73786800	-2.53708100	-0.19360600
C	-1.51217200	-3.58312500	-0.69541500
C	-1.97667400	-2.28425000	-2.67902200
H	-1.07787400	-0.32246800	-2.74811500
H	-0.25248800	-2.63047500	0.77661000
H	-1.62945500	-4.49572100	-0.11617600
H	-2.45677900	-2.18229200	-3.64918000
H	-2.73449200	-4.27436200	-2.33325400

Zero-point correction= 0.129193 (Hartree/Particle)

Thermal correction to Energy= 0.136712

Thermal correction to Enthalpy= 0.137656

Thermal correction to Gibbs Free Energy= 0.095926

Sum of electronic and zero-point Energies= -669.142429

Sum of electronic and thermal Energies= -669.134911

Sum of electronic and thermal Enthalpies= -669.133967

Sum of electronic and thermal Free Energies= -669.175696

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -669.404350915

9

H	0.81150000	-0.15603400	0.31016700
C	0.35440800	0.00463400	1.28263100
C	-0.79956300	0.35841600	3.79596200
C	0.14815700	-1.10692500	2.11322100
C	-0.02269600	1.27749100	1.69749100
C	-0.60128300	1.45613500	2.95756100
C	-0.43131300	-0.91976200	3.37588900
H	0.13332800	2.13126800	1.04304300
H	-0.89480400	2.45022900	3.28556400
H	-0.58203200	-1.75962300	4.04816000
H	-1.24074400	0.49612800	4.77969600
C	0.58817300	-2.44353500	1.59850500
0	1.30471300	-2.50459400	0.59928900
C	0.13610200	-3.67100400	2.29334500
H	-0.57078200	-3.58237000	3.11278500
C	0.58757700	-4.87014800	1.87816800
H	1.28785000	-4.86634300	1.04132900
C	0.24952200	-6.19057900	2.41487700
C	-0.32489700	-8.77632100	3.35260000
C	0.83580500	-7.31923000	1.81849800
C	-0.63302700	-6.38063000	3.49382000
C	-0.91576700	-7.66127300	3.95649500
C	0.55234800	-8.60259700	2.28168300
H	1.51886900	-7.17690200	0.98313000
H	-1.09899500	-5.52323700	3.97342000

H -1.59932600 -7.79421400 4.79122400

H 1.01479300 -9.46443900 1.80753100

H -0.54929300 -9.77533200 3.71774100

Zero-point correction= 0.226711 (Hartree/Particle)

Thermal correction to Energy= 0.239788

Thermal correction to Enthalpy= 0.240732

Thermal correction to Gibbs Free Energy= 0.184991

Sum of electronic and zero-point Energies= -653.037361

Sum of electronic and thermal Energies= -653.024285

Sum of electronic and thermal Enthalpies= -653.023340

Sum of electronic and thermal Free Energies= -653.079081

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -653.426863838

SMA-2b-Binary-8

H 0.07448200 2.91306400 0.74008100

S -0.09790400 2.73228500 -0.57931900

C -0.78646900 4.39610600 -0.93723900

H 0.03753300 5.11523300 -0.93851800

H -1.18213700 4.32278100 -1.95505200

C -1.85315600 4.78899100 0.04840900

C -3.80048400 5.48166200 1.94428200

C -1.50033300 5.50238500 1.20079100

C -3.19186700 4.42463200 -0.14585300

C -4.16054300 4.76941000 0.79755200

C -2.46815400 5.84878400 2.14462800

H -0.46025200 5.78921800 1.35256600

H -3.47645400 3.86899100 -1.03902200

H -5.19507500 4.47849200 0.63392200

H -2.18241100 6.40720200 3.03300700

H -4.55673500 5.75150200 2.67764800

H 0.52465400 -2.24691000 -2.57584400

C	0.51350700	-2.24699900	-1.49157900
C	0.48013000	-2.23640000	1.42420600
C	-0.64490100	-2.40588500	-0.74064900
C	1.65692100	-2.09506100	-0.71618200
C	1.64106500	-2.08306100	0.67384000
C	-0.66285500	-2.39928700	0.64950600
H	0.46697800	-2.22395000	2.50844800
0	-1.92519700	-2.55923500	-1.20519400
0	-1.95629300	-2.54432100	1.08149200
0	2.94569700	-1.91499500	-1.15204100
0	2.91828900	-1.88069600	1.13296700
C	-2.73191500	-2.88009700	-0.07419500
C	3.77324900	-2.05414200	-0.00226800
C	-4.04349100	-2.12239600	-0.05732700
C	-6.65673000	-1.17017700	0.04618800
C	-5.08854700	-3.00261600	0.21892300
C	-4.26128500	-0.75880700	-0.22678100
C	-5.59146500	-0.29054800	-0.19376700
C	-6.40725200	-2.52693100	0.27102500
H	-7.67332600	-0.78951800	0.06653200
C	4.90178300	-1.04553500	0.05566400
C	7.25991800	0.40981600	0.32574400
C	6.07728500	-1.69460700	0.43485100
C	4.86202400	0.33027300	-0.14534000
C	6.06546100	1.05610400	-0.02311700
C	7.26737100	-0.96593100	0.57039500
H	8.17506200	0.98752300	0.41389100
C	-4.58497200	-4.39821200	0.46849700
H	-5.21252600	-5.16030500	-0.00496600
H	-4.59331800	-4.59373400	1.54864700
C	4.48945600	-3.41299200	0.01129500

H 3.87398300 -4.17285100 0.50070000
H 4.64360900 -3.70127400 -1.03398400
C 5.84375800 -3.15926900 0.68858900
H 5.79581700 -3.33169900 1.77175700
H 6.64952400 -3.78617700 0.29324400
C -3.15545700 -4.35814000 -0.09381100
H -2.43894600 -4.97481400 0.45543200
H -3.15929100 -4.67196200 -1.14287500
I 3.05838300 1.33181000 -0.54824900
I -2.66213100 0.59218000 -0.43504500
C -7.48558200 -3.43351600 0.54917100
N -8.34507600 -4.18353000 0.77498300
C -5.88488700 1.10113900 -0.40435400
N -6.14158500 2.22144600 -0.58275200
C 8.47814300 -1.63524300 0.95601900
N 9.44803900 -2.19532000 1.26850800
C 6.10280100 2.47602400 -0.24307300
N 6.16416700 3.62430500 -0.41559300
Zero-point correction= 0.468242 (Hartree/Particle)
Thermal correction to Energy= 0.509022
Thermal correction to Enthalpy= 0.509967
Thermal correction to Gibbs Free Energy= 0.388154
Sum of electronic and zero-point Energies= -2854.914963
Sum of electronic and thermal Energies= -2854.874183
Sum of electronic and thermal Enthalpies= -2854.873239
Sum of electronic and thermal Free Energies= -2854.995051
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2856.07923927

SMA-2b-Binary-9
C -0.26996300 3.44472100 1.11283700
H -0.33590600 4.47068000 1.46631100

C	-0.85474600	2.42381400	1.77286100
H	-0.71608200	1.42189300	1.36225700
C	0.48770800	3.15995000	-0.11733500
0	0.25404200	2.13529200	-0.78431600
C	1.57126300	4.08305200	-0.54823200
C	3.69933500	5.68663700	-1.39534600
C	2.07009700	5.09284000	0.28888100
C	2.14968000	3.88382200	-1.81285900
C	3.20848700	4.68094500	-2.23466100
C	3.13049500	5.89167800	-0.13653400
H	1.65090700	5.24353700	1.28017400
H	1.75430800	3.09755900	-2.45081000
H	3.65560300	4.51872200	-3.21191400
H	3.51803900	6.66856800	0.51739100
H	4.52883400	6.30864100	-1.72295400
C	-1.66606400	2.49311000	2.98938100
C	-3.28894900	2.52204100	5.27834100
C	-2.42383700	1.36363400	3.34431800
C	-1.73076700	3.63909800	3.80189900
C	-2.53460800	3.65030400	4.93767900
C	-3.23451200	1.37929200	4.47803300
H	-2.39075200	0.48136400	2.70523300
H	-1.13808700	4.51578000	3.55007500
H	-2.57219800	4.53860200	5.56340900
H	-3.82136500	0.50156700	4.73714800
H	-3.91483100	2.53535200	6.16735300
C	-1.28711400	-2.80518800	-0.17815300
C	0.95887800	-2.19809300	1.20731900
C	-1.34698400	-2.02801900	0.97120600
C	-0.10186500	-3.32043300	-0.68913800
C	1.01793100	-2.97649000	0.05818600

C	-0.22615700	-1.67812600	1.71651900
H	-0.05308600	-3.91255100	-1.59611400
H	-0.27056600	-1.05525900	2.60419600
0	-2.54325400	-2.92185100	-0.71097400
0	-2.64756500	-1.64598100	1.18809900
0	2.22967100	-1.99869400	1.68138800
0	2.32451700	-3.28061800	-0.21501800
C	-3.44836100	-2.33315400	0.22970200
C	3.10755900	-2.77719100	0.87419400
C	-4.42530200	-1.44588700	-0.52131400
C	-6.53748700	-0.25322700	-1.89043400
C	-5.65146900	-2.10443300	-0.61616900
C	-4.20737900	-0.21587200	-1.13816200
C	-5.29130900	0.38479900	-1.81392600
C	-6.71887600	-1.50676500	-1.30115200
H	-7.35602900	0.22970800	-2.41541800
C	4.28590300	-1.99797500	0.31571700
C	6.71178600	-1.01591800	-0.63739900
C	4.29940700	-0.75920100	-0.31890700
C	5.44235300	-2.76760400	0.44063400
C	6.66658400	-2.27612100	-0.03510300
C	5.53713000	-0.26487700	-0.78375800
H	7.65291300	-0.61561400	-1.00206500
C	-4.34377500	-3.37918600	0.90507100
H	-4.59165100	-2.99060400	1.89869900
H	-3.81294100	-4.32822300	1.01855100
C	-5.61013900	-3.45721000	0.04164400
H	-6.51590800	-3.66992000	0.61879500
H	-5.52643700	-4.23020700	-0.73351600
C	5.15452400	-4.10350800	1.07065100
H	5.91437600	-4.39284100	1.80382400

H 5.14420400 -4.87384700 0.28841000
C 3.76307200 -3.90078000 1.68699400
H 3.85865100 -3.53319600 2.71434100
H 3.13473300 -4.79536400 1.68872200
I 2.54929000 0.35987200 -0.61738300
I -2.33202700 0.72915200 -1.08361400
C -7.98142600 -2.18480700 -1.38980200
N -8.99589700 -2.75022500 -1.44855700
C -5.15056100 1.66642800 -2.44976300
N -5.07110300 2.70179600 -2.97316400
C 5.62538200 1.01801900 -1.42799000
N 5.72356500 2.05121600 -1.95297800
C 7.85738800 -3.06722100 0.09970000
N 8.81045500 -3.72267000 0.21948600

Zero-point correction= 0.565518 (Hartree/Particle)
Thermal correction to Energy= 0.611866
Thermal correction to Enthalpy= 0.612810
Thermal correction to Gibbs Free Energy= 0.479335
Sum of electronic and zero-point Energies= -2838.802047
Sum of electronic and thermal Energies= -2838.755699
Sum of electronic and thermal Enthalpies= -2838.754755
Sum of electronic and thermal Free Energies= -2838.888230
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -2840.10470731

SMA-2b-enol-complex

H -0.42778300 3.60585500 -1.50145600
C -0.99093200 3.65239300 -0.57267100
C -0.23614400 3.65610200 0.72234400
H -0.89726700 3.97682600 1.53553800
C -2.33773200 3.65960800 -0.62776100
C -3.10140400 3.53725600 -1.89246100

C	-4.55584400	3.31682300	-4.28006300
C	-2.63572200	2.72151500	-2.93436300
C	-4.31394500	4.22538800	-2.05185600
C	-5.03425100	4.11780200	-3.24087100
C	-3.35592600	2.61793800	-4.12311700
H	-1.71877000	2.15245300	-2.79505300
H	-4.68398100	4.85879500	-1.24791400
H	-5.96806800	4.66261100	-3.35652000
H	-2.98778000	1.97967400	-4.92275500
H	-5.11948400	3.23104500	-5.20596600
C	1.02655000	4.48864200	0.73857100
C	3.39889900	5.98696300	0.84685100
C	1.24848700	5.39364600	1.78190700
C	2.00888800	4.33885500	-0.25072100
C	3.18763000	5.08052200	-0.19733000
C	2.42676200	6.14332400	1.83488500
H	0.49052000	5.51048000	2.55572100
H	1.85365000	3.62868900	-1.06201600
H	3.94561400	4.94494400	-0.96486800
H	2.58393400	6.84498600	2.65083500
H	4.31933600	6.56440400	0.88887800
S	0.16317200	1.88618700	1.06952400
C	0.93976800	2.00053800	2.71665400
H	1.96826500	2.36237400	2.60174900
H	0.37262100	2.74894000	3.28528800
C	0.91243700	0.66450600	3.41680300
C	0.86527700	-1.77057600	4.81600100
C	2.09049100	-0.06483500	3.61311500
C	-0.29585400	0.14770900	3.90660000
C	-0.32077700	-1.05950700	4.60363400
C	2.06923500	-1.27467300	4.31215200

H	3.03097400	0.32958300	3.23207900
H	-1.21672500	0.70891900	3.75098100
H	-1.26302400	-1.44180000	4.98908400
H	2.99484600	-1.82393900	4.46772000
H	0.84849800	-2.70691700	5.36899100
C	-0.95444500	-3.08865800	-0.78752800
C	1.47651200	-2.74105700	0.35563500
C	-0.82673100	-2.95055300	0.58888300
C	0.12834300	-3.07160300	-1.65882600
C	1.35021600	-2.89417500	-1.01989700
C	0.39148700	-2.74173600	1.22573600
H	0.02865800	-3.17631500	-2.73350100
H	0.48781100	-2.59944000	2.29687800
0	-2.28083200	-3.20931500	-1.10878300
0	-2.07225100	-3.01316200	1.16397800
0	2.80364100	-2.57256000	0.66803400
0	2.59049500	-2.81001900	-1.59771100
C	-2.99822100	-3.31547800	0.12808100
C	3.53517900	-2.84926900	-0.52136800
C	-4.20131600	-2.38916300	0.07481900
C	-6.66315100	-1.11569900	-0.22992500
C	-5.34112800	-3.14205800	-0.20747200
C	-4.25076300	-1.00401200	0.18487900
C	-5.50585800	-0.37339300	0.03895600
C	-6.58204700	-2.50554300	-0.36096200
H	-7.61689000	-0.60836000	-0.33862600
C	4.64866700	-1.86238000	-0.81465100
C	6.93826300	-0.46656100	-1.56374600
C	4.61869800	-0.47137500	-0.78564500
C	5.77424800	-2.56202400	-1.24932000
C	6.93075100	-1.86285400	-1.62441900

C	5.78959200	0.22464000	-1.15264500
H	7.82871500	0.08931600	-1.84203300
C	-3.62297100	-4.70406800	0.30401200
H	-3.72010400	-4.87787400	1.38134000
H	-2.97929400	-5.47713900	-0.12419200
C	-5.01409700	-4.60578400	-0.34025800
H	-5.76108600	-5.24718000	0.13846800
H	-4.98563300	-4.87266400	-1.40491700
C	5.52471000	-4.04584800	-1.28620900
H	6.37482500	-4.62318500	-0.90839900
H	5.35532200	-4.35458600	-2.32609800
C	4.25697300	-4.20125100	-0.43401600
H	4.52834100	-4.34912600	0.61684500
H	3.59776900	-5.01561100	-0.74710800
I	2.87172700	0.57065500	-0.24375300
I	-2.52814600	0.14637300	0.55107900
C	-7.75458700	-3.28300300	-0.64886700
N	-8.69242000	-3.93044700	-0.88033600
C	-5.59279600	1.05552700	0.16083500
N	-5.62308600	2.21364000	0.26530300
C	5.83246100	1.66166500	-1.12694700
N	5.89540900	2.82290600	-1.11735600
C	8.09123700	-2.58302100	-2.06806400
N	9.02096300	-3.18414200	-2.42382300
0	-3.06289400	3.82110900	0.51233800
H	-3.96639800	3.46340900	0.39479600

Zero-point correction= 0.699947 (Hartree/Particle)

Thermal correction to Energy= 0.754168

Thermal correction to Enthalpy= 0.755112

Thermal correction to Gibbs Free Energy= 0.605620

Sum of electronic and zero-point Energies= -3507.926232

Sum of electronic and thermal Energies= -3507.872012

Sum of electronic and thermal Enthalpies= -3507.871068

Sum of electronic and thermal Free Energies= -3508.020560

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3509.53180277

SMA-2b-product-complex-2

H	2.19321200	2.13409900	-1.22794400
C	1.68906000	3.10161000	-1.15330100
H	0.82179500	3.06737700	-1.82614100
C	1.20854200	3.35155600	0.28430300
H	0.56125300	4.23540800	0.28850600
C	2.56731900	4.25857700	-1.60694500
0	2.12867100	5.39830700	-1.51051300
C	3.93410700	4.01050700	-2.15540500
C	6.52795300	3.71163800	-3.16817000
C	4.57749800	2.76514000	-2.09566300
C	4.60654500	5.10411700	-2.72527500
C	5.89160700	4.95586600	-3.23533800
C	5.87257400	2.62125200	-2.59453200
H	4.09231500	1.90058600	-1.64963400
H	4.09787100	6.06392900	-2.75706900
H	6.40170900	5.80618500	-3.68105100
H	6.36784100	1.65592900	-2.52626500
H	7.53560600	3.59489900	-3.56007800
C	2.34685300	3.56691900	1.25836500
C	4.45616800	4.01487700	3.05917500
C	2.33219800	4.67820900	2.10911800
C	3.43318600	2.68123100	1.31919200
C	4.48123200	2.90422900	2.21032500
C	3.37946600	4.90066400	3.00745500
H	1.49538200	5.37362800	2.05966400

H	3.46716600	1.81118000	0.66629400
H	5.31894900	2.21073300	2.23344700
H	3.35372400	5.76893500	3.66161200
H	5.27381200	4.18901900	3.75452100
S	0.19255500	1.89080900	0.72277700
C	-0.35874200	2.28033900	2.41580700
H	0.44815700	2.85194000	2.89087500
H	-1.25190100	2.91316100	2.36622700
C	-0.63395000	1.01411400	3.18747600
C	-1.11272900	-1.30307500	4.69515500
C	0.43147200	0.19860300	3.59439700
C	-1.94041400	0.64819800	3.52730300
C	-2.17977500	-0.50203100	4.28414700
C	0.19519600	-0.95434500	4.34105200
H	1.44948000	0.48538000	3.32900400
H	-2.77034100	1.27859300	3.21202200
H	-3.19928600	-0.76890300	4.55264000
H	1.03034400	-1.57502900	4.65696200
H	-1.29712700	-2.19594200	5.28825300
C	-2.68548400	-2.35492100	-1.03451800
C	-0.57411000	-3.18550100	0.44103000
C	-2.66987400	-2.18744300	0.34530600
C	-1.63884600	-2.93210600	-1.74498300
C	-0.57951000	-3.33480700	-0.94008200
C	-1.60676100	-2.58305900	1.14910800
H	-1.64417700	-3.04727500	-2.82313200
H	-1.58533800	-2.43603000	2.22311600
0	-3.85375800	-1.84017900	-1.53532300
0	-3.83237300	-1.56883400	0.73527800
0	0.60671800	-3.67375700	0.94189100
0	0.60759200	-3.89222500	-1.33831300

C	-4.69073500	-1.58873900	-0.40096600
C	1.31489600	-4.25572000	-0.14598300
C	-5.44836400	-0.29564200	-0.62305800
C	-7.22855600	1.77206700	-1.17472400
C	-6.77373200	-0.59029200	-0.94291100
C	-4.97020900	1.01111900	-0.62253600
C	-5.88551200	2.05192500	-0.88470300
C	-7.67461600	0.44845000	-1.21878300
H	-7.91505100	2.58943400	-1.37366800
C	2.75461500	-3.78587400	-0.25843900
C	5.49057900	-3.40803100	-0.62163900
C	3.26750700	-2.49739100	-0.16092900
C	3.56872800	-4.87598800	-0.56473200
C	4.94662000	-4.68987300	-0.74930400
C	4.65714600	-2.31902500	-0.33131000
H	6.55730500	-3.24948800	-0.74843300
C	-5.79621000	-2.64383600	-0.24668300
H	-6.01075200	-2.72396100	0.82438700
H	-5.45963200	-3.61746100	-0.61350000
C	-7.01742000	-2.07486000	-0.98341400
H	-7.96996500	-2.35612000	-0.52262400
H	-7.05055900	-2.40313400	-2.03045300
C	2.76785200	-6.14544800	-0.67992100
H	3.27081100	-7.00078500	-0.21733700
H	2.62264200	-6.38468200	-1.74154400
C	1.44287800	-5.77637700	0.00451300
H	1.50529800	-5.98629200	1.07786300
H	0.56517200	-6.28284600	-0.40570100
I	2.03128700	-0.84045600	0.22060600
I	-2.93394400	1.42916300	-0.28890300
C	-9.04036100	0.14535900	-1.54278600

N -10.14232500 -0.12066200 -1.80183900
C -5.46819100 3.42745200 -0.86978600
N -5.15993900 4.54867600 -0.86205700
C 5.24232700 -1.01108300 -0.21013800
N 5.71985700 0.04545500 -0.10904800
C 5.78533300 -5.81320700 -1.06052900
N 6.44773400 -6.73566900 -1.31049600
Zero-point correction= 0.700007 (Hartree/Particle)
Thermal correction to Energy= 0.754446
Thermal correction to Enthalpy= 0.755390
Thermal correction to Gibbs Free Energy= 0.602691
Sum of electronic and zero-point Energies= -3507.940211
Sum of electronic and thermal Energies= -3507.885772
Sum of electronic and thermal Enthalpies= -3507.884828
Sum of electronic and thermal Free Energies= -3508.037528
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3509.54060087

SMA-2b-product-complex
H -1.73498900 3.31747800 -0.17153900
C -0.65316700 3.38566900 0.00297600
H -0.42596400 4.42058500 0.27378400
C -0.28447700 2.43381400 1.15884600
H -0.41988000 1.40057400 0.80058700
C 0.03420700 2.91807400 -1.26560800
0 -0.29914000 1.81651800 -1.72170600
C 1.09760800 3.70857500 -1.93239400
C 3.16110800 5.07227300 -3.23935200
C 1.59578600 4.91038800 -1.40401800
C 1.64306600 3.20016800 -3.12474000
C 2.66908000 3.87715100 -3.77419400
C 2.62440900 5.58701400 -2.05761300

H	1.19795600	5.32130900	-0.48030400
H	1.24701400	2.27200100	-3.52800400
H	3.09116300	3.47328000	-4.69048200
H	3.00920000	6.51433700	-1.64170300
H	3.96529800	5.60151100	-3.74468300
C	-1.15615400	2.65452500	2.37639500
C	-2.83339900	3.07528500	4.58881300
C	-2.11054500	1.69628200	2.73677500
C	-1.05143800	3.82862200	3.13457300
C	-1.88520600	4.03906700	4.23156800
C	-2.94427100	1.90425000	3.83910000
H	-2.21126900	0.78792000	2.14413200
H	-0.30353700	4.57289300	2.86474100
H	-1.79402400	4.95457200	4.81146600
H	-3.67794700	1.14813500	4.10892700
H	-3.47996100	3.23832300	5.44779800
S	1.49461000	2.66200000	1.49233900
C	1.77433400	1.22354200	2.56945300
H	1.13155500	1.31468100	3.45428900
H	1.49035800	0.32206000	2.01242300
C	3.23092400	1.16209600	2.94963100
C	5.96021500	1.07685700	3.59715700
C	3.74387500	1.97808300	3.96571100
C	4.09938200	0.30913700	2.25957700
C	5.45644200	0.26286900	2.58039400
C	5.10052900	1.93421300	4.28928900
H	3.07269500	2.64669700	4.50323300
H	3.69695800	-0.32654800	1.47355300
H	6.11740300	-0.40807000	2.03517900
H	5.48767100	2.56892300	5.08304900
H	7.01719100	1.04346400	3.85063400

C	-1.98215300	-2.96094800	0.04732800
C	0.46778900	-2.36430200	1.03143700
C	-1.83391800	-2.06004600	1.09384300
C	-0.91260400	-3.61646800	-0.55092100
C	0.31982600	-3.27312100	-0.00811900
C	-0.60136500	-1.71028000	1.63356300
H	-1.02611200	-4.30868800	-1.37769600
H	-0.48793200	-0.99264000	2.44020900
0	-3.30525100	-3.03872800	-0.29710300
0	-3.06415500	-1.55804400	1.43423300
0	1.80365600	-2.19452400	1.29328300
0	1.55567400	-3.70132800	-0.41421200
C	-4.03252700	-2.27319700	0.67054400
C	2.51543900	-3.12197300	0.47631800
C	-5.02653100	-1.37848400	-0.04668900
C	-7.20162100	-0.11000400	-1.23478100
C	-6.30714000	-1.91203400	0.10164500
C	-4.79186400	-0.24429000	-0.81966200
C	-5.90593900	0.39847200	-1.40140500
C	-7.40603700	-1.27573500	-0.49244600
H	-8.04160400	0.40351600	-1.69266400
C	3.63151100	-2.49133800	-0.33878800
C	5.94061900	-1.76810900	-1.71992800
C	3.60024000	-1.35259000	-1.14035300
C	4.77058700	-3.29191400	-0.25296400
C	5.93684000	-2.92906600	-0.94219000
C	4.78015900	-0.98828500	-1.82404900
H	6.83730600	-1.46861300	-2.25415000
C	-4.90892100	-3.15480100	1.56904000
H	-4.97876500	-2.64976900	2.53843900
H	-4.45073500	-4.13675400	1.71397400

C -6.28833800 -3.18972200 0.89616300
H -7.11627600 -3.25075600 1.60993900
H -6.38404700 -4.04060400 0.20912300
C 4.52785200 -4.51620600 0.58693600
H 5.36713500 -4.73857500 1.25388300
H 4.39640000 -5.38306900 -0.07369900
C 3.23415500 -4.16896200 1.33683400
H 3.47396800 -3.67984700 2.28724600
H 2.58176400 -5.02356800 1.53416100
I 1.87433200 -0.18176400 -1.36192000
I -2.85601000 0.50318600 -1.16624500
C -8.72433600 -1.82220000 -0.33258600
N -9.78391200 -2.27948900 -0.18977800
C -5.74911800 1.59185600 -2.18740100
N -5.65775000 2.55943700 -2.82587800
C 4.82095600 0.18223100 -2.65850700
N 4.88071600 1.11873100 -3.34539500
C 7.10931400 -3.75248000 -0.84645800
N 8.04805900 -4.43253800 -0.75451700

Zero-point correction= 0.700249 (Hartree/Particle)
Thermal correction to Energy= 0.754472
Thermal correction to Enthalpy= 0.755416
Thermal correction to Gibbs Free Energy= 0.604610
Sum of electronic and zero-point Energies= -3507.946063
Sum of electronic and thermal Energies= -3507.891840
Sum of electronic and thermal Enthalpies= -3507.890896
Sum of electronic and thermal Free Energies= -3508.041702
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3509.54430040

SMA-2b-tertiary

C -0.50188200 2.07396700 2.01458500

H	-0.48776900	3.14056100	1.77704300
C	0.69118500	1.44394800	2.02097500
H	0.77630100	0.38563100	2.25151400
C	1.90483200	2.23661500	1.72116800
0	1.81160400	3.35709700	1.20925500
H	0.29485100	2.88278900	-0.48675700
C	3.25676400	1.69037700	2.06176600
C	5.84242000	0.79901600	2.67425400
C	3.46605100	0.37573300	2.50161600
C	4.35913900	2.54746700	1.91255000
C	5.64209400	2.11033600	2.22843600
C	4.75594900	-0.06931900	2.79631800
H	2.63778300	-0.31837600	2.60239600
H	4.18501600	3.55624600	1.54784900
H	6.48748300	2.78559600	2.11827500
H	4.90838000	-1.09450800	3.12711400
H	6.84512400	0.45351400	2.91666400
C	-1.83130400	1.51499500	2.25350900
C	-4.45240400	0.55025500	2.52799100
C	-2.93319200	2.35742100	2.03289100
C	-2.06162500	0.17648300	2.61901500
C	-3.36208400	-0.29872000	2.75607500
C	-4.23649300	1.88030900	2.16092300
H	-2.75330200	3.39001500	1.73961500
H	-1.22184600	-0.49508700	2.78539800
H	-3.52904700	-1.33896600	3.02473500
H	-5.07699600	2.54308900	1.96518600
H	-5.46647100	0.16870700	2.62936700
S	-0.23948000	2.31412000	-1.58257600
C	-1.10567800	3.79491500	-2.22233100
H	-0.35362600	4.51093300	-2.56668900

H	-1.66433900	3.44186100	-3.09518500
C	-2.02647500	4.42155700	-1.20780600
C	-3.73134900	5.66871700	0.64292000
C	-1.51153300	5.31006100	-0.25293800
C	-3.39869200	4.14371000	-1.20756000
C	-4.24825100	4.76658500	-0.28997000
C	-2.35807800	5.93271300	0.66595900
H	-0.44185400	5.52041400	-0.24084000
H	-3.80723500	3.44751800	-1.93888500
H	-5.31245900	4.54394200	-0.31061600
H	-1.94785900	6.63068400	1.39210800
H	-4.39321300	6.16140000	1.35142200
H	0.19985200	-3.03875300	-2.85643500
C	0.22533500	-2.89932900	-1.78147100
C	0.29083200	-2.51770500	1.10774400
C	-0.91282800	-2.90863300	-0.98434400
C	1.39957700	-2.70096500	-1.06524200
C	1.43088800	-2.51077700	0.31077100
C	-0.88461800	-2.72370900	0.39325500
H	0.31693500	-2.37990200	2.18384300
0	-2.21217100	-3.06856600	-1.38976500
0	-2.16543800	-2.76452300	0.87814200
0	2.67802900	-2.63430100	-1.55849500
0	2.72848300	-2.31050400	0.70652500
C	-2.99654000	-3.19431000	-0.20844600
C	3.54635300	-2.60743400	-0.43285900
C	-4.26511100	-2.36604100	-0.23825900
C	-6.80868700	-1.24904700	-0.06659900
C	-5.32585400	-3.13248700	0.24326500
C	-4.42720600	-1.02935500	-0.59212100
C	-5.72508600	-0.48038400	-0.51426400

C	-6.61056900	-2.57557100	0.32800400
H	-7.79786000	-0.80399500	-0.01587700
C	4.65052600	-1.57394800	-0.53272900
C	6.96806500	-0.03421200	-0.44793300
C	5.84099800	-2.13811400	-0.07411600
C	4.57663200	-0.23758700	-0.91531000
C	5.75882300	0.53025000	-0.87805700
C	7.01221500	-1.36852200	-0.03590900
H	7.86538300	0.57702500	-0.42507500
C	-4.87285200	-4.50755300	0.65487000
H	-5.57655900	-5.28929500	0.35118800
H	-4.79279300	-4.54663600	1.74917800
C	4.29788900	-3.93417700	-0.26715900
H	3.70347800	-4.64963600	0.30773000
H	4.46153400	-4.33534300	-1.27319200
C	5.64220400	-3.56158200	0.37324200
H	5.58930500	-3.58741100	1.47006400
H	6.46484000	-4.21682600	0.06929000
C	-3.49962600	-4.63285800	-0.02097200
H	-2.77362100	-5.23053300	0.53690000
H	-3.61508800	-5.06056900	-1.02262000
I	2.76845700	0.65610500	-1.49967000
I	-2.79091300	0.19067300	-1.08038300
C	-7.70475900	-3.36670700	0.81630500
N	-8.57783700	-4.02357200	1.21471000
C	-5.96166900	0.89894800	-0.84277100
N	-6.18390900	2.01320000	-1.09259100
C	8.23789200	-1.94859700	0.43668400
N	9.22033700	-2.43505900	0.82460300
C	5.75833400	1.92128900	-1.24093000
N	5.79428300	3.05100500	-1.51471000

Zero-point correction= 0.695851 (Hartree/Particle)
Thermal correction to Energy= 0.751008
Thermal correction to Enthalpy= 0.751952
Thermal correction to Gibbs Free Energy= 0.601982
Sum of electronic and zero-point Energies= -3507.933357
Sum of electronic and thermal Energies= -3507.878201
Sum of electronic and thermal Enthalpies= -3507.877257
Sum of electronic and thermal Free Energies= -3508.027226
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3509.53377515

SMA-2b-TS

C	-0.35879000	2.60012400	1.32079800
H	-0.44318200	3.62674600	0.96698700
C	0.90419800	2.18707500	1.81266000
H	0.98121800	1.35932900	2.50957400
C	2.05466700	2.82048700	1.38546300
0	2.01160300	3.64775500	0.34251900
H	1.26810000	3.34986800	-0.26131100
C	3.38686400	2.61279800	1.96694800
C	5.94595200	2.17582300	3.00772900
C	3.54261700	2.09832100	3.26455600
C	4.52322800	2.91885400	1.20086600
C	5.79680200	2.69396800	1.71849800
C	4.81762100	1.88194500	3.77976400
H	2.66687500	1.88670100	3.87343800
H	4.39647700	3.31225500	0.19634300
H	6.67069400	2.92168700	1.11242800
H	4.93326200	1.48919900	4.78662900
H	6.94007700	2.00442100	3.41341100
C	-1.61691500	2.00819800	1.76987500
C	-4.08642600	0.95728400	2.57199100

C	-2.79182100	2.76722800	1.63649800
C	-1.69443100	0.71153000	2.30883400
C	-2.92206700	0.19362500	2.71274500
C	-4.02064300	2.24499800	2.03065300
H	-2.72714600	3.77020400	1.21951300
H	-0.79898100	0.09733000	2.37819300
H	-2.97666200	-0.81674300	3.10947200
H	-4.92389600	2.83820300	1.90769100
H	-5.04552700	0.54418000	2.87716200
S	-0.17870900	1.97083800	-1.10523600
C	-0.94434700	3.18563000	-2.25612400
H	-0.14244200	3.72687100	-2.77001600
H	-1.50476000	2.61780300	-3.00791300
C	-1.86225600	4.15550100	-1.55662100
C	-3.55860600	5.96974000	-0.23460200
C	-1.33341200	5.25585200	-0.86516500
C	-3.25094100	3.97782700	-1.57629900
C	-4.09510000	4.87906300	-0.92214100
C	-2.17234800	6.15530500	-0.20550100
H	-0.25245700	5.40571700	-0.84956900
H	-3.67557200	3.12798500	-2.10866800
H	-5.17034300	4.71918300	-0.94903100
H	-1.74604900	7.00582700	0.32168300
H	-4.21415800	6.67375600	0.27269700
H	-0.00270000	-3.35148400	-2.65708600
C	0.03557200	-3.15961200	-1.59062300
C	0.13756800	-2.62622900	1.27294600
C	-1.09523200	-3.09380900	-0.78677300
C	1.22086300	-2.95745800	-0.89407900
C	1.27191400	-2.69712200	0.47012500
C	-1.04926400	-2.83619500	0.57835600

H	0.17476700	-2.42566900	2.33840100
0	-2.40135100	-3.23302000	-1.17591700
0	-2.32790900	-2.80703200	1.07214900
0	2.49440300	-2.94981500	-1.40117000
0	2.57985200	-2.51098400	0.84133000
C	-3.18489100	-3.25619800	0.01253300
C	3.37114000	-2.92362700	-0.27875600
C	-4.41165900	-2.36927700	-0.05774000
C	-6.88698800	-1.10903700	0.08628100
C	-5.50814800	-3.05835200	0.45817600
C	-4.50134200	-1.04202300	-0.47325900
C	-5.76581000	-0.41901800	-0.39668700
C	-6.76118000	-2.43015200	0.52477500
H	-7.84886300	-0.60696300	0.12948500
C	4.54078600	-1.98063900	-0.47163900
C	6.97050800	-0.64492700	-0.69033000
C	5.71746200	-2.61778000	-0.07925000
C	4.53281300	-0.66240600	-0.92072300
C	5.77531200	-0.00632900	-1.05200200
C	6.94462100	-1.94718100	-0.18444100
H	7.91364100	-0.11803600	-0.80035200
C	-5.12703200	-4.43567400	0.93075600
H	-5.86537100	-5.19406100	0.65024300
H	-5.06163000	-4.43390700	2.02664600
C	4.03078600	-4.29404300	-0.05438500
H	3.42805400	-4.91088500	0.61780000
H	4.08365700	-4.78443700	-1.03211800
C	5.44829000	-3.99766500	0.45733400
H	5.48848900	-3.97041400	1.55407300
H	6.19039500	-4.72922300	0.12142600
C	-3.75468800	-4.65767800	0.27764300

H -3.06087900 -5.25377000 0.87662100
H -3.87993300 -5.13729500 -0.69896600
I 2.72270500 0.36434400 -1.26474300
I -2.78901700 0.06081100 -1.01088600
C -7.89472900 -3.13981900 1.04697300
N -8.80081300 -3.73151400 1.47312600
C -5.93431300 0.95825400 -0.77275700
N -6.10916100 2.07365200 -1.05347400
C 8.15736600 -2.60169600 0.21843600
N 9.12882500 -3.14817500 0.55011200
C 5.86022900 1.33679200 -1.55781300
N 5.96730500 2.42319600 -1.95991300
Zero-point correction= 0.698395 (Hartree/Particle)
Thermal correction to Energy= 0.752152
Thermal correction to Enthalpy= 0.753096
Thermal correction to Gibbs Free Energy= 0.605871
Sum of electronic and zero-point Energies= -3507.903062
Sum of electronic and thermal Energies= -3507.849305
Sum of electronic and thermal Enthalpies= -3507.848361
Sum of electronic and thermal Free Energies= -3507.995586
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3509.50500299

SMA-UN-Binary
C -0.61266600 1.87881000 1.73505400
H -0.66807900 2.85704100 1.25615800
C 0.61850600 1.37459700 1.94994800
H 0.76620200 0.40700500 2.42127300
C 1.80007900 2.14091900 1.50253200
0 1.68794200 3.10182600 0.73299300
H 0.27764500 2.65934000 -0.90825400
C 3.15725300 1.73253200 1.97672200

C	5.74766200	1.06793500	2.79887700
C	3.35291600	0.86646600	3.06166900
C	4.27129900	2.26838600	1.31379600
C	5.55962000	1.93379100	1.71739700
C	4.64498000	0.54009000	3.47228800
H	2.50400000	0.46000500	3.60450200
H	4.10221000	2.94352000	0.47951900
H	6.41794800	2.34575300	1.19304200
H	4.79027900	-0.12556100	4.31902500
H	6.75387700	0.80690300	3.11726300
C	-1.90547000	1.27315900	2.05527900
C	-4.44640700	0.20475300	2.57705900
C	-3.06268800	1.91082800	1.57818500
C	-2.04009500	0.08999000	2.80277200
C	-3.30111900	-0.43713300	3.06113500
C	-4.32491200	1.37960000	1.83364600
H	-2.95823000	2.82460000	0.99493000
H	-1.15524800	-0.41124300	3.18861900
H	-3.39567400	-1.35022500	3.64337600
H	-5.21013700	1.88387700	1.45415600
H	-5.42947000	-0.21145800	2.78264500
S	-0.53700300	2.35070600	-1.93400000
C	-1.11302400	4.05437900	-2.27272600
H	-0.24097700	4.67815900	-2.49130100
H	-1.70714900	3.98074700	-3.18879200
C	-1.93238400	4.64320400	-1.15436300
C	-3.44656000	5.71748400	0.95441400
C	-1.30134900	5.14516500	-0.00788000
C	-3.32882300	4.68517200	-1.23103800
C	-4.08321600	5.21982800	-0.18412100
C	-2.05231600	5.67698500	1.04089400

H -0.21470500 5.10015600 0.06571200
H -3.82534200 4.29788300 -2.11926700
H -5.16756600 5.25028400 -0.26031700
H -1.54927100 6.06279500 1.92431200
H -4.03209700 6.13526700 1.76960600
Zero-point correction= 0.356758 (Hartree/Particle)
Thermal correction to Energy= 0.379242
Thermal correction to Enthalpy= 0.380186
Thermal correction to Gibbs Free Energy= 0.299724
Sum of electronic and zero-point Energies= -1322.190212
Sum of electronic and thermal Energies= -1322.167728
Sum of electronic and thermal Enthalpies= -1322.166783
Sum of electronic and thermal Free Energies= -1322.247245
E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -1322.84137003

SMA-UN-TS
C -0.40928400 3.06174300 1.52877100
H -0.83264700 2.75004800 2.48312300
C 0.33614600 2.14131600 0.81382600
H 0.55742000 2.29321500 -0.23750000
C 0.87068300 1.02122600 1.47891300
0 0.92389000 1.00691100 2.78228500
H 0.98895400 1.98731200 3.18331400
C 1.43225800 -0.14577900 0.79126300
C 2.50848300 -2.38968500 -0.47793100
C 1.14570800 -0.39705700 -0.56127900
C 2.25475000 -1.03440200 1.50423200
C 2.79255200 -2.14861100 0.86893300
C 1.68349300 -1.51504200 -1.19042100
H 0.48665800 0.26836300 -1.11248000
H 2.47058500 -0.83296600 2.54911200

H	3.43448000	-2.82928000	1.42135600
H	1.45561800	-1.70925500	-2.23480300
H	2.92748700	-3.26211200	-0.97270100
C	-0.91828000	4.31885600	1.00149100
C	-1.99646600	6.71150000	0.02682700
C	-2.02812100	4.91113300	1.63122400
C	-0.35009700	4.94788600	-0.12235900
C	-0.88657900	6.13598100	-0.60287000
C	-2.56779900	6.09834300	1.14325600
H	-2.46840300	4.41542000	2.49446400
H	0.52422100	4.51305500	-0.60033800
H	-0.43972500	6.62173000	-1.46609900
H	-3.42989500	6.54467300	1.63131100
H	-2.41204200	7.64121000	-0.35337600
S	1.39271500	3.77631600	3.69900000
C	-0.07471700	4.26230700	4.66469400
H	0.27970200	4.83231400	5.53428400
H	-0.68557400	4.96155500	4.07702000
C	-0.96743900	3.13477600	5.14501600
C	-2.68059900	1.10813900	6.09875200
C	-0.45258600	1.90891000	5.58705900
C	-2.35634800	3.32430600	5.18844200
C	-3.20771800	2.32324500	5.65987500
C	-1.29907800	0.90670900	6.06206400
H	0.62261000	1.74517300	5.55117100
H	-2.77086600	4.27579600	4.85580200
H	-4.28182500	2.49300600	5.68100900
H	-0.87758400	-0.03660200	6.40201800
H	-3.33958200	0.32392600	6.46350400

Zero-point correction= 0.357990 (Hartree/Particle)

Thermal correction to Energy= 0.378600

Thermal correction to Enthalpy= 0.379544

Thermal correction to Gibbs Free Energy= 0.305929

Sum of electronic and zero-point Energies= -1322.156370

Sum of electronic and thermal Energies= -1322.135761

Sum of electronic and thermal Enthalpies= -1322.134817

Sum of electronic and thermal Free Energies= -1322.208432

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -1322.80862027

1-catalyzed Sulfa-Michael Addition Reaction

SMA-1-Binary-8

H	-0.12584700	3.70771400	0.08636800
S	-0.34270500	2.99611700	-1.02951400
C	-1.76473700	3.96914700	-1.65760300
H	-1.37559600	4.88840300	-2.10373600
H	-2.19529100	3.35826800	-2.45673100
C	-2.77744600	4.27558400	-0.58878000
C	-4.61958600	4.86453400	1.44034700
C	-2.64436000	5.44173000	0.17364100
C	-3.84175100	3.40510400	-0.32522900
C	-4.76035300	3.69956200	0.68291500
C	-3.55942100	5.73565100	1.18471700
H	-1.82018500	6.12316200	-0.03367500
H	-3.95368700	2.49795500	-0.91717600
H	-5.58706500	3.02183400	0.87305800
H	-3.44790400	6.64655100	1.76761500
H	-5.33679300	5.09359400	2.22447000
N	-0.58754600	-0.47632600	-0.38738700
H	-0.66562500	0.53145200	-0.55451400
C	0.65799900	-0.93988200	-0.06261700
S	0.96046400	-2.39673400	0.68864100
N	1.62561900	-0.04304800	-0.43888900
H	1.35508100	0.63305700	-1.15313500

C	3.01111400	-0.07880400	-0.17271600
C	5.78328200	0.00186000	0.27614200
C	3.52862700	-0.44258600	1.07476700
C	3.87758400	0.34420200	-1.18377900
C	5.25015400	0.38511700	-0.95071600
C	4.90534500	-0.40718500	1.27826800
H	2.86449400	-0.74023600	1.87763900
H	3.47576200	0.64109200	-2.14953700
H	6.85422800	0.02785200	0.45078800
C	-1.82582400	-1.14028400	-0.27011100
C	-4.36890900	-2.32399400	-0.11325700
C	-2.91975700	-0.40006900	0.18300800
C	-2.00398200	-2.47169300	-0.66221800
C	-3.26661100	-3.04816600	-0.56651600
C	-4.17879100	-0.99527400	0.24966500
H	-2.78511100	0.63779100	0.48345900
H	-1.16851200	-3.04375400	-1.04875000
H	-5.34966300	-2.78376200	-0.05069900
C	5.45218600	-0.74172500	2.63922600
C	6.17129300	0.79107300	-2.06754900
F	7.30718000	1.33099800	-1.60217100
F	5.59718400	1.69096300	-2.88093600
F	6.52185500	-0.25604200	-2.83329400
F	6.68538000	-1.26439400	2.56250000
F	4.67669700	-1.62204800	3.28733900
F	5.54154000	0.34883300	3.42105600
C	-5.34218200	-0.15725700	0.69832400
C	-3.43585100	-4.49744900	-0.93178200
F	-2.57505600	-4.87267800	-1.88980200
F	-4.67504800	-4.75448500	-1.37745200
F	-3.22472000	-5.30570100	0.12021400

F -5.74342700 0.69349300 -0.26843500

F -5.02432600 0.59884300 1.76114300

F -6.40471100 -0.90007700 1.03023500

Zero-point correction= 0.374427 (Hartree/Particle)

Thermal correction to Energy= 0.411180

Thermal correction to Enthalpy= 0.412124

Thermal correction to Gibbs Free Energy= 0.297302

Sum of electronic and zero-point Energies= -3025.427388

Sum of electronic and thermal Energies= -3025.390635

Sum of electronic and thermal Enthalpies= -3025.389691

Sum of electronic and thermal Free Energies= -3025.504513

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3026.63661775

SMA-1-Binary-9

C -2.24645200 2.45259800 -0.48590100

H -1.83124500 1.54923900 -0.93737600

C -1.37088900 3.35864200 -0.00095500

H -1.69737600 4.30937800 0.41089700

C 0.07034200 3.06292900 -0.04112500

0 0.46678700 1.88939200 -0.13263000

C 1.06003700 4.16973400 0.02419500

C 2.99590500 6.18531900 0.09050600

C 0.69036300 5.50911400 -0.16855300

C 2.40933100 3.84993300 0.24466600

C 3.37222700 4.85213700 0.28066300

C 1.65774400 6.51178600 -0.13640800

H -0.34548600 5.77168700 -0.36482500

H 2.68763800 2.81088300 0.39747800

H 4.41407600 4.59605700 0.45174900

H 1.36763100 7.54719300 -0.29248000

H 3.74793600 6.96984200 0.11716100

C	-3.70662200	2.52610600	-0.49653100
C	-6.51152400	2.49442500	-0.48485500
C	-4.41543300	1.48793800	-1.12465200
C	-4.42767800	3.55593500	0.13384100
C	-5.81797800	3.53858100	0.13683600
C	-5.80812800	1.46927700	-1.11912600
H	-3.85904600	0.68224200	-1.60304500
H	-3.89795800	4.36373700	0.63334100
H	-6.36653900	4.33571300	0.63171300
H	-6.34160400	0.65254400	-1.59886400
H	-7.59841400	2.48152700	-0.47160300
N	-0.57796100	-0.84147000	0.09438100
H	-0.46542700	0.17176900	0.21583800
C	0.57456200	-1.57663600	0.03059000
S	0.61615200	-3.24713200	0.04686200
N	1.66223000	-0.75238000	-0.04549100
H	1.44400700	0.24140800	-0.16538600
C	3.04480500	-0.99688200	-0.02422400
C	5.86166100	-1.16958100	0.03691600
C	3.66724500	-2.15842200	0.44734400
C	3.84272200	0.07011800	-0.46252900
C	5.22789500	-0.01606400	-0.41911500
C	5.06045700	-2.22599000	0.46100800
H	3.07852700	-2.99381900	0.80367500
H	3.36504600	0.97433600	-0.83388200
H	6.94405200	-1.24034400	0.06629500
C	-1.91237300	-1.30096400	0.12608000
C	-4.63316700	-2.00066600	0.15434700
C	-2.79437000	-0.67186500	1.00832900
C	-2.39391200	-2.27408000	-0.75736700
C	-3.74186700	-2.62020900	-0.72204700

C	-4.14368800	-1.02189100	1.01246600
H	-2.42402400	0.10410100	1.67482700
H	-1.72595700	-2.73838200	-1.47371500
H	-5.68603500	-2.26412800	0.15328500
C	5.71571300	-3.45567100	1.02927400
C	6.03651000	1.14993300	-0.91561700
F	7.26660100	1.16641300	-0.38469200
F	5.44738900	2.32053700	-0.61073400
F	6.18393700	1.13057100	-2.25038500
F	6.91955700	-3.67558800	0.47882900
F	4.97360400	-4.55470700	0.83313500
F	5.90957200	-3.34846400	2.35567500
C	-5.07503700	-0.32340300	1.96481300
C	-4.24801100	-3.69893900	-1.64005900
F	-3.51708700	-3.78443700	-2.76116900
F	-5.52186400	-3.48073900	-2.00321500
F	-4.21270600	-4.90850900	-1.05688300
F	-4.74558900	0.96813100	2.11971100
F	-5.04934600	-0.87798800	3.18919200
F	-6.34681600	-0.36949600	1.54132200

Zero-point correction= 0.472380 (Hartree/Particle)

Thermal correction to Energy= 0.515441

Thermal correction to Enthalpy= 0.516386

Thermal correction to Gibbs Free Energy= 0.385570

Sum of electronic and zero-point Energies= -3009.333577

Sum of electronic and thermal Energies= -3009.290516

Sum of electronic and thermal Enthalpies= -3009.289572

Sum of electronic and thermal Free Energies= -3009.420387

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3010.66924381

SMA-1-enol-complex

C	1.44836600	-3.51531000	-1.36650800
H	1.04140700	-4.52297600	-1.37340700
C	0.56449500	-2.51071500	-1.52600900
0	0.91098800	-1.18888700	-1.60415500
H	1.85565700	-1.10131100	-1.32089100
C	-0.89385100	-2.72897600	-1.66445400
C	-3.64986400	-3.14482100	-1.97448500
C	-1.54114500	-3.75362300	-0.95689500
C	-1.64482200	-1.90595000	-2.51843600
C	-3.01465200	-2.11775600	-2.67485000
C	-2.91044400	-3.96016300	-1.11387100
H	-0.96873000	-4.37278500	-0.26945600
H	-1.14727500	-1.10896800	-3.06661800
H	-3.58556300	-1.47693100	-3.34198600
H	-3.40676600	-4.74283500	-0.54647700
H	-4.72015700	-3.29885700	-2.08237900
C	2.94861700	-3.40002400	-1.29114300
H	3.34809200	-3.11761400	-2.27643200
C	3.63952300	-4.67795300	-0.85831000
C	5.01920200	-6.98340800	-0.03744700
C	4.91436700	-4.96526700	-1.36316800
C	3.06405700	-5.56040600	0.06304400
C	3.75142400	-6.70547100	0.47222200
C	5.59996200	-6.10841000	-0.95927100
H	5.36756100	-4.27996300	-2.07817000
H	2.07086200	-5.36033600	0.46114000
H	3.29081000	-7.38147700	1.18837600
H	6.58586200	-6.31912400	-1.36617200
H	5.55157900	-7.87715200	0.27801000
S	3.53195200	-1.97815800	-0.25644900
C	2.73617700	-2.34999000	1.34901200

H	3.49325500	-2.76585700	2.02016400
H	1.97748000	-3.11740900	1.15950400
C	2.09378700	-1.12168400	1.93613100
C	0.89234500	1.18271000	2.99758700
C	2.85086700	-0.19977300	2.66977300
C	0.72850600	-0.87478300	1.73465100
C	0.12822200	0.26280900	2.27581400
C	2.25512600	0.94945100	3.19251400
H	3.91312200	-0.38212900	2.82396600
H	0.13273500	-1.59610300	1.17198800
H	-0.93819500	0.43261100	2.13997800
H	2.85623800	1.66283000	3.74964000
H	0.42404900	2.07467100	3.40621300
N	-1.75120700	0.71426300	-0.50933200
H	-1.20489300	-0.12051800	-0.73491800
C	-1.04567500	1.87694400	-0.35159800
N	0.22682000	1.74697500	-0.82762200
H	0.49296600	0.81128900	-1.14449600
S	-1.64004700	3.24958800	0.38827200
C	-3.07827500	0.44326300	-0.11269200
C	-5.69490800	-0.26396500	0.61159700
C	-3.32956900	-0.78429800	0.50786600
C	-4.13699900	1.31169600	-0.38965200
C	-5.42916500	0.95302200	-0.01100300
C	-4.63191300	-1.13123700	0.85401200
H	-2.50590900	-1.46924500	0.70024200
H	-3.95553200	2.24766600	-0.90506000
H	-6.70889700	-0.53596200	0.89049900
C	1.31469900	2.62083600	-0.59282500
C	3.56919500	4.22765900	-0.15663100
C	1.26783600	3.98055900	-0.90560000

C	2.48632000	2.06256500	-0.07937800
C	3.60397000	2.86530600	0.13154600
C	2.39349200	4.76925200	-0.67227100
H	0.37149600	4.41122100	-1.33702800
H	2.51331000	1.00122100	0.15942600
H	4.44269100	4.85145000	0.00654000
C	4.84525800	2.26728100	0.73356000
C	2.32142100	6.24327400	-0.96143200
C	-6.55786500	1.91620400	-0.25650500
C	-4.92717100	-2.47470100	1.46055300
F	-5.73587200	-2.36480500	2.52655500
F	-5.55630200	-3.28508200	0.58867800
F	-3.81661000	-3.11035300	1.85856500
F	-7.72179200	1.27575700	-0.44674800
F	-6.73833700	2.75025200	0.78108500
F	-6.33505800	2.68000700	-1.33634700
F	1.50962100	6.50704100	-1.99671600
F	3.52807200	6.75238200	-1.25324400
F	1.84955800	6.93649000	0.08835900
F	5.95444400	2.86195900	0.26790800
F	4.94859600	0.95536600	0.47173700
F	4.87141200	2.39979100	2.07215400

Zero-point correction= 0.606717 (Hartree/Particle)

Thermal correction to Energy= 0.657180

Thermal correction to Enthalpy= 0.658124

Thermal correction to Gibbs Free Energy= 0.515114

Sum of electronic and zero-point Energies= -3678.485796

Sum of electronic and thermal Energies= -3678.435334

Sum of electronic and thermal Enthalpies= -3678.434390

Sum of electronic and thermal Free Energies= -3678.577400

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3680.09158034

SMA-1-product-complex

H	-1.35670800	-1.73704500	-0.27788400
C	-1.02309600	-2.77911100	-0.17034700
C	-2.10720800	-3.70568600	-0.67892100
C	-4.13219700	-5.43707100	-1.55698400
C	-3.33474700	-3.19731300	-1.11364400
C	-1.90141600	-5.09203900	-0.69019200
C	-2.90523100	-5.95224400	-1.13206300
C	-4.34554000	-4.05872800	-1.54409800
H	-3.50155800	-2.12186900	-1.11795400
H	-0.94882000	-5.49982100	-0.35271100
H	-2.73094400	-7.02528400	-1.14085100
H	-5.29896100	-3.64793700	-1.86452700
H	-4.91799300	-6.10796300	-1.89483600
C	-0.74387300	-3.06611100	1.32447000
C	0.11847200	-2.00009200	1.95861500
0	-0.38100800	-0.88237600	2.13995000
S	0.46595000	-2.99168700	-1.21657600
C	1.23625800	-1.33602000	-1.11915600
H	1.18921900	-0.96667900	-0.09031700
H	0.66636500	-0.64682200	-1.75510600
C	2.67650500	-1.43123700	-1.55562100
C	5.36262500	-1.63071100	-2.34487200
C	3.70635200	-1.17353800	-0.64465200
C	3.00585300	-1.79578300	-2.86797300
C	4.34039300	-1.90191900	-3.25803300
C	5.04263100	-1.26009700	-1.03821200
H	3.46162500	-0.88862500	0.37840800
H	2.21018700	-1.99406600	-3.58483700
H	4.58311800	-2.18658200	-4.27893200

H	5.82629300	-1.03460200	-0.31855600
H	6.40261700	-1.70365700	-2.65344700
H	-1.70417300	-3.03167700	1.85534600
H	-0.32832600	-4.07029400	1.44178400
C	1.53596300	-2.23653800	2.32206900
C	4.26028600	-2.48130200	2.89698800
C	2.24758200	-3.36557100	1.88872100
C	2.19712900	-1.24310500	3.06602800
C	3.55086800	-1.36426500	3.35462200
C	3.60881200	-3.48011700	2.17256300
H	1.75571700	-4.13811100	1.30581400
H	1.62882500	-0.38653400	3.42053500
H	4.05772700	-0.59086800	3.92450700
H	4.16057700	-4.34727400	1.82095000
H	5.32202800	-2.57214800	3.11177900
N	-1.69453600	1.32888800	0.84133300
H	-1.44776200	0.45320900	1.31593500
C	-0.64703600	2.04330400	0.32794300
S	-0.79141300	3.31465900	-0.74503300
N	0.54460900	1.57470500	0.81443500
H	0.48307300	0.90265800	1.58523300
C	1.86157100	1.86326000	0.40179900
C	4.56077100	2.22115500	-0.30694400
C	2.21230100	2.10377500	-0.93107400
C	2.86564600	1.79239000	1.37466200
C	4.19960100	1.94875500	1.00996200
C	3.55102500	2.29978000	-1.26166000
H	1.45226700	2.12717900	-1.70331900
H	2.59923300	1.60678500	2.41170200
H	5.60272500	2.35053000	-0.58392800
C	-3.07646800	1.48288100	0.61993600

C	-5.86431200	1.59938800	0.25745400
C	-3.83952100	0.30988500	0.59046100
C	-3.71641200	2.72093800	0.50543700
C	-5.09710500	2.75975900	0.31801800
C	-5.21614900	0.37516500	0.40299500
H	-3.34756900	-0.65277000	0.71706800
H	-3.14938300	3.64089700	0.57683600
H	-6.93907400	1.64705600	0.11448100
C	3.92059800	2.47592700	-2.70796200
C	5.28126100	1.70948100	2.02306700
F	5.74769100	0.44595800	1.94072400
F	4.84913200	1.88122100	3.28185100
F	6.33241200	2.51950400	1.83912600
F	5.05939800	3.17101200	-2.84956700
F	2.96449100	3.11791900	-3.39486600
F	4.10793400	1.29087200	-3.31341200
C	-6.00346400	-0.89976200	0.28697100
C	-5.76555700	4.09692800	0.14846900
F	-5.14977300	5.05388600	0.85893500
F	-7.04816000	4.06422600	0.54025700
F	-5.75914100	4.49928400	-1.13337900
F	-5.45342300	-1.89687400	0.99524400
F	-6.06941300	-1.32131500	-0.99154000
F	-7.26608300	-0.74767500	0.70880100

Zero-point correction= 0.607669 (Hartree/Particle)

Thermal correction to Energy= 0.658037

Thermal correction to Enthalpy= 0.658981

Thermal correction to Gibbs Free Energy= 0.515471

Sum of electronic and zero-point Energies= -3678.504927

Sum of electronic and thermal Energies= -3678.454560

Sum of electronic and thermal Enthalpies= -3678.453615

Sum of electronic and thermal Free Energies= -3678.597125

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3680.10373408

SMA-1-tertiary-8

C	0.30575900	2.18718300	1.19395900
H	0.09172000	3.14664300	0.71929100
C	1.56885200	1.72319000	1.11093000
H	1.87097000	0.80440500	1.60670400
C	2.56733100	2.45033900	0.30185300
0	2.22795400	3.33647000	-0.49124700
H	0.45983600	2.86020400	-1.58998400
C	4.00729700	2.07676800	0.42437200
C	6.72902900	1.45231500	0.56933600
C	4.51072500	1.37399200	1.52727300
C	4.87817800	2.46221000	-0.60663000
C	6.23015700	2.14414900	-0.53938700
C	5.87166000	1.07454100	1.60309700
H	3.85206800	1.06791900	2.33570600
H	4.47101100	3.00332800	-1.45643600
H	6.89608700	2.42642000	-1.35065400
H	6.25503100	0.52930000	2.46131400
H	7.78606100	1.20331500	0.62232900
C	-0.83212800	1.54796500	1.85567300
C	-3.09324400	0.41469500	3.07235900
C	-2.01345900	2.29261900	2.00781000
C	-0.80466800	0.21702700	2.31047200
C	-1.92681400	-0.34282100	2.91267000
C	-3.13652300	1.73377200	2.61640500
H	-2.03486400	3.31928800	1.64807400
H	0.09113800	-0.38725400	2.17445200
H	-1.89809400	-1.37711500	3.24640900

H	-4.04672300	2.32039500	2.71715700
H	-3.97034800	-0.03171100	3.53261500
S	-0.42059200	2.12727700	-2.29825400
C	-1.63015400	3.44493500	-2.68159400
H	-1.13012500	4.17770800	-3.32155100
H	-2.40295700	2.95294800	-3.27968400
C	-2.23322800	4.11265700	-1.47391100
C	-3.39796200	5.45680900	0.69880400
C	-1.52913500	5.12131000	-0.80150600
C	-3.51293500	3.76561400	-1.02797900
C	-4.09556600	4.43641900	0.05001500
C	-2.10703600	5.79041000	0.27787800
H	-0.52777500	5.39001400	-1.13794500
H	-4.06150400	2.97650300	-1.53918400
H	-5.09518200	4.16346400	0.37795500
H	-1.55568400	6.58022600	0.78204800
H	-3.85435200	5.98690200	1.53101300
N	-1.32712900	-0.98089900	-0.81801000
H	-1.19387700	0.01610500	-1.01420900
C	-0.20559700	-1.67486400	-0.45838200
S	-0.20837800	-3.16097900	0.29850100
N	0.92533500	-0.97378400	-0.78987600
H	0.80096400	-0.22563000	-1.47213300
C	2.27583700	-1.27512300	-0.51709800
C	5.01345100	-1.71180300	-0.04711900
C	2.70350200	-1.78130400	0.71555700
C	3.22073700	-0.95652400	-1.49588000
C	4.57577600	-1.17697900	-1.25438200
C	4.06136600	-2.00039800	0.92895800
H	1.98550800	-1.99161900	1.50130500
H	2.89456100	-0.53923600	-2.44632000

H	6.06915800	-1.87956400	0.13802900
C	-2.67683900	-1.35785100	-0.65686600
C	-5.40348200	-1.95538200	-0.37310000
C	-3.57081500	-0.37409400	-0.22439400
C	-3.14752800	-2.63468600	-0.97566700
C	-4.50226600	-2.91893200	-0.82001800
C	-4.92182300	-0.68116600	-0.08313300
H	-3.20159500	0.62504200	0.00166800
H	-2.46893400	-3.38958400	-1.35470900
H	-6.45854300	-2.18815400	-0.26549400
C	4.50379200	-2.45085500	2.29284900
C	5.56056700	-0.87529600	-2.35020000
F	6.80994500	-0.74425800	-1.88315400
F	5.24615500	0.25808200	-2.99849200
F	5.58807100	-1.85046600	-3.27533900
F	5.72845700	-2.99297100	2.27228400
F	3.66380200	-3.35484300	2.81686400
F	4.54651900	-1.42055700	3.16252500
C	-5.87242300	0.35233500	0.45318100
C	-5.00023800	-4.30753900	-1.11309300
F	-4.24131600	-4.92852900	-2.02784700
F	-6.26064200	-4.29345700	-1.57439900
F	-4.99893700	-5.08072000	-0.01407100
F	-5.44784300	1.60256100	0.20875900
F	-6.02815900	0.25064000	1.78538700
F	-7.09405400	0.22742800	-0.08642900

Zero-point correction= 0.602853 (Hartree/Particle)

Thermal correction to Energy= 0.654563

Thermal correction to Enthalpy= 0.655507

Thermal correction to Gibbs Free Energy= 0.510032

Sum of electronic and zero-point Energies= -3678.491620

Sum of electronic and thermal Energies= -3678.439910

Sum of electronic and thermal Enthalpies= -3678.438966

Sum of electronic and thermal Free Energies= -3678.584441

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3680.09141250

SMA-1-tertiary-9

C	0.75149400	3.72210300	0.34470000
H	0.94303600	2.82983300	-0.25347800
C	0.32317500	3.52801000	1.61258200
H	0.10693200	4.35998100	2.27493500
C	0.11306200	2.15674800	2.08475100
0	0.16695200	1.20590200	1.27627900
H	-1.17001800	1.73443800	-0.51302600
C	-0.19007600	1.88492000	3.51490100
C	-0.77537600	1.27200400	6.18367900
C	-0.07663500	2.86885000	4.50919500
C	-0.58906600	0.58719200	3.87755200
C	-0.88533900	0.28339300	5.20132800
C	-0.36638200	2.56040000	5.83681400
H	0.25350500	3.87273900	4.26109200
H	-0.66327800	-0.18193800	3.11197000
H	-1.19940600	-0.72135700	5.47034300
H	-0.27131300	3.32701900	6.60082200
H	-1.00547100	1.03590700	7.21939200
C	0.98319900	4.98597900	-0.34638000
C	1.41947900	7.33648200	-1.80785800
C	1.25655800	4.93179200	-1.72391500
C	0.93513000	6.23838600	0.29244000
C	1.15364500	7.40266400	-0.43520900
C	1.46947600	6.09933600	-2.45218400
H	1.29013700	3.96109600	-2.21657900

H	0.73741500	6.29682300	1.36019800
H	1.11940200	8.36690200	0.06506200
H	1.67550000	6.04193400	-3.51793500
H	1.58968200	8.25072700	-2.37084700
S	-2.02025300	2.04484100	-1.50752700
C	-1.28496200	0.92673600	-2.75435300
H	-1.33918300	-0.10176300	-2.38048100
H	-1.94025000	0.99882300	-3.62773900
C	0.13076800	1.29043400	-3.11422400
C	2.77876100	1.96730100	-3.75638900
C	1.18840300	0.89288100	-2.28532900
C	0.41416200	2.03319300	-4.26524300
C	1.73077400	2.37060000	-4.58610000
C	2.50531500	1.22732200	-2.60271100
H	0.96695100	0.32354700	-1.38102300
H	-0.40342100	2.34259500	-4.91411900
H	1.93790400	2.94221300	-5.48770400
H	3.32103500	0.89957600	-1.96323300
H	3.80482500	2.22311600	-4.00845800
N	-1.28320000	-1.16344100	0.28510400
H	-1.08572300	-0.35828700	0.88570200
C	-0.21934000	-1.99414800	0.05022100
S	-0.27852100	-3.38502900	-0.86882100
N	0.90685300	-1.51460400	0.66471700
H	0.81334100	-0.58560800	1.09104500
C	2.24577600	-1.93276700	0.51780800
C	4.97138900	-2.59143100	0.31051200
C	2.64337500	-3.27369100	0.52449900
C	3.21439900	-0.92696200	0.43558500
C	4.56236700	-1.26137700	0.33429700
C	3.99720300	-3.58252400	0.41125100

H	1.90761400	-4.06184500	0.62728000
H	2.90585600	0.11763600	0.44874900
H	6.02175600	-2.84973300	0.22427000
C	-2.65674600	-1.33061900	0.01040900
C	-5.43564100	-1.44308400	-0.42350800
C	-3.54589400	-0.76740000	0.93603700
C	-3.16165500	-1.93332200	-1.14517700
C	-4.54257200	-1.99027600	-1.33773700
C	-4.91611400	-0.82543500	0.71341800
H	-3.15543300	-0.28103800	1.82790100
H	-2.49036400	-2.33888000	-1.89191300
H	-6.50641600	-1.48291700	-0.59560200
C	4.42231100	-5.02382000	0.48054800
C	5.57094400	-0.15565100	0.19447700
F	6.80869400	-0.56091400	0.50587100
F	5.27189200	0.88781300	0.98338500
F	5.62066700	0.31955600	-1.06546600
F	5.56011000	-5.23878600	-0.19684800
F	3.48907200	-5.84464300	-0.02141300
F	4.64494700	-5.41595100	1.74757500
C	-5.85817800	-0.26323900	1.74133700
C	-5.06342800	-2.68996000	-2.56316300
F	-4.27608900	-2.47480300	-3.62866000
F	-6.29979600	-2.28221400	-2.88459800
F	-5.12259200	-4.02115100	-2.38898100
F	-5.29237800	0.72329200	2.45248400
F	-6.25314400	-1.20009100	2.62105500
F	-6.97005100	0.22949800	1.17590800

Zero-point correction= 0.602612 (Hartree/Particle)

Thermal correction to Energy= 0.654299

Thermal correction to Enthalpy= 0.655244

Thermal correction to Gibbs Free Energy= 0.501635

Sum of electronic and zero-point Energies= -3678.485795

Sum of electronic and thermal Energies= -3678.434108

Sum of electronic and thermal Enthalpies= -3678.433163

Sum of electronic and thermal Free Energies= -3678.586772

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3680.08541025

SMA-1-TS

C	-0.32603700	2.22444800	-0.86218900
H	-0.25580800	3.28407100	-0.62270100
C	-1.61403900	1.65897200	-0.98396200
H	-1.76325900	0.75679900	-1.56749900
C	-2.70738200	2.22276000	-0.34784100
0	-2.53743300	3.14779900	0.58882700
H	-1.63862000	3.00235800	1.02161100
C	-4.09905900	1.84080900	-0.61674200
C	-6.75448600	1.10924900	-1.09690100
C	-4.45426800	1.22281200	-1.82719700
C	-5.08692800	2.09438600	0.34892500
C	-6.40711500	1.72268700	0.11005800
C	-5.77738700	0.86101600	-2.06467700
H	-3.69968700	1.04219100	-2.58835800
H	-4.80534400	2.56313800	1.28684900
H	-7.16461000	1.90543400	0.86727400
H	-6.04385400	0.38045400	-3.00201800
H	-7.78684600	0.82392300	-1.28294900
C	0.84003400	1.66496900	-1.54605200
C	3.08704500	0.69197300	-2.90976700
C	1.95074300	2.49536500	-1.77560800
C	0.87223800	0.33673800	-2.00816500
C	1.98701500	-0.14345300	-2.68732600

C	3.06924100	2.01146900	-2.44963900
H	1.92084400	3.52462700	-1.42500600
H	0.02716400	-0.32589400	-1.83228600
H	2.00378800	-1.17399900	-3.03280300
H	3.92703100	2.66017000	-2.60918200
H	3.96115800	0.30925400	-3.42915000
S	0.06960200	1.90684800	1.62481600
C	1.16742600	3.12002200	2.45120900
H	0.55991900	3.72399400	3.13333900
H	1.89359800	2.56155300	3.05080100
C	1.88978700	4.01069300	1.47375900
C	3.23350200	5.67862300	-0.34707300
C	1.22613200	5.08853200	0.87013000
C	3.22844200	3.77383400	1.14519000
C	3.89915400	4.60249600	0.24188800
C	1.89140400	5.91796100	-0.03313400
H	0.18157900	5.27710000	1.12066300
H	3.74900000	2.93628900	1.60631300
H	4.94011900	4.40365600	-0.00072500
H	1.36702200	6.75592200	-0.48623200
H	3.75457700	6.32864800	-1.04558400
N	-0.81728900	-1.16277300	0.93493200
H	-0.66830500	-0.41920400	1.62314500
C	0.31590100	-1.80194400	0.50793900
S	0.33501600	-3.22235300	-0.36978000
N	1.42404100	-1.09546300	0.88472500
H	1.24261000	-0.11454000	1.14872400
C	2.78104500	-1.39008100	0.65484300
C	5.52538400	-1.81264000	0.23346800
C	3.32485500	-2.66549100	0.82379100
C	3.61329000	-0.32169600	0.29678200

C	4.97083400	-0.54141300	0.08832700
C	4.68835300	-2.86005700	0.60519700
H	2.69571700	-3.49335600	1.13001000
H	3.18571200	0.67231400	0.17090200
H	6.58452200	-1.98016800	0.06350500
C	-2.17360800	-1.40496600	0.65227100
C	-4.93890200	-1.67543500	0.19086700
C	-3.09783900	-1.05159500	1.64193900
C	-2.63727000	-1.85816900	-0.58760500
C	-4.00851700	-1.99146100	-0.79588300
C	-4.46282800	-1.19468100	1.40679900
H	-2.74263500	-0.66205100	2.59414700
H	-1.93818200	-2.08470300	-1.38626200
H	-6.00277400	-1.77194700	0.00569800
C	5.26871200	-4.22520700	0.85125100
C	5.85437900	0.58166300	-0.37785900
F	7.07041400	0.52012500	0.18669900
F	5.33735300	1.78704700	-0.09302700
F	6.04870400	0.54677400	-1.70873700
F	6.41745900	-4.40797900	0.18368100
F	4.42362300	-5.19831300	0.47962100
F	5.53814900	-4.42433600	2.15374900
C	-5.41602000	-0.82996500	2.51104700
C	-4.46668400	-2.44067700	-2.15569600
F	-3.93111200	-1.67503300	-3.12589200
F	-5.79846000	-2.37902800	-2.29013400
F	-4.09459200	-3.70294500	-2.41990000
F	-5.12506300	0.37341600	3.03487200
F	-5.35907400	-1.71006100	3.52511100
F	-6.68800300	-0.79055700	2.09226600

Zero-point correction= 0.604879 (Hartree/Particle)

Thermal correction to Energy= 0.655023

Thermal correction to Enthalpy= 0.655967

Thermal correction to Gibbs Free Energy= 0.515043

Sum of electronic and zero-point Energies= -3678.466194

Sum of electronic and thermal Energies= -3678.416051

Sum of electronic and thermal Enthalpies= -3678.415106

Sum of electronic and thermal Free Energies= -3678.556030

E(RMN15/6-311+G(2d,p)+Def2-TZVPD(I)) = -3680.06862939

References

1. S. H. Jungbauer and S. M. Huber, *J. Am. Chem. Soc.*, 2015, **137**, 12110-12120.
2. S. H. Jungbauer, S. M. Walter, S. Schindler, L. Rout, F. Kniep and S. M. Huber, *Chem. Commun.*, 2014, **50**, 6281-6284.