Electronic Supplementary Information for

Predicting the Origin of Selectivity in NHC-Catalyzed Ring Opening of Formylcyclopropane: A Theoretical Investigation

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Content

Part 1: Energy profiles for the other three pathways

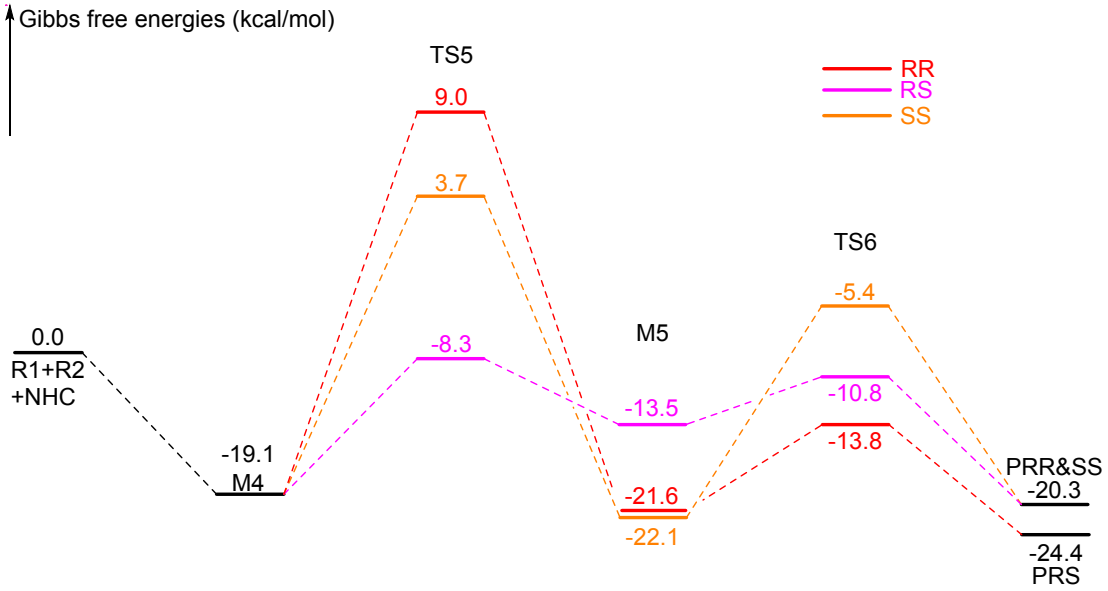
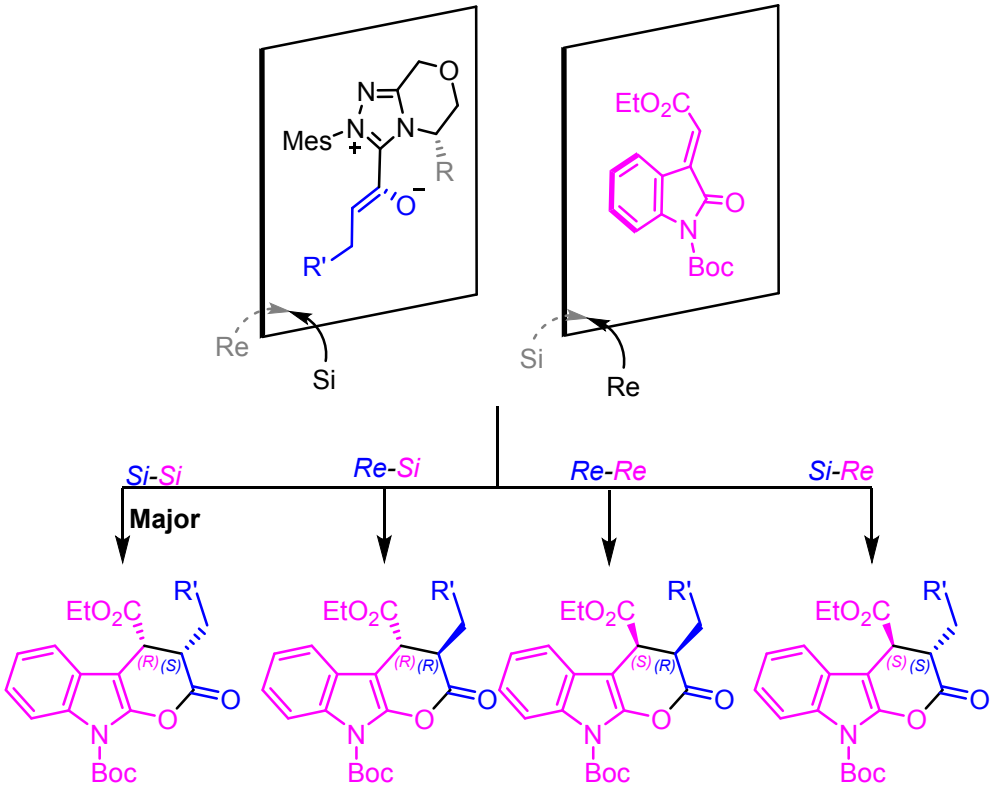


Fig. S1 Energy profiles involved in other three possible pathways of the NHC-catalyzed ring-opening/[4+2] cycloaddition reaction of formylcyclopropane and alkylideneoxindole.

Part 2: Stereochemical possibilities for the [4+2]cycloaddition



Scheme S1 Illustration of stereochemistry of NHC-catalyzed ring-opening/[4+2] cycloaddition reaction of formylcyclopropane.

Part 3: NCI plots of TS5RR and TS5SS

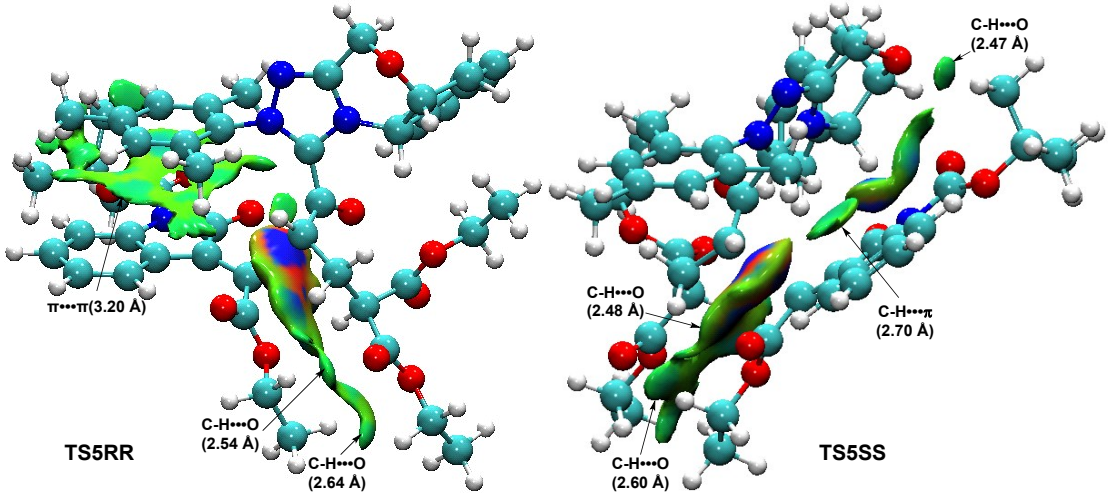


Fig. S2 NCI analysis of stereoselective transition states **TS5RR** and **TS5SS** (distance in Å).

Part 4: local reactivity indexes

For disclosing the origin of chemoselectivity, we have also performed the local reactivity analysis, pioneered by Domingo and coworkers, the nucleophilic (P_k^-) and electrophilc (P_k^+) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studies molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P^- (r) = \rho_S^{rc} (r) \; for\ the\ electrophilic\ attacks \qquad (3)$$

$$P^+ (r) = \rho_S^{ra} (r) \; for\ the\ nucleophilic\ attacks \qquad (4)$$

where $\rho_S^{rc}(r)$ is the ASD of the radical cation and $\rho_S^{ra}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^- and electrophilic P_k^+ Parr functions of the neutral system, respectively.

Part 5: Computational equation for ee value calculation

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

$$\frac{[TS5SR]}{[TS5RS]} = \frac{e^{-G^{\neq}_{[TS5SR]}/RT}}{e^{-G^{\neq}_{[TS5SR]}/RT}} = e^{\Delta G^{\neq}/RT} \quad (1)$$

$$ee\% = \frac{[TS5SR] - [TS5RS]}{[TS5SR] + [TS5RS]} \times 100\% = \frac{\frac{[TS5SR]}{[TS5RS]} - 1}{\frac{[TS5SR]}{[TS5RS]} + 1} \times 100\% \quad (2)$$

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

As depicted in **Figure 1** of the main text and Figure S1, the relative Gibbs free energy barriers of **TS5RS** and **TS5SR** are 10.8 and 6.0 kcal/mol, separately. Based on the above expression (equation 1), the $\Delta G^{\neq}$is 4.8 kcal/mol (20160 J/mol), the [TS5SR]/[TS5RS] can be calculated to be 3418.6. Then, the ee % value can be obtained by equation 2, which is 99.9% and in agreement with experimental observations.

Part 6: Solvent effects on chemoselective transition states

Table S1. Energy barriers in different solvents of chemoselective transition states

	DMSO	Cyclohexene	MeCN	THF	Toluene
M4	-1816.737787	-1816.721939	-1816.737447	-1816.732674	-1816.723856
R2	-1089.469655	-1089.462228	-1089.470763	-1089.464532	-1089.463328
M4+R2	-2906.207442 (0.0)	-2906.184167 (0.0)	-2906.20821 (0.0)	-2906.197206 (0.0)	-2906.187184 (0.0)
TS5-CO	-2906.169375 (23.9)	-2906.147737 (22.9)	-2906.168889 (24.7)	-2906.16121 (22.6)	-2906.150052 (23.3)
TS5SR	-2906.196536 (6.8)	-2906.176749 (4.7)	-2906.195918 (7.7)	-2906.189346 (4.9)	-2906.181248 (3.7)

Part 7: Cartesian coordinates of all the stationary points

R1

Zero-point correction=			0.236758 (Hartree/Particle)
Thermal correction to Energy=			0.252968
Thermal correction to Enthalpy=			0.253912
Thermal correction to Gibbs Free Energy=			0.191348
Sum of electronic and zero-point Energies=			-765.075900
Sum of electronic and thermal Energies=			-765.059690
Sum of electronic and thermal Enthalpies=			-765.058746
Sum of electronic and thermal Free Energies=			-765.121310
C	-0.02430900	-0.84936300	0.26010200
C	0.54875700	-2.24445300	0.03289400
C	0.63630800	-1.58177700	1.38005600
H	-0.18571100	-3.03037000	-0.09822500
H	-0.00534100	-1.96664700	2.16311900
H	1.61653100	-1.21670900	1.66585900
C	1.80874800	-2.34132800	-0.75001200
O	2.67033300	-1.48957600	-0.71438400
H	1.92942600	-3.25037800	-1.36466600
C	-1.52247700	-0.80821700	0.31315600
O	-2.19978900	-1.74245500	0.67726700
O	-2.00394800	0.37778200	-0.04581800
C	0.65716700	0.31374200	-0.42097400
O	0.54250800	0.54622800	-1.59984500
O	1.36848600	1.04936200	0.42854300
C	2.11366800	2.12760800	-0.16838700
C	2.88836400	2.80606800	0.93788700
H	1.41132000	2.80699400	-0.65909500
H	2.76997200	1.70470300	-0.93450000
H	3.46930200	3.63356700	0.52486700
H	2.21031300	3.20282900	1.69665100
H	3.57547900	2.10266700	1.41320200
C	-3.43986200	0.51584600	0.00160600
C	-3.76619400	1.92486100	-0.43622800
H	-3.77363500	0.30993200	1.02198400
H	-3.87957900	-0.23529600	-0.65966400
H	-4.84841700	2.07021800	-0.42498200
H	-3.31072500	2.65341200	0.23782900
H	-3.40068500	2.10643200	-1.44907800

R2

Zero-point correction=			0.341535 (Hartree/Particle)

Thermal correction to Energy= 0.362775
Thermal correction to Enthalpy= 0.363719
Thermal correction to Gibbs Free Energy= 0.290607
Sum of electronic and zero-point Energies= -1089.413985
Sum of electronic and thermal Energies= -1089.392745
Sum of electronic and thermal Enthalpies= -1089.391801
Sum of electronic and thermal Free Energies= -1089.464913

C	-0.50290400	1.65124000	0.00001200
C	0.89517400	1.46473100	-0.00000100
C	1.74287100	2.57211800	-0.00002200
C	1.18567600	3.84825600	-0.00002700
C	-0.19679300	4.01296000	-0.00001400
C	-1.06556900	2.91950400	0.00000600
C	-0.20300900	-0.64735300	0.00002200
C	1.15197900	0.02785400	0.00000800
H	2.81387500	2.42549800	-0.00003500
H	1.83427900	4.71723000	-0.00004500
H	-0.61945400	5.01253200	-0.00001900
H	-2.13535300	3.05652600	0.00001500
C	2.21567800	-0.79080300	0.00000200
H	2.01062700	-1.85748700	0.00001100
C	3.64418000	-0.40792100	-0.00000900
O	4.09300700	0.71862800	0.00002000
O	4.41087400	-1.50300200	-0.00001900
C	5.83149800	-1.27244600	0.00000800
C	6.50564400	-2.62515200	-0.00001500
H	6.08834300	-0.68242600	0.88426000
H	6.08836800	-0.68238200	-0.88420700
H	7.58982300	-2.49460700	0.00000600
H	6.22450700	-3.19595600	0.88758100
H	6.22453600	-3.19590900	-0.88765100
O	-0.40329600	-1.83474500	0.00003400
N	-1.16366400	0.38835500	0.00003200
C	-2.56277600	0.24101400	0.00006000
O	-3.30760200	1.19464800	0.00001700
O	-2.90487900	-1.03239800	0.00005600
C	-4.31960000	-1.42613300	-0.00002000
C	-4.99741900	-0.92198700	1.26845700
C	-4.99724700	-0.92216600	-1.26866200
C	-4.23056700	-2.94666300	0.00009200
H	-4.43299200	-1.24297200	2.14836100
H	-5.08090400	0.16467600	1.27036400
H	-6.00046500	-1.35281600	1.32886700
H	-4.43268700	-1.24325600	-2.14844200

H	-6.00027700	-1.35302200	-1.32916000
H	-5.08075200	0.16449500	-1.27072300
H	-5.23583400	-3.37469300	0.00005100
H	-3.69780200	-3.29569400	-0.88793100
H	-3.69792700	-3.29557100	0.88823700

NHC

Zero-point correction= 0.383740 (Hartree/Particle)
Thermal correction to Energy= 0.403897
Thermal correction to Enthalpy= 0.404842
Thermal correction to Gibbs Free Energy= 0.333957
Sum of electronic and zero-point Energies= -1051.532980
Sum of electronic and thermal Energies= -1051.512823
Sum of electronic and thermal Enthalpies= -1051.511878
Sum of electronic and thermal Free Energies= -1051.582763

C	-3.78315900	0.57348400	-0.37315100
C	-2.93275300	0.62429600	0.73392500
C	-2.74379600	1.80356900	1.44450800
C	-3.43242000	2.94467800	1.03620500
C	-4.29135100	2.89655400	-0.06400000
C	-4.47240600	1.71213100	-0.77712700
C	-3.78730300	-0.80545000	-0.98394000
C	-3.22858600	-1.67038600	0.16725300
C	-2.30593000	-0.72646700	0.98128800
H	-2.06951200	1.83115800	2.29430000
H	-3.30419100	3.87611200	1.57796200
H	-4.82589200	3.79178700	-0.36581200
H	-5.14087400	1.68050900	-1.63231700
H	-3.12846200	-0.82931200	-1.86003200
H	-4.05742100	-1.95361200	0.82067700
H	-4.77448600	-1.14303600	-1.30692200
H	-2.26773000	-0.99922700	2.03854700
N	-0.94311500	-0.80531700	0.44599700
O	-2.61582000	-2.88974800	-0.19796800
C	0.10052300	0.00658200	0.81300800
C	-0.53606500	-1.74167000	-0.46833800
N	1.07813100	-0.51827100	0.04685100
N	0.72268200	-1.59150800	-0.74724300
C	-1.48404400	-2.75306500	-1.03491400
H	-1.77156800	-2.46892700	-2.05540300
H	-1.00129400	-3.73066100	-1.08190900
C	2.43007600	-0.05145600	-0.00273900
C	2.69982800	1.16298200	-0.64004300
C	3.43283800	-0.82892300	0.58244100

C	4.02449900	1.59739500	-0.67585400
C	4.74378100	-0.35790100	0.51658500
C	5.05772600	0.84895000	-0.10991400
H	4.25465300	2.54170400	-1.16376400
H	5.53740200	-0.94558900	0.97225700
C	3.09558200	-2.12388200	1.27205100
H	2.75659900	-2.87412400	0.55209000
H	2.28358300	-1.97929200	1.99142200
H	3.96550000	-2.51678500	1.80121200
C	6.48636000	1.32153500	-0.19808800
H	6.95558100	0.96293600	-1.12017800
H	7.07915500	0.94846100	0.64029100
H	6.54264900	2.41255800	-0.20314400
C	1.59116300	1.96882900	-1.26348500
H	0.87720200	2.30157600	-0.50505200
H	1.03109500	1.36443000	-1.98408800
H	1.99331700	2.84225900	-1.77966200

$^{i}Pr_2NEt$

Zero-point correction= 0.264640 (Hartree/Particle)
Thermal correction to Energy= 0.276196
Thermal correction to Enthalpy= 0.277140
Thermal correction to Gibbs Free Energy= 0.228935
Sum of electronic and zero-point Energies= -370.600137
Sum of electronic and thermal Energies= -370.588581
Sum of electronic and thermal Enthalpies= -370.587637
Sum of electronic and thermal Free Energies= -370.635841

N	-0.04412200	0.13715000	-0.14280700
C	-1.31105500	-0.50668100	0.24015200
C	-1.56317800	-1.79884000	-0.53563700
C	-2.47482200	0.45279100	-0.02008500
H	-1.31032700	-0.75306600	1.32005000
H	-0.87741500	-2.60286800	-0.25933600
H	-2.57903900	-2.14857800	-0.33436900
H	-1.47150900	-1.61593400	-1.61170500
H	-2.37727500	1.38894600	0.53462100
H	-2.52204800	0.69193800	-1.08757600
H	-3.41941100	-0.01179000	0.27670300
C	1.10725800	-0.77273800	-0.26510100
C	1.51679100	-1.45862700	1.04526300
C	2.29412300	-0.05785800	-0.91061900
H	0.80615400	-1.55397700	-0.96954200
H	0.67974700	-2.01043200	1.48426800
H	2.33084200	-2.16746800	0.86713700

H	1.86601000	-0.73109400	1.78520900
H	1.98960600	0.41130000	-1.85002700
H	2.71454000	0.71531700	-0.25961000
H	3.09034900	-0.77748900	-1.12112500
C	0.24234600	1.32348500	0.67879100
C	0.19859100	2.61431700	-0.13347800
H	1.22800900	1.23199400	1.14773500
H	-0.46689200	1.38433000	1.51460400
H	0.40186000	3.48456000	0.49857800
H	0.94657400	2.58452600	-0.93088400
H	-0.78125200	2.74463700	-0.60078600

$^{i}Pr_2NEt\square H^{+}$

Zero-point correction= 0.280360 (Hartree/Particle)
Thermal correction to Energy= 0.292062
Thermal correction to Enthalpy= 0.293006
Thermal correction to Gibbs Free Energy= 0.244254
Sum of electronic and zero-point Energies= -371.042637
Sum of electronic and thermal Energies= -371.030936
Sum of electronic and thermal Enthalpies= -371.029991
Sum of electronic and thermal Free Energies= -371.078743

N	-0.03239400	0.13957600	-0.15640900
C	-1.37307100	-0.47442400	0.24415000
C	-1.65056400	-1.75716700	-0.52735800
C	-2.47226700	0.55316400	-0.00290800
H	-1.28023200	-0.68225200	1.31368700
H	-0.98395700	-2.57625700	-0.25539000
H	-2.66977900	-2.07272000	-0.29683800
H	-1.59257000	-1.58955500	-1.60761200
H	-2.32681700	1.48222100	0.55042300
H	-2.55151000	0.78340000	-1.07038100
H	-3.42357900	0.12592000	0.31825500
C	1.11913300	-0.85756200	-0.26298400
C	1.40616000	-1.51586700	1.07727000
C	2.33498300	-0.17555500	-0.87573600
H	0.76264200	-1.60769500	-0.96974700
H	0.53619800	-2.03999200	1.47899800
H	2.19627500	-2.25397700	0.92614400
H	1.76183300	-0.80048700	1.82256700
H	2.09334700	0.29374100	-1.83391300
H	2.77917100	0.57139300	-0.21335500
H	3.09123900	-0.94019100	-1.06344000
C	0.31240800	1.34561400	0.70172400
C	0.33858400	2.62080800	-0.12099000

H	1.28216900	1.15932800	1.15881400
H	-0.42190700	1.39588700	1.50527600
H	0.57790600	3.46119300	0.53259100
H	1.10375300	2.57045400	-0.90000500
H	-0.62971800	2.81871600	-0.58796000
H	-0.16990300	0.48977500	-1.11226500

TS1

Zero-point correction= 0.622987 (Hartree/Particle)
Thermal correction to Energy= 0.660397
Thermal correction to Enthalpy= 0.661341
Thermal correction to Gibbs Free Energy= 0.550490
Sum of electronic and zero-point Energies= -1816.617397
Sum of electronic and thermal Energies= -1816.579987
Sum of electronic and thermal Enthalpies= -1816.579043
Sum of electronic and thermal Free Energies= -1816.689893
Imaginary frequency=-103.66 cm^{-1}

C	-5.00497100	-2.01324200	0.07969800
C	-3.67567400	-1.60363400	0.15163500
C	-2.92180300	-1.76533400	1.31089400
C	-3.52986800	-2.37413800	2.40785200
C	-4.85818700	-2.80208600	2.33946700
C	-5.60635000	-2.62182800	1.17793300
C	-5.60131900	-1.69410100	-1.26823800
C	-4.57381000	-0.76439500	-1.95284300
C	-3.23725800	-0.97053000	-1.15291900
H	-1.89290800	-1.41110500	1.37494700
H	-2.96803700	-2.51260400	3.32586100
H	-5.31552200	-3.27058600	3.20517800
H	-6.64343900	-2.94100500	1.13419500
H	-6.57329500	-1.19575600	-1.20475700
H	-4.43003900	-1.02398200	-3.00218300
H	-5.74046200	-2.60503000	-1.86009200
H	-2.55195200	-1.61284300	-1.71234900
N	-2.56701300	0.30051900	-0.93084800
O	-5.00376900	0.59106700	-1.98423200
C	-1.24065300	0.56031500	-0.80924900
C	-3.29264300	1.42234200	-0.63018000
N	-1.25364600	1.84975900	-0.43994100
N	-2.50873800	2.41222200	-0.33092500
C	-4.77443500	1.33301200	-0.79666200
H	-5.23704900	0.85363300	0.07696400
H	-5.21090800	2.32216800	-0.93261600
C	-0.09796500	2.63068600	-0.11259400

C	0.19643100	2.84047100	1.23940200
C	0.69448000	3.12596200	-1.14654500
C	1.34462800	3.56937300	1.53959000
C	1.83245200	3.85620000	-0.79593100
C	2.17342300	4.08201800	0.53642200
H	1.60121300	3.74090500	2.58267300
H	2.46910600	4.24848200	-1.58523700
C	0.36066300	2.83795500	-2.58536400
H	-0.69104700	3.04752400	-2.79998900
H	0.53622700	1.78047100	-2.81222400
H	0.98059600	3.43970100	-3.25195500
C	3.40822800	4.86485700	0.90251300
H	3.14538600	5.76766000	1.46176500
H	3.96599200	5.16507600	0.01340500
H	4.07052300	4.26979900	1.53784100
C	-0.69268700	2.27728200	2.31485300
H	-0.78402500	1.19368300	2.19029900
H	-1.69473100	2.71315400	2.26201200
H	-0.27545900	2.48376500	3.30231300
C	2.72199000	-0.98316000	-0.54743800
C	1.33721700	-0.52597200	-1.01469000
C	2.35886500	0.47809100	-0.63012600
H	1.14767100	-0.68717100	-2.07129700
H	2.83215200	1.04934500	-1.42022100
H	2.21776800	0.97332900	0.32536600
C	0.19996100	-0.83583300	-0.07684900
O	0.28688400	-0.59461800	1.13552300
H	-0.44902900	-1.65643700	-0.43760400
C	3.61244200	-1.49113000	-1.63186700
O	3.52919200	-1.13723200	-2.78805200
O	4.53496100	-2.34204000	-1.18072900
C	2.80920400	-1.66286900	0.79346600
O	2.56856400	-2.83541600	0.96413700
O	3.17271200	-0.82584900	1.76350000
C	3.03944900	-1.33197100	3.10129300
C	3.23964700	-0.16266300	4.03867800
H	3.78013300	-2.12149900	3.25852900
H	2.04260800	-1.77058500	3.19859000
H	3.13792500	-0.49422000	5.07440200
H	4.23315700	0.27266800	3.90896500
H	2.49110600	0.60920800	3.84281700
C	5.45479100	-2.85073900	-2.16572600
C	6.41862900	-3.76561200	-1.44546400
H	5.96217800	-2.00549000	-2.63860600

H	4.88409800	-3.37614400	-2.93638500
H	7.13715400	-4.17707500	-2.15761600
H	6.96668100	-3.21755800	-0.67594600
H	5.88439400	-4.59225100	-0.97230800

M1

Zero-point correction= 0.625003 (Hartree/Particle)
Thermal correction to Energy= 0.662098
Thermal correction to Enthalpy= 0.663043
Thermal correction to Gibbs Free Energy= 0.553140
Sum of electronic and zero-point Energies= -1816.627849
Sum of electronic and thermal Energies= -1816.590753
Sum of electronic and thermal Enthalpies= -1816.589809
Sum of electronic and thermal Free Energies= -1816.699712

C	4.42644700	-1.65998400	-0.16376500
C	3.13093600	-1.60929000	0.35986800
C	2.19657900	-2.59450600	0.04637800
C	2.58347000	-3.62514700	-0.80798600
C	3.87236500	-3.66993800	-1.34174400
C	4.80556300	-2.68705600	-1.02159600
C	5.26951400	-0.52344800	0.34884500
C	4.49752600	-0.10234400	1.61435900
C	3.00575200	-0.45245200	1.33239500
H	1.18310400	-2.57097100	0.43200200
H	1.87042700	-4.40571200	-1.05463900
H	4.15319300	-4.48462000	-2.00198900
H	5.81437800	-2.72827500	-1.42082900
H	5.31157800	0.28273600	-0.39225400
H	4.81154800	-0.74034600	2.44329200
H	6.29749100	-0.80940600	0.58114700
H	2.46727400	-0.71592800	2.24531700
N	2.34163500	0.76358400	0.79466200
O	4.70816200	1.21864200	2.06477600
C	1.04964800	0.91799200	0.43459300
C	2.93666700	1.99533500	0.69723900
N	0.93075200	2.20055600	0.10140800
N	2.09900500	2.89171500	0.26722000
C	4.35332600	2.21053800	1.12660000
H	5.02237600	2.21699700	0.25862400
H	4.43257000	3.17724100	1.62532900
C	-0.23838700	2.88630100	-0.38094600
C	-0.54616500	2.78914900	-1.73888000
C	-0.99615300	3.61903300	0.53364600
C	-1.69063900	3.45437500	-2.17610600

C	-2.13289600	4.26144100	0.04693900
C	-2.49296900	4.18900800	-1.30070500
H	-1.96359600	3.39225700	-3.22668800
H	-2.75086200	4.83206800	0.73549600
C	-0.59269900	3.70656900	1.98134200
H	0.37045500	4.21508600	2.08633500
H	-0.48211200	2.71240400	2.42650500
H	-1.33948100	4.25628600	2.55556000
C	-3.70935500	4.91863200	-1.80860200
H	-3.43699000	5.91844300	-2.16211900
H	-4.45667300	5.03817400	-1.02124900
H	-4.16800100	4.38698700	-2.64533500
C	0.31143600	1.97174300	-2.66511700
H	0.32233300	0.92483200	-2.33123300
H	1.34388400	2.33762400	-2.65978100
H	-0.06779100	2.02912800	-3.68687500
C	-2.40521600	-0.88587900	0.32488100
C	-1.38364300	0.20456300	0.61203600
C	-2.33136400	0.36826700	-0.51459900
H	-1.57379700	0.76238600	1.52674400
H	-3.14488500	1.07758800	-0.41118300
H	-1.90530500	0.21339100	-1.49960400
C	0.05546300	-0.23219000	0.28759600
O	0.20996400	-0.76468800	-0.92641100
H	0.33487300	-0.90662500	1.14007700
C	-3.54357200	-0.96963800	1.27909200
O	-3.99364500	-0.02018900	1.88454200
O	-4.04267800	-2.20652700	1.37047300
C	-1.83981900	-2.18421200	-0.18859200
O	-1.25834900	-2.97072800	0.52879900
O	-2.08442400	-2.39359300	-1.48098000
C	-1.27340800	-3.41623100	-2.07792600
C	-1.55169700	-3.40231400	-3.56426700
H	-1.51498800	-4.38157500	-1.62304400
H	-0.23228100	-3.16612600	-1.84875600
H	-0.94652600	-4.16285600	-4.06320200
H	-2.60508200	-3.61185400	-3.76543800
H	-1.30194700	-2.42660200	-3.98758300
C	-5.16852800	-2.36558500	2.25199400
C	-5.57669800	-3.82027500	2.19622800
H	-5.96940100	-1.69903200	1.92017000
H	-4.87076700	-2.05948000	3.25870500
H	-6.42922100	-3.99027100	2.85737200
H	-5.86303900	-4.10047900	1.18017900

H	-4.75363800	-4.46252300	2.51712500

M02

Zero-point correction= 0.905990 (Hartree/Particle)
Thermal correction to Energy= 0.956276
Thermal correction to Enthalpy= 0.957220
Thermal correction to Gibbs Free Energy= 0.820989
Sum of electronic and zero-point Energies= -2187.711525
Sum of electronic and thermal Energies= -2187.661239
Sum of electronic and thermal Enthalpies= -2187.660295
Sum of electronic and thermal Free Energies= -2187.796526

C	-4.59694800	-1.24973000	-0.20969500
C	-3.65774100	-0.86323600	0.75397300
C	-3.63509900	0.44568900	1.23259200
C	-4.48372900	1.38385500	0.64808600
C	-5.34556800	1.01966800	-0.38837700
C	-5.42566700	-0.30667200	-0.80814400
C	-4.62333200	-2.74815900	-0.35898500
C	-3.98254400	-3.17437100	0.98173700
C	-2.91055900	-2.08436300	1.24810400
H	-2.98057100	0.73021100	2.04585500
H	-4.48937000	2.40465800	1.01576700
H	-5.99011300	1.76773400	-0.83864200
H	-6.14613100	-0.60568300	-1.56301500
H	-4.03068700	-3.07219200	-1.22225700
H	-4.72608900	-3.06999900	1.77482000
H	-5.63060300	-3.15081900	-0.47916600
H	-2.57869300	-2.03151800	2.28407400
N	-1.70395400	-2.48234700	0.42769500
O	-3.50521000	-4.49210600	1.07656400
C	-0.55604100	-1.83997900	0.12048600
C	-1.56939900	-3.75107000	-0.10100600
N	0.17462200	-2.69169900	-0.58738800
N	-0.44122400	-3.89261200	-0.73001000
C	-2.59613200	-4.83007100	0.06008200
H	-3.09708500	-5.00665500	-0.89943900
H	-2.09148900	-5.75064400	0.35748200
C	1.50547600	-2.50826800	-1.11240900
C	1.66802700	-2.07754200	-2.42938700
C	2.57060500	-2.87703300	-0.27892100
C	2.97930200	-1.98515900	-2.90406500
C	3.85153700	-2.78479100	-0.81038800
C	4.07380600	-2.33154600	-2.11585300
H	3.13950500	-1.64521900	-3.92405100

H	4.69980400	-3.07060500	-0.19293600
C	2.32006700	-3.35369800	1.12681900
H	1.60713300	-4.18326600	1.14399200
H	1.91272000	-2.54478600	1.74659300
H	3.24998900	-3.68860400	1.58850700
C	5.47762300	-2.19277500	-2.64078100
H	6.11259800	-3.00895800	-2.28874900
H	5.91970100	-1.25456800	-2.28858200
H	5.49430500	-2.18117100	-3.73206600
C	0.51354200	-1.72742000	-3.33257000
H	-0.45563100	-1.92266700	-2.86954100
H	0.57113400	-2.31125500	-4.25431700
H	0.55335100	-0.66827800	-3.60926000
C	-0.67841100	1.83501400	-0.93506900
C	-0.23731400	0.39165600	-0.82384300
C	-1.51417200	0.71985600	-1.52151300
H	0.59865100	0.19389200	-1.49057200
H	-1.52659200	0.65799300	-2.60434400
H	-2.45089800	0.51495300	-1.01541000
C	-0.11002800	-0.44340800	0.45510500
O	-0.85817300	-0.06428100	1.56771200
H	0.96698400	-0.49044300	0.70430900
C	0.14416600	2.61175900	-1.93023500
O	0.56305100	2.13128400	-2.95831000
O	0.38385600	3.85089600	-1.51817500
C	-1.20601000	2.66027300	0.20746600
O	-0.82584300	2.59901600	1.36309800
O	-2.12098100	3.51230100	-0.21547700
C	-2.59428400	4.47809600	0.75087300
C	-3.69121900	5.27167300	0.08121800
H	-1.74584700	5.10219900	1.04463700
H	-2.94320900	3.94058700	1.63699700
H	-4.08312100	6.01480300	0.77835300
H	-3.30775600	5.78836500	-0.80092500
H	-4.51030600	4.61650800	-0.22637800
C	1.23066200	4.65465700	-2.36951900
C	1.43332100	5.97601200	-1.66598200
H	0.73667600	4.76781500	-3.33776400
H	2.16989900	4.11611000	-2.52451000
H	2.06685900	6.62269400	-2.27625500
H	0.47568800	6.47654800	-1.50633600
H	1.91757200	5.82547200	-0.69828300
N	2.97130700	0.45572400	1.86605100
C	3.50540300	1.41859500	0.88512800

C	2.49297100	2.50646700	0.53622100
C	3.89714900	0.67986400	-0.39576300
H	4.40524200	1.92185200	1.27965300
H	2.30574400	3.20630900	1.35438300
H	2.85953200	3.08387900	-0.31750000
H	1.53757200	2.05247000	0.26102500
H	4.70919600	-0.03473400	-0.23953800
H	3.03353200	0.12283900	-0.78256500
H	4.22272600	1.39214900	-1.15902500
C	2.22727500	1.06409000	2.98700100
C	3.03385100	2.00698400	3.89147400
C	1.51060200	0.01074700	3.83205100
H	1.43753600	1.65889900	2.51415900
H	3.64257600	2.70644800	3.31017500
H	2.35583000	2.59200900	4.52029200
H	3.69689900	1.44532800	4.55654700
H	0.99755300	-0.71757500	3.19709300
H	2.19241100	-0.51948800	4.50318000
H	0.75875500	0.50144500	4.45705600
C	3.96379100	-0.55898100	2.24864500
C	5.37271400	-0.08569600	2.63005100
H	4.06150000	-1.26238700	1.41425700
H	3.54633400	-1.14078600	3.07381600
H	5.96132400	-0.94868300	2.95414300
H	5.89475300	0.36453400	1.78091400
H	5.36637000	0.64224700	3.44390100
H	-0.63879000	0.86375700	1.77405800

TS2

Zero-point correction= 0.903271 (Hartree/Particle)
Thermal correction to Energy= 0.952520
Thermal correction to Enthalpy= 0.953464
Thermal correction to Gibbs Free Energy= 0.821987
Sum of electronic and zero-point Energies= -2187.676141
Sum of electronic and thermal Energies= -2187.626892
Sum of electronic and thermal Enthalpies= -2187.625948
Sum of electronic and thermal Free Energies= -2187.757425
Imaginary frequency= -959.66 cm^{-1}

C	4.59553300	0.94654500	0.26392600
C	3.34080800	1.18733200	-0.30501100
C	2.70903300	2.41543600	-0.13375200
C	3.31238100	3.36830000	0.68429900
C	4.53367600	3.10237000	1.30585200
C	5.19388200	1.89484100	1.08599800

C	5.16448100	-0.35214700	-0.24491000
C	4.37651700	-0.50564600	-1.56426900
C	2.96227300	0.04662400	-1.22737400
H	1.77261500	2.65031800	-0.63284300
H	2.83481600	4.33252700	0.82728000
H	4.98901600	3.85701200	1.93947000
H	6.16983600	1.71002100	1.52434100
H	4.95359800	-1.17235400	0.45117400
H	4.80360700	0.17692700	-2.30274800
H	6.24304000	-0.32138400	-0.41178400
H	2.40462500	0.38197200	-2.10804800
N	2.17475800	-1.07176300	-0.64229500
O	4.39455600	-1.77407800	-2.17219000
C	0.84737800	-1.06251500	-0.28495500
C	2.50145000	-2.39223900	-0.87816600
N	0.48915000	-2.36413700	-0.26662700
N	1.51080400	-3.19472400	-0.65833900
C	3.85641800	-2.79471700	-1.36024900
H	4.51105900	-3.02145400	-0.50961900
H	3.76396000	-3.69293900	-1.97126400
C	-0.69266000	-2.91395600	0.32760000
C	-0.89926400	-2.70972200	1.69594700
C	-1.58478300	-3.62093100	-0.48109700
C	-2.06335300	-3.23971400	2.25063700
C	-2.72987200	-4.13681400	0.12321100
C	-2.98819000	-3.94935000	1.48226800
H	-2.24876700	-3.09774000	3.31258900
H	-3.44005500	-4.69188600	-0.48465600
C	-1.31859100	-3.79613500	-1.95226800
H	-2.16518700	-4.28095200	-2.44036800
H	-0.42288200	-4.40033100	-2.12134000
H	-1.14867900	-2.82788300	-2.43517900
C	-4.25423900	-4.48151900	2.10219700
H	-4.11512700	-4.69292700	3.16474700
H	-4.58272900	-5.39726200	1.60548100
H	-5.06283400	-3.74881100	2.01282200
C	0.09680300	-1.94998700	2.53378200
H	0.14338600	-0.88864900	2.25743400
H	1.10319500	-2.36398000	2.40710200
H	-0.16937200	-2.01980200	3.59000300
C	-2.26188300	1.24070900	-0.06575100
C	-1.46194700	-0.06404000	-0.12419100
C	-2.29186800	0.24845800	1.07392000
H	-1.87255000	-0.78398900	-0.82680400

H	-3.21864900	-0.29460600	1.21766400
H	-1.74948400	0.57138300	1.95541300
C	0.02150600	0.07232300	-0.06112600
O	0.47797300	1.00982200	0.97215900
H	0.54295600	1.13730800	-0.27922800
C	-3.46828000	1.27235500	-0.93581000
O	-4.14359700	0.29860500	-1.19272500
O	-3.74336100	2.50167500	-1.38291100
C	-1.46630300	2.51027600	0.04642000
O	-0.82015400	2.96382300	-0.87590600
O	-1.55322500	3.08130700	1.24565600
C	-0.58886900	4.11746600	1.49044900
C	-0.77973700	4.58812600	2.91440200
H	-0.73611600	4.92333800	0.76614700
H	0.40190300	3.67899200	1.32865100
H	-0.05238100	5.36988800	3.14534500
H	-1.78309600	4.99605500	3.05724700
H	-0.63459000	3.76171600	3.61359100
C	-4.90805300	2.61823900	-2.22044700
C	-5.02406800	4.07004900	-2.62584700
H	-5.78028200	2.27725300	-1.65575300
H	-4.78555900	1.95757400	-3.08313400
H	-5.89903400	4.20495200	-3.26553100
H	-5.13502600	4.70766700	-1.74601700
H	-4.13681200	4.38709600	-3.17814200

M2

Zero-point correction= 0.624937 (Hartree/Particle)
Thermal correction to Energy= 0.662009
Thermal correction to Enthalpy= 0.662954
Thermal correction to Gibbs Free Energy= 0.555339
Sum of electronic and zero-point Energies= -1816.642486
Sum of electronic and thermal Energies= -1816.605414
Sum of electronic and thermal Enthalpies= -1816.604470
Sum of electronic and thermal Free Energies= -1816.712084

C	-4.88476300	-0.43778900	-0.58673800
C	-3.85448300	0.39882200	-1.02629200
C	-3.26627200	0.20163500	-2.27506800
C	-3.70596100	-0.86249700	-3.06207600
C	-4.72203000	-1.70827300	-2.61458700
C	-5.32548500	-1.49475400	-1.37656900
C	-5.38575400	-0.02417500	0.77097900
C	-4.78992000	1.39235700	0.93801400
C	-3.53086000	1.44551500	0.02479400

H	-2.49042800	0.87304000	-2.62560400
H	-3.25640700	-1.03047400	-4.03566000
H	-5.05319700	-2.53095800	-3.24071200
H	-6.13047800	-2.13932400	-1.03576800
H	-5.01701900	-0.71324700	1.53924500
H	-5.50232100	2.12582100	0.55413300
H	-6.47591200	-0.01471800	0.84535600
H	-3.35162800	2.43596600	-0.39251000
N	-2.36075300	1.06902900	0.85048100
O	-4.52634000	1.78623800	2.26863900
C	-1.16251100	0.56197100	0.33636600
C	-2.54074600	0.46394200	2.08256000
N	-0.74514900	-0.34066300	1.30131000
N	-1.61887700	-0.38260100	2.37904900
C	-3.67086500	0.90407000	2.96631600
H	-4.20638300	0.03246800	3.36100800
H	-3.27340600	1.46669000	3.81499900
C	0.29286600	-1.30517600	1.18789900
C	1.59968500	-0.94596800	1.52027100
C	-0.03616400	-2.58444100	0.71784200
C	2.58967200	-1.92585700	1.41236000
C	0.98278300	-3.52664400	0.61602100
C	2.30128300	-3.21351800	0.96499100
H	3.61156100	-1.66774400	1.68144500
H	0.75004000	-4.52369900	0.24878600
C	-1.45329700	-2.88215600	0.30289200
H	-1.76816500	-2.20564200	-0.50202600
H	-2.14715600	-2.73059500	1.13540900
H	-1.54826600	-3.90955700	-0.05253100
C	3.38955400	-4.24648300	0.82218500
H	3.61148800	-4.42747200	-0.23504800
H	3.08687100	-5.20166500	1.25966800
H	4.31205100	-3.92157000	1.31020900
C	1.93152900	0.44987900	1.97673900
H	1.77254600	0.55626000	3.05503900
H	1.29321400	1.18723900	1.47913100
H	2.97577400	0.68217000	1.75200300
C	2.05431700	0.81680800	-1.46447800
C	0.55582600	0.25602200	-1.46827000
C	1.15492700	0.79399800	-2.69718500
H	0.59906600	-0.82422400	-1.36724700
H	1.47294200	0.09914800	-3.46434100
H	0.80550900	1.76567400	-3.02628200
C	-0.56498600	0.95545600	-0.82012500

O	-1.11392100	2.06155600	-1.46658000
H	-0.47140600	2.77797700	-1.32205000
C	3.05254900	-0.29368900	-1.44519300
O	2.88634900	-1.30733200	-2.09595800
O	4.11288100	-0.10773900	-0.65875400
C	2.24272600	2.14792500	-0.83607100
O	1.37499600	3.00791500	-0.83753600
O	3.42400300	2.34684200	-0.26238100
C	3.59395800	3.60748500	0.41093400
C	4.98251700	3.60136900	1.00855400
H	2.81584100	3.70299800	1.17416200
H	3.45735100	4.41476200	-0.31352600
H	5.16452100	4.54407800	1.52900800
H	5.09047100	2.78215100	1.72355700
H	5.73674100	3.48368100	0.22732200
C	5.08900900	-1.16278400	-0.67953600
C	6.17057500	-0.78070200	0.30552000
H	5.47712100	-1.26179600	-1.69741700
H	4.59759900	-2.10316500	-0.41433100
H	6.94244100	-1.55324400	0.32844000
H	6.63303000	0.16702500	0.02020300
H	5.75764900	-0.67233500	1.31233200

TS3

Zero-point correction= 0.624420 (Hartree/Particle)
Thermal correction to Energy= 0.660929
Thermal correction to Enthalpy= 0.661873
Thermal correction to Gibbs Free Energy= 0.555061
Sum of electronic and zero-point Energies= -1816.641657
Sum of electronic and thermal Energies= -1816.605148
Sum of electronic and thermal Enthalpies= -1816.604204
Sum of electronic and thermal Free Energies= -1816.711016
Imaginary frequency= -357.21 cm^{-1}

C	-5.64875300	-0.39725600	0.21501100
C	-4.32722600	-0.39377800	0.65284100
C	-3.97082900	0.16007300	1.88008300
C	-4.97114100	0.72392500	2.66795800
C	-6.29977200	0.72500100	2.23332800
C	-6.64798100	0.16307100	1.00743300
C	-5.78314200	-1.06511500	-1.12902200
C	-4.33464800	-1.35585300	-1.59511000
C	-3.41054200	-1.04680200	-0.35618100
H	-2.93586000	0.14685300	2.21099700
H	-4.71937200	1.16343800	3.62771900

H	-7.06785600	1.16827300	2.85921100
H	-7.68144400	0.16563400	0.67350700
H	-6.29485000	-0.43903300	-1.86777500
H	-4.21341400	-2.40062900	-1.88153700
H	-6.35334000	-1.99585200	-1.05185000
H	-2.97581900	-1.96273300	0.03616200
N	-2.30333200	-0.16802500	-0.73818800
O	-3.98809600	-0.63318900	-2.76621300
C	-1.08836100	0.07036600	-0.12815300
C	-2.46946500	0.78855900	-1.70872300
N	-0.58209700	1.12883400	-0.83507700
N	-1.45408800	1.57477100	-1.81321500
C	-3.71779100	0.73395100	-2.52425100
H	-4.54917400	1.22245700	-1.99593200
H	-3.56726200	1.22950100	-3.48312100
C	0.70701400	1.73351500	-0.74089100
C	1.82489600	1.04129600	-1.21240300
C	0.79104000	3.02166600	-0.19581400
C	3.06062800	1.68614600	-1.13209000
C	2.04363500	3.62456000	-0.14345700
C	3.18872500	2.97231600	-0.61056800
H	3.94198200	1.16405800	-1.49671100
H	2.13201300	4.62405100	0.27594900
C	-0.44343300	3.70657300	0.32630800
H	-0.95424000	3.07561400	1.06168100
H	-1.15637400	3.89898400	-0.48051600
H	-0.18731800	4.65464900	0.80172700
C	4.53009100	3.65581000	-0.54029300
H	4.85001100	3.77863400	0.49971900
H	4.48331800	4.65337800	-0.98585100
H	5.29720000	3.08174400	-1.06607300
C	1.70695000	-0.33151800	-1.81906800
H	1.29275300	-0.26880500	-2.83114200
H	1.04591400	-0.97899600	-1.23398200
H	2.69044000	-0.80461000	-1.86818500
C	2.18739200	-1.18539900	1.54920900
C	0.61672600	-0.18566500	1.65754500
C	1.22339900	-1.00395200	2.70623900
H	1.00139400	0.82245700	1.55273300
H	1.67198300	-0.47775700	3.54263400
H	0.67585000	-1.90230900	2.97447300
C	-0.56040100	-0.58508600	0.98173400
O	-1.26736200	-1.68815400	1.45231700
H	-0.70340600	-2.45380900	1.23237100

C	3.33430800	-0.27707000	1.56933000
O	3.39319200	0.68120300	2.32803600
O	4.31660000	-0.54748300	0.69218000
C	2.00755000	-2.35040000	0.70409000
O	0.95865900	-2.99584400	0.64899800
O	3.05217900	-2.68508500	-0.06407600
C	2.82549000	-3.74274300	-1.00567500
C	4.09919100	-3.89703200	-1.80713500
H	1.97277000	-3.47649000	-1.63890900
H	2.56635200	-4.65767100	-0.46542700
H	3.98042600	-4.69270400	-2.54597900
H	4.33845800	-2.96842800	-2.33178300
H	4.93671400	-4.15082100	-1.15339200
C	5.46215600	0.30818000	0.77653300
C	6.41566800	-0.11532200	-0.31919800
H	5.91297200	0.20369100	1.76841700
H	5.14207200	1.34755100	0.66642500
H	7.31210000	0.50875400	-0.29579500
H	6.71317200	-1.15853700	-0.18902400
H	5.94882600	-0.01326800	-1.30299900

M3

Zero-point correction= 0.625288 (Hartree/Particle)
Thermal correction to Energy= 0.661829
Thermal correction to Enthalpy= 0.662773
Thermal correction to Gibbs Free Energy= 0.557221
Sum of electronic and zero-point Energies= -1816.655152
Sum of electronic and thermal Energies= -1816.618612
Sum of electronic and thermal Enthalpies= -1816.617667
Sum of electronic and thermal Free Energies= -1816.723220

C	5.28075200	0.40067700	0.77851000
C	4.09954800	1.08650300	0.47952600
C	3.53125800	1.97354000	1.39016600
C	4.15596300	2.14479500	2.62468100
C	5.32721400	1.45079800	2.93238800
C	5.90249700	0.57903400	2.00898000
C	5.71983500	-0.46107000	-0.37675300
C	4.92826900	0.14935100	-1.55265500
C	3.64136800	0.74494800	-0.92106000
H	2.63187800	2.52222800	1.13198300
H	3.73215900	2.83228900	3.34913000
H	5.80220100	1.60124000	3.89663500
H	6.82420300	0.05528100	2.24287600
H	5.44577000	-1.50704600	-0.19718400

H	5.49327500	0.99031500	-1.96024800
H	6.79634100	-0.43346500	-0.55702600
H	3.22778200	1.58741100	-1.47535800
N	2.60622200	-0.32135600	-0.93659100
O	4.67759000	-0.69890100	-2.65365600
C	1.38613900	-0.30818500	-0.36482700
C	2.74299000	-1.53627100	-1.55282000
N	0.84477400	-1.49681300	-0.64271400
N	1.68563700	-2.27586900	-1.37968200
C	3.97371600	-1.87777300	-2.33526300
H	4.59034200	-2.58963100	-1.77401100
H	3.68133200	-2.34732200	-3.27570000
C	-0.47363100	-1.97180400	-0.30742200
C	-0.56983800	-2.98949700	0.64691400
C	-1.57917100	-1.40485200	-0.94511000
C	-1.84398300	-3.46138900	0.94669000
C	-2.83540000	-1.89956700	-0.58811600
C	-2.98445300	-2.93537200	0.33383900
H	-1.94976300	-4.25989800	1.67670500
H	-3.71566900	-1.46899600	-1.05878000
C	-1.43739500	-0.34157000	-2.00181800
H	-0.86165900	-0.71828500	-2.85403800
H	-0.93345000	0.55616200	-1.63058800
H	-2.42399000	-0.03846400	-2.35846400
C	-4.34000900	-3.51464100	0.64630000
H	-4.39454800	-4.55580300	0.31387100
H	-5.13651700	-2.95811900	0.14713800
H	-4.53361300	-3.50573000	1.72283200
C	0.65710200	-3.54681400	1.31905000
H	1.25876100	-2.74957700	1.76819000
H	1.29478300	-4.07246300	0.60265800
H	0.37336300	-4.24467200	2.10768600
C	-2.27902200	1.74477600	1.01723500
C	-0.09784000	0.68522100	1.31007700
C	-0.97613500	1.80397600	1.79136100
H	-0.26872000	-0.30744100	1.71688800
H	-1.18295900	1.68525900	2.85574300
H	-0.47964600	2.76536300	1.62763200
C	0.74284300	0.83751700	0.27769000
O	1.00695900	2.00147200	-0.37207500
H	0.09313600	2.47838900	-0.49575200
C	-3.27369200	0.87147000	1.57067600
O	-3.13119500	0.25666000	2.62924800
O	-4.42613000	0.74187900	0.85745800

C	-2.27531300	2.35123500	-0.24613500
O	-1.27105700	2.93089200	-0.76051200
O	-3.41862600	2.33697500	-0.96916100
C	-3.35822900	2.92100200	-2.27017100
C	-4.70433700	2.67749400	-2.91970900
H	-2.54565600	2.46198600	-2.84312800
H	-3.13713800	3.98994800	-2.18611000
H	-4.72146900	3.10622600	-3.92453000
H	-4.90344800	1.60509000	-2.99412200
H	-5.50371600	3.13517800	-2.33196000
C	-5.38511400	-0.14919400	1.41914400
C	-6.50633500	-0.29815400	0.41225000
H	-5.75227400	0.25251000	2.37023400
H	-4.90594400	-1.10801700	1.63735000
H	-7.26805000	-0.98285700	0.79399100
H	-6.97573600	0.66772600	0.20961600
H	-6.12572300	-0.69545800	-0.53337000

TS4

Zero-point correction= 0.620375 (Hartree/Particle)
Thermal correction to Energy= 0.657403
Thermal correction to Enthalpy= 0.658347
Thermal correction to Gibbs Free Energy= 0.550201
Sum of electronic and zero-point Energies= -1816.642003
Sum of electronic and thermal Energies= -1816.604974
Sum of electronic and thermal Enthalpies= -1816.604030
Sum of electronic and thermal Free Energies= -1816.712176
Imaginary frequency= -1187.49 cm^{-1}

C	4.29733800	1.08691000	0.82069300
C	3.07272500	1.31856600	0.18673300
C	2.15755400	2.23502400	0.69892900
C	2.47312200	2.89673200	1.88331400
C	3.68630800	2.65358100	2.53063500
C	4.61114500	1.75401800	1.99993600
C	5.13211700	0.09938500	0.04405000
C	4.47157300	0.15507500	-1.35078500
C	2.98463000	0.49499500	-1.07913300
H	1.21992800	2.43340700	0.19138700
H	1.76052400	3.60761100	2.28924900
H	3.92024300	3.18100400	3.45017700
H	5.56365200	1.58535400	2.49309400
H	5.05604200	-0.89904800	0.49111700
H	4.89171900	0.99615700	-1.90642900
H	6.19198900	0.35859400	0.00276000

H	2.48185000	0.99507000	-1.90695700
N	2.28130900	-0.79892900	-0.87346000
O	4.65001000	-0.96922900	-2.18806700
C	1.03345800	-0.99285900	-0.41147200
C	2.81195500	-2.03751100	-1.11390300
N	0.85452900	-2.31049400	-0.38672300
N	1.96150700	-2.98086200	-0.82200800
C	4.20475300	-2.19111700	-1.64399200
H	4.86628000	-2.55387600	-0.84790700
H	4.20687800	-2.92629500	-2.45020500
C	-0.35605500	-3.01590000	-0.05994600
C	-1.45749100	-2.87791900	-0.91197900
C	-0.36106600	-3.81607400	1.08335500
C	-2.60594500	-3.59049400	-0.57569200
C	-1.53898200	-4.50443500	1.37452900
C	-2.66689400	-4.40174900	0.56106000
H	-3.47848400	-3.51277200	-1.22124800
H	-1.57226300	-5.13254100	2.26069600
C	0.85418900	-3.92862600	1.96470900
H	1.24944300	-2.94095200	2.22310700
H	1.65504900	-4.47657100	1.46042100
H	0.60611900	-4.45168300	2.88906600
C	-3.94238100	-5.12570700	0.90337200
H	-3.77159500	-5.90165900	1.65176200
H	-4.38050000	-5.58826400	0.01536200
H	-4.68215200	-4.42546600	1.30581100
C	-1.41707100	-2.00030600	-2.13545400
H	-0.49213500	-2.14526300	-2.70240900
H	-1.47512100	-0.93944500	-1.86678400
H	-2.25775800	-2.23340000	-2.79122400
C	-1.85735200	2.10555300	0.33333600
C	-0.48908000	0.13153600	1.12733400
C	-1.32958700	1.30905600	1.53886000
H	-0.30758400	-0.67465600	1.83173400
H	-2.15224800	0.97306800	2.17807800
H	-0.70995400	1.98595800	2.13963500
C	0.09111600	0.08919300	-0.08671100
O	-0.01452700	0.98432500	-1.06276200
C	-3.09504900	1.60182500	-0.29049100
O	-3.76328000	2.11710400	-1.16555000
O	-3.38222700	0.35712700	0.18189800
C	-1.58979600	3.55027700	0.40805900
O	-0.70186700	4.04054300	1.09433000
O	-2.33996700	4.31662800	-0.40436400

C	-2.00626700	5.70941600	-0.42133400
C	-2.93647300	6.37878600	-1.40954800
H	-0.95637600	5.82390300	-0.70832800
H	-2.11873500	6.12109700	0.58631700
H	-2.71875600	7.44814800	-1.46130900
H	-2.81117700	5.94880800	-2.40587200
H	-3.97775700	6.24977900	-1.10540600
C	-4.47386800	-0.34058700	-0.41991800
C	-4.99286600	-1.33312200	0.60037000
H	-4.10796000	-0.84729800	-1.32215400
H	-5.24260800	0.37320100	-0.72277800
H	-5.77173300	-1.95902600	0.15602100
H	-4.18202700	-1.97920300	0.94714100
H	-5.41513600	-0.81004200	1.46178900
H	-0.94879100	1.69519200	-0.56776200

M4

Zero-point correction= 0.625366 (Hartree/Particle)
Thermal correction to Energy= 0.662819
Thermal correction to Enthalpy= 0.663763
Thermal correction to Gibbs Free Energy= 0.553853
Sum of electronic and zero-point Energies= -1816.662069
Sum of electronic and thermal Energies= -1816.624616
Sum of electronic and thermal Enthalpies= -1816.623672
Sum of electronic and thermal Free Energies= -1816.733582

C	4.81425600	-1.66496800	-0.81902700
C	3.58390600	-1.82761000	-0.17598700
C	2.62822500	-2.71826500	-0.65872000
C	2.92210800	-3.43534000	-1.81790200
C	4.14488200	-3.26732000	-2.47043800
C	5.10303500	-2.38495200	-1.97286000
C	5.68204900	-0.67147400	-0.09073200
C	5.02007000	-0.62614000	1.30297900
C	3.52417600	-0.96101200	1.06260400
H	1.68847700	-2.83877200	-0.12803400
H	2.19438100	-4.13675100	-2.21333100
H	4.35743700	-3.83804200	-3.36903100
H	6.06028800	-2.26821300	-2.47193100
H	5.64237600	0.30272100	-0.59204700
H	5.42932000	-1.43353200	1.91409600
H	6.73210100	-0.96547300	-0.03258500
H	3.02521100	-1.43460700	1.90746600
N	2.81638600	0.32018700	0.82589000
O	5.22508400	0.55061400	2.05883900

C	1.53713400	0.49362300	0.44175100
C	3.36838500	1.56409400	0.96967900
N	1.37302700	1.81270600	0.35222300
N	2.50856600	2.49869800	0.68196400
C	4.78213500	1.73444800	1.43349500
H	5.42278100	2.02187700	0.59125700
H	4.82360900	2.53046500	2.17850300
C	0.15762100	2.52306500	0.06262500
C	-0.83767300	2.54991900	1.04137600
C	0.04100100	3.15145800	-1.17779900
C	-2.00024800	3.25579800	0.73825700
C	-1.14255500	3.84258300	-1.43177200
C	-2.16759700	3.90849700	-0.48547000
H	-2.79555300	3.29236400	1.47899100
H	-1.26681800	4.33826900	-2.39138900
C	1.14684700	3.06597600	-2.19568000
H	1.40852500	2.02314400	-2.40456800
H	2.05249200	3.56196700	-1.83469800
H	0.84336400	3.53714500	-3.13154500
C	-3.42118900	4.69600100	-0.76624200
H	-3.61210100	4.76736500	-1.83953900
H	-3.32948400	5.71421700	-0.37457500
H	-4.29187000	4.23910400	-0.28793900
C	-0.65427300	1.84755800	2.35947400
H	0.27670200	2.16388700	2.84165800
H	-0.61529000	0.76158000	2.22567000
H	-1.48737500	2.07233000	3.02609400
C	-2.29029000	-1.72814300	0.22029400
C	-0.28581400	-0.58360200	-0.76121400
C	-1.29099400	-1.68170000	-0.94748500
H	-0.23104000	0.23564500	-1.46953400
H	-1.83989400	-1.56289500	-1.88481200
H	-0.80086000	-2.66321600	-0.97977900
C	0.53155200	-0.61338600	0.32729900
O	0.60641000	-1.47141600	1.27500100
C	-3.05026500	-0.42564200	0.38103400
O	-3.15795600	0.19888800	1.40963500
O	-3.61739800	-0.06725300	-0.77949200
C	-3.27205200	-2.87527400	0.06417000
O	-3.08016100	-3.86023400	-0.60915700
O	-4.38319100	-2.67780700	0.78452700
C	-5.37200400	-3.72181500	0.72199100
C	-6.54513500	-3.27718700	1.56578800
H	-4.92506700	-4.64834100	1.09315700

H	-5.65040800	-3.87687600	-0.32413700
H	-7.32581700	-4.04068500	1.54456100
H	-6.23726600	-3.12263500	2.60222900
H	-6.96146500	-2.34306600	1.18190300
C	-4.45835600	1.09874200	-0.76886400
C	-4.46142300	1.67147100	-2.16872500
H	-4.06745800	1.80853700	-0.03801800
H	-5.45880600	0.78790200	-0.45023600
H	-5.14099600	2.52573800	-2.22010500
H	-3.45638200	2.00744600	-2.44001400
H	-4.79083300	0.92335100	-2.89360600
H	-1.72553900	-1.88183200	1.14709100

TS5RR

Zero-point correction= 0.969770 (Hartree/Particle)
Thermal correction to Energy= 1.028575
Thermal correction to Enthalpy= 1.029519
Thermal correction to Gibbs Free Energy= 0.877734
Sum of electronic and zero-point Energies= -2906.064540
Sum of electronic and thermal Energies= -2906.005735
Sum of electronic and thermal Enthalpies= -2906.004791
Sum of electronic and thermal Free Energies= -2906.156575
Imaginary frequency= -313.60 cm^{-1}

C	2.90630800	2.33653400	0.30404000
C	1.16583700	0.89112800	-1.05506800
C	2.38417500	1.80459500	-1.03886500
H	0.74137900	0.75856400	-2.04488800
H	3.21896800	1.28927100	-1.53116300
H	2.17945900	2.67067700	-1.67373700
C	1.17559000	-0.24168200	-0.21908300
O	1.72644300	-0.35648900	0.89052600
C	3.65176100	1.34980600	1.19324100
O	3.60208800	1.35658800	2.39673400
O	4.46153300	0.54627300	0.48468700
C	3.84782100	3.51329600	0.03386500
O	4.05267700	4.00079900	-1.05389000
O	4.41050500	3.96169300	1.15758900
C	5.32701200	5.06512500	1.00887800
C	5.75728300	5.47686500	2.39784100
H	4.81701000	5.87352400	0.47749300
H	6.16880200	4.73497800	0.39375200
H	6.46518000	6.30590200	2.33232800
H	4.89566600	5.79971500	2.98646900
H	6.24140100	4.64499300	2.91363900

C	5.18823300	-0.41874200	1.26711000
C	6.17650600	-1.10386100	0.35052800
H	4.46399000	-1.11944300	1.69589200
H	5.69026200	0.09665800	2.08920100
H	6.69267000	-1.90005200	0.89266000
H	5.67361700	-1.54876000	-0.51266100
H	6.91791100	-0.39406100	-0.02291800
H	2.10910000	2.73888800	0.93340500
C	-4.04949100	1.51609600	-0.10782100
C	-2.96850300	2.13432500	-0.78625800
C	-3.23454000	2.97228500	-1.87072100
C	-4.55492900	3.20641600	-2.24996700
C	-5.60602400	2.62362200	-1.54811100
C	-5.36656500	1.77398300	-0.46533700
C	-2.09605700	0.69895900	0.84710500
C	-1.74224700	1.71137200	-0.13147900
H	-2.41748100	3.42554700	-2.41674100
H	-4.76197200	3.85284100	-3.09692900
H	-6.63217000	2.82150500	-1.84137000
H	-6.19174700	1.32062400	0.06256000
C	-0.42223600	2.13195600	-0.13331500
H	0.11540800	1.95815900	0.79459700
C	-0.03761300	3.33876600	-0.91639600
O	-0.24616400	3.50344100	-2.09985200
O	0.60424700	4.23014500	-0.15483800
C	1.09290300	5.40963500	-0.82598300
C	1.72371600	6.28429400	0.23368300
H	0.25589900	5.90149500	-1.32755800
H	1.81870900	5.09690500	-1.58271900
H	2.19213200	7.15327600	-0.23384800
H	0.97446300	6.63242700	0.94785800
H	2.48919500	5.72974000	0.78419800
O	-1.32938400	0.00713800	1.49702700
N	-3.52499300	0.64128300	0.88349000
C	-4.20524000	-0.22726200	1.73626200
O	-3.65914000	-1.00637500	2.48029700
O	-5.52822400	-0.06876900	1.61609400
C	-6.44392100	-0.75330800	2.53103000
C	-6.38522100	-2.26090100	2.31305200
C	-6.13209100	-0.36364200	3.97252400
C	-7.80278700	-0.20301200	2.11440700
H	-6.62893300	-2.50539400	1.27444800
H	-5.39856600	-2.65522700	2.55880800
H	-7.12789600	-2.74145900	2.95613600

H	-6.09885000	0.72558600	4.06533700
H	-6.92839400	-0.73900000	4.62100900
H	-5.18171100	-0.78161600	4.30297500
H	-8.58678000	-0.65147200	2.72947100
H	-7.83223900	0.88206300	2.24518400
H	-8.00949700	-0.43747500	1.06589500
C	4.31883400	-4.28963400	0.30806900
C	3.32433000	-3.33888400	0.52222900
C	2.66923000	-3.22650700	1.74653700
C	3.03639700	-4.09604700	2.76963600
C	4.03768300	-5.05060800	2.56580800
C	4.68594100	-5.15381800	1.33747300
C	4.86156800	-4.21767200	-1.09573900
C	3.94378700	-3.21864500	-1.84023500
C	3.09736100	-2.50188000	-0.71680900
H	1.91017200	-2.46272200	1.88821900
H	2.54399100	-4.02988400	3.73411300
H	4.31103000	-5.72063700	3.37465600
H	5.45833500	-5.90091500	1.18226800
H	4.84856200	-5.18388800	-1.61012800
H	4.51762400	-2.47608900	-2.39644900
H	5.89824700	-3.86613000	-1.10320100
H	3.41178800	-1.46290600	-0.57723100
N	1.68159400	-2.47320800	-1.09361800
O	3.15008600	-3.85627800	-2.83015700
C	0.73189500	-1.54204800	-0.86519300
C	1.10935300	-3.48567400	-1.80508800
N	-0.37454800	-2.03057900	-1.42859300
N	-0.14570800	-3.24521000	-2.03041800
C	2.02133300	-4.54706800	-2.32456900
H	2.29139400	-5.25952500	-1.53390000
H	1.55148800	-5.08259800	-3.14844100
C	-1.76300700	-1.63140300	-1.37244400
C	-2.55240600	-2.31243000	-0.43445900
C	-2.29336500	-0.79882500	-2.35718600
C	-3.93029900	-2.17366600	-0.54357800
C	-3.68515700	-0.67044100	-2.39882500
C	-4.51440800	-1.37097200	-1.52856500
H	-4.56487000	-2.70130100	0.16456300
H	-4.12489800	-0.00369900	-3.13721200
C	-1.44018300	-0.03388000	-3.33148900
H	-1.96083100	0.07871700	-4.28450500
H	-0.48489500	-0.53016300	-3.52174300
H	-1.23785400	0.97259100	-2.94220500

C	-6.01282600	-1.26590800	-1.62145100
H	-6.45035100	-2.21937800	-1.93456900
H	-6.31402600	-0.49386300	-2.33244400
H	-6.42997800	-1.01085600	-0.64276600
C	-1.92791500	-3.13594500	0.65775800
H	-1.30904500	-2.49039100	1.28873400
H	-1.30582000	-3.94130100	0.25415300
H	-2.70376600	-3.57391500	1.28728500

TS5RS

Zero-point correction= 0.968120 (Hartree/Particle)
Thermal correction to Energy= 1.028245
Thermal correction to Enthalpy= 1.029190
Thermal correction to Gibbs Free Energy= 0.871596
Sum of electronic and zero-point Energies= -2906.086230
Sum of electronic and thermal Energies= -2906.026105
Sum of electronic and thermal Enthalpies= -2906.025161
Sum of electronic and thermal Free Energies= -2906.182755
Imaginary frequency= -268.24 cm^{-1}

C	-2.74551100	-0.69564900	2.32054000
C	-2.06875200	0.29213400	0.05999400
C	-2.50562300	-0.93909400	0.81302100
H	-2.84853100	0.95527500	-0.29669700
H	-1.75423200	-1.72646900	0.72177300
H	-3.43982100	-1.32083700	0.39135700
C	-0.79512500	0.81394800	0.35058900
O	0.16011300	0.12168600	0.76606900
C	-1.42190000	-0.39169600	3.01225900
O	-1.08305000	0.70373600	3.40058100
O	-0.68590000	-1.49499400	3.09655700
C	-3.37459900	-1.90366900	3.00185600
O	-4.04224500	-1.83112600	4.00734200
O	-3.07546600	-3.04879700	2.38566200
C	-3.51057800	-4.25992500	3.03125700
C	-2.71015800	-5.39517000	2.43335100
H	-3.34101100	-4.16231000	4.10598500
H	-4.58591200	-4.37575400	2.86407000
H	-2.99532200	-6.33784200	2.90579500
H	-1.64284900	-5.22768500	2.59615200
H	-2.88863000	-5.47869200	1.35782200
C	0.69818300	-1.35169500	3.45936000
C	1.37599100	-2.64212000	3.05715900
H	1.10652500	-0.50224300	2.90762600
H	0.76358500	-1.15212100	4.53310300

H	2.44287500	-2.59254700	3.28707100
H	1.25268500	-2.80167600	1.98194100
H	0.94256000	-3.49284600	3.58923100
H	-3.40494500	0.15745100	2.49214600
C	1.59447600	-2.69519400	-0.95613800
C	0.17819200	-2.64132800	-0.96127400
C	-0.53200100	-3.73060700	-0.44521500
C	0.15446600	-4.84648800	0.02543100
C	1.54648200	-4.88419600	0.00814600
C	2.28365900	-3.80158500	-0.47177800
C	1.00675100	-0.58261100	-1.71038500
C	-0.21560000	-1.34721600	-1.50358600
H	-1.61238700	-3.70114100	-0.40001800
H	-0.40580600	-5.69044900	0.41579100
H	2.07305600	-5.75514400	0.38470400
H	3.36277000	-3.82499100	-0.45537300
C	-1.38872300	-0.65456300	-1.78179700
H	-1.23478100	0.28601500	-2.30368400
C	-2.73484500	-1.20149300	-2.09950900
O	-3.61508100	-0.53749700	-2.60456500
O	-2.88898900	-2.48471900	-1.75915000
C	-4.21169100	-3.03443000	-1.89877800
C	-4.29171700	-4.23298700	-0.97883000
H	-4.94071400	-2.26575100	-1.63017000
H	-4.36913900	-3.30157800	-2.94771500
H	-5.28112800	-4.69067300	-1.04636000
H	-4.11918800	-3.91808300	0.05564300
H	-3.54289900	-4.98290900	-1.24856400
O	1.11431100	0.58227500	-2.06855600
N	2.10357500	-1.46018400	-1.44011900
C	3.40096100	-1.17030600	-1.86747900
O	3.74592800	-0.09289600	-2.29557400
O	4.18217800	-2.24397600	-1.75147000
C	5.54647800	-2.24209300	-2.28034400
C	6.39451300	-1.16740800	-1.60722900
C	5.49950600	-2.07563100	-3.79472100
C	6.04386000	-3.63175600	-1.90057100
H	6.23206400	-1.18050900	-0.52528900
H	6.16114500	-0.17596900	-1.99463600
H	7.45002500	-1.38007400	-1.79868300
H	4.88069300	-2.85868400	-4.24140600
H	6.51212400	-2.16379200	-4.19751900
H	5.09800900	-1.09853700	-4.06693800
H	7.04903200	-3.78662200	-2.29978300

H	5.38024900	-4.39705300	-2.31170500
H	6.07897400	-3.74132500	-0.81284500
C	3.57358100	2.89234100	2.47707700
C	2.72070400	2.30154900	1.54584700
C	3.20296400	1.66121700	0.40993600
C	4.58443000	1.62060500	0.22402400
C	5.44892500	2.19454600	1.15904400
C	4.95124700	2.83536700	2.29291000
C	2.79001800	3.53549300	3.59491000
C	1.33931600	3.59666600	3.07155000
C	1.28201700	2.48854300	1.96554200
H	2.52998200	1.23230400	-0.33015500
H	4.97743000	1.14318900	-0.66597500
H	6.52119500	2.15255600	0.99356600
H	5.62544600	3.29360800	3.01045700
H	3.13811900	4.53889800	3.85497200
H	0.60858900	3.37984800	3.85234700
H	2.83365800	2.92515700	4.50362300
H	0.84003100	1.57949400	2.37347400
N	0.43038900	2.92016300	0.85461600
O	0.99272600	4.89905800	2.60919300
C	-0.50052200	2.26997600	0.12972300
C	0.42270700	4.22689300	0.46112400
N	-1.04214100	3.21083300	-0.65576100
N	-0.47390900	4.43836500	-0.45666800
C	1.26911500	5.17350800	1.24639900
H	2.33107400	5.04360900	1.00320700
H	0.97366300	6.20258600	1.04487400
C	-2.19280500	3.11422600	-1.51562600
C	-2.00747100	2.95334900	-2.88939600
C	-3.44848800	3.26462100	-0.91762000
C	-3.15729400	2.85172900	-3.67129400
C	-4.56384100	3.15358800	-1.74411700
C	-4.43519600	2.92552600	-3.11613700
H	-3.04818500	2.71162100	-4.74370600
H	-5.55410200	3.25076700	-1.30685400
C	-3.57509100	3.53851400	0.55837500
H	-3.04221900	4.45524700	0.82986900
H	-3.14943800	2.72488700	1.15733900
H	-4.62304900	3.65281200	0.83803300
C	-5.65316200	2.74426300	-3.98187200
H	-5.86464000	1.67773300	-4.11020600
H	-5.50026000	3.17215400	-4.97527000
H	-6.53363900	3.20852900	-3.53291900

C	-0.63037300	2.93389500	-3.49379600
H	-0.00623700	2.15319200	-3.05030800
H	-0.13059900	3.89319500	-3.32370900
H	-0.69232800	2.76642300	-4.57024300

TS5SR

Zero-point correction= 0.968653 (Hartree/Particle)
Thermal correction to Energy= 1.028525
Thermal correction to Enthalpy= 1.029469
Thermal correction to Gibbs Free Energy= 0.873019
Sum of electronic and zero-point Energies= -2906.094902
Sum of electronic and thermal Energies= -2906.035031
Sum of electronic and thermal Enthalpies= -2906.034086
Sum of electronic and thermal Free Energies= -2906.190537
Imaginary frequency= -266.38 cm^{-1}

C	-2.38049400	0.60388600	2.11664900
C	-1.83561800	-0.46114900	-0.12952200
C	-2.33367800	0.76897200	0.58538900
H	-2.56739100	-1.22469000	-0.36503500
H	-1.69131400	1.62436300	0.36062900
H	-3.34271900	1.01458200	0.24377900
C	-0.48508400	-0.81799700	0.03700900
O	0.41478600	-0.00669300	0.35113000
C	-0.97733400	0.50612400	2.70159100
O	-0.50068400	-0.49149900	3.19460000
O	-0.34606700	1.67160100	2.59256200
C	-3.07649600	1.74945500	2.84363400
O	-3.17039600	1.79755500	4.04898300
O	-3.55365900	2.68343200	2.02410300
C	-4.17947200	3.81507500	2.66027900
C	-4.64461200	4.74144000	1.56059700
H	-3.44604300	4.28869100	3.31838300
H	-5.00714700	3.45595000	3.27773700
H	-5.10055800	5.63345400	1.99542500
H	-3.79956300	5.04975700	0.93963700
H	-5.38586700	4.24624900	0.92884400
C	1.05155700	1.68077400	2.93679000
C	1.65296000	2.93392200	2.34108800
H	1.50920100	0.77890300	2.52405000
H	1.13756400	1.65537200	4.02764600
H	2.68671200	3.03965900	2.68159600
H	1.64670200	2.88072700	1.24841100
H	1.09625500	3.82119700	2.65323700
H	-2.90502400	-0.31585200	2.39457200

C	1.02834700	3.02698100	-1.51221900
C	-0.35328900	2.72772000	-1.56472800
C	-1.26673900	3.73054400	-1.22079300
C	-0.80736300	4.99768200	-0.87748500
C	0.55636000	5.28556400	-0.88333900
C	1.49075700	4.30240900	-1.20436100
C	0.85062500	0.81593000	-2.19942900
C	-0.49266000	1.34495000	-1.99863500
H	-2.32598700	3.51549300	-1.21663500
H	-1.52211700	5.77103400	-0.61349100
H	0.90388600	6.28258300	-0.63339900
H	2.54696400	4.52804700	-1.19990400
C	-1.50390200	0.39841300	-2.10910000
H	-1.17468500	-0.53517500	-2.55801000
C	-2.95906600	0.60328600	-2.34483400
O	-3.72476700	-0.30650000	-2.59195200
O	-3.34647100	1.87720100	-2.27152900
C	-4.74796300	2.12655900	-2.49041400
C	-4.94884800	3.62428500	-2.43946400
H	-5.31868500	1.60520400	-1.71591000
H	-5.02912400	1.70578000	-3.45921400
H	-5.99798900	3.86172700	-2.62871800
H	-4.67779300	4.02050700	-1.45766300
H	-4.33707800	4.11922000	-3.19724200
O	1.16663900	-0.30378000	-2.57652600
N	1.76812800	1.86719000	-1.86448200
C	3.10873700	1.60574500	-1.58382400
O	3.67907300	0.58517300	-1.90271000
O	3.65326500	2.61318900	-0.90552500
C	5.00322100	2.50093700	-0.34927100
C	5.03252500	1.36960500	0.67177100
C	6.02927900	2.31265700	-1.46147400
C	5.18911800	3.85197200	0.33029300
H	4.25034900	1.51583700	1.42350500
H	4.88206300	0.40179200	0.19296400
H	6.00211200	1.36278100	1.17767900
H	5.90181800	3.08679400	-2.22341300
H	7.03163900	2.41230200	-1.03603400
H	5.93545500	1.33221700	-1.92750200
H	6.16039600	3.88509700	0.82982600
H	5.14812400	4.65905000	-0.40666200
H	4.40418600	4.01427600	1.07392500
C	4.52732500	-2.21335200	0.75658400
C	3.17343200	-1.92638500	0.91357100

C	2.60174500	-1.73127500	2.16632200
C	3.42828700	-1.82264400	3.28525800
C	4.79023600	-2.10089600	3.13979700
C	5.34954500	-2.29834700	1.87746900
C	4.88452000	-2.35144200	-0.70449200
C	3.53253500	-2.39965600	-1.45245000
C	2.50009200	-1.82183500	-0.43121500
H	1.54238500	-1.50195400	2.26815000
H	3.00993400	-1.67371100	4.27568900
H	5.41980600	-2.16744600	4.02152800
H	6.40785100	-2.51846400	1.77229500
H	5.47403300	-3.24568300	-0.92777500
H	3.52695400	-1.77253400	-2.34246500
H	5.45975100	-1.48255200	-1.04540700
H	2.26776400	-0.79642900	-0.69062500
N	1.24889600	-2.57964200	-0.47277100
O	3.22078700	-3.71109100	-1.91783700
C	-0.03563000	-2.20910600	-0.31592200
C	1.26907000	-3.92761400	-0.67021500
N	-0.73481900	-3.34864100	-0.41984900
N	0.06735300	-4.42844900	-0.65022300
C	2.59053100	-4.55310400	-0.97395500
H	3.18277100	-4.66229400	-0.05503700
H	2.44976000	-5.53307100	-1.42904900
C	-2.14389200	-3.56665100	-0.22581100
C	-2.97411100	-3.65308800	-1.34278500
C	-2.59880900	-3.69637400	1.09105400
C	-4.33412500	-3.85889100	-1.10340000
C	-3.96380800	-3.89745900	1.27279900
C	-4.84429100	-3.97395700	0.18900500
H	-5.00836600	-3.92783600	-1.95338400
H	-4.34983200	-4.00379300	2.28342300
C	-1.64651000	-3.59503600	2.25185300
H	-1.30597500	-2.56210300	2.39639200
H	-0.76126600	-4.21900100	2.09252600
H	-2.13345100	-3.91907900	3.17300300
C	-6.32162000	-4.15838500	0.41874800
H	-6.80617500	-3.19055300	0.58278800
H	-6.51030100	-4.77482100	1.30058300
H	-6.80035400	-4.62733500	-0.44329500
C	-2.45881000	-3.47318200	-2.74520500
H	-3.03278300	-4.09058600	-3.43926900
H	-1.40443000	-3.74024600	-2.83767900
H	-2.58883900	-2.42771500	-3.04577500

TS5SS

Zero-point correction=	0.968142 (Hartree/Particle)
Thermal correction to Energy=	1.027932
Thermal correction to Enthalpy=	1.028876
Thermal correction to Gibbs Free Energy=	0.871711
Sum of electronic and zero-point Energies=	-2906.069044
Sum of electronic and thermal Energies=	-2906.009254
Sum of electronic and thermal Enthalpies=	-2906.008310
Sum of electronic and thermal Free Energies=	-2906.165475

Imaginary frequency= -224.33 cm^{-1}

C	-3.65108100	-0.01598400	-0.71084200
C	-1.42988500	-0.81441500	0.37082000
C	-2.93673000	-0.91883300	0.30938900
H	-0.89843400	-1.69696800	0.71184400
H	-3.37134500	-0.71135400	1.29809300
H	-3.21387300	-1.95139600	0.08201300
C	-0.90035800	0.44065800	0.69682200
O	-1.50499900	1.53170300	0.69921200
C	-3.86622200	1.43955700	-0.30675200
O	-3.68963100	2.38194300	-1.03992200
O	-4.41939800	1.51901000	0.91065300
C	-5.03771500	-0.58418000	-1.01346300
O	-5.48426600	-1.61590900	-0.56777000
O	-5.71596400	0.20641700	-1.85146700
C	-7.05678900	-0.21450800	-2.17160000
C	-7.59612100	0.75785800	-3.19532900
H	-7.01989900	-1.23843500	-2.55430800
H	-7.64721700	-0.21894600	-1.25109400
H	-8.61882300	0.48260700	-3.46184600
H	-6.98395100	0.74138600	-4.09990900
H	-7.60185500	1.77422800	-2.79573500
C	-4.73507600	2.84228100	1.37883400
C	-3.51316600	3.52915300	1.95581600
H	-5.15499800	3.41382300	0.54765800
H	-5.50714600	2.68866000	2.13480600
H	-3.79360100	4.52075200	2.32291600
H	-2.73820300	3.62931600	1.19414700
H	-3.10586800	2.94994200	2.78837400
H	-3.11379200	0.01807500	-1.66276900
C	2.98820500	-2.22900000	-1.26504500
C	1.66445400	-2.73227400	-1.23033300
C	1.44786000	-4.05211300	-0.82854900
C	2.53732100	-4.84474400	-0.47398200

C	3.83065200	-4.32827500	-0.49985300
C	4.07388000	-3.01066900	-0.89413400
C	1.59865200	-0.49510200	-1.92770000
C	0.77428200	-1.66050800	-1.64219100
H	0.43953800	-4.44133100	-0.78686500
H	2.37202100	-5.87169000	-0.16401500
H	4.67063100	-4.95234700	-0.21278800
H	5.08003500	-2.61916400	-0.91317000
C	-0.58561900	-1.45479600	-1.70302200
H	-0.89094500	-0.52953100	-2.18071000
C	-1.58780400	-2.55067500	-1.75200500
O	-1.53944300	-3.60063900	-1.14838400
O	-2.59480800	-2.22270600	-2.57031000
C	-3.64459400	-3.20070100	-2.71189800
C	-4.59883300	-2.66521300	-3.75567900
H	-3.19817300	-4.15360400	-3.00759600
H	-4.13024100	-3.32893800	-1.74047300
H	-5.46874300	-3.32115000	-3.83456900
H	-4.11370000	-2.60718900	-4.73248500
H	-4.94052300	-1.66221000	-3.48446100
O	1.22524200	0.60187200	-2.31869100
N	2.94676100	-0.86429400	-1.66494600
C	4.00539000	0.04459300	-1.78807100
O	3.84811200	1.24197300	-1.81968800
O	5.16632100	-0.59832600	-1.86953700
C	6.43093300	0.14694100	-1.86323100
C	6.56675000	0.89985600	-0.54505000
C	6.50782100	1.06464600	-3.07863100
C	7.46993100	-0.96265500	-1.96511200
H	6.49205800	0.19846500	0.29202800
H	5.79765200	1.66607000	-0.43814500
H	7.55147900	1.37399100	-0.50495500
H	6.29510500	0.49762500	-3.98924500
H	7.52196500	1.46625300	-3.15397800
H	5.80335800	1.89136100	-2.99802600
H	8.47160200	-0.52630200	-1.98302600
H	7.32264600	-1.54091500	-2.88094300
H	7.40157600	-1.63621600	-1.10625200
C	0.96209500	4.72492600	0.53800300
C	0.55967200	3.56095400	-0.12313300
C	-0.60384600	3.53601600	-0.88459800
C	-1.39754900	4.67933000	-0.92549700
C	-1.01882100	5.83111200	-0.23099100
C	0.17000300	5.86783900	0.49587600

C	2.32173500	4.54259500	1.16266300
C	2.86778300	3.36558700	0.32748000
C	1.62747300	2.49743200	-0.01556500
H	-0.89971300	2.64063000	-1.41914200
H	-2.32272600	4.66126700	-1.49108100
H	-1.64875100	6.71453500	-0.27260800
H	0.48080400	6.77518100	1.00507400
H	2.23253100	4.28495400	2.22519100
H	3.22516700	3.74745200	-0.63124500
H	2.95913000	5.42635500	1.08933200
H	1.77350400	1.93325200	-0.93539400
N	1.45241900	1.47755800	1.07535600
O	3.96124300	2.66200200	0.87044300
C	0.49992000	0.53316300	1.27699100
C	2.42772800	1.24292200	2.01231000
N	0.91500200	-0.17405900	2.33199600
N	2.11617300	0.25111500	2.79502000
C	3.68535800	2.04929400	2.10289300
H	3.59403200	2.78009000	2.91662700
H	4.51658600	1.38164300	2.33625200
C	0.22322500	-1.22706100	3.03189900
C	-0.97035600	-0.93048800	3.69583700
C	0.80502200	-2.49949300	3.02474900
C	-1.62011400	-1.99040700	4.33035300
C	0.11258100	-3.51741000	3.67561600
C	-1.10538800	-3.28559400	4.31906900
H	-2.55183700	-1.78984900	4.85324300
H	0.53641900	-4.51851400	3.67772100
C	2.13189800	-2.75959100	2.36370100
H	2.94931600	-2.36548500	2.97491500
H	2.19616600	-2.28353200	1.38034400
H	2.28479300	-3.83063900	2.22659200
C	-1.84698400	-4.41885300	4.97805100
H	-2.57114800	-4.04807000	5.70615000
H	-1.15764900	-5.09723000	5.48655400
H	-2.39259900	-5.00368300	4.23071600
C	-1.55555600	0.45729100	3.75177300
H	-2.09299600	0.59113600	4.69274700
H	-2.25856200	0.63190500	2.93038100
H	-0.78468500	1.22999900	3.68466200

M5RR

Zero-point correction= 0.972993 (Hartree/Particle)

Thermal correction to Energy= 1.031805

Thermal correction to Enthalpy= 1.032750
Thermal correction to Gibbs Free Energy= 0.878679
Sum of electronic and zero-point Energies= -2906.113716
Sum of electronic and thermal Energies= -2906.054904
Sum of electronic and thermal Enthalpies= -2906.053960
Sum of electronic and thermal Free Energies= -2906.208030

C	-2.78834900	2.26132600	-0.10759600
C	-0.50213600	1.14103800	0.53632900
C	-1.95462800	1.47692700	0.91812000
H	0.07688300	1.08384900	1.46016700
H	-2.50705000	0.57025000	1.18797500
H	-1.93776200	2.08833900	1.82643100
C	-0.43555100	-0.24444500	-0.16531400
O	-1.19902900	-0.41637700	-1.16704900
C	-2.94983000	1.59876400	-1.47153800
O	-2.40920400	1.97564400	-2.48101900
O	-3.83750800	0.59798700	-1.41114400
C	-4.18037100	2.51418700	0.45731400
O	-4.59420300	2.08855100	1.50933900
O	-4.89783500	3.27306100	-0.37467200
C	-6.25564600	3.53611100	0.02902000
C	-6.89505000	4.36547100	-1.06073400
H	-6.23781200	4.05860100	0.98946900
H	-6.76504800	2.57919400	0.17332700
H	-7.93041500	4.58820300	-0.79399500
H	-6.35985400	5.30835700	-1.19225000
H	-6.88909500	3.82405200	-2.00920300
C	-3.94346700	-0.22484100	-2.58947000
C	-5.18963700	-1.06864400	-2.44331800
H	-3.02900800	-0.82494900	-2.63889500
H	-3.99186800	0.42227600	-3.46784300
H	-5.27807600	-1.74555800	-3.29627000
H	-5.14987800	-1.67717000	-1.53542700
H	-6.08214400	-0.44011600	-2.39902700
H	-2.33720200	3.23853200	-0.30877900
C	3.85393300	1.52720600	-0.86412200
C	2.82165400	2.48408700	-0.71831900
C	3.13430300	3.84763700	-0.73603800
C	4.45959300	4.23374600	-0.88830800
C	5.46973100	3.27645300	-1.02847400
C	5.18273100	1.91305800	-1.02495700
C	1.86488400	0.44230200	-0.63338900
C	1.58166300	1.77134000	-0.56820700
H	2.34762000	4.59167200	-0.65261400

H	4.71370000	5.28878700	-0.90225700
H	6.50031200	3.59488500	-1.14498100
H	5.97233600	1.18422900	-1.13504000
C	0.18796300	2.24129000	-0.28750100
H	-0.36300600	2.44673000	-1.21151100
C	0.22658800	3.50700900	0.55486300
O	0.55632400	3.54750400	1.71924400
O	-0.14476100	4.58839600	-0.13937500
C	-0.10717300	5.83873800	0.57783600
C	-0.51431200	6.92387000	-0.39172800
H	0.90613500	5.98550600	0.96365000
H	-0.78609000	5.76822500	1.43223400
H	-0.50315300	7.89178200	0.11402100
H	0.17707200	6.96505800	-1.23645300
H	-1.52157500	6.74208000	-0.77308700
O	1.04731000	-0.58621700	-0.48727000
N	3.24601500	0.24888200	-0.83191400
C	3.82622200	-0.97805300	-1.16876600
O	3.19493100	-1.94462500	-1.52111900
O	5.15206900	-0.90664700	-1.04055800
C	6.01283300	-1.92103900	-1.65848000
C	5.86593200	-3.25453800	-0.93551600
C	5.69564400	-2.03064800	-3.14594700
C	7.40866100	-1.34842100	-1.44663700
H	6.16921100	-3.15699800	0.11112800
H	4.83869200	-3.61733700	-0.98917500
H	6.52469300	-3.98835300	-1.40824300
H	5.70953900	-1.03697700	-3.60367100
H	6.46337400	-2.64173000	-3.62780000
H	4.72239900	-2.49110400	-3.31611300
H	8.15662500	-2.05868800	-1.80744200
H	7.52941500	-0.40990000	-1.99468500
H	7.58423800	-1.16404800	-0.38310600
C	-3.94424900	-4.12427000	-0.60248900
C	-2.87903600	-3.23557600	-0.71808300
C	-1.87889800	-3.40937100	-1.67197600
C	-1.95704000	-4.51833000	-2.51033500
C	-3.01785300	-5.42188400	-2.39586200
C	-4.02014800	-5.22942900	-1.44775800
C	-4.91313300	-3.69357300	0.46820400
C	-4.25699200	-2.46833800	1.15394400
C	-2.99557300	-2.10741000	0.27931500
H	-1.08700300	-2.66984900	-1.75876600
H	-1.19241100	-4.67924100	-3.26317300

H	-3.06345500	-6.28134800	-3.05719600
H	-4.84597100	-5.93002500	-1.36821900
H	-5.10906300	-4.47510900	1.21001800
H	-4.92825900	-1.60826100	1.17404900
H	-5.88172600	-3.41875500	0.03814900
H	-3.10124800	-1.13955400	-0.21145400
N	-1.79332000	-2.01623900	1.12685600
O	-3.96086100	-2.71294400	2.52064900
C	-0.65930400	-1.31367300	0.96853000
C	-1.65569800	-2.76674400	2.26223700
N	0.10664500	-1.65377100	2.00920800
N	-0.50231500	-2.56260500	2.82735100
C	-2.83956700	-3.55265700	2.71648400
H	-2.92556500	-4.49208300	2.15298900
H	-2.76002600	-3.77917500	3.77927700
C	1.48348900	-1.28987100	2.23396800
C	2.44526000	-2.12736400	1.65288700
C	1.80239800	-0.15542900	2.97570700
C	3.77334100	-1.74685600	1.77274700
C	3.15563600	0.20309800	3.03090000
C	4.14301800	-0.55882800	2.41500700
H	4.53885000	-2.37071800	1.32065000
H	3.43166400	1.10470700	3.57220700
C	0.77913100	0.65997900	3.72591500
H	1.02486800	0.66103200	4.79152300
H	-0.23147100	0.25898600	3.61746800
H	0.78014000	1.69780700	3.37850900
C	5.57977800	-0.11096100	2.39106600
H	6.26113000	-0.95872000	2.50423400
H	5.78825200	0.61574700	3.17895000
H	5.79786300	0.36081200	1.42586600
C	2.03404300	-3.36223400	0.90075000
H	1.48991900	-3.07768400	-0.00547300
H	1.39116600	-4.00252600	1.51225700
H	2.91336400	-3.93350700	0.59919000

M5RS

Zero-point correction=	0.971975 (Hartree/Particle)
Thermal correction to Energy=	1.031221
Thermal correction to Enthalpy=	1.032165
Thermal correction to Gibbs Free Energy=	0.875273
Sum of electronic and zero-point Energies=	-2906.096486
Sum of electronic and thermal Energies=	-2906.037240
Sum of electronic and thermal Enthalpies=	-2906.036296

Sum of electronic and thermal Free Energies= -2906.193188

C	3.87321600	0.62013600	-0.74206900
C	1.70144600	-0.30913400	0.23990400
C	2.45008000	0.13582700	-1.04700400
H	2.37832100	-0.18909700	1.09118000
H	1.90844100	0.94622600	-1.53554000
H	2.51763300	-0.67978700	-1.77221400
C	0.56957400	0.76150900	0.42674000
O	1.00135700	1.95269400	0.28943300
C	3.81639700	1.80425500	0.20826900
O	3.96384000	1.71615500	1.40666100
O	3.54124100	2.93480100	-0.43816300
C	4.61791700	0.98426300	-2.01217800
O	4.20417300	0.81537600	-3.13460400
O	5.81763600	1.50331200	-1.73143900
C	6.61076200	1.90629800	-2.86301200
C	7.87755600	2.53017200	-2.32300400
H	6.81538800	1.02513600	-3.47790400
H	6.02803900	2.60986600	-3.46402200
H	8.51375300	2.84845100	-3.15171600
H	8.43220700	1.81211800	-1.71502100
H	7.64363700	3.40250000	-1.70882300
C	3.15096600	4.04928700	0.38351500
C	2.33856000	4.98391400	-0.48341500
H	2.56061600	3.66050000	1.21493200
H	4.05544900	4.52500500	0.77617500
H	2.05391500	5.86897500	0.09119400
H	1.43153200	4.47472800	-0.81916300
H	2.91031400	5.30741200	-1.35659400
H	4.43396000	-0.17131500	-0.23276500
C	-2.09366100	-2.72261800	-1.16084400
C	-0.83300300	-3.13140500	-0.67021700
C	-0.57549200	-4.48842500	-0.45366600
C	-1.57409100	-5.41352200	-0.72796600
C	-2.81678000	-4.99496300	-1.22098400
C	-3.09532600	-3.64921600	-1.44650600
C	-0.81838300	-0.87610400	-0.75356900
C	-0.04236800	-1.95314200	-0.44334700
H	0.39123500	-4.80496000	-0.07191400
H	-1.39108900	-6.47060500	-0.56304900
H	-3.58452400	-5.73174500	-1.43371300
H	-4.05883700	-3.33983100	-1.82544900
C	1.30403100	-1.80571500	0.16961100
H	1.28633200	-2.21926000	1.18011100

C	2.44485300	-2.58451500	-0.46334700
O	3.55966300	-2.60822100	0.01479300
O	2.10928800	-3.23495700	-1.57716200
C	3.15418000	-4.00468000	-2.20001300
C	2.53234000	-4.72433600	-3.37517100
H	3.95258400	-3.32198300	-2.50625500
H	3.56649500	-4.69727300	-1.46120900
H	3.28683200	-5.33287300	-3.87844500
H	2.12591400	-4.00903800	-4.09333100
H	1.72366000	-5.37700900	-3.03769900
O	-0.51388900	0.40981900	-0.67904900
N	-2.08503900	-1.30970800	-1.20415200
C	-3.16494800	-0.45067700	-1.45788600
O	-3.20489200	0.69761900	-1.09603800
O	-4.10708000	-1.09917200	-2.14193700
C	-5.36292600	-0.42594000	-2.48150300
C	-5.07805700	0.71666000	-3.44856100
C	-6.07555800	0.04433700	-1.21759800
C	-6.15807600	-1.53215500	-3.16382900
H	-4.54229500	0.34049600	-4.32475800
H	-4.48417500	1.49561300	-2.96816300
H	-6.02628200	1.14710100	-3.78326300
H	-6.14851600	-0.77862100	-0.50045500
H	-7.08924200	0.35794400	-1.48177800
H	-5.55536800	0.88251800	-0.75402300
H	-7.11398800	-1.13627800	-3.51515200
H	-6.35598500	-2.34966000	-2.46466500
H	-5.60474700	-1.92519100	-4.02065600
C	-3.13584100	3.72016700	-0.07112000
C	-1.80675900	3.28832200	-0.12130400
C	-1.16251200	3.13203000	-1.34577300
C	-1.87683000	3.38708100	-2.51399100
C	-3.20791100	3.80279900	-2.46260900
C	-3.84738800	3.97507400	-1.23730300
C	-3.59159100	3.90789100	1.34940300
C	-2.24112800	4.09396400	2.06326600
C	-1.22380000	3.21374600	1.27771200
H	-0.13254300	2.79931100	-1.36994000
H	-1.38822300	3.27008100	-3.47625800
H	-3.74502800	4.00770900	-3.38431900
H	-4.87605000	4.32107500	-1.19132800
H	-4.12399500	3.01563700	1.69941300
H	-1.91360500	5.12525400	1.91031900
H	-4.25070800	4.76667600	1.49409500

H	-0.20421800	3.58995800	1.32726800
N	-1.16155800	1.85914600	1.93229400
O	-2.24151900	3.90855900	3.46097300
C	-0.37941200	0.77635800	1.66555900
C	-1.76923400	1.61203900	3.13635900
N	-0.58089800	-0.05434800	2.68697900
N	-1.43671200	0.45162100	3.61661100
C	-2.63232400	2.61116400	3.83798500
H	-3.69138600	2.41940800	3.62853400
H	-2.47315700	2.51140800	4.91240000
C	0.04712300	-1.31225800	2.97218000
C	-0.67572700	-2.48427500	2.73297900
C	1.33604700	-1.28681500	3.50774000
C	-0.01384000	-3.68751700	2.96579300
C	1.95332400	-2.52038400	3.72195600
C	1.30232900	-3.72284600	3.43854500
H	-0.53477400	-4.61932900	2.75860200
H	2.96589800	-2.53972000	4.11528800
C	2.01406200	0.01305700	3.86088200
H	1.43958000	0.54171600	4.62859700
H	2.11617500	0.68749400	3.00422100
H	3.01462300	-0.17659100	4.25187500
C	1.99972000	-5.04445000	3.62833800
H	1.39184100	-5.72452700	4.23092000
H	2.96674400	-4.91674500	4.11777500
H	2.17022100	-5.52692900	2.66076700
C	-2.10302900	-2.44675500	2.25780400
H	-2.24655300	-1.69227400	1.47831400
H	-2.77260500	-2.19851900	3.08763900
H	-2.39348600	-3.41702600	1.84961700

M5SR

Zero-point correction= 0.972326 (Hartree/Particle)
Thermal correction to Energy= 1.030783
Thermal correction to Enthalpy= 1.031727
Thermal correction to Gibbs Free Energy= 0.876217
Sum of electronic and zero-point Energies= -2906.102288
Sum of electronic and thermal Energies= -2906.043831
Sum of electronic and thermal Enthalpies= -2906.042887
Sum of electronic and thermal Free Energies= -2906.198397

C	3.39460800	0.36678100	-1.38521300
C	1.42157300	0.20577100	0.20932700
C	1.90867500	0.68546000	-1.17607300
H	2.22945500	-0.34907000	0.69600100

H	1.33939900	0.18150200	-1.96005200
H	1.75560300	1.76047900	-1.30081700
C	0.28420000	-0.82024100	-0.04387300
O	0.57144300	-1.77646800	-0.82663400
C	3.55957700	-1.14099600	-1.45540900
O	4.02684900	-1.82001800	-0.57030900
O	3.05324000	-1.61407300	-2.59272000
C	3.94522300	1.05764800	-2.61897900
O	3.43458100	2.00987600	-3.16061000
O	5.10274700	0.51465300	-3.00595000
C	5.73197800	1.12056200	-4.15121100
C	6.99892300	0.34458000	-4.42983600
H	5.93313800	2.17099500	-3.92291900
H	5.03313400	1.08504800	-4.99139900
H	7.51113800	0.77488900	-5.29310900
H	7.67194600	0.38440900	-3.57060200
H	6.76963300	-0.70097900	-4.64686100
C	2.84182300	-3.03481200	-2.67909700
C	1.62488200	-3.24573600	-3.55077600
H	2.68421900	-3.42139700	-1.67070600
H	3.74618500	-3.48946500	-3.09605200
H	1.41885900	-4.31425000	-3.65555000
H	0.77007000	-2.76267400	-3.07235800
H	1.77739100	-2.82175700	-4.54669500
H	3.98496200	0.71446500	-0.52878300
C	-2.29322600	3.05788300	0.57100600
C	-1.03223200	3.06438000	1.20837700
C	-0.70117500	4.10187800	2.08464700
C	-1.62524400	5.11352100	2.31014700
C	-2.86868600	5.09643600	1.66914500
C	-3.22170900	4.07379100	0.79243500
C	-1.12144500	1.20719600	-0.07096900
C	-0.30829400	1.89644000	0.77579000
H	0.26748000	4.11403500	2.57541100
H	-1.38154800	5.92530600	2.98797700
H	-3.58074500	5.89368000	1.85523000
H	-4.18685300	4.07521700	0.30843600
C	1.04642200	1.38903100	1.13716700
H	1.07520900	1.04658400	2.17486800
C	2.18878400	2.38982800	1.05197600
O	3.29197300	2.16111900	1.50034200
O	1.88296900	3.50129300	0.38276300
C	2.96998300	4.41429000	0.14217400
C	2.41746300	5.54811400	-0.69028600

H	3.76643900	3.87248800	-0.37711900
H	3.36118600	4.75611800	1.10432100
H	3.20208600	6.28335800	-0.88154900
H	2.04925100	5.17322100	-1.64781400
H	1.59517400	6.04234000	-0.16761100
O	-0.89698300	0.04359400	-0.66150800
N	-2.35048600	1.89171700	-0.23290000
C	-3.34356600	1.50816900	-1.13876700
O	-3.26951400	0.51796900	-1.83013000
O	-4.35653000	2.36606900	-1.10689600
C	-5.55208400	2.13567400	-1.92485100
C	-5.18864800	2.18283700	-3.40418300
C	-6.20980200	0.82032400	-1.52139300
C	-6.43697800	3.31790300	-1.54903700
H	-4.65563700	3.11064500	-3.62939800
H	-4.56904400	1.33283300	-3.68830000
H	-6.10843400	2.16318500	-3.99489600
H	-6.37041900	0.79906800	-0.43941100
H	-7.18346800	0.74521700	-2.01302400
H	-5.60174600	-0.03602800	-1.81357200
H	-7.37628300	3.26642600	-2.10466500
H	-6.66226200	3.30223600	-0.47912300
H	-5.93770700	4.25973300	-1.79240800
C	-3.25970500	-3.92953100	-0.74807800
C	-2.60527200	-2.70277600	-0.90208800
C	-1.99781600	-2.37126600	-2.11031700
C	-2.01874900	-3.30640000	-3.14293100
C	-2.63940000	-4.54590200	-2.97683100
C	-3.27421500	-4.86306400	-1.77861400
C	-3.94117800	-4.01983800	0.58945900
C	-4.04455600	-2.53204800	0.97731100
C	-2.81426900	-1.83562800	0.32490100
H	-1.53053700	-1.40441600	-2.23292800
H	-1.55246600	-3.06360800	-4.09272100
H	-2.64573200	-5.25910300	-3.79544800
H	-3.78654900	-5.81240200	-1.65525300
H	-3.32771600	-4.59105200	1.29503500
H	-4.92224900	-2.10570100	0.48521200
H	-4.92338700	-4.49580700	0.54822000
H	-3.00829300	-0.79648000	0.07486700
N	-1.69459500	-1.83791600	1.32312800
O	-4.21058300	-2.25586700	2.34959100
C	-0.42088000	-1.37527900	1.24072300
C	-1.85201400	-2.32789100	2.59699900

N	0.13623400	-1.67711600	2.41748500
N	-0.74902800	-2.25508800	3.27650600
C	-3.17241200	-2.77948400	3.14122600
H	-3.21021500	-3.87272300	3.20816000
H	-3.28741100	-2.37299000	4.14707300
C	1.48430400	-1.48343100	2.89019000
C	2.49783700	-2.30301900	2.38255800
C	1.69389400	-0.52700400	3.88814000
C	3.79077200	-2.06237500	2.84199400
C	3.00597700	-0.33528100	4.31784200
C	4.06394700	-1.08014500	3.79619800
H	4.60380500	-2.66134300	2.44044800
H	3.20318500	0.41998500	5.07422700
C	0.55904400	0.25782500	4.49680100
H	0.09572800	-0.31081100	5.30875400
H	-0.22948800	0.48056700	3.77156900
H	0.92745500	1.20050300	4.90611700
C	5.47299500	-0.86171500	4.28175200
H	5.73431000	-1.60015400	5.04675900
H	5.59075900	0.13072700	4.72125700
H	6.18988600	-0.96722200	3.46439800
C	2.19904000	-3.40863000	1.40779900
H	1.78583100	-3.01222900	0.47504300
H	1.46732800	-4.10246900	1.83668200
H	3.11133700	-3.96047500	1.17844300

M5SS

Zero-point correction= 0.970706 (Hartree/Particle)
Thermal correction to Energy= 1.030113
Thermal correction to Enthalpy= 1.031057
Thermal correction to Gibbs Free Energy= 0.871660
Sum of electronic and zero-point Energies= -2906.108493
Sum of electronic and thermal Energies= -2906.049085
Sum of electronic and thermal Enthalpies= -2906.048141
Sum of electronic and thermal Free Energies= -2906.207539

C	3.24150100	0.63694000	-0.94989400
C	1.05111500	0.80825300	0.49995400
C	2.50045200	0.30423400	0.34839500
H	0.88747000	1.06111500	1.55077200
H	2.53006600	-0.78181700	0.45026500
H	3.10413900	0.69641800	1.17273800
C	0.05004700	-0.27678400	0.07707800
O	0.03261800	-0.62729400	-1.13040000
C	2.64086100	0.00955300	-2.20043800

O	2.16260600	0.62412200	-3.12174200
O	2.79192300	-1.31861600	-2.17697500
C	4.67933300	0.13875600	-0.84341800
O	5.16563900	-0.39223900	0.12579600
O	5.34126500	0.36571700	-1.98148100
C	6.70425400	-0.09906800	-2.02317100
C	7.24322600	0.21555800	-3.39972900
H	7.26768900	0.40502800	-1.23323100
H	6.71131400	-1.17216700	-1.81216500
H	8.27844500	-0.12397100	-3.47578700
H	7.21523500	1.29080400	-3.58847300
H	6.65414000	-0.29010400	-4.16803900
C	2.35507600	-2.01323100	-3.35720400
C	2.83015500	-3.44334800	-3.22792800
H	1.26555800	-1.92932100	-3.42261900
H	2.78876800	-1.51957200	-4.23107300
H	2.56557800	-4.00648800	-4.12611400
H	2.37732500	-3.93281000	-2.36089600
H	3.91629500	-3.47195200	-3.11252600
H	3.28372300	1.71453400	-1.13817500
C	-2.76065400	3.40368900	-0.52142000
C	-1.37372600	3.62734300	-0.70545000
C	-0.93264500	4.85217400	-1.21686700
C	-1.86952200	5.83188300	-1.52217300
C	-3.23383700	5.60235900	-1.32044200
C	-3.69915100	4.38825700	-0.81767100
C	-1.60890000	1.54584400	0.13228600
C	-0.67431500	2.44532500	-0.27525400
H	0.12725000	5.02367200	-1.37817400
H	-1.53829800	6.78591200	-1.92010600
H	-3.95199100	6.38012900	-1.55860900
H	-4.75603500	4.22443300	-0.66697500
C	0.78523700	2.10195700	-0.30154900
H	1.11228500	1.98396200	-1.34021300
C	1.59609300	3.22275900	0.33521800
O	1.66234800	3.43773700	1.52347300
O	2.23246500	3.96411900	-0.58225000
C	2.96829700	5.09456800	-0.07583500
C	3.58558700	5.79507000	-1.26457300
H	2.27476800	5.74032800	0.47078100
H	3.72107000	4.73260900	0.62954300
H	4.15679700	6.66232500	-0.92645400
H	2.81132300	6.13769600	-1.95509400
H	4.25884800	5.12295800	-1.80135200

O	-1.41316300	0.33279100	0.58969800
N	-2.90709400	2.08979300	-0.01136200
C	-4.07487300	1.35196600	0.18634900
O	-4.08731600	0.18717800	0.51535700
O	-5.14457200	2.10923800	-0.03966500
C	-6.49294000	1.54499900	0.06587500
C	-6.75967700	1.10276600	1.50010000
C	-6.66693300	0.41197600	-0.93991100
C	-7.37422500	2.73192900	-0.30381800
H	-6.55244200	1.92539000	2.19008900
H	-6.14740300	0.24307500	1.77121600
H	-7.81421900	0.83036000	1.59754100
H	-6.38632900	0.75299500	-1.94028700
H	-7.71930600	0.11597300	-0.96007500
H	-6.06162300	-0.45448400	-0.67233200
H	-8.42590000	2.43877300	-0.26085500
H	-7.14735700	3.07482200	-1.31698800
H	-7.21269600	3.55791400	0.39424500
C	-2.89650000	-4.29263600	-1.53734100
C	-1.80122200	-3.47020400	-1.28473400
C	-0.60312500	-3.61285900	-1.97420900
C	-0.52021600	-4.60890400	-2.94545000
C	-1.61611600	-5.43354600	-3.21300400
C	-2.81142200	-5.28246200	-2.51233400
C	-4.05855300	-3.92620300	-0.64737800
C	-3.45197600	-3.01200000	0.43912900
C	-2.12715900	-2.46926200	-0.20140800
H	0.22475000	-2.94493400	-1.74943600
H	0.40155900	-4.74864400	-3.50044700
H	-1.53175800	-6.20485400	-3.97196900
H	-3.65734400	-5.93153500	-2.71803000
H	-4.54710000	-4.78849400	-0.18501900
H	-4.10104700	-2.17583000	0.69725400
H	-4.82180900	-3.37994800	-1.21281500
H	-2.27097800	-1.45720000	-0.58094700
N	-1.06856000	-2.40751100	0.81004300
O	-3.25348800	-3.71028800	1.66715400
C	-0.10379200	-1.50160500	1.04157000
C	-0.95736900	-3.38619500	1.75367600
N	0.54873000	-1.96334600	2.11103300
N	0.02317700	-3.14289500	2.57180700
C	-2.03458300	-4.42057100	1.78672200
H	-1.89942800	-5.15619600	0.98348600
H	-2.03618200	-4.93264600	2.74868000

C	1.60234200	-1.34482300	2.87250300
C	2.90039500	-1.84225300	2.73817900
C	1.25893900	-0.29995300	3.73344400
C	3.89972700	-1.21026500	3.47430800
C	2.29859900	0.30503200	4.43857200
C	3.61906500	-0.13331900	4.31818600
H	4.92411700	-1.55887400	3.37360700
H	2.06822900	1.13401800	5.10248600
C	-0.17468200	0.12866400	3.91234800
H	-0.76212600	-0.68810900	4.34503200
H	-0.65155700	0.40068600	2.96444700
H	-0.23293400	0.98613100	4.58392500
C	4.71975800	0.52152400	5.11098700
H	4.47292400	1.55859200	5.34729500
H	5.66342800	0.50426600	4.56132600
H	4.87773200	-0.00714100	6.05658500
C	3.20514600	-2.99972100	1.82525900
H	2.78474100	-2.85116300	0.82416900
H	2.77804800	-3.92653600	2.22011400
H	4.28332000	-3.12714600	1.72207100

TS6RR

Zero-point correction= 0.971164 (Hartree/Particle)
Thermal correction to Energy= 1.030018
Thermal correction to Enthalpy= 1.030962
Thermal correction to Gibbs Free Energy= 0.876176
Sum of electronic and zero-point Energies= -2906.099655
Sum of electronic and thermal Energies= -2906.040801
Sum of electronic and thermal Enthalpies= -2906.039857
Sum of electronic and thermal Free Energies= -2906.194643
Imaginary frequency= -133.44 cm^{-1}

C	-2.81501200	2.21388800	-0.62493200
C	-0.50906900	1.28424800	0.20794600
C	-1.98302700	1.58032300	0.49844400
H	-0.00625400	1.12235200	1.16295500
H	-2.47023900	0.65852400	0.83526100
H	-2.03206500	2.27147900	1.34584200
C	-0.33257400	-0.01028800	-0.59245300
O	-1.13768300	-0.42095900	-1.40440000
C	-3.10736400	1.30580500	-1.80893200
O	-2.71881300	1.50675800	-2.93234900
O	-3.89573600	0.28641900	-1.44395200
C	-4.13149900	2.73561700	-0.06120000
O	-4.38842500	2.84972400	1.11451300

O	-4.95934400	3.09949600	-1.04155100
C	-6.22379600	3.65550800	-0.62953800
C	-7.01246000	3.95124200	-1.88450300
H	-6.02920700	4.55712900	-0.04148900
H	-6.72823400	2.93153700	0.01580800
H	-7.98014600	4.38114200	-1.61715800
H	-6.47785900	4.66336600	-2.51668600
H	-7.18416400	3.03575700	-2.45483200
C	-4.11578400	-0.73073600	-2.43930000
C	-5.29620500	-1.56280000	-1.99130300
H	-3.19433800	-1.31820700	-2.51100800
H	-4.30077700	-0.24955200	-3.40200700
H	-5.44951900	-2.39013800	-2.68819200
H	-5.12419000	-1.98657600	-0.99838000
H	-6.20593000	-0.95913700	-1.95510100
H	-2.30521100	3.09174700	-1.03340100
C	3.94791400	1.61455100	-0.88735400
C	2.95798500	2.60461600	-0.68829400
C	3.33070600	3.94838700	-0.58424700
C	4.67336800	4.28313400	-0.68429300
C	5.64239900	3.29330500	-0.88785900
C	5.29717300	1.94997300	-0.99568200
C	1.91993000	0.61515300	-0.79290000
C	1.68022800	1.94172600	-0.63742800
H	2.58098300	4.71629100	-0.42622900
H	4.97618900	5.32211800	-0.60439800
H	6.68812600	3.57270300	-0.96288700
H	6.05616500	1.19705000	-1.14768600
C	0.28572900	2.44615300	-0.44625400
H	-0.17258400	2.74965100	-1.39494800
C	0.21321800	3.60756500	0.52903000
O	0.92423500	3.73435600	1.49917500
O	-0.78926600	4.43800500	0.22710800
C	-1.06669300	5.49001300	1.17456900
C	-2.45699300	6.00235300	0.87370700
H	-0.30286800	6.26408600	1.05903400
H	-0.98858600	5.07878300	2.18376800
H	-2.69737500	6.83143000	1.54285700
H	-2.52491700	6.35731900	-0.15723200
H	-3.19336500	5.20907900	1.02763300
O	1.03079400	-0.39069500	-0.80973800
N	3.28530800	0.36598800	-0.96818700
C	3.82154400	-0.88106800	-1.31432000
O	3.14906200	-1.82410800	-1.65209400

O	5.14861300	-0.85136900	-1.21551400
C	5.96090400	-1.92653600	-1.79877100
C	5.72248300	-3.24009500	-1.06360900
C	5.66342700	-2.03768500	-3.28972100
C	7.38175400	-1.42984800	-1.56538500
H	5.93598600	-3.12726600	0.00340200
H	4.69757300	-3.58633000	-1.19689000
H	6.40581200	-3.99420700	-1.46398300
H	5.76835100	-1.05899600	-3.76651800
H	6.38366800	-2.72232000	-3.74520100
H	4.65768400	-2.41942100	-3.46763600
H	8.09592800	-2.17280800	-1.92828400
H	7.55556100	-0.49192300	-2.10004900
H	7.55722300	-1.26800200	-0.49805200
C	-3.68636000	-4.39170400	-0.22715600
C	-2.67956200	-3.44319900	-0.38092800
C	-1.68466800	-3.58398100	-1.34579700
C	-1.71526200	-4.70987700	-2.16504600
C	-2.72330100	-5.66766400	-2.01689800
C	-3.71520900	-5.51523700	-1.05105600
C	-4.64724600	-4.00792900	0.86788800
C	-4.05684100	-2.72552600	1.50781400
C	-2.84059800	-2.30148800	0.59645700
H	-0.92323700	-2.81636400	-1.46178800
H	-0.95387300	-4.84378600	-2.92635900
H	-2.73280200	-6.53992700	-2.66274700
H	-4.49567400	-6.26203700	-0.93946300
H	-4.75834700	-4.78676900	1.62974000
H	-4.79021800	-1.91788700	1.53021300
H	-5.64837800	-3.81462800	0.46892500
H	-3.03657500	-1.35852000	0.07589600
N	-1.64002400	-2.09872600	1.40241900
O	-3.70841800	-2.91536700	2.87130600
C	-0.57414000	-1.30752900	1.13081700
C	-1.40545200	-2.80484700	2.55263200
N	0.24228900	-1.58174700	2.15609400
N	-0.24616300	-2.50325400	3.05611800
C	-2.51630900	-3.65780200	3.06724800
H	-2.54843000	-4.62123500	2.53893300
H	-2.40383700	-3.84180300	4.13538900
C	1.56686600	-1.04649700	2.28269100
C	2.61056900	-1.79300400	1.71984300
C	1.76341200	0.20207600	2.87257000
C	3.88345800	-1.23768900	1.74200900

C	3.05429800	0.74036200	2.82167600
C	4.11834000	0.04101200	2.25960100
H	4.70950100	-1.79175400	1.30361400
H	3.22149000	1.73333400	3.23279400
C	0.65710500	0.96071500	3.56153000
H	0.82519900	0.96174000	4.64280000
H	-0.32460200	0.51737600	3.37924100
H	0.64231300	2.00122600	3.22442500
C	5.50355700	0.63032300	2.21258100
H	6.09008300	0.32056200	3.08400800
H	5.46704500	1.72224500	2.19865900
H	6.02958000	0.29498100	1.31424900
C	2.32966600	-3.12289600	1.07567100
H	1.74576900	-2.97247200	0.16136000
H	1.75881300	-3.77368000	1.74406400
H	3.26107500	-3.62391300	0.80521100

TS6RS

Zero-point correction= 0.970323 (Hartree/Particle)
Thermal correction to Energy= 1.029660
Thermal correction to Enthalpy= 1.030604
Thermal correction to Gibbs Free Energy= 0.873257
Sum of electronic and zero-point Energies= -2906.107069
Sum of electronic and thermal Energies= -2906.047732
Sum of electronic and thermal Enthalpies= -2906.046788
Sum of electronic and thermal Free Energies= -2906.204136
Imaginary frequency= -81.96 cm^{-1}

C	2.94165900	2.69685400	0.09674100
C	1.07487300	1.06864200	-0.50240800
C	1.45816500	2.35199600	0.28913400
H	1.96245400	0.69639900	-1.01808100
H	1.27455700	2.21916800	1.35897200
H	0.85396700	3.20980000	-0.01888600
C	0.72853800	0.02295800	0.55124200
O	1.57374500	-0.43643600	1.29411300
C	3.80163400	1.50310100	0.48405100
O	4.32297600	0.75898400	-0.31854900
O	3.83700500	1.33692700	1.80024200
C	3.32324100	3.92723800	0.90021700
O	2.53892700	4.64975900	1.46662600
O	4.64351800	4.12054200	0.88230500
C	5.12304200	5.26185000	1.62045600
C	6.62891900	5.27757700	1.49202000
H	4.66341300	6.16260700	1.20437500

H	4.79744900	5.16382400	2.65963500
H	7.03582700	6.12940200	2.04112100
H	6.92518500	5.36561700	0.44452900
H	7.05904400	4.36137800	1.90234700
C	4.40341400	0.09587100	2.27431900
C	3.86526500	-0.13857900	3.66614300
H	4.09633400	-0.70105700	1.59347100
H	5.49329500	0.18887200	2.25190300
H	4.28068300	-1.06693000	4.06605100
H	2.77800400	-0.23113900	3.62069600
H	4.13178100	0.68093600	4.33771500
H	3.14391100	2.89841300	-0.96085300
C	-3.59482000	1.23669500	-0.35730700
C	-2.68479600	1.56567300	-1.38644300
C	-3.16164400	2.09317400	-2.59112700
C	-4.52551500	2.29721800	-2.74355300
C	-5.41154000	1.99778400	-1.70063300
C	-4.96331500	1.46884100	-0.49540100
C	-1.51204900	0.64514400	0.28655100
C	-1.35965200	1.21429500	-0.93453200
H	-2.47007900	2.33878300	-3.39073100
H	-4.90904200	2.70084200	-3.67508500
H	-6.47360000	2.17905900	-1.83011800
H	-5.65923600	1.24173200	0.29829400
C	-0.01325800	1.28917900	-1.57632600
H	0.10343600	0.49805300	-2.32712700
C	0.34255500	2.57396900	-2.30602600
O	1.36861900	2.69506800	-2.93976000
O	-0.54377800	3.55121700	-2.13739100
C	-0.24494900	4.80348200	-2.78588000
C	-1.41291100	5.72547400	-2.51997900
H	0.69287500	5.18996400	-2.37631800
H	-0.09792700	4.61560800	-3.85284000
H	-1.24186200	6.68881000	-3.00506600
H	-1.53510400	5.89210300	-1.44758100
H	-2.33663500	5.29376400	-2.91268100
O	-0.56898700	0.10656100	1.08059000
N	-2.85065500	0.64792300	0.69147200
C	-3.30663200	0.12886800	1.91299400
O	-2.59644000	-0.45327300	2.69480600
O	-4.60122300	0.39135400	2.06622700
C	-5.26544200	0.13005200	3.34977500
C	-4.55137000	0.88352900	4.46715300
C	-5.33246000	-1.36933200	3.61054300

C	-6.65820100	0.70519400	3.12547400
H	-4.43460700	1.93599400	4.19373000
H	-3.57181300	0.45461800	4.67610600
H	-5.16089400	0.83028900	5.37310000
H	-5.86067700	-1.87283900	2.79567800
H	-5.88921400	-1.54367900	4.53541700
H	-4.33394000	-1.79548200	3.71568800
H	-7.26022200	0.56846400	4.02699800
H	-7.15897200	0.19706900	2.29624900
H	-6.59887400	1.77353900	2.90131800
C	4.50913900	-3.69398900	-0.15267400
C	3.31109200	-3.05989100	0.16707500
C	2.67410100	-3.27706900	1.38499700
C	3.26853700	-4.15020900	2.29434200
C	4.47181100	-4.78826800	1.98231900
C	5.10095200	-4.56513000	0.75837000
C	4.98517900	-3.28432000	-1.52466000
C	3.77744600	-2.56510700	-2.16621000
C	2.86272500	-2.15606400	-0.96235600
H	1.74824300	-2.75870700	1.61739300
H	2.79302500	-4.33661600	3.25193400
H	4.91890100	-5.46943300	2.69955500
H	6.03230100	-5.06914700	0.51756400
H	5.29844200	-4.12613800	-2.14905000
H	4.08360100	-1.68103700	-2.72715600
H	5.83423000	-2.59628100	-1.44944500
H	3.01966000	-1.10769800	-0.70102000
N	1.45652600	-2.35478200	-1.29140800
O	3.11217800	-3.38071600	-3.12568500
C	0.35708800	-1.67096800	-0.87490400
C	1.07508800	-3.47401800	-1.98267600
N	-0.63228900	-2.44196700	-1.35179600
N	-0.21809600	-3.56299200	-2.04519000
C	2.16069900	-4.29350200	-2.60221800
H	2.60982200	-4.97143700	-1.86367800
H	1.77280100	-4.88178800	-3.43387500
C	-2.02976200	-2.28211700	-1.06919600
C	-2.49315700	-2.67527000	0.18992000
C	-2.86907600	-1.76625000	-2.05821200
C	-3.85905300	-2.54730200	0.43905800
C	-4.22357800	-1.63959400	-1.75540300
C	-4.73366000	-2.02212500	-0.51482900
H	-4.24475100	-2.86049800	1.40632400
H	-4.89205500	-1.21248500	-2.49928100

C	-2.31830400	-1.34866300	-3.39387600
H	-3.11559400	-0.97952600	-4.04127300
H	-1.81322600	-2.18178700	-3.89113400
H	-1.58396900	-0.54607400	-3.27211000
C	-6.19297000	-1.84229000	-0.19013900
H	-6.62140700	-2.75523400	0.23408000
H	-6.76775000	-1.56719900	-1.07702900
H	-6.31451700	-1.04442900	0.55065500
C	-1.54714200	-3.18012000	1.24679000
H	-0.97031700	-2.34461600	1.65946200
H	-0.84464200	-3.91408100	0.83956700
H	-2.10247600	-3.64382100	2.06446700

TS6SR

Zero-point correction= 0.971218 (Hartree/Particle)
Thermal correction to Energy= 1.030461
Thermal correction to Enthalpy= 1.031406
Thermal correction to Gibbs Free Energy= 0.872936
Sum of electronic and zero-point Energies= -2906.090707
Sum of electronic and thermal Energies= -2906.031464
Sum of electronic and thermal Enthalpies= -2906.030520
Sum of electronic and thermal Free Energies= -2906.188990
Imaginary frequency= -122.41 cm^{-1}

C	3.63551900	0.25041000	-1.32058100
C	1.48225800	0.21055000	0.03517400
C	2.19645800	0.76957600	-1.22783400
H	2.17527700	-0.43909100	0.57747100
H	1.66389100	0.47502400	-2.13611200
H	2.21749500	1.86280300	-1.22556700
C	0.36825100	-0.70072200	-0.48649200
O	0.64282700	-1.69451300	-1.13961200
C	3.61947000	-1.26419800	-1.45183700
O	3.91535900	-2.03171300	-0.56652400
O	3.17006000	-1.62292900	-2.65375700
C	4.37643900	0.88671300	-2.48263300
O	3.98430600	1.83816200	-3.11522300
O	5.54269300	0.27389700	-2.70087600
C	6.34156200	0.80161800	-3.77739000
C	7.59073100	-0.04516800	-3.86419600
H	6.56734600	1.84951700	-3.56122400
H	5.75223000	0.76489200	-4.69756000
H	8.22994800	0.32307500	-4.66956200
H	8.15106900	-0.00149000	-2.92781500
H	7.33564300	-1.08664800	-4.07166200

C	2.81857500	-3.00911000	-2.82601200
C	1.77775700	-3.06674300	-3.92087700
H	2.42375700	-3.37954900	-1.87860100
H	3.72623900	-3.56563100	-3.07931000
H	1.48095700	-4.10380500	-4.09676400
H	0.90081100	-2.49472900	-3.60828100
H	2.16560000	-2.65311400	-4.85490500
H	4.18054000	0.48694700	-0.39965300
C	-2.28025100	3.00408600	0.20777600
C	-1.07332400	3.01462100	0.94217300
C	-0.84128800	4.02486700	1.88127600
C	-1.80200300	5.00988600	2.06055100
C	-2.98513500	4.99624700	1.31183300
C	-3.24375700	3.99856700	0.37782200
C	-1.04129200	1.19815000	-0.37787000
C	-0.29414400	1.87006600	0.53254900
H	0.08031100	4.03587000	2.45363100
H	-1.63543300	5.79862300	2.78695800
H	-3.72406100	5.77653900	1.46076100
H	-4.16272400	4.00009400	-0.18877400
C	1.01843800	1.32902200	0.99469200
H	0.91948400	0.90216300	1.99557600
C	2.16995400	2.31274800	1.12321700
O	3.25031400	1.99368000	1.56927700
O	1.89168100	3.52964300	0.65919300
C	2.96030400	4.49381700	0.71958600
C	2.39758600	5.80634900	0.22377700
H	3.78552500	4.13319800	0.09802300
H	3.31484100	4.55709100	1.75183600
H	3.16796400	6.57923700	0.26736000
H	2.05501400	5.71251200	-0.80888100
H	1.55303500	6.11697900	0.84361100
O	-0.76591900	0.03667600	-0.98697000
N	-2.25880700	1.85659700	-0.62258200
C	-3.21279800	1.42826300	-1.55624000
O	-3.11201700	0.39786600	-2.17959400
O	-4.21352200	2.29533600	-1.62416900
C	-5.39514000	1.99775400	-2.44519100
C	-5.00054500	1.92516800	-3.91509000
C	-6.05663000	0.71695500	-1.94752200
C	-6.28773700	3.20337200	-2.18135000
H	-4.47149900	2.83650400	-4.20691400
H	-4.36668900	1.06110900	-4.11305900
H	-5.90736800	1.84533800	-4.52069700

H	-6.23390800	0.78269400	-0.86978600
H	-7.02255400	0.60067700	-2.44623500
H	-5.44367500	-0.15929300	-2.16082900
H	-7.21177900	3.11001100	-2.75679400
H	-6.54289900	3.26556000	-1.11980600
H	-5.78115800	4.12518100	-2.47953200
C	-3.52160400	-3.85164200	-0.23303500
C	-2.79711200	-2.70674900	-0.58449900
C	-2.11639700	-2.64227600	-1.79603100
C	-2.12523400	-3.76453600	-2.62424600
C	-2.81802700	-4.91899800	-2.25873100
C	-3.53314500	-4.96635800	-1.06302500
C	-4.26197000	-3.64680000	1.06047500
C	-4.28565600	-2.10709500	1.16306300
C	-2.98499000	-1.62387400	0.46109000
H	-1.59839500	-1.73932500	-2.08594400
H	-1.59608300	-3.73278300	-3.57155200
H	-2.81775900	-5.78036200	-2.91950700
H	-4.10183000	-5.85069400	-0.79145400
H	-3.71404800	-4.10454700	1.89179700
H	-5.11982800	-1.73107200	0.56544400
H	-5.26910500	-4.06947200	1.05953300
H	-3.08725200	-0.62977700	0.02825700
N	-1.90607900	-1.56506400	1.48038300
O	-4.47484300	-1.57301900	2.45419000
C	-0.57763500	-1.30152200	1.30546600
C	-2.13357600	-1.81827400	2.81294400
N	-0.08545800	-1.48274500	2.54204800
N	-1.02784600	-1.79103700	3.48959000
C	-3.50645200	-2.00354400	3.38382300
H	-3.66330300	-3.04554400	3.68710400
H	-3.60673400	-1.37530700	4.27067100
C	1.28885500	-1.41608000	2.95065600
C	2.19935800	-2.31778700	2.38974600
C	1.66048600	-0.45884800	3.90467700
C	3.53799500	-2.19421200	2.76508400
C	3.00721800	-0.38551700	4.25010800
C	3.96040100	-1.23252200	3.68066300
H	4.26423400	-2.87056300	2.32282900
H	3.32217100	0.36160100	4.97487300
C	0.65511100	0.46410700	4.54675700
H	0.12596200	-0.04498600	5.35711500
H	-0.10796600	0.80273500	3.83850600
H	1.15863600	1.34068900	4.95913900

C	5.41679000	-1.08735000	4.03663500
H	5.54494600	-0.88680300	5.10332700
H	5.86099400	-0.24982900	3.48902400
H	5.97900900	-1.98815300	3.78243500
C	1.76543000	-3.38537800	1.42087900
H	1.54396600	-2.96075400	0.43673600
H	0.86433800	-3.89388800	1.77830300
H	2.56000100	-4.12407900	1.30203400

TS6SS

Zero-point correction= 0.970550 (Hartree/Particle)
Thermal correction to Energy= 1.029938
Thermal correction to Enthalpy= 1.030882
Thermal correction to Gibbs Free Energy= 0.873837
Sum of electronic and zero-point Energies= -2906.085448
Sum of electronic and thermal Energies= -2906.026060
Sum of electronic and thermal Enthalpies= -2906.025115
Sum of electronic and thermal Free Energies= -2906.182161
Imaginary frequency= -186.77 cm^{-1}

C	3.50350100	0.02447800	-1.10943900
C	1.24443900	0.47182900	0.12135900
C	2.63854200	-0.17462000	0.14424200
H	0.97129200	0.68948400	1.15168000
H	2.54430300	-1.24823000	0.30783300
H	3.19313500	0.22921800	0.99793000
C	0.19180000	-0.52099600	-0.45122500
O	0.53575800	-1.48855300	-1.11481400
C	2.83342500	-0.55185900	-2.34683900
O	2.22248700	0.10847100	-3.15524600
O	2.98730500	-1.87216500	-2.40273200
C	4.86542000	-0.62189600	-0.90918000
O	5.23607600	-1.17780600	0.09692300
O	5.62061400	-0.47782600	-2.00270600
C	6.92917900	-1.07576100	-1.94663600
C	7.60185300	-0.80883100	-3.27384700
H	7.47838100	-0.63494200	-1.10992100
H	6.81360900	-2.14530800	-1.75005000
H	8.60188300	-1.24791600	-3.27466100
H	7.69389800	0.26515000	-3.44988600
H	7.02792400	-1.24992100	-4.09170900
C	2.17029600	-2.57473500	-3.35838000
C	1.97368900	-3.97684600	-2.82843500
H	1.22082000	-2.04454200	-3.44665500
H	2.68357900	-2.56058600	-4.32510100

H	1.38693300	-4.56445300	-3.53916200
H	1.43141800	-3.93026700	-1.88128700
H	2.93334300	-4.47593500	-2.67283100
H	3.67996100	1.08606200	-1.31390600
C	-2.20194800	3.44284900	-0.46889200
C	-0.80325100	3.63136200	-0.36414200
C	-0.29560100	4.91218900	-0.12378800
C	-1.18270600	5.97158300	0.00895700
C	-2.56371300	5.76763100	-0.09975800
C	-3.09462100	4.50448400	-0.34505500
C	-1.16695600	1.44799900	-0.76996700
C	-0.17882100	2.34789900	-0.55626500
H	0.77585400	5.07752600	-0.06181400
H	-0.80152100	6.97027100	0.19531600
H	-3.24046300	6.60861400	0.00821700
H	-4.16238300	4.35530600	-0.42640800
C	1.23654600	1.86577900	-0.54383200
H	1.63304300	1.82895300	-1.56319900
C	2.11364100	2.78207900	0.29493100
O	2.08169000	2.84391800	1.50265300
O	2.92768700	3.52473600	-0.46221100
C	3.78847000	4.43515800	0.25198700
C	4.57340800	5.21256800	-0.77903400
H	3.16689400	5.08442700	0.87552800
H	4.43435600	3.85118200	0.91351000
H	5.24655600	5.91148500	-0.27796800
H	3.90152300	5.78077000	-1.42607300
H	5.16999900	4.53913200	-1.39820700
O	-1.04117500	0.13353700	-0.95933500
N	-2.42435300	2.07132300	-0.73466100
C	-3.60179700	1.46969800	-1.19398900
O	-3.60672100	0.46348000	-1.86554800
O	-4.66095600	2.13999900	-0.76247800
C	-6.01510100	1.66470500	-1.07893500
C	-6.21077600	0.25593300	-0.52443800
C	-6.24773100	1.73942300	-2.58230700
C	-6.89465600	2.66370200	-0.33908300
H	-5.86732600	0.20480700	0.51440600
H	-5.67240800	-0.48209500	-1.12049400
H	-7.27632700	0.01231800	-0.54469400
H	-6.05557500	2.75381700	-2.94230100
H	-7.29118200	1.49046900	-2.79311100
H	-5.60498300	1.03882300	-3.11564000
H	-7.94647900	2.41716300	-0.50112800

H	-6.71490600	3.67720700	-0.70800400
H	-6.68763300	2.63506900	0.73368100
C	-3.06698800	-4.10780800	-0.32334500
C	-2.62234900	-2.83867400	-0.71416600
C	-2.01660100	-2.64257500	-1.94989000
C	-1.80295100	-3.75368500	-2.76580600
C	-2.20077400	-5.02736000	-2.35783800
C	-2.85092200	-5.21257400	-1.13740100
C	-3.82309100	-4.03119300	0.97859000
C	-4.21228300	-2.53659100	0.99966200
C	-3.02622600	-1.80881000	0.31799700
H	-1.72161700	-1.65002900	-2.26404300
H	-1.33007400	-3.62273200	-3.73436400
H	-2.02563000	-5.87894000	-3.00830100
H	-3.19904700	-6.19677000	-0.83868700
H	-3.17325000	-4.29529200	1.82151300
H	-5.08048700	-2.39657100	0.35039700
H	-4.69706000	-4.68491500	1.01617400
H	-3.30329300	-0.85257500	-0.11884000
N	-1.99767800	-1.55885500	1.36087700
O	-4.58053200	-1.98735700	2.24433000
C	-0.70634000	-1.14610500	1.21834400
C	-2.24623900	-1.75600800	2.69920100
N	-0.24829400	-1.17341600	2.47717300
N	-1.18266200	-1.54007400	3.41024300
C	-3.59149600	-2.14066700	3.23670600
H	-3.56076900	-3.16665600	3.62377100
H	-3.85136900	-1.47520200	4.06181900
C	1.10621000	-0.99389400	2.92176000
C	2.00822600	-2.03889100	2.70205200
C	1.45538700	0.19690100	3.56022700
C	3.32088000	-1.85054700	3.12598900
C	2.78642300	0.34414800	3.95262400
C	3.72865000	-0.66310100	3.73891200
H	4.04977600	-2.63803100	2.95124900
H	3.09182900	1.27133100	4.43072400
C	0.43432300	1.27847700	3.78867800
H	-0.38426100	0.91243300	4.41498200
H	0.00212000	1.61939900	2.84128100
H	0.89402400	2.14103800	4.27238900
C	5.17160300	-0.47582200	4.12944300
H	5.32054800	0.46291400	4.66640500
H	5.80571800	-0.46492800	3.23751700
H	5.51608500	-1.29607300	4.76537900

C	1.57799600	-3.29244700	1.98526400
H	1.33737100	-3.07759500	0.93649700
H	0.68173300	-3.72275200	2.44358900
H	2.37335900	-4.03890800	2.01048400

PRR

Zero-point correction= 0.584203 (Hartree/Particle)
Thermal correction to Energy= 0.622574
Thermal correction to Enthalpy= 0.623518
Thermal correction to Gibbs Free Energy= 0.509490
Sum of electronic and zero-point Energies= -1854.552973
Sum of electronic and thermal Energies= -1854.514602
Sum of electronic and thermal Enthalpies= -1854.513658
Sum of electronic and thermal Free Energies= -1854.627686

C	-2.96679400	-1.39686900	-0.37583800
C	-0.70070600	-0.25829600	-0.63855800
C	-2.11326800	-0.42934500	-1.20065000
H	-0.72279200	-0.27617000	0.46224800
H	-2.61891200	0.54120500	-1.21343900
H	-2.06620900	-0.78740300	-2.23175000
C	0.17314100	-1.43753800	-1.01806800
O	-0.22650800	-2.47512000	-1.46614200
C	-3.06207600	-0.90675100	1.05988900
O	-2.51315700	-1.42810300	2.00183000
O	-3.77164900	0.21910700	1.13025100
C	-4.35666500	-1.53154100	-0.97483900
O	-4.69539000	-1.07968100	-2.04189000
O	-5.15648600	-2.22871000	-0.16584600
C	-6.50928600	-2.42059000	-0.62607700
C	-7.24089500	-3.19607800	0.44535600
H	-6.47876500	-2.95860200	-1.57750200
H	-6.95704100	-1.43929400	-0.80455200
H	-8.27389700	-3.36639200	0.13445000
H	-6.76456800	-4.16432200	0.61341600
H	-7.24783800	-2.64037800	1.38551400
C	-3.81699800	0.85637200	2.42304400
C	-4.44455400	2.21659600	2.22879600
H	-2.79551800	0.92995800	2.80157900
H	-4.39732500	0.22092600	3.09834800
H	-4.53246800	2.72237400	3.19296300
H	-3.81540300	2.82124600	1.57238500
H	-5.44125400	2.12755300	1.79066500
H	-2.50671500	-2.38902600	-0.34595100
C	3.53080200	1.45873900	0.07569000

C	2.31957900	2.10755900	-0.25334200
C	2.25063800	3.50464300	-0.20872500
C	3.37886900	4.21645800	0.17133100
C	4.56828100	3.55511000	0.50425400
C	4.66694900	2.16925800	0.46110700
C	2.00480100	-0.10240400	-0.46276600
C	1.36048100	1.08061300	-0.58976400
H	1.33495500	4.01697800	-0.48071000
H	3.34078200	5.30011500	0.20839600
H	5.43763100	4.13359700	0.79832500
H	5.58569900	1.65961000	0.71091400
C	-0.08392000	1.10253900	-1.00184200
H	-0.18878700	1.31366500	-2.07299900
C	-0.85246300	2.17804700	-0.23844100
O	-1.34895800	2.01657400	0.85250000
O	-0.90300300	3.31783400	-0.92428800
C	-1.55038000	4.42895800	-0.26694500
C	-1.41696500	5.62715600	-1.17820300
H	-1.06823100	4.58563100	0.70214200
H	-2.59579500	4.16179000	-0.09072800
H	-1.90484700	6.48999700	-0.72010400
H	-0.36587700	5.87371300	-1.34661500
H	-1.88957400	5.43200100	-2.14303000
O	1.51702700	-1.33353900	-0.75761600
N	3.32849400	0.06886700	-0.05825600
C	4.31134500	-0.90293100	0.20593600
O	5.44825400	-0.59926600	0.48089500
O	3.80312500	-2.11561900	0.11345000
C	4.64621600	-3.30487600	0.29118800
C	5.73710100	-3.32429800	-0.77227700
C	5.20604700	-3.33407000	1.70794000
C	3.65167000	-4.43753800	0.07376400
H	5.29338700	-3.22855800	-1.76700800
H	6.45772800	-2.52064800	-0.61953600
H	6.26329300	-4.28122100	-0.72150200
H	4.39478200	-3.23808600	2.43464900
H	5.70117400	-4.29501300	1.87154000
H	5.92937100	-2.53427200	1.86644900
H	4.16170000	-5.39895000	0.16858000
H	2.85152500	-4.38778300	0.81655200
H	3.20861000	-4.36767100	-0.92282300

PRS

Zero-point correction= 0.584794 (Hartree/Particle)

Thermal correction to Energy= 0.623058
Thermal correction to Enthalpy= 0.624002
Thermal correction to Gibbs Free Energy= 0.510363
Sum of electronic and zero-point Energies= -1854.547056
Sum of electronic and thermal Energies= -1854.508792
Sum of electronic and thermal Enthalpies= -1854.507848
Sum of electronic and thermal Free Energies= -1854.621487

C	2.54561700	-0.23838900	0.62259100
C	0.65500800	-0.17685600	-1.15913800
C	1.10012400	-0.60127000	0.26266000
H	1.46398100	-0.34444300	-1.87335900
H	1.01136300	-1.68692400	0.35053100
H	0.43122300	-0.16239400	1.00923100
C	-0.43472900	-1.15220100	-1.56724600
O	-0.25482000	-2.14750900	-2.20822100
C	3.54418400	-0.62904900	-0.45694400
O	4.43898300	0.07312600	-0.86033300
O	3.29275000	-1.86151900	-0.90039000
C	2.93830300	-0.94317600	1.91974000
O	2.19229500	-1.61537200	2.58823600
O	4.21570900	-0.71013100	2.21761000
C	4.70299000	-1.32606300	3.42886500
C	6.15161200	-0.92455200	3.58257600
H	4.08666700	-0.98171000	4.26343900
H	4.57996100	-2.40865500	3.33873400
H	6.56239400	-1.37517700	4.48854300
H	6.24398600	0.16070800	3.66191900
H	6.73883000	-1.26508900	2.72712800
C	4.11913700	-2.34008300	-1.98198700
C	3.48239900	-3.61418800	-2.48754500
H	4.16193000	-1.56476900	-2.75172200
H	5.13109100	-2.49816700	-1.59910000
H	4.05331500	-4.00265800	-3.33350300
H	2.45782900	-3.41842700	-2.81267300
H	3.46119500	-4.37380600	-1.70313300
H	2.68098900	0.83118700	0.80396600
C	-3.18590300	1.94532100	0.36537700
C	-1.93361300	2.47635900	-0.01709600
C	-1.67507000	3.83761900	0.18162600
C	-2.65752400	4.62622900	0.76100500
C	-3.88719900	4.07710200	1.14921700
C	-4.17325900	2.73065600	0.96012200
C	-1.95697100	0.29769500	-0.54183200
C	-1.16491200	1.39365500	-0.59033900

H	-0.71844600	4.25943100	-0.10197000
H	-2.47013800	5.68299500	0.92051200
H	-4.63783100	4.71445600	1.60477600
H	-5.12321800	2.30712200	1.25187200
C	0.16711700	1.29286700	-1.26383700
H	0.08303600	1.54770000	-2.32790700
C	1.24185700	2.19497000	-0.68877800
O	1.18718400	2.76597400	0.37586500
O	2.29805700	2.21977500	-1.50136500
C	3.42829200	3.00758000	-1.06710900
C	4.41412000	3.03750400	-2.21111900
H	3.06925500	4.00341000	-0.79531900
H	3.85803400	2.53324600	-0.18021400
H	5.28876800	3.62531500	-1.92393200
H	3.96484500	3.49333000	-3.09637400
H	4.73761900	2.02324100	-2.45149500
O	-1.69592200	-0.92517700	-1.07466400
N	-3.19285900	0.57173400	0.04131100
C	-4.26096100	-0.30066500	0.31696100
O	-5.32637000	0.10532500	0.71797300
O	-3.91372000	-1.55231400	0.08748400
C	-4.89219300	-2.64112700	0.21062300
C	-6.03138400	-2.41796900	-0.77658500
C	-5.37551700	-2.74322100	1.65202600
C	-4.06632400	-3.86077200	-0.17628500
H	-5.63279400	-2.28787900	-1.78642800
H	-6.62583500	-1.54464600	-0.50714300
H	-6.67963100	-3.29818400	-0.77332600
H	-4.52120500	-2.82144500	2.32999500
H	-5.98145600	-3.64727100	1.75730300
H	-5.97888100	-1.87937700	1.93054100
H	-4.69444300	-4.75422300	-0.15015800
H	-3.23563000	-3.99373900	0.52133400
H	-3.66115100	-3.74057900	-1.18409100

PSR

Zero-point correction=	0.584794 (Hartree/Particle)
Thermal correction to Energy=	0.623058
Thermal correction to Enthalpy=	0.624002
Thermal correction to Gibbs Free Energy=	0.510363
Sum of electronic and zero-point Energies=	-1854.547056
Sum of electronic and thermal Energies=	-1854.508792
Sum of electronic and thermal Enthalpies=	-1854.507848
Sum of electronic and thermal Free Energies=	-1854.621487

C	-2.54561700	-0.23838900	0.62259100
C	-0.65500800	-0.17685600	-1.15913800
C	-1.10012400	-0.60127000	0.26266000
H	-1.46398100	-0.34444300	-1.87335900
H	-1.01136300	-1.68692400	0.35053100
H	-0.43122300	-0.16239400	1.00923100
C	0.43472900	-1.15220100	-1.56724600
O	0.25482000	-2.14750900	-2.20822100
C	-3.54418400	-0.62904900	-0.45694400
O	-4.43898300	0.07312600	-0.86033300
O	-3.29275000	-1.86151900	-0.90039000
C	-2.93830300	-0.94317600	1.91974000
O	-2.19229500	-1.61537200	2.58823600
O	-4.21570900	-0.71013100	2.21761000
C	-4.70299000	-1.32606300	3.42886500
C	-6.15161200	-0.92455200	3.58257600
H	-4.08666700	-0.98171000	4.26343900
H	-4.57996100	-2.40865500	3.33873400
H	-6.56239400	-1.37517700	4.48854300
H	-6.24398600	0.16070800	3.66191900
H	-6.73883000	-1.26509000	2.72712800
C	-4.11913700	-2.34008300	-1.98198700
C	-3.48239900	-3.61418800	-2.48754500
H	-4.16193000	-1.56476900	-2.75172200
H	-5.13109100	-2.49816700	-1.59910000
H	-4.05331500	-4.00265800	-3.33350300
H	-2.45782900	-3.41842600	-2.81267300
H	-3.46119500	-4.37380600	-1.70313300
H	-2.68098900	0.83118700	0.80396700
C	3.18590300	1.94532100	0.36537700
C	1.93361300	2.47635900	-0.01709600
C	1.67507000	3.83761900	0.18162600
C	2.65752400	4.62622900	0.76100500
C	3.88719900	4.07710200	1.14921700
C	4.17325900	2.73065600	0.96012200
C	1.95697000	0.29769500	-0.54183200
C	1.16491200	1.39365500	-0.59033900
H	0.71844600	4.25943100	-0.10197000
H	2.47013800	5.68299500	0.92051300
H	4.63783100	4.71445600	1.60477600
H	5.12321800	2.30712200	1.25187300
C	-0.16711700	1.29286700	-1.26383700
H	-0.08303600	1.54769900	-2.32790700
C	-1.24185700	2.19497000	-0.68877800

O	-1.18718400	2.76597400	0.37586500
O	-2.29805700	2.21977500	-1.50136500
C	-3.42829200	3.00758000	-1.06710900
C	-4.41412000	3.03750400	-2.21111900
H	-3.06925500	4.00341000	-0.79531900
H	-3.85803400	2.53324600	-0.18021400
H	-5.28876800	3.62531500	-1.92393300
H	-3.96484500	3.49333000	-3.09637400
H	-4.73761900	2.02324100	-2.45149500
O	1.69592200	-0.92517700	-1.07466400
N	3.19285900	0.57173400	0.04131100
C	4.26096100	-0.30066500	0.31696100
O	5.32637000	0.10532500	0.71797300
O	3.91372000	-1.55231400	0.08748400
C	4.89219400	-2.64112700	0.21062300
C	6.03138400	-2.41796900	-0.77658500
C	5.37551700	-2.74322100	1.65202600
C	4.06632400	-3.86077200	-0.17628500
H	5.63279400	-2.28787900	-1.78642800
H	6.62583500	-1.54464600	-0.50714300
H	6.67963100	-3.29818300	-0.77332600
H	4.52120500	-2.82144500	2.32999500
H	5.98145600	-3.64727100	1.75730300
H	5.97888100	-1.87937600	1.93054100
H	4.69444300	-4.75422300	-0.15015800
H	3.23563000	-3.99373900	0.52133400
H	3.66115100	-3.74057900	-1.18409100

PSS

Zero-point correction= 0.584203 (Hartree/Particle)
Thermal correction to Energy= 0.622574
Thermal correction to Enthalpy= 0.623518
Thermal correction to Gibbs Free Energy= 0.509490
Sum of electronic and zero-point Energies= -1854.552973
Sum of electronic and thermal Energies= -1854.514602
Sum of electronic and thermal Enthalpies= -1854.513658
Sum of electronic and thermal Free Energies= -1854.627686

C	2.96679400	-1.39686900	-0.37583800
C	0.70070600	-0.25829600	-0.63855800
C	2.11326800	-0.42934500	-1.20065000
H	0.72279200	-0.27617000	0.46224800
H	2.61891200	0.54120500	-1.21343900
H	2.06620900	-0.78740300	-2.23175000
C	-0.17314100	-1.43753800	-1.01806800

O	0.22650800	-2.47512000	-1.46614200
C	3.06207600	-0.90675100	1.05988900
O	2.51315700	-1.42810300	2.00183000
O	3.77164900	0.21910700	1.13025100
C	4.35666500	-1.53154100	-0.97483900
O	4.69539000	-1.07968100	-2.04189000
O	5.15648600	-2.22871000	-0.16584600
C	6.50928600	-2.42059000	-0.62607700
C	7.24089500	-3.19607800	0.44535600
H	6.47876500	-2.95860200	-1.57750200
H	6.95704100	-1.43929400	-0.80455200
H	8.27389700	-3.36639200	0.13445000
H	6.76456800	-4.16432200	0.61341600
H	7.24783800	-2.64037800	1.38551400
C	3.81699800	0.85637200	2.42304400
C	4.44455400	2.21659600	2.22879600
H	2.79551800	0.92995800	2.80157900
H	4.39732500	0.22092500	3.09834700
H	4.53246800	2.72237400	3.19296300
H	3.81540300	2.82124600	1.57238500
H	5.44125400	2.12755300	1.79066500
H	2.50671500	-2.38902600	-0.34595100
C	-3.53080200	1.45873900	0.07569000
C	-2.31957900	2.10755900	-0.25334200
C	-2.25063800	3.50464300	-0.20872500
C	-3.37886900	4.21645800	0.17133100
C	-4.56828100	3.55511000	0.50425400
C	-4.66694900	2.16925800	0.46110700
C	-2.00480100	-0.10240400	-0.46276600
C	-1.36048100	1.08061300	-0.58976400
H	-1.33495500	4.01697800	-0.48071000
H	-3.34078200	5.30011500	0.20839600
H	-5.43763100	4.13359700	0.79832500
H	-5.58569900	1.65961000	0.71091400
C	0.08392000	1.10253900	-1.00184200
H	0.18878700	1.31366500	-2.07299900
C	0.85246300	2.17804700	-0.23844100
O	1.34895800	2.01657400	0.85250000
O	0.90300300	3.31783400	-0.92428800
C	1.55038000	4.42895800	-0.26694500
C	1.41696500	5.62715600	-1.17820300
H	1.06823100	4.58563100	0.70214200
H	2.59579500	4.16179000	-0.09072800
H	1.90484700	6.48999700	-0.72010400

H	0.36587700	5.87371300	-1.34661600
H	1.88957500	5.43200100	-2.14303000
O	-1.51702700	-1.33353900	-0.75761600
N	-3.32849400	0.06886700	-0.05825600
C	-4.31134500	-0.90293100	0.20593600
O	-5.44825400	-0.59926600	0.48089500
O	-3.80312500	-2.11561900	0.11345000
C	-4.64621600	-3.30487600	0.29118800
C	-5.73710100	-3.32429800	-0.77227700
C	-5.20604700	-3.33407000	1.70794000
C	-3.65167000	-4.43753800	0.07376400
H	-5.29338700	-3.22855800	-1.76700800
H	-6.45772800	-2.52064800	-0.61953600
H	-6.26329300	-4.28122100	-0.72150200
H	-4.39478200	-3.23808600	2.43464900
H	-5.70117400	-4.29501300	1.87154000
H	-5.92937100	-2.53427200	1.86644900
H	-4.16170000	-5.39895000	0.16858000
H	-2.85152500	-4.38778300	0.81655200
H	-3.20861000	-4.36767000	-0.92282300