Electronic Supporting Information for

Theoretical study on NHC-catalyzed C-S bond cleavage/annulation cascade reaction: Mechanism, stereoselectivity, and role of catalyst

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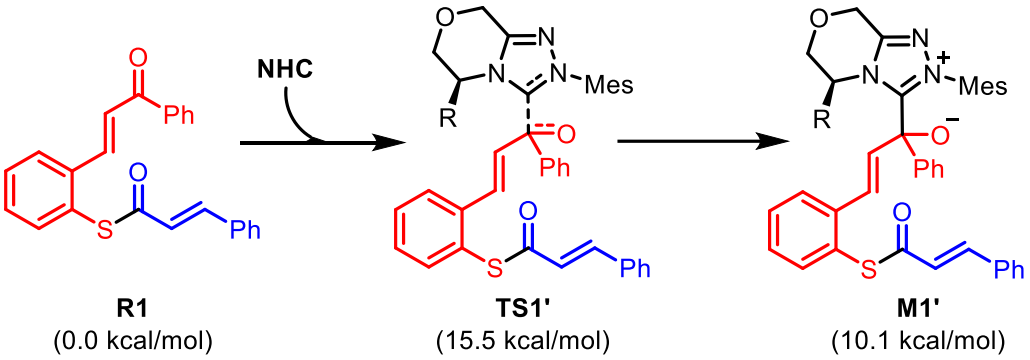
Content

Part 1: Another adsorption mode



Scheme S1 Another possible adsorption mode

Part 2: Scan results of C-S bond

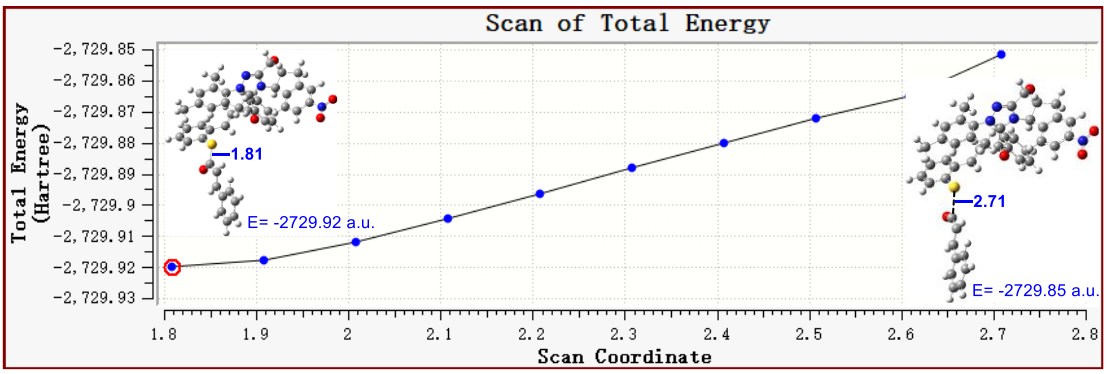


Fig. S1 Scan coordinates involved in C-S bond cleavage

Part 3: Conformational search for TS2s

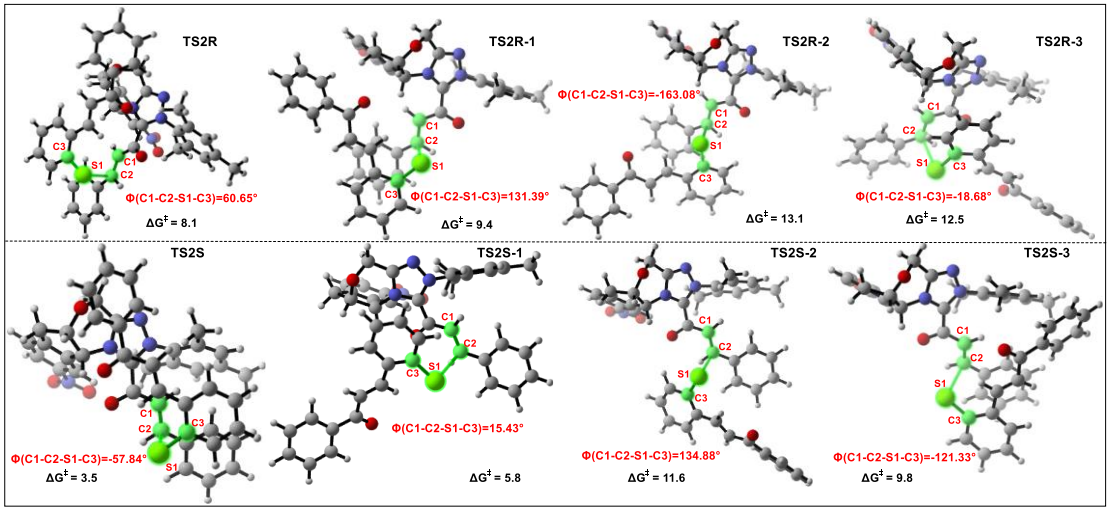
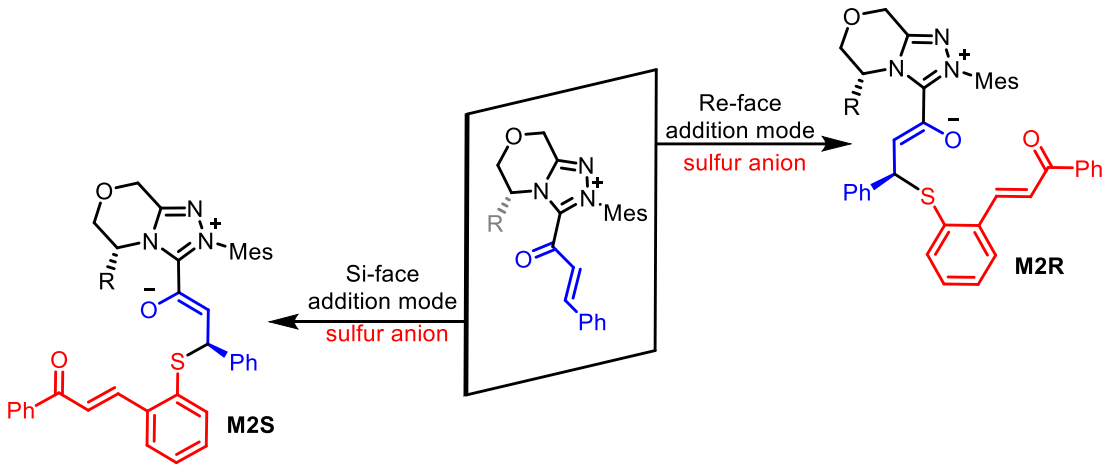


Fig. S2 Different conformations of the transition states involved in C-S bond formation step

By rotating dihedral angle Φ1(C1-C2-S1-C3) from 0~360° at intervals of 90° in the two transition states **TS2R** and **TS2S**, we have respectively constructed eight (4×2=8) initial structures of **TS2R** and **TS2S**, and then located the optimized structures of the eight conformations, which are summarized in **Fig. S2**. The relative Gibbs free energies depicted in **Fig. S2** show that we have selected the conformations of the transition states **TS2R** and **TS2S** with the lowest energies among all the conformers, and we just discussed the conformations with the lowest energies in the main text of the revised manuscript.

Part 4: Stereocontrolling Mode



Scheme S2 Illustration of the stereocontrolling mode

Part 5: Calculation equation for ee value prediction

The predicted ee value is calculated using Boltzmann distribution of stereoselective transition states with the following expressions:

$$\frac{[TS2S]}{[TS2R]} = \frac{e^{-G^{\neq}_{[TS2R]}/RT}}{e^{-G^{\neq}_{[TS2S]}/RT}} = e^{\Delta G^{\neq}/RT} \quad (1)$$

$$\text{ee}\% = \frac{[TS2S]-[TS2R]}{[TS2S]+[TS2R]} \times 100\% = \frac{[TS2S]/[TS2R]^{-1}}{[TS2S]/[TS2R]^{+1}} \times 100\% \quad (2)$$

In the above expression, the $\Delta G^{\neq}$ is the difference in the Gibbs free energies between the competing stereoselective transition states.

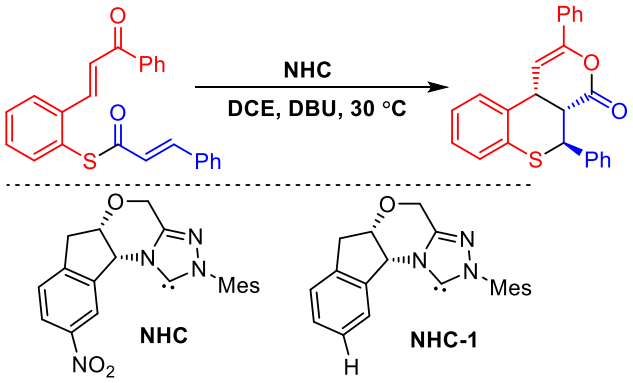
Part 6: Distortion/interaction analysis

Table S2 Distortion/interaction analysis of stereochemical transition states **TS2R** and **TS2S** (energies in kcal/mol)

	$\Delta E^{\neq}$	E_{dist}			E_{int}
		$M1_{acylazolium\text{-}part}$	$M1_{sulfa\text{-}part}$	Total	
TS2R	7.5	6.7	0.4	7.1	-0.3
TS2S	2.9	0.1	0.9	1.0	-1.9

Part 7: Substituent effect on NHC catalyst

Table S3 Substituent effect on NHC catalyst



Energy barrier	NHC	NHC-1
$\Delta G^{\neq}_{TS1}$	18.2	19.4
$\Delta G^{\neq}_{TS2R}$	8.1	8.7
$\Delta G^{\neq}_{TS2S}$	3.5	3.9
$\Delta G^{\neq}_{TS3R}$	18.1	19.1
$\Delta G^{\neq}_{TS3S}$	15.5	16.0

Part 8: Cartesian coordinates of all optimized structures

R1

Zero-point correction= 0.353750 (Hartree/Particle)
Thermal correction to Energy= 0.377262
Thermal correction to Enthalpy= 0.378206
Thermal correction to Gibbs Free Energy= 0.294485
Sum of electronic and zero-point Energies= -1473.201229
Sum of electronic and thermal Energies= -1473.177716
Sum of electronic and thermal Enthalpies= -1473.176772
Sum of electronic and thermal Free Energies= -1473.260493

C	-0.54717300	4.79242700	0.64412800
C	0.31175300	3.91121400	-0.00155500
C	-0.15913300	2.68554200	-0.47423800
C	-1.50848400	2.32208600	-0.30251900
C	-2.36138900	3.23890800	0.33107400
C	-1.89010400	4.45539900	0.80422900
H	-0.17217000	5.74269300	1.00867300
H	1.35705300	4.16586000	-0.14091300
H	-3.41436500	2.99601200	0.43145600
H	-2.57297700	5.14662200	1.28668300
C	-2.02740200	1.03229100	-0.78007000
C	-3.09261000	0.39700000	-0.27157400
H	-1.50413800	0.54535200	-1.59930100
H	-3.63932200	0.80010300	0.57394700
C	-3.53977200	-0.88872700	-0.87004500
O	-3.08951500	-1.28075000	-1.93665100
S	0.99089300	1.59461000	-1.29100300
C	2.09655400	1.18591000	0.08683800
O	1.96577900	1.65233100	1.19245700
C	3.14984000	0.24110300	-0.33065100
C	4.05633600	-0.16953900	0.56981200
H	3.14308600	-0.09341600	-1.36337700
H	3.96190100	0.22965800	1.57895800
C	5.16112900	-1.10444500	0.34569900
C	5.99234500	-1.42983600	1.42582800
C	5.41788500	-1.68829800	-0.90443000
C	7.05120100	-2.31774300	1.26638900
H	5.80143900	-0.98109300	2.39670500
C	6.47468300	-2.57348900	-1.06329600

H	4.79069700	-1.44971000	-1.75739600
C	7.29408100	-2.89175500	0.02142800
H	7.68425800	-2.56166800	2.11298100
H	6.66182600	-3.01902700	-2.03472900
H	8.11785800	-3.58632900	-0.10655700
C	-4.57084200	-1.69591400	-0.14494400
C	-5.24958100	-2.68944200	-0.85979200
C	-4.85224500	-1.51012300	1.21201700
C	-6.20903800	-3.47275600	-0.23223700
H	-5.01121900	-2.82814300	-1.90913800
C	-5.80435500	-2.30525400	1.84347600
H	-4.31611500	-0.76547800	1.79060500
C	-6.48780500	-3.28059500	1.12148600
H	-6.73970600	-4.23490300	-0.79329900
H	-6.01157400	-2.16288000	2.89876000
H	-7.23617400	-3.89384000	1.61322500

NHC

Zero-point correction=	0.386931 (Hartree/Particle)
Thermal correction to Energy=	0.410496
Thermal correction to Enthalpy=	0.411440
Thermal correction to Gibbs Free Energy=	0.331047
Sum of electronic and zero-point Energies=	-1255.959304
Sum of electronic and thermal Energies=	-1255.935739
Sum of electronic and thermal Enthalpies=	-1255.934795
Sum of electronic and thermal Free Energies=	-1256.015188

C	3.31345400	0.82919800	0.66558100
C	2.56588000	0.37578300	-0.42634600
C	2.66545500	-0.93006500	-0.87935800
C	3.55406500	-1.75937300	-0.20463500
C	4.32060700	-1.33682600	0.87840900
C	4.19791900	-0.02409100	1.32003600
C	2.98784900	2.26707200	0.97332800
C	2.32569200	2.74417300	-0.33942700
C	1.68258500	1.47624300	-0.96039200
H	2.07994000	-1.30085500	-1.71145000
H	4.99804700	-2.03401300	1.35499200
H	4.78628600	0.32297500	2.16263900
H	2.28884700	2.31052900	1.81692400
H	3.11058100	3.07693100	-1.02282700
H	3.86068000	2.86665300	1.23827800
H	1.65712600	1.51780800	-2.05133800
N	0.30860100	1.34308700	-0.47433000
O	1.43919300	3.83622400	-0.23766600

C	-0.50259600	0.25642800	-0.68755900
C	-0.35512000	2.32263000	0.21755700
N	-1.62068400	0.68303800	-0.06867600
N	-1.56578100	1.94468400	0.49218000
C	0.30999700	3.61226900	0.58565500
H	0.58424800	3.60508200	1.64822000
H	-0.37440900	4.44569200	0.42036600
C	-2.83958600	-0.06057400	0.03887900
C	-2.91147300	-1.10520400	0.96395200
C	-3.91600500	0.29359100	-0.77817700
C	-4.11083200	-1.81063500	1.05413200
C	-5.09741300	-0.43589300	-0.65011300
C	-5.21106500	-1.49124400	0.25630200
H	-4.18944500	-2.62577300	1.76966100
H	-5.94771300	-0.17489600	-1.27578300
C	-3.78658000	1.42312700	-1.76471800
H	-3.65614700	2.37966100	-1.25049000
H	-2.90839100	1.27849600	-2.40189300
C	-1.72869000	-1.44579000	1.83119400
H	-0.87813400	-1.76217200	1.22071400
H	-1.40388100	-0.57215500	2.40515900
H	-1.97936500	-2.24655300	2.52882000
H	-4.67220800	1.48568300	-2.39910500
C	-6.48639700	-2.28872600	0.35301800
H	-6.45621100	-3.14974000	-0.32268600
H	-6.63733400	-2.67081300	1.36535900
H	-7.35333500	-1.68379500	0.07816400
N	3.69492500	-3.14720700	-0.65917300
O	4.46444200	-3.87308000	-0.05291500
O	3.03448000	-3.50145800	-1.62037400

TS1

Zero-point correction=	0.743114 (Hartree/Particle)
Thermal correction to Energy=	0.789684
Thermal correction to Enthalpy=	0.790629
Thermal correction to Gibbs Free Energy=	0.660979
Sum of electronic and zero-point Energies=	-2729.168954
Sum of electronic and thermal Energies=	-2729.122384
Sum of electronic and thermal Enthalpies=	-2729.121440
Sum of electronic and thermal Free Energies=	-2729.251090

C	-5.70919600	-0.90385600	0.40831500
C	-4.66684200	-0.22250400	-0.23322400
C	-4.42331600	1.11681200	0.02267900
C	-5.21467400	1.72416300	0.98915300

C	-6.22762400	1.06203600	1.67738800
C	-6.48755400	-0.26944200	1.37211200
C	-5.85064700	-2.29381300	-0.14984500
C	-5.14735000	-2.13850400	-1.51794000
C	-4.00663400	-1.11712600	-1.25803600
H	-3.64600900	1.66996600	-0.48512900
H	-6.80725500	1.59673600	2.41936500
H	-7.29692400	-0.79434300	1.86768700
H	-5.33376800	-3.01461100	0.49491000
H	-5.84243400	-1.66157100	-2.21311200
H	-6.88739900	-2.62008900	-0.25053600
H	-3.69558900	-0.59173700	-2.16239700
N	-2.83556200	-1.86462100	-0.74102400
O	-4.72925500	-3.31999800	-2.15418900
C	-1.66744000	-1.38179000	-0.21822800
C	-2.74568300	-3.23519000	-0.82705700
N	-0.97059500	-2.50160800	0.00700500
N	-1.61127400	-3.65681200	-0.36418600
C	-3.83680300	-4.09522400	-1.38507400
H	-4.35403400	-4.61925000	-0.57182300
H	-3.40163800	-4.84385700	-2.04865800
C	0.35034600	-2.63031500	0.55603100
C	0.53796000	-2.40952000	1.92231700
C	1.38547000	-2.98233600	-0.31199000
C	1.83055300	-2.56207900	2.42124900
C	2.65793900	-3.13662600	0.23927400
C	2.89692800	-2.93367700	1.59853200
H	2.01181600	-2.37502900	3.47692300
H	3.48121600	-3.41373300	-0.41408500
C	1.13798200	-3.15717000	-1.78595200
H	0.53910000	-4.05149500	-1.98123900
H	0.59151700	-2.29681700	-2.18734500
C	-0.60797100	-1.98975000	2.80396300
H	-0.96900500	-0.99264300	2.52639000
H	-1.44951000	-2.68342800	2.71120400
H	-0.29509300	-1.96375000	3.84907900
H	2.08481000	-3.22976200	-2.32146000
C	4.28393900	-3.08951900	2.16565100
H	4.46277500	-2.36157200	2.96102900
H	4.42400900	-4.08990700	2.58812600
H	5.04202200	-2.94332500	1.39098200
N	-4.97439200	3.13819600	1.28683600
O	-5.61587500	3.65148000	2.18848300
O	-4.14540200	3.73252200	0.61782700

C	-0.77871700	5.05439200	-1.31423700
C	-1.33912900	3.78183900	-1.37552400
C	-0.54236200	2.66633300	-1.64451600
C	0.84786900	2.82793200	-1.83666500
C	1.39103700	4.11862500	-1.77787300
C	0.58908100	5.22303300	-1.52176400
H	-1.41037100	5.91135600	-1.10401700
H	-2.40222400	3.64484200	-1.20424100
H	2.45409400	4.25142100	-1.95505800
H	1.02924700	6.21409200	-1.48501400
C	1.70744200	1.66259200	-2.07060600
C	2.99510300	1.55239900	-1.71117800
H	1.24247700	0.78934800	-2.52235500
H	3.50794500	2.35339900	-1.18985300
C	3.68486000	0.25201100	-1.90330400
O	3.08272800	-0.73092000	-2.31829100
S	-1.30102400	1.04933000	-1.68709100
C	-1.07853800	0.61031300	0.19699300
O	-1.83962900	1.11029300	1.00367000
C	0.37613400	0.41289800	0.47731300
C	0.89997000	1.07723100	1.51595900
H	0.96140200	-0.17507700	-0.22349500
H	0.20936400	1.66732200	2.11637300
C	2.30580200	1.12097300	1.93287200
C	2.67186300	1.99906000	2.96255700
C	3.30010000	0.32133900	1.35102500
C	3.99088900	2.08452200	3.39607800
H	1.90863900	2.62152400	3.42202900
C	4.61962300	0.40654000	1.78300000
H	3.03413600	-0.38850400	0.57192500
C	4.96964900	1.28821400	2.80561100
H	4.25404000	2.77147100	4.19416000
H	5.37887000	-0.21497900	1.31509200
H	6.00042500	1.35163600	3.13985000
C	5.11954400	0.12840300	-1.49265900
C	5.62801700	-1.16096400	-1.30175500
C	5.94004900	1.23376800	-1.25252500
C	6.92927000	-1.34450000	-0.84947400
H	4.97745100	-2.00492800	-1.50534000
C	7.24685900	1.05008000	-0.80879500
H	5.57277600	2.24145700	-1.41403000
C	7.73865100	-0.23590200	-0.59651400
H	7.31423700	-2.34697400	-0.69209800
H	7.87937600	1.91171300	-0.62288500

H	8.75343300	-0.37551000	-0.23791500

M1

Zero-point correction=	0.744706 (Hartree/Particle)
Thermal correction to Energy=	0.791910
Thermal correction to Enthalpy=	0.792854
Thermal correction to Gibbs Free Energy=	0.662824
Sum of electronic and zero-point Energies=	-2729.198352
Sum of electronic and thermal Energies=	-2729.151147
Sum of electronic and thermal Enthalpies=	-2729.150203
Sum of electronic and thermal Free Energies=	-2729.280234

C	-5.56485800	-1.33821000	0.31796800
C	-4.50799800	-0.64843600	-0.28288800
C	-4.45758500	0.73604900	-0.29806000
C	-5.47865300	1.40138700	0.36468000
C	-6.52679100	0.74512400	1.00926800
C	-6.57671900	-0.64314800	0.97748200
C	-5.44052000	-2.81794500	0.06277800
C	-4.54074400	-2.81562200	-1.19382100
C	-3.58792000	-1.60889300	-0.99055300
H	-3.64980300	1.26513200	-0.79006300
H	-7.29277600	1.32622100	1.50718600
H	-7.40074800	-1.16981900	1.44600900
H	-4.95692200	-3.31438300	0.91287500
H	-5.15975100	-2.56139100	-2.05724700
H	-6.39766400	-3.31123100	-0.11407300
H	-3.18567200	-1.21185400	-1.92235600
N	-2.40798000	-2.07751700	-0.19929600
O	-3.90013300	-4.01797700	-1.53791400
C	-1.34143000	-1.39689200	0.28336100
C	-2.07513800	-3.40858700	-0.12788400
N	-0.45494500	-2.32236900	0.64726500
N	-0.89397600	-3.58268400	0.38709600
C	-3.00877600	-4.49529000	-0.56005400
H	-3.53775400	-4.88561300	0.31912300
H	-2.43168900	-5.30763500	-1.00263100
C	0.83839600	-2.13661000	1.25792800
C	0.90107600	-1.81673000	2.61466200
C	1.96104100	-2.28075700	0.43848500
C	2.17104300	-1.62013200	3.15615200
C	3.20724300	-2.08987800	1.03359800
C	3.32697900	-1.75007500	2.38438000
H	2.25683900	-1.36322400	4.20878700
H	4.10459900	-2.20360300	0.42943300

C	1.81324300	-2.58074600	-1.02899700
H	1.25482300	-3.50703000	-1.19104900
H	1.26816200	-1.77276100	-1.53633500
C	-0.34312100	-1.66036300	3.44763500
H	-0.83336000	-0.70084900	3.24697500
H	-1.06647000	-2.45460800	3.24255000
H	-0.09386900	-1.68901700	4.50916200
H	2.79181500	-2.67650200	-1.50101200
C	4.68056800	-1.48300200	2.98630000
H	4.92018300	-0.41577600	2.91150900
H	4.70534600	-1.75474300	4.04392100
H	5.46355100	-2.03121800	2.45785800
N	-5.45441300	2.86740300	0.38313100
O	-6.34129800	3.44656700	0.98687500
O	-4.54814700	3.43247600	-0.20559700
C	-0.77202900	4.31876900	-1.37139100
C	-1.31568400	3.07152900	-1.65491700
C	-0.50733000	1.98186900	-2.02550500
C	0.89344100	2.19943000	-2.10500600
C	1.42466600	3.46477000	-1.81602300
C	0.60634300	4.52465900	-1.45353200
H	-1.42962200	5.13447700	-1.08413100
H	-2.38939600	2.92580600	-1.58046400
H	2.49919700	3.61245700	-1.89163800
H	1.03547900	5.49683500	-1.23352200
C	1.78042500	1.09774400	-2.47842500
C	3.03493800	0.92657500	-2.02194800
H	1.37534200	0.34120800	-3.14736100
H	3.43932200	1.60968700	-1.28323000
C	3.81524400	-0.25106000	-2.45437300
O	3.47262100	-0.93261300	-3.41282300
S	-1.21286100	0.38857300	-2.25233800
C	-1.23408700	0.06482000	0.67182800
O	-2.22221900	0.56334600	1.18551100
C	0.09837400	0.67453000	0.65626700
C	0.27501400	1.84447500	1.29048800
H	0.89832500	0.18360800	0.11175400
H	-0.60271600	2.31520800	1.73109300
C	1.55015400	2.54388700	1.45042600
C	1.53795400	3.92164800	1.70453100
C	2.78164700	1.87239800	1.39979400
C	2.72507800	4.62534300	1.87274600
H	0.58447300	4.44084000	1.74852000
C	3.96651000	2.57585900	1.59402500

H	2.80681000	0.79489300	1.24098100
C	3.94349700	3.95246700	1.82081300
H	2.69962100	5.69460200	2.05545800
H	4.91578800	2.04821200	1.59313500
H	4.87260000	4.49222600	1.97199300
C	5.00291000	-0.67000400	-1.63611900
C	5.56984900	-1.92248600	-1.89894900
C	5.51589800	0.10603200	-0.59295900
C	6.61063500	-2.40352200	-1.11269400
H	5.16621800	-2.51030500	-2.71716200
C	6.56562300	-0.36966900	0.18749500
H	5.10608800	1.08647200	-0.38327800
C	7.10663300	-1.62907000	-0.06338100
H	7.03616800	-3.38123000	-1.31393000
H	6.95870700	0.24017600	0.99526100
H	7.91691100	-2.00408700	0.55384900

TS2R

Zero-point correction= 0.744880 (Hartree/Particle)
Thermal correction to Energy= 0.791062
Thermal correction to Enthalpy= 0.792006
Thermal correction to Gibbs Free Energy= 0.663568
Sum of electronic and zero-point Energies= -2729.186284
Sum of electronic and thermal Energies= -2729.140102
Sum of electronic and thermal Enthalpies= -2729.139158
Sum of electronic and thermal Free Energies= -2729.267597

C	0.48786800	1.08594000	3.81043000
C	0.61560000	0.33213500	2.64416700
C	1.19682000	-0.92791900	2.65640500
C	1.66272400	-1.39229100	3.87818500
C	1.57413600	-0.65648500	5.05656700
C	0.97661600	0.59789500	5.02138300
C	-0.22734500	2.38240500	3.54685200
C	-0.74146800	2.28554400	2.08999800
C	-0.01759700	1.03552800	1.46229500
H	1.28545500	-1.55068900	1.77205300
H	1.95632300	-1.07659300	5.97841400
H	0.88064700	1.17920900	5.93194800
H	-1.06013100	2.55300000	4.23582900
H	-0.47619300	3.17387300	1.51876400
H	0.45586700	3.23031000	3.65163100
H	0.69771400	1.36137600	0.70465800
N	-0.98507700	0.13047100	0.82642200
O	-2.14982000	2.21695200	1.99428100

C	-0.84071400	-0.82284100	-0.11659300
C	-2.23436300	-0.02947200	1.36140600
N	-1.96479700	-1.53892800	-0.07455600
N	-2.84980600	-1.04507600	0.83083200
C	-2.70071300	0.97023800	2.36960500
H	-2.39732200	0.67236100	3.38312000
H	-3.78709400	1.05793400	2.33108300
C	-2.23487800	-2.80048600	-0.71927100
C	-3.33698000	-2.90092500	-1.57081800
C	-1.40535300	-3.88336100	-0.40462700
C	-3.57858000	-4.14631100	-2.14864100
C	-1.69526200	-5.10332300	-1.01231000
C	-2.76780800	-5.25198500	-1.89156500
H	-4.42609900	-4.25067600	-2.82135500
H	-1.06936600	-5.96173000	-0.78265400
C	-0.25182100	-3.77356700	0.56017500
H	0.62776700	-3.31460300	0.09279000
H	-0.51353400	-3.18090700	1.44308200
C	-4.24386100	-1.73310700	-1.84887100
H	-3.67629900	-0.81199400	-2.00153100
H	-4.84849200	-1.93259500	-2.73518800
H	-4.92341600	-1.56903300	-1.00557700
H	0.04620400	-4.76506700	0.90373300
C	-3.03645600	-6.57388200	-2.56134500
H	-2.51820900	-6.62658000	-3.52414100
H	-2.68327000	-7.40635400	-1.94889100
H	-4.10318000	-6.70991100	-2.75256900
N	2.25795400	-2.73345700	3.92352500
O	2.71936400	-3.11558900	4.98345700
O	2.25206300	-3.39133500	2.89711300
C	4.10298900	3.72043400	-1.33727800
C	3.82068000	2.75210000	-2.28354400
C	2.51604300	2.23800300	-2.47038300
C	1.48599700	2.74545100	-1.62279400
C	1.80221600	3.72873400	-0.66170600
C	3.08640300	4.21751600	-0.51150300
H	5.12000200	4.08578300	-1.22874500
H	4.61368700	2.35773000	-2.91154600
H	1.01556200	4.11172600	-0.01716300
H	3.30131300	4.97059700	0.23919600
C	0.12174600	2.24376900	-1.73550900
C	-0.98972700	2.79061300	-1.19095100
H	-0.00192400	1.33676400	-2.32636600
H	-0.96470500	3.74094000	-0.66836700

C	-2.27276800	2.07790600	-1.27505200
O	-2.33613300	0.92037500	-1.68697200
S	2.24699100	1.01347900	-3.67634100
C	0.24087600	-1.03093500	-1.16435200
O	-0.14687900	-1.53238100	-2.21419700
C	1.57865400	-0.63882400	-0.85319400
C	2.56697100	-0.86916900	-1.78351800
H	1.81081000	-0.17685600	0.09573800
H	2.31692000	-1.50367200	-2.62732200
C	3.98799200	-0.62309400	-1.53240900
C	4.94465500	-1.28765400	-2.31412200
C	4.42558700	0.24737200	-0.52457200
C	6.30077000	-1.10938000	-2.07878700
H	4.60976900	-1.94594800	-3.11100900
C	5.78520200	0.42789400	-0.29090000
H	3.70311100	0.80917300	0.06148600
C	6.72470500	-0.25144600	-1.06234900
H	7.02947600	-1.63486700	-2.68721400
H	6.11107800	1.11027000	0.48765200
H	7.78476100	-0.10812100	-0.87904400
C	-3.51206300	2.75437300	-0.77864900
C	-4.58989000	1.94705500	-0.39858000
C	-3.62344800	4.14368600	-0.68060600
C	-5.75496100	2.52033100	0.09627500
H	-4.48976100	0.86905600	-0.49073000
C	-4.79799400	4.71782700	-0.20181900
H	-2.80712000	4.78407700	-0.99860300
C	-5.85962700	3.90819200	0.19527800
H	-6.58393600	1.88964100	0.40076900
H	-4.88385000	5.79753700	-0.13813100
H	-6.77054900	4.35701500	0.57823900

TS2R-1

Zero-point correction=	0.743425 (Hartree/Particle)
Thermal correction to Energy=	0.790382
Thermal correction to Enthalpy=	0.791326
Thermal correction to Gibbs Free Energy=	0.659397
Sum of electronic and zero-point Energies=	-2729.183556
Sum of electronic and thermal Energies=	-2729.136600
Sum of electronic and thermal Enthalpies=	-2729.135656
Sum of electronic and thermal Free Energies=	-2729.267584

C	-0.81642900	-3.60171400	-0.13172600
C	-0.01270700	-2.51022300	0.20488300
C	0.41671400	-2.29786700	1.50443500

C	-0.01618900	-3.20809200	2.46299800
C	-0.83475400	-4.29286400	2.16790400
C	-1.23547500	-4.49511600	0.85026500
C	-1.10724900	-3.61791200	-1.60655800
C	-0.11539700	-2.60900300	-2.22331200
C	0.31482700	-1.69216100	-1.02618400
H	1.06569600	-1.47713400	1.79119800
H	-1.13264200	-4.96686700	2.96108600
H	-1.85676200	-5.34737100	0.59510300
H	-0.99039600	-4.60382500	-2.06390200
H	-0.58172300	-2.00835200	-3.00378800
H	-2.13301200	-3.27413500	-1.77854600
H	-0.24128300	-0.75506600	-1.05359300
N	1.74770800	-1.40450100	-1.08055900
O	0.98431400	-3.24196400	-2.86447200
C	2.46899700	-0.32335900	-0.73384000
C	2.62962500	-2.37843200	-1.46063800
N	3.74085500	-0.68302000	-0.90391400
N	3.85868000	-1.96132300	-1.36158800
C	2.04877900	-3.63827600	-2.01917700
H	1.71664100	-4.30752500	-1.21446500
H	2.78893900	-4.15487600	-2.62943800
C	4.92972500	0.06152100	-0.56824200
C	5.58292800	0.75979600	-1.58421500
C	5.37483000	0.01143500	0.75129000
C	6.75351700	1.42743500	-1.23774600
C	6.55276600	0.69867200	1.04659500
C	7.25360500	1.40325800	0.06782300
H	7.28529600	1.98565200	-2.00404300
H	6.92789100	0.68101000	2.06640300
C	4.60253600	-0.72914000	1.81154300
H	3.67830800	-0.19753400	2.06564300
H	4.32880600	-1.73556900	1.48038600
C	5.00616300	0.80875400	-2.97106900
H	4.02214000	1.28760200	-2.93851300
H	5.65233600	1.38075400	-3.63801200
H	4.87981200	-0.19555700	-3.38621600
H	5.19402500	-0.81794100	2.72359900
C	8.53936500	2.11375700	0.40162200
H	8.62792700	2.28843400	1.47567400
H	9.40097800	1.51637700	0.08691400
H	8.60120700	3.07548300	-0.11315900
N	0.42826900	-3.01970100	3.84862100
O	-0.00289500	-3.78286700	4.69471800

O	1.20697200	-2.10990800	4.07626200
C	-3.46162100	5.98808900	-0.44751400
C	-2.23954400	5.46898600	-0.84387600
C	-2.03569500	4.08397600	-1.01151800
C	-3.13514900	3.22097700	-0.74041200
C	-4.36191500	3.76805200	-0.32597000
C	-4.53629900	5.13389300	-0.18104200
H	-3.57796700	7.06191100	-0.33238700
H	-1.40412000	6.13447500	-1.03803600
H	-5.18293200	3.09901800	-0.08455800
H	-5.48987500	5.53221200	0.14930200
C	-2.96774000	1.77583900	-0.83088100
C	-3.93648100	0.83707700	-0.85063200
H	-1.93769200	1.42655100	-0.87922100
H	-4.99044800	1.09315200	-0.85138000
C	-3.56918200	-0.58269600	-0.81280100
O	-2.41154300	-0.96224000	-0.62653500
S	-0.46041100	3.50101800	-1.50382900
C	2.01459700	1.07043400	-0.34320400
O	2.72888200	1.98956300	-0.75525000
C	0.82654200	1.17400500	0.41729900
C	0.35624900	2.43918600	0.74020800
H	0.25742400	0.28746200	0.66275300
H	1.05738900	3.26000600	0.63569300
C	-0.82307500	2.69016400	1.56889300
C	-1.09341000	4.00275000	1.98475100
C	-1.71348200	1.67119400	1.93974700
C	-2.21199300	4.29005000	2.75488500
H	-0.42473700	4.80087400	1.67282700
C	-2.83060700	1.95813900	2.71565200
H	-1.55554600	0.65085400	1.59938200
C	-3.08394100	3.26599900	3.12419800
H	-2.41221700	5.31289100	3.05713400
H	-3.51393800	1.16000900	2.98766600
H	-3.96205400	3.48949200	3.72177800
C	-4.65262200	-1.60420600	-0.96729400
C	-4.46452700	-2.86525400	-0.39053600
C	-5.82165200	-1.34282000	-1.68740200
C	-5.43573100	-3.85025200	-0.52536200
H	-3.55433400	-3.04876500	0.17381800
C	-6.78661200	-2.33552400	-1.83574700
H	-5.96933200	-0.37511000	-2.15638600
C	-6.59734100	-3.58618700	-1.25148600
H	-5.29059400	-4.82240700	-0.06516900

H	-7.68596800	-2.13193900	-2.40737600
H	-7.35475600	-4.35544600	-1.36227000

TS2R-2

Zero-point correction= 0.743839 (Hartree/Particle)
Thermal correction to Energy= 0.790973
Thermal correction to Enthalpy= 0.791917
Thermal correction to Gibbs Free Energy= 0.657527
Sum of electronic and zero-point Energies= -2729.169771
Sum of electronic and thermal Energies= -2729.122637
Sum of electronic and thermal Enthalpies= -2729.121693
Sum of electronic and thermal Free Energies= -2729.256083

C	-2.05495900	4.30552100	-1.22675300
C	-2.16611300	3.07139600	-0.58317400
C	-2.33150400	2.98083400	0.79013400
C	-2.34274200	4.17686900	1.49776200
C	-2.20320200	5.42151600	0.89289100
C	-2.06204000	5.48652300	-0.48963000
C	-1.96688100	4.12375700	-2.71895700
C	-2.39772700	2.66258900	-2.96651500
C	-2.13406300	1.94458100	-1.59638700
H	-2.47413700	2.04382200	1.31741600
H	-2.22432200	6.31558400	1.50307700
H	-1.97643800	6.44863400	-0.98251400
H	-2.60829500	4.81043900	-3.27701900
H	-1.81654700	2.19201400	-3.75904800
H	-0.93859000	4.27542200	-3.06319900
H	-1.17367400	1.42284200	-1.61246700
N	-3.18478000	0.96628200	-1.32388800
O	-3.74726900	2.55635200	-3.39741300
C	-3.16844300	-0.25389400	-0.76280000
C	-4.49037100	1.26418800	-1.60956600
N	-4.44056800	-0.63711800	-0.71423300
N	-5.28057900	0.29680000	-1.24178900
C	-4.73880800	2.51841400	-2.38549300
H	-4.70607700	3.39872500	-1.73144600
H	-5.71131200	2.47132300	-2.87402500
C	-4.96889900	-1.82173000	-0.08533000
C	-5.28580600	-2.91415100	-0.89358700
C	-5.15003800	-1.79456700	1.29678500
C	-5.82735900	-4.02802900	-0.25944500
C	-5.69494200	-2.93740800	1.88252300
C	-6.03829100	-4.05595400	1.12254700
H	-6.08781400	-4.89762200	-0.85719600

H	-5.85568400	-2.94982500	2.95717400
C	-4.75330500	-0.59580200	2.11893900
H	-3.66332900	-0.53794500	2.22461300
H	-5.09479000	0.33892000	1.66316800
C	-5.01310000	-2.87965000	-2.37151200
H	-3.93914600	-2.75339200	-2.54290800
H	-5.33588300	-3.80800900	-2.84413900
H	-5.53205400	-2.04602800	-2.85372900
H	-5.17884900	-0.66267800	3.12084000
C	-6.60407700	-5.28824400	1.77843000
H	-5.82447500	-6.04595400	1.90527900
H	-7.01283600	-5.06020300	2.76473100
H	-7.39470600	-5.73024800	1.16749600
N	-2.53496900	4.11777200	2.95234100
O	-2.51785900	5.16580700	3.57192900
O	-2.70370400	3.02149500	3.45741800
C	2.56043400	-5.03116600	-0.09489300
C	1.91942300	-3.99973100	-0.76395800
C	2.52554000	-2.73777300	-0.95258700
C	3.82865400	-2.55151400	-0.41173600
C	4.46533600	-3.61454900	0.25231300
C	3.84924100	-4.84448600	0.41625700
H	2.05644400	-5.98469300	0.03386000
H	0.91863400	-4.14636300	-1.16129900
H	5.44679000	-3.44810300	0.68795600
H	4.35396700	-5.64431800	0.94781300
C	4.47008400	-1.23922300	-0.46938300
C	5.78907100	-0.98985700	-0.37042500
H	3.80329200	-0.38894200	-0.59997500
H	6.51084900	-1.79467100	-0.28102300
C	6.28069400	0.40272200	-0.37702100
O	5.52080100	1.36292000	-0.33390200
S	1.62900300	-1.47102400	-1.75815200
C	-1.97970100	-1.11507500	-0.37649300
O	-2.05117400	-2.29420200	-0.71364500
C	-0.91749200	-0.45671700	0.30603800
C	0.22728100	-1.16273800	0.58881700
H	-1.01417900	0.59190300	0.56066300
H	0.19680900	-2.23695700	0.42639400
C	1.35134400	-0.65038600	1.36877400
C	2.19658900	-1.56151200	2.01613600
C	1.60428600	0.72530600	1.50026100
C	3.26340200	-1.10883000	2.78832900
H	2.01854000	-2.62784100	1.90066500

C	2.67155000	1.17290200	2.26305100
H	0.97756300	1.44280200	0.97776900
C	3.50347600	0.25535700	2.91195700
H	3.91421300	-1.82584200	3.27867800
H	2.86742100	2.23672000	2.34751600
H	4.34090300	0.60868800	3.50513800
C	7.76338300	0.64004600	-0.42278900
C	8.23648700	1.89510000	-0.02519600
C	8.67161000	-0.32343400	-0.87181100
C	9.59598800	2.17826800	-0.05771300
H	7.51735800	2.63486000	0.31067900
C	10.03321000	-0.03467800	-0.91799900
H	8.32298100	-1.29207600	-1.21374100
C	10.49721000	1.21197800	-0.50549500
H	9.95601400	3.15021800	0.26371100
H	10.73107400	-0.78295100	-1.27906700
H	11.55956300	1.43238300	-0.53529700

TS2R-3

Zero-point correction=			0.744337 (Hartree/Particle)
Thermal correction to Energy=			0.791272
Thermal correction to Enthalpy=			0.792216
Thermal correction to Gibbs Free Energy=			0.658424
Sum of electronic and zero-point Energies=			-2729.172436
Sum of electronic and thermal Energies=			-2729.125501
Sum of electronic and thermal Enthalpies=			-2729.124557
Sum of electronic and thermal Free Energies=			-2729.258349
C	-5.29302600	-0.36313400	-1.83705400
C	-4.18512900	-0.20623000	-1.00464500
C	-4.31296100	-0.17945400	0.37687700
C	-5.59841100	-0.28520300	0.88889700
C	-6.72939100	-0.40906700	0.08730200
C	-6.57339800	-0.45229800	-1.29342500
C	-4.88194900	-0.44619000	-3.28162900
C	-3.33782600	-0.54849500	-3.27026000
C	-2.90007400	-0.16840700	-1.80532800
H	-3.46763200	-0.09594100	1.05263100
H	-7.70489900	-0.48928800	0.55034600
H	-7.43944200	-0.57309300	-1.93499800
H	-5.31676900	-1.30876300	-3.79541200
H	-2.89488500	0.15536400	-3.97391600
H	-5.19721100	0.44744200	-3.82807600
H	-2.40589900	0.80343000	-1.80400800
N	-1.96001700	-1.15209900	-1.25627400

O	-2.85577900	-1.81381900	-3.68079700
C	-1.03864000	-1.06713500	-0.27440200
C	-2.08490200	-2.47399800	-1.57958000
N	-0.66985100	-2.32706000	-0.03350700
N	-1.30531400	-3.21317000	-0.84663700
C	-2.99328600	-2.83416100	-2.71005100
H	-4.02948800	-2.93266400	-2.35824500
H	-2.68003300	-3.77629800	-3.15847300
C	0.14977600	-2.83321600	1.04043200
C	1.33686600	-3.48652800	0.71185000
C	-0.32207800	-2.69311900	2.34851100
C	2.08822100	-4.00085800	1.76653100
C	0.46833700	-3.22754200	3.36352400
C	1.67519300	-3.87558300	3.09338000
H	3.02185900	-4.51054500	1.54312800
H	0.12817900	-3.13814800	4.39195600
C	-1.62193400	-1.99914700	2.66453900
H	-1.51232800	-0.90862200	2.62649700
H	-2.41676100	-2.28562200	1.96771500
C	1.78069700	-3.63527500	-0.71760800
H	1.62970000	-2.70508000	-1.27212600
H	2.83870700	-3.89871400	-0.76111400
H	1.20884700	-4.41856500	-1.22438400
H	-1.95305300	-2.25668400	3.67147700
C	2.52604100	-4.40921500	4.21555200
H	3.21787500	-3.63813200	4.56928500
H	1.91244900	-4.71709300	5.06497400
H	3.12198200	-5.26377200	3.88798600
N	-5.76230900	-0.28982100	2.34809400
O	-6.89591100	-0.29799100	2.79201400
O	-4.75322700	-0.29037000	3.03185300
C	0.14785900	0.21295700	-3.21525400
C	0.15757300	1.40786900	-2.49732400
C	1.24673100	1.78333500	-1.68375700
C	2.33437800	0.86701500	-1.59341800
C	2.30656400	-0.32670300	-2.32007000
C	1.22425300	-0.66627000	-3.12881300
H	-0.69662900	-0.03867800	-3.85146600
H	-0.66584000	2.11148100	-2.59492600
H	3.13771400	-1.01988500	-2.22030100
H	1.22237400	-1.60077800	-3.68086400
C	3.44659400	1.13719500	-0.68069000
C	4.71344400	0.71678800	-0.83743200
H	3.21058600	1.73303300	0.19807500

H	5.01501900	0.16354900	-1.72097400
C	5.72130500	1.00205100	0.20761800
O	5.40890300	1.48091400	1.29007900
S	1.21512200	3.30507500	-0.83399100
C	-0.41412000	0.13484900	0.42376400
O	0.69202100	-0.06367300	0.91250800
C	-1.16149600	1.35430500	0.47395800
C	-0.57288600	2.46102300	1.03132800
H	-2.15553400	1.40886800	0.05533200
H	0.35950600	2.31102100	1.56462100
C	-1.25735100	3.74176000	1.23935400
C	-0.74967700	4.63579400	2.19034200
C	-2.41649900	4.09246100	0.53272000
C	-1.39524000	5.84090600	2.44673300
H	0.15611900	4.37589900	2.73093600
C	-3.05871700	5.29721900	0.78580900
H	-2.80635500	3.42928000	-0.23423000
C	-2.55290300	6.17342900	1.74698500
H	-0.99349100	6.52170100	3.18996600
H	-3.95240100	5.55927400	0.22893000
H	-3.05596400	7.11484400	1.94238300
C	7.15999200	0.67479200	-0.06858000
C	8.02635900	0.57625700	1.02536800
C	7.66313400	0.49655200	-1.36077200
C	9.37125200	0.28666100	0.83473500
H	7.61978500	0.72914800	2.01952100
C	9.01458100	0.22002900	-1.55260300
H	7.01362900	0.59672000	-2.22394700
C	9.86719300	0.10834600	-0.45714200
H	10.03538000	0.20265200	1.68882600
H	9.40203300	0.09362300	-2.55815500
H	10.91860400	-0.11380000	-0.60972000

TS2S

Zero-point correction=	0.743372 (Hartree/Particle)
Thermal correction to Energy=	0.790015
Thermal correction to Enthalpy=	0.790959
Thermal correction to Gibbs Free Energy=	0.661537
Sum of electronic and zero-point Energies=	-2729.195036
Sum of electronic and thermal Energies=	-2729.148393
Sum of electronic and thermal Enthalpies=	-2729.147449
Sum of electronic and thermal Free Energies=	-2729.276870

C	-4.91352500	1.49504900	-0.96008600

C	-3.52138400	1.52557900	-0.88275100
C	-2.82862400	2.71235200	-0.69817200
C	-3.58938700	3.86784300	-0.58525800
C	-4.97964000	3.87733700	-0.66897900
C	-5.64968300	2.67480700	-0.86168100
C	-5.41048000	0.08690400	-1.14837100
C	-4.18780200	-0.81942100	-0.87177100
C	-2.94295300	0.13095000	-0.97556300
H	-1.74696100	2.75522400	-0.64996400
H	-5.51314300	4.81459400	-0.57300200
H	-6.73268200	2.65911500	-0.91905800
H	-6.23445700	-0.17204300	-0.47738200
H	-4.07986000	-1.61617800	-1.60712000
H	-5.76657500	-0.05658500	-2.17336600
H	-2.38669800	-0.04948200	-1.89311100
N	-2.02304800	-0.08550200	0.15429100
O	-4.29617800	-1.50000100	0.36797500
C	-0.71538800	0.20015300	0.29782400
C	-2.50609900	-0.39431100	1.39361800
N	-0.46677300	0.06901100	1.60458600
N	-1.57118300	-0.31488700	2.29938700
C	-3.95062400	-0.75726600	1.51281500
H	-4.55589900	0.15494500	1.61920100
H	-4.10580700	-1.39309700	2.38506800
C	0.73827100	0.43911100	2.30525100
C	1.04907100	1.79929800	2.39421600
C	1.56003900	-0.57668700	2.79539700
C	2.27290200	2.12741300	2.97348500
C	2.77468400	-0.19283500	3.36088400
C	3.15352200	1.14894200	3.43984300
H	2.55106100	3.17551600	3.04798400
H	3.44479500	-0.96205500	3.73525500
C	1.16137400	-2.02084800	2.67792800
H	0.27607700	-2.23405600	3.28544600
H	0.91958600	-2.26487600	1.63769500
C	0.14225300	2.86884900	1.84319100
H	0.31164300	3.00697600	0.76846400
H	-0.91534000	2.63372700	1.99651000
H	0.34795300	3.82470200	2.32711100
H	1.97334000	-2.67218400	3.00421700
C	4.50044200	1.54039000	3.98544500
H	5.17747700	1.78935400	3.16135300
H	4.42594000	2.42170400	4.62685100
H	4.94995600	0.72735600	4.55846000

N	-2.88869300	5.13584400	-0.35204700
O	-3.54944200	6.15919500	-0.33930000
O	-1.68238400	5.09565700	-0.17697200
C	5.37884800	-2.50594800	-0.80412100
C	4.86512800	-1.75719600	-1.84712300
C	3.47594900	-1.66666200	-2.10070000
C	2.60687100	-2.37891300	-1.21814400
C	3.15658700	-3.13366000	-0.16108400
C	4.51968600	-3.20206300	0.05622700
H	6.45316400	-2.54132100	-0.64722100
H	5.53412800	-1.20057500	-2.49641100
H	2.49215200	-3.68530800	0.49771100
H	4.91562000	-3.79023100	0.87749000
C	1.16682500	-2.34340900	-1.42675000
C	0.21727500	-3.04054300	-0.76001100
H	0.82738100	-1.69444400	-2.23369000
H	0.45525000	-3.75097400	0.02562500
C	-1.19402400	-2.91413100	-1.14231700
O	-1.57027300	-2.24959400	-2.10758000
S	2.91584700	-0.66522400	-3.41055300
C	0.19638100	0.67126100	-0.82372000
O	-0.37963600	1.08974400	-1.82835000
C	1.60142300	0.63335500	-0.58322300
C	2.46179900	1.25121200	-1.45258700
H	1.96900600	0.12459000	0.29546200
H	2.03466800	1.81790600	-2.27489700
C	3.87851900	1.47011800	-1.15890900
C	4.59792900	2.39611600	-1.92875000
C	4.53248100	0.81699900	-0.10315100
C	5.92804000	2.67510900	-1.64606100
H	4.09971900	2.89303100	-2.75668600
C	5.86693600	1.09421200	0.17661200
H	4.00838100	0.07624200	0.49544700
C	6.56623500	2.02492700	-0.58846000
H	6.47002600	3.39690200	-2.24815300
H	6.36430400	0.57168600	0.98807400
H	7.60670700	2.23998500	-0.36683100
C	-2.20900000	-3.62753800	-0.30530300
C	-3.35734500	-4.13316600	-0.92013800
C	-2.06693800	-3.71939700	1.08136200
C	-4.35595200	-4.72184900	-0.15527900
H	-3.45113400	-4.05438100	-1.99931900
C	-3.08207200	-4.28253300	1.85067400
H	-1.17824400	-3.32251400	1.56532800

C	-4.22414100	-4.78602500	1.23221800
H	-5.24149400	-5.12588600	-0.63514100
H	-2.97832200	-4.33326600	2.92993000
H	-5.01055400	-5.23509700	1.83062100

TS2S-1

Zero-point correction= 0.743247 (Hartree/Particle)
Thermal correction to Energy= 0.790462
Thermal correction to Enthalpy= 0.791406
Thermal correction to Gibbs Free Energy= 0.656679
Sum of electronic and zero-point Energies= -2729.185998
Sum of electronic and thermal Energies= -2729.138783
Sum of electronic and thermal Enthalpies= -2729.137839
Sum of electronic and thermal Free Energies= -2729.272566

C	1.35167700	4.38303700	0.19279800
C	0.63610700	3.22203400	0.48171400
C	-0.10244000	3.09661100	1.65027800
C	-0.09236400	4.18241100	2.51409100
C	0.62341300	5.35128900	2.26528700
C	1.35492100	5.45156200	1.08848000
C	2.05113000	4.27927400	-1.13390200
C	1.53126000	2.97132100	-1.77744200
C	0.75581200	2.20954500	-0.63702500
H	-0.65226600	2.19576900	1.89657900
H	0.59037300	6.16129600	2.98299300
H	1.91060400	6.35668300	0.86843600
H	1.84825800	5.13271800	-1.78820300
H	2.35099800	2.34571900	-2.12753500
H	3.13521500	4.23141000	-0.99601400
H	1.27213100	1.29786600	-0.33597400
N	-0.59147900	1.82650000	-1.09325300
O	0.75148300	3.20646500	-2.93732600
C	-1.43997100	0.88333700	-0.64669100
C	-1.28490100	2.60224900	-1.97807200
N	-2.60408300	1.13747400	-1.25055800
N	-2.51821100	2.20146900	-2.09566100
C	-0.54694900	3.69692800	-2.67583100
H	-0.53009300	4.60384900	-2.05548100
H	-1.02515400	3.92788800	-3.62726900
C	-3.88586400	0.53608000	-0.98266400
C	-4.47473700	0.77196100	0.26339700
C	-4.45926800	-0.26860100	-1.96967100
C	-5.69022200	0.13793000	0.51528700
C	-5.67555100	-0.87563800	-1.66543400

C	-6.29754000	-0.69338700	-0.42751600
H	-6.17223300	0.29708600	1.47623900
H	-6.14264800	-1.51328400	-2.41121600
C	-3.76324700	-0.51147100	-3.28098200
H	-3.53933500	0.42637700	-3.79605800
H	-2.81416400	-1.03189300	-3.11474200
C	-3.82120300	1.63463900	1.31191300
H	-3.06911100	1.06576100	1.87140300
H	-3.33260000	2.51225800	0.87788800
H	-4.56374400	1.98401700	2.03050400
H	-4.38018300	-1.13107600	-3.93224400
C	-7.58326700	-1.40592600	-0.10176100
H	-7.37235700	-2.34070300	0.42819000
H	-8.21908300	-0.79679700	0.54423200
H	-8.13957700	-1.65421700	-1.00762100
N	-0.88785200	4.09273900	3.74438300
O	-0.78055600	4.99218200	4.55902600
O	-1.61866400	3.12635800	3.88026500
C	0.03201900	-0.78476800	-3.11933300
C	-0.16528600	-1.81251100	-2.20015600
C	0.83021200	-2.18875700	-1.27042800
C	2.04186900	-1.43562400	-1.27976400
C	2.22624400	-0.41807000	-2.22329200
C	1.23441000	-0.07936700	-3.13995100
H	-0.74950000	-0.53797800	-3.83382100
H	-1.08388800	-2.39256300	-2.21723800
H	3.16376600	0.13353400	-2.21462500
H	1.39217700	0.72325600	-3.85312400
C	3.08424800	-1.71837100	-0.29132200
C	4.40537800	-1.55058100	-0.47373900
H	2.74714300	-2.11210900	0.66551500
H	4.79859500	-1.24351200	-1.43694700
C	5.35013200	-1.86670300	0.62070700
O	4.96369600	-2.29909300	1.69881800
S	0.56587300	-3.53332200	-0.19981700
C	-1.08025800	-0.19570000	0.35121400
O	-0.10338700	0.04287600	1.06523800
C	-1.89042800	-1.36968800	0.36366000
C	-1.53660900	-2.40495000	1.18399400
H	-2.69460600	-1.46561600	-0.35248500
H	-0.72319700	-2.23340500	1.88168100
C	-2.33561600	-3.61889500	1.38743900
C	-1.82581400	-4.63192300	2.21084000
C	-3.60848700	-3.78382900	0.82246000

C	-2.55736900	-5.78711300	2.45311800
H	-0.83820200	-4.50735200	2.64686200
C	-4.34092800	-4.94034700	1.06596900
H	-4.04130600	-3.00010800	0.20630900
C	-3.81825000	-5.94537600	1.87837800
H	-2.14673900	-6.56405200	3.08951300
H	-5.32601300	-5.05570200	0.62511200
H	-4.39308100	-6.84614400	2.06784800
C	6.82049400	-1.67890100	0.38244700
C	7.70723800	-2.31892000	1.25517100
C	7.32962300	-0.88444200	-0.64919700
C	9.07947300	-2.18300700	1.09030000
H	7.29558000	-2.92414600	2.05592500
C	8.70544000	-0.73769600	-0.80644500
H	6.66254800	-0.35659900	-1.32223800
C	9.58088800	-1.39085800	0.05722300
H	9.76021500	-2.69177600	1.76512500
H	9.09282000	-0.11224600	-1.60394000
H	10.65297700	-1.28136800	-0.07234100

TS2S-2

Zero-point correction= 0.742676 (Hartree/Particle)
Thermal correction to Energy= 0.789477
Thermal correction to Enthalpy= 0.790421
Thermal correction to Gibbs Free Energy= 0.655101
Sum of electronic and zero-point Energies= -2729.175051
Sum of electronic and thermal Energies= -2729.128250
Sum of electronic and thermal Enthalpies= -2729.127306
Sum of electronic and thermal Free Energies= -2729.262627

C	5.95993300	-2.46262200	-0.93666600
C	4.83250500	-1.80953400	-0.44092500
C	4.50207000	-1.84319300	0.90635800
C	5.35599900	-2.55659000	1.73632900
C	6.48796700	-3.22549600	1.27634400
C	6.79287400	-3.17853600	-0.07834400
C	6.08976200	-2.27416100	-2.42340900
C	5.04635500	-1.19557000	-2.79681000
C	4.09189000	-1.09069900	-1.54717600
H	3.61752800	-1.35470800	1.29845600
H	7.11128000	-3.76439800	1.97863700
H	7.67319200	-3.68707200	-0.45626000
H	7.09057400	-1.95683200	-2.73061100
H	4.46753700	-1.48034300	-3.67437900
H	5.87196900	-3.20996700	-2.94697700

H	3.11525700	-1.53261600	-1.74276600
N	3.87659000	0.31754300	-1.18964000
O	5.64719100	0.03814200	-3.15762500
C	2.82966800	0.93954700	-0.62297400
C	4.86550500	1.24802000	-1.33912300
N	3.22308100	2.20065800	-0.44007900
N	4.49047200	2.41187100	-0.88990300
C	6.09690800	0.82380700	-2.07001900
H	6.77513900	0.26945800	-1.40743200
H	6.61856800	1.69281900	-2.46917800
C	2.48072600	3.25926300	0.19260800
C	2.23113400	3.16734100	1.56301500
C	2.00285400	4.29331700	-0.61834300
C	1.44071700	4.16879100	2.12680600
C	1.21784200	5.26467100	-0.00296700
C	0.91735300	5.21075800	1.36145900
H	1.22467300	4.12648400	3.19103900
H	0.82376100	6.07874900	-0.60562200
C	2.30221500	4.33507000	-2.09312300
H	3.36761000	4.50191800	-2.27368700
H	2.03184500	3.39227300	-2.58035300
C	2.74939600	2.02623400	2.39855500
H	2.07066300	1.16697200	2.34592600
H	3.73894000	1.69457300	2.07209400
H	2.81757000	2.32648700	3.44511300
H	1.74066400	5.13841500	-2.57101000
C	0.01513600	6.24245700	1.98473900
H	-1.03215500	5.94182900	1.87445700
H	0.21811000	6.35346500	3.05176200
H	0.13368700	7.21516000	1.50266600
N	5.04809100	-2.60395500	3.17099200
O	5.75734100	-3.29196400	3.88409500
O	4.10128000	-1.94893300	3.57068300
C	-1.25273300	-4.15828200	0.80242600
C	-0.99166400	-3.14648700	-0.10905800
C	-2.02707600	-2.44769300	-0.76929100
C	-3.36667000	-2.79088000	-0.42596200
C	-3.60636100	-3.83128800	0.48899200
C	-2.57050200	-4.51937100	1.09903700
H	-0.42615200	-4.67319800	1.28378800
H	0.03181700	-2.85263400	-0.32302300
H	-4.63351500	-4.11156800	0.70567700
H	-2.78111800	-5.32347900	1.79620900
C	-4.48861100	-2.05294500	-1.00441500

C	-5.72427800	-1.95086400	-0.47937000
H	-4.28302000	-1.49719000	-1.91617300
H	-5.97917300	-2.42509100	0.46244300
C	-6.75255200	-1.14646500	-1.16938500
O	-6.60207800	-0.74763200	-2.31765700
S	-1.61182000	-1.16896200	-1.89403600
C	1.53172000	0.25849900	-0.24824500
O	1.63244500	-0.94846100	-0.00133300
C	0.35828900	1.05642900	-0.24158800
C	-0.83464100	0.48750800	0.13619400
H	0.41908700	2.07844600	-0.59132500
H	-0.79410000	-0.51100500	0.56344800
C	-2.08438200	1.23413500	0.31569800
C	-3.21384200	0.55558200	0.79550200
C	-2.18478100	2.60795000	0.04988900
C	-4.41943500	1.22130000	0.97460100
H	-3.13986400	-0.50848000	1.00371700
C	-3.38829800	3.27609100	0.24174200
H	-1.32110500	3.16558900	-0.30049700
C	-4.51030900	2.58478400	0.69764800
H	-5.29132600	0.67624200	1.32356100
H	-3.45261100	4.33905700	0.03247600
H	-5.45134200	3.10674200	0.83798000
C	-8.01835100	-0.81123500	-0.43238400
C	-9.10697800	-0.35239100	-1.18166400
C	-8.13776400	-0.91012700	0.95749900
C	-10.30049300	-0.01436300	-0.55687800
H	-8.99363200	-0.27068700	-2.25755300
C	-9.33030000	-0.55889400	1.58541700
H	-7.29998900	-1.24155100	1.56211000
C	-10.41343500	-0.11729200	0.82994700
H	-11.14363000	0.33005500	-1.14692600
H	-9.41253300	-0.63046500	2.66498600
H	-11.34432200	0.14844700	1.32079300

TS2S-3

Zero-point correction=	0.744499 (Hartree/Particle)
Thermal correction to Energy=	0.789907
Thermal correction to Enthalpy=	0.790851
Thermal correction to Gibbs Free Energy=	0.665475
Sum of electronic and zero-point Energies=	-2729.186912
Sum of electronic and thermal Energies=	-2729.141504
Sum of electronic and thermal Enthalpies=	-2729.140560
Sum of electronic and thermal Free Energies=	-2729.265935

C	-6.19185600	0.38618600	-1.36073200
C	-4.94612900	0.53391400	-0.75174300
C	-4.81928000	1.01060700	0.54518800
C	-5.99808800	1.32580600	1.20732800
C	-7.25906400	1.19643500	0.62959100
C	-7.35677700	0.72237400	-0.67298400
C	-6.05154700	-0.14811800	-2.76017100
C	-4.57859300	-0.60184600	-2.88142000
C	-3.83453900	0.09051000	-1.67833200
H	-3.85374900	1.14594200	1.01822700
H	-8.13781600	1.46115000	1.20375800
H	-8.32920500	0.60741600	-1.13939300
H	-6.72411800	-0.98413700	-2.97205200
H	-4.13288600	-0.28130900	-3.82237600
H	-6.26736200	0.63699500	-3.49144600
H	-3.21847500	0.92593900	-2.00783400
N	-2.95539000	-0.87239800	-1.00190000
O	-4.44860200	-2.01512000	-2.89334100
C	-1.79303500	-0.71436900	-0.34385200
C	-3.31972100	-2.18167100	-0.87117000
N	-1.50867600	-1.91635400	0.16189800
N	-2.45117600	-2.84423600	-0.16235500
C	-4.52621200	-2.63635700	-1.62488500
H	-5.44708900	-2.37416200	-1.08670900
H	-4.49464000	-3.71529000	-1.77219200
C	-0.38963100	-2.27388000	0.99613600
C	-0.34349000	-1.76206300	2.29672600
C	0.60400600	-3.08828000	0.44611600
C	0.79402700	-2.05229600	3.04749400
C	1.71540200	-3.35222800	1.24577600
C	1.83564100	-2.82819100	2.53407500
H	0.86541400	-1.66272300	4.05976000
H	2.50773700	-3.98057900	0.84508800
C	0.51731200	-3.62994500	-0.95602300
H	-0.49925200	-3.92739100	-1.21756900
H	0.86280600	-2.87723600	-1.67443400
C	-1.44925400	-0.91279600	2.86698400
H	-1.31002400	0.13995200	2.59675600
H	-2.43389600	-1.22688500	2.50939800
H	-1.44696200	-0.97690400	3.95619700
H	1.16904700	-4.50023600	-1.05320500
C	3.07740300	-3.07765000	3.34780600
H	2.85260800	-3.10740400	4.41628100
H	3.55718800	-4.01581900	3.05989200

H	3.80376700	-2.27352200	3.18341600
N	-5.90744900	1.81589600	2.58827200
O	-6.94159500	2.12890800	3.15209400
O	-4.80227800	1.87928300	3.09782900
C	4.55196600	5.25966700	-1.12309000
C	3.19784800	4.99324900	-1.25760300
C	2.71590200	3.69203600	-1.50294600
C	3.67392100	2.64779600	-1.61205700
C	5.04118600	2.93709600	-1.47106300
C	5.48743300	4.22574300	-1.22585400
H	4.88319400	6.27670800	-0.93333800
H	2.47365600	5.79630100	-1.15801000
H	5.76248300	2.13181200	-1.58038800
H	6.54849800	4.42866500	-1.12519500
C	3.23094100	1.27808400	-1.85703100
C	3.90097000	0.16440400	-1.50600300
H	2.25298500	1.15855100	-2.31945600
H	4.83760300	0.22418300	-0.96171100
C	3.33355400	-1.16342400	-1.78522000
O	2.35776800	-1.31969900	-2.51448200
S	0.99191000	3.39081200	-1.54898800
C	-1.11358500	0.62082600	-0.13282700
O	-1.87664600	1.59534500	-0.21766900
C	0.26520800	0.64334500	0.18038200
C	0.79578100	1.84598700	0.60924700
H	0.86720000	-0.24849300	0.05062500
H	0.08473100	2.63945100	0.81219700
C	2.12323000	1.99497500	1.21594000
C	2.58513600	3.27813300	1.54174200
C	2.93176300	0.89038700	1.52690300
C	3.82968200	3.46171800	2.13061800
H	1.96423700	4.13403900	1.29240100
C	4.17060400	1.07333400	2.13051400
H	2.58566600	-0.11861300	1.31227300
C	4.62858200	2.35820500	2.42315900
H	4.17816600	4.46430900	2.35610400
H	4.78224700	0.21213700	2.38354700
H	5.60046500	2.49596100	2.88643700
C	3.98096600	-2.35597300	-1.14507000
C	3.79045200	-3.60989900	-1.73392700
C	4.73718300	-2.25484400	0.02717200
C	4.35171600	-4.74726500	-1.16418100
H	3.19797000	-3.67044600	-2.64141900
C	5.29158100	-3.39492900	0.60368300

H	4.87480100	-1.29039500	0.50669000
C	5.10226900	-4.64065400	0.00767400
H	4.20791200	-5.71631800	-1.63108900
H	5.86868100	-3.31190200	1.51914100
H	5.54032100	-5.52765400	0.45417600

M2R

Zero-point correction=	0.745131 (Hartree/Particle)
Thermal correction to Energy=	0.790913
Thermal correction to Enthalpy=	0.791857
Thermal correction to Gibbs Free Energy=	0.665315
Sum of electronic and zero-point Energies=	-2729.196130
Sum of electronic and thermal Energies=	-2729.150348
Sum of electronic and thermal Enthalpies=	-2729.149404
Sum of electronic and thermal Free Energies=	-2729.275946

C	0.52494400	1.69708900	3.52988700
C	0.50879500	0.74967900	2.50629700
C	1.00245200	-0.53318200	2.69370000
C	1.53464700	-0.82010600	3.94359400
C	1.59078400	0.10764500	4.97958600
C	1.07617900	1.38276900	4.77020600
C	-0.12405800	2.97887600	3.08026700
C	-0.85815400	2.62101600	1.76657300
C	-0.16386900	1.30449400	1.26683400
H	0.97867500	-1.29211700	1.91800700
H	2.01712100	-0.18230400	5.93177600
H	1.09121500	2.11249700	5.57255200
H	-0.83016300	3.38409500	3.80974100
H	-0.74888300	3.40649900	1.01729800
H	0.63458000	3.74601900	2.89391500
H	0.53979600	1.53053400	0.46207500
N	-1.14391000	0.34664000	0.75580200
O	-2.25759500	2.50104300	1.94249200
C	-1.03331400	-0.67770600	-0.12278400
C	-2.35799700	0.22301700	1.37857100
N	-2.17198200	-1.36355500	0.01079600
N	-3.01099800	-0.80806800	0.93762000
C	-2.72752500	1.24981700	2.39929000
H	-2.30342900	0.98118500	3.37743400
H	-3.81219300	1.31704000	2.48680700
C	-2.50441900	-2.65871200	-0.52667300
C	-3.57595800	-2.76067600	-1.41351100
C	-1.77643300	-3.76193200	-0.07351200

C	-3.90530300	-4.03531400	-1.87083500
C	-2.14647800	-5.01364100	-0.56281800
C	-3.20508700	-5.16970700	-1.45808200
H	-4.72805100	-4.14160600	-2.57348300
H	-1.59325900	-5.88893500	-0.23152800
C	-0.63623900	-3.62083800	0.90083800
H	0.25507500	-3.20950100	0.41252500
H	-0.89783200	-2.95760900	1.73279000
C	-4.33820400	-1.54444800	-1.86269500
H	-4.96181600	-1.15825200	-1.04882500
H	-3.65643400	-0.74572200	-2.16886600
H	-4.99194100	-1.79415700	-2.70008200
H	-0.37044900	-4.59289800	1.31910100
C	-3.60407500	-6.53869300	-1.94497700
H	-4.35034400	-6.98214800	-1.27771800
H	-4.04194000	-6.48940600	-2.94443100
H	-2.74501900	-7.21253200	-1.97485800
N	2.04341300	-2.17628900	4.18238100
O	2.57519400	-2.40473800	5.25434600
O	1.90146200	-2.99984500	3.29517300
C	4.53750300	3.14714900	-2.40768600
C	4.16314000	1.88284300	-2.84368800
C	2.82405500	1.47476800	-2.81587000
C	1.83186500	2.36126000	-2.33442300
C	2.23663500	3.63429100	-1.89490100
C	3.56600000	4.02590000	-1.92828000
H	5.58056100	3.44470500	-2.43777200
H	4.90941200	1.18308100	-3.20556400
H	1.49317300	4.33666000	-1.53280900
H	3.84556000	5.01692200	-1.58639700
C	0.41691400	1.96984300	-2.30311400
C	-0.59319100	2.69387100	-1.78106000
H	0.16513600	1.00460500	-2.73785600
H	-0.42438000	3.66097300	-1.32219400
C	-1.95605800	2.12511000	-1.74427800
O	-2.19567600	1.01626500	-2.21081000
S	2.43963300	-0.16264100	-3.38120500
C	0.04731800	-1.03997800	-1.11601400
O	-0.34601400	-1.67369900	-2.12540800
C	1.34274700	-0.67753800	-0.80296700
C	2.41628800	-1.11826400	-1.71832700
H	1.60182600	-0.15881100	0.10706400
H	2.16701100	-2.10764300	-2.11928700
C	3.80209300	-1.12152300	-1.13238600

C	4.68979600	-2.15315400	-1.45318200
C	4.24342900	-0.09869100	-0.28620900
C	5.98141500	-2.17066800	-0.93711500
H	4.35943600	-2.94944800	-2.11536200
C	5.53755600	-0.11155400	0.22919900
H	3.57672500	0.72434900	-0.04091200
C	6.41007400	-1.14807000	-0.09231000
H	6.65288800	-2.98449200	-1.19232100
H	5.86410000	0.69207900	0.88196100
H	7.41717000	-1.16003700	0.31203800
C	-3.03257400	2.88420400	-1.03178700
C	-4.15694300	2.16518700	-0.61105600
C	-2.94144700	4.24859900	-0.74069600
C	-5.15870900	2.79034400	0.11967600
H	-4.21531200	1.10847100	-0.85216300
C	-3.95288700	4.87786100	-0.02036100
H	-2.09764000	4.83595900	-1.08818700
C	-5.05415700	4.14866900	0.42078800
H	-6.02196800	2.22279200	0.45276600
H	-3.88029900	5.93845700	0.19652500
H	-5.83616900	4.64022300	0.99075100

M2S

Zero-point correction=	0.745279 (Hartree/Particle)
Thermal correction to Energy=	0.791982
Thermal correction to Enthalpy=	0.792926
Thermal correction to Gibbs Free Energy=	0.663357
Sum of electronic and zero-point Energies=	-2729.207436
Sum of electronic and thermal Energies=	-2729.160734
Sum of electronic and thermal Enthalpies=	-2729.159789
Sum of electronic and thermal Free Energies=	-2729.289358

C	-4.94426700	1.39374700	-0.88923800
C	-3.55328600	1.47743300	-0.85973900
C	-2.89678700	2.69158600	-0.72317200
C	-3.69798900	3.81841000	-0.59911200
C	-5.09050400	3.77534500	-0.62969800
C	-5.72162400	2.54632200	-0.78098400
C	-5.39045600	-0.03494300	-1.05160400
C	-4.12830800	-0.88628700	-0.78091700
C	-2.92259700	0.10471300	-0.95016700
H	-1.81391500	2.75300700	-0.74434700
H	-5.65480900	4.69392700	-0.52900400
H	-6.80467700	2.48973000	-0.80108300
H	-6.19394400	-0.31915400	-0.36634900

H	-4.01656500	-1.70757100	-1.48899600
H	-5.75335900	-0.20421200	-2.07062700
H	-2.38883800	-0.05460200	-1.88642200
N	-1.95501500	-0.06492500	0.13926100
O	-4.18454400	-1.52346000	0.48740400
C	-0.64397500	0.23746300	0.19640800
C	-2.36534100	-0.36846900	1.40756800
N	-0.31785000	0.10862800	1.48921900
N	-1.38369300	-0.28170900	2.25614800
C	-3.79822500	-0.74560800	1.59770800
H	-4.41289400	0.16018400	1.70545300
H	-3.91013300	-1.36167100	2.49065400
C	0.89427200	0.53728100	2.14042800
C	1.14785500	1.91098900	2.21211000
C	1.75129800	-0.42967300	2.66535900
C	2.32688600	2.30390700	2.84101500
C	2.91705800	0.01724800	3.28837500
C	3.21947100	1.37624400	3.38363800
H	2.55671000	3.36460800	2.90468900
H	3.60691600	-0.71618500	3.69781100
C	1.43895300	-1.89430300	2.52548800
H	0.55059900	-2.16365700	3.10590800
H	1.23917400	-2.14348200	1.47642500
C	0.21878000	2.92409700	1.59771500
H	0.38110400	2.98415500	0.51511800
H	-0.83305700	2.66985600	1.76482600
H	0.39903100	3.91423900	2.01877900
H	2.27678100	-2.50295200	2.86898900
C	4.47718800	1.84576900	4.06661500
H	4.95180900	2.64959000	3.49775200
H	4.25216400	2.23751400	5.06369000
H	5.19511800	1.03076500	4.18057200
N	-3.04022600	5.11705100	-0.41802400
O	-3.73839300	6.11670000	-0.41277100
O	-1.82934100	5.12763300	-0.27480000
C	5.39879900	-2.72749200	-0.81945500
C	4.87206200	-1.81516400	-1.72685700
C	3.49530300	-1.74887700	-1.96460700
C	2.62167000	-2.61581900	-1.26733300
C	3.17792800	-3.53208300	-0.35851400
C	4.54535000	-3.58969400	-0.13303700
H	6.46964800	-2.76394300	-0.64859100
H	5.52531100	-1.13085300	-2.25882800
H	2.52719000	-4.22171100	0.16982200

H	4.94597600	-4.30944500	0.57303100
C	1.17093100	-2.56379300	-1.48276500
C	0.23478200	-3.19689500	-0.75183300
H	0.82253200	-1.95078900	-2.31003900
H	0.48138200	-3.82816200	0.09551300
C	-1.19271000	-3.06274900	-1.10272900
O	-1.57551400	-2.45600200	-2.09841500
S	2.90284200	-0.52739500	-3.11622300
C	0.18511600	0.70628500	-0.97132300
O	-0.45999600	1.31382300	-1.88032600
C	1.52084000	0.42351600	-0.85934800
C	2.49425500	0.86242900	-1.87760300
H	1.86484000	-0.17380400	-0.02670600
H	2.01695100	1.59211100	-2.53898400
C	3.78897100	1.41654400	-1.32693400
C	4.53986400	2.31590400	-2.09186600
C	4.27686200	1.03950500	-0.07285600
C	5.74357600	2.82691200	-1.61823800
H	4.17297000	2.61340500	-3.07136900
C	5.48603300	1.54535400	0.40225300
H	3.71607300	0.35074700	0.55162600
C	6.22337500	2.44050700	-0.36659200
H	6.30780400	3.52858400	-2.22463300
H	5.84782700	1.23339600	1.37798600
H	7.16313200	2.83695800	0.00448800
C	-2.18749900	-3.69765200	-0.18675800
C	-3.36416600	-4.22335400	-0.72617000
C	-1.99135800	-3.70339700	1.19628700
C	-4.33836600	-4.75105500	0.11118400
H	-3.49918900	-4.21067500	-1.80368200
C	-2.98243300	-4.20414000	2.03646500
H	-1.08206400	-3.28387000	1.61953300
C	-4.15243900	-4.73097400	1.49387400
H	-5.24656400	-5.17128400	-0.30842800
H	-2.83872400	-4.18801900	3.11216300
H	-4.91886500	-5.13181600	2.14958700

TS3R

Zero-point correction=	0.744917 (Hartree/Particle)
Thermal correction to Energy=	0.790315
Thermal correction to Enthalpy=	0.791259
Thermal correction to Gibbs Free Energy=	0.665823
Sum of electronic and zero-point Energies=	-2729.175438
Sum of electronic and thermal Energies=	-2729.130040

Sum of electronic and thermal Enthalpies= -2729.129096

Sum of electronic and thermal Free Energies= -2729.254532

C	-2.08051700	-1.05442000	3.23137400
C	-1.55548200	-0.43004700	2.09921000
C	-1.97694100	0.83257900	1.70289600
C	-2.97213100	1.42235100	2.46966700
C	-3.55555600	0.80797000	3.57265700
C	-3.09373500	-0.44363600	3.96688500
C	-1.40802600	-2.37866600	3.48022900
C	-0.20596700	-2.42244300	2.50664700
C	-0.50042900	-1.30096200	1.45103700
H	-1.57889300	1.35854600	0.83835600
H	-4.33629800	1.32364600	4.11867500
H	-3.51006300	-0.92527500	4.84496400
H	-1.06259000	-2.49519700	4.51141300
H	-0.14330500	-3.38762000	2.00063100
H	-2.09394000	-3.20510100	3.26989800
H	-0.84987000	-1.78298500	0.54219200
N	0.69707800	-0.50712900	1.13744400
O	1.04492800	-2.29106500	3.15813900
C	0.98535800	0.34434500	0.11879500
C	1.57568700	-0.22858500	2.14965600
N	2.01390300	1.07403000	0.55960800
N	2.39711700	0.72082100	1.81559500
C	1.44745000	-0.96789200	3.44209400
H	0.72751500	-0.45341400	4.09465800
H	2.41318100	-1.01144500	3.94560500
C	2.63746800	2.24399500	-0.01762300
C	3.92778700	2.11724300	-0.52530900
C	1.94261400	3.45310100	0.05174200
C	4.54098100	3.28154500	-0.98792500
C	2.60083700	4.58421000	-0.42430800
C	3.89745100	4.51824900	-0.94071000
H	5.54565700	3.21531100	-1.39761400
H	2.08720200	5.54182500	-0.38952700
C	0.53320600	3.52703000	0.57477900
H	-0.17155800	3.12785200	-0.16552200
H	0.40880100	2.95797400	1.50228100
C	4.59184100	0.77165800	-0.60544300
H	4.67502900	0.30387900	0.38143300
H	3.99811800	0.09968500	-1.23522500
H	5.59412500	0.86087300	-1.02867400
H	0.25013700	4.56093700	0.77812800
C	4.59511200	5.76762700	-1.41226800

H	5.08225900	6.27578800	-0.57371900
H	5.36449800	5.53555000	-2.15173700
H	3.88702000	6.47093400	-1.85640300
N	-3.40040300	2.77806200	2.11820500
O	-4.52750400	3.11766500	2.43508800
O	-2.59970400	3.48746500	1.53700500
C	-4.04916900	-4.11372100	-1.72643300
C	-3.82569400	-3.03065700	-2.56809800
C	-2.56747400	-2.42434000	-2.62817000
C	-1.50287500	-2.89894600	-1.83372700
C	-1.76134500	-3.98185200	-0.97934400
C	-3.01205500	-4.58540900	-0.92544300
H	-5.02835200	-4.57950900	-1.69014500
H	-4.62820300	-2.63701200	-3.18396200
H	-0.96023300	-4.39081700	-0.37343300
H	-3.17277200	-5.42960800	-0.26305100
C	-0.16324300	-2.25656200	-1.90006100
C	0.89956400	-2.70206800	-1.09830600
H	0.12109200	-1.86914900	-2.87692800
H	0.75873600	-3.40824000	-0.28982200
C	2.18486700	-2.13851000	-1.31380100
O	2.37640100	-1.23635000	-2.15705800
S	-2.33193800	-1.08333400	-3.76097800
C	0.31939700	0.54659200	-1.22259500
O	0.78506400	1.43983800	-1.93706600
C	-0.81394300	-0.27819800	-1.50530000
C	-1.63558400	0.23434500	-2.65913000
H	-1.42811000	-0.55428900	-0.65790800
H	-0.97454600	0.79521700	-3.32332500
C	-2.68603100	1.17157500	-2.09856500
C	-2.44894600	2.54905600	-2.12797700
C	-3.81732600	0.69069800	-1.43259100
C	-3.33221700	3.43066900	-1.50774700
H	-1.55708200	2.92229400	-2.62476300
C	-4.69544700	1.57222300	-0.80744600
H	-4.00585100	-0.38017900	-1.39841700
C	-4.45777200	2.94571400	-0.84683800
H	-3.13327700	4.49749800	-1.53058700
H	-5.56693800	1.18667900	-0.28655000
H	-5.13380000	3.63030000	-0.34432200
C	3.35338400	-2.58497000	-0.47902600
C	4.63373400	-2.52113300	-1.03896700
C	3.21483400	-2.99491400	0.84897800
C	5.75193400	-2.86647200	-0.28881400

H	4.73298600	-2.18526500	-2.06663700
C	4.33604600	-3.32087200	1.60968000
H	2.23482000	-3.03417000	1.31206500
C	5.60599600	-3.26169800	1.04173200
H	6.73983200	-2.82034600	-0.73649100
H	4.21279100	-3.61810200	2.64681600
H	6.47968600	-3.51943500	1.63191100

TS3S

Zero-point correction=	0.745795 (Hartree/Particle)
Thermal correction to Energy=	0.790826
Thermal correction to Enthalpy=	0.791770
Thermal correction to Gibbs Free Energy=	0.668057
Sum of electronic and zero-point Energies=	-2729.188317
Sum of electronic and thermal Energies=	-2729.143287
Sum of electronic and thermal Enthalpies=	-2729.142343
Sum of electronic and thermal Free Energies=	-2729.266056

C	-5.07490400	1.02416000	-0.83131500
C	-3.68598000	1.14039600	-0.86878400
C	-3.05912200	2.37748500	-0.88634500
C	-3.88260100	3.49418700	-0.84387200
C	-5.27296500	3.41743800	-0.81066800
C	-5.87639000	2.16523400	-0.80952200
C	-5.49289900	-0.42213900	-0.82360400
C	-4.19525800	-1.22204700	-0.55836100
C	-3.02437300	-0.21934900	-0.85068200
H	-1.98126100	2.47540500	-0.94599500
H	-5.85749700	4.32822500	-0.77957100
H	-6.95750800	2.08277700	-0.77801700
H	-6.24372400	-0.64923800	-0.06122400
H	-4.09283400	-2.08462800	-1.21575500
H	-5.91936800	-0.69882000	-1.79303900
H	-2.50146700	-0.47455400	-1.77187800
N	-2.03534100	-0.26608000	0.23200000
O	-4.16481100	-1.77465200	0.74828100
C	-0.72781700	0.03061900	0.23155400
C	-2.41075100	-0.44307900	1.53156100
N	-0.36887700	0.06966500	1.51841700
N	-1.41206000	-0.23790400	2.34382500
C	-3.81726500	-0.88276200	1.78392700
H	-4.48619000	-0.01116500	1.82982800
H	-3.87388700	-1.42633500	2.72730700
C	0.83582400	0.63706200	2.08080600
C	1.08017600	1.99994300	1.87710300

C	1.68823700	-0.19251600	2.81465700
C	2.24075800	2.52712500	2.44308900
C	2.82972100	0.38832000	3.36060900
C	3.12033000	1.74327300	3.18762700
H	2.46257500	3.58001300	2.28986400
H	3.51200300	-0.23708300	3.93080700
C	1.40411500	-1.66082700	2.96760000
H	2.19747000	-2.14877800	3.53501500
H	0.45239600	-1.83118700	3.47975200
C	0.15825800	2.88438800	1.07724100
H	0.33602900	2.77743700	0.00031400
H	-0.89656200	2.66232300	1.27009000
H	0.32944600	3.93141000	1.33121900
H	1.34096700	-2.13593100	1.98183700
C	4.34814600	2.34904900	3.81344000
H	5.18561100	1.64714600	3.79440000
H	4.64653300	3.25789600	3.28708200
H	4.15661300	2.60824100	4.85986400
N	-3.24883000	4.81700600	-0.81949900
O	-3.97079000	5.79817600	-0.85458300
O	-2.03161400	4.86384900	-0.75718000
C	5.69755000	-2.77843100	-1.53540200
C	5.14347500	-1.78204800	-2.32920600
C	3.76942200	-1.53165800	-2.29347500
C	2.92049500	-2.28143000	-1.45282700
C	3.50945600	-3.26128400	-0.63991400
C	4.87627500	-3.50990600	-0.67909000
H	6.76474500	-2.97090900	-1.57130700
H	5.77208000	-1.17480700	-2.97227300
H	2.88455600	-3.86397700	0.00879600
H	5.29898100	-4.28314500	-0.04586100
C	1.45260200	-2.04943100	-1.45007400
C	0.59434900	-2.80730300	-0.62881700
H	1.03586300	-1.78640300	-2.42170400
H	0.95483900	-3.35632100	0.23117600
C	-0.78194600	-2.85133200	-0.94417400
O	-1.28608000	-2.25743100	-1.92886200
S	3.10809100	-0.19552300	-3.24315900
C	0.10330100	0.35395800	-0.98448200
O	-0.48300800	0.95392100	-1.89666800
C	1.47085500	-0.03528200	-0.93022700
C	2.37309900	0.77436100	-1.81906700
H	1.86248800	-0.24933100	0.05657800
H	1.76219400	1.50929700	-2.35246400

C	3.44337900	1.48993100	-1.02701000
C	3.59252200	2.87257700	-1.16018800
C	4.27391900	0.80697700	-0.12907600
C	4.55144700	3.56177800	-0.42058800
H	2.94881600	3.41424100	-1.84871900
C	5.23941600	1.49294500	0.60009100
H	4.16160300	-0.26547000	0.01015900
C	5.38245300	2.87232000	0.45816000
H	4.64948600	4.63690400	-0.53494600
H	5.87629900	0.94807800	1.29092800
H	6.13522900	3.40487200	1.03125600
C	-1.70642000	-3.62184000	-0.04152400
C	-2.79582000	-4.29665800	-0.59889200
C	-1.55001700	-3.61418500	1.34661200
C	-3.70723300	-4.95863400	0.21540200
H	-2.91549700	-4.28653100	-1.67848500
C	-2.47199900	-4.26142200	2.16634200
H	-0.71647200	-3.07532800	1.78890700
C	-3.55038800	-4.93748000	1.60146200
H	-4.54478200	-5.48861000	-0.22796600
H	-2.34798400	-4.23572500	3.24489000
H	-4.26766600	-5.44621400	2.23799700

M3R

Zero-point correction=			0.746365 (Hartree/Particle)
Thermal correction to Energy=			0.791194
Thermal correction to Enthalpy=			0.792139
Thermal correction to Gibbs Free Energy=			0.667665
Sum of electronic and zero-point Energies=			-2729.191995
Sum of electronic and thermal Energies=			-2729.147166
Sum of electronic and thermal Enthalpies=			-2729.146221
Sum of electronic and thermal Free Energies=			-2729.270695
C	-2.49747800	-0.64965000	3.33908200
C	-1.90203800	-0.14278200	2.18352200
C	-2.34816600	1.02289800	1.58151200
C	-3.45516000	1.62952000	2.16045200
C	-4.12342100	1.11321900	3.26516300
C	-3.62672200	-0.03628900	3.87375900
C	-1.73255700	-1.83950500	3.85805300
C	-0.39801400	-1.83301300	3.07729800
C	-0.70457500	-0.98138200	1.79604000
H	-1.87554200	1.46809400	0.70907100
H	-4.98819000	1.63518500	3.65772600

H	-4.09976000	-0.42649800	4.76822000
H	-1.54415600	-1.79142900	4.93375000
H	-0.09152300	-2.84173700	2.79473300
H	-2.27712700	-2.76822000	3.65935100
H	-0.91304200	-1.65413700	0.96526000
N	0.41840400	-0.11451400	1.44965200
O	0.69208900	-1.32908200	3.83181400
C	0.91206300	0.34413800	0.27643200
C	1.10363700	0.51384400	2.45250600
N	1.82981700	1.25605600	0.62297200
N	1.97496400	1.35176500	1.97690600
C	0.82609100	0.08186500	3.85640000
H	-0.07238000	0.57618600	4.24825500
H	1.67523600	0.32587400	4.49371900
C	2.46549400	2.26726200	-0.19378600
C	3.75214700	2.04667900	-0.67937300
C	1.74743600	3.44682600	-0.40149300
C	4.33566400	3.08392100	-1.40552500
C	2.37590600	4.44945700	-1.13773900
C	3.66802200	4.28684200	-1.64089900
H	5.33700200	2.94225500	-1.80421500
H	1.84295300	5.37909800	-1.31991600
C	0.34337500	3.61438800	0.11801800
H	-0.35754600	2.97297200	-0.43054700
H	0.26777700	3.36571100	1.18163300
C	4.43806500	0.72627500	-0.48782500
H	4.35332300	0.36321600	0.54180300
H	3.97746600	-0.02813700	-1.13803400
H	5.49750600	0.80105600	-0.74107400
H	0.00493300	4.64349700	-0.01227800
C	4.33908100	5.39958800	-2.40327800
H	4.89438900	6.05185000	-1.72141000
H	5.04843100	5.00487800	-3.13387700
H	3.60637000	6.01640600	-2.92820900
N	-3.89838200	2.90975300	1.60845000
O	-5.09026700	3.16360300	1.64452600
O	-3.04396000	3.64515500	1.14820600
C	-3.20883900	-5.07698200	-1.90817700
C	-3.22503200	-3.91645200	-2.67807900
C	-2.14580900	-3.03349900	-2.62760700
C	-1.04636100	-3.29061000	-1.79015400
C	-1.05882000	-4.44771900	-1.01223800
C	-2.12532900	-5.34337400	-1.07635100
H	-4.04666100	-5.76490500	-1.95519600

H	-4.07104800	-3.69428400	-3.32141000
H	-0.20860300	-4.65709700	-0.36994200
H	-2.10965400	-6.24560400	-0.47367500
C	0.05457400	-2.26290100	-1.73708000
C	1.09978500	-2.40381900	-0.65999500
H	0.58298100	-2.23245100	-2.70173400
H	0.80443200	-2.77088900	0.31725500
C	2.45777000	-2.25236000	-0.95501300
O	2.91138000	-1.96796900	-2.09529900
S	-2.13692800	-1.64673400	-3.74128500
C	0.60470300	0.00162000	-1.16030900
O	1.33670600	0.48316400	-2.00103600
C	-0.58957300	-0.87319800	-1.54501800
C	-1.31495000	-0.30569600	-2.76934100
H	-1.31410700	-0.91493200	-0.72521600
H	-0.55922600	0.09783200	-3.44821500
C	-2.27463400	0.79062500	-2.36328500
C	-1.91509800	2.12774500	-2.54408000
C	-3.48902900	0.49148100	-1.73703300
C	-2.76048100	3.15124900	-2.11506500
H	-0.96666700	2.36640900	-3.02053900
C	-4.33138200	1.51138800	-1.30590200
H	-3.77519700	-0.54880300	-1.59798800
C	-3.97143900	2.84514700	-1.50139500
H	-2.46850400	4.18692200	-2.25788200
H	-5.26991000	1.26909500	-0.81590400
H	-4.62203900	3.63929900	-1.14845400
C	3.45027700	-2.35852100	0.18633000
C	4.79863500	-2.53882200	-0.13378300
C	3.10152700	-2.20928500	1.53250600
C	5.77176600	-2.56907000	0.85976300
H	5.06089000	-2.62653700	-1.18305800
C	4.07220800	-2.22513900	2.53101500
H	2.06670800	-2.05903900	1.82056200
C	5.41301700	-2.40513300	2.19758500
H	6.81463600	-2.71147800	0.59250600
H	3.77481100	-2.09091300	3.56716300
H	6.17266700	-2.41605100	2.97308000

M3S

Zero-point correction= 0.747496 (Hartree/Particle)
Thermal correction to Energy= 0.792843
Thermal correction to Enthalpy= 0.793787
Thermal correction to Gibbs Free Energy= 0.668300

Sum of electronic and zero-point Energies= -2729.202915
Sum of electronic and thermal Energies= -2729.157569
Sum of electronic and thermal Enthalpies= -2729.156625
Sum of electronic and thermal Free Energies= -2729.282112

C	-5.05108300	1.02165900	-0.85378600
C	-3.65805200	1.08377800	-0.89333600
C	-2.99382900	2.29415900	-1.02656100
C	-3.77864000	3.43583400	-1.11319400
C	-5.17071700	3.40867200	-1.09087200
C	-5.81411800	2.18346100	-0.96203600
C	-5.52229200	-0.39653200	-0.68375900
C	-4.25429800	-1.21420600	-0.34012200
C	-3.04375300	-0.28930500	-0.72499100
H	-1.91394100	2.36605700	-1.07004500
H	-5.72485100	4.33609900	-1.16273200
H	-6.89747000	2.13925300	-0.93080700
H	-6.27324700	-0.50722500	0.10410400
H	-4.18969800	-2.13524500	-0.91739800
H	-5.96983600	-0.76373900	-1.61254800
H	-2.53214800	-0.67847900	-1.60849000
N	-2.05892400	-0.25109400	0.36853700
O	-4.23729100	-1.64715600	1.00906900
C	-0.73487500	-0.01943200	0.36655400
C	-2.45143300	-0.28991300	1.67601300
N	-0.38803500	0.13866100	1.64653600
N	-1.45624400	-0.04825600	2.48032600
C	-3.87254100	-0.66595900	1.95481600
H	-4.51880100	0.22215500	1.90728200
H	-3.95013400	-1.11018100	2.94725200
C	0.84645300	0.66543600	2.17123800
C	1.20122600	1.97729100	1.83735000
C	1.60534900	-0.13719000	3.03252000
C	2.37049500	2.48491100	2.40485300
C	2.75863600	0.42331500	3.57154700
C	3.15195100	1.73191500	3.27689300
H	2.67023800	3.49917800	2.15716600
H	3.36682000	-0.17922000	4.24149500
C	1.21329500	-1.55642600	3.34272700
H	1.89416600	-1.98537400	4.07872800
H	0.19426800	-1.61743100	3.73395700
C	0.37354800	2.83885100	0.91719900
H	0.59666700	2.63527800	-0.13773000
H	-0.70076300	2.69783200	1.07367000
H	0.60060700	3.89225700	1.08741800

H	1.26219200	-2.17138700	2.43812000
C	4.38533600	2.31535600	3.91280000
H	5.22597500	1.61916000	3.84655400
H	4.67338500	3.24986000	3.42774000
H	4.20858900	2.51757500	4.97391400
N	-3.09929900	4.73198700	-1.21786800
O	-3.78586300	5.72589300	-1.37626100
O	-1.88240900	4.74536300	-1.13382500
C	5.46736400	-3.19112500	-2.01628100
C	5.06880000	-1.98500200	-2.58695300
C	3.76192400	-1.53396700	-2.40620300
C	2.83959700	-2.26903900	-1.64105600
C	3.26486800	-3.46383000	-1.06153200
C	4.56574400	-3.92735100	-1.25239000
H	6.48213400	-3.54753600	-2.16034100
H	5.76553700	-1.39022400	-3.16935900
H	2.55786200	-4.04503400	-0.47846400
H	4.87434200	-4.86580300	-0.80275000
C	1.44572600	-1.71323000	-1.47061200
C	0.50370800	-2.48487300	-0.59130300
H	0.97976700	-1.62695700	-2.46262400
H	0.87027500	-2.85395100	0.36099700
C	-0.79772900	-2.74426800	-0.98919800
O	-1.31589700	-2.38938400	-2.09789000
S	3.21813300	-0.02511500	-3.16438300
C	0.08956200	0.17221300	-0.87611700
O	-0.48771700	0.61330100	-1.84510800
C	1.54109400	-0.25834300	-0.90606600
C	2.39643300	0.75532500	-1.69806600
H	1.91953700	-0.34252000	0.11720000
H	1.73486400	1.48784800	-2.17069200
C	3.41078100	1.47946800	-0.84351600
C	3.51747700	2.86996300	-0.91664000
C	4.28748100	0.77689600	-0.00812400
C	4.48550300	3.54875300	-0.17881000
H	2.84320200	3.42567900	-1.56397100
C	5.25977400	1.45271200	0.72045500
H	4.21738900	-0.30606600	0.06342400
C	5.36408800	2.84071300	0.63645800
H	4.55511300	4.62991200	-0.24737600
H	5.93819200	0.89346900	1.35776100
H	6.12622800	3.36527400	1.20425500
C	-1.70012200	-3.46647300	-0.01230800
C	-2.75675500	-4.22628200	-0.52180400

C	-1.55434500	-3.37859500	1.37595900
C	-3.63443900	-4.89157700	0.32883300
H	-2.87622800	-4.27097500	-1.60021900
C	-2.43333900	-4.03552200	2.23247400
H	-0.76126400	-2.76520000	1.79379000
C	-3.47566200	-4.79830400	1.71061000
H	-4.44543700	-5.48372600	-0.08522500
H	-2.30849800	-3.94385900	3.30788400
H	-4.16336900	-5.31174200	2.37557700

TS4R

Zero-point correction=	0.747984 (Hartree/Particle)
Thermal correction to Energy=	0.791355
Thermal correction to Enthalpy=	0.792299
Thermal correction to Gibbs Free Energy=	0.672673
Sum of electronic and zero-point Energies=	-2729.196483
Sum of electronic and thermal Energies=	-2729.153112
Sum of electronic and thermal Enthalpies=	-2729.152168
Sum of electronic and thermal Free Energies=	-2729.271794

C	-1.95618200	-1.11524600	3.31583000
C	-1.44148600	-0.50117800	2.17351000
C	-1.83679600	0.77278500	1.79067100
C	-2.80704800	1.38264200	2.57411000
C	-3.39338400	0.77318400	3.67818500
C	-2.95098100	-0.48864400	4.06326900
C	-1.27600000	-2.43375000	3.57563000
C	-0.12272300	-2.51870300	2.54445200
C	-0.41585100	-1.38504500	1.50162000
H	-1.43133100	1.29850000	0.92877200
H	-4.15513400	1.30349200	4.23707900
H	-3.36285300	-0.96215900	4.94786000
H	-0.87285200	-2.49767600	4.59118200
H	-0.11886200	-3.48238800	2.03237900
H	-1.96834000	-3.27110600	3.44952000
H	-0.77935700	-1.84573600	0.58645000
N	0.79073200	-0.60820900	1.18934100
O	1.16040400	-2.42436300	3.13429100
C	1.07657200	0.24292000	0.17548200
C	1.65992000	-0.32045100	2.21011300
N	2.06261100	1.01649900	0.63667500
N	2.45076300	0.65808700	1.89465400
C	1.55840500	-1.11164700	3.47506400
H	0.84650200	-0.63496900	4.16400700
H	2.53262200	-1.17023900	3.96003900

C	2.67673200	2.19002900	0.05935900
C	3.97470900	2.07452500	-0.44148400
C	1.97382400	3.39325800	0.10994300
C	4.57370400	3.23374400	-0.92710500
C	2.61879500	4.52390100	-0.39257100
C	3.91193200	4.46404300	-0.91078400
H	5.58126000	3.17240400	-1.33131800
H	2.09426400	5.47583700	-0.37145800
C	0.56993900	3.47713400	0.64159400
H	-0.15112500	3.22887400	-0.14702000
H	0.39998500	2.79140100	1.47697100
C	4.65837000	0.73839600	-0.48143000
H	4.79902300	0.33155500	0.52539200
H	4.03200800	0.03245700	-1.03426800
H	5.63471900	0.81556000	-0.96334000
H	0.34833200	4.48604400	0.99439500
C	4.59793000	5.70120400	-1.42955800
H	5.42226800	5.99181200	-0.77078300
H	5.02107400	5.52647300	-2.42239600
H	3.90399500	6.54151700	-1.49385300
N	-3.19580100	2.75507000	2.24556500
O	-4.31769600	3.11882700	2.55471200
O	-2.36892600	3.45275900	1.68757100
C	-4.38275200	-3.85098700	-1.83841100
C	-4.13135900	-2.76010400	-2.66546800
C	-2.85791200	-2.19216800	-2.69717400
C	-1.81199500	-2.70095800	-1.90720900
C	-2.09879800	-3.77175400	-1.05775500
C	-3.36777800	-4.34834100	-1.02719700
H	-5.37183800	-4.29653700	-1.81619700
H	-4.91985400	-2.33894100	-3.28148500
H	-1.32473400	-4.17864900	-0.41620900
H	-3.56006500	-5.18692300	-0.36593000
C	-0.47042500	-2.00068000	-1.98032200
C	0.64905800	-2.67799400	-1.24949900
H	-0.18851700	-1.92553200	-3.04365400
H	0.54658500	-3.68724500	-0.87250100
C	1.85999700	-2.06447000	-1.25511300
O	2.00179800	-0.86532700	-1.76479700
S	-2.52256000	-0.82624400	-3.77316900
C	0.47855100	0.37385300	-1.22247000
O	0.69542500	1.43405700	-1.79235100
C	-0.73822300	-0.50501600	-1.57647200
C	-1.54293000	0.26553200	-2.65129200

H	-1.37646600	-0.52174600	-0.68481000
H	-0.82973500	0.74613500	-3.32326300
C	-2.41742700	1.32596700	-2.01430500
C	-2.13828800	2.68058200	-2.20089300
C	-3.50377700	0.96381100	-1.20854600
C	-2.93234000	3.65644500	-1.59835400
H	-1.28304800	2.96584500	-2.80670500
C	-4.29506100	1.93603500	-0.60555600
H	-3.73372200	-0.08996200	-1.05962600
C	-4.01183000	3.28789100	-0.80137600
H	-2.69950600	4.70617200	-1.74714700
H	-5.13054600	1.64089300	0.02269300
H	-4.61604400	4.04543700	-0.31212300
C	3.06847700	-2.69271000	-0.63885800
C	4.31315800	-2.53535100	-1.25917700
C	2.99722000	-3.42056800	0.55228600
C	5.45823700	-3.09864200	-0.70634900
H	4.36664800	-1.96544200	-2.18204000
C	4.14416200	-3.97925800	1.11237600
H	2.04309800	-3.52384900	1.05914400
C	5.37727800	-3.82136500	0.48399300
H	6.41616200	-2.97397900	-1.20191600
H	4.07448900	-4.52857500	2.04635300
H	6.27190900	-4.25370800	0.92091800

TS4S

Zero-point correction=			0.748111 (Hartree/Particle)
Thermal correction to Energy=			0.792680
Thermal correction to Enthalpy=			0.793624
Thermal correction to Gibbs Free Energy=			0.667970
Sum of electronic and zero-point Energies=			-2729.208466
Sum of electronic and thermal Energies=			-2729.163897
Sum of electronic and thermal Enthalpies=			-2729.162953
Sum of electronic and thermal Free Energies=			-2729.288606
C	5.18163700	-0.15331100	0.52949100
C	3.85048500	-0.37735800	0.17899900
C	3.47881000	-1.47991300	-0.57954900
C	4.49623900	-2.33914800	-0.97127800
C	5.83545400	-2.14426400	-0.64039400
C	6.18146900	-1.03425600	0.11946300
C	5.32941700	1.09926900	1.34832500
C	3.88807900	1.55885900	1.67086500
C	2.95220000	0.70798700	0.73058800
H	2.45013900	-1.66736700	-0.86419100

H	6.57880300	-2.85458500	-0.97948000
H	7.21745200	-0.86117900	0.39044700
H	5.89091800	0.93800000	2.27370800
H	3.74814500	2.61649900	1.44830000
H	5.85900000	1.87013800	0.78044100
H	2.50668100	1.33657900	-0.04191300
N	1.83536500	0.14548100	1.49293300
O	3.58338100	1.44754200	3.05174600
C	0.55975100	-0.07976500	1.13620100
C	1.95108700	-0.17782800	2.81338100
N	-0.03421600	-0.54491000	2.23432200
N	0.82000500	-0.59827900	3.30028500
C	3.24856100	0.14021400	3.47887900
H	4.01994500	-0.59417500	3.20858200
H	3.12848200	0.15412000	4.56128300
C	-1.41751000	-0.90087300	2.39646400
C	-1.83712400	-2.15526600	1.95304600
C	-2.27099500	0.06336600	2.94058100
C	-3.20738900	-2.41442100	2.00315400
C	-3.62638100	-0.25153500	2.97765000
C	-4.11208500	-1.46856600	2.48889300
H	-3.57309000	-3.36979400	1.63573000
H	-4.32662900	0.47925000	3.37511300
C	-1.73439100	1.37588500	3.44954900
H	-1.19900700	1.23004400	4.39298900
H	-1.03284300	1.82518600	2.73706600
C	-0.85697200	-3.14572400	1.38434400
H	-0.52078600	-2.84114700	0.38424700
H	0.02584800	-3.23915000	2.02351800
H	-1.32245400	-4.12673900	1.28154100
H	-2.55028600	2.07929300	3.62586100
C	-5.59530200	-1.72414000	2.46266400
H	-5.81835800	-2.75855500	2.19531100
H	-6.04899600	-1.50990000	3.43395200
H	-6.07044100	-1.06753900	1.72538400
N	4.13920500	-3.50803400	-1.78333200
O	5.01973200	-4.30423400	-2.05783400
O	2.97831800	-3.62018600	-2.14137500
C	-6.37459700	1.05638300	-0.78691100
C	-5.50877800	0.59694800	-1.77463100
C	-4.12942100	0.76688000	-1.62763100
C	-3.60169800	1.37830300	-0.48494700
C	-4.48667900	1.81778000	0.50092900
C	-5.86338200	1.67049400	0.35522400

H	-7.44536200	0.92591100	-0.90670000
H	-5.89662000	0.10437900	-2.66117400
H	-4.07957600	2.28994100	1.39189500
H	-6.53321100	2.02729900	1.13106800
C	-2.11381500	1.50956200	-0.28992300
C	-1.43226400	2.63552800	-1.00364500
H	-1.94297500	1.65789200	0.78249600
H	-1.91173000	3.16431500	-1.81741600
C	-0.17840000	2.90197500	-0.54350000
O	0.31644500	2.20397000	0.45038700
S	-3.05128300	0.27300500	-2.94513700
C	0.06494500	0.13528600	-0.27594200
O	0.92050700	0.02180300	-1.14486100
C	-1.42808100	0.13869400	-0.60028200
C	-1.57601500	-0.37206100	-2.05264100
H	-1.91659500	-0.58959000	0.05285600
H	-0.73858600	0.01521900	-2.63349500
C	-1.52567700	-1.88853600	-2.05224300
C	-0.34840000	-2.55418000	-2.40127300
C	-2.62454000	-2.63836000	-1.61657500
C	-0.27120700	-3.94607600	-2.32065700
H	0.51636000	-1.98002700	-2.72275900
C	-2.54889500	-4.02434000	-1.53683900
H	-3.54452500	-2.12609000	-1.34145100
C	-1.36992300	-4.68284000	-1.88942400
H	0.65260400	-4.44595300	-2.59293700
H	-3.41055100	-4.59292300	-1.19984900
H	-1.31091800	-5.76485000	-1.82699100
C	0.70151900	3.96508500	-1.11926800
C	1.79776500	4.39826200	-0.36606200
C	0.48240600	4.54283000	-2.37565500
C	2.65150500	5.38684800	-0.84698200
H	1.95118900	3.94760700	0.60923800
C	1.33418800	5.53168000	-2.85823100
H	-0.34712400	4.20244000	-2.98816100
C	2.42240800	5.95818600	-2.09672300
H	3.49519900	5.71304800	-0.24584700
H	1.15506900	5.96577700	-3.83726900
H	3.08776200	6.72631100	-2.47805000

M5R

Zero-point correction=	0.748095 (Hartree/Particle)
Thermal correction to Energy=	0.792810
Thermal correction to Enthalpy=	0.793754

Thermal correction to Gibbs Free Energy= 0.670503
Sum of electronic and zero-point Energies= -2729.200644
Sum of electronic and thermal Energies= -2729.155929
Sum of electronic and thermal Enthalpies= -2729.154985
Sum of electronic and thermal Free Energies= -2729.278236

C	-2.30578300	-0.98849100	3.13829500
C	-1.63180300	-0.37788200	2.07950300
C	-1.86409800	0.94346000	1.73004200
C	-2.84815400	1.60799600	2.45179800
C	-3.59252600	1.01043400	3.46250800
C	-3.30558400	-0.30358900	3.82303600
C	-1.76071100	-2.37191800	3.38658500
C	-0.44230500	-2.43281300	2.58023100
C	-0.60642600	-1.32384200	1.49276300
H	-1.31978900	1.46393400	0.94508800
H	-4.35073500	1.58695000	3.97871200
H	-3.83760600	-0.77138100	4.64420400
H	-1.57335400	-2.57759700	4.44368400
H	-0.30907500	-3.40747500	2.10751500
H	-2.45698400	-3.13309300	3.01856200
H	-0.94577400	-1.79201500	0.57090200
N	0.64800800	-0.60878200	1.25118000
O	0.71812200	-2.26335900	3.37819900
C	1.10927900	0.10617100	0.19528500
C	1.39537400	-0.25881600	2.34642200
N	2.09386000	0.85064200	0.70201000
N	2.29209200	0.62467500	2.03712100
C	1.08975000	-0.92408600	3.65134600
H	0.29842300	-0.37982700	4.18384100
H	1.98231200	-0.94751500	4.27605000
C	2.86624400	1.91614500	0.10304300
C	4.17306100	1.65460600	-0.29513000
C	2.28180200	3.18285300	0.05782600
C	4.91755800	2.73275100	-0.77561500
C	3.06612600	4.22541800	-0.42725200
C	4.38417600	4.01963600	-0.84376400
H	5.93903600	2.55784700	-1.10436600
H	2.63655500	5.22249700	-0.48567100
C	0.85026800	3.38135700	0.46848700
H	0.19867300	2.83980700	-0.22799200
H	0.65853000	3.00796800	1.48078900
C	4.72422900	0.25815300	-0.24506300
H	4.69494600	-0.15123100	0.77059700
H	4.11559000	-0.39504200	-0.87500600

H	5.75639600	0.23281000	-0.59858500
H	0.57473600	4.43707700	0.44146300
C	5.22043300	5.17385000	-1.33311100
H	5.71126600	5.67815800	-0.49430300
H	6.00052100	4.83398700	-2.01779500
H	4.60574700	5.91540800	-1.84862600
N	-3.06956400	3.02597300	2.16547800
O	-4.18536900	3.47878800	2.35833700
O	-2.12114600	3.66919000	1.75470800
C	-4.73441800	-3.35909700	-1.84004600
C	-4.32744900	-2.33551500	-2.69220000
C	-2.98777000	-1.94921200	-2.72257800
C	-2.03467500	-2.58088200	-1.90407000
C	-2.46860900	-3.58343700	-1.03611900
C	-3.80665500	-3.97574500	-1.00648000
H	-5.77612900	-3.66193600	-1.81972100
H	-5.04566600	-1.82817500	-3.32890900
H	-1.75987100	-4.08360400	-0.38365300
H	-4.12036400	-4.76514900	-0.33135200
C	-0.61727000	-2.07146000	-1.99559100
C	0.42360700	-2.82666900	-1.22053500
H	-0.32410300	-2.11087900	-3.05788100
H	0.24847900	-3.82088600	-0.82644300
C	1.64702500	-2.28126700	-1.16151400
O	1.86372500	-1.05906500	-1.70812600
S	-2.44127200	-0.67929800	-3.83325900
C	0.79430800	0.05730000	-1.35992500
O	1.09761700	1.13542100	-1.93422400
C	-0.63121500	-0.55450000	-1.64367900
C	-1.33041700	0.30083100	-2.72376900
H	-1.23772800	-0.42884400	-0.74154000
H	-0.55745800	0.68659900	-3.39103600
C	-2.07414800	1.46649200	-2.10482400
C	-1.57956700	2.76483200	-2.23404400
C	-3.25064100	1.26161700	-1.37397800
C	-2.25139900	3.84052400	-1.65306600
H	-0.64490800	2.91833000	-2.76472400
C	-3.92090700	2.33314600	-0.79286200
H	-3.64753200	0.25420900	-1.26417800
C	-3.42382900	3.62903200	-0.93423600
H	-1.84886800	4.84361500	-1.75544100
H	-4.82847300	2.15819600	-0.22163800
H	-3.93629400	4.46069500	-0.46051100
C	2.83056700	-2.90559300	-0.51730700

C	4.04867600	-2.95901000	-1.20483400
C	2.75958800	-3.41463100	0.78194100
C	5.17017800	-3.52201000	-0.60627500
H	4.10771300	-2.55091100	-2.20972900
C	3.88513300	-3.97402400	1.38366500
H	1.82875600	-3.34678300	1.33658500
C	5.09113200	-4.03037700	0.69089400
H	6.10847300	-3.56338800	-1.15027600
H	3.81871700	-4.35569500	2.39757300
H	5.96889800	-4.46367700	1.15944700

M5S

Zero-point correction=	0.748862 (Hartree/Particle)
Thermal correction to Energy=	0.793515
Thermal correction to Enthalpy=	0.794459
Thermal correction to Gibbs Free Energy=	0.669162
Sum of electronic and zero-point Energies=	-2729.214914
Sum of electronic and thermal Energies=	-2729.170260
Sum of electronic and thermal Enthalpies=	-2729.169316
Sum of electronic and thermal Free Energies=	-2729.294613

C	-5.25057700	-0.10991800	-0.62759200
C	-3.91197200	-0.24307000	-0.26218500
C	-3.49781900	-1.19131400	0.66311800
C	-4.48757100	-2.00261000	1.20076300
C	-5.83589900	-1.89526800	0.86522100
C	-6.22222800	-0.93443900	-0.06114100
C	-5.42524800	0.98854200	-1.64219100
C	-3.99466600	1.33134600	-2.11680400
C	-3.04386300	0.74667200	-1.00971900
H	-2.45749600	-1.26305300	0.96464400
H	-6.55554200	-2.56236300	1.32273700
H	-7.26529400	-0.83797800	-0.34292600
H	-6.04807200	0.69829000	-2.49291600
H	-3.84336600	2.40624300	-2.21295900
H	-5.89178300	1.86393200	-1.17907300
H	-2.64207600	1.52430700	-0.36119500
N	-1.90597800	0.06915300	-1.63489400
O	-3.72551100	0.81980300	-3.41534000
C	-0.63729400	-0.09838500	-1.21640600
C	-2.08403700	-0.69100600	-2.75547700
N	-0.11216700	-0.96737700	-2.08384300
N	-1.00170200	-1.33997300	-3.06119500
C	-3.39279700	-0.55572500	-3.46479700
H	-4.16130000	-1.18545400	-2.99652300

H	-3.28903500	-0.84077700	-4.51136900
C	1.16958900	-1.61714400	-2.03216500
C	1.34434900	-2.61926700	-1.07398000
C	2.16417500	-1.21324900	-2.92467200
C	2.61478400	-3.18709300	-0.98026900
C	3.41285900	-1.81573600	-2.79012300
C	3.66041800	-2.78222500	-1.81141700
H	2.79078800	-3.94550900	-0.22200400
H	4.21921000	-1.50887900	-3.45226700
C	1.88793100	-0.18496600	-3.98925700
H	1.19305800	-0.58236900	-4.73507300
H	1.42804900	0.71782600	-3.57451400
C	0.22346900	-3.01077900	-0.14739200
H	-0.03265100	-2.19161100	0.53810000
H	-0.68000600	-3.26808900	-0.71081300
H	0.51396500	-3.86757000	0.46238300
H	2.81130900	0.09980300	-4.49648600
C	5.04653100	-3.34782400	-1.64926100
H	5.05579100	-4.18672300	-0.95095500
H	5.44773200	-3.68897400	-2.60733600
H	5.72279800	-2.57646900	-1.26596300
N	-4.08799100	-3.02614900	2.17372400
O	-4.96712300	-3.67966300	2.71023600
O	-2.89754500	-3.17181300	2.39269800
C	6.39045500	0.64778400	-0.02004000
C	5.58239800	0.76061000	1.10810900
C	4.22393200	1.05146000	0.96607700
C	3.66252000	1.22130600	-0.30717200
C	4.48231900	1.08314400	-1.42600700
C	5.84044400	0.80441600	-1.29082500
H	7.44649300	0.42584100	0.09543100
H	5.99933700	0.61750400	2.10031000
H	4.04511600	1.20316800	-2.41469200
H	6.46503400	0.70830300	-2.17317900
C	2.18787300	1.48755800	-0.43021000
C	1.73479700	2.85021900	0.02930700
H	1.90708600	1.36034800	-1.48749400
H	2.43322200	3.59275400	0.39529800
C	0.40836400	3.02492800	0.08611400
O	-0.41696800	2.03246600	-0.34621100
S	3.20797500	1.26013900	2.40459500
C	-0.15060900	0.58586800	0.11363700
O	-0.94498300	0.24715900	1.06054000
C	1.38501400	0.43501800	0.36600100

C	1.62995900	0.43999300	1.89490100
H	1.70117100	-0.54448000	0.00942400
H	0.85627200	1.04929600	2.36626300
C	1.54976800	-0.96942400	2.45262600
C	0.43761000	-1.37295300	3.19325400
C	2.56029300	-1.90047100	2.19079800
C	0.33494600	-2.68169300	3.66244000
H	-0.36545200	-0.66300000	3.36010900
C	2.46265800	-3.20575500	2.66346700
H	3.43226700	-1.59795300	1.61352800
C	1.34698800	-3.60148300	3.40140200
H	-0.54398000	-2.98263600	4.22379200
H	3.25864500	-3.91541400	2.45635200
H	1.26817100	-4.62005700	3.76819100
C	-0.29616200	4.21372000	0.61241100
C	-1.51304900	4.03929300	1.28103600
C	0.23581800	5.50005200	0.48066600
C	-2.18025400	5.13463400	1.81943700
H	-1.90339900	3.03132700	1.39257700
C	-0.43465100	6.59415700	1.01908400
H	1.16817900	5.64058800	-0.05846600
C	-1.64424000	6.41514400	1.68845500
H	-3.11919600	4.99005600	2.34470700
H	-0.01688600	7.58974600	0.90755500
H	-2.16779600	7.27020900	2.10402800

TS5R

Zero-point correction=			0.746815 (Hartree/Particle)
Thermal correction to Energy=			0.791410
Thermal correction to Enthalpy=			0.792354
Thermal correction to Gibbs Free Energy=			0.668057
Sum of electronic and zero-point Energies=			-2729.199048
Sum of electronic and thermal Energies=			-2729.154454
Sum of electronic and thermal Enthalpies=			-2729.153509
Sum of electronic and thermal Free Energies=			-2729.277806
C	-2.39829900	-1.09496700	3.11091000
C	-1.69600000	-0.43998600	2.09993900
C	-1.89693700	0.90216300	1.81753800
C	-2.88075300	1.54716700	2.55573200
C	-3.64968000	0.91161800	3.52556700
C	-3.39296900	-0.42481100	3.81986000
C	-1.89241800	-2.50536600	3.28203000
C	-0.59263400	-2.57825100	2.44228300
C	-0.67660900	-1.35747200	1.46555200

H	-1.32286600	1.44262500	1.06841600
H	-4.40642400	1.47376000	4.05949600
H	-3.94750800	-0.92361800	4.60740800
H	-1.68843000	-2.76215100	4.32540500
H	-0.54159700	-3.51018000	1.87582200
H	-2.62334700	-3.22695900	2.90243400
H	-0.99861300	-1.70816400	0.48463700
N	0.59815900	-0.67460200	1.33320500
O	0.59005600	-2.58324400	3.22647400
C	1.05465400	0.11873400	0.32200600
C	1.38560900	-0.51316400	2.44335700
N	2.11320500	0.70493300	0.90210600
N	2.34250400	0.32778100	2.20908700
C	1.04357400	-1.31119000	3.66079500
H	0.28034700	-0.79423000	4.25923200
H	1.92771400	-1.46959300	4.27802600
C	2.94883200	1.72500800	0.33599900
C	4.30758300	1.46240200	0.16256300
C	2.36846400	2.96421400	0.03651300
C	5.09679100	2.48313000	-0.37302300
C	3.19860400	3.94746400	-0.49290400
C	4.56168400	3.72410300	-0.70886300
H	6.15675200	2.29692900	-0.52902600
H	2.77220500	4.91739400	-0.73846300
C	0.90778200	3.22894400	0.28631500
H	0.29205900	2.65847700	-0.41725400
H	0.61898100	2.94725700	1.30481300
C	4.91966600	0.14757400	0.56504900
H	5.22142900	0.17337600	1.61712800
H	4.21731100	-0.67978200	0.44664300
H	5.80607400	-0.06267200	-0.03741300
H	0.68252100	4.28906200	0.15189100
C	5.43216700	4.82106400	-1.26589600
H	5.61360100	5.59244200	-0.51059200
H	6.40020500	4.43333400	-1.58963500
H	4.95245800	5.30748600	-2.11925200
N	-3.08487600	2.97744900	2.32416600
O	-4.19500400	3.43719100	2.53652100
O	-2.13204200	3.62548600	1.93090200
C	-4.74001700	-3.23277200	-1.70753400
C	-4.40388500	-2.21027400	-2.59084600
C	-3.07119500	-1.82414300	-2.73046000
C	-2.05568600	-2.45387000	-1.98961700
C	-2.41706400	-3.45607700	-1.08879100

C	-3.74788000	-3.84857200	-0.95065600
H	-5.77653700	-3.53533800	-1.60209000
H	-5.17185400	-1.70252400	-3.16601000
H	-1.65670000	-3.95347500	-0.49449000
H	-4.00520600	-4.63723100	-0.25125300
C	-0.64936200	-1.94501200	-2.19687600
C	0.44088900	-2.66851600	-1.46012300
H	-0.43415500	-2.02058400	-3.27583400
H	0.31555700	-3.67948800	-1.09048600
C	1.63811600	-2.08444000	-1.37463300
O	1.84256900	-0.83496900	-1.90723800
S	-2.61938600	-0.55359000	-3.88252100
C	0.81387000	0.13719000	-1.73597400
O	1.09013600	1.24811100	-2.15691800
C	-0.63003000	-0.43244100	-1.85657600
C	-1.43354500	0.43348000	-2.85967300
H	-1.11505900	-0.29976500	-0.88869800
H	-0.74050700	0.84288000	-3.59694900
C	-2.13286000	1.57827300	-2.15496900
C	-1.66944700	2.88518400	-2.30641400
C	-3.23099400	1.34298500	-1.31921900
C	-2.29060800	3.93987500	-1.63690200
H	-0.79927000	3.06812500	-2.92992300
C	-3.85481400	2.39424200	-0.65613500
H	-3.60339600	0.32881900	-1.18917700
C	-3.38421200	3.69839100	-0.81111300
H	-1.91082700	4.94971900	-1.75680100
H	-4.70489000	2.19588900	-0.00887600
H	-3.85716000	4.51228400	-0.27007100
C	2.85071500	-2.65509500	-0.74918400
C	4.07170100	-2.60093700	-1.43105200
C	2.80201000	-3.20704100	0.53411800
C	5.22375400	-3.10887500	-0.84217900
H	4.11044600	-2.15219600	-2.41880900
C	3.96164000	-3.70166400	1.12728600
H	1.86409400	-3.21911700	1.08257100
C	5.17232700	-3.65536900	0.44031700
H	6.16623300	-3.06913900	-1.37889600
H	3.91711100	-4.11394000	2.13035300
H	6.07558600	-4.03919500	0.90347700

TS6S

Zero-point correction=	0.747610 (Hartree/Particle)
Thermal correction to Energy=	0.792063

Thermal correction to Enthalpy= 0.793007
Thermal correction to Gibbs Free Energy= 0.668560
Sum of electronic and zero-point Energies= -2729.210437
Sum of electronic and thermal Energies= -2729.165984
Sum of electronic and thermal Enthalpies= -2729.165040
Sum of electronic and thermal Free Energies= -2729.289487

C	5.29112200	-0.47481300	-0.51191200
C	3.91267800	-0.64831600	-0.61402800
C	3.34733200	-1.84750400	-1.02157300
C	4.23187200	-2.87878000	-1.30756500
C	5.61662900	-2.74564300	-1.21901200
C	6.15352000	-1.52678800	-0.82071700
C	5.62197400	0.92262000	-0.05536800
C	4.27336800	1.54081400	0.39385000
C	3.16584500	0.59648900	-0.19536200
H	2.27221600	-1.96445400	-1.13413000
H	6.24834400	-3.59216500	-1.45682000
H	7.22879100	-1.40658200	-0.74184900
H	6.34648700	0.94817500	0.76430700
H	4.13982700	2.55327800	0.00859200
H	6.04797600	1.50123200	-0.88129400
H	2.64501800	1.06055800	-1.03242200
N	2.17518200	0.25784300	0.82634900
O	4.18860800	1.68566100	1.80389000
C	0.89319500	-0.15407000	0.67534700
C	2.57461900	0.02576100	2.11797400
N	0.59848300	-0.62750500	1.89364500
N	1.62221000	-0.51531500	2.81177500
C	3.94474000	0.48031700	2.50627900
H	4.69263300	-0.29030500	2.27113100
H	3.98844800	0.69676700	3.57361000
C	-0.60468000	-1.31627800	2.26018200
C	-0.87402900	-2.54135300	1.64131500
C	-1.46297300	-0.73136000	3.19770100
C	-2.08195800	-3.16577200	1.95707000
C	-2.65524500	-1.39633500	3.47996200
C	-2.98256100	-2.60801200	2.86518800
H	-2.32425400	-4.10975600	1.47563300
H	-3.34902600	-0.95345400	4.19056400
C	-1.11732400	0.58066900	3.85219500
H	-0.32567000	0.44801100	4.59499300
H	-0.74750000	1.30587000	3.11803600
C	0.08233000	-3.15409000	0.64945000
H	0.05605500	-2.63034800	-0.31439300

H	1.11367300	-3.10818600	1.01453800
H	-0.17349700	-4.20047800	0.47509200
H	-1.99211400	1.00286200	4.35011300
C	-4.27514200	-3.30732000	3.19766200
H	-4.55310000	-4.01607100	2.41451300
H	-4.18264900	-3.86424000	4.13562100
H	-5.08924400	-2.58861600	3.32287100
N	3.67728700	-4.17512700	-1.71345700
O	4.45724800	-5.05897100	-2.02631400
O	2.46484400	-4.30271800	-1.71149800
C	-5.70530700	3.08919300	-0.36453400
C	-4.94105100	2.70988900	-1.46463200
C	-3.72428000	2.05473400	-1.27694900
C	-3.26858200	1.75462300	0.01195100
C	-4.06489800	2.10876100	1.10215000
C	-5.27190000	2.77864300	0.92230800
H	-6.64824400	3.60444000	-0.51542400
H	-5.28890200	2.91152900	-2.47313300
H	-3.72256200	1.86063000	2.10507100
H	-5.87370200	3.05166900	1.78286700
C	-1.89701500	1.14233000	0.25241000
C	-0.88825500	2.26383200	0.28665400
H	-1.93869600	0.71863800	1.26176000
H	-1.07692400	3.07714100	0.98059500
C	0.19771200	2.31570900	-0.48672500
O	0.49617600	1.32942500	-1.39460700
S	-2.75992200	1.52144800	-2.66811000
C	-0.00113400	0.02763700	-1.13340200
O	0.45240300	-0.84690300	-1.87567400
C	-1.47696100	-0.00356100	-0.71180300
C	-2.34283800	-0.13741200	-1.97461700
H	-1.57393400	-0.95465300	-0.18389300
H	-1.72932800	-0.60381000	-2.75047900
C	-3.59161500	-0.97764800	-1.77812000
C	-4.26715700	-1.45355700	-2.90758800
C	-4.09140500	-1.30718400	-0.51554200
C	-5.40707000	-2.23789300	-2.78217700
H	-3.88930100	-1.19954300	-3.89496300
C	-5.23758100	-2.09177400	-0.38692600
H	-3.59353500	-0.96385300	0.38763500
C	-5.89873600	-2.55975400	-1.51681900
H	-5.91137400	-2.60200400	-3.67172400
H	-5.60967800	-2.33353500	0.60422800
H	-6.78905900	-3.17230800	-1.41677200

C	1.25376800	3.35069800	-0.42307000
C	1.94502800	3.71976300	-1.58398700
C	1.62046200	3.91934400	0.80105700
C	2.96378000	4.66527200	-1.52277300
H	1.67614000	3.26030900	-2.53004300
C	2.63868800	4.86699200	0.85915100
H	1.12639900	3.59199900	1.71130800
C	3.31004800	5.24487800	-0.30185000
H	3.48907500	4.95052600	-2.42853800
H	2.92110100	5.29547000	1.81530900
H	4.10840800	5.97837300	-0.25413100

PR

Zero-point correction= 0.359131 (Hartree/Particle)
Thermal correction to Energy= 0.379884
Thermal correction to Enthalpy= 0.380828
Thermal correction to Gibbs Free Energy= 0.307845
Sum of electronic and zero-point Energies= -1473.238198
Sum of electronic and thermal Energies= -1473.217445
Sum of electronic and thermal Enthalpies= -1473.216500
Sum of electronic and thermal Free Energies= -1473.289484

C	2.21192600	4.08363000	0.71497200
C	2.76252500	3.09888600	-0.10010100
C	1.94657300	2.09412800	-0.61961300
C	0.57284300	2.05909600	-0.33080600
C	0.04774900	3.02909600	0.52246300
C	0.85785500	4.04137200	1.03371500
H	2.84529900	4.86846600	1.11483400
H	3.82351100	3.09912600	-0.32923900
H	-1.00166400	3.00217700	0.79602500
H	0.42864700	4.79240800	1.68846900
C	-0.23029200	0.92139900	-0.92780200
C	-1.68157700	0.92312400	-0.56027900
H	-0.12862600	0.98630000	-2.02327500
H	-2.22377000	1.86033900	-0.54004000
C	-2.35828600	-0.20103100	-0.31847300
O	-1.78697800	-1.45755200	-0.47816100
S	2.63130100	0.85968600	-1.69302900
C	-0.46604000	-1.60177400	-0.75315500
O	-0.07717800	-2.67068500	-1.14120600
C	0.41778400	-0.40223600	-0.46591900
C	1.83334500	-0.66580400	-1.02217300
H	0.46751400	-0.35047500	0.63128200
H	1.73451300	-1.30159100	-1.90532300

C	2.70543600	-1.38141300	-0.01214900
C	3.02457600	-2.72577300	-0.20076600
C	3.17251300	-0.72419900	1.13085100
C	3.80189900	-3.40571900	0.73574100
H	2.64914000	-3.24220200	-1.07932200
C	3.94669000	-1.40201600	2.06580400
H	2.93561600	0.32696200	1.28200200
C	4.26434600	-2.74633600	1.87029600
H	4.04351200	-4.45174400	0.57608300
H	4.30516100	-0.88097000	2.94792400
H	4.86889900	-3.27469300	2.60037500
C	-3.78042500	-0.30070000	0.06568500
C	-4.50412300	-1.46809300	-0.20029200
C	-4.42103600	0.77212100	0.69773100
C	-5.85034200	-1.55103900	0.14246000
H	-4.01013100	-2.30480200	-0.68082200
C	-5.76685300	0.68679500	1.03295400
H	-3.85889500	1.66605000	0.94904700
C	-6.48643200	-0.47459900	0.75538700
H	-6.40298200	-2.45957400	-0.07312400
H	-6.25155400	1.52319300	1.52561000
H	-7.53568000	-0.54155500	1.02371200

PS

Zero-point correction=	0.358751 (Hartree/Particle)
Thermal correction to Energy=	0.379714
Thermal correction to Enthalpy=	0.380659
Thermal correction to Gibbs Free Energy=	0.306782
Sum of electronic and zero-point Energies=	-1473.239386
Sum of electronic and thermal Energies=	-1473.218423
Sum of electronic and thermal Enthalpies=	-1473.217478
Sum of electronic and thermal Free Energies=	-1473.291355

C	-3.95448900	3.44569900	-0.81457400
C	-3.77935900	2.10409200	-1.11895400
C	-2.75698300	1.36032400	-0.51382100
C	-1.90459800	1.97037800	0.41330500
C	-2.09406300	3.32782400	0.69833200
C	-3.10286100	4.06774800	0.09799300
H	-4.75127200	4.00495500	-1.29368200
H	-4.43427600	1.62025900	-1.83806500
H	-1.42940600	3.80172100	1.41719400
H	-3.22768900	5.11733700	0.34104800
C	-0.76238400	1.26101400	1.11894600
C	0.57633300	1.63577800	0.52657900

H	-0.78475400	1.59279300	2.16701100
H	0.66649600	2.55028400	-0.04730500
C	1.63425200	0.83195600	0.65304500
O	1.55828900	-0.36090400	1.36512700
S	-2.67182200	-0.35528100	-0.97263400
C	0.35773200	-0.87917000	1.74641000
O	0.35044600	-1.80391300	2.51095700
C	-0.87781300	-0.26896600	1.11600200
C	-1.02978500	-0.81808000	-0.32153700
H	-1.72494900	-0.60563000	1.71858500
H	-0.27573700	-0.34632200	-0.95828500
C	-0.86962200	-2.31821200	-0.40850600
C	0.24972300	-2.84833900	-1.05198700
C	-1.78867300	-3.18431300	0.19125900
C	0.44848400	-4.22637600	-1.10140800
H	0.96946800	-2.17705400	-1.51402800
C	-1.59081000	-4.55999600	0.14061300
H	-2.66154700	-2.77875300	0.69585700
C	-0.47241600	-5.08387200	-0.50630900
H	1.32168500	-4.62771700	-1.60531600
H	-2.30999400	-5.22532400	0.60713300
H	-0.32019200	-6.15756000	-0.54501400
C	2.98399500	1.04731400	0.09622600
C	3.82738400	-0.04370700	-0.14063600
C	3.42959100	2.33714300	-0.21548000
C	5.08636700	0.15321700	-0.70014100
H	3.49229700	-1.04365800	0.11198900
C	4.68699900	2.52845800	-0.77561000
H	2.80017900	3.19435200	0.00156000
C	5.51862900	1.43705200	-1.02223600
H	5.73046000	-0.70027700	-0.88520800
H	5.02308300	3.53337400	-1.00904300
H	6.50163000	1.58844400	-1.45602700

TS4S'

Zero-point correction=	0.746306 (Hartree/Particle)
Thermal correction to Energy=	0.790979
Thermal correction to Enthalpy=	0.791923
Thermal correction to Gibbs Free Energy=	0.667645
Sum of electronic and zero-point Energies=	-2729.181938
Sum of electronic and thermal Energies=	-2729.137266
Sum of electronic and thermal Enthalpies=	-2729.136321
Sum of electronic and thermal Free Energies=	-2729.260599

C	4.86824900	-0.38389900	-0.23970500

C	3.49555900	-0.56769300	-0.39756700
C	2.95427100	-1.81870900	-0.66263000
C	3.84706200	-2.87756500	-0.74619700
C	5.22477600	-2.73177100	-0.59630500
C	5.74127400	-1.46699400	-0.34416900
C	5.19725400	1.05864600	0.03233000
C	3.83697400	1.75970100	0.26672000
C	2.74077100	0.73054400	-0.20099900
H	1.89049500	-1.96166400	-0.81965000
H	5.86534400	-3.60142900	-0.67119500
H	6.81024700	-1.33062200	-0.21958400
H	5.85029600	1.19076200	0.90065000
H	3.74518400	2.67383400	-0.31976400
H	5.71106500	1.50316800	-0.82550400
H	2.23003000	1.05629400	-1.10755800
N	1.72407400	0.56205700	0.84176500
O	3.67498300	2.18698500	1.60975700
C	0.44363700	0.15601100	0.75074200
C	2.03926400	0.62312400	2.16931400
N	0.05603400	-0.05357300	2.00989400
N	1.04223100	0.25045200	2.91300200
C	3.39135300	1.14749500	2.52578600
H	4.14075100	0.34429900	2.48367000
H	3.38129200	1.57043900	3.52994600
C	-1.10419600	-0.77890500	2.45074300
C	-1.21581500	-2.11816600	2.05780600
C	-2.04681400	-0.12693400	3.25141400
C	-2.36663900	-2.79968800	2.45464500
C	-3.17489700	-0.85782700	3.61828800
C	-3.35661800	-2.18519400	3.22205100
H	-2.48898500	-3.83660000	2.15147900
H	-3.93450400	-0.37465500	4.22808500
C	-1.84270200	1.29010700	3.71615100
H	-1.18760500	1.30487800	4.59344200
H	-1.37223900	1.90796600	2.94565900
C	-0.16865700	-2.80317800	1.21577500
H	-0.26665000	-2.54353100	0.15329800
H	0.84443800	-2.54125800	1.53936500
H	-0.28036100	-3.88640400	1.28666900
H	-2.79855600	1.73393000	4.00101900
C	-4.59796400	-2.93391300	3.63093000
H	-4.60054300	-3.94795700	3.22718400
H	-4.67087300	-2.99842800	4.72045500
H	-5.49482200	-2.41952600	3.27434200

N	3.30617800	-4.21879800	-0.99758500
O	4.09751600	-5.13229800	-1.15907500
O	2.09419500	-4.34912500	-1.02662600
C	-5.55977700	3.45314000	-1.84870500
C	-5.37433400	2.10770900	-2.13172000
C	-4.26744000	1.41842800	-1.61806200
C	-3.33025900	2.08371600	-0.82193700
C	-3.52706500	3.44659000	-0.56457500
C	-4.62794100	4.13020000	-1.06018900
H	-6.42267800	3.97425800	-2.25061700
H	-6.08552300	1.57795000	-2.75902200
H	-2.79240900	3.96093200	0.05151900
H	-4.76020000	5.18400400	-0.83821500
C	-2.10102300	1.43085700	-0.23336400
C	-0.78946600	2.02181600	-0.72210100
H	-2.13038000	1.57267600	0.85463100
H	-0.70857000	2.12747600	-1.80019700
C	-0.04074900	2.91091900	0.11338300
O	-0.24863000	3.01242300	1.33809900
S	-4.16468400	-0.31968500	-1.97782400
C	-0.28773100	0.02226500	-0.56786700
O	0.39759500	-0.44089800	-1.50527900
C	-1.83951400	-0.05585000	-0.51447400
C	-2.36013000	-0.60435800	-1.84392100
H	-2.22167600	-0.71551100	0.26875100
H	-1.87109300	-0.09993500	-2.68152000
C	-2.11688200	-2.09898300	-1.93441600
C	-1.18011000	-2.60971400	-2.83522000
C	-2.77290000	-2.97968700	-1.06816300
C	-0.89104500	-3.97122400	-2.85780800
H	-0.65131600	-1.92614200	-3.49123200
C	-2.48771500	-4.34282300	-1.09313200
H	-3.50217800	-2.59432200	-0.35948700
C	-1.54086200	-4.84133600	-1.98489400
H	-0.14887200	-4.35273900	-3.55163500
H	-3.00291000	-5.01334800	-0.41176800
H	-1.30916700	-5.90150600	-1.99939300
C	1.12217700	3.67826400	-0.46977000
C	1.83309500	4.52245700	0.38930900
C	1.52437600	3.58118300	-1.80809400
C	2.91554200	5.26240300	-0.07483400
H	1.51887500	4.57486500	1.42548700
C	2.61523500	4.31198100	-2.27200800
H	0.99819500	2.92799400	-2.49681000

C	3.31036200	5.15797500	-1.40794700
H	3.45685000	5.91503900	0.60270800
H	2.92025400	4.22412000	-3.30973900
H	4.15693000	5.73127700	-1.77249800

M4S'

Zero-point correction= 0.747570 (Hartree/Particle)
Thermal correction to Energy= 0.792587
Thermal correction to Enthalpy= 0.793531
Thermal correction to Gibbs Free Energy= 0.667013
Sum of electronic and zero-point Energies= -2729.213272
Sum of electronic and thermal Energies= -2729.168256
Sum of electronic and thermal Enthalpies= -2729.167311
Sum of electronic and thermal Free Energies= -2729.293830

C	-4.87296100	-0.28426500	0.22189600
C	-3.49941400	-0.46446800	0.37182900
C	-2.95080000	-1.69267100	0.71432400
C	-3.84459600	-2.74449300	0.86424900
C	-5.22397300	-2.60591500	0.71628400
C	-5.74553600	-1.35799900	0.39861600
C	-5.19709300	1.14751500	-0.11236300
C	-3.83669100	1.81715700	-0.42443000
C	-2.74566200	0.81868600	0.10528800
H	-1.88263800	-1.79853200	0.88645000
H	-5.86350500	-3.46953000	0.84871400
H	-6.81630800	-1.22928100	0.28128300
H	-5.87751900	1.24857500	-0.96345800
H	-3.73029800	2.77869300	0.07928000
H	-5.67448100	1.63853000	0.74134100
H	-2.23878700	1.16926500	1.00110700
N	-1.72279800	0.59304700	-0.92563800
O	-3.69237200	2.12174900	-1.80428300
C	-0.43508400	0.20510300	-0.81954200
C	-2.07544800	0.50323300	-2.24347300
N	-0.08414300	-0.13962800	-2.06008900
N	-1.09537200	0.05472800	-2.96696900
C	-3.43390800	0.99728800	-2.62339300
H	-4.18759300	0.20865700	-2.49301100
H	-3.43985800	1.32330300	-3.66310800
C	1.07576400	-0.88507400	-2.46664700
C	1.17872300	-2.20391800	-2.00607000
C	2.01532900	-0.28026800	-3.30056900
C	2.31713000	-2.91481100	-2.37728700
C	3.13545300	-1.03950700	-3.64290800

C	3.30772400	-2.34552200	-3.18286900
H	2.43525900	-3.93500600	-2.02001600
H	3.89223500	-0.59461800	-4.28395400
C	1.81654100	1.11647100	-3.82595200
H	1.10315800	1.10947600	-4.65635900
H	1.41643800	1.78652500	-3.05923400
C	0.13119900	-2.80929900	-1.10732500
H	0.17127400	-2.37704400	-0.09758800
H	-0.87754900	-2.64686200	-1.50363100
H	0.29257400	-3.88331900	-1.00339300
H	2.76121500	1.52126800	-4.19318500
C	4.55000600	-3.12448300	-3.52796900
H	4.33125500	-4.18958500	-3.63261500
H	4.99526200	-2.76667500	-4.45859700
H	5.29947800	-3.01702500	-2.73715800
N	-3.30845200	-4.07146300	1.18786600
O	-4.10187300	-4.96857700	1.42074600
O	-2.09728600	-4.20987600	1.19944300
C	5.56890800	3.42022200	1.92401000
C	5.35729600	2.07693700	2.20307600
C	4.27761100	1.39233200	1.63057900
C	3.39582100	2.06199800	0.77471400
C	3.61750800	3.42075600	0.51967100
C	4.69152500	4.10014300	1.07884800
H	6.41037500	3.93703900	2.37396800
H	6.02665600	1.54602900	2.87391200
H	2.92957200	3.93798800	-0.14609000
H	4.84488000	5.15172700	0.86009400
C	2.20449700	1.40187200	0.13508900
C	0.83168200	1.88046300	0.62314500
H	2.25487000	1.54220600	-0.95158200
H	0.83946000	2.08853200	1.69354800
C	0.11913100	2.91108300	-0.17963500
O	0.39563000	3.08692100	-1.36285400
S	4.13264900	-0.34221500	1.99430600
C	0.31039900	0.29428400	0.52962500
O	-0.44138500	-0.16217900	1.48883400
C	1.85771200	-0.06418700	0.44348100
C	2.32475800	-0.59340300	1.79562500
H	2.18527200	-0.77309500	-0.31647500
H	1.81907300	-0.06216500	2.60542300
C	2.03597300	-2.07674000	1.91002100
C	1.00507700	-2.53020000	2.73546100
C	2.74183900	-3.00372800	1.13626900

C	0.68520200	-3.88440000	2.78506300
H	0.43108900	-1.80599600	3.30293400
C	2.42487700	-4.35897800	1.18899000
H	3.53938000	-2.66129900	0.48112400
C	1.39338900	-4.80309700	2.01299200
H	-0.13064600	-4.22158200	3.41628000
H	2.98290300	-5.06615700	0.58232800
H	1.13886900	-5.85764900	2.04991200
C	-1.01406700	3.67548400	0.43649000
C	-1.66572400	4.63252000	-0.35029700
C	-1.44985000	3.44948600	1.74758800
C	-2.72662400	5.36481400	0.16817500
H	-1.32291900	4.78314100	-1.36821200
C	-2.52343100	4.17251800	2.26102700
H	-0.97704100	2.68779900	2.36059400
C	-3.15633700	5.13548100	1.47614500
H	-3.22369200	6.10935600	-0.44476500
H	-2.86286900	3.98702200	3.27457600
H	-3.98684000	5.70412100	1.88236700

NHC-1

Zero-point correction= 0.383858 (Hartree/Particle)

Thermal correction to Energy= 0.404862

Thermal correction to Enthalpy= 0.405806

Thermal correction to Gibbs Free Energy= 0.332284

Sum of electronic and zero-point Energies= -1051.533150

Sum of electronic and thermal Energies= -1051.512145

Sum of electronic and thermal Enthalpies= -1051.511201

Sum of electronic and thermal Free Energies= -1051.584723

C	3.78441600	0.57427900	-0.36965900
C	2.93196400	0.62700500	0.73577200
C	2.74268500	1.80720000	1.44478500
C	3.43259500	2.94748400	1.03626700
C	4.29327000	2.89753600	-0.06252200
C	4.47499200	1.71208800	-0.77382700
C	3.78962000	-0.80567300	-0.97813100
C	3.22866000	-1.66851800	0.17351600
C	2.30425000	-0.72319500	0.98390900
H	2.06760600	1.83611900	2.29392100
H	4.82880600	3.79210100	-0.36453700
H	5.14512700	1.67897500	-1.62764500
H	3.13257400	-0.83102000	-1.85551600
H	4.05610000	-1.95042300	0.82926000
H	4.77747200	-1.14374600	-1.29849000

H	2.26360100	-0.99417600	2.04152500
N	0.94254400	-0.80294500	0.44567600
O	2.61667600	-2.88862100	-0.19067200
C	-0.10213300	0.00901900	0.80941600
C	0.53736700	-1.74142200	-0.46730800
N	-1.07829700	-0.51789400	0.04291300
N	-0.72112700	-1.59260300	-0.74830500
C	1.48669000	-2.75357200	-1.03032900
H	1.77629800	-2.47096400	-2.05061500
H	1.00416100	-3.73129600	-1.07674400
C	-2.43068000	-0.05252100	-0.00778100
C	-2.70239300	1.15713800	-0.65241600
C	-3.43324600	-0.83144800	0.57684200
C	-4.02865100	1.58776300	-0.69370700
C	-4.74495200	-0.36469800	0.50532100
C	-5.06006100	0.84221600	-0.12162500
H	-4.26129900	2.52526500	-1.19323500
H	-5.53908000	-0.95667500	0.95470300
C	-3.09543400	-2.12726400	1.26464200
H	-2.76231800	-2.87876500	0.54322000
H	-2.27910700	-1.98446400	1.97941300
C	-1.59570000	1.95882000	-1.28471700
H	-0.88129000	2.29924000	-0.53010000
H	-1.03565000	1.34912200	-2.00083000
H	-1.99964800	2.82742200	-1.80757700
H	-3.96342700	-2.51769700	1.79873100
C	-6.48218900	1.34052900	-0.15486600
H	-6.72048700	1.89238500	0.76024900
H	-6.64566100	2.01413900	-0.99911800
H	-7.18956700	0.51133700	-0.23148100
H	3.30413400	3.87960600	1.57677400

$TS1_{NHC-1}$

Zero-point correction= 0.740219 (Hartree/Particle)
Thermal correction to Energy= 0.784188
Thermal correction to Enthalpy= 0.785132
Thermal correction to Gibbs Free Energy= 0.661020
Sum of electronic and zero-point Energies= -2524.739888
Sum of electronic and thermal Energies= -2524.695920
Sum of electronic and thermal Enthalpies= -2524.694975
Sum of electronic and thermal Free Energies= -2524.819087

C	-6.18343800	-0.23346800	0.52154500
C	-5.02979700	0.47706600	0.17104100
C	-4.68371800	1.64637000	0.83754800

C	-5.48666600	2.07190700	1.89619400
C	-6.62216400	1.34975500	2.26481900
C	-6.98430200	0.19457300	1.57281300
C	-6.39931100	-1.39983500	-0.40408100
C	-5.55200600	-0.97900400	-1.62286400
C	-4.36972000	-0.15691000	-1.03554200
H	-3.79635700	2.19906800	0.55568000
H	-7.23843800	1.69875000	3.08755100
H	-7.88321400	-0.35247900	1.84043900
H	-6.02713600	-2.32459600	0.05161900
H	-6.13889300	-0.28594200	-2.23020500
H	-7.44607300	-1.56106800	-0.67044500
H	-3.97794600	0.56978100	-1.74853000
N	-3.26587200	-1.09388600	-0.70745400
O	-5.15983100	-2.00888900	-2.50067800
C	-2.07519500	-0.83809900	-0.08387600
C	-3.29325100	-2.41735900	-1.07907100
N	-1.48923800	-2.04424700	-0.08372400
N	-2.21884300	-3.03166400	-0.69556100
C	-4.40931900	-3.02322900	-1.87230900
H	-5.03514400	-3.65688800	-1.23247900
H	-3.98558100	-3.65005000	-2.65852700
C	-0.20384800	-2.41482100	0.43703500
C	0.01605300	-2.35473000	1.81567700
C	0.77110700	-2.83549300	-0.47286600
C	1.27493800	-2.73614200	2.27933300
C	2.00713000	-3.22190100	0.04519100
C	2.27675800	-3.17777500	1.41298100
H	1.47965600	-2.67874900	3.34571800
H	2.78153900	-3.55387100	-0.64198600
C	0.51276400	-2.84976700	-1.95605100
H	-0.12987000	-3.68923700	-2.23454300
H	0.01176100	-1.92911100	-2.27238700
C	-1.05154800	-1.86787300	2.75958300
H	-1.22871600	-0.79384900	2.63247100
H	-2.00120000	-2.38107900	2.58043500
H	-0.75204600	-2.04669000	3.79381100
H	1.45588000	-2.91912500	-2.49897200
C	3.62961900	-3.57946600	1.93949600
H	3.90311000	-2.98055900	2.81168600
H	3.63625400	-4.63254900	2.23975400
H	4.40015200	-3.44430600	1.17529200
C	-0.40605500	5.53079900	-0.46693300
C	-1.13420200	4.35852400	-0.64359300

C	-0.51027600	3.18996200	-1.08669600
C	0.87861400	3.19526400	-1.34676200
C	1.59450900	4.38634600	-1.16490100
C	0.96258200	5.54420900	-0.73030800
H	-0.90655300	6.43147300	-0.12656200
H	-2.19951700	4.33823600	-0.43772200
H	2.65661200	4.40125700	-1.39053400
H	1.53436700	6.45756700	-0.60342400
C	1.55530200	1.97149100	-1.78850400
C	2.83198900	1.63940800	-1.54507100
H	0.94799800	1.23894000	-2.31517600
H	3.48562500	2.27777700	-0.96023000
C	3.30636800	0.29472100	-1.96036000
O	2.53962700	-0.51959400	-2.45966100
S	-1.48919700	1.70684600	-1.26360200
C	-1.20888400	1.00405300	0.52943100
O	-1.83115700	1.50785400	1.44488600
C	0.21910200	0.58539100	0.66840100
C	0.89871100	1.05698000	1.72230100
H	0.67095700	0.00561900	-0.13118800
H	0.33901900	1.66541800	2.43079900
C	2.32059700	0.86364600	2.02568100
C	2.88402400	1.57711900	3.09291300
C	3.14007900	-0.01153500	1.29879500
C	4.22773200	1.43008100	3.42153500
H	2.25643400	2.25432000	3.66610300
C	4.48320700	-0.16044000	1.62732300
H	2.71438300	-0.59836800	0.48879000
C	5.03180000	0.56026200	2.68801500
H	4.64684200	1.99305700	4.24957000
H	5.10588500	-0.83683000	1.04753100
H	6.08103700	0.44220000	2.93997300
C	4.72340000	-0.09626700	-1.67642000
C	5.02736600	-1.46199400	-1.67650100
C	5.72214100	0.83108700	-1.36933300
C	6.30418700	-1.89889000	-1.34491100
H	4.23913000	-2.16371700	-1.92839000
C	7.00495700	0.39452200	-1.04957500
H	5.51227300	1.89526200	-1.38333900
C	7.29425200	-0.96816400	-1.02557000
H	6.52981300	-2.96039000	-1.33314800
H	7.77781300	1.11875100	-0.81447600
H	8.29163600	-1.30561700	-0.76246800
H	-5.22929100	2.97944200	2.43260200

$M1_{NHC-1}$

Zero-point correction=			0.741187 (Hartree/Particle)
Thermal correction to Energy=			0.786191
Thermal correction to Enthalpy=			0.787135
Thermal correction to Gibbs Free Energy=			0.661842
Sum of electronic and zero-point Energies=			-2524.771517
Sum of electronic and thermal Energies=			-2524.726513
Sum of electronic and thermal Enthalpies=			-2524.725569
Sum of electronic and thermal Free Energies=			-2524.850862
C	-6.06676500	-0.33990300	0.36645300
C	-4.92127200	0.28190800	-0.13896900
C	-4.73538600	1.65423400	-0.02391000
C	-5.69131500	2.39685100	0.66389900
C	-6.81643700	1.77334400	1.20877600
C	-7.01983400	0.40286800	1.05476400
C	-6.10107200	-1.79421500	-0.02837400
C	-5.17058800	-1.77481200	-1.25970300
C	-4.09560100	-0.70543200	-0.92720400
H	-3.85649900	2.12056400	-0.45751000
H	-7.55363300	2.36756800	1.73962100
H	-7.91497000	-0.07061700	1.44612400
H	-5.70419900	-2.42743100	0.77418400
H	-5.73146500	-1.37611900	-2.10825900
H	-7.09982600	-2.15815600	-0.27712300
H	-3.62953300	-0.26864600	-1.81076900
N	-2.98422800	-1.38707100	-0.18368100
O	-4.65943500	-3.00989800	-1.70030400
C	-1.83915200	-0.89355600	0.34146600
C	-2.83890000	-2.75331700	-0.18976800
N	-1.09802700	-1.95305800	0.66548100
N	-1.70496000	-3.12081600	0.33073300
C	-3.88144900	-3.67636000	-0.73722000
H	-4.49257100	-4.06910400	0.08513200
H	-3.38674400	-4.51471300	-1.22866600
C	0.20017700	-1.97761000	1.29207400
C	0.30422200	-1.64527500	2.64321400
C	1.29385100	-2.31408600	0.48769900
C	1.58801900	-1.62279200	3.18903900
C	2.55123300	-2.29237100	1.08703700
C	2.71584300	-1.93114200	2.42781100
H	1.70595800	-1.35862100	4.23677200
H	3.42380900	-2.55649200	0.49412100
C	1.11492000	-2.63447000	-0.97187900

H	0.42097300	-3.46679600	-1.11436800
H	0.70837200	-1.76839000	-1.51118300
C	-0.90126400	-1.29362700	3.47488000
H	-1.18360300	-0.24418700	3.33517500
H	-1.76658100	-1.90972000	3.21552800
H	-0.68234700	-1.43900200	4.53370500
H	2.07165400	-2.89468500	-1.42598400
C	4.09508600	-1.83494600	3.02284600
H	4.50581900	-0.83250800	2.85310400
H	4.07724300	-2.00886900	4.10083100
H	4.77727200	-2.55013500	2.55731100
C	-0.17886500	4.71768200	-1.31500800
C	-0.96408500	3.60086500	-1.57109400
C	-0.40026600	2.36881900	-1.95155600
C	1.01501600	2.30343600	-2.05576200
C	1.79299300	3.44194800	-1.79588700
C	1.21113100	4.64615300	-1.43075200
H	-0.65364300	5.65104700	-1.02533000
H	-2.04427800	3.66508400	-1.47748500
H	2.87306900	3.37324700	-1.89958300
H	1.82858900	5.51618500	-1.23294100
C	1.66046700	1.04743200	-2.43415400
C	2.87700300	0.64479800	-2.02110200
H	1.08885300	0.37395400	-3.06959600
H	3.43811500	1.24618400	-1.31468600
C	3.40038000	-0.66411200	-2.45960600
O	2.90281400	-1.27343900	-3.39861700
S	-1.42189800	0.95981100	-2.17329500
C	-1.50016400	0.52249300	0.76723500
O	-2.38568800	1.15332100	1.31799400
C	-0.08996800	0.91946300	0.71792600
C	0.28265000	2.04429400	1.34914000
H	0.60587700	0.31311200	0.14648100
H	-0.50066300	2.63771000	1.81875200
C	1.65075400	2.54719100	1.46941900
C	1.84760700	3.90111400	1.76965000
C	2.77098500	1.71298500	1.32944100
C	3.12999000	4.42429200	1.89421000
H	0.98159900	4.54730500	1.88435800
C	4.05216200	2.23489600	1.47565500
H	2.63464400	0.65034900	1.13358800
C	4.23625700	3.59132300	1.74846700
H	3.26619100	5.47832100	2.11329100
H	4.91597200	1.58032100	1.40376800

H	5.23854700	3.99118600	1.86235800
C	4.50780300	-1.30112500	-1.66868100
C	4.81049800	-2.64046300	-1.93990700
C	5.19218400	-0.64213900	-0.64244800
C	5.75747500	-3.31830900	-1.18161100
H	4.27684100	-3.13587400	-2.74444000
C	6.14904900	-1.31684800	0.11087700
H	4.98890500	0.39931800	-0.42361300
C	6.42520200	-2.65777100	-0.14931800
H	5.97637500	-4.36006300	-1.39178100
H	6.67447400	-0.79748600	0.90641700
H	7.16344800	-3.18562300	0.44599700
H	-5.56614700	3.46930800	0.77071400

$TS2R_{NHC-1}$

Zero-point correction= 0.741641 (Hartree/Particle)
Thermal correction to Energy= 0.784602
Thermal correction to Enthalpy= 0.785547
Thermal correction to Gibbs Free Energy= 0.664647
Sum of electronic and zero-point Energies= -2524.762183
Sum of electronic and thermal Energies= -2524.719221
Sum of electronic and thermal Enthalpies= -2524.718277
Sum of electronic and thermal Free Energies= -2524.839176

C	-0.53218200	-2.13761500	3.60715800
C	-0.61623000	-1.00110400	2.80655300
C	-1.07625300	0.21079600	3.31680200
C	-1.47861300	0.26317000	4.64835500
C	-1.41411100	-0.87877400	5.45074100
C	-0.93822600	-2.08324100	4.93812000
C	0.02915500	-3.30972600	2.84701800
C	0.48887600	-2.73655400	1.48588100
C	-0.12224200	-1.28804400	1.40420200
H	-1.11367300	1.10474700	2.69907100
H	-1.72931800	-0.82335100	6.48754900
H	-0.87648400	-2.96469900	5.56885600
H	0.87124100	-3.78741500	3.35787400
H	0.11071800	-3.33111200	0.65547300
H	-0.73130400	-4.08118100	2.69301400
H	-0.90840000	-1.26233300	0.64658400
N	0.90569100	-0.30725700	1.02261600
O	1.89432900	-2.75899100	1.31492300
C	0.83704000	0.88743000	0.40538100
C	2.19420300	-0.45488800	1.45581600
N	2.05012100	1.42877400	0.53728800

N	2.91073300	0.59473000	1.17796400
C	2.58495900	-1.76830400	2.05102000
H	2.34288400	-1.80451400	3.12190200
H	3.65459000	-1.93357400	1.91822200
C	2.47014100	2.76979600	0.21457700
C	3.54409000	2.94536500	-0.66300400
C	1.81740900	3.83329900	0.84751000
C	3.93455500	4.25606800	-0.93110600
C	2.24965000	5.12199600	0.53901600
C	3.29633600	5.35356800	-0.35270400
H	4.76210200	4.42095800	-1.61652500
H	1.75874400	5.96500500	1.01829700
C	0.70058900	3.62729100	1.83848900
H	-0.25671500	3.44746300	1.33596600
H	0.89925400	2.78026800	2.50295000
C	4.27357700	1.78571100	-1.28520000
H	3.58248200	1.00670900	-1.61471900
H	4.85997400	2.12903800	-2.13929100
H	4.96082100	1.33530900	-0.56137500
H	0.58274700	4.51861700	2.45662900
C	3.72081100	6.75710900	-0.69656900
H	3.22017400	7.09462300	-1.60971900
H	3.46178200	7.45560300	0.10193900
H	4.79762900	6.81184300	-0.87188400
C	-4.75076800	-2.48588700	-1.64837500
C	-4.39428500	-1.30089300	-2.26728500
C	-3.04429000	-0.91081000	-2.42556500
C	-2.04657800	-1.78164200	-1.89525600
C	-2.43622800	-2.98236900	-1.26617400
C	-3.76535400	-3.34111100	-1.13923900
H	-5.80094100	-2.74470200	-1.54850400
H	-5.16154100	-0.63498100	-2.65054300
H	-1.67211500	-3.64048800	-0.86089500
H	-4.03852500	-4.26665500	-0.64367600
C	-0.63495700	-1.42636800	-1.97996500
C	0.41842800	-2.25412100	-1.79216100
H	-0.42113600	-0.38654200	-2.22359500
H	0.28979300	-3.32206400	-1.64816100
C	1.78129900	-1.70499500	-1.74011000
O	1.98164700	-0.49184200	-1.70243800
S	-2.67204800	0.59284600	-3.21677700
C	-0.27321800	1.51127600	-0.42184300
O	0.10257200	2.24517400	-1.33006200
C	-1.62859500	1.20113700	-0.09281400

C	-2.63139100	1.80411800	-0.81663200
H	-1.85720200	0.51510900	0.71008800
H	-2.35079200	2.63156100	-1.45957000
C	-4.05561200	1.64463000	-0.51769800
C	-4.96643700	2.59220600	-1.00865900
C	-4.54078900	0.57725300	0.25019300
C	-6.32010200	2.49161200	-0.71993100
H	-4.59797700	3.40678500	-1.62618400
C	-5.89808100	0.47674500	0.54001800
H	-3.86067800	-0.19362300	0.60221100
C	-6.78943500	1.43322300	0.06016900
H	-7.01240700	3.23363900	-1.10391800
H	-6.26039500	-0.35826300	1.13117700
H	-7.84808900	1.35129300	0.28480000
C	2.94017100	-2.64766000	-1.66680100
C	4.13078500	-2.18210500	-1.09775000
C	2.87063300	-3.95711800	-2.14719800
C	5.23267500	-3.02170600	-0.99498200
H	4.16882400	-1.15939600	-0.73164200
C	3.98172500	-4.79233200	-2.06025400
H	1.96065600	-4.32208800	-2.61301400
C	5.15911800	-4.32876900	-1.47881400
H	6.15088500	-2.66011600	-0.54331600
H	3.92718600	-5.80451300	-2.44706100
H	6.02127900	-4.98387900	-1.40515000
H	-1.84099200	1.19692200	5.06454000

$TS2S_{NHC-1}$

Zero-point correction= 0.740671 (Hartree/Particle)
Thermal correction to Energy= 0.784768
Thermal correction to Enthalpy= 0.785712
Thermal correction to Gibbs Free Energy= 0.663037
Sum of electronic and zero-point Energies= -2524.768703
Sum of electronic and thermal Energies= -2524.724606
Sum of electronic and thermal Enthalpies= -2524.723662
Sum of electronic and thermal Free Energies= -2524.846337

C	-4.85046300	2.34359600	-1.14272500
C	-3.46592200	2.25433100	-1.02036100
C	-2.67251000	3.39141800	-0.90425300
C	-3.29445700	4.63733500	-0.90598100
C	-4.68276100	4.73449200	-1.02942900
C	-5.46906700	3.59106100	-1.15186200
C	-5.47480200	0.97757500	-1.26609200
C	-4.35229000	-0.01428200	-0.88959900

C	-3.02177700	0.80655100	-1.02509400
H	-1.59276800	3.30728400	-0.82622600
H	-5.15358000	5.71240400	-1.02816700
H	-6.54791100	3.67092300	-1.24518500
H	-6.33797300	0.83146300	-0.61014600
H	-4.30582600	-0.87379400	-1.55750500
H	-5.81033900	0.79725000	-2.29254000
H	-2.47639800	0.52023600	-1.92263100
N	-2.13458800	0.55086200	0.12546800
O	-4.55697000	-0.58367400	0.39634900
C	-0.80226700	0.66977700	0.26713400
C	-2.65579800	0.36514900	1.37324900
N	-0.57389000	0.56306400	1.58076600
N	-1.72070600	0.36139100	2.28298300
C	-4.13424900	0.18918200	1.49399600
H	-4.62510800	1.17262500	1.52924400
H	-4.37031500	-0.36308000	2.40422500
C	0.66802400	0.80528900	2.27344400
C	1.15496900	2.11493400	2.29769500
C	1.35192100	-0.28276100	2.81727000
C	2.41342600	2.30984400	2.86219800
C	2.60711000	-0.03268900	3.36960500
C	3.15963500	1.24963300	3.38088000
H	2.82636500	3.31508300	2.88493300
H	3.17122300	-0.86362900	3.78472200
C	0.76938600	-1.66673000	2.76124700
H	-0.14109500	-1.73373200	3.36518400
H	0.50607600	-1.92221900	1.72876800
C	0.39031900	3.26262800	1.69318700
H	0.57575300	3.32116200	0.61393200
H	-0.68798000	3.16611700	1.85049400
H	0.71629600	4.20632700	2.13278600
H	1.48564100	-2.40332400	3.12761100
C	4.54916500	1.48790100	3.90800600
H	5.24745900	1.60881900	3.07287900
H	4.59266000	2.40007600	4.50784400
H	4.89304000	0.65065900	4.51814400
C	4.92236000	-2.83285500	-0.73250900
C	4.49424200	-2.07013200	-1.80345200
C	3.12471000	-1.81377800	-2.05096800
C	2.18486000	-2.37513700	-1.13266200
C	2.64766000	-3.14465900	-0.04484000
C	3.99363900	-3.37623200	0.16562700
H	5.98558800	-2.99767200	-0.58233100

H	5.22041500	-1.63452800	-2.48322100
H	1.92565200	-3.57232600	0.64495000
H	4.32257600	-3.97163800	1.01084100
C	0.75814400	-2.17527100	-1.33785900
C	-0.26499500	-2.72199000	-0.64055600
H	0.49277200	-1.52779000	-2.17270200
H	-0.11141800	-3.41870600	0.17764900
C	-1.65166900	-2.45072400	-1.03890700
O	-1.94625700	-1.80286100	-2.04274100
S	2.67897000	-0.79692300	-3.39402400
C	0.17108800	0.97609600	-0.85909100
O	-0.32925600	1.44433600	-1.88008000
C	1.55807600	0.74641600	-0.60534900
C	2.49597700	1.21242900	-1.48574300
H	1.84614800	0.20702300	0.28460200
H	2.15135700	1.80235200	-2.32969200
C	3.93109000	1.23845300	-1.19934000
C	4.77798900	1.97778800	-2.03784400
C	4.48628500	0.57994400	-0.09243000
C	6.13734200	2.07203100	-1.77322800
H	4.35485900	2.47278400	-2.90778100
C	5.84913300	0.67366900	0.17198500
H	3.86123700	-0.02481200	0.55971000
C	6.67695500	1.42120900	-0.66267000
H	6.77790000	2.65099000	-2.43033900
H	6.26723800	0.14889100	1.02570500
H	7.73967300	1.49200000	-0.45399300
C	-2.74386700	-2.99190700	-0.17002600
C	-3.94007700	-3.40274000	-0.76334900
C	-2.61740700	-3.01014500	1.22096800
C	-5.00018600	-3.82794700	0.02699500
H	-4.02196300	-3.38200600	-1.84602900
C	-3.69099700	-3.40710400	2.01414300
H	-1.69111900	-2.68355500	1.68668900
C	-4.88016100	-3.81869500	1.41699400
H	-5.92417800	-4.15977100	-0.43560400
H	-3.59714000	-3.39925000	3.09545000
H	-5.71394800	-4.13753100	2.03442000
H	-2.69691600	5.53831300	-0.81547800

$M2R_{NHC-1}$

Zero-point correction= 0.742517 (Hartree/Particle)

Thermal correction to Energy= 0.786621

Thermal correction to Enthalpy= 0.787565

Thermal correction to Gibbs Free Energy= 0.664033
Sum of electronic and zero-point Energies= -2524.771066
Sum of electronic and thermal Energies= -2524.726962
Sum of electronic and thermal Enthalpies= -2524.726018
Sum of electronic and thermal Free Energies= -2524.849550

C	-0.62135400	-2.49613000	3.26009600
C	-0.53109700	-1.28275300	2.58119600
C	-0.86614500	-0.08014700	3.19733200
C	-1.31861600	-0.11390300	4.51458900
C	-1.42716400	-1.32875200	5.19481000
C	-1.07750300	-2.52688800	4.57452300
C	-0.17194700	-3.63993800	2.38726600
C	0.52963000	-2.97206500	1.18390300
C	-0.01299700	-1.49957600	1.17321700
H	-0.77635500	0.86436100	2.66633700
H	-1.77819100	-1.33812800	6.22158600
H	-1.14786200	-3.46767600	5.11195300
H	0.51775600	-4.32529700	2.88770800
H	0.28172400	-3.46763900	0.24328500
H	-1.02991700	-4.22850500	2.04536900
H	-0.79028300	-1.39511800	0.41265400
N	1.05167700	-0.54540900	0.85305100
O	1.94254200	-3.06636900	1.26219800
C	1.03669300	0.67734600	0.27406500
C	2.31272400	-0.74999500	1.34497900
N	2.27525300	1.15121100	0.44613300
N	3.08396900	0.26689900	1.10654300
C	2.59762500	-2.05959800	2.00601500
H	2.26459300	-2.03691300	3.05301200
H	3.66737000	-2.26839100	1.97423700
C	2.77189100	2.48054500	0.19067700
C	3.79476900	2.64507600	-0.74407300
C	2.24976100	3.53546900	0.94390300
C	4.28877300	3.93556000	-0.93007900
C	2.77827800	4.80499400	0.71864500
C	3.79519600	5.02421000	-0.21158000
H	5.07717900	4.09121800	-1.66210800
H	2.38558900	5.64360800	1.28859500
C	1.15768800	3.32577300	1.95919200
H	0.18702100	3.18645700	1.47016100
H	1.34978000	2.44208500	2.57710400
C	4.33775400	1.48195000	-1.52664300
H	4.92267200	0.82058900	-0.87849800
H	3.52514400	0.89252800	-1.96124200

H	4.98982500	1.83449200	-2.32764600
H	1.08403800	4.19144300	2.61929700
C	4.36756000	6.40394600	-0.40958800
H	5.15038600	6.60581700	0.32883500
H	4.81206300	6.50888600	-1.40156100
H	3.59824100	7.17043700	-0.29123600
C	-5.21168900	-1.62684000	-2.37508500
C	-4.68192300	-0.34705100	-2.47466600
C	-3.29796100	-0.13437500	-2.47652600
C	-2.42002900	-1.23888700	-2.37252700
C	-2.98084100	-2.52460600	-2.26835100
C	-4.35312600	-2.72094000	-2.26798700
H	-6.28713500	-1.77077300	-2.37594400
H	-5.33811200	0.51486800	-2.53928200
H	-2.32873300	-3.38930600	-2.20220100
H	-4.75444200	-3.72594400	-2.18963100
C	-0.96353000	-1.05256700	-2.38255700
C	-0.04371800	-2.01629600	-2.17953400
H	-0.59799700	-0.04425100	-2.56566300
H	-0.32773900	-3.04223200	-1.97673600
C	1.38829000	-1.65919300	-2.13081200
O	1.76049800	-0.50239400	-2.29879500
S	-2.71349200	1.53769100	-2.58559300
C	-0.04998500	1.42539800	-0.46307400
O	0.35175100	2.26855400	-1.30247600
C	-1.35387100	1.13898900	-0.11123100
C	-2.43053100	1.93884300	-0.73061800
H	-1.60238400	0.42423800	0.65760400
H	-2.09436100	2.97500600	-0.85482500
C	-3.75388600	1.89441400	-0.01567800
C	-4.54206900	3.04656700	0.06815200
C	-4.23879000	0.71107500	0.55182100
C	-5.77669800	3.02297100	0.70886000
H	-4.17926800	3.97006000	-0.37626200
C	-5.47586100	0.68349100	1.19131500
H	-3.65343900	-0.20217800	0.47942700
C	-6.24807700	1.83917500	1.27450900
H	-6.37069400	3.92965800	0.76776000
H	-5.83715300	-0.24501200	1.62252300
H	-7.21065500	1.81814600	1.77552800
C	2.38393800	-2.71961200	-1.77599000
C	3.62946100	-2.30202600	-1.29389100
C	2.10778900	-4.08664900	-1.86927300
C	4.57399500	-3.23343300	-0.88410800

H	3.82914900	-1.23734700	-1.22899100
C	3.05922300	-5.02045400	-1.46907400
H	1.16242500	-4.43597600	-2.27147200
C	4.28657100	-4.59597100	-0.96608900
H	5.53301700	-2.90031300	-0.49997800
H	2.84163900	-6.08034400	-1.54965100
H	5.02202300	-5.32639100	-0.64384900
H	-1.58484400	0.81068400	5.01560800

$M2S_{NHC-1}$

Zero-point correction= 0.742109 (Hartree/Particle)
Thermal correction to Energy= 0.786141
Thermal correction to Enthalpy= 0.787085
Thermal correction to Gibbs Free Energy= 0.664404
Sum of electronic and zero-point Energies= -2524.780266
Sum of electronic and thermal Energies= -2524.736234
Sum of electronic and thermal Enthalpies= -2524.735289
Sum of electronic and thermal Free Energies= -2524.857971

C	4.84668900	-2.39891100	-1.01095200
C	3.45822400	-2.31498900	-0.94421600
C	2.66308600	-3.45136300	-0.83295500
C	3.29230700	-4.69289300	-0.77398100
C	4.68534400	-4.78602200	-0.83481600
C	5.47167100	-3.64229900	-0.95972200
C	5.46366800	-1.03087800	-1.15554300
C	4.32557200	-0.04378800	-0.81613100
C	3.00493100	-0.87025600	-0.99417400
H	1.58137900	-3.35213600	-0.82352100
H	5.16001000	-5.76098200	-0.78451000
H	6.55378000	-3.71947100	-1.00875900
H	6.31623800	-0.86042800	-0.49187800
H	4.30262600	0.82053200	-1.48016900
H	5.81042300	-0.87133400	-2.18209600
H	2.48693500	-0.61977000	-1.91949700
N	2.07312800	-0.59136100	0.10698000
O	4.49055100	0.51791800	0.48076400
C	0.73112900	-0.67469900	0.16379000
C	2.52886100	-0.38759300	1.37852100
N	0.43070900	-0.51990200	1.46127900
N	1.54778900	-0.32916600	2.23108500
C	4.00353000	-0.24142100	1.56381100
H	4.47389100	-1.23351400	1.62227700
H	4.21527600	0.31137000	2.47974700
C	-0.83693500	-0.74395700	2.11040900

C	-1.32835500	-2.05185200	2.15659100
C	-1.51244100	0.34533800	2.66185300
C	-2.55888000	-2.24743100	2.78029100
C	-2.73802900	0.09560600	3.27970700
C	-3.27514300	-1.19097000	3.34614400
H	-2.97034700	-3.25284100	2.82097900
H	-3.28655100	0.92931700	3.71092800
C	-0.94849000	1.73519400	2.55811700
H	-0.02696600	1.82978900	3.14173100
H	-0.70818300	1.96925700	1.51457400
C	-0.58518000	-3.19818900	1.52563100
H	-0.73185700	-3.19292500	0.43922700
H	0.49064100	-3.13910000	1.71954600
H	-0.95199700	-4.14958500	1.91339500
H	-1.66673600	2.47248100	2.91996000
C	-4.59243000	-1.44444800	4.03167300
H	-5.14445500	-2.24473800	3.53284100
H	-4.43337600	-1.75009900	5.07092200
H	-5.21340500	-0.54570200	4.04119300
C	-4.86812500	3.09710200	-0.69076300
C	-4.47738300	2.15875900	-1.63887800
C	-3.12435800	1.92537400	-1.90605300
C	-2.13480100	2.64794400	-1.19804300
C	-2.55470600	3.59286300	-0.24703600
C	-3.89981600	3.81648600	0.00810600
H	-5.92249800	3.26489200	-0.49727100
H	-5.22141000	1.58416100	-2.18115300
H	-1.81275300	4.17231500	0.29325400
H	-4.19371900	4.55481600	0.74696500
C	-0.70707300	2.41289900	-1.44321900
C	0.31851500	2.90625000	-0.72474100
H	-0.45859200	1.76818100	-2.28190900
H	0.17540800	3.55619800	0.13249800
C	1.70872200	2.56910900	-1.09156800
O	1.99372100	1.95696100	-2.11573200
S	-2.71306700	0.67674700	-3.10678800
C	-0.16141900	-0.98473100	-1.01119300
O	0.38253700	-1.65982700	-1.93657200
C	-1.44208700	-0.51088400	-0.89024400
C	-2.46111400	-0.79385100	-1.91823800
H	-1.70614600	0.10599200	-0.04295000
H	-2.06975900	-1.54931600	-2.60669000
C	-3.81048700	-1.21784900	-1.38501600
C	-4.64941500	-2.00689600	-2.18005700

C	-4.26040500	-0.83166900	-0.11927800
C	-5.90171100	-2.40390800	-1.72507200
H	-4.31103600	-2.30875200	-3.16844200
C	-5.51826300	-1.22332100	0.33716300
H	-3.63005400	-0.22928500	0.52863100
C	-6.34277300	-2.01050500	-0.46135800
H	-6.53363200	-3.02284000	-2.35439600
H	-5.85006900	-0.90892700	1.32274300
H	-7.31963600	-2.31961200	-0.10334700
C	2.78877600	2.99643000	-0.15115400
C	4.03356200	3.36202800	-0.66924000
C	2.59260500	2.96211100	1.23148900
C	5.07405000	3.69184300	0.18933900
H	4.16813100	3.38269900	-1.74667700
C	3.64539100	3.26367200	2.09145400
H	1.62915200	2.66316300	1.63684300
C	4.88323400	3.63218300	1.57011000
H	6.03692600	3.98967100	-0.21302500
H	3.49762300	3.21468000	3.16569300
H	5.70087400	3.87863500	2.24011100
H	2.69677500	-5.59585800	-0.68559900

$TS3R_{NHC-1}$

Zero-point correction= 0.743161 (Hartree/Particle)
Thermal correction to Energy= 0.785822
Thermal correction to Enthalpy= 0.786766
Thermal correction to Gibbs Free Energy= 0.668520
Sum of electronic and zero-point Energies= -2524.749113
Sum of electronic and thermal Energies= -2524.706452
Sum of electronic and thermal Enthalpies= -2524.705507
Sum of electronic and thermal Free Energies= -2524.823754

C	-2.17038900	-0.92349900	3.44880600
C	-1.67101100	-0.25426200	2.33327100
C	-1.89815100	1.10891700	2.14657600
C	-2.64270700	1.79507400	3.10265700
C	-3.14605800	1.12796900	4.22169200
C	-2.91488400	-0.23381700	4.40192700
C	-1.80382600	-2.38449300	3.42857500
C	-0.79156800	-2.53916500	2.27033000
C	-0.89189700	-1.20362700	1.44507300
H	-1.51365000	1.64103700	1.27842500
H	-3.72049000	1.67734900	4.96049000
H	-3.30348100	-0.74886200	5.27517300
H	-1.35463700	-2.73124700	4.36443000

H	-1.04910900	-3.38015600	1.62386100
H	-2.68538500	-3.00591800	3.24371000
H	-1.38641400	-1.42275900	0.50172100
N	0.44475300	-0.64790900	1.14934100
O	0.51652600	-2.84165200	2.72538800
C	0.86785800	0.28385800	0.25806000
C	1.43510200	-0.78103400	2.08388200
N	2.07718500	0.65515800	0.69153800
N	2.44486700	-0.00680200	1.82003900
C	1.23745400	-1.73273300	3.21770900
H	0.70758600	-1.23339000	4.04121200
H	2.20224100	-2.08835200	3.57908800
C	2.93611800	1.73198000	0.25212900
C	4.10936300	1.40831700	-0.42235900
C	2.58273000	3.03278100	0.61733700
C	4.95985300	2.46457200	-0.75242200
C	3.46524800	4.04931300	0.26375000
C	4.65649100	3.78370400	-0.41747000
H	5.88053600	2.24570500	-1.28710600
H	3.21712800	5.07470800	0.52685500
C	1.28611100	3.32275000	1.32386100
H	0.44571900	3.21555100	0.62741600
H	1.11841500	2.64033000	2.16401200
C	4.40703800	-0.01266100	-0.80848100
H	4.39601600	-0.67672200	0.06242200
H	3.64367400	-0.37943200	-1.50376500
H	5.38634800	-0.08679000	-1.28526400
H	1.27761200	4.34377900	1.70860400
C	5.60354700	4.90514500	-0.75781300
H	6.20258300	5.18254400	0.11551400
H	6.29024000	4.61429500	-1.55533600
H	5.05824200	5.79646900	-1.07759400
C	-5.17217500	-2.49501100	-1.78227400
C	-4.75939300	-1.33749100	-2.43185000
C	-3.40111900	-1.02376700	-2.53155700
C	-2.42464300	-1.87321900	-1.97020900
C	-2.86988300	-3.02531100	-1.30496400
C	-4.22119300	-3.33792800	-1.21296100
H	-6.22889100	-2.73134800	-1.71505300
H	-5.48869500	-0.65950200	-2.86449100
H	-2.14555100	-3.71412300	-0.88448900
H	-4.52872200	-4.24449500	-0.70226300
C	-0.97853800	-1.54213900	-2.07479400
C	0.00093800	-2.35603100	-1.48810600

H	-0.67808500	-1.04109300	-2.99350400
H	-0.24547500	-3.14993400	-0.79404400
C	1.36571300	-2.06660900	-1.75643300
O	1.71349800	-1.09251800	-2.45728900
S	-2.93876800	0.42997700	-3.43302900
C	0.19127600	0.88283400	-0.95385100
O	0.82351100	1.76142900	-1.55095700
C	-1.12183300	0.41345700	-1.26085200
C	-1.85508000	1.31358000	-2.22184100
H	-1.73589200	0.11681000	-0.42052900
H	-1.11347700	1.80719300	-2.85378000
C	-2.57778800	2.36050900	-1.39503500
C	-1.89531000	3.54196500	-1.08510600
C	-3.82241700	2.12132000	-0.80746100
C	-2.44318500	4.46255100	-0.19381300
H	-0.91984700	3.71836000	-1.53090800
C	-4.37202500	3.04471900	0.07842600
H	-4.35818700	1.20413200	-1.03944900
C	-3.68369000	4.21617200	0.39145200
H	-1.90095300	5.37380900	0.03977300
H	-5.33872000	2.84656400	0.53116900
H	-4.11277200	4.93261600	1.08487300
C	2.44186300	-2.91965200	-1.14339800
C	3.65297600	-3.06740700	-1.82736500
C	2.29568500	-3.51220600	0.11299900
C	4.69345500	-3.80207700	-1.27031200
H	3.76342900	-2.58735700	-2.79505400
C	3.34486400	-4.23043300	0.68297700
H	1.37364500	-3.39073900	0.67104400
C	4.54381400	-4.38099600	-0.00876300
H	5.62630900	-3.91864300	-1.81319600
H	3.22226200	-4.66823600	1.66916900
H	5.36089900	-4.94316000	0.43240400
H	-2.83247400	2.85466400	2.96736700

$TS3S_{NHC-1}$

Zero-point correction= 0.742294 (Hartree/Particle)
Thermal correction to Energy= 0.785203
Thermal correction to Enthalpy= 0.786148
Thermal correction to Gibbs Free Energy= 0.666689
Sum of electronic and zero-point Energies= -2524.761615
Sum of electronic and thermal Energies= -2524.718705
Sum of electronic and thermal Enthalpies= -2524.717761
Sum of electronic and thermal Free Energies= -2524.837220

C	4.98000400	-2.06102100	-1.15848200
C	3.59023300	-1.96905100	-1.16975900
C	2.78977400	-3.09622800	-1.33300400
C	3.41016100	-4.33595400	-1.46779700
C	4.80369600	-4.43665900	-1.44959800
C	5.59737300	-3.30149500	-1.30098900
C	5.61501200	-0.70314500	-1.00355300
C	4.45607900	0.24424400	-0.61910300
C	3.14388600	-0.53363000	-0.98665600
H	1.70913200	-2.99708700	-1.37298900
H	5.27219400	-5.41002300	-1.55502000
H	6.68015300	-3.38302000	-1.29087900
H	6.39536000	-0.67108600	-0.23714300
H	4.47759600	1.18242400	-1.17233500
H	6.07128900	-0.38069000	-1.94500900
H	2.65777400	-0.10111100	-1.86038100
N	2.17929800	-0.44299900	0.11942600
O	4.52613900	0.64364700	0.74235600
C	0.84090500	-0.51144700	0.12279800
C	2.58897600	-0.46930700	1.42005700
N	0.48961600	-0.62342000	1.40892200
N	1.57680100	-0.58690700	2.23346600
C	4.05053200	-0.29359900	1.68176400
H	4.57023300	-1.25991700	1.61092000
H	4.20180500	0.12491100	2.67713400
C	-0.79011400	-1.02581400	1.94761600
C	-1.28687300	-2.28719500	1.60188700
C	-1.46282100	-0.14877400	2.80348700
C	-2.51382100	-2.66000300	2.15012700
C	-2.68183700	-0.57427100	3.32515500
C	-3.21963900	-1.82447900	3.01332700
H	-2.93089300	-3.62791300	1.88383400
H	-3.22868300	0.09298800	3.98659900
C	-0.91214800	1.21616400	3.10782400
H	-1.59952200	1.77539500	3.74367300
H	0.05683700	1.15144700	3.61168800
C	-0.56779100	-3.21953000	0.66234200
H	-0.78049800	-2.96439200	-0.38295600
H	0.51728000	-3.19478000	0.80385900
H	-0.90486200	-4.24439500	0.82533000
H	-0.76620300	1.77558000	2.17684300
C	-4.52672300	-2.26679300	3.61489200
H	-5.22238500	-1.42854400	3.70329100
H	-4.99491800	-3.04287800	3.00598800

H	-4.36889300	-2.67270800	4.61947700
C	-5.06207400	3.47936400	-1.13639300
C	-4.68375600	2.50511400	-2.05124400
C	-3.36831400	2.03518800	-2.08093700
C	-2.40112400	2.53779800	-1.18519000
C	-2.81688900	3.49833300	-0.25117000
C	-4.12541400	3.96599000	-0.22549500
H	-6.08388200	3.84397200	-1.12229900
H	-5.40760900	2.08568100	-2.74245400
H	-2.09698600	3.91294800	0.44510200
H	-4.41190400	4.71960900	0.50100300
C	-0.99006100	2.07907100	-1.25455000
C	-0.00718900	2.59118500	-0.38640300
H	-0.63773400	1.85941800	-2.26158100
H	-0.25853800	3.09522300	0.53758400
C	1.35345500	2.44627200	-0.74263600
O	1.73696400	1.89129600	-1.80057900
S	-2.94184300	0.73051300	-3.19383600
C	-0.04525700	-0.55150100	-1.09696400
O	0.42280300	-1.12505600	-2.09008100
C	-1.33205400	0.04100900	-0.95821400
C	-2.35902300	-0.50392600	-1.90945700
H	-1.67512800	0.20265200	0.05592100
H	-1.87617200	-1.25672700	-2.54026300
C	-3.52204100	-1.13529000	-1.17955800
C	-3.87616400	-2.45619800	-1.46586800
C	-4.23671000	-0.44658400	-0.19051300
C	-4.92222600	-3.07905300	-0.78820300
H	-3.32503600	-3.00156600	-2.22788500
C	-5.28877000	-1.06433600	0.47771700
H	-3.96581200	0.57454500	0.06659600
C	-5.63630300	-2.38192800	0.18265700
H	-5.17943000	-4.10737800	-1.02270100
H	-5.83394900	-0.51701100	1.24116200
H	-6.45554300	-2.86170500	0.70930200
C	2.40637900	2.95742500	0.20278400
C	3.58210800	3.50103000	-0.32158000
C	2.27555700	2.82948400	1.58764900
C	4.60526300	3.91676200	0.52226500
H	3.67932100	3.58437700	-1.40030700
C	3.30774400	3.22668100	2.43503900
H	1.37299600	2.38799200	2.00119300
C	4.47268600	3.77396600	1.90359200
H	5.51104600	4.34705600	0.10597300

H	3.20178300	3.10702700	3.50929800
H	5.27633400	4.08817300	2.56231000
H	2.80755300	-5.22975500	-1.59274700

$M3R_{NHC-1}$

Zero-point correction= 0.744343 (Hartree/Particle)
Thermal correction to Energy= 0.786503
Thermal correction to Enthalpy= 0.787447
Thermal correction to Gibbs Free Energy= 0.669788
Sum of electronic and zero-point Energies= -2524.767797
Sum of electronic and thermal Energies= -2524.725637
Sum of electronic and thermal Enthalpies= -2524.724693
Sum of electronic and thermal Free Energies= -2524.842352

C	-2.49741900	-0.47996100	3.63453800
C	-1.90754800	0.08033700	2.50366500
C	-2.11016500	1.41326200	2.15945900
C	-2.93168200	2.18727000	2.97694100
C	-3.53059900	1.63142200	4.10945900
C	-3.31986400	0.29567200	4.44612600
C	-2.11199200	-1.92822600	3.79405300
C	-0.95860700	-2.15404400	2.79214800
C	-1.05447600	-0.94410700	1.78713200
H	-1.64488500	1.85559400	1.27947800
H	-4.16259900	2.25001900	4.73826700
H	-3.77964700	-0.13027000	5.33250000
H	-1.78243100	-2.18134600	4.80590500
H	-1.06478300	-3.09608600	2.25179200
H	-2.95352900	-2.58472300	3.55141300
H	-1.49697400	-1.28546100	0.85205000
N	0.27730700	-0.39891900	1.49951900
O	0.30649400	-2.25358900	3.42727200
C	0.84050900	0.15120500	0.40051500
C	1.19678300	-0.31530700	2.50843200
N	2.04651800	0.57676300	0.80460700
N	2.28579400	0.27150600	2.11085600
C	0.88401500	-1.01264900	3.79133300
H	0.21262900	-0.41197500	4.41817600
H	1.80449700	-1.21504300	4.33785300
C	2.98348900	1.45917600	0.14274400
C	3.98938600	0.92267600	-0.65847700
C	2.85378800	2.82296900	0.41483800
C	4.88716700	1.82480400	-1.22773500
C	3.77320600	3.68144800	-0.18565700
C	4.79344700	3.19984800	-1.00745200

H	5.67915800	1.43914600	-1.86479900
H	3.69291600	4.74931500	0.00103600
C	1.78194600	3.33959800	1.33778500
H	0.78486200	3.00787000	1.02850500
H	1.94512600	2.98664500	2.36095100
C	4.07160100	-0.55102900	-0.92566800
H	3.91172000	-1.13633300	-0.01422300
H	3.30070900	-0.85101100	-1.64638300
H	5.04934200	-0.81268400	-1.33569300
H	1.78177200	4.43070700	1.34881700
C	5.79664600	4.14445800	-1.61674800
H	6.65673900	4.27205000	-0.95139200
H	6.16977500	3.76279000	-2.56955100
H	5.35871000	5.13090100	-1.78413700
C	-5.20096400	-2.52724000	-2.45925400
C	-4.79222000	-1.25918700	-2.86559000
C	-3.45128400	-0.89127100	-2.75282500
C	-2.50678200	-1.78000400	-2.21029500
C	-2.93979500	-3.03709700	-1.79161500
C	-4.27425500	-3.41758400	-1.92481500
H	-6.24364700	-2.81214300	-2.55498700
H	-5.51036400	-0.55502700	-3.27492200
H	-2.21169500	-3.72896400	-1.37906800
H	-4.58875900	-4.40604200	-1.60619700
C	-1.08796100	-1.29760800	-2.05973500
C	-0.13680700	-2.12681200	-1.23436700
H	-0.62746700	-1.17793800	-3.05192400
H	-0.50314100	-2.63495900	-0.34884800
C	1.14881500	-2.40970200	-1.70586100
O	1.60631700	-2.00669000	-2.80766800
S	-2.94756200	0.67100100	-3.44083100
C	0.35345500	0.30849200	-1.01841000
O	1.17436600	0.68246300	-1.83415900
C	-1.11213400	0.10134900	-1.41161000
C	-1.59105700	1.23609000	-2.32567900
H	-1.75596600	0.08743000	-0.52517300
H	-0.76594900	1.48160900	-2.99964900
C	-1.94974600	2.45729100	-1.50426500
C	-0.94408000	3.38173100	-1.20464300
C	-3.22063400	2.63420100	-0.95044000
C	-1.20570200	4.46469600	-0.36549100
H	0.04866400	3.25057600	-1.63088700
C	-3.48222600	3.71726500	-0.11683000
H	-4.00638800	1.91913800	-1.17780100

C	-2.47548600	4.63518000	0.18044700
H	-0.41731400	5.17847000	-0.14733000
H	-4.47405400	3.84291200	0.30633600
H	-2.68242500	5.48088000	0.82859300
C	2.08589700	-3.17841400	-0.79718800
C	3.21805700	-3.76859200	-1.36514600
C	1.91972500	-3.25626700	0.58923900
C	4.15487700	-4.42441100	-0.57252600
H	3.35257000	-3.67729400	-2.43813100
C	2.86054300	-3.89848900	1.38984800
H	1.06326600	-2.79274700	1.06619800
C	3.98291400	-4.48711900	0.81033200
H	5.02762000	-4.88002900	-1.03077400
H	2.71339600	-3.92888900	2.46559800
H	4.72005200	-4.98734400	1.43064700
H	-3.10195000	3.22941100	2.72835400

$M3S_{NHC-1}$

Zero-point correction=			0.745368 (Hartree/Particle)
Thermal correction to Energy=			0.787854
Thermal correction to Enthalpy=			0.788798
Thermal correction to Gibbs Free Energy=			0.671581
Sum of electronic and zero-point Energies=			-2524.775607
Sum of electronic and thermal Energies=			-2524.733121
Sum of electronic and thermal Enthalpies=			-2524.732177
Sum of electronic and thermal Free Energies=			-2524.849393
C	4.99362900	-1.77497200	-1.46073900
C	3.60571100	-1.65278400	-1.45907400
C	2.79054600	-2.70168600	-1.87687200
C	3.39008800	-3.88794900	-2.29229100
C	4.78139000	-4.01498300	-2.29517400
C	5.59154600	-2.95958100	-1.88356900
C	5.65450600	-0.51053000	-0.97919700
C	4.51019800	0.35404600	-0.40355500
C	3.18336100	-0.29147700	-0.94559700
H	1.71058200	-2.59270100	-1.88812900
H	5.23423700	-4.94610600	-2.62073600
H	6.67263300	-3.06088000	-1.88453800
H	6.41625000	-0.68364300	-0.21273000
H	4.56174000	1.38846200	-0.73914900
H	6.14325600	0.01180200	-1.80770500
H	2.71925900	0.36102800	-1.68809300
N	2.21064600	-0.44971800	0.15263500
O	4.56688200	0.44574600	1.01162200

C	0.86790100	-0.48333200	0.15945400
C	2.61837900	-0.77568900	1.41366200
N	0.51428700	-0.88103300	1.38530000
N	1.60803600	-1.05241000	2.18776600
C	4.08217600	-0.68207900	1.70539400
H	4.59130500	-1.60877600	1.40410000
H	4.23898600	-0.51823800	2.77174800
C	-0.77688900	-1.33196600	1.84067300
C	-1.33073700	-2.46817700	1.24158600
C	-1.38712200	-0.65654100	2.90576500
C	-2.54352500	-2.93314500	1.75214100
C	-2.59138000	-1.16825700	3.37717000
C	-3.17791700	-2.30930500	2.82217200
H	-2.99756900	-3.80980600	1.29891500
H	-3.08403800	-0.66323800	4.20421500
C	-0.78712500	0.58815900	3.50132900
H	-1.37289600	0.91771300	4.36031700
H	0.24425700	0.42458400	3.82519400
C	-0.66865400	-3.19114800	0.09692400
H	-0.88342300	-2.70638200	-0.86377300
H	0.41799900	-3.24745600	0.21619400
H	-1.05395600	-4.20959300	0.02849500
H	-0.78284300	1.39770000	2.76377100
C	-4.46214700	-2.85335000	3.38783600
H	-5.22560600	-2.07199700	3.44257200
H	-4.84889000	-3.66770900	2.77236000
H	-4.30437500	-3.23161200	4.40258600
C	-4.85914100	3.98536700	-1.17529300
C	-4.64936400	2.88481900	-2.00249600
C	-3.41778700	2.23171800	-1.98409000
C	-2.38497400	2.65429000	-1.12893000
C	-2.62229300	3.74593200	-0.29471900
C	-3.84612100	4.41318700	-0.32133800
H	-5.81492100	4.49904600	-1.19248700
H	-5.43557800	2.52856000	-2.66082300
H	-1.82665000	4.08689500	0.35976300
H	-4.00766500	5.26799500	0.32776300
C	-1.08189200	1.89069900	-1.14365300
C	-0.02733600	2.31486700	-0.16249200
H	-0.64757500	1.96059600	-2.15098900
H	-0.32393500	2.49292900	0.86599200
C	1.29388300	2.47311100	-0.54817400
O	1.74495800	2.32164600	-1.72989900
S	-3.10899100	0.85818800	-3.06388900

C	0.00315700	-0.24608700	-1.04723100
O	0.48640000	-0.51497100	-2.12411100
C	-1.37051600	0.37521500	-0.89424400
C	-2.39378100	-0.31732500	-1.82176900
H	-1.69860000	0.28663000	0.14575700
H	-1.87102200	-1.03512300	-2.46178200
C	-3.49667000	-1.02856900	-1.07204100
C	-3.86130300	-2.32694700	-1.43548200
C	-4.20325600	-0.39023800	-0.04567800
C	-4.91533700	-2.97583700	-0.79491800
H	-3.32119500	-2.83023500	-2.23392700
C	-5.26140500	-1.03361900	0.58677300
H	-3.93341500	0.61987400	0.25342200
C	-5.62238500	-2.32778300	0.21442200
H	-5.18495800	-3.98558100	-1.08843200
H	-5.80344000	-0.52359200	1.37750500
H	-6.44776300	-2.82770900	0.71164500
C	2.29860900	2.80889400	0.53328400
C	3.45397300	3.51178600	0.17989600
C	2.14880300	2.40645800	1.86440900
C	4.42473800	3.81539000	1.12983200
H	3.57554000	3.80147500	-0.85976200
C	3.11865000	2.70088100	2.81810900
H	1.27572000	1.82875300	2.15207200
C	4.26136400	3.40921600	2.45328900
H	5.31320300	4.36813200	0.83850400
H	2.98646900	2.36627900	3.84335300
H	5.02232000	3.63790300	3.19320200
H	2.77240700	-4.71830900	-2.61798400