Electronic Supplementary Information For

Mechanistic Studies on N-Heterocyclic Carbene-Catalyzed Reaction of Isatin-Derived Enal with Hydrazone

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Content

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Part 1: IRC calculations of representative transition states

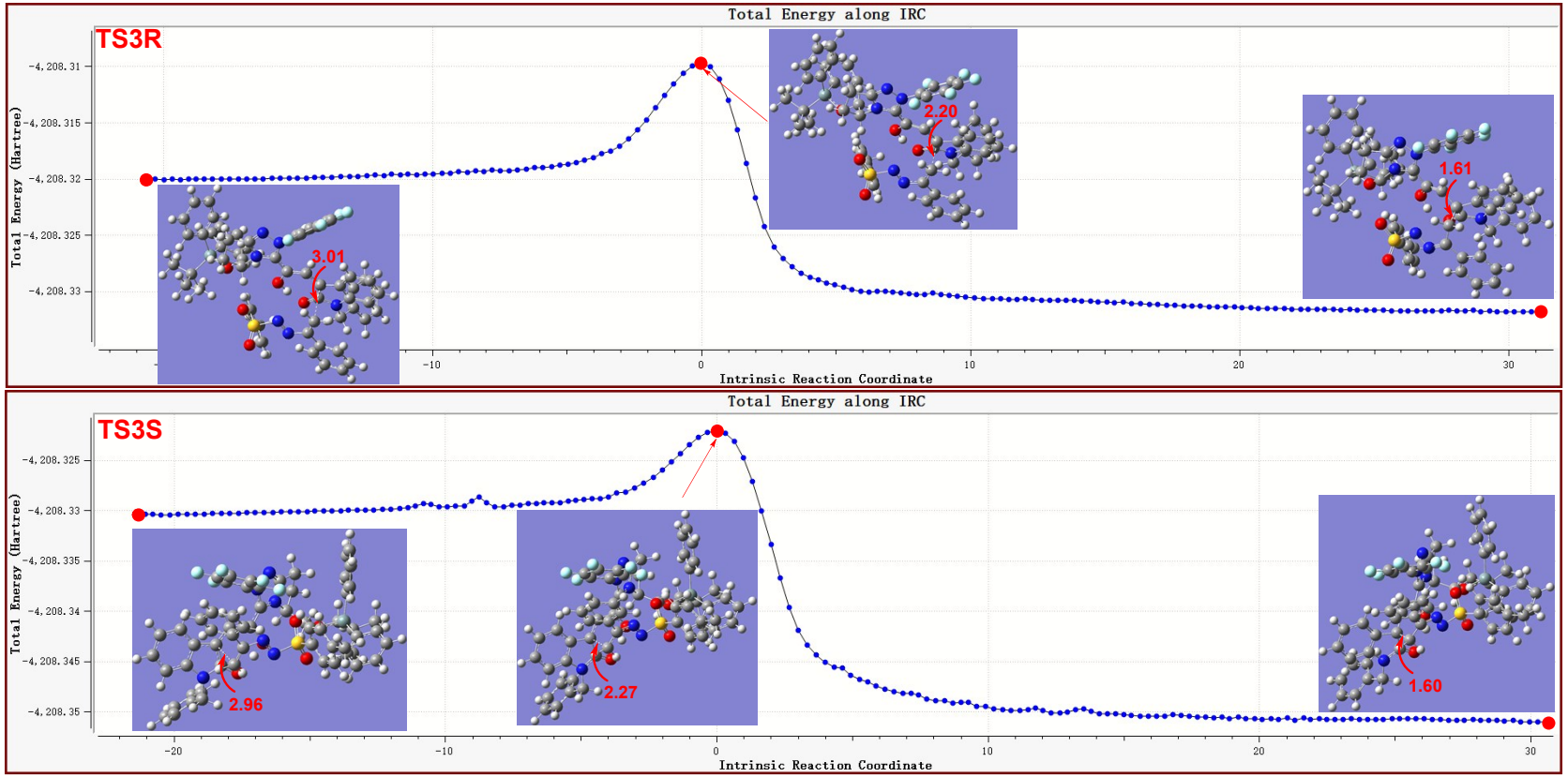


Fig. S1 IRC results of**TS3R** and **TS3S**.

Part 2: Energy barrier of the direct [1,2]-proton transfer process

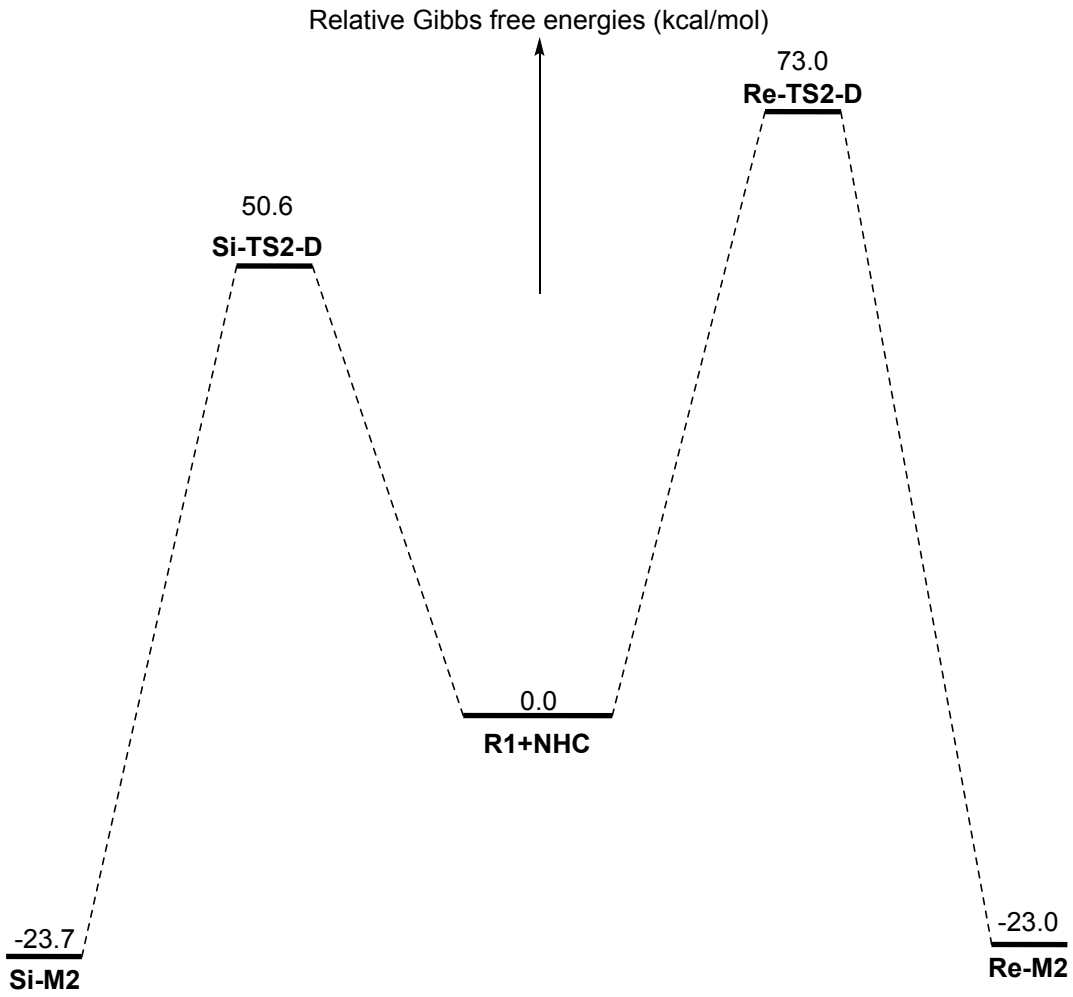


Fig. S2 Energy barrier of direct [1,2]-proton transfer process.

Part 3: Energy barrier of *R*-configured pathway

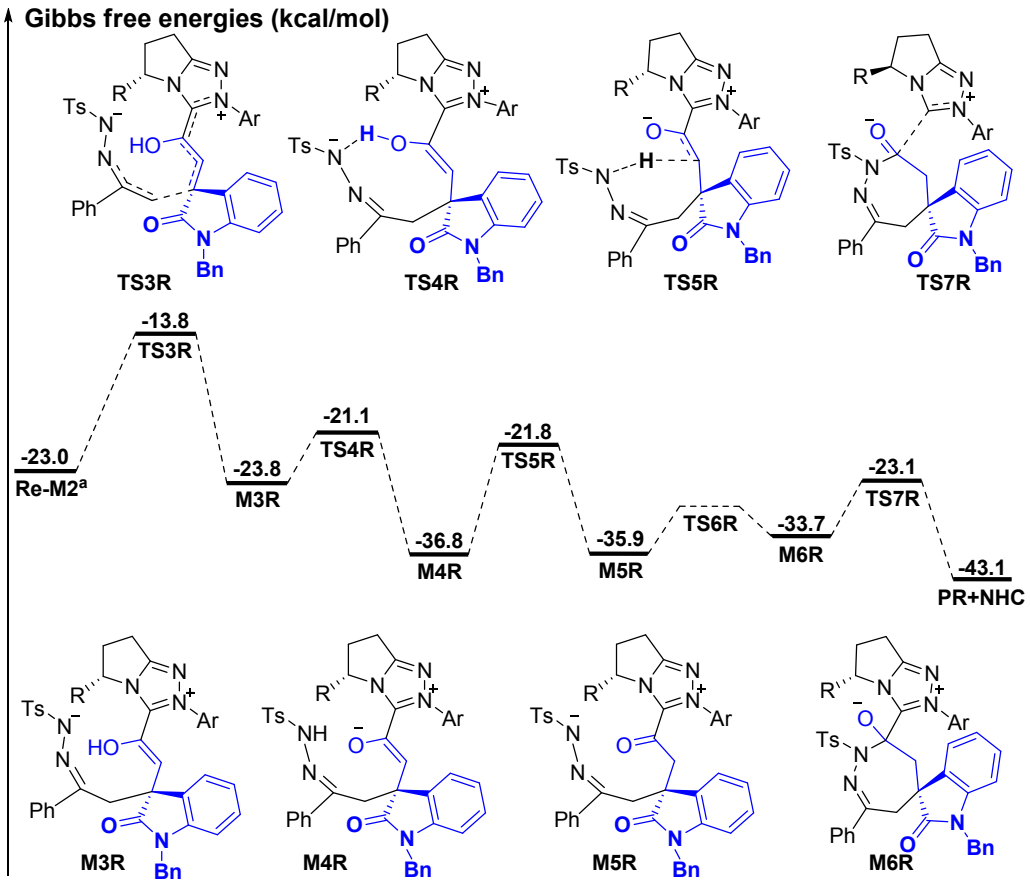
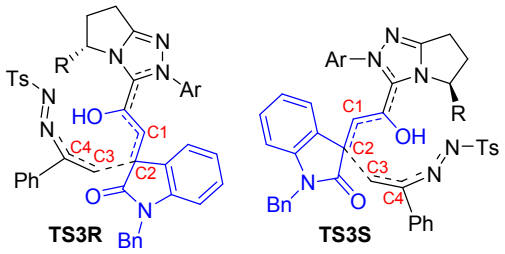


Fig. S3 Energy barrier of *R*-configured pathway involved in the reaction.

Part 4: Conformational search for TS3s

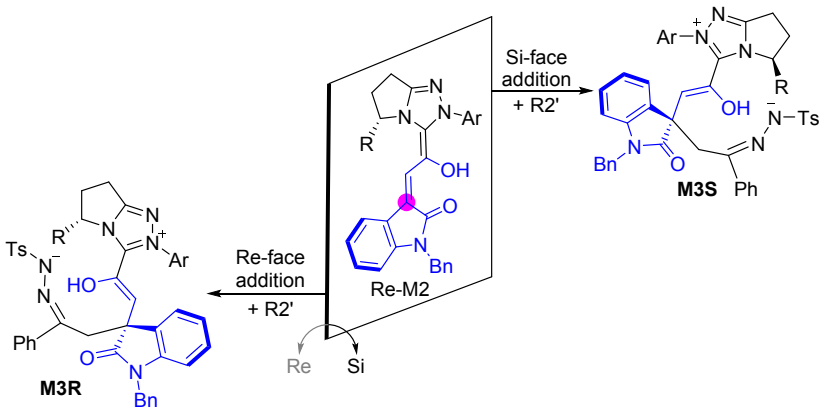
Table S1 Different conformations of the transition states involved in C-C bond formation step



	R	S
TS3	9.2	5.0
TS3-90	13.9	8.3
TS3-180	14.3	11.8
TS3-270	27.1	15.7

To confirm the reliability of the calculated results, we have additionally considered and investigated the different conformations of TS3s in the C-C bond formation step of the revised manuscript. By rotating dihedral angle Φ1(C1-C2-C3-C4) from 0~360° at intervals of 90° based on the original transition states **TS3R** and **TS3S**, we have constructed eight (4×2=8) initial structures of TS3s and located eight conformations after the optimization, which are summarized in **Table S1**. As an important note, the initial structures by rotating the dihedral Φ1 with 90° would lead to the same conformations of those with Φ1=0°/360° after the structural optimizations. The relative Gibbs free energies depicted in **Table S1** show that the original conformations of the transition states **TS3R** and **TS3S** indeed have the lowest energies among their conformers, and thus only these two transition states are discussed in the main text of the revised manuscript.

Part 5: Illustration of Stereoselectivity



Scheme S1 Illustration of Stereoselectivity

Part 6: Computational equation for ee value calculation

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

$$\frac{[TS3S]}{[TS3R]} = \frac{e^{-G^{\neq}_{[TS3R]}/RT}}{e^{-G^{\neq}_{[TS3S]}/RT}} = e^{\Delta G^{\neq}/_{RT}} \quad (1)$$

$$ee\% = \frac{[TS3S] - [TS3R]}{[TS3S] + [TS3R]} \times 100\% = \frac{\frac{[TS3S]}{[TS3R]} - 1}{\frac{[TS3S]}{[TS3R]} + 1} \times 100\% \quad (2)$$

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

For this reaction, we have first identified the lowest energy conformer of the competing stereoselective pathways by conformer search. The computational results show that the **TS3R** and **TS3S** have the lowest energy among the R- and S-configured transition states, respectively. Thus, the transition states **TS3R** and **TS3S** are selected to perform the Boltzmann analysis. As depicted in **Fig. 2** of the main text and **Table S1**, the relative Gibbs free energy barriers of **TS3R** and **TS3S** are 9.2 and 5.0 kcal/mol, separately. Based on the above expression (equation 1), the $\Delta G^{\neq}$ is 4.2 kcal/mol (17640J/mol), the [TS3S]/[TS3R] can be calculated to be 1236.3. Then, the ee% value can be obtained by equation 2, which is 99.8% and in good agreement with experimental observations.

Part 7: Distances of C-C bond involved in TS3R and TS3S

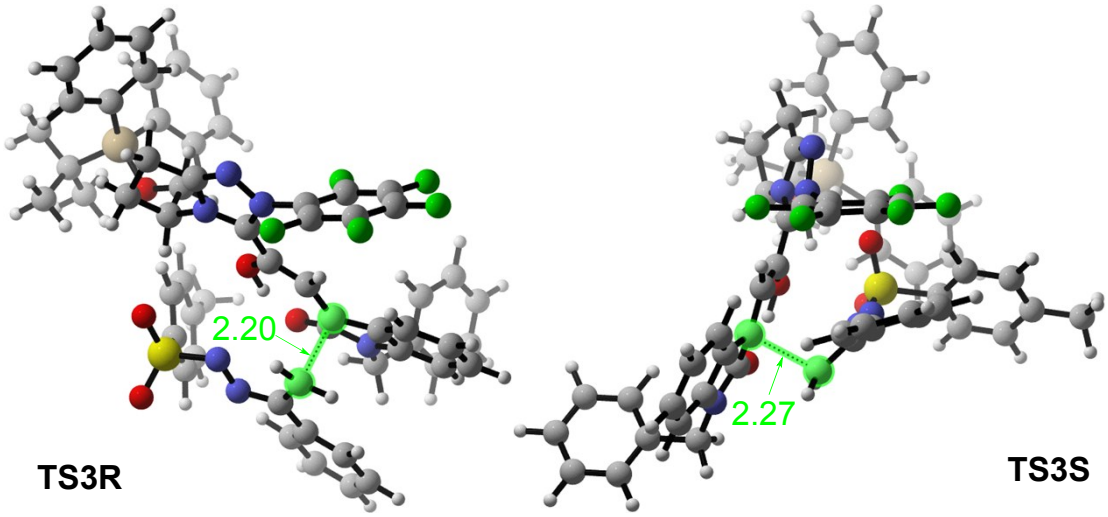


Fig.S4 3D-structures of the stereocontrol transition states **TS3R** and **TS3S**

Part 8: Distortion-interaction analysis

The distortion/interaction analysis is a fragment approach to understand organic reactions,in which the height of the energetic barrier is described interms of the original reactants. According to Houk's definition, the activationenergy of the transition state is decomposed into to two main components: the distortion ($\Delta E_{dist}^{\neq}$) and the interaction($\Delta E_{int}^{\neq}$) energy. The distortion energy involves geometric andelectronic changes to deform the reactants into their transitionstate geometry, which involves bond stretching, angle decreaseor increase, dihedral changes and so on. The interaction energy includes exchange-repulsive and stabilizing electrostatic, polarization, and orbital effects in the transition state structure. The interaction energy is recovered by the relationship: $\Delta E^{\neq} = \Delta E_{dist}^{\neq} + \Delta E_{int}^{\neq}$.

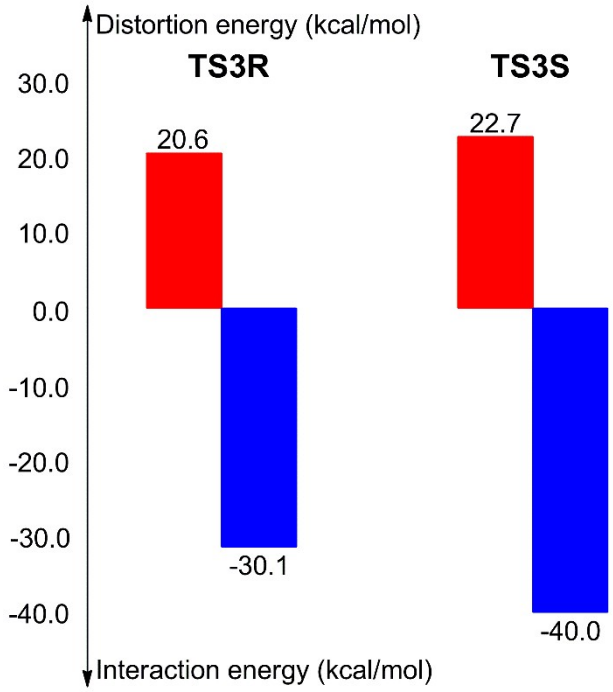


Fig.S5 Distortion and interaction energies for the stereocontrol transition states **TS3R** and **TS3S**

Part 9: Cartesian coordinates of all the stationary points

R1

Total energy= -860.503250

Zero-point correction= 0.261342 (Hartree/Particle)

Thermal correction to Energy= 0.277428

Thermal correction to Enthalpy= 0.278373

Thermal correction to Gibbs Free Energy= 0.215780

Sum of electronic and zero-point Energies= -860.241909

Sum of electronic and thermal Energies= -860.225822

Sum of electronic and thermal Enthalpies= -860.224878

Sum of electronic and thermal Free Energies= -860.287470

C	-0.25204400	1.08292000	-0.44096500
C	-1.54802900	1.22932400	0.08130200
C	-1.97378000	2.46390400	0.55093500
C	-1.09176300	3.54363300	0.49251900
C	0.19261300	3.37906600	-0.02620800
C	0.63792500	2.14236900	-0.50265500
C	-1.17611800	-1.01119900	-0.61326800
C	-2.20293000	-0.07649200	0.00136400
H	-2.97319300	2.58802300	0.95684500
H	-1.40567900	4.51589800	0.85509800
H	0.86687900	4.22861500	-0.05886900
H	1.64238500	2.01535000	-0.89118300
N	-0.05824600	-0.24053300	-0.85652200
O	-1.27072800	-2.19895800	-0.85551900
C	-3.44785600	-0.40765200	0.38169100
C	-4.04698100	-1.75581500	0.27086400
O	-5.18301700	-1.96054400	0.64725600
H	-3.42133000	-2.54988000	-0.16262400
H	-4.10291700	0.34836500	0.81096300
C	1.15634400	-0.75833200	-1.45270500
H	1.40389800	-0.16221300	-2.33837400
H	0.91324800	-1.77238400	-1.78360400
C	2.32441800	-0.77362100	-0.48900600
C	3.56982900	-0.28515700	-0.88006800
C	2.16799800	-1.29756000	0.79579900
C	4.65064200	-0.32231800	-0.00135500
H	3.69515000	0.12803800	-1.87817200
C	3.24451200	-1.33253900	1.67509000
H	1.19784100	-1.68017500	1.10319200
C	4.48911200	-0.84509000	1.27802400
H	5.61558100	0.06181700	-0.31625600

H	3.11398200	-1.74265300	2.67136300
H	5.32848000	-0.87170300	1.96522500

R2

Total energy= -1237.666833

Zero-point correction= 0.264401 (Hartree/Particle)

Thermal correction to Energy= 0.282554

Thermal correction to Enthalpy= 0.283498

Thermal correction to Gibbs Free Energy= 0.214201

Sum of electronic and zero-point Energies= -1237.402432

Sum of electronic and thermal Energies= -1237.384279

Sum of electronic and thermal Enthalpies= -1237.383335

Sum of electronic and thermal Free Energies= -1237.452631

C	-1.63868100	-1.73629900	-0.37487500
C	-1.97988500	-2.95220800	-0.81150400
H	-3.01032100	-3.19391600	-1.04312700
H	-1.22071800	-3.70829600	-0.97525100
C	-2.55062200	-0.59492800	-0.12993900
C	-3.89328900	-0.81694100	0.19486000
C	-2.07714000	0.72113200	-0.21214100
C	-4.75265700	0.25412200	0.40764300
H	-4.26070600	-1.83295600	0.30258200
C	-2.94160700	1.78931000	0.00403100
H	-1.03411900	0.90262300	-0.45160700
C	-4.28021700	1.56179200	0.31102500
H	-5.79106100	0.06707500	0.66116100
H	-2.56424300	2.80460800	-0.06776900
H	-4.95139900	2.39689400	0.48324800
N	-0.26094800	-1.37393000	-0.21326500
N	0.50677200	-2.26547100	0.13982200
S	2.17645900	-1.65299000	0.23378400
O	2.84457500	-2.19546200	-0.93936300
O	2.60976300	-1.99871600	1.57735600
C	2.04241400	0.10550400	0.08806000
C	2.10294600	0.68971200	-1.17207100
C	1.80069000	0.85616000	1.23549100
C	1.92404000	2.06441900	-1.27788400
H	2.29571800	0.07577400	-2.04561200
C	1.62264400	2.22700700	1.10790200
H	1.76138900	0.36990700	2.20470800
C	1.67587100	2.84736400	-0.14609800
H	1.97920200	2.53777600	-2.25364100
H	1.43959800	2.82838800	1.99373400
C	1.44996700	4.33104700	-0.26712700

H	1.96074800	4.87180000	0.53317400
H	1.80763800	4.71122500	-1.22575200
H	0.38263200	4.56301200	-0.19046900

TMEDA

Total energy= -347.585116
Zero-point correction= 0.225851 (Hartree/Particle)
Thermal correction to Energy= 0.235659
Thermal correction to Enthalpy= 0.236604
Thermal correction to Gibbs Free Energy= 0.192546
Sum of electronic and zero-point Energies= -347.359265
Sum of electronic and thermal Energies= -347.349457
Sum of electronic and thermal Enthalpies= -347.348513
Sum of electronic and thermal Free Energies= -347.392571

C	-0.40690400	-0.64585500	0.96777400
C	0.40690400	0.64585500	0.96777400
H	-0.08290700	-1.23751700	1.84829900
H	-1.46810400	-0.41577100	1.12265900
H	0.08290700	1.23751700	1.84829900
H	1.46810400	0.41577100	1.12265900
N	-0.29962800	-1.41682900	-0.26056300
N	0.29962800	1.41682900	-0.26056300
C	1.08080000	2.63479400	-0.14870800
H	1.05066500	3.18277600	-1.09450600
H	0.71252300	3.30576700	0.65058300
H	2.12355300	2.38713400	0.07155200
C	-1.08080000	1.71818000	-0.59802300
H	-1.60460100	2.26700800	0.20794000
H	-1.10336900	2.33773900	-1.49866200
H	-1.61702000	0.79112300	-0.81018100
C	1.08080000	-1.71818000	-0.59802300
H	1.60460100	-2.26700800	0.20794000
H	1.10336900	-2.33773900	-1.49866200
H	1.61702000	-0.79112300	-0.81018100
C	-1.08080000	-2.63479400	-0.14870800
H	-1.05066500	-3.18277600	-1.09450600
H	-0.71252300	-3.30576700	0.65058300
H	-2.12355300	-2.38713400	0.07155200

TMEDA□H^+

Total energy= -348.021032
Zero-point correction= 0.240492 (Hartree/Particle)
Thermal correction to Energy= 0.250732
Thermal correction to Enthalpy= 0.251676

Thermal correction to Gibbs Free Energy= 0.205702
Sum of electronic and zero-point Energies= -347.780539
Sum of electronic and thermal Energies= -347.770300
Sum of electronic and thermal Enthalpies= -347.769356
Sum of electronic and thermal Free Energies= -347.815330

C	-0.73192400	0.28731900	1.08646100
C	0.67904000	-0.31053600	1.12023700
H	-1.31267900	-0.11900100	1.92683200
H	-0.68286100	1.37120700	1.22403000
H	1.29165500	0.09642700	1.92686900
H	0.64987400	-1.39749600	1.21668300
N	-1.33242800	0.00517200	-0.21651500
N	1.33312500	-0.00326500	-0.19558900
C	2.36435800	-1.00394100	-0.57971700
H	2.77445700	-0.73225100	-1.55162000
H	3.15320700	-0.99796300	0.17347300
H	1.90134400	-1.98879500	-0.63204900
C	1.87204200	1.38530100	-0.24842600
H	2.69087900	1.46768100	0.46695200
H	2.23171600	1.58402200	-1.25710600
H	1.07881100	2.08751200	0.00341900
C	-1.89224400	-1.34733600	-0.27215800
H	-2.72723700	-1.47049700	0.43335500
H	-2.25398600	-1.54759500	-1.28244800
H	-1.12806800	-2.09224400	-0.03445700
C	-2.34962800	0.99307400	-0.57909500
H	-2.71919900	0.77370700	-1.58269000
H	-3.20155400	0.98137200	0.11631000
H	-1.91149100	1.99388800	-0.58349800
H	0.51039300	-0.04660800	-0.84313900

NHC

Total energy= -2110.060380
Zero-point correction= 0.497294 (Hartree/Particle)
Thermal correction to Energy= 0.532164
Thermal correction to Enthalpy= 0.533108
Thermal correction to Gibbs Free Energy= 0.428659
Sum of electronic and zero-point Energies= -2109.563086
Sum of electronic and thermal Energies= -2109.528216
Sum of electronic and thermal Enthalpies= -2109.527272
Sum of electronic and thermal Free Energies= -2109.631721

C	0.10433000	-2.48184500	0.48851100
C	-0.67471100	-2.47946800	-0.85127900
C	-0.23411300	-1.19458900	-1.58615900

C	1.32329700	-1.70188500	0.10887400
C	2.19412900	-0.26097900	-1.41693200
H	-0.44613100	-1.95443800	1.27696500
H	0.33560100	-3.48442000	0.84947800
H	-0.38122100	-3.34834000	-1.44596200
H	-0.22164100	-1.31672600	-2.67079800
N	2.50170200	-1.46429700	0.58393700
N	3.00820400	-0.58150600	-0.36888100
N	1.12157800	-1.02085600	-1.06904400
C	4.31927900	-0.09989600	-0.19736800
C	4.70220500	0.50088800	0.99998100
C	5.26156700	-0.21424400	-1.21707600
C	5.99579800	0.96805200	1.18254200
C	6.55228500	0.26906100	-1.04869500
C	6.92056700	0.85688100	0.15324500
F	4.94850800	-0.80178600	-2.36447700
F	7.44362200	0.15164900	-2.02888900
F	8.15788300	1.30976100	0.31978400
F	6.34483500	1.54079400	2.33103400
F	3.82527800	0.64747500	1.98587300
H	-1.75597600	-2.50953700	-0.71230200
C	-1.06235500	0.03357300	-1.20356200
H	-0.93400400	0.21390800	-0.12566400
H	-0.67524200	0.91095400	-1.73518800
O	-2.41444700	-0.18393900	-1.54282000
Si	-3.65675400	-0.01486700	-0.42859500
C	-5.15986100	-0.77833400	-1.28347100
C	-5.58396600	0.16827800	-2.42046200
C	-4.81248800	-2.14105900	-1.90186000
C	-6.32175200	-0.91687000	-0.29043400
H	-5.88599700	1.14897500	-2.03999500
H	-4.77413100	0.31808600	-3.14279800
H	-6.43766600	-0.26376300	-2.95824000
H	-4.55406300	-2.89476000	-1.15107600
H	-5.67655000	-2.52463800	-2.45996500
H	-3.97051300	-2.05459600	-2.59531400
H	-7.21288300	-1.29634900	-0.80671100
H	-6.08876800	-1.60765900	0.52668900
H	-6.58625700	0.05084200	0.15219500
C	-3.90159900	1.81699600	-0.11500700
C	-4.59597400	2.29413000	1.00665400
C	-3.42810600	2.75158000	-1.04717800
C	-4.81579800	3.65695900	1.18897000
H	-4.95943200	1.59217000	1.75524900

C	-3.63937900	4.11644200	-0.86684400
H	-2.88740900	2.40306700	-1.92474600
C	-4.33543700	4.56929800	0.25131300
H	-5.35551300	4.00799600	2.06307200
H	-3.26065300	4.82611500	-1.59576900
H	-4.50138300	5.63254900	0.39448700
C	-3.15688100	-0.81891200	1.20449100
C	-3.40065000	-2.16922200	1.50404100
C	-2.42887200	-0.07041400	2.14513200
C	-2.93203900	-2.75019400	2.67988200
H	-3.96579000	-2.78660900	0.81141900
C	-1.95344900	-0.64472800	3.32295100
H	-2.23195700	0.98290700	1.95735500
C	-2.20344800	-1.98813800	3.59095500
H	-3.13686800	-3.79610000	2.88590600
H	-1.38848700	-0.04391400	4.02854300
H	-1.83393300	-2.43865700	4.50676200

Re-TS1

Total energy= -2970.571684

Zero-point correction= 0.760493 (Hartree/Particle)

Thermal correction to Energy= 0.811901

Thermal correction to Enthalpy= 0.812846

Thermal correction to Gibbs Free Energy= 0.669462

Sum of electronic and zero-point Energies= -2969.811191

Sum of electronic and thermal Energies= -2969.759783

Sum of electronic and thermal Enthalpies= -2969.758838

Sum of electronic and thermal Free Energies= -2969.902222

Imaginary frequency= -186.05 cm^{-1}

C	-2.35140700	-0.73044500	-2.76800200
C	-2.44407900	0.77709900	-2.41836800
C	-1.76726900	0.92852800	-1.03732400
C	-1.10565200	-1.11432800	-2.03384100
C	0.31095800	-0.52100300	-0.41932400
H	-3.20563200	-1.29171600	-2.36995000
H	-2.28642300	-0.92178200	-3.83919900
H	-1.88538400	1.35801000	-3.15660900
H	-1.26385600	1.88988500	-0.91823200
N	-0.25831400	-2.09513300	-2.01006200
N	0.61071100	-1.69971900	-1.00219000
N	-0.78279200	-0.15596000	-1.10441100
C	1.71238800	-2.51842000	-0.67134200
C	1.51063200	-3.75870300	-0.07263300
C	3.01252500	-2.08489400	-0.90795300

C	2.59329000	-4.54184500	0.30346800
C	4.10162700	-2.85105000	-0.52010800
C	3.88691300	-4.08108200	0.08810700
F	3.23133000	-0.90463900	-1.47706200
F	5.33572200	-2.41025900	-0.72536400
F	4.92051200	-4.82040900	0.46693800
F	2.39880100	-5.72136100	0.88332800
F	0.28083800	-4.19339100	0.15652000
H	-3.47090800	1.14175100	-2.39696300
C	-2.71722600	0.66652900	0.13578900
H	-3.10515300	-0.35929400	0.04221700
H	-2.17062900	0.71502400	1.08344800
O	-3.75372600	1.62655700	0.09043100
Si	-5.37396400	1.19830700	0.10377800
C	-6.28453600	2.80246000	-0.31171300
C	-6.15260500	3.73908600	0.90178600
C	-5.65225600	3.49919700	-1.52564700
C	-7.77004000	2.51727300	-0.56846500
H	-6.62611300	3.31617000	1.79322100
H	-5.10237700	3.94114600	1.13874800
H	-6.63855200	4.69857900	0.68260700
H	-5.75062800	2.91596900	-2.44668200
H	-6.14820000	4.46299200	-1.69968600
H	-4.58781800	3.68997200	-1.35939700
H	-8.30781700	3.45666700	-0.75006900
H	-7.92062900	1.87119300	-1.43993000
H	-8.23815800	2.03180400	0.29589300
C	-5.80272300	0.59638700	1.82574900
C	-6.96640200	-0.14112700	2.09153500
C	-4.97032400	0.93172400	2.90304900
C	-7.29182700	-0.52480300	3.38972900
H	-7.62081500	-0.43292000	1.27168700
C	-5.28739200	0.54442900	4.20280100
H	-4.06056500	1.49858200	2.71857400
C	-6.45028900	-0.18170300	4.44640300
H	-8.19627000	-1.09494000	3.57822100
H	-4.62679000	0.80543600	5.02348900
H	-6.69938800	-0.48470100	5.45872800
C	-5.65845200	-0.23496100	-1.09408900
C	-5.95783100	-0.06176600	-2.45534600
C	-5.47947500	-1.55148700	-0.63571800
C	-6.06350100	-1.14730000	-3.32158900
H	-6.11238000	0.93589600	-2.85711700
C	-5.58051500	-2.64339900	-1.49651500

H	-5.26081600	-1.72940300	0.41489800
C	-5.87147300	-2.44212100	-2.84324600
H	-6.29797100	-0.98276500	-4.36869500
H	-5.43322800	-3.64840200	-1.11395000
H	-5.95129400	-3.28949000	-3.51699100
C	5.20652800	0.61979700	0.50273600
C	4.43022000	-0.16788200	1.36962400
C	5.03594700	-1.14603100	2.14603600
C	6.41613000	-1.32849900	2.04265300
C	7.17125700	-0.53501200	1.17854100
C	6.57925200	0.45749300	0.39406200
C	3.04978900	1.32808100	0.15712500
C	3.03293200	0.23611300	1.18790300
H	4.44410000	-1.76216000	2.81750000
H	6.90537400	-2.09099500	2.63882800
H	8.24358600	-0.68828900	1.11307300
H	7.17070200	1.08149800	-0.26758500
N	4.37941900	1.51505800	-0.18400500
O	2.11430500	1.93560600	-0.33563800
C	1.92163600	-0.32756500	1.68148000
C	0.49556500	0.08182700	1.39263800
O	-0.41934500	-0.49101400	2.03469700
H	0.41418400	1.14753300	1.11182000
H	2.00236100	-1.17088100	2.36902700
C	4.81342600	2.39821900	-1.24247600
H	3.89747800	2.82276100	-1.66529100
H	5.30669800	1.81054600	-2.02680900
C	5.73784400	3.49648600	-0.75962100
C	6.85511600	3.85674600	-1.51208100
C	5.46904100	4.17548700	0.42992800
C	7.68992400	4.88866500	-1.08859200
H	7.07424400	3.32475200	-2.43477200
C	6.30281600	5.20396800	0.85590400
H	4.60385900	3.89032700	1.02270600
C	7.41503100	5.56431100	0.09656400
H	8.55785100	5.15907000	-1.68150900
H	6.08569500	5.72517100	1.78280200
H	8.06621900	6.36545100	0.43085400

Re-M1

Total energy= -2970.579141

Zero-point correction= 0.762138 (Hartree/Particle)

Thermal correction to Energy= 0.813445

Thermal correction to Enthalpy= 0.814389

Thermal correction to Gibbs Free Energy= 0.673274
Sum of electronic and zero-point Energies= -2969.817003
Sum of electronic and thermal Energies= -2969.765696
Sum of electronic and thermal Enthalpies= -2969.764752
Sum of electronic and thermal Free Energies= -2969.905867

C	-1.89505100	0.48061100	-2.73760700
C	-2.05691700	1.71683000	-1.81306300
C	-1.53128400	1.28396300	-0.42637200
C	-0.75572800	-0.23312200	-2.07609700
C	0.41594000	-0.41497300	-0.22395100
H	-2.78700100	-0.15662400	-2.72357500
H	-1.68094800	0.74502600	-3.77328600
H	-1.43805800	2.53637100	-2.18618000
H	-1.05607200	2.10184900	0.11826200
N	0.04039300	-1.22780100	-2.32016900
N	0.78367400	-1.31238600	-1.15410400
N	-0.53839900	0.28952400	-0.82694300
C	1.64325600	-2.40443000	-0.90130400
C	1.11798000	-3.56458500	-0.33823500
C	3.01504600	-2.28969800	-1.09897700
C	1.96757000	-4.60019200	0.02853000
C	3.87084700	-3.31118500	-0.71928800
C	3.33828800	-4.46576700	-0.15607500
F	3.52071200	-1.16883700	-1.59893600
F	5.18296100	-3.19254000	-0.88319100
F	4.14753700	-5.45253400	0.20367300
F	1.48033900	-5.71719300	0.55653600
F	-0.18333200	-3.69862300	-0.17875700
H	-3.08907600	2.06177600	-1.75265900
C	-2.57044700	0.57097400	0.44668200
H	-2.93116400	-0.31202200	-0.10255700
H	-2.09344700	0.19950900	1.36197700
O	-3.61325600	1.47622200	0.73341800
Si	-5.22148300	1.14971000	0.38790800
C	-6.08912900	2.81320700	0.62338300
C	-6.08023600	3.12938200	2.12907800
C	-5.34019800	3.93788600	-0.10757000
C	-7.54123200	2.72944000	0.13479300
H	-6.63629300	2.38140600	2.70280000
H	-5.05908700	3.17045300	2.52329800
H	-6.54747000	4.10709300	2.30394600
H	-5.34694400	3.81317000	-1.19505500
H	-5.81743700	4.90249900	0.10898700
H	-4.29761100	3.99389400	0.21951700

H	-8.05592700	3.68104000	0.31994200
H	-7.60359700	2.51834600	-0.93814000
H	-8.09598900	1.94678900	0.66525400
C	-5.84832400	-0.12788200	1.60564600
C	-7.04484000	-0.82390800	1.37558000
C	-5.15595400	-0.37576800	2.79869100
C	-7.53876400	-1.73115100	2.30858600
H	-7.59126700	-0.66620200	0.44704900
C	-5.64102500	-1.28971100	3.73192500
H	-4.22415200	0.14955900	2.99611000
C	-6.83449900	-1.96486500	3.48806300
H	-8.46640800	-2.26041000	2.11413400
H	-5.08702700	-1.47760400	4.64616800
H	-7.21389400	-2.67708500	4.21424800
C	-5.36127700	0.39070600	-1.33811100
C	-5.53976900	1.14634800	-2.50792400
C	-5.20568500	-0.99865000	-1.48445800
C	-5.54902100	0.54929800	-3.76622500
H	-5.67443300	2.22270100	-2.44507100
C	-5.21180400	-1.60425300	-2.74017900
H	-5.08499100	-1.62139300	-0.60059500
C	-5.38096600	-0.82899700	-3.88440100
H	-5.69131500	1.15809600	-4.65375300
H	-5.08566600	-2.67915700	-2.82300700
H	-5.38713600	-1.29650800	-4.86413000
C	5.33163100	0.54305000	0.42783700
C	4.64362400	-0.40561400	1.20411500
C	5.34843400	-1.40635800	1.85618600
C	6.73961900	-1.43998900	1.73237800
C	7.40602500	-0.48318400	0.96847800
C	6.71105000	0.53007200	0.30115600
C	3.11947900	1.09586800	0.19328200
C	3.21381900	-0.10007100	1.08948700
H	4.82730700	-2.15069200	2.45200700
H	7.30537600	-2.21547400	2.23698200
H	8.48757200	-0.52118900	0.88876500
H	7.23145200	1.28258000	-0.28200600
N	4.41322600	1.42460400	-0.15628200
O	2.11825500	1.69171500	-0.18054200
C	2.15030200	-0.76916200	1.55594200
C	0.67347600	-0.47260900	1.28335500
O	-0.17488900	-1.40905400	1.69070200
H	0.49621900	0.57938200	1.62734800
H	2.29237200	-1.65004400	2.18387300

C	4.75414100	2.49820400	-1.06366300
H	3.80615200	2.83211100	-1.49655800
H	5.37656800	2.09950400	-1.87354000
C	5.45978400	3.64966000	-0.37842100
C	6.61065200	4.20839200	-0.93077900
C	4.94163500	4.18115200	0.80438100
C	7.23633300	5.29077700	-0.31458300
H	7.01990800	3.79504100	-1.84960800
C	5.56531800	5.25953300	1.42171100
H	4.04420700	3.74561800	1.23676700
C	6.71430100	5.81778800	0.86249000
H	8.13350000	5.71692900	-0.75205400
H	5.15543100	5.66638800	2.34059000
H	7.20161400	6.65812200	1.34612900

Si-TS1

Total energy= -2970.568327

Zero-point correction= 0.760382 (Hartree/Particle)

Thermal correction to Energy= 0.811976

Thermal correction to Enthalpy= 0.812920

Thermal correction to Gibbs Free Energy= 0.667741

Sum of electronic and zero-point Energies= -2969.807944

Sum of electronic and thermal Energies= -2969.756351

Sum of electronic and thermal Enthalpies= -2969.755407

Sum of electronic and thermal Free Energies= -2969.900586

Imaginary frequency= -156.58 cm^{-1}

C	-1.91090600	-0.71749800	-2.65869600
C	-2.07404300	0.73629400	-2.14623500
C	-1.56832000	0.72695400	-0.68618200
C	-0.75296700	-1.17791100	-1.83101300
C	0.45436100	-0.77566500	0.00044000
H	-2.79530200	-1.32625800	-2.43515800
H	-1.71576800	-0.77843800	-3.72938200
H	-1.44260300	1.40305500	-2.73904900
H	-1.08850800	1.66797900	-0.40673000
N	0.11917000	-2.13692900	-1.83262100
N	0.85083800	-1.86367000	-0.68618000
N	-0.57265700	-0.34709000	-0.75183900
C	1.94284400	-2.68831800	-0.34252700
C	1.94438600	-3.39077900	0.85503500
C	3.06328000	-2.73433500	-1.16300900
C	3.05033600	-4.14403900	1.22684700
C	4.16510200	-3.49355700	-0.80810700
C	4.15594800	-4.19839100	0.38920300

F	3.10464100	-2.00442200	-2.27025800
F	5.24187800	-3.52300700	-1.58879500
F	5.21315800	-4.92152000	0.73696600
F	3.05139300	-4.81674400	2.37320900
F	0.89523300	-3.32817600	1.66520400
H	-3.10210300	1.09278900	-2.20561700
C	-2.63946900	0.35501200	0.34224200
H	-2.99826600	-0.66175200	0.11974500
H	-2.18496900	0.34345400	1.33944900
O	-3.68064300	1.30805900	0.26823100
Si	-5.28285000	0.88266800	0.02566700
C	-6.15311600	2.52500500	-0.32420400
C	-6.20420800	3.31717000	0.99365900
C	-5.37171000	3.35640300	-1.35270300
C	-7.58453600	2.27130000	-0.81546900
H	-6.78482200	2.79274400	1.75887100
H	-5.19954400	3.49450800	1.39295200
H	-6.67436700	4.29373000	0.82050200
H	-5.32384000	2.87792800	-2.33615500
H	-5.86077600	4.32950100	-1.49040700
H	-4.34625500	3.53594300	-1.01590400
H	-8.10467300	3.22570400	-0.96787600
H	-7.60358600	1.72395600	-1.76390400
H	-8.16189900	1.69536900	-0.08271500
C	-5.92211300	0.08418000	1.59470700
C	-7.11271800	-0.65841900	1.61307500
C	-5.23533200	0.26537200	2.80330800
C	-7.60540300	-1.19576200	2.79911100
H	-7.65522800	-0.83274600	0.68525500
C	-5.71936600	-0.27743700	3.99146300
H	-4.30889600	0.83523700	2.81265800
C	-6.90678100	-1.00513600	3.98978400
H	-8.52764800	-1.76832800	2.79509700
H	-5.17025000	-0.13436000	4.91672400
H	-7.28592600	-1.42768200	4.91515500
C	-5.39522700	-0.40107900	-1.35674400
C	-5.51585200	-0.06584900	-2.71508400
C	-5.27240700	-1.76397500	-1.03690300
C	-5.50120200	-1.04023600	-3.70986800
H	-5.62372200	0.97416800	-3.01061700
C	-5.25485500	-2.74586800	-2.02647500
H	-5.19580900	-2.06586300	0.00542800
C	-5.36669500	-2.38408000	-3.36628200
H	-5.59775500	-0.75211100	-4.75202800

H	-5.15557300	-3.79090200	-1.75039700
H	-5.35322500	-3.14561500	-4.13988900
C	3.79204700	3.04033500	-0.21783200
C	2.59499500	3.12299300	0.51519600
C	2.02647800	4.36226700	0.76849300
C	2.66281000	5.50737700	0.28351400
C	3.85221100	5.40608500	-0.43663000
C	4.44100800	4.16559300	-0.69914400
C	3.27802000	0.86833800	0.30384400
C	2.20456700	1.75262500	0.86510300
H	1.10447200	4.44133300	1.33711200
H	2.23117300	6.48395700	0.47379800
H	4.33704200	6.30721600	-0.79787300
H	5.37697200	4.08847800	-1.24222100
N	4.16218600	1.69663900	-0.35562100
O	3.39226400	-0.34628300	0.38060100
C	1.10277400	1.31146600	1.49095900
C	0.74101400	-0.11718600	1.85263900
O	-0.31315300	-0.29305300	2.49797900
H	1.62569800	-0.76001400	2.00407900
H	0.35897500	2.03372800	1.83187500
C	5.32020500	1.21327100	-1.07958700
H	5.33990000	1.68390700	-2.06894500
H	5.15780100	0.13948700	-1.21765800
C	6.61928500	1.47069600	-0.34702400
C	7.66913700	2.14650800	-0.96509700
C	6.77523700	1.01483400	0.96417100
C	8.86549900	2.36610200	-0.28413100
H	7.55172400	2.50267100	-1.98604800
C	7.96671300	1.23426900	1.64539700
H	5.95683200	0.48247300	1.44310900
C	9.01512100	1.91119800	1.02180700
H	9.67681600	2.89496400	-0.77399600
H	8.08078800	0.87502900	2.66312200
H	9.94487100	2.08305900	1.55442200

Si-M1

Total energy= -2970.577162

Zero-point correction= 0.762060 (Hartree/Particle)

Thermal correction to Energy= 0.813613

Thermal correction to Enthalpy= 0.814557

Thermal correction to Gibbs Free Energy= 0.671386

Sum of electronic and zero-point Energies= -2969.815102

Sum of electronic and thermal Energies= -2969.763549

Sum of electronic and thermal Enthalpies= -2969.762605

Sum of electronic and thermal Free Energies= -2969.905777

C	1.75145300	0.75737500	-2.60014100
C	1.89020500	-0.70974300	-2.11979700
C	1.42973900	-0.71723800	-0.64471600
C	0.64126200	1.24043400	-1.72170100
C	-0.50134000	0.87003100	0.12323600
H	2.66030100	1.33706800	-2.39888300
H	1.51699400	0.84527900	-3.66105600
H	1.22752500	-1.35073000	-2.70665800
H	0.93976200	-1.65262700	-0.36527800
N	-0.16082800	2.25673500	-1.65113500
N	-0.86781300	2.00611800	-0.48954100
N	0.45241900	0.37732800	-0.67394600
C	-1.93767500	2.85301400	-0.12904500
C	-1.90739600	3.56496500	1.06436100
C	-3.03238400	2.97751400	-0.97926000
C	-2.97051200	4.38689800	1.41598300
C	-4.08662100	3.81095000	-0.64237200
C	-4.05296300	4.51339900	0.55648400
F	-3.07905400	2.29566500	-2.11215700
F	-5.13337700	3.93375700	-1.45255000
F	-5.06376800	5.30831500	0.88206300
F	-2.94718400	5.06248300	2.55986500
F	-0.87233800	3.44867900	1.88012500
H	2.90798200	-1.08787400	-2.21185300
C	2.53879200	-0.37596600	0.35641600
H	2.90309200	0.64015800	0.13923500
H	2.11462600	-0.36336500	1.36529400
O	3.56073200	-1.34432400	0.21918000
Si	5.16079200	-0.93647800	-0.06087600
C	5.99762000	-2.58385600	-0.46513100
C	6.07369600	-3.39869800	0.83782400
C	5.17703100	-3.38895100	-1.48436400
C	7.41884500	-2.34194400	-0.99093900
H	6.68405600	-2.89597700	1.59443500
H	5.07812500	-3.56764200	1.26267200
H	6.52369800	-4.37914100	0.63532600
H	5.11518900	-2.89952400	-2.46170100
H	5.64478000	-4.36919400	-1.64380400
H	4.15669900	-3.55366000	-1.12503300
H	7.92234400	-3.30084000	-1.16895100
H	7.42059200	-1.78252600	-1.93249200
H	8.02257800	-1.78286100	-0.26639400

C	5.85698700	-0.17722200	1.50335500
C	7.05746400	0.54934700	1.50361100
C	5.20191200	-0.37517600	2.72698200
C	7.59054500	1.05455500	2.68641200
H	7.57645400	0.73612800	0.56483100
C	5.72668500	0.13505700	3.91212100
H	4.26756300	-0.93145600	2.75046800
C	6.92323300	0.84720200	3.89220900
H	8.51985200	1.61534600	2.66837300
H	5.20146300	-0.02007200	4.84919700
H	7.33331000	1.24547500	4.81514400
C	5.25128500	0.36835100	-1.42470100
C	5.32589200	0.05148200	-2.79083100
C	5.15606200	1.72795000	-1.08196900
C	5.29390900	1.04027200	-3.77095200
H	5.41063100	-0.98535200	-3.10443100
C	5.12226200	2.72426300	-2.05675200
H	5.11269900	2.01565700	-0.03375400
C	5.18833500	2.38067500	-3.40450300
H	5.35435900	0.76603500	-4.81958200
H	5.04534000	3.76624100	-1.76259900
H	5.16128100	3.15361200	-4.16633900
C	-3.63812000	-3.21648300	-0.02279500
C	-2.49780900	-3.13346200	0.79528100
C	-1.97543100	-4.28421000	1.36630200
C	-2.60370900	-5.50625600	1.11366700
C	-3.73763700	-5.56778900	0.30480900
C	-4.27771300	-4.41837500	-0.27922300
C	-3.10149400	-0.98941900	0.00143500
C	-2.10810500	-1.71909000	0.85060900
H	-1.09482200	-4.23660800	2.00002900
H	-2.20822700	-6.41508300	1.55396000
H	-4.21608300	-6.52531000	0.12658900
H	-5.17035300	-4.46205500	-0.89433700
N	-3.97036300	-1.93797400	-0.49369800
O	-3.17116700	0.21081300	-0.22586700
C	-1.11212300	-1.11325400	1.51392700
C	-0.77406500	0.38718600	1.55821200
O	0.32843700	0.67958300	2.22848700
H	-1.72128800	0.90460900	1.85697200
H	-0.44222700	-1.70284100	2.14139800
C	-5.09508000	-1.62838900	-1.35049400
H	-5.04038500	-2.24425300	-2.25556900
H	-4.96309800	-0.58193600	-1.64351400

C	-6.42924100	-1.82990600	-0.66207200
C	-7.46491100	-2.50611900	-1.30448000
C	-6.63749100	-1.32161200	0.62149100
C	-8.69833400	-2.66923600	-0.67634800
H	-7.30558100	-2.90978000	-2.30165500
C	-7.86631100	-1.48593200	1.25112300
H	-5.83001800	-0.79627600	1.12547900
C	-8.90044500	-2.16018900	0.60264300
H	-9.49742300	-3.19913300	-1.18486000
H	-8.01833300	-1.08728100	2.24901900
H	-9.85880000	-2.29004200	1.09485800

Re-TS2-D

Total energy= -2970.494776

Zero-point correction= 0.756672 (Hartree/Particle)

Thermal correction to Energy= 0.794849

Thermal correction to Enthalpy= 0.795793

Thermal correction to Gibbs Free Energy= 0.691901

Sum of electronic and zero-point Energies= -2969.738104

Sum of electronic and thermal Energies= -2969.699927

Sum of electronic and thermal Enthalpies= -2969.698983

Sum of electronic and thermal Free Energies= -2969.802876

Imaginary frequency= -1747.08 cm^{-1}

C	-2.54808100	-3.95372900	-1.83174800
C	-2.98694000	-2.60989100	-2.46597800
C	-2.18782200	-1.49707500	-1.74742000
C	-1.19026000	-3.60910600	-1.31106800
C	0.20651600	-2.00303400	-0.80215200
H	-3.18689900	-4.24530900	-1.00546200
H	-2.51812300	-4.77148700	-2.53804700
H	-2.73257400	-2.60936900	-3.51924900
H	-1.87107200	-0.71052200	-2.40874100
N	-0.18264700	-4.24254700	-0.87038900
N	0.70371300	-3.22852400	-0.52764300
N	-1.01332700	-2.25853000	-1.29189600
C	2.03913300	-3.57562600	-0.24730900
C	2.45220300	-3.83743900	1.04589300
C	2.95162800	-3.72106100	-1.27795400
C	3.74747100	-4.21964400	1.31139800
C	4.24967200	-4.10179500	-1.02474400
C	4.64319500	-4.35328400	0.27229300
F	2.57943100	-3.49188500	-2.51446000
F	5.11107800	-4.23464000	-2.01050800
F	5.87738200	-4.71860000	0.51946400

F	4.13221500	-4.45756000	2.54765600
F	1.61093200	-3.69519200	2.04482300
H	-4.05040000	-2.44001100	-2.37963100
C	-2.90579100	-0.87645000	-0.55637400
H	-3.26557400	-1.65257900	0.11630800
H	-2.19847900	-0.25081300	-0.02919300
O	-3.97449100	-0.12781500	-1.05997300
Si	-5.05883500	0.81098200	-0.22220900
C	-6.25331300	1.45149700	-1.57370500
C	-5.47997800	2.44805600	-2.46486700
C	-6.75532100	0.31158300	-2.48281300
C	-7.45741100	2.18787600	-0.95534000
H	-5.14397300	3.31536900	-1.90762200
H	-4.60943600	1.98712200	-2.92141000
H	-6.12482800	2.80099400	-3.26751300
H	-7.34760200	-0.42500900	-1.95090200
H	-7.38575200	0.71936300	-3.27079600
H	-5.92938300	-0.20771900	-2.95585800
H	-8.09275900	2.59026400	-1.74195400
H	-8.07121600	1.53593600	-0.34194200
H	-7.14204000	3.02335200	-0.33700400
C	-4.12799000	2.23865600	0.59552600
C	-4.70398000	2.99091600	1.62446100
C	-2.85175000	2.60636100	0.16197500
C	-4.04112700	4.06673500	2.19055300
H	-5.67970000	2.73148700	1.99928600
C	-2.17904000	3.67679500	0.73240300
H	-2.36313500	2.05214200	-0.61903300
C	-2.77400600	4.41051200	1.74448500
H	-4.50751600	4.63047100	2.97969000
H	-1.19215000	3.92890900	0.38703900
H	-2.25329200	5.24172900	2.18725600
C	-5.84820600	-0.23604100	1.15320800
C	-7.04957400	-0.93608400	1.01033500
C	-5.17035600	-0.38231700	2.36914700
C	-7.55211300	-1.73548300	2.02480200
H	-7.61477100	-0.86151400	0.10061900
C	-5.66246100	-1.18456300	3.38624300
H	-4.24651400	0.14392500	2.53342200
C	-6.85799300	-1.86279600	3.21641300
H	-8.48334400	-2.25590500	1.88421500
H	-5.11630100	-1.27453800	4.30890400
H	-7.24628200	-2.48241900	4.00572800
C	4.54496600	1.77635400	0.93803500

C	3.67683700	0.81420800	1.46049000
C	3.79263500	0.42853700	2.77968600
C	4.78736900	0.99935500	3.56772000
C	5.64009600	1.95001200	3.03387100
C	5.52966800	2.35751500	1.70674000
C	3.18486300	1.22120900	-0.81216800
C	2.76083700	0.42314100	0.37972800
H	3.12416100	-0.30123000	3.20193100
H	4.88894300	0.70506400	4.59674500
H	6.40095900	2.39007800	3.65389800
H	6.18571300	3.10839700	1.30906100
N	4.24043300	1.99979400	-0.40913400
O	2.75371900	1.18448700	-1.93345500
C	1.79353700	-0.49343800	0.39218500
C	0.82707500	-0.73312000	-0.69282400
O	-0.04012300	0.37008900	-1.08524100
H	0.98439600	-0.18353200	-1.69975900
H	1.67986700	-1.06812700	1.29937100
C	4.98359200	2.85792900	-1.30822000
H	4.69651500	2.56704500	-2.30902900
H	6.04163900	2.64806900	-1.19661700
C	4.72783500	4.34038400	-1.10740600
C	3.42810300	4.83523900	-1.05458700
C	5.78760900	5.23038000	-1.01814300
C	3.19935700	6.19118800	-0.90910800
H	2.59625700	4.15784400	-1.13349000
C	5.56023400	6.59242100	-0.87522000
H	6.79938500	4.86348200	-1.06077200
C	4.26584600	7.07535600	-0.81819900
H	2.18966300	6.56045200	-0.87010200
H	6.39378800	7.26906100	-0.80524800
H	4.08554300	8.12977300	-0.70465400

Si-TS2-D

Total energy= -2970.506036

Zero-point correction= 0.757180 (Hartree/Particle)

Thermal correction to Energy= 0.808669

Thermal correction to Enthalpy= 0.809613

Thermal correction to Gibbs Free Energy= 0.667424

Sum of electronic and zero-point Energies= -2969.748856

Sum of electronic and thermal Energies= -2969.697367

Sum of electronic and thermal Enthalpies= -2969.696423

Sum of electronic and thermal Free Energies= -2969.838612

Imaginary frequency= -1700.75 cm^{-1}

C	2.91426500	2.80069800	-1.60151800
C	2.74224200	1.47147900	-2.37666700
C	1.60968000	0.70052500	-1.65242300
C	1.52095800	3.01117700	-1.10412900
C	-0.43177100	2.06076200	-0.69827200
H	3.60312900	2.68723900	-0.75511100
H	3.26299900	3.62418300	-2.22374900
H	2.42701100	1.68572900	-3.40069100
H	0.96940000	0.14681600	-2.34488800
N	0.77111100	4.00751500	-0.76176700
N	-0.45177900	3.40454400	-0.50159000
N	0.84984300	1.81349200	-1.06985800
C	-1.49471400	4.12374600	0.10655500
C	-2.13229500	3.59064700	1.22343900
C	-1.92649300	5.34146300	-0.40997300
C	-3.19524300	4.25745600	1.81261500
C	-2.97899400	6.02001600	0.18479100
C	-3.61908700	5.47030600	1.28922700
F	-1.34728700	5.85587100	-1.48932700
F	-3.39285200	7.18333800	-0.31228100
F	-4.63414400	6.11651600	1.85160100
F	-3.79436400	3.75052800	2.88621500
F	-1.66724400	2.48192200	1.78683900
H	3.65692500	0.87980900	-2.41290600
C	2.12911500	-0.23014100	-0.55259800
H	2.55636300	0.39002100	0.25050200
H	1.29835900	-0.80431000	-0.12903800
O	3.07885900	-1.11151700	-1.10466200
Si	4.52761000	-1.37980300	-0.29320800
C	5.50786600	-2.54633600	-1.41062700
C	4.88873900	-3.95010700	-1.29142400
C	5.42515100	-2.11092000	-2.88184800
C	6.97071400	-2.60132600	-0.94826800
H	4.96016400	-4.34103700	-0.27198600
H	3.83228300	-3.95140200	-1.58197000
H	5.41939200	-4.64215300	-1.95766400
H	5.89690100	-1.14059400	-3.06504400
H	5.94349400	-2.84511600	-3.51193200
H	4.38580600	-2.04932900	-3.21780100
H	7.52710200	-3.33008900	-1.55113600
H	7.47035300	-1.63208000	-1.04771900
H	7.04834800	-2.91459300	0.09981700
C	4.08803100	-2.18570000	1.34061900
C	4.94903500	-2.18251800	2.44772500

C	2.87695300	-2.88767300	1.44822600
C	4.61265100	-2.85305800	3.62174900
H	5.89243800	-1.64156200	2.39781100
C	2.53463500	-3.55717600	2.61980800
H	2.19486700	-2.92052400	0.60040300
C	3.40348500	-3.53964100	3.70863100
H	5.29116700	-2.83887100	4.46885200
H	1.59384400	-4.09662800	2.67603400
H	3.13986400	-4.06175500	4.62306300
C	5.32424400	0.29931500	0.03524300
C	6.11724200	0.94883100	-0.92516100
C	5.04046900	0.99966900	1.21997600
C	6.60124200	2.23794600	-0.71877400
H	6.36619000	0.44537400	-1.85516400
C	5.52078000	2.29096600	1.43439200
H	4.43799200	0.52712400	1.99278300
C	6.30152700	2.91267100	0.46334300
H	7.21384200	2.71454000	-1.47758300
H	5.28688200	2.80921200	2.35895500
H	6.67811400	3.91739800	0.62718300
C	-2.86960500	-3.38341400	-0.06484000
C	-1.93000900	-2.52489300	0.53754600
C	-1.16956200	-2.97635300	1.60793600
C	-1.35337200	-4.28552000	2.06004800
C	-2.28944200	-5.12176700	1.45207100
C	-3.06840600	-4.68222500	0.37789100
C	-3.02892000	-1.41434300	-1.23665800
C	-2.01102300	-1.24287900	-0.15825400
H	-0.44882700	-2.32150400	2.09177300
H	-0.77886200	-4.65007100	2.90551800
H	-2.42585100	-6.13170100	1.82478500
H	-3.81018400	-5.32683700	-0.08221300
N	-3.50030800	-2.71548900	-1.11732400
O	-3.36291000	-0.63426700	-2.11345600
C	-1.27028400	-0.13003400	0.01423700
C	-1.54432800	1.16035800	-0.63491200
O	-2.82829500	1.75911500	-0.52788800
H	-2.20614200	1.10279400	-1.59792200
H	-0.45669100	-0.17377200	0.74047800
C	-4.50377100	-3.28591300	-1.98599000
H	-4.10847300	-4.19479500	-2.45559400
H	-4.66700400	-2.54316900	-2.77330900
C	-5.80070300	-3.59721900	-1.26611400
C	-6.29820300	-2.72445900	-0.29709100

C	-6.52201900	-4.74816700	-1.58200300
C	-7.50321300	-2.99765200	0.34159600
H	-5.73467400	-1.83080500	-0.04249700
C	-7.73102100	-5.02117800	-0.94589400
H	-6.13395100	-5.43638500	-2.32921300
C	-8.22352900	-4.14625400	0.01810000
H	-7.88108200	-2.31225800	1.09346100
H	-8.28355500	-5.92040300	-1.19925500
H	-9.16284100	-4.35890600	0.51832100

Re-M02

Total energy= -3318.687825

Zero-point correction= 1.005122 (Hartree/Particle)

Thermal correction to Energy= 1.067487

Thermal correction to Enthalpy= 1.068431

Thermal correction to Gibbs Free Energy= 0.904415

Sum of electronic and zero-point Energies= -3317.682703

Sum of electronic and thermal Energies= -3317.620338

Sum of electronic and thermal Enthalpies= -3317.619394

Sum of electronic and thermal Free Energies= -3317.783410

C	-2.98671600	-0.13127200	-2.92016400
C	-3.40621600	1.14791100	-2.15680000
C	-2.57492200	1.16791400	-0.85574600
C	-1.58886500	-0.31288600	-2.42669400
C	-0.12324900	0.19568400	-0.87977000
H	-3.59349300	-0.99776500	-2.63092700
H	-3.03367500	-0.02697600	-4.00394300
H	-3.17061600	2.02832900	-2.75896500
H	-2.29437400	2.16748500	-0.52818600
N	-0.53974800	-1.00577800	-2.75174900
N	0.36980700	-0.67910700	-1.77653400
N	-1.36524000	0.43514700	-1.29592800
C	1.64459300	-1.30544300	-1.78839400
C	1.89919000	-2.36625100	-0.92274100
C	2.63364900	-0.88076900	-2.66892400
C	3.15303100	-2.95376900	-0.87579300
C	3.89234500	-1.46579300	-2.63278600
C	4.14601400	-2.49557900	-1.73550700
F	2.39488600	0.10423200	-3.51846300
F	4.86341600	-1.02287200	-3.41922800
F	5.36429400	-3.00778700	-1.65754100
F	3.41885500	-3.90928000	0.00025900
F	0.96485200	-2.75000000	-0.06360800
H	-4.47170800	1.16742000	-1.93004600

C	-3.22435900	0.38345900	0.29110500
H	-3.32250000	-0.66959900	-0.01743900
H	-2.56323400	0.43091600	1.16250900
O	-4.46773600	0.96870200	0.57713800
Si	-5.90415300	0.08678200	0.60381600
C	-7.24865500	1.40663400	0.72301100
C	-7.17424800	2.01832500	2.13311600
C	-7.02372600	2.53171400	-0.29915700
C	-8.62955200	0.76637200	0.52215300
H	-7.37256200	1.27388600	2.91018100
H	-6.18991900	2.45904100	2.32641100
H	-7.92316100	2.81448100	2.22843700
H	-7.10444600	2.18708800	-1.33483600
H	-7.78278700	3.31167600	-0.16010700
H	-6.03922300	2.99202900	-0.17065600
H	-9.41466200	1.52087700	0.65497500
H	-8.74399700	0.33644600	-0.47841100
H	-8.81130600	-0.02918700	1.25403600
C	-5.87196200	-1.01530700	2.11667900
C	-6.71067200	-2.13449200	2.22601100
C	-5.05299600	-0.69078000	3.20800800
C	-6.73319900	-2.90370100	3.38649400
H	-7.34816000	-2.41491700	1.38950600
C	-5.06735500	-1.46024000	4.36901200
H	-4.40248100	0.17974700	3.14875900
C	-5.90934000	-2.56651600	4.45837400
H	-7.38961000	-3.76538200	3.45430100
H	-4.42767700	-1.19598600	5.20525800
H	-5.92404800	-3.16569300	5.36329300
C	-5.96534300	-1.02398000	-0.92327600
C	-6.51118000	-0.61394500	-2.15095100
C	-5.37201700	-2.29730000	-0.87381100
C	-6.45759900	-1.42839400	-3.27967500
H	-6.99199500	0.35661100	-2.23666600
C	-5.31477600	-3.11947400	-1.99885300
H	-4.96022700	-2.66114200	0.06504900
C	-5.85568500	-2.68340000	-3.20584000
H	-6.89201400	-1.08738000	-4.21408200
H	-4.85492600	-4.10026800	-1.92965000
H	-5.81789100	-3.32119000	-4.08316000
C	4.72148800	-1.24035100	1.36175100
C	3.41344600	-1.31195900	1.86692000
C	3.08534400	-2.27750600	2.80783200
C	4.08248300	-3.15312400	3.24028300

C	5.37586400	-3.06654200	2.72622500
C	5.72056900	-2.10697700	1.76975400
C	3.57541000	0.36000600	0.19057000
C	2.61466000	-0.31599300	1.14529000
H	2.07502800	-2.35485100	3.19787000
H	3.84905900	-3.91166800	3.97883800
H	6.13498400	-3.75911600	3.07368400
H	6.72803100	-2.03814400	1.37408100
N	4.79515400	-0.22792500	0.38592600
O	3.34210700	1.23735400	-0.63459200
C	1.29181100	-0.11529700	1.17406100
C	0.55482100	0.87008200	0.29893800
O	-0.42348300	1.53631300	1.02844200
H	1.26930400	1.56428800	-0.15747800
H	0.66744000	-0.67566000	1.86797800
C	5.97712000	0.09063100	-0.39482700
H	5.65533700	0.83522300	-1.12993700
H	6.29552600	-0.80595800	-0.94128800
C	7.11692500	0.61493800	0.45263500
C	6.87223900	1.46012300	1.53533600
C	8.43028600	0.26730700	0.13828700
C	7.92965900	1.95428100	2.29221500
H	5.84885900	1.72485900	1.78931400
C	9.48966300	0.76596200	0.89202200
H	8.62581800	-0.39782000	-0.69917200
C	9.24098400	1.60934600	1.97116600
H	7.73005600	2.60809100	3.13504600
H	10.50817600	0.48922700	0.64009800
H	10.06520500	1.99294700	2.56332100
C	1.34506600	4.19947600	-0.97565200
C	0.91988000	4.85854000	0.32964100
H	1.61751800	5.00296400	-1.68553600
H	2.25029800	3.60020200	-0.81960400
H	1.69814600	5.57600400	0.63483100
H	0.00575100	5.43866700	0.17439500
N	0.32789900	3.31987600	-1.55534800
N	0.66636400	3.89592500	1.41104400
C	-0.14446800	4.50109200	2.47161300
H	-0.33313800	3.75601300	3.24845200
H	0.35895800	5.36609200	2.92782800
H	-1.10265000	4.82637100	2.05931600
C	1.92089200	3.38839400	1.97861000
H	2.48201600	4.18631200	2.48661900
H	1.69396800	2.59804700	2.69973500

H	2.54955200	2.96420400	1.19097000
C	-0.85648600	4.06612400	-1.95680800
H	-0.61418100	4.92404400	-2.60810700
H	-1.52414300	3.40352400	-2.51435900
H	-1.40191800	4.43529400	-1.08389600
C	0.90304200	2.63749200	-2.70934100
H	1.19640500	3.33692100	-3.51121400
H	1.79136400	2.08091100	-2.39919100
H	0.17518100	1.93347000	-3.13082000
H	-0.12196400	2.51090400	1.06300700

Re-TS2

Total energy= -3318.649940

Zero-point correction= 1.001633 (Hartree/Particle)

Thermal correction to Energy= 1.063678

Thermal correction to Enthalpy= 1.064623

Thermal correction to Gibbs Free Energy= 0.900796

Sum of electronic and zero-point Energies= -3317.648307

Sum of electronic and thermal Energies= -3317.586261

Sum of electronic and thermal Enthalpies= -3317.585317

Sum of electronic and thermal Free Energies= -3317.749144

Imaginary frequency= -1253.43 cm^{-1}

C	3.22763000	-2.90961300	0.71502700
C	3.32930900	-1.67700000	1.64614300
C	2.24156100	-0.69448900	1.15923600
C	1.76804000	-2.88904000	0.39117300
C	-0.06753600	-1.65547600	0.34419000
H	3.81449200	-2.77298200	-0.20201000
H	3.53825200	-3.84182300	1.18598500
H	3.10868400	-1.97760400	2.67475500
H	1.80188400	-0.11067900	1.96655300
N	0.86992600	-3.70999700	-0.04465400
N	-0.28068200	-2.93406700	-0.08085500
N	1.24325700	-1.64308500	0.63972400
C	-1.48795500	-3.57411900	-0.45654500
C	-1.96591600	-3.50047900	-1.76304700
C	-2.15466400	-4.39522000	0.44840900
C	-3.12920200	-4.15482000	-2.13659700
C	-3.30970700	-5.07205600	0.08539000
C	-3.79273100	-4.95425200	-1.21264300
F	-1.70235000	-4.51747300	1.69362200
F	-3.94359700	-5.83218800	0.96554100
F	-4.89781200	-5.58570000	-1.56241200
F	-3.59894800	-4.02582600	-3.36823700

F	-1.34536700	-2.73269100	-2.65137100
H	4.31498100	-1.21270100	1.62816700
C	2.70871800	0.24299400	0.04442000
H	3.01621700	-0.36109000	-0.82265900
H	1.86857000	0.87797700	-0.25379900
O	3.76722500	1.01911100	0.55294900
Si	5.24217000	1.14376000	-0.25493100
C	6.36975700	2.00827400	0.98968700
C	5.92904800	3.48044900	1.07577300
C	6.23546600	1.38569900	2.38818300
C	7.82791900	1.94784000	0.51342800
H	6.04219400	3.99480800	0.11664400
H	4.88202900	3.56993800	1.38731000
H	6.54506600	4.00570100	1.81643900
H	6.57978900	0.34723600	2.42530300
H	6.84438600	1.95246200	3.10387700
H	5.19652300	1.40934900	2.73289100
H	8.47017400	2.50993100	1.20285900
H	8.20500400	0.92093900	0.46616800
H	7.94429600	2.39531900	-0.48053600
C	4.94580600	2.18413800	-1.78149000
C	5.82315600	2.19168800	-2.87620200
C	3.83622300	3.04180400	-1.81565700
C	5.60134300	3.02993100	-3.96591900
H	6.68597300	1.52811100	-2.88372200
C	3.60656100	3.87728800	-2.90523800
H	3.14623000	3.05629500	-0.97449300
C	4.49155200	3.87279200	-3.98060300
H	6.29024200	3.02452900	-4.80457200
H	2.74041600	4.53134000	-2.91608000
H	4.31607600	4.52425600	-4.83093800
C	5.77767600	-0.58402500	-0.79415600
C	6.53299800	-1.43992800	0.02447200
C	5.34076400	-1.09096500	-2.03029400
C	6.83152900	-2.74346900	-0.36434400
H	6.90234900	-1.08836900	0.98372700
C	5.63331100	-2.39553000	-2.42623000
H	4.76997700	-0.45247500	-2.70136200
C	6.37847500	-3.22478600	-1.59142600
H	7.42376900	-3.38051800	0.28490100
H	5.28495900	-2.76084700	-3.38702600
H	6.61261400	-4.23930500	-1.89791900
C	-5.03926000	1.47519700	-1.07577700
C	-4.14973500	0.47292700	-1.49525300

C	-4.32662300	-0.13668000	-2.73000200
C	-5.40139800	0.26409900	-3.52626700
C	-6.27103000	1.26540100	-3.09467600
C	-6.10269200	1.89373500	-1.85734800
C	-3.55658300	1.25126600	0.65382500
C	-3.15528600	0.31301600	-0.43165000
H	-3.64456100	-0.90931300	-3.07699100
H	-5.55691500	-0.20208100	-4.49279600
H	-7.09475400	1.56898400	-3.73189400
H	-6.77045100	2.68315000	-1.52937400
N	-4.66878500	1.92029300	0.20528200
O	-3.05016400	1.38176700	1.76340700
C	-2.09795200	-0.51472600	-0.40916300
C	-1.00461300	-0.56830600	0.58965600
O	-0.31156900	0.65096800	0.73626000
H	-1.45046500	-0.75085400	1.93472800
H	-1.99890400	-1.15091400	-1.28338800
C	-5.37362800	2.92960900	0.96815700
H	-4.90839100	2.93240800	1.95859500
H	-6.42009600	2.62609000	1.08794000
C	-5.29837400	4.30199800	0.33105600
C	-4.09895000	4.76394800	-0.21318400
C	-6.42427200	5.12385400	0.30025400
C	-4.02748300	6.03347700	-0.77650700
H	-3.22183000	4.12166700	-0.20110500
C	-6.35310200	6.39719000	-0.26053700
H	-7.36342300	4.76474500	0.71417200
C	-5.15436900	6.85375100	-0.80030800
H	-3.09174300	6.38440900	-1.19972000
H	-7.23606200	7.02759200	-0.28119200
H	-5.09736300	7.84285700	-1.24275400
C	-1.79504600	0.13551600	4.16472200
C	-0.46875200	0.80884700	4.48692300
H	-2.19771700	-0.27140200	5.10269900
H	-2.51483200	0.84878800	3.76478400
H	-0.66061800	1.52070900	5.30708300
H	0.23880900	0.07449100	4.88302500
N	-1.72561200	-0.98990700	3.19244600
N	0.15621700	1.48818800	3.34955500
C	1.57261600	1.74611600	3.62795100
H	2.05443100	2.15636900	2.73545200
H	1.69970100	2.45899900	4.45687600
H	2.08043000	0.81524000	3.89851200
C	-0.51119100	2.76822300	3.06593200

H	-0.42419400	3.45597000	3.92102900
H	-0.03581400	3.22832400	2.19577400
H	-1.56167300	2.60360100	2.82655700
C	-0.72160500	-1.99860400	3.57259300
H	-0.87809400	-2.33677200	4.60266800
H	-0.80704100	-2.85360100	2.90095000
H	0.28062200	-1.57287800	3.47876700
C	-3.06413900	-1.59711100	3.06681400
H	-3.37316100	-2.05398400	4.01262400
H	-3.76675300	-0.81396900	2.77891400
H	-3.03252600	-2.36384400	2.28916600
H	-0.22764600	0.87069000	1.69768100

Re-M2

Total energy= -2970.627722

Zero-point correction= 0.762679 (Hartree/Particle)

Thermal correction to Energy= 0.814043

Thermal correction to Enthalpy= 0.814987

Thermal correction to Gibbs Free Energy= 0.671831

Sum of electronic and zero-point Energies= -2969.865043

Sum of electronic and thermal Energies= -2969.813679

Sum of electronic and thermal Enthalpies= -2969.812735

Sum of electronic and thermal Free Energies= -2969.955891

C	-3.15665400	-2.82292100	-1.16572500
C	-3.24443500	-1.63336700	-2.15111900
C	-2.14686000	-0.64105300	-1.70733800
C	-1.70206000	-2.79232000	-0.82074400
C	0.15981400	-1.58132000	-0.80608600
H	-3.75554500	-2.64713600	-0.26353300
H	-3.46287500	-3.77446700	-1.60010000
H	-3.02313100	-1.98057500	-3.16368100
H	-1.70652400	-0.08752300	-2.53512500
N	-0.83702900	-3.60211900	-0.30985800
N	0.33250100	-2.84591800	-0.28577400
N	-1.16200500	-1.57309700	-1.13717900
C	1.46690600	-3.41300300	0.31629500
C	2.02058600	-2.85864700	1.47064000
C	2.03299200	-4.56933800	-0.21551500
C	3.14136000	-3.42217900	2.06063300
C	3.13882400	-5.15625200	0.38445600
C	3.69344100	-4.57852200	1.51910200
F	1.52231400	-5.11498800	-1.30969300
F	3.67485200	-6.25747400	-0.12878100
F	4.75510000	-5.13062600	2.08873500

F	3.67367700	-2.88135600	3.14927100
F	1.49757200	-1.75234900	1.98035600
H	-4.22577200	-1.15852800	-2.15721600
C	-2.60980900	0.32843800	-0.61716500
H	-2.89140000	-0.25278700	0.27451300
H	-1.77379600	0.98410800	-0.35485500
O	-3.69449200	1.08257000	-1.11403900
Si	-5.14222300	1.21461400	-0.27859600
C	-6.31088500	2.06438800	-1.49808700
C	-5.88747800	3.54056400	-1.60034900
C	-6.20096800	1.43755400	-2.89666700
C	-7.75711200	1.99246400	-0.98958500
H	-5.99195000	4.05947600	-0.64250200
H	-4.84674500	3.63961200	-1.92804800
H	-6.52067100	4.05438600	-2.33499400
H	-6.53295800	0.39460500	-2.92159900
H	-6.83265500	1.99407400	-3.60106200
H	-5.17077900	1.47127200	-3.26336600
H	-8.41926900	2.55026200	-1.66414300
H	-8.12522200	0.96260100	-0.93483800
H	-7.85472500	2.43823900	0.00742100
C	-4.82916000	2.28105300	1.22971200
C	-5.70040300	2.31690000	2.32861200
C	-3.71639400	3.13489900	1.23887700
C	-5.47100000	3.17917600	3.39782900
H	-6.56478700	1.65561500	2.35538000
C	-3.47859400	3.99442500	2.30823500
H	-3.03082100	3.12704500	0.39420500
C	-4.35840500	4.01846500	3.38756600
H	-6.15552100	3.19479500	4.24018500
H	-2.60921800	4.64421800	2.29954900
H	-4.17634900	4.68889700	4.22178300
C	-5.68265700	-0.49890500	0.30276600
C	-6.44736200	-1.36543900	-0.49539900
C	-5.24102900	-0.98549300	1.54497300
C	-6.75301800	-2.65892800	-0.08042100
H	-6.81445000	-1.03102300	-1.46163300
C	-5.54027800	-2.28019800	1.96714500
H	-4.65704800	-0.34015600	2.19769700
C	-6.29656000	-3.11974000	1.15316400
H	-7.34941400	-3.30546600	-0.71650600
H	-5.18442700	-2.63151500	2.93049200
H	-6.53283200	-4.12777700	1.47913800
C	5.47930200	1.34222500	-1.09118900

C	4.83649600	0.10511700	-0.87128500
C	5.61298800	-1.01091200	-0.57006400
C	6.99934500	-0.87357000	-0.49043600
C	7.61217800	0.36222100	-0.70555100
C	6.85362100	1.49572800	-1.00947900
C	3.24476800	1.73632200	-1.32709000
C	3.40933300	0.32781600	-1.01951900
H	5.14993200	-1.97982100	-0.39783200
H	7.60924200	-1.73911700	-0.25267800
H	8.69119600	0.44822100	-0.63099500
H	7.32034000	2.46402000	-1.15994900
N	4.50444700	2.29596700	-1.38353500
O	2.20505700	2.41141200	-1.50545600
C	2.41349000	-0.62976500	-0.86261300
C	1.04044300	-0.50774900	-1.02420400
O	0.39718400	0.61826800	-1.45237200
H	1.05128100	1.39005500	-1.49141900
H	2.77663800	-1.62046300	-0.60781600
C	4.75255800	3.69262400	-1.66962200
H	3.82429000	4.07993000	-2.09881100
H	5.53945400	3.76582600	-2.42875600
C	5.13521200	4.48501400	-0.43755300
C	6.31804100	5.21936900	-0.39292700
C	4.28350500	4.49057500	0.66989600
C	6.65085800	5.95481500	0.74401100
H	6.98323500	5.21729200	-1.25343600
C	4.61432600	5.22147200	1.80507100
H	3.35876600	3.91973500	0.62831700
C	5.79992900	5.95587800	1.84422100
H	7.57568400	6.52238800	0.76930200
H	3.94767200	5.22146800	2.66162200
H	6.05805600	6.52564600	2.73114600

Si-M02

Total energy= -3318.670359

Zero-point correction= 1.004718 (Hartree/Particle)

Thermal correction to Energy= 1.066910

Thermal correction to Enthalpy= 1.067854

Thermal correction to Gibbs Free Energy= 0.905276

Sum of electronic and zero-point Energies= -3317.665641

Sum of electronic and thermal Energies= -3317.603449

Sum of electronic and thermal Enthalpies= -3317.602505

Sum of electronic and thermal Free Energies= -3317.765083

C	-0.07829700	-3.76171400	1.93902100

C	0.86740100	-2.69533200	2.54525300
C	0.53192200	-1.36648800	1.83406600
C	-1.24218300	-2.91721200	1.53281500
C	-1.94183300	-0.89233800	1.08129300
H	0.35449900	-4.23497200	1.04914200
H	-0.35601300	-4.54580300	2.64316900
H	0.66649300	-2.59057300	3.61381700
H	0.65682200	-0.49953000	2.48556600
N	-2.46713200	-3.08748900	1.13365500
N	-2.88755800	-1.81036700	0.85547700
N	-0.89856900	-1.58737000	1.53042200
C	-4.19805300	-1.59632600	0.36474700
C	-4.60071200	-2.22373700	-0.81065900
C	-5.10525500	-0.82538900	1.08478400
C	-5.90469800	-2.08539100	-1.26331500
C	-6.41517800	-0.69922700	0.64953200
C	-6.80891400	-1.32571700	-0.52835400
F	-4.70869200	-0.20997600	2.19346000
F	-7.29563600	-0.00106700	1.35126200
F	-8.05292800	-1.19342400	-0.95068500
F	-6.28577200	-2.66406300	-2.39088100
F	-3.73144400	-2.92829100	-1.51664600
H	1.91939300	-2.94698900	2.41691900
C	1.27708300	-1.14423200	0.51002500
H	1.01280500	-1.95877900	-0.18188200
H	0.93690000	-0.20277600	0.06051200
O	2.65015100	-1.10179400	0.78636100
Si	3.77265900	-2.13773800	0.06904100
C	5.31802500	-1.90501700	1.12717200
C	5.85735900	-0.48998600	0.84976400
C	4.98528600	-2.00807000	2.62375800
C	6.38840400	-2.93583600	0.74265200
H	6.16881400	-0.37684700	-0.19393900
H	5.10694600	0.27868500	1.07062600
H	6.73076900	-0.29609800	1.48480700
H	4.64623000	-3.00818300	2.91304300
H	5.88176600	-1.78891500	3.21711600
H	4.20885000	-1.29019000	2.90648200
H	7.30696800	-2.75305400	1.31410300
H	6.06652700	-3.96234700	0.94776200
H	6.64453200	-2.86941200	-0.32105800
C	4.04423300	-1.56331600	-1.68930000
C	4.60662600	-2.40265100	-2.66286600
C	3.76976600	-0.23417800	-2.04060200

C	4.89056200	-1.92772100	-3.94044700
H	4.81876800	-3.44321000	-2.42381200
C	4.05395100	0.24832100	-3.31547600
H	3.33153100	0.43498900	-1.30338900
C	4.61589800	-0.60057400	-4.26652100
H	5.32540700	-2.59100000	-4.68138200
H	3.84247300	1.28517800	-3.55975400
H	4.83967300	-0.22905000	-5.26159500
C	3.05413000	-3.88223800	0.00924300
C	3.24308700	-4.83927600	1.02029700
C	2.22679400	-4.23765600	-1.07086400
C	2.62444700	-6.08616600	0.96571000
H	3.88506700	-4.61679900	1.86838800
C	1.60268700	-5.48286700	-1.13214800
H	2.07770600	-3.53393600	-1.88727300
C	1.79917100	-6.40873700	-0.11047000
H	2.79208400	-6.80938800	1.75743800
H	0.97229800	-5.73225300	-1.97971900
H	1.31938100	-7.38119900	-0.15697600
C	1.48782500	3.79324900	1.80805300
C	0.64740400	2.89327000	2.47910800
C	0.83631400	2.64854800	3.83215800
C	1.86058100	3.32229300	4.50017800
C	2.68674400	4.21238000	3.81452400
C	2.51801800	4.46088600	2.44993100
C	0.00791600	3.09160300	0.19700100
C	-0.27599800	2.33146500	1.48184300
H	0.19368300	1.95758400	4.37111300
H	2.01610200	3.15132700	5.55935500
H	3.48233800	4.72183800	4.34767200
H	3.17244900	5.13916000	1.91309400
N	1.10414200	3.88282500	0.46247700
O	-0.62350700	3.11318100	-0.84405200
C	-1.15233800	1.34092200	1.69397100
C	-1.94824800	0.56339600	0.67013600
O	-1.39827900	0.52976500	-0.60184800
H	-2.99604500	0.91605400	0.65532000
H	-1.27819000	1.00638000	2.72584600
C	1.66494700	4.81240400	-0.49255600
H	1.61922200	5.82518900	-0.07374300
H	1.00359400	4.78455500	-1.36350100
C	3.08925600	4.48471400	-0.89731500
C	3.85095400	5.47329300	-1.52356200
C	3.64751500	3.22349200	-0.69195500

C	5.14471500	5.20131600	-1.95511900
H	3.42458500	6.46162400	-1.67723700
C	4.94607300	2.95141100	-1.11991000
H	3.07031700	2.45449300	-0.18383300
C	5.69559800	3.93679300	-1.75585200
H	5.72444400	5.97793400	-2.44339900
H	5.36909400	1.96441900	-0.95824000
H	6.70601800	3.72313600	-2.08834100
C	-4.77764100	3.03536200	-1.46401900
C	-3.52477800	2.98464800	-2.32991100
H	-5.12785800	4.08441000	-1.45879400
H	-5.57281100	2.44832800	-1.93646200
H	-3.82695200	3.30046700	-3.34260900
H	-2.76986300	3.69441200	-1.97825900
N	-4.60802500	2.53900100	-0.10047300
N	-2.87407600	1.66905400	-2.39611100
C	-1.83472500	1.69062900	-3.43093700
H	-1.29600000	0.73941400	-3.41993500
H	-2.26475700	1.84678600	-4.43100900
H	-1.12998100	2.49278900	-3.20447700
C	-3.81618700	0.57605400	-2.63005600
H	-4.38122800	0.70395900	-3.56593500
H	-3.25749500	-0.36343400	-2.68459600
H	-4.51387000	0.52013900	-1.78925600
C	-3.68563800	3.38809700	0.64628400
H	-4.03311100	4.43536700	0.68731900
H	-3.60191600	3.01852000	1.67340600
H	-2.69509900	3.36368800	0.18546100
C	-5.90358100	2.52769700	0.56818800
H	-5.80448600	2.08996500	1.56520600
H	-6.32498200	3.54195800	0.67543900
H	-6.61411100	1.92738400	-0.00697300
H	-1.96373700	1.13640900	-1.21348800

Si-TS2

Total energy=	-3318.639137
Zero-point correction=	1.001489 (Hartree/Particle)
Thermal correction to Energy=	1.063332
Thermal correction to Enthalpy=	1.064277
Thermal correction to Gibbs Free Energy=	0.903194
Sum of electronic and zero-point Energies=	-3317.637648
Sum of electronic and thermal Energies=	-3317.575804
Sum of electronic and thermal Enthalpies=	-3317.574860
Sum of electronic and thermal Free Energies=	-3317.735943

Imaginary frequency= -1077.23 cm^{-1}

C	0.32167300	3.99533200	1.83059100
C	-0.68346800	3.03428400	2.51381700
C	-0.40804900	1.62990100	1.93264400
C	1.42395400	3.05708200	1.45390500
C	1.96597700	0.95594700	1.06681100
H	-0.09691100	4.43795500	0.91811000
H	0.65636500	4.80403900	2.48019900
H	-0.50833600	3.01969200	3.59173300
H	-0.56919000	0.83677100	2.66446800
N	2.60538300	3.13245200	0.91753200
N	2.93098000	1.81630600	0.69607600
N	1.02067700	1.75375000	1.58594700
C	4.17513900	1.49946700	0.10587900
C	4.31325600	1.50567900	-1.27753700
C	5.28868500	1.27200600	0.90786500
C	5.55083700	1.25094400	-1.85553500
C	6.52580500	1.00875500	0.33966000
C	6.65505800	1.00496900	-1.04628800
F	5.15878000	1.25903200	2.22802700
F	7.56962100	0.73927100	1.11041500
F	7.82734200	0.74498600	-1.59501500
F	5.66970500	1.20376100	-3.17397400
F	3.26522300	1.72725600	-2.04848600
H	-1.71962100	3.32280800	2.33539800
C	-1.17049500	1.31713800	0.64316600
H	-0.89543300	2.07321900	-0.10912300
H	-0.85577100	0.33890000	0.25636600
O	-2.54251500	1.33300700	0.93619200
Si	-3.60136600	2.14874100	-0.09317600
C	-5.27935500	2.04979200	0.76968000
C	-5.81082000	0.61616700	0.59122700
C	-5.15233300	2.33351500	2.27422200
C	-6.26040400	3.03474300	0.11850500
H	-5.97542900	0.37886300	-0.46457600
H	-5.11495100	-0.12521200	1.00222800
H	-6.76708400	0.50864600	1.11858700
H	-4.83382400	3.35922800	2.48555500
H	-6.12687200	2.19347600	2.75888800
H	-4.43692200	1.65338100	2.74587800
H	-7.25361700	2.93029900	0.57272000
H	-5.94148700	4.07471000	0.24377600
H	-6.36878500	2.84230900	-0.95549500
C	-3.58919900	1.21709700	-1.71475800

C	-4.01531100	1.78448700	-2.92539000
C	-3.21894900	-0.13628900	-1.71103900
C	-4.06940200	1.02440100	-4.09107900
H	-4.30199700	2.83411900	-2.96112900
C	-3.26925200	-0.90090100	-2.87372400
H	-2.89800600	-0.60843900	-0.78352900
C	-3.69609600	-0.31866500	-4.06455000
H	-4.40301800	1.47754700	-5.01945100
H	-2.98945100	-1.95072800	-2.84082400
H	-3.74060200	-0.91165300	-4.97292100
C	-2.90741100	3.88571900	-0.34810200
C	-3.14840400	4.93081100	0.55904500
C	-2.01888300	4.14019300	-1.40661300
C	-2.52608100	6.16973100	0.42467900
H	-3.83562400	4.78321100	1.38767800
C	-1.39213200	5.37779000	-1.54877100
H	-1.81714900	3.36003300	-2.13760400
C	-1.64378700	6.39443900	-0.63060400
H	-2.73406800	6.96093900	1.13805000
H	-0.71223400	5.54880800	-2.37743300
H	-1.16074200	7.36024500	-0.74036600
C	-1.79986200	-3.40093700	2.16799500
C	-0.89623400	-2.48272100	2.73239800
C	-1.03735100	-2.11231200	4.06317800
C	-2.06974700	-2.67385200	4.81740600
C	-2.95723100	-3.58084300	4.23960600
C	-2.83888600	-3.95589600	2.89856600
C	-0.32885000	-2.89779200	0.47891500
C	0.02486100	-2.07033900	1.66777200
H	-0.35110200	-1.40423600	4.52129800
H	-2.18447200	-2.39973500	5.86028300
H	-3.75856300	-4.00220200	4.83720200
H	-3.54172200	-4.64772500	2.44516200
N	-1.45859700	-3.61759000	0.82752700
O	0.26944200	-3.04581700	-0.57918300
C	0.96784800	-1.10272000	1.76842400
C	1.85079400	-0.49142000	0.78275200
O	1.49660500	-0.55765100	-0.57986300
H	3.07377300	-1.34276400	0.85720700
H	1.12147900	-0.71001200	2.77858700
C	-2.02765300	-4.62621000	-0.04176200
H	-2.27629800	-5.50006000	0.57277800
H	-1.23606700	-4.92241100	-0.73557100
C	-3.24723400	-4.17620600	-0.82163400

C	-3.51007300	-4.76560700	-2.06000100
C	-4.14208600	-3.23167300	-0.31555800
C	-4.65383000	-4.42703700	-2.77797400
H	-2.81255000	-5.49488600	-2.46429200
C	-5.28697100	-2.89268400	-1.03371800
H	-3.94322300	-2.75397900	0.64050500
C	-5.54718200	-3.48986200	-2.26388900
H	-4.84308100	-4.89093900	-3.74078400
H	-5.97315500	-2.15362100	-0.63224300
H	-6.43606300	-3.21925600	-2.82398600
C	4.78811500	-2.30349300	-0.31268500
C	4.20824800	-3.05729800	-1.50369900
H	5.73786800	-2.77756400	-0.03587700
H	5.00143400	-1.26111800	-0.57623100
H	4.99670700	-3.10376100	-2.27371300
H	4.00652400	-4.09215300	-1.21531700
N	3.92011700	-2.26450400	0.89827100
N	2.98029200	-2.47019600	-2.03359600
C	2.17981200	-3.47739200	-2.73194100
H	1.25623600	-3.01594100	-3.08589400
H	2.72453800	-3.90316400	-3.58976400
H	1.90309000	-4.27393300	-2.03954700
C	3.28467800	-1.37226800	-2.95044600
H	3.75604900	-1.73724100	-3.87651000
H	2.36927300	-0.83186100	-3.20068500
H	3.96956400	-0.66896900	-2.47650300
C	3.14050600	-3.50351700	1.11169300
H	3.80333800	-4.37462100	1.10462700
H	2.64911900	-3.43328700	2.08290800
H	2.37721400	-3.58543600	0.33308200
C	4.71827500	-1.94762900	2.09806800
H	4.04014700	-1.66586000	2.90778200
H	5.30999700	-2.81617000	2.40011200
H	5.38856600	-1.11368700	1.88878000
H	1.81199700	-1.41451600	-0.95132500

Si-M2

Total energy= -2970.627197

Zero-point correction= 0.762181 (Hartree/Particle)

Thermal correction to Energy= 0.813668

Thermal correction to Enthalpy= 0.814613

Thermal correction to Gibbs Free Energy= 0.670187

Sum of electronic and zero-point Energies= -2969.865016

Sum of electronic and thermal Energies= -2969.813529

Sum of electronic and thermal Enthalpies= -2969.812584

Sum of electronic and thermal Free Energies= -2969.957010

C	2.97537900	2.84925000	-1.28632800
C	2.90695800	1.55011800	-2.12110100
C	1.71501400	0.75654900	-1.54418100
C	1.53187100	3.03215700	-0.93965300
C	-0.46750200	2.07054100	-0.78050500
H	3.57041000	2.71245200	-0.37469000
H	3.38034100	3.69875500	-1.83582300
H	2.69771200	1.79503800	-3.16523700
H	1.21922300	0.15811300	-2.31290300
N	0.77446200	4.00100100	-0.55588500
N	-0.47876400	3.40601100	-0.45066000
N	0.84818800	1.85038600	-1.09291800
C	-1.53597900	4.18643100	0.04924700
C	-2.21202000	3.81783300	1.20902300
C	-1.87902700	5.37662200	-0.58465700
C	-3.23636500	4.60493100	1.70981500
C	-2.88506200	6.18411700	-0.07453600
C	-3.56563400	5.79410400	1.07065600
F	-1.25287200	5.74702500	-1.69488300
F	-3.20647200	7.32168000	-0.68427600
F	-4.53373300	6.56045400	1.55804700
F	-3.88250800	4.24612800	2.81499400
F	-1.87164700	2.70482900	1.84368200
H	3.82514600	0.96433700	-2.07907300
C	2.11194500	-0.11452900	-0.34876900
H	2.56161900	0.53801900	0.41450400
H	1.22915900	-0.58262400	0.10434000
O	3.00788200	-1.10245600	-0.79844100
Si	4.46594200	-1.38939100	-0.00846100
C	5.40181200	-2.55019800	-1.16901900
C	4.74508500	-3.93891100	-1.07450300
C	5.30540100	-2.07406700	-2.62672700
C	6.87061600	-2.65744200	-0.73610500
H	4.82543700	-4.35817100	-0.06698600
H	3.68304000	-3.90224000	-1.34291600
H	5.24149400	-4.62816100	-1.76942100
H	5.79125100	-1.10717100	-2.79112400
H	5.80039300	-2.79978500	-3.28473100
H	4.26219300	-1.98439900	-2.94387500
H	7.39578300	-3.38361600	-1.36940300
H	7.39506500	-1.69970300	-0.81916500
H	6.95952000	-3.00146100	0.30119800

C	4.06502200	-2.20957000	1.62573600
C	4.97728300	-2.24609100	2.69085800
C	2.83905100	-2.87374900	1.78072800
C	4.67692500	-2.92373100	3.86976600
H	5.93185800	-1.72983800	2.60377300
C	2.53132100	-3.54804400	2.95955200
H	2.11740400	-2.86680700	0.96593100
C	3.45196500	-3.57429500	4.00424200
H	5.39466700	-2.94249800	4.68392900
H	1.57550300	-4.05194600	3.06268400
H	3.21485000	-4.10043000	4.92362100
C	5.29483700	0.27166500	0.33532600
C	6.11709800	0.91458800	-0.60426300
C	5.01217400	0.96213300	1.52646100
C	6.62488700	2.19069600	-0.37537200
H	6.36930000	0.41694600	-1.53663900
C	5.51728700	2.23985400	1.76400700
H	4.39076900	0.49190400	2.28565000
C	6.32286000	2.85731700	0.81070200
H	7.25914200	2.66266600	-1.11914500
H	5.28291600	2.75080700	2.69249300
H	6.71800200	3.85195000	0.99181500
C	-3.20721500	-3.28301600	-1.42244800
C	-1.98688500	-2.57535700	-1.39871700
C	-0.79654000	-3.27261100	-1.59219800
C	-0.84645600	-4.65063700	-1.80859900
C	-2.06563900	-5.33041900	-1.82878800
C	-3.27119000	-4.65131500	-1.63196100
C	-3.74767100	-1.09819300	-1.02764000
C	-2.30422500	-1.18057700	-1.15396400
H	0.16214000	-2.75707600	-1.57675700
H	0.07677800	-5.20069200	-1.96072700
H	-2.08093400	-6.40256200	-1.99424800
H	-4.22105000	-5.17670100	-1.62978900
N	-4.24606900	-2.37533800	-1.20517400
O	-4.48023300	-0.11261800	-0.79943600
C	-1.38358000	-0.14605400	-1.07198600
C	-1.57646100	1.21044200	-0.83694600
O	-2.78054600	1.80763700	-0.63748500
H	-3.51055500	1.11270000	-0.67423100
H	-0.35578100	-0.46050100	-1.20321600
C	-5.65046200	-2.70895700	-1.15153400
H	-5.95491200	-3.16504900	-2.10142200
H	-6.17870400	-1.75571000	-1.05147300

C	-5.99665400	-3.63628600	-0.00374900
C	-6.96677100	-4.62448500	-0.17011900
C	-5.36409100	-3.50429700	1.23314000
C	-7.30929700	-5.46503200	0.88649100
H	-7.45375000	-4.73958900	-1.13558000
C	-5.70221900	-4.34519600	2.28847700
H	-4.59866300	-2.74368100	1.36145800
C	-6.67652700	-5.32731200	2.11864000
H	-8.06426500	-6.23170200	0.74373300
H	-5.20306800	-4.23547500	3.24608500
H	-6.93698200	-5.98442600	2.94211800

TS3R

Total energy= -4208.309711

Zero-point correction= 1.028737 (Hartree/Particle)

Thermal correction to Energy= 1.098488

Thermal correction to Enthalpy= 1.099433

Thermal correction to Gibbs Free Energy= 0.915847

Sum of electronic and zero-point Energies= -4207.280974

Sum of electronic and thermal Energies= -4207.211222

Sum of electronic and thermal Enthalpies= -4207.210278

Sum of electronic and thermal Free Energies= -4207.393863

Imaginary frequency= -365.58 cm^{-1}

C	-3.85683500	-2.95744200	-1.45449100
C	-3.77773100	-1.51119700	-2.00396100
C	-2.63219200	-0.82743800	-1.23028600
C	-2.42831500	-3.18497500	-1.07305600
C	-0.48069600	-2.23902800	-0.66620700
H	-4.49698600	-3.02025100	-0.56562500
H	-4.21045500	-3.68502700	-2.18464900
H	-3.51677900	-1.52898100	-3.06504900
H	-2.09722700	-0.09872900	-1.83780900
N	-1.65087700	-4.19157300	-0.82642700
N	-0.43297900	-3.59586400	-0.56024500
N	-1.76344600	-1.99101300	-0.97576200
C	0.63082300	-4.41711200	-0.13174200
C	1.18172100	-4.25498200	1.13875700
C	1.11133700	-5.42460500	-0.96304900
C	2.22583900	-5.06228300	1.56140800
C	2.14006200	-6.25418800	-0.53611200
C	2.69508600	-6.06956300	0.72419200
F	0.59700800	-5.59206100	-2.17079400
F	2.59380900	-7.21788200	-1.32638400
F	3.67818500	-6.85616400	1.13201500

F	2.76059500	-4.89716500	2.76281800
F	0.73428400	-3.28943800	1.92820000
H	-4.71366300	-0.96561800	-1.88852500
C	-3.05994600	-0.22930800	0.11236000
H	-3.49769500	-1.01869500	0.74324500
H	-2.17616400	0.17218700	0.61892600
O	-3.98019000	0.80662200	-0.14626300
Si	-5.51758300	0.87009200	0.52289400
C	-6.39543800	2.20601300	-0.48178700
C	-5.75359500	3.55707500	-0.12146900
C	-6.20227100	1.97775100	-1.98932100
C	-7.88760600	2.24203100	-0.12599000
H	-5.85923300	3.78913000	0.94326500
H	-4.68734700	3.56948500	-0.37379700
H	-6.23916500	4.35870200	-0.69232500
H	-6.68217700	1.06034600	-2.34408200
H	-6.64857900	2.81074900	-2.54735300
H	-5.14023000	1.92721100	-2.24960800
H	-8.38595000	3.04885600	-0.67800000
H	-8.39410400	1.30329900	-0.37524200
H	-8.03802300	2.43373000	0.94297200
C	-5.33376600	1.35574300	2.32408500
C	-6.39406400	1.23427900	3.23493400
C	-4.12795400	1.90535600	2.78211700
C	-6.25890100	1.65848900	4.55404400
H	-7.33562800	0.79187000	2.91344300
C	-3.98469900	2.32616800	4.10233700
H	-3.28884100	1.99805400	2.09561300
C	-5.05281300	2.20610400	4.98778600
H	-7.08990100	1.55896000	5.24533500
H	-3.04197500	2.74521900	4.44026700
H	-4.94508900	2.53506000	6.01667200
C	-6.29692000	-0.84978300	0.47272800
C	-7.04808200	-1.32647400	-0.61376500
C	-6.05341000	-1.74288500	1.53054600
C	-7.52125100	-2.63571300	-0.65369300
H	-7.26996700	-0.67103300	-1.45117100
C	-6.52210100	-3.05560900	1.49792200
H	-5.49337600	-1.40571000	2.40028000
C	-7.25492900	-3.50504300	0.40244600
H	-8.10049200	-2.97517600	-1.50662000
H	-6.31775700	-3.72435400	2.32825700
H	-7.62229600	-4.52603100	0.37363400
C	4.99352500	-0.11202800	0.68053000

C	4.29703100	-1.19069000	0.10318800
C	4.93080100	-2.41946300	-0.02935800
C	6.25043600	-2.54959900	0.41239100
C	6.92759100	-1.46465000	0.96856600
C	6.30541700	-0.22087300	1.11249300
C	2.91752300	0.69194300	0.18864700
C	2.98292200	-0.68795700	-0.31298400
H	4.41669100	-3.26721700	-0.47712000
H	6.75527400	-3.50511900	0.31620300
H	7.95302600	-1.58564100	1.30145700
H	6.82131500	0.62342700	1.55808400
N	4.14715400	0.99934500	0.71583200
O	1.98926500	1.51149500	0.09436300
C	1.85573400	-1.55248700	-0.47105100
C	0.53230400	-1.22815800	-0.49594700
O	-0.00853500	-0.00123600	-0.38502800
H	0.72401600	0.69540700	-0.30873600
H	2.10796800	-2.59257700	-0.64665000
C	4.53256400	2.32809800	1.14023500
H	3.67812100	2.97333000	0.91397100
H	5.37307000	2.66504000	0.52165800
C	4.89521200	2.40541600	2.60785000
C	5.88335600	3.29774600	3.02514300
C	4.24346600	1.61839900	3.55776000
C	6.20854700	3.41252800	4.37417900
H	6.40049400	3.90355600	2.28452900
C	4.57058700	1.72835500	4.90588500
H	3.48232500	0.91358200	3.23362100
C	5.55260600	2.62664900	5.31806600
H	6.97989800	4.10926800	4.68711600
H	4.05975100	1.10913800	5.63659000
H	5.80893400	2.70937900	6.36939200
C	3.31743400	1.29355000	-2.53204800
C	3.49633500	-0.07921300	-2.36035000
H	4.49463800	-0.48939100	-2.26913000
H	2.74333600	-0.73191100	-2.78837500
C	4.37155400	2.29015300	-2.22939900
C	5.72765900	1.93632800	-2.16939300
C	4.02814800	3.62351900	-1.96039100
C	6.70232300	2.87953900	-1.85908200
H	6.03535700	0.91494100	-2.37220500
C	5.00456100	4.56849900	-1.66338400
H	2.97987000	3.90147000	-1.96901000
C	6.34848500	4.20468000	-1.60884800

H	7.74452700	2.57704100	-1.82186800
H	4.71146400	5.59422000	-1.45979400
H	7.10991100	4.94179200	-1.37437200
N	2.10588500	1.80202700	-2.87108400
N	1.11830800	0.99309400	-2.92477200
S	-0.25802600	1.84892400	-3.47249700
O	-1.34687900	0.86846600	-3.45613100
O	0.02998700	2.56323900	-4.71411200
C	-0.56918300	3.05950700	-2.20918600
C	-1.51844800	2.81598500	-1.22348400
C	0.18559300	4.23103700	-2.21169300
C	-1.69609300	3.75748100	-0.21383600
H	-2.13409000	1.92422900	-1.25476100
C	0.00023300	5.15441500	-1.19115300
H	0.89529300	4.40755600	-3.01280700
C	-0.93465400	4.92787100	-0.17460900
H	-2.44698300	3.58064500	0.55221200
H	0.58401400	6.07092200	-1.18539800
C	-1.10488100	5.92283900	0.94314300
H	-2.07729200	5.81082900	1.42792900
H	-0.33230600	5.77935700	1.70549300
H	-1.01763600	6.94821100	0.57556100

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Total energy= -4208.298879

Zero-point correction= 1.028303 (Hartree/Particle)

Thermal correction to Energy= 1.098178

Thermal correction to Enthalpy= 1.099122

Thermal correction to Gibbs Free Energy= 0.912465

Sum of electronic and zero-point Energies= -4207.270576

Sum of electronic and thermal Energies= -4207.200701

Sum of electronic and thermal Enthalpies= -4207.199757

Sum of electronic and thermal Free Energies= -4207.386414

Imaginary frequency= -385.79 cm^{-1}

C	5.18765900	1.88194400	-1.98886100
C	4.69880900	0.55221700	-2.61274100
C	3.55003700	0.05514500	-1.70922700
C	3.93510900	2.36475600	-1.33239800
C	1.92436700	1.82795300	-0.60815900
H	5.96241100	1.71925100	-1.23041900
H	5.57073700	2.59175200	-2.72178200
H	4.30977900	0.73825100	-3.61668000
H	2.77364800	-0.48401300	-2.24853900
N	3.48793200	3.47342600	-0.83435300

N	2.22985900	3.13278200	-0.37776800
N	3.02393000	1.34606000	-1.21741100
C	1.49289500	4.09002000	0.35137600
C	1.28500700	3.91536500	1.71810100
C	0.99185100	5.22298000	-0.28211500
C	0.55848600	4.84697400	2.44244700
C	0.27682700	6.16900200	0.44011200
C	0.06140800	5.97639900	1.79971000
F	1.18286800	5.39516800	-1.58080900
F	-0.20488800	7.24836000	-0.16057100
F	-0.62283900	6.87395300	2.48894900
F	0.35145000	4.67921700	3.74021400
F	1.75532600	2.83173800	2.31732200
H	5.48812400	-0.19637600	-2.68224400
C	4.02989200	-0.76256800	-0.50418900
H	4.66060600	-0.11683600	0.12682800
H	3.15775200	-1.07328100	0.07918100
O	4.73573100	-1.88460400	-0.97630600
Si	6.27955300	-2.26007700	-0.43092100
C	6.84355700	-3.66957800	-1.55448600
C	6.04105900	-4.92397700	-1.16413100
C	6.55436600	-3.35827000	-3.03090200
C	8.33886500	-3.94367400	-1.34390100
H	6.24066200	-5.22863500	-0.13217300
H	4.96290300	-4.76008800	-1.26817600
H	6.31846400	-5.75679100	-1.82263400
H	7.11725400	-2.49558000	-3.40143700
H	6.83748500	-4.21852200	-3.65075200
H	5.49017000	-3.16182600	-3.19202100
H	8.64850200	-4.81031400	-1.94141900
H	8.96082400	-3.09250700	-1.64016200
H	8.55869300	-4.17278000	-0.29448500
C	6.13819500	-2.81237300	1.35277800
C	7.24172900	-2.82617100	2.21878200
C	4.91245800	-3.29777200	1.83204200
C	7.12770200	-3.31216300	3.51865700
H	8.20111800	-2.44241100	1.87611700
C	4.79146900	-3.77967800	3.13310300
H	4.04487800	-3.30187000	1.17538800
C	5.90051400	-3.78848300	3.97608000
H	7.99240300	-3.31666900	4.17479900
H	3.83489100	-4.14949600	3.48844900
H	5.80844600	-4.16599300	4.98968200
C	7.34226700	-0.69692100	-0.47762800

C	8.06868300	-0.29857900	-1.61201100
C	7.35590000	0.16443200	0.63306300
C	8.76731000	0.90593200	-1.64319900
H	8.09511900	-0.93472300	-2.49219800
C	8.05168400	1.37262300	0.60998600
H	6.82026300	-0.11767800	1.53685200
C	8.75720500	1.74616200	-0.53119300
H	9.32361800	1.18654500	-2.53200300
H	8.04558900	2.01775500	1.48285000
H	9.30235400	2.68450500	-0.55285400
C	-3.81031400	0.64682700	1.02286100
C	-2.93216700	1.65263500	0.58369300
C	-3.37333200	2.96857300	0.53127500
C	-4.67611400	3.26011400	0.93573100
C	-5.52863500	2.24674100	1.37796000
C	-5.10579100	0.91786300	1.43452800
C	-1.86298100	-0.42180000	0.53908300
C	-1.70934100	0.98660400	0.14047900
H	-2.72502800	3.75912200	0.15983200
H	-5.03669800	4.28220000	0.89080000
H	-6.54113800	2.49410800	1.67984600
H	-5.76225700	0.12850900	1.78634100
N	-3.14749600	-0.58344700	0.96908400
O	-1.01536100	-1.33740300	0.51511800
C	-0.44769300	1.64622900	-0.00361200
C	0.73218900	1.06038000	-0.35834000
O	0.92600700	-0.25165100	-0.60796600
H	0.16639000	-0.79795600	-0.16831500
H	-0.47261900	2.72703700	0.08204000
C	-3.76305100	-1.86892400	1.23092400
H	-3.12021700	-2.62090900	0.75901900
H	-4.72987400	-1.88207100	0.71504600
C	-3.94660400	-2.14928000	2.70471800
C	-5.20217000	-2.46582300	3.21949900
C	-2.84507200	-2.10646700	3.56297600
C	-5.36030900	-2.73634500	4.57816100
H	-6.05924000	-2.50134800	2.55002000
C	-3.00159900	-2.37282100	4.91828800
H	-1.86607500	-1.86817300	3.15339100
C	-4.26084600	-2.68821700	5.42906400
H	-6.34280800	-2.97921800	4.97086800
H	-2.14091100	-2.33880900	5.57882600
H	-4.38237600	-2.89546300	6.48751400
C	-3.57894000	0.32119300	-2.07855400

C	-2.22119200	0.62019800	-1.92649100
H	-1.87914500	1.61615800	-2.17964000
H	-1.49869500	-0.18045100	-2.06083900
C	-4.62134400	1.36154200	-2.23745900
C	-4.32836000	2.62382100	-2.77240600
C	-5.94159900	1.10402900	-1.84439200
C	-5.31187400	3.59866100	-2.89023300
H	-3.32275300	2.84619400	-3.11746600
C	-6.92782600	2.07629900	-1.97240500
H	-6.18031700	0.13351500	-1.41910600
C	-6.61883700	3.33202500	-2.48815500
H	-5.05903700	4.56755900	-3.31072700
H	-7.94226600	1.85406700	-1.65388400
H	-7.38756300	4.09240200	-2.58291900
N	-4.03322500	-0.96089000	-2.09364000
N	-3.21391900	-1.89291400	-1.80842900
S	-3.92471200	-3.41998200	-2.12594900
O	-3.15056600	-4.36989000	-1.33133800
O	-4.02929000	-3.59968800	-3.57280400
C	-5.57977200	-3.38537400	-1.46669500
C	-5.84012700	-4.06113800	-0.27940100
C	-6.58291600	-2.68392200	-2.13448200
C	-7.12649500	-4.02390200	0.25172300
H	-5.03914900	-4.60258600	0.21464100
C	-7.85744700	-2.64762600	-1.58269700
H	-6.35798600	-2.17462300	-3.06457500
C	-8.14713900	-3.31430400	-0.38613700
H	-7.33984500	-4.55492800	1.17554200
H	-8.64475100	-2.09654900	-2.09002200
C	-9.54309400	-3.29179900	0.17937200
H	-9.54641700	-3.55306000	1.23973100
H	-9.99937200	-2.30542500	0.06399200
H	-10.18097200	-4.01149700	-0.34381600

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Total energy=	-4208.302788
Zero-point correction=	1.028358 (Hartree/Particle)
Thermal correction to Energy=	1.097185
Thermal correction to Enthalpy=	1.098129
Thermal correction to Gibbs Free Energy=	0.917130
Sum of electronic and zero-point Energies=	-4207.274430
Sum of electronic and thermal Energies=	-4207.205604
Sum of electronic and thermal Enthalpies=	-4207.204659
Sum of electronic and thermal Free Energies=	-4207.385659

Imaginary frequency= -395.83 cm^{-1}

C	-4.53337300	-3.05259100	-0.77885700
C	-4.61820200	-2.01785800	-1.92644900
C	-3.70300600	-0.84803100	-1.50667000
C	-3.15423800	-2.79028400	-0.26880100
C	-1.44831400	-1.39043700	-0.22159300
H	-5.26681800	-2.84917800	0.01022400
H	-4.66313000	-4.08284700	-1.10972900
H	-4.23357600	-2.45974800	-2.84901100
H	-3.22737700	-0.34630700	-2.34673200
N	-2.28926400	-3.39518300	0.47920500
N	-1.22321000	-2.51777000	0.51433100
N	-2.69251600	-1.57871500	-0.71215100
C	-0.10077700	-2.88341000	1.28697700
C	0.35643600	-2.06625800	2.32010500
C	0.52588500	-4.10686700	1.06062500
C	1.48547600	-2.41105300	3.04632200
C	1.64489200	-4.46857600	1.79794500
C	2.12655800	-3.61746700	2.78359400
F	0.05922700	-4.93324700	0.13813900
F	2.25605800	-5.62224300	1.56208700
F	3.19885200	-3.95784000	3.48131700
F	1.93793800	-1.61226200	4.00259600
F	-0.25565000	-0.91621800	2.56844100
H	-5.63553100	-1.67245200	-2.10888600
C	-4.39894000	0.17621700	-0.60096500
H	-4.70872700	-0.32770900	0.32773700
H	-3.68306400	0.96388300	-0.34723800
O	-5.49685300	0.71529000	-1.29761200
Si	-7.06397300	0.70450600	-0.69403800
C	-8.12914200	1.21003200	-2.17045300
C	-7.84903400	2.69617700	-2.45547600
C	-7.76001300	0.40374900	-3.42523300
C	-9.61598700	1.03170000	-1.83468100
H	-8.13270400	3.33132500	-1.61061400
H	-6.78926200	2.86992100	-2.67144100
H	-8.42729100	3.01866900	-3.33056400
H	-7.98930000	-0.66224300	-3.32700100
H	-8.33099500	0.77678900	-4.28514400
H	-6.69535100	0.50174100	-3.65817100
H	-10.23405600	1.37345600	-2.67445700
H	-9.87059800	-0.01465800	-1.63516200
H	-9.90034500	1.62121400	-0.95528100
C	-7.17849800	1.95259900	0.69743300

C	-8.23369600	1.90853400	1.62110400
C	-6.24567900	2.99361500	0.80523600
C	-8.35718400	2.87283700	2.61729600
H	-8.96305800	1.10183800	1.56900600
C	-6.36074900	3.95781300	1.80437800
H	-5.42191400	3.04907800	0.09657100
C	-7.41814100	3.89817500	2.70928700
H	-9.18048300	2.82349900	3.32297400
H	-5.62760900	4.75496900	1.87716100
H	-7.51029600	4.64984100	3.48701900
C	-7.43720300	-0.99485200	0.04355900
C	-7.98175000	-2.05709100	-0.69593000
C	-7.08803400	-1.25165400	1.38096800
C	-8.15904600	-3.31980900	-0.13422300
H	-8.27688300	-1.90403400	-1.73018500
C	-7.25889000	-2.51314700	1.95001000
H	-6.68424200	-0.44896400	1.99439000
C	-7.79299900	-3.55084500	1.19030200
H	-8.58630500	-4.12148700	-0.72840200
H	-6.97966700	-2.68328000	2.98506100
H	-7.92983000	-4.53379900	1.62988200
C	3.20086100	2.44741800	0.30152400
C	2.81972100	1.09763300	0.37162900
C	3.67848000	0.16481000	0.93634100
C	4.90650000	0.60608900	1.43670100
C	5.25753200	1.95360600	1.37069300
C	4.40711100	2.90401800	0.79674800
C	1.17496100	2.32891500	-0.73161400
C	1.55983200	0.96130300	-0.35524100
H	3.41743100	-0.89085000	0.96419300
H	5.60599200	-0.10784500	1.86144500
H	6.21457500	2.27550000	1.76728800
H	4.69051800	3.94908500	0.73300300
N	2.19933300	3.15943100	-0.37270300
O	0.15190600	2.71368200	-1.33651700
C	0.65807100	-0.12742300	-0.13150300
C	-0.65328600	-0.22346200	-0.49284800
O	-1.37682600	0.72041700	-1.14114500
H	-0.80967700	1.55710800	-1.29213300
H	1.11942200	-1.00262600	0.31143700
C	2.29523000	4.55284500	-0.76098900
H	1.46437200	4.73203800	-1.44963100
H	3.23330700	4.69629100	-1.30911500
C	2.22554800	5.49753900	0.41942500

C	3.14925900	6.53277100	0.55157900
C	1.21847200	5.35340000	1.37574300
C	3.06717000	7.41963500	1.62343000
H	3.93917000	6.64336900	-0.18726000
C	1.13652500	6.23565100	2.44724900
H	0.49920800	4.54448200	1.27375800
C	2.06080800	7.27218300	2.57288100
H	3.79401100	8.21993500	1.71860600
H	0.35144200	6.11564700	3.18708200
H	1.99775100	7.95899800	3.41077100
C	3.33759600	-0.46572700	-2.12650800
C	2.31798900	0.46651700	-2.31343200
H	1.33280600	0.16052700	-2.64791900
H	2.62422900	1.46841200	-2.60332200
C	3.07395900	-1.89404700	-1.86701700
C	1.88794200	-2.51113100	-2.29496900
C	4.00146600	-2.67522100	-1.15753200
C	1.65092000	-3.85830900	-2.04806700
H	1.15321400	-1.94025400	-2.85484700
C	3.75855300	-4.02124100	-0.90490500
H	4.91323900	-2.20522200	-0.80110100
C	2.58531600	-4.62488100	-1.35370100
H	0.73127000	-4.31444900	-2.40186900
H	4.48720100	-4.60257600	-0.34683200
H	2.39307000	-5.67342700	-1.15138500
N	4.64857900	-0.09308900	-2.06390200
N	4.93597900	1.14278200	-2.10643300
S	6.63394500	1.33264600	-2.26807300
O	6.91156400	2.71139700	-1.87780700
O	7.02418200	0.86928800	-3.59978600
C	7.40807700	0.25606500	-1.07960700
C	8.02042800	0.82347500	0.02966900
C	7.41570000	-1.12379100	-1.28177200
C	8.62747000	-0.00624100	0.96886000
H	8.01801700	1.90245800	0.13944800
C	8.01112000	-1.93799300	-0.32701400
H	6.96336100	-1.54154000	-2.17385800
C	8.61905000	-1.39363100	0.81145800
H	9.11620900	0.43084400	1.83516600
H	8.01838100	-3.01531800	-0.47179600
C	9.25041500	-2.29717300	1.83854100
H	8.48394300	-2.84454900	2.39642800
H	9.89907100	-3.03782800	1.36301800
H	9.84657600	-1.72857700	2.55503600

TS3R-270

Total energy= -4208.284364

Zero-point correction= 1.029350 (Hartree/Particle)

Thermal correction to Energy= 1.098599

Thermal correction to Enthalpy= 1.099543

Thermal correction to Gibbs Free Energy= 0.918954

Sum of electronic and zero-point Energies= -4207.255013

Sum of electronic and thermal Energies= -4207.185765

Sum of electronic and thermal Enthalpies= -4207.184820

Sum of electronic and thermal Free Energies= -4207.365409

Imaginary frequency= -395.16 cm^{-1}

C	-3.08125400	-3.28595700	-0.04946000
C	-3.29824000	-2.39453500	-1.29291000
C	-2.66089300	-1.02791300	-0.96453600
C	-1.83518500	-2.68414500	0.51096600
C	-0.49179300	-0.93967100	0.56076700
H	-3.89895500	-3.18749300	0.67455000
H	-2.95794000	-4.34296200	-0.28575200
H	-2.77401400	-2.82335700	-2.14993300
H	-2.19820200	-0.56146100	-1.83287900
N	-0.92465200	-3.02045200	1.36733800
N	-0.07984600	-1.93346000	1.39261500
N	-1.61013200	-1.43809100	-0.00420100
C	1.11133500	-2.09365000	2.14183700
C	1.43860100	-1.24878800	3.19519800
C	1.95696300	-3.15809600	1.84299400
C	2.62590300	-1.41688200	3.89131500
C	3.12177400	-3.35734100	2.56319500
C	3.46634900	-2.47832500	3.57795200
F	1.69428200	-3.95297700	0.81546700
F	3.95017000	-4.33878400	2.22101300
F	4.59833900	-2.63951600	4.24058100
F	2.95183500	-0.57187800	4.86472300
F	0.62870600	-0.23823200	3.50789900
H	-4.35089400	-2.28050500	-1.55134700
C	-3.61208400	-0.05867900	-0.25534700
H	-3.89183000	-0.48982300	0.71882000
H	-3.08691600	0.88529100	-0.07715900
O	-4.73901900	0.15474100	-1.07383900
Si	-6.30365300	-0.07758600	-0.51062700
C	-7.37919100	0.07638600	-2.05630300
C	-7.38749400	1.55784900	-2.47381600
C	-6.79866200	-0.74306300	-3.21914700

C	-8.81640400	-0.36575600	-1.74906800
H	-7.83128900	2.19500200	-1.70258000
H	-6.37529200	1.92445700	-2.67726800
H	-7.97737200	1.67649200	-3.39170100
H	-6.81184900	-1.82050400	-3.02728300
H	-7.39290100	-0.56991900	-4.12567300
H	-5.76528000	-0.45140500	-3.42924900
H	-9.45281800	-0.20817100	-2.62917600
H	-8.87423800	-1.42535200	-1.47884000
H	-9.24609800	0.21596900	-0.92488100
C	-6.67229800	1.27720800	0.72929200
C	-7.71320800	1.16991900	1.66364600
C	-5.92938200	2.46637100	0.69867600
C	-8.00353400	2.21421500	2.53759100
H	-8.29701900	0.25265200	1.71788400
C	-6.21143900	3.51171000	1.57448400
H	-5.12195100	2.57330300	-0.02288600
C	-7.25017200	3.38569300	2.49403000
H	-8.81151400	2.11358300	3.25542900
H	-5.62266500	4.42300100	1.54094200
H	-7.47147100	4.19902400	3.17808700
C	-6.40569000	-1.73465400	0.39045800
C	-6.70249300	-2.94103700	-0.26479700
C	-6.09900500	-1.80383800	1.76069500
C	-6.68576900	-4.15991800	0.40848700
H	-6.95313500	-2.93880400	-1.32178300
C	-6.07927300	-3.01999000	2.44239600
H	-5.87954800	-0.89025900	2.30916100
C	-6.37114300	-4.20156100	1.76546100
H	-6.92203900	-5.07578800	-0.12396900
H	-5.83807600	-3.04337300	3.50045100
H	-6.35714100	-5.14990900	2.29325000
C	3.39668700	3.74319900	0.18870600
C	3.14385100	2.50610600	0.79886300
C	3.92940600	2.10199300	1.87009300
C	4.94308700	2.94973700	2.31567300
C	5.18133100	4.17408300	1.68957000
C	4.40656500	4.59419200	0.60675500
C	1.57276200	2.89778400	-0.88523900
C	2.02534700	1.87516900	0.07854400
H	3.77664100	1.13314900	2.34173900
H	5.56580800	2.64355100	3.14892100
H	5.98114700	4.81336100	2.04827400
H	4.57099900	5.55448300	0.12902900

N	2.46492200	3.92989600	-0.84469100
O	0.59969100	2.87371200	-1.66943100
C	1.21082000	0.86529600	0.69018800
C	0.05915800	0.35173100	0.18420400
O	-0.69615900	0.90679400	-0.78156700
H	-0.22806400	1.70791800	-1.20469300
H	1.69210500	0.33456000	1.49820900
C	2.41652500	5.07681500	-1.73055300
H	1.74090200	4.80012900	-2.54477400
H	3.41521100	5.23479600	-2.15184200
C	1.93130400	6.33369900	-1.04097200
C	2.66703700	7.51470500	-1.11293400
C	0.72303300	6.32091500	-0.34075600
C	2.20333600	8.67424800	-0.49415100
H	3.60932700	7.52768300	-1.65569200
C	0.26072900	7.47556000	0.28013100
H	0.14672500	5.40009800	-0.29185000
C	1.00040400	8.65567800	0.20402400
H	2.78539600	9.58837600	-0.55309800
H	-0.67856200	7.45773400	0.82361500
H	0.63909500	9.55638000	0.68980200
C	2.48593700	-0.54584600	-1.45177700
C	3.04126700	0.75018100	-1.51136300
H	2.80671700	1.36009100	-2.37883300
H	3.98550700	0.97696800	-1.03756900
C	1.36605700	-0.97774100	-2.32877300
C	0.74767000	-0.11420000	-3.24331000
C	0.89090500	-2.29720400	-2.24411400
C	-0.30159400	-0.55231300	-4.04568300
H	1.05316900	0.92507400	-3.31084600
C	-0.16612400	-2.72908500	-3.03761000
H	1.36294000	-2.97836000	-1.54345200
C	-0.76719200	-1.86176900	-3.95015700
H	-0.76256300	0.14009600	-4.74341200
H	-0.50773200	-3.75808200	-2.95802200
H	-1.58172800	-2.20351600	-4.58178400
N	2.62121300	-1.31297900	-0.35382900
N	3.53139700	-1.28099400	0.55238800
S	5.20036300	-0.94649300	0.29371900
O	5.77845300	-1.57338500	1.48360800
O	5.65139200	0.41546500	-0.03002200
C	5.53052200	-1.97272800	-1.12414200
C	5.98341700	-1.39949100	-2.30343200
C	5.30329600	-3.34498100	-1.01968200

C	6.22424000	-2.22252500	-3.40184700
H	6.15172600	-0.32851200	-2.34684800
C	5.54307600	-4.14702800	-2.12491800
H	4.94032800	-3.76333800	-0.08545600
C	6.00693500	-3.59829600	-3.32869300
H	6.58540100	-1.78779800	-4.32943700
H	5.37422200	-5.21842300	-2.05881500
C	6.24951400	-4.48817900	-4.51955200
H	5.30340100	-4.87011900	-4.91547100
H	6.75752200	-3.94910500	-5.32145900
H	6.86121000	-5.35189100	-4.24454200

TS3S

Total energy= -4208.322043

Zero-point correction= 1.029861 (Hartree/Particle)

Thermal correction to Energy= 1.098870

Thermal correction to Enthalpy= 1.099814

Thermal correction to Gibbs Free Energy= 0.921606

Sum of electronic and zero-point Energies= -4207.292182

Sum of electronic and thermal Energies= -4207.223173

Sum of electronic and thermal Enthalpies= -4207.222229

Sum of electronic and thermal Free Energies= -4207.400437

Imaginary frequency= -326.46 cm^{-1}

C	5.44826200	2.19551500	0.46591500
C	4.82814300	1.22480800	-0.34614100
C	5.59845300	0.51807400	-1.26490200
C	6.96965800	0.77407000	-1.33645600
C	7.56562600	1.72597900	-0.50887000
C	6.80708800	2.45968100	0.40722500
C	3.22214400	2.31108700	0.93855300
C	3.41024800	1.19809100	0.00926900
H	5.14553500	-0.22077500	-1.92243300
H	7.57796400	0.22818500	-2.04993300
H	8.63201100	1.91078000	-0.58349300
H	7.25904700	3.22510000	1.02982000
N	4.46778600	2.79935200	1.25740400
O	2.17220600	2.75737100	1.44308900
C	2.40215100	0.65444000	-0.85033300
C	1.05599300	0.80570700	-0.75880800
O	0.36612600	1.57425600	0.09432600
H	1.00208800	2.04514500	0.73418800
H	2.77140200	0.03762200	-1.65840500
C	4.69320400	3.87407300	2.20403100
H	3.78062700	3.94234900	2.80280600

H	5.51895800	3.59193700	2.86607000
C	4.98666400	5.19551700	1.52640300
C	6.13658700	5.91981400	1.83239500
C	4.08750500	5.70253900	0.58487900
C	6.39015000	7.13961100	1.20672200
H	6.83886600	5.52783900	2.56453600
C	4.34038900	6.91678400	-0.04239600
H	3.18630500	5.13893500	0.35549900
C	5.49361000	7.63811400	0.26720700
H	7.28962900	7.69562400	1.45099900
H	3.63654900	7.30519800	-0.77163000
H	5.68993800	8.58608900	-0.22331800
C	2.71188900	-1.38607800	1.41736000
C	3.40368900	-0.23327000	1.77220600
H	4.48596100	-0.25389700	1.85361800
H	2.86700000	0.49165100	2.37437300
C	3.38940500	-2.60515000	0.93344000
C	4.62127600	-2.53703700	0.27073300
C	2.84549400	-3.87038800	1.20375100
C	5.30121000	-3.69745700	-0.09202300
H	5.05427700	-1.56595700	0.04767500
C	3.52873400	-5.02781400	0.84692000
H	1.88949300	-3.93101200	1.71673000
C	4.76484400	-4.94756000	0.20559500
H	6.25518500	-3.62072300	-0.60519000
H	3.09632300	-5.99784800	1.07285500
H	5.29604000	-5.85160700	-0.07309800
N	1.35307700	-1.44747300	1.47782000
N	0.75237000	-0.44156700	1.99043800
S	-0.92535400	-0.65269600	1.83531300
O	-1.52242800	0.51180100	2.48599700
O	-1.26942200	-0.96229300	0.43981900
C	-1.31944900	-2.08705300	2.80645400
C	-1.64409900	-1.92294100	4.15010500
C	-1.23736700	-3.35065600	2.22968500
C	-1.90179200	-3.04878000	4.92207300
H	-1.69128000	-0.92463600	4.57258300
C	-1.49426900	-4.46598800	3.02043700
H	-0.98109900	-3.44829800	1.18077400
C	-1.83174600	-4.33219000	4.37006300
H	-2.15972900	-2.93281900	5.97122500
H	-1.43384000	-5.45828300	2.58204000
C	-2.13938400	-5.54144800	5.21400800
H	-1.73141900	-6.45098700	4.76824900

H	-3.22130600	-5.67532500	5.31574400
H	-1.72608000	-5.43464500	6.21999300
C	-2.81181400	0.31896600	-3.59343300
C	-2.73066800	1.79875300	-3.14446500
C	-1.89846800	1.79217400	-1.84337700
C	-1.52179600	-0.20514800	-3.05327700
C	0.16995500	0.15315200	-1.70303000
H	-3.65269300	-0.20477500	-3.12608800
H	-2.88669800	0.19427200	-4.67367100
H	-2.20863900	2.38467700	-3.90548800
H	-1.31536600	2.70138700	-1.69721200
N	-0.74916100	-1.22541600	-3.25321300
N	0.31284000	-0.99516900	-2.40136000
N	-1.00075600	0.65201000	-2.12153200
C	1.22702800	-2.06535800	-2.23187100
C	0.77570200	-3.22100800	-1.59830400
C	2.46183100	-2.08832200	-2.87183000
C	1.54963200	-4.37123200	-1.59394400
C	3.25838300	-3.22206000	-2.84066500
C	2.77799400	-4.37864100	-2.24099400
F	2.90358600	-1.01104500	-3.51864400
F	4.44999600	-3.21785000	-3.42536100
F	3.49191500	-5.49138600	-2.28944700
F	1.10822500	-5.47004200	-0.99513300
F	-0.42163900	-3.24308600	-1.03774600
H	-3.71103200	2.24235200	-2.97416400
C	-2.73838000	1.47933500	-0.59630600
H	-3.11675500	0.44928900	-0.66881900
H	-2.10400500	1.52953000	0.29148900
O	-3.78314200	2.42870800	-0.51871900
Si	-5.38807900	1.97406100	-0.34215200
C	-6.33623000	3.60877500	-0.38429700
C	-6.06002600	4.33576700	0.94331000
C	-5.85045900	4.50581900	-1.53266400
C	-7.84327000	3.34901200	-0.51208600
H	-6.42180300	3.76113100	1.80172600
H	-4.98934500	4.51814500	1.08474100
H	-6.57092400	5.30734800	0.94557600
H	-6.06481900	4.08249100	-2.51928600
H	-6.35826800	5.47790800	-1.48211900
H	-4.77278600	4.68182700	-1.46652900
H	-8.39122500	4.29963700	-0.48260100
H	-8.09660200	2.84429900	-1.45074300
H	-8.21363500	2.73143600	0.31461400

C	-5.57924000	1.07526700	1.28817500
C	-6.74218300	0.35516900	1.60796500
C	-4.53712700	1.09921100	2.22319500
C	-6.86117500	-0.31031400	2.82425100
H	-7.55801200	0.29456600	0.88920100
C	-4.64309300	0.41607700	3.43337400
H	-3.61574000	1.63134500	2.00678400
C	-5.80724900	-0.28255400	3.73749000
H	-7.76760100	-0.86108600	3.05624100
H	-3.80634100	0.42971700	4.12405600
H	-5.89297700	-0.81441400	4.68036400
C	-5.84591300	0.74052900	-1.70105300
C	-6.25742800	1.12517500	-2.98783100
C	-5.69228300	-0.63524000	-1.45684700
C	-6.49517700	0.18564000	-3.98825000
H	-6.39654900	2.17720700	-3.22218600
C	-5.92840700	-1.58242000	-2.45288300
H	-5.38203900	-0.97462000	-0.47150100
C	-6.32800800	-1.17233700	-3.72211700
H	-6.81446700	0.51217200	-4.97310400
H	-5.79727300	-2.63805700	-2.23688400
H	-6.51126300	-1.90703700	-4.49998600

TS3S-90

Total energy= -4208.313266

Zero-point correction= 1.029388 (Hartree/Particle)

Thermal correction to Energy= 1.098788

Thermal correction to Enthalpy= 1.099732

Thermal correction to Gibbs Free Energy= 0.918104

Sum of electronic and zero-point Energies= -4207.283878

Sum of electronic and thermal Energies= -4207.214478

Sum of electronic and thermal Enthalpies= -4207.213534

Sum of electronic and thermal Free Energies= -4207.395162

Imaginary frequency= -347.63 cm^{-1}

C	4.05703900	2.35210500	-0.39459100
C	3.43200100	1.13482700	-0.71735100
C	4.20844300	-0.00765200	-0.86917600
C	5.59321500	0.09849800	-0.70665900
C	6.18843500	1.31427800	-0.37244400
C	5.42328400	2.47194900	-0.21249400
C	1.83804300	2.82529100	-0.55956700
C	1.98748100	1.36514500	-0.71112400
H	3.75580000	-0.96666300	-1.10266000
H	6.21207700	-0.78404700	-0.83697900

H	7.26387700	1.36799700	-0.23634600
H	5.87968100	3.42348400	0.03946700
N	3.07531800	3.34095700	-0.27989600
O	0.80894500	3.52934700	-0.61052300
C	1.04274800	0.47748600	-1.33125600
C	-0.30408000	0.67617700	-1.38887400
O	-0.95373800	1.75022800	-0.86411700
H	-0.31528800	2.53466900	-0.76438800
H	1.45278700	-0.45862200	-1.69292100
C	3.31738700	4.71395100	0.11320300
H	2.33548500	5.14172900	0.33661000
H	3.90964200	4.70507600	1.03618900
C	4.01577600	5.52056800	-0.95994300
C	5.18430400	6.22438400	-0.67692600
C	3.47821200	5.57485700	-2.24766500
C	5.81168300	6.97900000	-1.66679400
H	5.60747300	6.17909700	0.32403200
C	4.10329900	6.32522100	-3.23687800
H	2.56510400	5.02565800	-2.46479900
C	5.27240200	7.02923300	-2.94805500
H	6.72315800	7.52137000	-1.43669600
H	3.67959800	6.36342000	-4.23545800
H	5.76082900	7.61234800	-3.72216200
C	2.53967500	0.49792700	1.95921000
C	1.44688000	1.17256100	1.40872700
H	1.26609300	2.21041100	1.66398500
H	0.56633800	0.59359500	1.15285700
C	3.67217100	1.19238200	2.61124200
C	3.55680700	2.51813200	3.05536200
C	4.91502000	0.55870100	2.75011000
C	4.64846400	3.19291400	3.59165400
H	2.60459000	3.03670500	2.98866900
C	6.00120900	1.23104700	3.29784100
H	5.02078800	-0.46288800	2.40146900
C	5.88090600	2.55497900	3.71371900
H	4.52984800	4.21927000	3.92752000
H	6.95535900	0.71973900	3.38697200
H	6.73276800	3.08021900	4.13368500
N	2.70959800	-0.81975400	1.69811400
N	1.80753900	-1.37369100	0.97197400
S	2.19676000	-2.97172100	0.57898300
O	0.94178900	-3.72256700	0.61632200
O	2.92774600	-2.94328300	-0.69801300
C	3.29396200	-3.62464300	1.80931300

C	2.77619900	-4.43912900	2.80712600
C	4.64945600	-3.30534300	1.75700100
C	3.64072300	-4.94885600	3.77221200
H	1.71777200	-4.67683400	2.81142600
C	5.49405800	-3.81648300	2.73167400
H	5.02371500	-2.66999800	0.95974300
C	5.00226100	-4.64205600	3.75120400
H	3.25155800	-5.59796300	4.55115200
H	6.55367800	-3.57729500	2.70430600
C	5.93239600	-5.17186400	4.81077800
H	6.21047000	-4.37703400	5.51016000
H	6.85498900	-5.55584600	4.36777100
H	5.46474500	-5.97521900	5.38336300
C	-4.64816500	-0.83096600	-2.79202600
C	-4.72700600	0.70164300	-2.60002300
C	-3.53380700	1.07271100	-1.69376800
C	-3.17633400	-1.05066500	-2.66904000
C	-1.24286800	-0.24209200	-1.97566700
H	-5.17109200	-1.37052300	-1.99335200
H	-5.04050800	-1.17308400	-3.74957300
H	-4.61149700	1.19923900	-3.56620700
H	-3.12631900	2.06033800	-1.89736800
N	-2.33371800	-1.98754300	-2.95662600
N	-1.12356900	-1.48221800	-2.52218400
N	-2.56392200	0.02830800	-2.08903000
C	-0.00205800	-2.32987100	-2.67616900
C	-0.03248700	-3.59132800	-2.08618100
C	1.03544400	-2.00362200	-3.54622200
C	0.98107800	-4.50248700	-2.33687700
C	2.06230700	-2.90133600	-3.78125600
C	2.02307800	-4.15517800	-3.18307300
F	1.04274700	-0.81230700	-4.13777600
F	3.06444200	-2.58091700	-4.59320200
F	3.00747000	-5.01344400	-3.40078600
F	0.97661300	-5.68800800	-1.74526100
F	-1.03804200	-3.92824500	-1.29917400
H	-5.66868000	1.02498900	-2.15591300
C	-3.83994600	0.92116000	-0.19971600
H	-4.07942500	-0.13362100	0.00481000
H	-2.94821300	1.19180000	0.37306600
O	-4.91270200	1.77636200	0.12386100
Si	-6.29155700	1.23379300	0.91325600
C	-7.48907200	2.69179500	0.79978200
C	-6.95874200	3.80028800	1.72634300

C	-7.54782000	3.25194700	-0.62952500
C	-8.88675600	2.26779000	1.27015200
H	-6.93138500	3.47698900	2.77150700
H	-5.94837000	4.11261900	1.44019500
H	-7.61304200	4.67901500	1.66081300
H	-7.97730400	2.54338700	-1.34474100
H	-8.17774800	4.15059200	-0.64862700
H	-6.55053600	3.52876600	-0.98481400
H	-9.56347400	3.13174700	1.26492800
H	-9.32196400	1.49719300	0.62510200
H	-8.86172800	1.87616200	2.29390200
C	-5.82891600	0.85893700	2.68890500
C	-6.63141100	0.05468200	3.51218500
C	-4.68110400	1.44040500	3.24622300
C	-6.30178200	-0.15789200	4.84802200
H	-7.51934100	-0.42233100	3.10065800
C	-4.34291800	1.22570300	4.58007400
H	-4.04649400	2.06911100	2.62512700
C	-5.15542400	0.42736200	5.38195000
H	-6.93338900	-0.78354100	5.47090500
H	-3.44683100	1.67756700	4.99358900
H	-4.89391700	0.25743900	6.42174400
C	-6.87465000	-0.37225300	0.11093500
C	-7.75934600	-0.41187900	-0.97926400
C	-6.34062800	-1.59489300	0.55423700
C	-8.08858700	-1.61129700	-1.60603100
H	-8.20414800	0.50609600	-1.35336300
C	-6.66258100	-2.79944800	-0.06952300
H	-5.66515500	-1.60888800	1.40681000
C	-7.53667800	-2.80836300	-1.15350600
H	-8.77626900	-1.61242500	-2.44588800
H	-6.23258900	-3.72802800	0.29225300
H	-7.79006500	-3.74401900	-1.64188100

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Total energy= -4208.307276

Zero-point correction= 1.029716 (Hartree/Particle)

Thermal correction to Energy= 1.099258

Thermal correction to Enthalpy= 1.100202

Thermal correction to Gibbs Free Energy= 0.917626

Sum of electronic and zero-point Energies= -4207.277560

Sum of electronic and thermal Energies= -4207.208018

Sum of electronic and thermal Enthalpies= -4207.207074

Sum of electronic and thermal Free Energies= -4207.389650

Imaginary frequency= -374.98 cm^{-1}

C	3.80253500	2.65015100	-0.85136100
C	3.22984400	1.46182500	-1.32431900
C	4.02129600	0.55834800	-2.02609700
C	5.36295400	0.86476900	-2.23820200
C	5.91343400	2.05572600	-1.75417800
C	5.13763000	2.97449700	-1.05059000
C	1.61183900	2.75839800	-0.25247500
C	1.84049000	1.43783300	-0.86027400
H	3.62253300	-0.39691900	-2.36080700
H	5.99457900	0.15407600	-2.75927700
H	6.96401200	2.26662200	-1.92454900
H	5.55255600	3.90398300	-0.67422600
N	2.81768200	3.39149300	-0.18641700
O	0.54917500	3.25240300	0.18832400
C	0.83384800	0.61003300	-1.44549800
C	-0.49690700	0.60551100	-1.15555200
O	-1.15322900	1.45412200	-0.32808600
H	-0.54020700	2.23178800	-0.08141100
H	1.18585800	-0.10003700	-2.18409200
C	3.05055500	4.64224500	0.50928100
H	2.19641600	4.78360000	1.17796200
H	3.94707400	4.52362800	1.12946300
C	3.18705800	5.81487800	-0.43659100
C	4.28541200	6.66927200	-0.36992500
C	2.18758300	6.05688700	-1.38226000
C	4.38797200	7.75521700	-1.23846300
H	5.06481500	6.48287700	0.36547700
C	2.28970100	7.13674600	-2.25097500
H	1.32756900	5.39260300	-1.42434900
C	3.39152100	7.98929300	-2.18059500
H	5.24939000	8.41311800	-1.18179900
H	1.50946600	7.31698100	-2.98377500
H	3.47166000	8.83166000	-2.86020400
C	3.26510000	0.61830700	1.55817800
C	1.92836400	0.59267800	1.15450100
H	1.20591500	1.27750700	1.58565700
H	1.53377000	-0.35197200	0.79935900
C	3.86700000	1.73478100	2.31848900
C	3.09468200	2.54621600	3.16141300
C	5.23572700	2.02018200	2.19223100
C	3.66743700	3.61156400	3.85074100
H	2.03607800	2.33901400	3.29107100
C	5.80577900	3.08209700	2.88548100

H	5.83517800	1.40421400	1.52891600
C	5.02637300	3.88649600	3.71782300
H	3.04824100	4.22487200	4.49849900
H	6.86596800	3.28745100	2.76947700
H	5.47431600	4.71569100	4.25616200
N	4.12278100	-0.34521900	1.13343000
N	3.64640300	-1.26205200	0.38492400
S	4.89384900	-2.32601700	-0.09095300
O	4.34923800	-3.01097600	-1.26578600
O	6.18806000	-1.65715600	-0.18044600
C	4.98398200	-3.49712000	1.24334200
C	4.21619700	-4.65527700	1.20590000
C	5.80565300	-3.20576200	2.32979700
C	4.27933000	-5.53795100	2.27932300
H	3.60305500	-4.87050400	0.33831700
C	5.85450800	-4.09849600	3.39226700
H	6.40272000	-2.30002000	2.32326200
C	5.09220100	-5.27224600	3.38398800
H	3.69241000	-6.45181000	2.25596800
H	6.49871300	-3.88659200	4.24115100
C	5.13657500	-6.21856400	4.55520800
H	4.80384600	-7.21865700	4.26933600
H	4.48286200	-5.86623900	5.35977700
H	6.14740900	-6.29443700	4.96313000
C	-4.68030400	-1.06463600	-2.85262000
C	-4.84682500	0.45674700	-2.61406800
C	-3.74421200	0.84745500	-1.60555400
C	-3.21236500	-1.22766600	-2.62272700
C	-1.38510900	-0.32452800	-1.79071600
H	-5.23971600	-1.65700600	-2.11891600
H	-4.98070500	-1.38351700	-3.85050900
H	-4.68516700	0.99538900	-3.55102400
H	-3.36392900	1.85904900	-1.74422200
N	-2.29551200	-2.10232500	-2.88536600
N	-1.14553400	-1.53489200	-2.36324600
N	-2.70658800	-0.13919200	-1.95881300
C	-0.02566200	-2.38744300	-2.19150600
C	-0.07156400	-3.33077700	-1.17028500
C	1.04142600	-2.40406400	-3.08575800
C	0.93484200	-4.27608200	-1.04058700
C	2.05943800	-3.33476100	-2.95671100
C	1.98120200	-4.29284700	-1.95223700
F	1.11126200	-1.48538900	-4.04421500
F	3.08198600	-3.32685800	-3.79396900

F	2.91341900	-5.22248900	-1.85002700
F	0.89168200	-5.18139200	-0.06882800
F	-1.09614300	-3.33282100	-0.32669100
H	-5.83343900	0.71722900	-2.23071700
C	-4.15920600	0.62645100	-0.14514100
H	-4.35802400	-0.44650500	0.00145200
H	-3.33109000	0.91691100	0.50720500
O	-5.29921100	1.41087500	0.11615500
Si	-6.69196300	0.76313700	0.79805000
C	-7.96388300	2.15290400	0.65448100
C	-7.57875400	3.24692200	1.66591800
C	-7.94795900	2.77330800	-0.75074000
C	-9.36387200	1.62451900	0.99535400
H	-7.61645800	2.87924700	2.69598200
H	-6.56994100	3.63108900	1.47854400
H	-8.27860500	4.08793600	1.58111700
H	-8.26627300	2.07074800	-1.52752200
H	-8.63728200	3.62669200	-0.78608400
H	-6.94796700	3.13335100	-1.01077100
H	-10.08964800	2.44753400	0.97906500
H	-9.70380400	0.86460100	0.28380700
H	-9.39074400	1.18292900	1.99867300
C	-6.31417400	0.34250800	2.58371000
C	-7.08658800	-0.57300200	3.31389500
C	-5.26337200	0.99737900	3.24304800
C	-6.82044300	-0.82594600	4.65709700
H	-7.89975300	-1.10513600	2.82348300
C	-4.99000400	0.74491600	4.58512700
H	-4.65374700	1.71400900	2.69647900
C	-5.76958400	-0.16734300	5.29243500
H	-7.42726800	-1.53836700	5.20711700
H	-4.17002900	1.25699600	5.07862300
H	-5.55728200	-0.36719300	6.33809800
C	-7.12449200	-0.83961000	-0.10342000
C	-7.93117700	-0.87935200	-1.25281700
C	-6.55109600	-2.04955000	0.32503100
C	-8.14700200	-2.06571800	-1.95007100
H	-8.40432000	0.02842400	-1.61676100
C	-6.76127500	-3.24114200	-0.36742700
H	-5.93421500	-2.06443100	1.22084800
C	-7.55863000	-3.24967100	-1.50940600
H	-8.77671400	-2.06715200	-2.83413700
H	-6.30542700	-4.16064700	-0.01404600
H	-7.72566200	-4.17565700	-2.05050000

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Total energy= -4208.304495

Zero-point correction= 1.029562 (Hartree/Particle)

Thermal correction to Energy= 1.098726

Thermal correction to Enthalpy= 1.099670

Thermal correction to Gibbs Free Energy= 0.921186

Sum of electronic and zero-point Energies= -4207.274933

Sum of electronic and thermal Energies= -4207.205769

Sum of electronic and thermal Enthalpies= -4207.204825

Sum of electronic and thermal Free Energies= -4207.383309

Imaginary frequency= -351.98 cm^{-1}

C	4.96626800	1.53940200	0.96788500
C	3.92894600	2.41605200	0.58773800
C	4.24028700	3.69570100	0.13963800
C	5.58043900	4.08090200	0.08604700
C	6.59473700	3.19576700	0.45763900
C	6.30294600	1.90591700	0.90517400
C	3.03754600	0.37795800	1.27689100
C	2.68163600	1.66459100	0.67261600
H	3.45826900	4.38998200	-0.16013500
H	5.83825100	5.07870400	-0.25303600
H	7.63044500	3.51412800	0.40180700
H	7.08777900	1.21850800	1.20258300
N	4.40392500	0.32987600	1.38497400
O	2.28133400	-0.55587900	1.60798600
C	1.38111200	2.26166900	0.71475400
C	0.19701700	1.67035300	1.04214300
O	0.00616800	0.42227500	1.50555600
H	0.91307000	-0.07204800	1.54888900
H	1.35373500	3.31313600	0.46850400
C	5.12731200	-0.88537900	1.70048500
H	4.36299300	-1.64755400	1.88856600
H	5.68411400	-1.20773800	0.81244700
C	6.05437900	-0.76077500	2.88941000
C	7.11984600	-1.65665500	3.00080300
C	5.86450500	0.19711000	3.88521300
C	7.97794700	-1.60174900	4.09444100
H	7.26837400	-2.40272400	2.22387100
C	6.72795900	0.25754700	4.97664600
H	5.04244300	0.90216700	3.80004900
C	7.78542900	-0.64126300	5.08555600
H	8.80066100	-2.30578000	4.17034300
H	6.57385000	1.01078000	5.74307800

H	8.45763100	-0.59274600	5.93627800
C	1.87945600	-0.27381800	-1.45762300
C	2.70677900	0.83963100	-1.35774400
H	2.37377400	1.79358000	-1.75193700
H	3.78166700	0.68578300	-1.32296200
C	0.45499400	-0.18221400	-1.84538500
C	0.03415000	0.75457400	-2.80200500
C	-0.49642500	-1.06254400	-1.31364000
C	-1.28908500	0.80141900	-3.22433100
H	0.76433800	1.41973800	-3.25662300
C	-1.82219200	-1.01546400	-1.73771100
H	-0.18023500	-1.78728300	-0.56843400
C	-2.22580100	-0.08308600	-2.69106400
H	-1.58810900	1.52009100	-3.98219000
H	-2.54131900	-1.71861900	-1.32741300
H	-3.25668300	-0.06083700	-3.03388000
N	2.33420000	-1.53057500	-1.18045300
N	3.56621200	-1.66163100	-0.89325200
S	3.91576500	-3.30232000	-0.55600300
O	5.37490600	-3.38533300	-0.60177200
O	3.21360200	-3.71995300	0.65731300
C	3.25884300	-4.24256700	-1.91527700
C	4.11898700	-4.67021000	-2.91812500
C	1.89495600	-4.53020700	-1.95528700
C	3.60108200	-5.40735400	-3.98004300
H	5.17609500	-4.43537600	-2.85262400
C	1.39672200	-5.25814100	-3.02552900
H	1.24901000	-4.18569100	-1.15562300
C	2.24010500	-5.70820600	-4.04947100
H	4.26583400	-5.75554400	-4.76530000
H	0.33504300	-5.48653600	-3.07131500
C	1.67854900	-6.51367400	-5.19177700
H	0.83589200	-5.99563800	-5.65835800
H	1.31201000	-7.48278500	-4.83942800
H	2.43437500	-6.69621100	-5.95816100
C	-4.37338800	2.63100200	2.19162900
C	-3.85085000	1.60619000	3.22670400
C	-2.58178600	0.96660000	2.61233800
C	-3.11683300	2.98258400	1.47063900
C	-1.03902500	2.40861700	1.02088700
H	-5.07818900	2.17982700	1.48406300
H	-4.84935300	3.50067000	2.64455800
H	-3.57745300	2.12409800	4.14892200
H	-1.81390900	0.75743900	3.35580000

N	-2.72195300	3.90371900	0.65335800
N	-1.41306000	3.55045300	0.37186600
N	-2.13024800	2.06597200	1.72959600
C	-0.85496900	4.10765800	-0.80483000
C	-1.47726100	3.81513100	-2.01815200
C	0.21526100	4.99498200	-0.79483100
C	-0.97959200	4.32151400	-3.20891500
C	0.73768800	5.48667700	-1.98270000
C	0.13375900	5.15452400	-3.18906300
F	0.79252300	5.34317000	0.35032900
F	1.79635200	6.28631300	-1.96135000
F	0.61794400	5.63481400	-4.32199400
F	-1.56057000	4.01713200	-4.36328000
F	-2.55346300	3.04548400	-2.03099300
H	-4.58645100	0.83807700	3.46451500
C	-2.86683400	-0.27764700	1.75043800
H	-3.26358900	0.06855800	0.78576300
H	-1.93009800	-0.80247600	1.55052900
O	-3.78026000	-1.11875100	2.42275200
Si	-5.06789000	-1.77970400	1.56793100
C	-6.05160700	-2.75474700	2.85063700
C	-5.20603900	-3.97357700	3.26048000
C	-6.31509400	-1.91438000	4.10972100
C	-7.37110100	-3.24414100	2.23725000
H	-5.01908300	-4.64293100	2.41519100
H	-4.23896100	-3.66903100	3.67523600
H	-5.73669700	-4.54492400	4.03264400
H	-6.93768200	-1.03594200	3.91393100
H	-6.83920600	-2.52380000	4.85713200
H	-5.37659600	-1.56945500	4.55493300
H	-7.90813000	-3.87480400	2.95695100
H	-8.03248300	-2.41705500	1.95887100
H	-7.19236300	-3.84747300	1.33927900
C	-4.32313300	-2.88368600	0.24916500
C	-4.93577200	-3.10430300	-0.99264900
C	-3.09615700	-3.51746600	0.50575100
C	-4.34163200	-3.92393400	-1.95013700
H	-5.88112900	-2.61626900	-1.22198500
C	-2.49932800	-4.34029900	-0.44603700
H	-2.59772100	-3.35297600	1.45909400
C	-3.12270200	-4.54037500	-1.67697900
H	-4.82479000	-4.07724900	-2.90994200
H	-1.54849100	-4.81864000	-0.23174900
H	-2.65723400	-5.17428100	-2.42523900

C	-5.98882000	-0.36363000	0.71952200
C	-7.10885500	0.26552200	1.28451500
C	-5.46867100	0.18848300	-0.46573000
C	-7.67824500	1.39756600	0.70396500
H	-7.55322000	-0.12908300	2.19320600
C	-6.01987900	1.33018200	-1.04310200
H	-4.61292300	-0.27952700	-0.94877700
C	-7.12836200	1.93769500	-0.45648400
H	-8.54767300	1.86015300	1.16026700
H	-5.58364800	1.74304100	-1.94776000
H	-7.56388100	2.82560300	-0.90369600

M3R

Total energy=	-4208.331581
Zero-point correction=	1.033572 (Hartree/Particle)
Thermal correction to Energy=	1.102758
Thermal correction to Enthalpy=	1.103703
Thermal correction to Gibbs Free Energy=	0.921794
Sum of electronic and zero-point Energies=	-4207.298009
Sum of electronic and thermal Energies=	-4207.228823
Sum of electronic and thermal Enthalpies=	-4207.227879
Sum of electronic and thermal Free Energies=	-4207.409787

C	-2.95908900	-2.73067800	-2.00695800
C	-3.26021300	-1.21060100	-1.98362600
C	-2.22221500	-0.58337900	-1.02732800
C	-1.49045000	-2.72713600	-1.74467300
C	0.21873700	-1.57123100	-1.02449000
H	-3.47543400	-3.26936100	-1.20287100
H	-3.20510500	-3.20677000	-2.95597500
H	-3.10095400	-0.78064300	-2.97420700
H	-1.90231900	0.41555000	-1.32473400
N	-0.48936900	-3.54619200	-1.86720500
N	0.57650900	-2.81287100	-1.40812500
N	-1.09503500	-1.52200800	-1.22393800
C	1.84132600	-3.43355300	-1.28354500
C	2.45843500	-3.51611400	-0.03761700
C	2.46457700	-3.98252000	-2.39981600
C	3.69952600	-4.11839400	0.09244600
C	3.69954400	-4.60490900	-2.27136700
C	4.31503400	-4.66750200	-1.02762600
F	1.88980000	-3.90899500	-3.58802600
F	4.29530100	-5.13056300	-3.33244000

F	5.49454100	-5.25379000	-0.90795900
F	4.29153800	-4.18557500	1.27628300
F	1.86643900	-2.99302600	1.02773600
H	-4.27579200	-0.99634700	-1.64948600
C	-2.65057300	-0.63391700	0.44431400
H	-2.73344400	-1.68825000	0.75359400
H	-1.88744300	-0.15311800	1.06272000
O	-3.88019500	0.04211600	0.56595700
Si	-5.20870300	-0.64385100	1.32800600
C	-6.61366600	0.56499500	0.96524000
C	-6.19479700	1.91846400	1.56838900
C	-6.83102200	0.75318400	-0.54501100
C	-7.91123600	0.08626300	1.62872400
H	-6.04752100	1.85255900	2.65145900
H	-5.26566100	2.28648500	1.11956900
H	-6.98052500	2.66242800	1.38186200
H	-7.37160300	-0.08429500	-0.99413700
H	-7.43753100	1.65108200	-0.72409500
H	-5.88315400	0.87842400	-1.08018300
H	-8.71613600	0.81019200	1.44900700
H	-8.23739800	-0.88158300	1.23041900
H	-7.79223000	-0.01478400	2.71335600
C	-4.83368900	-0.71505400	3.16308300
C	-5.54426200	-1.54309800	4.04467000
C	-3.84602100	0.12651900	3.69571000
C	-5.28051800	-1.52988500	5.41188000
H	-6.30796600	-2.21530100	3.65704700
C	-3.57452800	0.14024800	5.06183500
H	-3.28740700	0.78165500	3.03034400
C	-4.29299100	-0.68810800	5.92046400
H	-5.84163500	-2.17636100	6.07947400
H	-2.80566000	0.79733000	5.45597500
H	-4.08391500	-0.67858600	6.98568900
C	-5.43108100	-2.41122400	0.69987100
C	-6.16216400	-2.72840800	-0.45678800
C	-4.75908400	-3.46284700	1.34743300
C	-6.21773300	-4.03038200	-0.94890200
H	-6.69270700	-1.94953400	-0.99479400
C	-4.80475100	-4.76735800	0.85815400
H	-4.19378400	-3.25997200	2.25446700
C	-5.53474900	-5.05279400	-0.29312600
H	-6.79208000	-4.24687100	-1.84408900
H	-4.27468100	-5.55975900	1.37720300
H	-5.57423200	-6.06753700	-0.67643100

C	5.41202600	0.92798100	0.21127200
C	4.70540800	0.42420700	-0.88483700
C	5.38108100	-0.21807000	-1.90598400
C	6.76985500	-0.36381600	-1.80524900
C	7.45621700	0.14015800	-0.70365800
C	6.78565100	0.80039600	0.33107200
C	3.22839200	1.37776000	0.68434600
C	3.24815500	0.79955600	-0.73569600
H	4.84877600	-0.59410300	-2.77598900
H	7.31531900	-0.86893000	-2.59478700
H	8.53243000	0.01824200	-0.64105400
H	7.31563800	1.17862600	1.19876600
N	4.51055000	1.52975600	1.10823400
O	2.23786300	1.68207200	1.34459900
C	2.31368000	-0.35894400	-0.94779900
C	1.05004000	-0.47589700	-0.51585200
O	0.33537900	0.31712400	0.28762200
H	0.92763000	1.02834300	0.66568700
H	2.66505500	-1.09166800	-1.66576800
C	4.87584700	2.20602700	2.33975100
H	3.97269100	2.72612900	2.67247600
H	5.63319800	2.96274500	2.10515000
C	5.38416400	1.25549500	3.40141800
C	6.57871000	1.51335500	4.07098400
C	4.64526400	0.11734200	3.73217300
C	7.03244700	0.64761200	5.06434800
H	7.15761100	2.39734000	3.81440900
C	5.09873600	-0.74954900	4.71997300
H	3.70954600	-0.08167300	3.21495500
C	6.29371800	-0.48586100	5.38867800
H	7.96456400	0.85712500	5.57905800
H	4.51881700	-1.63152000	4.97207500
H	6.64687400	-1.16376400	6.15889000
C	1.79474800	2.89392300	-1.40487100
C	2.89592700	1.93499700	-1.77378300
H	3.81501100	2.49303000	-1.97199000
H	2.60130900	1.43214100	-2.69994200
C	2.10282600	4.08217300	-0.57261900
C	3.41140900	4.41382400	-0.19142200
C	1.06186500	4.90977700	-0.11714700
C	3.67053700	5.52991600	0.60271300
H	4.25245600	3.80607200	-0.51272200
C	1.32335200	6.02606800	0.66374800
H	0.04369700	4.65046200	-0.38823800

C	2.63076700	6.34524700	1.03408200
H	4.69582200	5.76274500	0.87641000
H	0.49826200	6.64876000	0.99736800
H	2.83300900	7.21433200	1.65187000
N	0.59421900	2.80479600	-1.87773400
N	0.22576000	1.67963000	-2.52883800
S	-1.02053400	2.01654600	-3.52931600
O	-1.69999000	0.73269900	-3.78895300
O	-0.60273100	2.79238600	-4.70471600
C	-2.19201800	3.06573600	-2.66643100
C	-3.40279300	2.54458400	-2.22801800
C	-1.88451100	4.41169600	-2.45636600
C	-4.30066200	3.37136300	-1.55456500
H	-3.64838100	1.50729600	-2.43793900
C	-2.78040100	5.21782200	-1.76752500
H	-0.95037400	4.81032300	-2.83454000
C	-3.99779200	4.70817200	-1.29990400
H	-5.25702200	2.97552400	-1.22594100
H	-2.53790900	6.26356300	-1.59511200
C	-4.95263200	5.58600300	-0.53324700
H	-5.08515800	6.55289900	-1.02636800
H	-5.93264300	5.11297300	-0.43462500
H	-4.57328700	5.78229500	0.47496000

M3S

Total energy= -4208.351969

Zero-point correction= 1.033916 (Hartree/Particle)

Thermal correction to Energy= 1.103069

Thermal correction to Enthalpy= 1.104014

Thermal correction to Gibbs Free Energy= 0.924730

Sum of electronic and zero-point Energies= -4207.318053

Sum of electronic and thermal Energies= -4207.248899

Sum of electronic and thermal Enthalpies= -4207.247955

Sum of electronic and thermal Free Energies= -4207.427238

C	-4.99401300	-2.76670600	0.96783500
C	-4.65418700	-1.55741200	0.35300000
C	-5.46484400	-1.05309600	-0.65082600
C	-6.63391300	-1.74443100	-0.99093600
C	-6.96688000	-2.93179100	-0.34631600
C	-6.14137600	-3.47190900	0.64316000
C	-2.95139100	-2.24293300	1.85090400
C	-3.33914400	-1.06655900	0.93418800
H	-5.20522900	-0.13966700	-1.17985200
H	-7.27918600	-1.35443900	-1.77030100

H	-7.87309900	-3.45924500	-0.62501200
H	-6.37726200	-4.41765900	1.11900800
N	-3.99750100	-3.12182000	1.88849300
O	-1.92423300	-2.36844100	2.49946600
C	-2.38272600	-0.76941100	-0.18756500
C	-1.06810100	-0.99488600	-0.28653600
O	-0.25252300	-1.67557300	0.53990100
H	-0.60171400	-1.62060000	1.45887000
H	-2.85442100	-0.24606900	-1.00390100
C	-3.95961800	-4.36535800	2.63759200
H	-3.18792500	-4.23141100	3.40016900
H	-4.92210700	-4.50159200	3.14110500
C	-3.64427700	-5.55305500	1.75309700
C	-4.49471800	-6.65523500	1.70424900
C	-2.48384400	-5.54636700	0.97381000
C	-4.19513700	-7.74317200	0.88573300
H	-5.39719100	-6.66416700	2.31104800
C	-2.18561300	-6.62994500	0.15573200
H	-1.81336000	-4.69060400	1.01805900
C	-3.04136400	-7.73046300	0.10903000
H	-4.86503200	-8.59635300	0.85369700
H	-1.28164100	-6.62019200	-0.44480200
H	-2.80611900	-8.57516000	-0.53038200
C	-2.94232500	1.48518100	1.34314300
C	-3.50781000	0.19554500	1.88894700
H	-4.56490200	0.29273500	2.14557400
H	-2.94044700	-0.02271800	2.79882200
C	-3.80788500	2.55620100	0.81256900
C	-5.12261200	2.30900400	0.39787500
C	-3.32681600	3.87599700	0.73068200
C	-5.92226100	3.33422700	-0.10640200
H	-5.53547800	1.30832500	0.47527200
C	-4.12896100	4.89790800	0.24221200
H	-2.31405500	4.07615000	1.06803700
C	-5.43304000	4.63348000	-0.18196900
H	-6.93539900	3.11325400	-0.42851600
H	-3.73571200	5.90883200	0.18940600
H	-6.05588300	5.43283300	-0.56994100
N	-1.66919400	1.71943400	1.38257000
N	-0.90432900	0.76880300	1.96157300
S	0.66677800	1.10129100	1.70073200
O	1.42878900	0.12511100	2.49452500
O	0.98982000	1.18741600	0.25687300
C	1.01123600	2.71660700	2.37735800

C	1.34325000	2.82098600	3.72365200
C	0.86619600	3.85231600	1.58567200
C	1.54781700	4.08049100	4.27840100
H	1.44158500	1.91855000	4.31923800
C	1.06694400	5.10398900	2.15676200
H	0.61082700	3.74350400	0.53746300
C	1.40798800	5.23654700	3.50685300
H	1.81741800	4.16822400	5.32740900
H	0.96266700	5.99673000	1.54506900
C	1.60001000	6.60245700	4.11414600
H	2.21215600	7.23875300	3.46943400
H	2.08390800	6.53722500	5.09109600
H	0.63666700	7.10431200	4.25076100
C	2.53614100	-0.87825100	-3.49449400
C	2.62172000	-2.21815500	-2.72296200
C	1.87593700	-1.97762200	-1.39501200
C	1.24179200	-0.33961000	-2.97593600
C	-0.31365900	-0.50251600	-1.44352700
H	3.35564300	-0.20117800	-3.22927000
H	2.52725600	-0.99858900	-4.57778200
H	2.11253800	-3.00278600	-3.28867800
H	1.40511000	-2.87096400	-0.98653100
N	0.38690400	0.57908700	-3.30145800
N	-0.59057400	0.46823300	-2.33756500
N	0.84503600	-1.01950100	-1.85504300
C	-1.58206600	1.48518700	-2.32303600
C	-1.19957100	2.78673600	-2.00552000
C	-2.86902200	1.25813700	-2.80013100
C	-2.09878100	3.83428300	-2.14245000
C	-3.78310800	2.29441600	-2.90652700
C	-3.37893600	3.59245000	-2.62341100
F	-3.25101100	0.02424600	-3.12526600
F	-5.02175000	2.04994200	-3.31874600
F	-4.21323700	4.60025300	-2.81379200
F	-1.73024600	5.07135200	-1.83697800
F	0.03713400	3.04381400	-1.62166500
H	3.64831600	-2.53181200	-2.53706000
C	2.73960800	-1.28193700	-0.33282300
H	3.02011400	-0.28231500	-0.69831900
H	2.15481500	-1.13926300	0.57875800
O	3.86810900	-2.09526300	-0.08344300
Si	5.42760300	-1.47892500	-0.11346900
C	6.51502500	-2.97714900	0.27521400
C	6.32679000	-3.29905600	1.76775000

C	6.08588000	-4.20558000	-0.54072000
C	7.98997600	-2.65138700	0.00692600
H	6.64781000	-2.46798100	2.40337200
H	5.27842400	-3.51595800	1.99921100
H	6.92163600	-4.18204500	2.03504600
H	6.25417900	-4.07576200	-1.61449600
H	6.67019600	-5.08045700	-0.22690500
H	5.02663700	-4.43132500	-0.38703200
H	8.62024600	-3.50828000	0.27768700
H	8.17274400	-2.41969700	-1.04820200
H	8.32530000	-1.79571700	0.60426700
C	5.58433800	-0.12995600	1.17388500
C	6.70991800	0.70931400	1.21387100
C	4.56609900	0.08036800	2.11295500
C	6.81765100	1.71965200	2.16448300
H	7.50452100	0.58766300	0.47907600
C	4.65996700	1.10557200	3.05250800
H	3.67181700	-0.53550100	2.11031900
C	5.78742600	1.92107400	3.08293300
H	7.69577400	2.35796700	2.18155100
H	3.84097800	1.26491000	3.74650400
H	5.86216200	2.72017900	3.81433500
C	5.73577700	-0.66390800	-1.79389700
C	6.08883800	-1.38750500	-2.94491800
C	5.51292600	0.71594800	-1.94237800
C	6.20313300	-0.76985000	-4.18801400
H	6.27547100	-2.45609900	-2.87819700
C	5.62859500	1.34291200	-3.18297600
H	5.24326200	1.31270000	-1.07466600
C	5.97076500	0.59923500	-4.30925900
H	6.47871900	-1.35434700	-5.06038600
H	5.44829200	2.40995600	-3.26785900
H	6.06149200	1.08326900	-5.27676100

TS4R

Total energy=	-4208.325535
Zero-point correction=	1.027419 (Hartree/Particle)
Thermal correction to Energy=	1.095699
Thermal correction to Enthalpy=	1.096643
Thermal correction to Gibbs Free Energy=	0.920114
Sum of electronic and zero-point Energies=	-4207.298116
Sum of electronic and thermal Energies=	-4207.229836
Sum of electronic and thermal Enthalpies=	-4207.228892
Sum of electronic and thermal Free Energies=	-4207.405421

Imaginary frequency= -1201.09 cm^{-1}

C	-2.64150400	-4.24262500	-1.57881300
C	-3.11160000	-2.95690400	-2.30891900
C	-2.29004700	-1.78373600	-1.71546100
C	-1.23868700	-3.87142900	-1.22361600
C	0.18310600	-2.22864700	-0.98157800
H	-3.21786800	-4.42437400	-0.66475700
H	-2.68903700	-5.13663500	-2.19987700
H	-2.89991000	-3.04674500	-3.37678900
H	-2.01201400	-1.03059600	-2.45576100
N	-0.12760800	-4.47047000	-0.90701200
N	0.75276500	-3.42600400	-0.75394600
N	-1.08397900	-2.51151100	-1.27259600
C	2.10855200	-3.63336700	-0.39611300
C	2.61430200	-3.03047600	0.75265800
C	2.96856500	-4.29715500	-1.26273100
C	3.97172300	-3.07728200	1.03273100
C	4.32583900	-4.36504900	-0.98079400
C	4.82207700	-3.75428900	0.16406800
F	2.49970100	-4.83180400	-2.38209400
F	5.15118100	-4.99891100	-1.80441300
F	6.11306700	-3.83984100	0.44277900
F	4.46258100	-2.50264400	2.12036000
F	1.78895100	-2.37288600	1.55402200
H	-4.17851700	-2.77087600	-2.18358500
C	-2.98871900	-1.08770000	-0.54641100
H	-3.13887200	-1.81188700	0.27089300
H	-2.36580800	-0.25988200	-0.19774500
O	-4.21341500	-0.62278100	-1.06097900
Si	-5.61889600	-0.55958700	-0.16011100
C	-6.94180700	-0.08423200	-1.42499800
C	-6.73688700	1.40380600	-1.76316000
C	-6.78846300	-0.88937300	-2.72427700
C	-8.34250900	-0.28545100	-0.83281100
H	-6.91400800	2.04485800	-0.89418900
H	-5.72068000	1.59843000	-2.12486700
H	-7.43981600	1.70143700	-2.55212800
H	-6.97287000	-1.95953000	-2.58439400
H	-7.51417700	-0.53233000	-3.46658300
H	-5.78580000	-0.76819200	-3.14499400
H	-9.10518100	0.06881300	-1.53822300
H	-8.54827300	-1.33957100	-0.61664500
H	-8.46765500	0.28032500	0.09819600
C	-5.42781200	0.77035200	1.14075800

C	-6.24273900	0.83480500	2.28052800
C	-4.50992400	1.80833100	0.91398200
C	-6.14879600	1.90363700	3.16826300
H	-6.95578100	0.03667200	2.48125300
C	-4.41833500	2.88229200	1.79698000
H	-3.86786500	1.78170500	0.03328600
C	-5.23741000	2.92917700	2.92321200
H	-6.78515200	1.93816500	4.04733400
H	-3.70972100	3.68182500	1.60086900
H	-5.16567100	3.76628000	3.61151500
C	-5.84598400	-2.23714900	0.67652700
C	-6.41156900	-3.33746700	0.01207800
C	-5.33489500	-2.45344300	1.96677700
C	-6.46823100	-4.59592200	0.60619900
H	-6.82305000	-3.21605000	-0.98608600
C	-5.38482300	-3.70999600	2.56711200
H	-4.89111400	-1.62359800	2.51246600
C	-5.95260800	-4.78404500	1.88694400
H	-6.91938600	-5.42751100	0.07355600
H	-4.98226600	-3.84914600	3.56567600
H	-5.99768900	-5.76324800	2.35363300
C	4.82599000	0.13882200	0.02990900
C	4.31139000	-0.04860200	-1.25903300
C	5.03366800	-0.76825800	-2.19372000
C	6.28131200	-1.29259600	-1.83204500
C	6.77431900	-1.10472800	-0.54274000
C	6.05188500	-0.38563000	0.41487000
C	2.78625000	1.18780100	0.06586200
C	2.89942100	0.50608500	-1.31873300
H	4.63723500	-0.92500600	-3.19426100
H	6.86222600	-1.85351000	-2.55625100
H	7.73404400	-1.53035100	-0.26859700
H	6.42545200	-0.25955900	1.42550200
N	3.92782000	0.89235800	0.78452100
O	1.87576200	1.87294300	0.47850400
C	2.00685600	-0.71650800	-1.36112200
C	0.75430900	-0.85634200	-0.85358600
O	-0.06369800	-0.03779000	-0.29827400
H	0.15364600	1.35445400	-1.25747900
H	2.44060400	-1.57127600	-1.86701800
C	4.17786100	1.42382600	2.11080500
H	3.47850900	2.25627700	2.23136100
H	5.19770200	1.82303200	2.14127800
C	3.97090600	0.39265000	3.19655500

C	5.00323800	0.03849000	4.06172700
C	2.72210900	-0.21875700	3.32800000
C	4.79607700	-0.92082200	5.05149700
H	5.97508800	0.51689100	3.96253200
C	2.51548800	-1.17831700	4.31277700
H	1.92002500	0.05494800	2.64489100
C	3.55173600	-1.53052200	5.17689300
H	5.60700300	-1.19211900	5.71997000
H	1.54388300	-1.65347200	4.40662300
H	3.38868000	-2.27935500	5.94548400
C	2.21667300	2.91545100	-2.12635200
C	2.62233600	1.50763500	-2.50220500
H	3.52245500	1.56387100	-3.11996500
H	1.82302600	1.09045800	-3.11666200
C	3.26873000	3.92700200	-1.84855800
C	4.60176900	3.54440100	-1.66817000
C	2.93229200	5.28151800	-1.71695800
C	5.57836700	4.49307900	-1.36913600
H	4.89417800	2.50062900	-1.75305000
C	3.90784100	6.22483500	-1.43012300
H	1.89469300	5.57169100	-1.83979700
C	5.23677800	5.83548400	-1.25436800
H	6.60718900	4.17650100	-1.22929500
H	3.63287200	7.27113700	-1.34045600
H	5.99778500	6.57592300	-1.02904300
N	0.99794100	3.30156200	-2.02813900
N	0.03893300	2.31860400	-2.17012100
S	-1.50058000	2.92034600	-1.87807200
O	-2.34064200	1.72395800	-1.80146200
O	-1.81481800	3.96040300	-2.84838400
C	-1.43217800	3.67993400	-0.26806700
C	-1.01740800	2.92227800	0.82461300
C	-1.77854900	5.02047200	-0.13701000
C	-0.95006900	3.53567400	2.07080000
H	-0.72275600	1.88237000	0.70371400
C	-1.71722800	5.61003300	1.12105600
H	-2.08369400	5.58053200	-1.01423400
C	-1.29815600	4.87899800	2.23778000
H	-0.62050900	2.95809400	2.92966700
H	-1.99096100	6.65517600	1.23826500
C	-1.20814800	5.54008700	3.58864100
H	-2.09145200	6.15339700	3.78646700
H	-1.11637500	4.80008600	4.38627100
H	-0.33457000	6.19785500	3.63871900

TS4S

Total energy= -4208.348930

Zero-point correction= 1.028905 (Hartree/Particle)

Thermal correction to Energy= 1.097578

Thermal correction to Enthalpy= 1.098522

Thermal correction to Gibbs Free Energy= 0.919467

Sum of electronic and zero-point Energies= -4207.320025

Sum of electronic and thermal Energies= -4207.251352

Sum of electronic and thermal Enthalpies= -4207.250408

Sum of electronic and thermal Free Energies= -4207.429463

Imaginary frequency= -655.10 cm^{-1}

C	5.39168900	-1.54112400	-1.33276900
C	4.59617500	-0.50688500	-0.82861200
C	5.13479100	0.38202300	0.08675900
C	6.48090300	0.26244000	0.44663400
C	7.26451800	-0.75385500	-0.09254400
C	6.72786700	-1.68354900	-0.98774400
C	3.29568300	-1.99574000	-2.15056000
C	3.17272700	-0.68616600	-1.32597600
H	4.52401700	1.17978000	0.50126800
H	6.90765200	0.96412900	1.15496300
H	8.30657300	-0.84087500	0.19781600
H	7.32445300	-2.50407300	-1.37170500
N	4.62158600	-2.37171400	-2.15441800
O	2.40513200	-2.58078300	-2.72719400
C	2.26621200	-0.85844200	-0.13405200
C	0.92425500	-0.96024400	-0.15457100
O	0.12823900	-1.07053600	-1.20253000
H	0.07803700	-0.02148100	-1.69038300
H	2.76816900	-0.89809000	0.82075200
C	5.09708600	-3.57943500	-2.80218900
H	4.33777700	-3.83667200	-3.54624000
H	6.03175700	-3.35457400	-3.32679000
C	5.29203800	-4.71997900	-1.82563700
C	6.51869300	-5.36922500	-1.70636200
C	4.21815100	-5.13314200	-1.03232000
C	6.67659000	-6.41975200	-0.80327300
H	7.35659100	-5.05399900	-2.32409500
C	4.37472500	-6.17872700	-0.13017700
H	3.25788300	-4.63341500	-1.13731300
C	5.60587800	-6.82405600	-0.01280200
H	7.63737800	-6.91696700	-0.71554600
H	3.53499000	-6.49505400	0.48048700

H	5.72769300	-7.63900000	0.69338600
C	2.26724800	1.71521200	-1.72679900
C	2.66616100	0.39773300	-2.34742100
H	3.46101900	0.53679300	-3.08663300
H	1.81202700	-0.03698400	-2.87148900
C	3.30959000	2.67801400	-1.27583600
C	4.58641600	2.71157600	-1.84585000
C	3.02815800	3.56827800	-0.22917400
C	5.56071100	3.58302500	-1.36547000
H	4.83985500	2.04038500	-2.65971200
C	4.00410200	4.42768900	0.26208500
H	2.02629500	3.57160400	0.18934000
C	5.28080400	4.43244100	-0.29995200
H	6.54658800	3.58502500	-1.81966000
H	3.76885700	5.09070600	1.08914100
H	6.04564800	5.09848100	0.08621800
N	1.05244200	2.07213800	-1.50120100
N	0.02545900	1.28770100	-1.95240200
S	-1.38626900	1.72536900	-1.21049200
O	-2.45655800	1.11594700	-2.00325500
O	-1.34163000	1.39719600	0.22757500
C	-1.52207200	3.49150700	-1.34957300
C	-2.15551500	4.02188900	-2.46606100
C	-0.99408300	4.31189100	-0.35644100
C	-2.25522000	5.40473400	-2.58981100
H	-2.57111300	3.35512700	-3.21418200
C	-1.10022800	5.68852200	-0.49774700
H	-0.52559700	3.86642900	0.51392900
C	-1.72715600	6.25319800	-1.61495700
H	-2.75256100	5.83181800	-3.45587700
H	-0.69338500	6.34099600	0.27026200
C	-1.82026000	7.75042000	-1.75385700
H	-2.25963500	8.20027000	-0.85900400
H	-2.43064900	8.03245500	-2.61398200
H	-0.82642300	8.18908100	-1.88569300
C	-2.59526400	-1.93018100	3.03111500
C	-2.65439600	-2.99826700	1.91067300
C	-1.95083500	-2.36202400	0.69110000
C	-1.32217500	-1.23403300	2.67841500
C	0.20399400	-0.91655900	1.13961400
H	-3.43379100	-1.22752200	2.97157100
H	-2.57021700	-2.35270700	4.03549600
H	-2.10119400	-3.88780700	2.22325600
H	-1.44140800	-3.08655000	0.05520400

N	-0.45057300	-0.47102200	3.26375300
N	0.50447200	-0.28017300	2.29342400
N	-0.95581100	-1.52114100	1.39047000
C	1.54806100	0.64557300	2.55474600
C	1.27619800	2.01035000	2.52696200
C	2.82285900	0.21995000	2.91789400
C	2.28347000	2.93147100	2.77454800
C	3.83951500	1.13419900	3.14934700
C	3.56643900	2.49497400	3.07124100
F	3.09448400	-1.07860800	2.98076100
F	5.06832400	0.71778100	3.42612200
F	4.53451800	3.37476500	3.26792500
F	2.02353400	4.23131900	2.68530900
F	0.06120400	2.44967000	2.25974900
H	-3.67340300	-3.29199500	1.66221100
C	-2.87882800	-1.47130700	-0.14879000
H	-3.19139500	-0.60276100	0.44899000
H	-2.33406900	-1.09319600	-1.01558000
O	-3.97074100	-2.26451200	-0.56600900
Si	-5.57609900	-1.88060300	-0.28002100
C	-6.51004100	-3.43877300	-0.81087200
C	-6.42515700	-3.52119700	-2.34524100
C	-5.86345600	-4.70506100	-0.22945400
C	-7.98325900	-3.34811700	-0.39165500
H	-6.90822500	-2.66410500	-2.82446500
H	-5.38477500	-3.55818100	-2.68589500
H	-6.92767700	-4.43275000	-2.69405900
H	-5.94579100	-4.75993700	0.86096200
H	-6.36269200	-5.59514600	-0.63432900
H	-4.80292600	-4.76157400	-0.49315800
H	-8.53272400	-4.22706500	-0.75295200
H	-8.10072400	-3.30340100	0.69651700
H	-8.46457700	-2.46075500	-0.81902200
C	-6.05993200	-0.40270700	-1.31758800
C	-7.25687000	0.29285800	-1.08213800
C	-5.24096700	0.01887200	-2.37158400
C	-7.63034600	1.36669900	-1.88367200
H	-7.89743200	0.00255100	-0.25076300
C	-5.60340500	1.10423300	-3.16727700
H	-4.29486600	-0.48211200	-2.55536900
C	-6.80029100	1.77283800	-2.92840900
H	-8.55971000	1.89339600	-1.68980400
H	-4.94262700	1.42860200	-3.96495800
H	-7.08455800	2.61808300	-3.54794200

C	-5.80184100	-1.38687300	1.53095800
C	-6.07710800	-2.30696700	2.55567200
C	-5.61714600	-0.04331600	1.90036600
C	-6.15433900	-1.91143700	3.88868700
H	-6.23669600	-3.35506700	2.31718700
C	-5.69018200	0.36054100	3.23318900
H	-5.41597300	0.70157500	1.13357400
C	-5.95703400	-0.57455900	4.23003200
H	-6.37073100	-2.64415900	4.66003800
H	-5.53785100	1.40404200	3.49012200
H	-6.01512100	-0.26288500	5.26829900

M4R

Total energy= -4208.352637

Zero-point correction= 1.032068 (Hartree/Particle)

Thermal correction to Energy= 1.101370

Thermal correction to Enthalpy= 1.102314

Thermal correction to Gibbs Free Energy= 0.922207

Sum of electronic and zero-point Energies= -4207.320569

Sum of electronic and thermal Energies= -4207.251267

Sum of electronic and thermal Enthalpies= -4207.250323

Sum of electronic and thermal Free Energies= -4207.430430

C	-2.66505900	-3.56226300	-2.02877000
C	-3.11493900	-2.16395000	-2.52761100
C	-2.23701100	-1.13638800	-1.78026000
C	-1.23465100	-3.29215900	-1.68459300
C	0.26349500	-1.74482900	-1.27681600
H	-3.21215600	-3.86869100	-1.12889400
H	-2.77159900	-4.34613600	-2.77845100
H	-2.92913100	-2.07958500	-3.60100000
H	-2.00905600	-0.23895600	-2.35803000
N	-0.14849300	-3.96959100	-1.45384700
N	0.77975000	-2.98940800	-1.19293400
N	-1.01763000	-1.94385700	-1.57966300
C	2.10976400	-3.32220800	-0.83634400
C	2.60791100	-2.92786000	0.40293200
C	2.95991400	-3.90465000	-1.76895000
C	3.95047200	-3.09612100	0.70554800
C	4.30235400	-4.09040500	-1.46836800
C	4.79238600	-3.68496200	-0.23329900
F	2.49975100	-4.24403300	-2.96508200
F	5.11708000	-4.64736200	-2.35576000
F	6.06654800	-3.88448600	0.06338400
F	4.43679200	-2.71706500	1.87739600

F	1.79872400	-2.33639100	1.26925300
H	-4.17264000	-1.97521400	-2.34568400
C	-2.78257500	-0.74223300	-0.40364200
H	-2.82586100	-1.63734600	0.23732400
H	-2.09057800	-0.02277000	0.04404300
O	-4.05752600	-0.16570100	-0.58020900
Si	-5.41509300	-0.70343500	0.24532500
C	-6.83816100	0.24471300	-0.55612200
C	-6.71117000	1.71749300	-0.12953000
C	-6.74678300	0.18392300	-2.08898800
C	-8.18550500	-0.30903600	-0.07399100
H	-6.78327800	1.83460800	0.95723900
H	-5.75860600	2.14721800	-0.45995900
H	-7.51683700	2.30521900	-0.58767400
H	-6.88351400	-0.82897700	-2.48086400
H	-7.53519100	0.80797600	-2.52910200
H	-5.78157900	0.55807700	-2.44344800
H	-9.00789800	0.27321000	-0.50874000
H	-8.32733800	-1.35620700	-0.36266700
H	-8.27723700	-0.24343300	1.01666800
C	-5.19382600	-0.24474800	2.04846000
C	-6.03658700	-0.73681400	3.05649100
C	-4.19260800	0.66681500	2.41064700
C	-5.89471800	-0.31857700	4.37701400
H	-6.80814500	-1.46480000	2.81069500
C	-4.04579400	1.09005400	3.72997600
H	-3.51644400	1.05246600	1.65088500
C	-4.90054600	0.59883200	4.71371100
H	-6.55718100	-0.70836800	5.14360600
H	-3.26357000	1.79842400	3.98628800
H	-4.78980400	0.92584400	5.74292700
C	-5.51554200	-2.58689800	0.13783500
C	-6.14172200	-3.26527700	-0.92095300
C	-4.87011000	-3.36601300	1.11305100
C	-6.11258200	-4.65464400	-1.01277500
H	-6.66450300	-2.70625700	-1.69209500
C	-4.83551500	-4.75745900	1.02802800
H	-4.39180300	-2.87760600	1.95924400
C	-5.45461300	-5.40384500	-0.03891600
H	-6.60676300	-5.15297600	-1.84082500
H	-4.32839200	-5.33396100	1.79533700
H	-5.43055300	-6.48679700	-0.10879400
C	5.04280000	0.17003700	0.25205000
C	4.54701100	0.20579800	-1.05676400

C	5.26052800	-0.38587600	-2.08338400
C	6.48095800	-1.00856700	-1.79236200
C	6.95660500	-1.04250900	-0.48340100
C	6.24206900	-0.45545900	0.56557300
C	3.02780200	1.25828800	0.42965400
C	3.15702600	0.81529900	-1.05104500
H	4.87551000	-0.37133300	-3.10022200
H	7.05364700	-1.47341700	-2.58764400
H	7.89457300	-1.54344400	-0.26729100
H	6.59768400	-0.50889200	1.58907700
N	4.15420500	0.82208100	1.10546100
O	2.12025000	1.87323300	0.94303000
C	2.21224900	-0.33827300	-1.30384200
C	0.87952000	-0.40234700	-1.03687500
O	0.03692200	0.47749400	-0.64257800
H	0.21748200	1.71462400	-1.51152400
H	2.67441300	-1.19760300	-1.76970000
C	4.39601800	1.12145200	2.50445600
H	3.74200800	1.96468200	2.74480700
H	5.43595100	1.44848500	2.61482900
C	4.10316700	-0.05666200	3.40501700
C	5.09868700	-0.64412100	4.18211100
C	2.80844000	-0.57868300	3.43652900
C	4.80990200	-1.75115100	4.97872000
H	6.10654100	-0.23519800	4.16431400
C	2.52033600	-1.68563800	4.22603300
H	2.03599600	-0.11524900	2.82663900
C	3.52108800	-2.27481800	4.99813400
H	5.59251400	-2.20517200	5.57841000
H	1.51316000	-2.09063100	4.23925300
H	3.29426700	-3.13938700	5.61401100
C	2.34726100	3.27003300	-1.51477100
C	2.97094000	2.00526400	-2.05586100
H	3.95075100	2.26832600	-2.46301300
H	2.34829000	1.65752300	-2.88159200
C	3.22155700	4.26088100	-0.82927000
C	4.54601200	3.94611900	-0.50492900
C	2.72130100	5.51628700	-0.46084300
C	5.35241300	4.86503600	0.16338600
H	4.96504500	2.97636700	-0.76273800
C	3.52906000	6.43498600	0.19382900
H	1.68822300	5.74970400	-0.69249100
C	4.84981600	6.11352000	0.51032100
H	6.37626300	4.60067700	0.40869700

H	3.12742300	7.40617700	0.46574000
H	5.47834700	6.83178100	1.02707800
N	1.10982600	3.57658100	-1.65429100
N	0.30831600	2.56813500	-2.17236300
S	-1.21047300	3.11153700	-2.58912200
O	-1.94839300	1.89228700	-2.91817800
O	-1.06177100	4.17277800	-3.57406900
C	-1.95699100	3.82799900	-1.14512900
C	-2.91473600	3.11058400	-0.43702100
C	-1.56847700	5.10844400	-0.75279500
C	-3.49111800	3.69950600	0.68713600
H	-3.22070800	2.12205800	-0.77435200
C	-2.14029000	5.66626600	0.38187500
H	-0.83717400	5.65055000	-1.34179000
C	-3.10630800	4.97017500	1.11754100
H	-4.25837400	3.16264100	1.23879400
H	-1.84073200	6.66108800	0.70018800
C	-3.71423100	5.58717000	2.34999000
H	-4.15474100	6.56274400	2.12497300
H	-4.49364600	4.94723300	2.76909500
H	-2.95208400	5.74272900	3.11964800

M4S

Total energy= -4208.354156
Zero-point correction= 1.032817 (Hartree/Particle)
Thermal correction to Energy= 1.101109
Thermal correction to Enthalpy= 1.102054
Thermal correction to Gibbs Free Energy= 0.925509
Sum of electronic and zero-point Energies= -4207.321339
Sum of electronic and thermal Energies= -4207.253047
Sum of electronic and thermal Enthalpies= -4207.252103
Sum of electronic and thermal Free Energies= -4207.428647

C	-2.39527100	4.68889900	-1.12819400
C	-3.29345400	3.66856000	-0.77943700
C	-4.41988600	3.97695500	-0.04091200
C	-4.65853100	5.30906300	0.32188200
C	-3.75404500	6.30499600	-0.02754300
C	-2.59676600	6.00721300	-0.75598900
C	-1.55078400	2.81925800	-2.11851700
C	-2.69545900	2.33356700	-1.19644200
H	-5.11240700	3.19968400	0.26940800
H	-5.54840200	5.56134900	0.88824700
H	-3.94169000	7.33150100	0.27027900
H	-1.88159100	6.78204500	-1.01145600

N	-1.35175900	4.15403300	-1.89685800
O	-0.99470600	2.17521300	-2.99399400
C	-2.17902300	1.69487600	0.07711000
C	-0.88206400	1.32533700	0.25299700
O	0.12384900	1.48828800	-0.50417400
H	-1.21220300	0.46687900	-2.34259200
H	-2.91892800	1.55073100	0.85292900
C	-0.32748100	4.91343200	-2.59785800
H	-0.14806000	4.38254600	-3.53741600
H	-0.73343000	5.90119100	-2.83675400
C	0.96198800	5.02855000	-1.81307300
C	1.44892900	6.26552200	-1.39663500
C	1.68378600	3.86729500	-1.51757000
C	2.64981200	6.34950300	-0.69157500
H	0.89208700	7.17061900	-1.62929000
C	2.88092400	3.95017600	-0.81272200
H	1.29177700	2.89982200	-1.81815100
C	3.36597000	5.19251100	-0.40010100
H	3.02270800	7.31766000	-0.37206200
H	3.43359800	3.03988300	-0.58799000
H	4.30329300	5.25710100	0.14490900
C	-3.63544200	-0.06966200	-1.50317000
C	-3.61113900	1.35392300	-2.01795700
H	-4.62747900	1.74758200	-2.06832000
H	-3.23371800	1.32540000	-3.04748100
C	-4.87928900	-0.63030700	-0.91111300
C	-5.85318600	0.19412800	-0.34028600
C	-5.10282900	-2.01579700	-0.93017000
C	-7.02304200	-0.34383600	0.19363800
H	-5.70346900	1.26802100	-0.30813400
C	-6.27287100	-2.55135600	-0.40791300
H	-4.34816500	-2.65848900	-1.37287000
C	-7.24298000	-1.71597600	0.14860200
H	-7.76151100	0.31436900	0.63984800
H	-6.43310600	-3.62460200	-0.43744400
H	-8.15632400	-2.13616300	0.55645300
N	-2.64186600	-0.87993400	-1.53993800
N	-1.47505900	-0.51516600	-2.13922100
S	-0.16702700	-1.43691900	-1.64110300
O	0.96422000	-0.92417700	-2.40236500
O	-0.09093200	-1.54020400	-0.18491000
C	-0.60515800	-3.04594700	-2.24944400
C	-0.22415100	-3.40186700	-3.54048500
C	-1.33708300	-3.90838000	-1.44214400

C	-0.58725600	-4.65150000	-4.02401600
H	0.34981400	-2.70604800	-4.14360900
C	-1.69690800	-5.15376900	-1.94788100
H	-1.61073200	-3.60690600	-0.43763800
C	-1.32922400	-5.54150700	-3.23827500
H	-0.29244600	-4.94517100	-5.02769800
H	-2.26930200	-5.83738600	-1.32737200
C	-1.71180400	-6.89249200	-3.78337100
H	-2.27698600	-6.79078900	-4.71428500
H	-2.32350900	-7.44982200	-3.07149000
H	-0.82120600	-7.48758600	-4.00612700
C	2.16236300	-0.12353300	3.69385900
C	2.75674000	1.11366500	2.97150400
C	2.02700200	1.19062200	1.61351800
C	0.77797400	-0.13798600	3.12380000
C	-0.52667600	0.61167000	1.52420500
H	2.69159400	-1.04433100	3.42069800
H	2.16424500	-0.03621600	4.78030300
H	2.53854900	2.01483000	3.55076900
H	1.90760300	2.20098800	1.22186800
N	-0.37570800	-0.66726700	3.39586400
N	-1.18810100	-0.18388400	2.38806400
N	0.71703600	0.64130100	2.00322000
C	-2.50268000	-0.70730000	2.31615600
C	-2.67136800	-2.05574000	2.01364000
C	-3.60645100	0.03256900	2.72852600
C	-3.92422400	-2.64472800	2.08744200
C	-4.86413800	-0.54817700	2.80360100
C	-5.01188900	-1.89997600	2.52241200
F	-3.46624000	1.31442500	3.04890500
F	-5.91241500	0.17072900	3.18858400
F	-6.19062400	-2.48368400	2.67458600
F	-4.07703800	-3.92780600	1.77968600
F	-1.62986700	-2.80451200	1.68861300
H	3.83517600	1.04154300	2.83355100
C	2.64092500	0.28686300	0.54019700
H	2.63594200	-0.75561300	0.89609900
H	2.02787600	0.34673600	-0.36202600
O	3.95459800	0.75317100	0.29426000
Si	5.29322000	-0.25043300	0.32271200
C	6.74580200	0.94325000	0.11488000
C	6.73449500	1.43119000	-1.34405100
C	6.58438300	2.16592000	1.03104500
C	8.07493400	0.23410000	0.40398700

H	6.87543900	0.60497600	-2.04784300
H	5.79056000	1.92935800	-1.59236400
H	7.54650300	2.15322400	-1.49991500
H	6.62907800	1.90585100	2.09356700
H	7.39374700	2.88236400	0.83838300
H	5.63103600	2.67253900	0.85005100
H	8.91295800	0.92489300	0.24459400
H	8.13043600	-0.12934300	1.43589700
H	8.22440000	-0.62181000	-0.26438200
C	5.15327400	-1.46974900	-1.09092700
C	6.02523100	-2.56437900	-1.20274300
C	4.15563800	-1.31249000	-2.06270500
C	5.91467500	-3.46417700	-2.25815400
H	6.78990600	-2.72794500	-0.44485200
C	4.02878400	-2.22278100	-3.11061900
H	3.45317600	-0.48559900	-1.99839400
C	4.91225100	-3.29346400	-3.21286500
H	6.59949100	-4.30347800	-2.33151500
H	3.23334700	-2.09113200	-3.83702500
H	4.81685400	-4.00232600	-4.02984300
C	5.27757700	-1.25560000	1.92538000
C	5.79269300	-0.78090800	3.14283400
C	4.63089600	-2.50299400	1.94031700
C	5.65592800	-1.50666600	4.32358200
H	6.30943000	0.17469100	3.17913600
C	4.48971700	-3.23617400	3.11803400
H	4.23255200	-2.91078300	1.01417400
C	4.99963900	-2.73612100	4.31329500
H	6.06434700	-1.11568200	5.25037500
H	3.98160100	-4.19528000	3.10029400
H	4.89183500	-3.30303600	5.23284400

TS5R

Total energy= -4208.328199

Zero-point correction= 1.028895 (Hartree/Particle)

Thermal correction to Energy= 1.097510

Thermal correction to Enthalpy= 1.098454

Thermal correction to Gibbs Free Energy= 0.921664

Sum of electronic and zero-point Energies= -4207.299304

Sum of electronic and thermal Energies= -4207.230690

Sum of electronic and thermal Enthalpies= -4207.229746

Sum of electronic and thermal Free Energies= -4207.406535

Imaginary frequency= -1214.07 cm^{-1}

C	2.21635400	0.63657000	3.11909200

C	2.68244100	1.16712600	1.73928100
C	1.92382000	0.34417300	0.66719900
C	0.82539100	0.21076100	2.78212700
C	-0.53742600	-0.32080000	1.16916300
H	2.80900200	-0.22787300	3.44356100
H	2.23772800	1.39347700	3.90213000
H	2.37701500	2.21103700	1.64748900
H	1.59369900	0.96568400	-0.17153000
N	-0.32595400	0.08916900	3.37628200
N	-1.17036800	-0.24403200	2.34814200
N	0.72973300	-0.04868500	1.44163200
C	-2.58065500	-0.25865300	2.49361400
C	-3.30504100	-1.37698600	2.09077600
C	-3.23988600	0.93882500	2.76900800
C	-4.68071700	-1.29795600	1.92612900
C	-4.61692000	1.02142100	2.61423400
C	-5.32790900	-0.09300200	2.18202500
F	-2.55194200	2.00467000	3.12734300
F	-5.25646600	2.15348000	2.86670200
F	-6.63997400	-0.01439900	2.03397200
F	-5.38307900	-2.34528200	1.52184900
F	-2.65709600	-2.49076700	1.76930600
H	3.76025400	1.08912200	1.60311200
C	2.66943700	-0.89131500	0.15922100
H	2.78320600	-1.60922000	0.98644900
H	2.08117200	-1.36474100	-0.63298600
O	3.91640900	-0.46471900	-0.34337500
Si	5.35746600	-1.15587400	0.15319400
C	6.68463900	-0.06843600	-0.64039200
C	6.73055500	-0.41159000	-2.13980100
C	6.31913400	1.41717000	-0.49962500
C	8.05959000	-0.34795000	-0.01973600
H	7.06302300	-1.44047200	-2.30922000
H	5.74614200	-0.29362000	-2.60717000
H	7.43155300	0.26048500	-2.65177200
H	6.28815500	1.74833000	0.54372000
H	7.06825400	2.03349300	-1.01363400
H	5.34045800	1.62179300	-0.94491600
H	8.83144300	0.23537500	-0.53797300
H	8.09542800	-0.08287900	1.04193900
H	8.33190700	-1.40617000	-0.11102700
C	5.40929300	-2.90627400	-0.51039400
C	6.28376800	-3.87662600	0.00077300
C	4.60124100	-3.24983900	-1.60486500

C	6.35451100	-5.14730200	-0.56416600
H	6.91045200	-3.64106000	0.85933400
C	4.66437700	-4.52156300	-2.16923600
H	3.91689800	-2.51093800	-2.01915400
C	5.54319200	-5.47005200	-1.65016000
H	7.03781000	-5.88604500	-0.15695000
H	4.02886900	-4.77295200	-3.01289000
H	5.59521700	-6.46124200	-2.09007000
C	5.38477400	-1.22691200	2.04134900
C	5.83852600	-0.16476800	2.84070200
C	4.83575200	-2.34050900	2.69908000
C	5.74234400	-0.20557300	4.22942200
H	6.27465600	0.71696600	2.37828200
C	4.73391000	-2.38906700	4.08891600
H	4.48810600	-3.19073900	2.11603900
C	5.18673600	-1.31943900	4.85659900
H	6.10201500	0.62966300	4.82218000
H	4.30449700	-3.26233100	4.56989600
H	5.11029800	-1.35370700	5.93884400
C	-5.01762600	-0.42786400	-1.83010400
C	-4.15297200	0.67522600	-1.82540300
C	-4.60578600	1.90909800	-1.39365300
C	-5.94411900	2.03171600	-0.99460900
C	-6.78853700	0.92505600	-0.99659300
C	-6.33544100	-0.33313700	-1.41049500
C	-3.00478600	-1.27183500	-2.53092300
C	-2.73715200	0.16040500	-2.03102500
H	-3.92387300	2.75333500	-1.33449700
H	-6.31667800	2.99327300	-0.65851100
H	-7.81369800	1.03081700	-0.65668200
H	-6.98202800	-1.20424400	-1.37966400
N	-4.32528300	-1.56490500	-2.26314900
O	-2.22737600	-2.03598900	-3.06899700
C	-2.19994000	0.13962700	-0.59188800
C	-1.03869800	-0.60992400	-0.24128700
O	-0.29219800	-1.31040700	-0.91358200
H	-1.85554500	1.46018300	-0.53192800
H	-2.98103700	0.15614800	0.15985300
C	-4.92261300	-2.85260200	-2.55787600
H	-4.27347300	-3.32086900	-3.30389800
H	-5.90495600	-2.68759300	-3.01277300
C	-5.03757800	-3.73745900	-1.33638900
C	-6.27093100	-4.23122400	-0.91751200
C	-3.88266900	-4.08149500	-0.62841300

C	-6.35518200	-5.06835900	0.19387200
H	-7.17064300	-3.96518700	-1.46767000
C	-3.96582200	-4.91935600	0.47798200
H	-2.91973900	-3.69666900	-0.95932500
C	-5.20206600	-5.41547800	0.89043100
H	-7.32061000	-5.44723800	0.51410000
H	-3.06481600	-5.18516200	1.02159400
H	-5.26410800	-6.06955400	1.75442000
C	-0.40066300	1.28099800	-2.47037800
C	-1.79753100	0.95226800	-2.98793800
H	-1.71101900	0.41228700	-3.93287500
H	-2.27180400	1.91936100	-3.19401400
C	0.81083400	0.67212700	-3.07571000
C	0.77510800	-0.62762300	-3.59240600
C	2.02645500	1.37058900	-3.06099600
C	1.94236600	-1.21767100	-4.07398400
H	-0.15224400	-1.19286200	-3.56473800
C	3.18453500	0.78008000	-3.54995400
H	2.04370200	2.38180300	-2.66571700
C	3.14724700	-0.51937200	-4.05653800
H	1.90780700	-2.23208500	-4.45998900
H	4.11806300	1.33529400	-3.54227000
H	4.05317000	-0.98249600	-4.43787300
N	-0.18640400	2.12382400	-1.51994200
N	-1.33572800	2.61424700	-0.92090000
S	-0.94082200	3.44500900	0.45829400
O	-0.09431900	2.62386800	1.34395300
O	-2.20858500	3.94563700	0.98247900
C	0.04817300	4.82158700	-0.06829500
C	1.40093200	4.63568200	-0.34852500
C	-0.55706200	6.06317800	-0.21672800
C	2.14958900	5.71871600	-0.78794500
H	1.84598000	3.65361000	-0.22707800
C	0.21138300	7.13925700	-0.65174600
H	-1.61095900	6.17521800	0.01500400
C	1.56777300	6.98341100	-0.94313300
H	3.20444400	5.58640300	-1.01334400
H	-0.25016500	8.11578400	-0.76678500
C	2.40451200	8.15103700	-1.39662900
H	1.77993500	8.99471600	-1.69642700
H	3.06339600	8.49028200	-0.59093300
H	3.03809200	7.87380500	-2.24318000

TS5S

Total energy= -4208.337820

Zero-point correction= 1.028162 (Hartree/Particle)

Thermal correction to Energy= 1.096886

Thermal correction to Enthalpy= 1.097830

Thermal correction to Gibbs Free Energy= 0.919828

Sum of electronic and zero-point Energies= -4207.309658

Sum of electronic and thermal Energies= -4207.240934

Sum of electronic and thermal Enthalpies= -4207.239990

Sum of electronic and thermal Free Energies= -4207.417993

Imaginary frequency= -836.04 cm^{-1}

C	-4.74912100	0.96546000	1.06270400
C	-3.49040800	1.33616800	0.57838900
C	-3.38172300	2.00729400	-0.63088900
C	-4.55406900	2.33444100	-1.32262100
C	-5.80093600	1.96588400	-0.82116500
C	-5.92106800	1.26860400	0.38409000
C	-3.27024800	0.03557400	2.55818200
C	-2.42508000	0.67680200	1.43613500
H	-2.40590500	2.24973400	-1.04706800
H	-4.48773400	2.86019100	-2.26941700
H	-6.69761000	2.21029900	-1.38159200
H	-6.88762700	0.94617700	0.75702500
N	-4.60298800	0.23501900	2.24880700
O	-2.86715800	-0.50837000	3.56290500
C	-1.75824000	-0.35930800	0.51203600
C	-1.12708900	-1.57625800	0.92915800
O	-0.73577400	-1.94687800	2.02203000
H	-0.69994500	0.24696800	0.20753000
H	-2.25623400	-0.42780000	-0.44603700
C	-5.69050100	-0.28110500	3.04777600
H	-5.23224700	-0.64533700	3.97278400
H	-6.37119700	0.53818400	3.30830100
C	-6.45489200	-1.39417000	2.35753600
C	-5.81930500	-2.22424500	1.43694900
C	-7.80105300	-1.61021800	2.65523200
C	-6.51566200	-3.26215900	0.82494900
H	-4.77603600	-2.04917200	1.19136100
C	-8.49788500	-2.65215800	2.04927300
H	-8.30576300	-0.95853500	3.36447100
C	-7.85598000	-3.48077700	1.13153300
H	-6.00832600	-3.89174500	0.10088000
H	-9.54480400	-2.81184600	2.28724800
H	-8.40040900	-4.28814200	0.65239400
C	-0.83429600	2.69892300	1.16624900

C	-1.35968400	1.60535500	2.08237000
H	-1.76719700	2.05572400	2.98947500
H	-0.52345500	0.96863400	2.39656800
C	-1.24878500	4.10773500	1.39203700
C	-2.45374300	4.41659700	2.03264300
C	-0.44437900	5.16009700	0.93276900
C	-2.84337200	5.74135100	2.21228300
H	-3.11021400	3.62087000	2.37274200
C	-0.83248800	6.48042000	1.11618900
H	0.48766800	4.92083500	0.43034600
C	-2.03375000	6.77786100	1.75943600
H	-3.78541500	5.96036300	2.70480700
H	-0.19332900	7.28329600	0.76190400
H	-2.33446400	7.81033000	1.90608300
N	-0.03767700	2.49091900	0.17810900
N	0.37479300	1.19251600	-0.02108900
S	0.71959200	0.92939300	-1.60260800
O	1.09705300	-0.49522500	-1.65529000
O	-0.38513800	1.37153500	-2.46728300
C	2.13836400	1.90532800	-2.01880200
C	3.39579400	1.30924700	-2.05408600
C	1.97447400	3.26966900	-2.23918100
C	4.50509700	2.10196900	-2.31573600
H	3.48955600	0.23968700	-1.89015800
C	3.10075500	4.04875400	-2.48398300
H	0.98002300	3.70199900	-2.21766100
C	4.37585000	3.47972300	-2.51877600
H	5.49449800	1.65262200	-2.35850700
H	2.98773000	5.11600700	-2.65369000
C	5.59891500	4.33271900	-2.72078700
H	6.33612700	3.82998200	-3.35190100
H	6.07665800	4.53384100	-1.75495900
H	5.34827300	5.29242900	-3.17764300
C	2.21064500	-4.22751300	-1.36912100
C	2.50018300	-4.29435900	0.15406100
C	1.68579600	-3.15221200	0.79694900
C	0.85868900	-3.58981600	-1.38389800
C	-0.58401900	-2.40306200	-0.25280900
H	2.91716300	-3.57324300	-1.89085100
H	2.22270300	-5.20306900	-1.85485300
H	2.16123200	-5.25370700	0.55185100
H	1.30443100	-3.38059400	1.79106500
N	-0.08891300	-3.34607100	-2.24239600
N	-0.98423100	-2.60829100	-1.52064200

N	0.56808300	-3.05864000	-0.16083900
C	-2.09539600	-2.00773500	-2.16251200
C	-3.37125600	-2.15564900	-1.62372400
C	-1.88930200	-1.13327000	-3.22827300
C	-4.42691700	-1.38778400	-2.08526700
C	-2.94661700	-0.36311900	-3.69712900
C	-4.20663600	-0.49051200	-3.12665200
F	-0.70663600	-1.02508000	-3.79339900
F	-2.75807700	0.48732300	-4.69373600
F	-5.21000000	0.24118400	-3.58231000
F	-5.63501200	-1.50382300	-1.55218600
F	-3.54589300	-2.97218000	-0.58466300
H	3.56074200	-4.17951600	0.37725200
C	2.40279700	-1.79988800	0.81160200
H	2.83974800	-1.60915500	-0.18036400
H	1.66657300	-1.00729300	0.99387000
O	3.37353500	-1.83247000	1.83012300
Si	4.88163100	-1.11245300	1.66084700
C	5.72861600	-1.42961900	3.32131500
C	4.83744300	-0.81150200	4.41131900
C	5.88602800	-2.93174900	3.59459600
C	7.10912900	-0.76120300	3.35305700
H	4.68743300	0.26127200	4.24766900
H	3.85416400	-1.29071700	4.44227500
H	5.31007200	-0.93932200	5.39371200
H	4.93686000	-3.46741200	3.48201800
H	6.62689100	-3.38539900	2.92866300
H	6.23606100	-3.08584000	4.62360100
H	7.60247300	-0.97082400	4.31096000
H	7.76189200	-1.13488800	2.55496400
H	7.03037800	0.32604700	3.25356100
C	4.69291100	0.72407100	1.33281600
C	5.80990900	1.52563000	1.03595800
C	3.43672500	1.34354700	1.37575900
C	5.67570000	2.88942800	0.79890300
H	6.80076200	1.07745900	0.97955000
C	3.29136200	2.70479300	1.10838900
H	2.54463200	0.76696400	1.60338000
C	4.41163900	3.47932900	0.82814100
H	6.55415700	3.49073600	0.58212100
H	2.29788900	3.14509000	1.11024100
H	4.30162900	4.53943700	0.61747200
C	5.70583500	-1.91098100	0.16060500
C	5.97492500	-3.28998400	0.12486000

C	5.96964700	-1.17201400	-1.00222600
C	6.48259200	-3.90270200	-1.01795200
H	5.77570100	-3.90254300	1.00076600
C	6.47728100	-1.77699300	-2.15086100
H	5.76930600	-0.10414800	-1.00872100
C	6.73424600	-3.14484000	-2.16039800
H	6.68320200	-4.96971000	-1.01755500
H	6.66812900	-1.18058000	-3.03811600
H	7.12910500	-3.61951000	-3.05322800

M5R

Total energy= -4208.352633

Zero-point correction= 1.032822 (Hartree/Particle)

Thermal correction to Energy= 1.102328

Thermal correction to Enthalpy= 1.103273

Thermal correction to Gibbs Free Energy= 0.923529

Sum of electronic and zero-point Energies= -4207.319812

Sum of electronic and thermal Energies= -4207.250305

Sum of electronic and thermal Enthalpies= -4207.249361

Sum of electronic and thermal Free Energies= -4207.429105

C	-2.45874500	-0.97178400	2.83157100
C	-2.88966200	-1.39984300	1.41012800
C	-2.08045300	-0.53033700	0.41589400
C	-1.06043000	-0.53753400	2.56212500
C	0.38402200	0.08100800	1.05731000
H	-3.04852000	-0.12564500	3.20536800
H	-2.50003200	-1.78219900	3.55836700
H	-2.59611600	-2.44084400	1.26115200
H	-1.72598300	-1.12228800	-0.42857000
N	0.05387900	-0.43983000	3.22281900
N	0.95192800	-0.06316400	2.26486700
N	-0.89847700	-0.20473200	1.24533800
C	2.31418400	0.06356300	2.62822300
C	2.98882300	1.26983000	2.47237800
C	2.96413900	-1.02970400	3.19833100
C	4.31278600	1.38962300	2.86115500
C	4.29004000	-0.91124400	3.59607700
C	4.95736100	0.29547700	3.42839600
F	2.32837200	-2.16895700	3.36680700
F	4.91863500	-1.94243100	4.13967500
F	6.21947100	0.40723000	3.80868300
F	4.95968800	2.53817200	2.71545700
F	2.36835200	2.30322700	1.90344800
H	-3.96055800	-1.29482700	1.24119800

C	-2.77647800	0.75342300	-0.05324600
H	-2.79885200	1.47630100	0.77740100
H	-2.20545000	1.19581600	-0.87839100
O	-4.07238300	0.42051400	-0.49456500
Si	-5.44157200	1.17588600	0.10160800
C	-6.86546000	0.23477800	-0.71181700
C	-6.89598700	0.63916100	-2.19613800
C	-6.62839200	-1.28144800	-0.63558000
C	-8.20314500	0.60634100	-0.05924100
H	-7.11937500	1.70313800	-2.32247600
H	-5.93527500	0.43499800	-2.68305500
H	-7.67043900	0.06479700	-2.72059900
H	-6.62545600	-1.65939900	0.39191700
H	-7.42765300	-1.80883500	-1.17209700
H	-5.67197200	-1.55079800	-1.09474900
H	-9.02843500	0.10709100	-0.58268000
H	-8.24542400	0.30847000	0.99364600
H	-8.38695300	1.68602900	-0.11061900
C	-5.38305300	2.96585000	-0.44600000
C	-6.16583700	3.96258800	0.15494100
C	-4.57728200	3.32144000	-1.53814500
C	-6.15042300	5.27095400	-0.32149700
H	-6.78762900	3.71724100	1.01430200
C	-4.55363500	4.63040800	-2.01367500
H	-3.96325600	2.56218400	-2.02062400
C	-5.34215000	5.60509300	-1.40644400
H	-6.76285100	6.03051000	0.15449700
H	-3.92046000	4.89012700	-2.85660600
H	-5.32548600	6.62561500	-1.77635900
C	-5.40644100	1.13005700	1.98955400
C	-5.92818800	0.06415100	2.74073100
C	-4.74830000	2.15376100	2.69260300
C	-5.79560300	0.01569300	4.12629500
H	-6.44881200	-0.74871300	2.24215100
C	-4.60724300	2.11106200	4.07918400
H	-4.34603800	3.00615200	2.14890000
C	-5.13053800	1.03987300	4.79853400
H	-6.21180800	-0.81940900	4.68107200
H	-4.09342600	2.91552400	4.59605400
H	-5.02432800	1.00361400	5.87817300
C	5.06498800	0.52604600	-2.38718400
C	4.17525400	-0.48174100	-2.00892700
C	4.64361400	-1.71411000	-1.59000200
C	6.02767200	-1.92685100	-1.57527100

C	6.90500700	-0.91278300	-1.95154900
C	6.43815300	0.34059000	-2.36162200
C	2.98429200	1.45517700	-2.67096100
C	2.76151300	0.06428400	-2.03860900
H	3.93957100	-2.47855000	-1.26666600
H	6.41958500	-2.88619800	-1.25526200
H	7.97501700	-1.09192800	-1.92282100
H	7.12486500	1.13322500	-2.63905700
N	4.33997500	1.66151000	-2.77982400
O	2.13896800	2.26782100	-2.99443800
C	2.40156600	0.27930600	-0.54155100
C	0.99434700	0.69381200	-0.20114500
O	0.31977000	1.52801900	-0.74905200
H	2.62812400	-0.64893800	-0.01459000
H	3.05788200	1.07383100	-0.15668700
C	4.91004800	2.96774700	-3.05185100
H	4.13560400	3.53160100	-3.57859200
H	5.77009000	2.85621000	-3.71933000
C	5.30291500	3.65867500	-1.76274000
C	6.61550900	4.05019100	-1.51659800
C	4.32697300	3.87560800	-0.78256300
C	6.95738000	4.65009700	-0.30430800
H	7.37711000	3.88536400	-2.27489400
C	4.66751400	4.46753400	0.42710300
H	3.29555000	3.58923700	-0.98170400
C	5.98639800	4.85384800	0.66975300
H	7.98466900	4.94828600	-0.12046700
H	3.90611200	4.62406600	1.18416700
H	6.25285900	5.31149900	1.61712400
C	0.40760800	-1.08920300	-2.30582000
C	1.77448900	-0.80370200	-2.87768700
H	1.66410700	-0.34249700	-3.86227900
H	2.25134700	-1.78037200	-3.01209400
C	-0.81232800	-0.49309100	-2.89685300
C	-0.80004600	0.80772700	-3.41798700
C	-2.01749600	-1.21266700	-2.90533200
C	-1.97400400	1.37992800	-3.90453300
H	0.11989200	1.38542400	-3.40137800
C	-3.18583800	-0.63629000	-3.38713100
H	-2.01494700	-2.23279800	-2.53147000
C	-3.16988900	0.66537100	-3.88791400
H	-1.95258400	2.39410800	-4.29296500
H	-4.11063600	-1.20605700	-3.38220900
H	-4.08181300	1.11580300	-4.26992100

N	0.24026900	-1.91206800	-1.31892700
N	1.36068800	-2.46577000	-0.78907200
S	0.95324600	-3.45346000	0.44200500
O	-0.04110900	-2.84816700	1.35531300
O	2.21540600	-3.92071700	1.02092200
C	0.12874600	-4.87109400	-0.26307700
C	-1.20694200	-4.76941200	-0.64133100
C	0.84287100	-6.04520600	-0.47703000
C	-1.82875400	-5.85841300	-1.24290000
H	-1.74665400	-3.84648100	-0.45455000
C	0.20534100	-7.12834900	-1.07170100
H	1.87979600	-6.09814100	-0.16229000
C	-1.13342500	-7.04947100	-1.46785600
H	-2.87239800	-5.78716200	-1.53729800
H	0.75309200	-8.05361000	-1.23081200
C	-1.80078200	-8.22431500	-2.13542000
H	-1.57094400	-9.15680500	-1.61303400
H	-2.88582900	-8.10329900	-2.16020700
H	-1.45213400	-8.33296400	-3.16745000

M5S

Total energy= -4208.363025
Zero-point correction= 1.034025 (Hartree/Particle)
Thermal correction to Energy= 1.102720
Thermal correction to Enthalpy= 1.103664
Thermal correction to Gibbs Free Energy= 0.927603
Sum of electronic and zero-point Energies= -4207.329000
Sum of electronic and thermal Energies= -4207.260305
Sum of electronic and thermal Enthalpies= -4207.259361
Sum of electronic and thermal Free Energies= -4207.435422

C	4.71027900	1.90596800	-1.19864700
C	3.51333400	1.77809800	-0.48997400
C	3.42141400	2.25095300	0.80927000
C	4.53128600	2.89201900	1.36900200
C	5.71080800	3.02960300	0.64218500
C	5.82528000	2.52753100	-0.65715000
C	3.33754600	0.72218500	-2.60924000
C	2.51228200	1.01462000	-1.33579400
H	2.50382000	2.12401100	1.37887300
H	4.47239000	3.27905300	2.38029200
H	6.56506800	3.52338600	1.09413000
H	6.75493700	2.60724400	-1.21029100
N	4.57614900	1.31246000	-2.46362300
O	3.00303100	0.05923400	-3.57009900

C	2.24597300	-0.32930700	-0.61853000
C	1.13000400	-1.15632200	-1.19577400
O	0.67299400	-1.07544200	-2.30880700
H	2.03362100	-0.15134700	0.44058400
H	3.16805800	-0.92274500	-0.68300000
C	5.69376600	0.96489600	-3.32420400
H	5.25406600	0.63206600	-4.26806600
H	6.29458400	1.85837600	-3.51975200
C	6.53552100	-0.12948000	-2.69853600
C	7.89031300	0.05616200	-2.43622900
C	5.92952600	-1.33785700	-2.33763800
C	8.63468200	-0.94794200	-1.81728000
H	8.36738300	0.99379200	-2.71193100
C	6.66728700	-2.33573900	-1.71262000
H	4.87684000	-1.49602200	-2.56223500
C	8.02333400	-2.14153300	-1.44893600
H	9.68906000	-0.78999600	-1.61409900
H	6.18291300	-3.26326500	-1.42517100
H	8.59823800	-2.91949800	-0.95701200
C	0.64121100	2.56217300	-0.53282700
C	1.24417800	1.83413500	-1.71021900
H	1.52028300	2.54738800	-2.49029200
H	0.50313600	1.16196200	-2.14860700
C	0.87739900	4.01736200	-0.33778700
C	1.86732600	4.71101100	-1.04600800
C	0.11690300	4.73339400	0.60185700
C	2.08376600	6.06984100	-0.83099100
H	2.50247200	4.18990900	-1.75555700
C	0.33461400	6.08786400	0.81522100
H	-0.64527500	4.20294500	1.16432300
C	1.31782000	6.76738300	0.09664500
H	2.86207300	6.58090200	-1.38915100
H	-0.26924800	6.61920800	1.54486000
H	1.48545100	7.82692800	0.26142100
N	-0.04806200	1.96930400	0.37749500
N	-0.35571000	0.64611700	0.22654700
S	-0.68611600	0.06791000	1.71296000
O	-1.26414300	-1.27790800	1.52686700
O	0.50398600	0.15341300	2.58384400
C	-1.95442400	1.07505600	2.45105900
C	-3.27786000	0.65218700	2.36193800
C	-1.62589100	2.28875800	3.04506700
C	-4.28136900	1.45834900	2.88247500
H	-3.50189800	-0.30702700	1.90456900

C	-2.64629100	3.09387800	3.54295800
H	-0.58591300	2.58829600	3.11460600
C	-3.98236300	2.69432900	3.46425700
H	-5.31854100	1.13490000	2.83024200
H	-2.40087000	4.04642100	4.00537100
C	-5.08956400	3.58997500	3.95187100
H	-4.71897500	4.34063900	4.65330800
H	-5.87867300	3.01575300	4.44416700
H	-5.54697400	4.11609100	3.10574000
C	-2.23231400	-4.44771600	-0.05415200
C	-2.50113400	-3.97891900	-1.50674900
C	-1.72456100	-2.65739900	-1.67777100
C	-0.89938000	-3.82820400	0.20877200
C	0.51630700	-2.27480800	-0.36264800
H	-2.95797400	-4.02872800	0.65122100
H	-2.22404400	-5.53136300	0.05998400
H	-2.12506600	-4.72390300	-2.21170700
H	-1.32367200	-2.50660100	-2.67881800
N	0.04139200	-3.91266300	1.10507500
N	0.92067100	-2.93975400	0.73093500
N	-0.61671000	-2.87485500	-0.72222200
C	2.06951800	-2.71906100	1.52764400
C	3.34315200	-2.83419700	0.97839400
C	1.92034400	-2.44482300	2.88636900
C	4.46828300	-2.60333000	1.75051000
C	3.04823100	-2.22620800	3.66701100
C	4.31373800	-2.30415500	3.09986400
F	0.73106200	-2.42317200	3.44349600
F	2.92329100	-1.96332500	4.95971900
F	5.38392400	-2.10086500	3.85059100
F	5.68147500	-2.69154200	1.22016800
F	3.48129900	-3.12947400	-0.31531000
H	-3.56207900	-3.81871900	-1.69974900
C	-2.50011200	-1.41873000	-1.23181500
H	-2.96314400	-1.61585000	-0.25351800
H	-1.79892400	-0.58909700	-1.09348900
O	-3.46094600	-1.12826400	-2.22550300
Si	-4.94167900	-0.45770700	-1.80355100
C	-5.84679500	-0.24737500	-3.44988600
C	-4.96985300	0.64652600	-4.34190200
C	-6.06041600	-1.59844400	-4.14607500
C	-7.20607800	0.43003400	-3.23031900
H	-4.79351900	1.62388800	-3.87971100
H	-3.99779800	0.18359200	-4.53759200

H	-5.46846600	0.81429900	-5.30534700
H	-5.12269100	-2.15682500	-4.24449400
H	-6.78227300	-2.21876500	-3.60504800
H	-6.46095000	-1.43698900	-5.15537400
H	-7.72914400	0.53399700	-4.18981100
H	-7.85013800	-0.15545000	-2.56324900
H	-7.09125200	1.43251900	-2.80589900
C	-4.68395000	1.19624200	-0.95674600
C	-5.75700700	1.89821200	-0.37918500
C	-3.41296700	1.78541000	-0.90090400
C	-5.56705800	3.13736100	0.22480600
H	-6.75827600	1.47020800	-0.39701000
C	-3.21198900	3.01552600	-0.27642300
H	-2.55402700	1.28690700	-1.34176800
C	-4.28987700	3.69496900	0.28065700
H	-6.41316600	3.66500600	0.65626400
H	-2.21107700	3.43313100	-0.23191300
H	-4.13517000	4.65486400	0.76583000
C	-5.74068500	-1.66107600	-0.58768600
C	-5.98947400	-2.99484100	-0.95531000
C	-5.98421500	-1.30397200	0.74667800
C	-6.46072300	-3.92744500	-0.03476800
H	-5.80751900	-3.31791300	-1.97770000
C	-6.45545500	-2.23104600	1.67495300
H	-5.79086000	-0.28425200	1.06923800
C	-6.69414700	-3.54550900	1.28531600
H	-6.64687000	-4.95089400	-0.34618400
H	-6.62854100	-1.92717400	2.70293100
H	-7.05980800	-4.27048000	2.00578400

TS6S

Total energy= -4208.342837

Zero-point correction= 1.034367 (Hartree/Particle)

Thermal correction to Energy= 1.102518

Thermal correction to Enthalpy= 1.103462

Thermal correction to Gibbs Free Energy= 0.926380

Sum of electronic and zero-point Energies= -4207.308470

Sum of electronic and thermal Energies= -4207.240319

Sum of electronic and thermal Enthalpies= -4207.239375

Sum of electronic and thermal Free Energies= -4207.416458

Imaginary frequency= -73.07 cm^{-1}

C	-4.52066400	3.28168300	-1.05676900

C	-4.42262900	1.96343400	-0.59123800
C	-5.32047100	1.50529600	0.35765400
C	-6.35842600	2.34646800	0.77741300
C	-6.45653700	3.64264400	0.28086300
C	-5.52655800	4.13941800	-0.63744100
C	-2.65787900	2.44530100	-2.10832600
C	-3.13360800	1.35899500	-1.11952300
H	-5.22276800	0.51058000	0.78613000
H	-7.07692400	1.98917300	1.50696100
H	-7.25746900	4.28972600	0.62354100
H	-5.57504100	5.16424000	-0.99048600
N	-3.47501700	3.54796000	-1.94295500
O	-1.76735400	2.35932700	-2.92175200
C	-2.23116200	1.27994600	0.13113400
C	-0.73622900	1.03475300	-0.00136800
O	0.01444500	1.86402000	-0.51945900
H	-2.30363700	2.22664900	0.68054500
H	-2.68905100	0.51906800	0.75810400
C	-3.21032600	4.82422400	-2.57120200
H	-2.51241900	4.61500600	-3.38725600
H	-4.13639700	5.21736100	-3.00449000
C	-2.61239500	5.81499100	-1.59340900
C	-3.15042000	7.09168700	-1.44997900
C	-1.50142900	5.44564400	-0.82799100
C	-2.58753600	7.99959600	-0.55407700
H	-4.01632500	7.37814500	-2.04244600
C	-0.94122900	6.35172700	0.06572300
H	-1.07251100	4.45000300	-0.93686200
C	-1.48242400	7.63004400	0.20543100
H	-3.01657400	8.99087900	-0.44729600
H	-0.07526400	6.06233100	0.65292300
H	-1.04337200	8.33394400	0.90522700
C	-2.95793200	-1.22811900	-1.08620900
C	-3.23446600	0.01989500	-1.88704100
H	-4.20266300	-0.04216800	-2.38849400
H	-2.44437800	0.05220300	-2.64795200
C	-4.02444900	-2.21127600	-0.78125100
C	-5.37163000	-1.83679700	-0.73009700
C	-3.68949300	-3.55251600	-0.53965600
C	-6.35479400	-2.76573500	-0.39531800
H	-5.65924200	-0.81271200	-0.94521200
C	-4.67203000	-4.47966300	-0.21824100
H	-2.64582300	-3.84835300	-0.60432200
C	-6.00829200	-4.08728800	-0.13379700

H	-7.39282600	-2.45317700	-0.34491600
H	-4.39514700	-5.51157200	-0.02750000
H	-6.77393700	-4.81103300	0.12656400
N	-1.76138900	-1.53078700	-0.71049600
N	-0.80288200	-0.59445100	-1.07301800
S	0.68760600	-1.34317200	-1.16855900
O	1.51723700	-0.48187200	-2.00802100
O	1.21677400	-1.72694300	0.15282100
C	0.37147800	-2.84348800	-2.07275900
C	0.33582400	-2.78036700	-3.46266300
C	0.15565800	-4.03567500	-1.39325800
C	0.07635600	-3.94152900	-4.17951000
H	0.51771800	-1.83402400	-3.96210600
C	-0.10303000	-5.18879300	-2.12858100
H	0.19090000	-4.04773400	-0.30942500
C	-0.14905100	-5.15756400	-3.52473400
H	0.05013700	-3.90811900	-5.26532600
H	-0.26949200	-6.12953300	-1.61119500
C	-0.44453400	-6.40247000	-4.32019700
H	-0.46094900	-7.28780500	-3.68157000
H	0.30635500	-6.55585800	-5.10010400
H	-1.41774800	-6.32313300	-4.81446400
C	2.68516400	0.46044000	3.42809000
C	2.92715800	1.80898300	2.70884100
C	2.16355200	1.71782800	1.36961700
C	1.34582500	0.09428400	2.88366300
C	-0.13465800	0.41511600	1.29951100
H	3.41930200	-0.29753100	3.13232100
H	2.68567600	0.53753000	4.51526700
H	2.51342800	2.62443100	3.30797500
H	1.75106200	2.66788500	1.03473700
N	0.37567900	-0.70581800	3.20094100
N	-0.55433800	-0.48366000	2.21535600
N	1.05530500	0.81141500	1.75656600
C	-1.75089400	-1.24221300	2.31709600
C	-1.70055500	-2.61985700	2.12503800
C	-2.93820000	-0.66361200	2.75246600
C	-2.82877700	-3.39777700	2.32982100
C	-4.08734600	-1.42857800	2.89918400
C	-4.02555000	-2.80154500	2.70572300
F	-2.99855300	0.64319700	2.99178700
F	-5.23436400	-0.84926500	3.24028000
F	-5.10849200	-3.54423700	2.86663800
F	-2.77502400	-4.71009000	2.13294500

F	-0.57620100	-3.20158700	1.75157100
H	3.98398300	2.00881400	2.53200500
C	2.96746100	1.05720500	0.24560600
H	3.11222700	-0.00659100	0.48660300
H	2.38333100	1.10970300	-0.67428700
O	4.19664100	1.74297000	0.09805800
Si	5.64534900	0.90129100	0.05336100
C	6.96361900	2.24796500	-0.11213100
C	6.87492700	2.80367300	-1.54394800
C	6.70581500	3.40230200	0.86790100
C	8.36140300	1.65777800	0.11582700
H	7.08935600	2.03277400	-2.29063000
H	5.87950700	3.20981600	-1.75365500
H	7.60441100	3.61382000	-1.67257500
H	6.80359100	3.09727600	1.91478300
H	7.43785000	4.20240300	0.69627900
H	5.70501200	3.82184600	0.72918100
H	9.12507400	2.43371000	-0.02368100
H	8.47610700	1.25068900	1.12618300
H	8.57592300	0.85426700	-0.59823200
C	5.62849800	-0.25552800	-1.42024300
C	6.59847400	-1.25899400	-1.57945000
C	4.63121100	-0.13873300	-2.39703700
C	6.57836800	-2.10820800	-2.68158100
H	7.36911900	-1.39299300	-0.82185700
C	4.59449200	-1.00032000	-3.49152900
H	3.85419700	0.61317200	-2.29604800
C	5.57139600	-1.98010300	-3.63809300
H	7.33742400	-2.87684200	-2.79012600
H	3.79453400	-0.90771300	-4.21899100
H	5.54576300	-2.65107300	-4.49132500
C	5.77206300	-0.17849500	1.60049500
C	6.25517400	0.29187400	2.83269000
C	5.27121400	-1.49114700	1.56089300
C	6.23627900	-0.50572200	3.97473300
H	6.65493000	1.29931900	2.91115700
C	5.24751200	-2.29552500	2.70007800
H	4.88753500	-1.89274300	0.62575700
C	5.72961100	-1.80256200	3.90998500
H	6.61918100	-0.11714900	4.91342200
H	4.84918500	-3.30337200	2.64033300
H	5.71325400	-2.42563000	4.79879400

M6R

Total energy= -4208.342837

Zero-point correction= 1.034367 (Hartree/Particle)

Thermal correction to Energy= 1.102518

Thermal correction to Enthalpy= 1.103462

Thermal correction to Gibbs Free Energy= 0.926380

Sum of electronic and zero-point Energies= -4207.308470

Sum of electronic and thermal Energies= -4207.240319

Sum of electronic and thermal Enthalpies= -4207.239375

Sum of electronic and thermal Free Energies= -4207.416458

C	-0.69882500	-2.46453500	4.03155600
C	-0.99377000	-3.29021100	2.74807200
C	-1.03164400	-2.28520000	1.57894600
C	-0.00409600	-1.27021900	3.46196400
C	0.50474000	-0.16963900	1.64843900
H	-1.60913500	-2.15141300	4.55135900
H	-0.06428500	-2.99669400	4.74040000
H	-0.17304200	-3.98645700	2.56692300
H	-0.61901700	-2.68646300	0.65438200
N	0.66066500	-0.23902600	3.89808700
N	0.96659200	0.44305800	2.75529100
N	-0.13866200	-1.23813900	2.10575100
C	1.66248400	1.67497500	2.83352200
C	0.98757700	2.84832200	2.50249300
C	3.01480800	1.72792600	3.16276900
C	1.65956400	4.05477400	2.40637500
C	3.68944100	2.94249600	3.09272400
C	3.01728300	4.09474200	2.70426200
F	3.67402900	0.64706100	3.52216300
F	4.98037500	3.00361300	3.39070500
F	3.67522600	5.23940100	2.60930500
F	1.02641900	5.15565900	2.03022000
F	-0.29756500	2.78818200	2.16630300
H	-1.93268100	-3.84260700	2.80706500
C	-2.39161000	-1.62343500	1.36269000
H	-2.75407900	-1.21183500	2.31838800
H	-2.25999600	-0.78918100	0.65806500
O	-3.29107000	-2.58301300	0.86363200
Si	-4.73339700	-2.04647500	0.17686100
C	-5.72759100	-3.61457400	-0.15709400
C	-4.90248600	-4.51479800	-1.08882000
C	-6.01572700	-4.35978100	1.15289800
C	-7.05257400	-3.24392600	-0.83746300
H	-4.66110100	-4.00585000	-2.02819500
H	-3.96247000	-4.82100400	-0.61876800

H	-5.47148800	-5.42113800	-1.33306900
H	-6.64948800	-3.76831300	1.82217600
H	-6.54371800	-5.29801200	0.93822900
H	-5.09083700	-4.61049300	1.68415400
H	-7.64937200	-4.14883300	-1.00980700
H	-7.65104800	-2.56480200	-0.21838700
H	-6.88665100	-2.76735800	-1.80950000
C	-4.32869800	-1.13409900	-1.40803900
C	-5.27970100	-0.38479500	-2.12127600
C	-3.03672000	-1.23785800	-1.94578700
C	-4.94780500	0.25037600	-3.31406300
H	-6.29978300	-0.30118700	-1.75157100
C	-2.69822800	-0.60975500	-3.14318000
H	-2.27407100	-1.81162800	-1.42394700
C	-3.65518400	0.13944300	-3.82314400
H	-5.69666100	0.82937500	-3.84566100
H	-1.68424200	-0.68394700	-3.52071600
H	-3.39558800	0.63503000	-4.75458300
C	-5.52789800	-0.92213400	1.46361600
C	-5.51921300	-1.34562500	2.80412800
C	-6.10401800	0.32402800	1.17887900
C	-6.07555300	-0.56770400	3.81510900
H	-5.05882900	-2.29845600	3.06160300
C	-6.66662700	1.10650900	2.18622900
H	-6.09713800	0.70511600	0.16101800
C	-6.65634300	0.66031000	3.50484600
H	-6.05652000	-0.91652300	4.84300700
H	-7.11313400	2.06576400	1.94118600
H	-7.09397100	1.26944300	4.28961300
C	0.89036800	3.82339600	-2.14235800
C	2.01622700	3.20039200	-1.58643600
C	2.97359900	3.94985700	-0.92940900
C	2.80595800	5.33902700	-0.84686100
C	1.67884900	5.94248400	-1.39809300
C	0.69704300	5.19333100	-2.05608400
C	0.62533700	1.59338300	-2.62445000
C	1.78932200	1.69863400	-1.62445100
H	3.83798700	3.46852200	-0.47713100
H	3.54988700	5.94288300	-0.33840200
H	1.55161600	7.01676000	-1.31271300
H	-0.19083500	5.66550500	-2.46347200
N	0.06867300	2.85709700	-2.73222400
O	0.23262700	0.61548800	-3.21854600
C	1.26858000	1.44438400	-0.18873900

C	0.58596700	0.15492100	0.16347400
O	-0.15052000	-0.48005700	-0.56086100
H	2.13043400	1.58117200	0.46382800
H	0.52652300	2.22269200	0.04366800
C	-1.22272500	3.08571700	-3.34560800
H	-1.39477900	2.22909100	-4.00597200
H	-1.18017100	3.98925100	-3.96237000
C	-2.33568900	3.17944800	-2.32158100
C	-3.26909000	4.21091400	-2.37655300
C	-2.45809100	2.19414100	-1.33587200
C	-4.32126800	4.26154800	-1.46261500
H	-3.17481800	4.97948400	-3.14012800
C	-3.50774900	2.24241300	-0.42539800
H	-1.74926600	1.36777200	-1.30596400
C	-4.44149100	3.27755000	-0.48662700
H	-5.04158500	5.07202900	-1.51292900
H	-3.61094000	1.46460600	0.32728100
H	-5.25806400	3.31309800	0.22886700
C	2.78268600	-0.64761600	-2.16959400
C	3.00962300	0.83984300	-1.97009000
H	3.49090200	1.26154900	-2.85565100
H	3.71805500	0.93375900	-1.13585300
C	2.84933500	-1.23080200	-3.53606800
C	2.71549100	-0.44563600	-4.68650200
C	3.07389600	-2.60630300	-3.69860900
C	2.80480600	-1.01196400	-5.95566900
H	2.51191500	0.61606500	-4.60132700
C	3.16178900	-3.17093000	-4.96320200
H	3.18275100	-3.21734700	-2.80975100
C	3.02997400	-2.37622100	-6.10186700
H	2.69245800	-0.38093100	-6.83205400
H	3.33961100	-4.23745900	-5.06354100
H	3.10259100	-2.81766300	-7.09087100
N	2.68825700	-1.47903000	-1.19179700
N	2.70076400	-0.97824000	0.08245900
S	2.74929700	-2.26747800	1.10665000
O	1.69129800	-3.26310600	0.85587400
O	2.80611600	-1.69861200	2.46160900
C	4.29744300	-3.09309500	0.80675300
C	4.35770100	-4.12404400	-0.12599300
C	5.43335700	-2.66460100	1.48379600
C	5.58183700	-4.72992600	-0.38165300
H	3.44788800	-4.44742700	-0.62106100
C	6.64995800	-3.28539600	1.21919800

H	5.34981300	-1.86730200	2.21571300
C	6.74242200	-4.31796700	0.28199200
H	5.64073600	-5.53967600	-1.10407700
H	7.54246800	-2.96740600	1.75111500
C	8.06653600	-4.96735100	-0.02645300
H	8.79157900	-4.79089300	0.77092600
H	7.95499700	-6.04664400	-0.15841400
H	8.48590900	-4.56549900	-0.95457400

M6S

Total energy= -4208.347068

Zero-point correction= 1.033899 (Hartree/Particle)

Thermal correction to Energy= 1.102419

Thermal correction to Enthalpy= 1.103363

Thermal correction to Gibbs Free Energy= 0.925244

Sum of electronic and zero-point Energies= -4207.313169

Sum of electronic and thermal Energies= -4207.244649

Sum of electronic and thermal Enthalpies= -4207.243705

Sum of electronic and thermal Free Energies= -4207.421824

C	-3.54281200	4.18750700	-0.93108200
C	-3.91511300	2.90713000	-0.49533000
C	-4.92584400	2.76699900	0.43779000
C	-5.60474000	3.90849300	0.88387200
C	-5.23239500	5.16928400	0.42826900
C	-4.18183100	5.33237400	-0.48046500
C	-2.16199600	2.76698900	-2.08665800
C	-2.91207700	1.91105200	-1.04289400
H	-5.17730300	1.79063500	0.84560400
H	-6.41042100	3.80918100	1.60293100
H	-5.75537500	6.04747600	0.79314800
H	-3.86612800	6.31764000	-0.80723400
N	-2.48752600	4.08789900	-1.83944700
O	-1.45901300	2.38050500	-2.99002300
C	-1.99219100	1.60761100	0.16198200
C	-0.66079600	0.89202000	-0.14967900
O	0.28675600	1.62447400	-0.59156500
H	-1.68943900	2.54925000	0.63116300
H	-2.60864500	1.07076500	0.88604500
C	-1.79574400	5.20095400	-2.45118800
H	-1.21712200	4.77259700	-3.27503500
H	-2.52407300	5.90196300	-2.87438600
C	-0.89006700	5.90186700	-1.45952200
C	-0.93917000	7.28556400	-1.30729100
C	0.00903600	5.15217600	-0.69251100

C	-0.09786900	7.92790300	-0.40042400
H	-1.64028500	7.86643200	-1.90252200
C	0.84661200	5.79684300	0.21163600
H	0.05698300	4.06706100	-0.80256100
C	0.79650700	7.18307300	0.36109900
H	-0.14590200	9.00645700	-0.28757800
H	1.54807800	5.21441100	0.80144100
H	1.45297800	7.67857100	1.06952700
C	-3.24475700	-0.65822400	-0.97963800
C	-3.45034600	0.63467600	-1.72830300
H	-4.50109700	0.75944000	-1.99555700
H	-2.87015300	0.51454600	-2.65343300
C	-4.39625200	-1.52926500	-0.64038500
C	-5.63552100	-0.99109500	-0.28124300
C	-4.23831100	-2.92027400	-0.68411700
C	-6.68780500	-1.82918900	0.07675500
H	-5.77967200	0.08500600	-0.27526000
C	-5.29832200	-3.75558600	-0.35036900
H	-3.27526000	-3.32894800	-0.98080000
C	-6.52079400	-3.21161600	0.04155700
H	-7.63922600	-1.40264800	0.37699100
H	-5.16721900	-4.83212000	-0.38660500
H	-7.34314200	-3.86373300	0.31724800
N	-2.08468300	-1.11667400	-0.67279400
N	-1.01995900	-0.29092600	-1.11194800
S	0.31440300	-1.31040000	-1.44978500
O	1.18327000	-0.62902500	-2.39748700
O	0.89191300	-1.83765900	-0.20789000
C	-0.50496100	-2.64210600	-2.29079700
C	-1.05063700	-2.39852700	-3.54794300
C	-0.58977000	-3.88721400	-1.68255400
C	-1.71201900	-3.43286100	-4.19747000
H	-0.95536900	-1.41534100	-3.99965500
C	-1.24502300	-4.91438900	-2.35606600
H	-0.15536400	-4.03319000	-0.69986600
C	-1.82212100	-4.69943300	-3.61087600
H	-2.14751200	-3.26028900	-5.17761900
H	-1.31521300	-5.89698500	-1.89776700
C	-2.57404600	-5.80073100	-4.31128300
H	-2.24681500	-6.78450600	-3.96843700
H	-2.43551800	-5.74718600	-5.39358300
H	-3.64753000	-5.71706200	-4.11166300
C	2.59460600	0.00201800	3.43458300
C	3.00377500	1.28910200	2.68109300

C	2.24876500	1.25351500	1.33531500
C	1.22515100	-0.21776100	2.88111900
C	-0.17684900	0.21908900	1.24558700
H	3.23703100	-0.84557300	3.16810800
H	2.59565800	0.10852500	4.51931100
H	2.68469900	2.16489000	3.25251900
H	1.94969500	2.23215900	0.96814600
N	0.16758200	-0.89826200	3.19801700
N	-0.70845200	-0.60197000	2.17555400
N	1.03869300	0.49174200	1.72640500
C	-1.99163700	-1.20141900	2.26955000
C	-2.13250500	-2.55524600	1.98179200
C	-3.07501100	-0.50303500	2.78831600
C	-3.33816900	-3.20001900	2.20753600
C	-4.30192500	-1.12932000	2.96639100
C	-4.42277700	-2.48618000	2.70269700
F	-2.95601500	0.78435800	3.10011500
F	-5.34425000	-0.44020000	3.41888100
F	-5.57787300	-3.10039900	2.91467400
F	-3.46737700	-4.49205600	1.92644300
F	-1.11428600	-3.23514200	1.48427200
H	4.07933300	1.35622500	2.51712600
C	2.97776000	0.48382000	0.23309700
H	3.04018700	-0.57822900	0.51389500
H	2.38429700	0.56822300	-0.68009600
O	4.25804200	1.05992500	0.05022100
Si	5.63416900	0.10969700	0.02956400
C	7.05275200	1.34274100	-0.18686300
C	7.02400200	1.82578700	-1.64706400
C	6.86190300	2.56160300	0.72830100
C	8.40197200	0.67104500	0.09896000
H	7.19743300	1.00290500	-2.34747000
H	6.06157300	2.28513800	-1.89729900
H	7.80803500	2.57782100	-1.80436600
H	6.91710000	2.30256500	1.79071100
H	7.65311100	3.29765500	0.53369500
H	5.89650700	3.04329400	0.54843900
H	9.21962000	1.38456300	-0.06646900
H	8.47160000	0.31319200	1.13184200
H	8.57343900	-0.18285800	-0.56668900
C	5.51024100	-1.09367400	-1.40172100
C	6.41840200	-2.15481100	-1.54407900
C	4.49839400	-0.95476500	-2.36196100
C	6.32824000	-3.03904900	-2.61479200

H	7.19664200	-2.30583500	-0.79746900
C	4.39235100	-1.84910800	-3.42556100
H	3.76766900	-0.15520900	-2.27625100
C	5.31083000	-2.88689000	-3.55624500
H	7.04184500	-3.85172000	-2.71052200
H	3.58563600	-1.73290200	-4.14228600
H	5.23145600	-3.58320500	-4.38562400
C	5.69089800	-0.92063200	1.61585100
C	6.19058400	-0.43227800	2.83460400
C	5.11674300	-2.20286200	1.62098500
C	6.11405500	-1.18233900	4.00589200
H	6.64820200	0.55275600	2.87932200
C	5.03601800	-2.96037400	2.78919200
H	4.72474100	-2.61797400	0.69537300
C	5.53345100	-2.44922600	3.98500200
H	6.51017900	-0.78067000	4.93350600
H	4.58365900	-3.94683800	2.76330700
H	5.47339500	-3.03561800	4.89666300

TS7R

Total energy= -4208.336424

Zero-point correction= 1.033470 (Hartree/Particle)

Thermal correction to Energy= 1.101451

Thermal correction to Enthalpy= 1.102395

Thermal correction to Gibbs Free Energy= 0.927902

Sum of electronic and zero-point Energies= -4207.302954

Sum of electronic and thermal Energies= -4207.234974

Sum of electronic and thermal Enthalpies= -4207.234029

Sum of electronic and thermal Free Energies= -4207.408522

Imaginary frequency= -107.34 cm^{-1}

C	-1.74667400	4.20823300	-1.27911800
C	-2.19094700	3.81985200	0.15972700
C	-1.59898800	2.41927900	0.43049900
C	-0.54586500	3.33894300	-1.47466100
C	0.64164600	1.64834500	-0.65698100
H	-2.50699000	3.96758500	-2.02832200
H	-1.50055200	5.26776600	-1.37373300
H	-1.77990800	4.53318100	0.87615700
H	-1.29569400	2.24833000	1.46467900
N	0.39436100	3.18427400	-2.35641500
N	1.11706000	2.13132400	-1.82760300
N	-0.43058000	2.42743300	-0.45807500
C	2.13120300	1.50764200	-2.59305200
C	1.88043500	0.24461900	-3.12583400

C	3.38263900	2.08269600	-2.78073000
C	2.88222400	-0.48176000	-3.75005300
C	4.39073700	1.37070000	-3.41698000
C	4.14211300	0.08765000	-3.88870300
F	3.64032600	3.30650500	-2.34665400
F	5.59257900	1.91249400	-3.57889000
F	5.11252000	-0.59690400	-4.47925100
F	2.64124000	-1.69803000	-4.21964300
F	0.67996500	-0.30717800	-2.97743000
H	-3.27601600	3.79517300	0.27405700
C	-2.52536000	1.30494100	-0.05321100
H	-2.77650300	1.49112100	-1.11067000
H	-1.99137700	0.34944800	0.02045800
O	-3.69087900	1.32039000	0.74168100
Si	-4.85225900	0.12534300	0.51346900
C	-6.30821700	0.64527200	1.59873200
C	-5.81832400	0.73321900	3.05173900
C	-6.84536500	2.01241800	1.15707300
C	-7.42294100	-0.40403600	1.49251300
H	-5.41866000	-0.22529300	3.39976800
H	-5.03228500	1.48707800	3.16204100
H	-6.65074000	1.01125100	3.71135600
H	-7.24785300	1.97891100	0.13909100
H	-7.65690600	2.32866700	1.82559100
H	-6.06378600	2.77981300	1.19370900
H	-8.28295600	-0.10130700	2.10362900
H	-7.77414500	-0.52032200	0.46009900
H	-7.08830800	-1.38234600	1.85384900
C	-4.13301400	-1.51536600	1.05264500
C	-4.75136200	-2.74941200	0.78931300
C	-2.93277100	-1.52206100	1.77903400
C	-4.18081900	-3.94435200	1.21615800
H	-5.69561800	-2.78490400	0.24960400
C	-2.35787900	-2.71521800	2.21340700
H	-2.41790300	-0.58950300	1.99616700
C	-2.98121500	-3.92653400	1.92617900
H	-4.67136200	-4.88773800	0.99670300
H	-1.41042600	-2.69178700	2.74105700
H	-2.53528600	-4.85993700	2.25908600
C	-5.26430400	0.17036400	-1.32571800
C	-5.39752100	1.43009800	-1.93531900
C	-5.41361500	-0.96302500	-2.13625200
C	-5.68338900	1.55473400	-3.29158500
H	-5.26361300	2.33005800	-1.33604700

C	-5.70624300	-0.84583300	-3.49464200
H	-5.27382400	-1.95423700	-1.71300400
C	-5.84387800	0.41257400	-4.07353600
H	-5.78096000	2.53887900	-3.73970600
H	-5.82317400	-1.73904000	-4.10156800
H	-6.06862500	0.50413100	-5.13158500
C	2.46744900	-3.67518500	-0.78171800
C	3.27801800	-2.59495300	-0.40543900
C	4.40206200	-2.27534200	-1.14397000
C	4.72977600	-3.06830700	-2.25150100
C	3.91279400	-4.13552600	-2.61586000
C	2.76027900	-4.45498800	-1.88989000
C	1.48315700	-2.83405200	1.10758600
C	2.54718400	-1.82143900	0.67216900
H	5.01305200	-1.41607500	-0.87665700
H	5.61138100	-2.83627500	-2.83899700
H	4.16604100	-4.72843400	-3.48864100
H	2.11270100	-5.27060000	-2.19410800
N	1.39663100	-3.78907500	0.11532100
O	0.82858800	-2.82255500	2.12936300
C	1.86180700	-0.69304400	-0.14290200
C	0.99374100	0.21869200	0.69288800
O	-0.10248400	-0.14169400	1.12241900
H	2.66637900	-0.11206200	-0.59858600
H	1.24189100	-1.14210100	-0.92438900
C	0.27301800	-4.69681800	0.00284600
H	-0.16491900	-4.75509900	1.00509000
H	0.63406100	-5.69375000	-0.27009100
C	-0.76095500	-4.20105600	-0.98850300
C	-1.28176200	-5.05257400	-1.95956700
C	-1.22624700	-2.88374700	-0.90507300
C	-2.26529800	-4.60283400	-2.84026900
H	-0.91737200	-6.07504600	-2.02842700
C	-2.20659300	-2.43682900	-1.78399100
H	-0.84099100	-2.20794700	-0.14169200
C	-2.72901600	-3.29439500	-2.75241000
H	-2.66193800	-5.27459800	-3.59510100
H	-2.57486200	-1.41665400	-1.70984100
H	-3.49219800	-2.93411400	-3.43634000
C	2.59596400	-0.69071700	3.01825200
C	3.37328300	-1.29528900	1.85120800
H	4.00624100	-2.09952500	2.23092600
H	4.04854300	-0.51084600	1.48385200
C	2.73716100	-1.30795400	4.36497100

C	2.87393300	-2.68958500	4.52454300
C	2.74777400	-0.48286100	5.49546200
C	3.00966100	-3.23832600	5.79580500
H	2.83819500	-3.34166200	3.65845000
C	2.89375800	-1.03305600	6.76313300
H	2.65419300	0.58885300	5.35800500
C	3.02398300	-2.41204500	6.91636900
H	3.10291000	-4.31340500	5.91050400
H	2.91167300	-0.38482800	7.63324000
H	3.13914300	-2.84145600	7.90659000
N	1.90925600	0.39349500	2.98158200
N	1.83920300	0.98824200	1.67975400
S	2.94237500	2.17684400	1.37039000
O	3.51420500	1.99646200	0.03555500
O	3.83420500	2.23913300	2.51860300
C	1.96056300	3.65870500	1.32792900
C	2.07261600	4.53907700	0.26166800
C	1.10164300	3.90905800	2.39815900
C	1.28890600	5.69295800	0.26047700
H	2.74150800	4.30810600	-0.55978800
C	0.34350200	5.07057900	2.38666700
H	1.02873500	3.19522600	3.21473700
C	0.42147800	5.97485100	1.31603700
H	1.35866700	6.38330200	-0.57560900
H	-0.32847100	5.28130900	3.21447000
C	-0.44712700	7.20566300	1.30014700
H	-0.44923000	7.69805700	2.27578000
H	-0.10495900	7.92272300	0.55153300
H	-1.48647000	6.94603400	1.06651300

TS7S

Total energy= -4208.344466

Zero-point correction= 1.032744 (Hartree/Particle)

Thermal correction to Energy= 1.101215

Thermal correction to Enthalpy= 1.102159

Thermal correction to Gibbs Free Energy= 0.922486

Sum of electronic and zero-point Energies= -4207.311722

Sum of electronic and thermal Energies= -4207.243251

Sum of electronic and thermal Enthalpies= -4207.242306

Sum of electronic and thermal Free Energies= -4207.421980

Imaginary frequency= -157.63 cm^{-1}

C	4.28732800	3.71913100	0.77806500
C	4.25852500	2.39855300	0.30886600
C	5.07835700	2.02467700	-0.74154200

C	5.97105600	2.96268600	-1.27488000
C	6.00061900	4.26352500	-0.78167000
C	5.14633300	4.66959500	0.24787800
C	2.66562200	2.70304600	2.04177700
C	3.12361300	1.66988000	0.99608400
H	5.01899100	1.02702000	-1.17019500
H	6.62703400	2.67797200	-2.09006300
H	6.68728900	4.98488200	-1.21259500
H	5.14395400	5.69425000	0.60408000
N	3.34600600	3.87784400	1.80002300
O	1.85812700	2.53079100	2.92769600
C	2.03132200	1.49307100	-0.08225800
C	0.68814300	0.90882200	0.37523300
O	-0.22139000	1.65713600	0.76575600
H	1.78478300	2.46692700	-0.51769700
H	2.47792300	0.88865600	-0.87180200
C	2.97421600	5.13407400	2.41966200
H	2.43090000	4.86671300	3.33047600
H	3.87811200	5.68080800	2.70716300
C	2.10448800	5.96747100	1.50119200
C	2.43915400	7.28410200	1.19480300
C	0.94849400	5.40318000	0.95083900
C	1.62903500	8.03965200	0.34807700
H	3.33874300	7.72252200	1.62069700
C	0.14256300	6.15719900	0.10522200
H	0.67558600	4.37532000	1.18778600
C	0.48060000	7.47645300	-0.19813300
H	1.89872300	9.06458300	0.11352600
H	-0.75632400	5.71591400	-0.31377300
H	-0.15128400	8.06265300	-0.85775700
C	3.09882100	-0.91054100	0.96866100
C	3.45145200	0.34547400	1.72458900
H	4.49668000	0.33078400	2.03783600
H	2.81579900	0.32759300	2.61974000
C	4.14523800	-1.89165500	0.59103900
C	5.44495600	-1.48741800	0.27050500
C	3.82785700	-3.25630200	0.57784000
C	6.40033700	-2.42957500	-0.10198800
H	5.71265700	-0.43551500	0.30326500
C	4.79004100	-4.19632100	0.22987100
H	2.82048000	-3.56085100	0.84823300
C	6.07548300	-3.78335100	-0.11975000
H	7.40041200	-2.10546700	-0.36986800
H	4.53487200	-5.25103500	0.22250900

H	6.82265200	-4.51659700	-0.40605000
N	1.88744500	-1.23807700	0.69210000
N	0.92403100	-0.33184900	1.19394000
S	-0.50270200	-1.22944200	1.53724300
O	-1.28440900	-0.47486700	2.50430200
O	-1.13116800	-1.68510500	0.29691800
C	0.19462200	-2.63901100	2.36063700
C	0.67156900	-2.48056200	3.65804700
C	0.23419500	-3.86466900	1.70810300
C	1.21572300	-3.58249100	4.30612600
H	0.60895900	-1.51197000	4.14485200
C	0.77340700	-4.95790000	2.37852400
H	-0.14353700	-3.94468900	0.69453300
C	1.27745100	-4.83075100	3.67682700
H	1.59444900	-3.47626300	5.31858300
H	0.80680500	-5.92561800	1.88562200
C	1.89907800	-6.00964200	4.37820500
H	1.50129800	-6.95217400	3.99619200
H	1.71970800	-5.96876100	5.45493900
H	2.98309100	-6.01793000	4.22379200
C	-2.74917200	0.41592900	-3.42890400
C	-2.98193500	1.70274800	-2.60101700
C	-2.20854600	1.49947300	-1.28060900
C	-1.40882800	-0.00382300	-2.92086000
C	0.08496800	0.20208400	-1.29378400
H	-3.49185500	-0.35592700	-3.19603700
H	-2.75485900	0.58335500	-4.50614100
H	-2.56466700	2.56101500	-3.13471100
H	-1.80319600	2.41959700	-0.86397600
N	-0.45996400	-0.80683700	-3.28720000
N	0.46336000	-0.65197500	-2.26722100
N	-1.10318600	0.63253600	-1.74384200
C	1.66278500	-1.39647200	-2.36380300
C	1.65014300	-2.76357800	-2.10523800
C	2.84294500	-0.80516900	-2.79804100
C	2.79155600	-3.52655200	-2.29483600
C	4.00307300	-1.55375700	-2.94645900
C	3.96550700	-2.92279700	-2.72952200
F	2.88607600	0.50025800	-3.05499500
F	5.13715000	-0.96173300	-3.31127600
F	5.05478200	-3.65522200	-2.91316800
F	2.78103300	-4.82906200	-2.02816900
F	0.54388800	-3.34531100	-1.66839600
H	-4.03704900	1.89526000	-2.40546900

C	-3.00439200	0.74421300	-0.21315600
H	-3.15178500	-0.29584700	-0.54200300
H	-2.41214100	0.72912400	0.70373600
O	-4.23594400	1.40795000	0.01258500
Si	-5.66836100	0.54333700	0.03475300
C	-7.00327200	1.83301700	0.40009600
C	-6.89073400	2.20809900	1.88813100
C	-6.79142400	3.10703100	-0.43147300
C	-8.39537000	1.24716900	0.13094500
H	-7.07895200	1.34799300	2.53820300
H	-5.89752100	2.60310600	2.12786600
H	-7.62889000	2.98402600	2.12991100
H	-6.93293500	2.93914200	-1.50389900
H	-7.51906800	3.87095600	-0.12694400
H	-5.78734200	3.51446800	-0.28227400
H	-9.16977700	1.97729600	0.40017200
H	-8.53253800	0.98463500	-0.92360800
H	-8.57276700	0.34561200	0.72936400
C	-5.55735700	-0.75152900	1.38630500
C	-6.47462100	-1.80953300	1.48996400
C	-4.53503800	-0.66840600	2.34189800
C	-6.37796500	-2.74588500	2.51570000
H	-7.26553900	-1.91609600	0.74905200
C	-4.42231700	-1.61358200	3.35916600
H	-3.80152500	0.13121900	2.29078900
C	-5.34734300	-2.64957700	3.44988800
H	-7.09777000	-3.55614800	2.58132800
H	-3.60497000	-1.53854700	4.06916800
H	-5.26299300	-3.38721000	4.24224900
C	-5.85979500	-0.36096500	-1.61413100
C	-6.34627700	0.27310900	-2.76911800
C	-5.41377100	-1.68693900	-1.74382100
C	-6.38115700	-0.37909100	-3.99871600
H	-6.70455100	1.29770400	-2.71554600
C	-5.44653900	-2.34789600	-2.97134600
H	-5.03260100	-2.21198700	-0.87102200
C	-5.92910900	-1.69373600	-4.10158600
H	-6.76295700	0.13539900	-4.87524300
H	-5.09177800	-3.37122500	-3.04401100
H	-5.95466700	-2.20532600	-5.05879500

PR+NHC

Total energy= -4208.364348

Zero-point correction= 1.032055 (Hartree/Particle)

Thermal correction to Energy= 1.101503
Thermal correction to Enthalpy= 1.102447
Thermal correction to Gibbs Free Energy= 0.923817
Sum of electronic and zero-point Energies= -4207.332292
Sum of electronic and thermal Energies= -4207.262845
Sum of electronic and thermal Enthalpies= -4207.261900
Sum of electronic and thermal Free Energies= -4207.440530

C	-1.17378200	-4.31107700	-2.81129000
C	-2.04832100	-3.02759200	-2.89728400
C	-1.83935100	-2.24708800	-1.57211800
C	-0.16506200	-3.91232600	-1.78435100
C	0.29539300	-2.42707100	-0.15167400
H	-1.74697800	-5.17493700	-2.46085700
H	-0.71338900	-4.57283300	-3.76412900
H	-1.69851400	-2.41331700	-3.72955800
H	-1.65881200	-1.18357900	-1.75415800
N	1.01797200	-4.27101900	-1.40393600
N	1.27404400	-3.34240500	-0.39945000
N	-0.61359500	-2.83984100	-1.06001000
C	2.57426800	-3.21564800	0.12036900
C	2.77302400	-2.93482400	1.47171300
C	3.69062100	-3.25000600	-0.71756600
C	4.04380400	-2.70159800	1.97512200
C	4.96723000	-3.04949600	-0.20981200
C	5.14731400	-2.79093000	1.14014200
F	3.55532000	-3.44158500	-2.02105700
F	6.01853600	-3.06286900	-1.02307200
F	6.36477200	-2.57831100	1.62024200
F	4.20320800	-2.37850600	3.25980900
F	1.74096300	-2.84792000	2.31154000
H	-3.10565700	-3.24672000	-3.05886400
C	-2.96310100	-2.39187100	-0.55929300
H	-3.21235700	-3.45311500	-0.41015200
H	-2.61428800	-1.98898200	0.40337100
O	-4.08448500	-1.68445300	-1.05177300
Si	-5.21779700	-1.04793700	0.00549400
C	-6.59326300	-0.38978900	-1.11222200
C	-5.98334100	0.65117500	-2.06316500
C	-7.20019300	-1.53631500	-1.93094800
C	-7.68688400	0.26773300	-0.26064000
H	-5.52218300	1.47759000	-1.51048300
H	-5.21665100	0.20220000	-2.70287200
H	-6.76411500	1.07078800	-2.71119300
H	-7.68904200	-2.27502700	-1.28682700

H	-7.95742900	-1.14410500	-2.62241800
H	-6.43668800	-2.05026000	-2.52505100
H	-8.50359900	0.62020900	-0.90400500
H	-8.11563000	-0.43562100	0.46321600
H	-7.30176100	1.13361600	0.28854000
C	-4.42221300	0.35067400	0.97258100
C	-5.05950000	0.98714700	2.05109500
C	-3.17431200	0.84852300	0.56458300
C	-4.46676300	2.06162300	2.70984900
H	-6.04079400	0.65104600	2.38008800
C	-2.58233500	1.92852200	1.21609500
H	-2.65168200	0.40340900	-0.28027000
C	-3.22316300	2.53175700	2.29440000
H	-4.97819800	2.53476300	3.54258800
H	-1.62934200	2.31203000	0.86070200
H	-2.75442500	3.37240200	2.79679200
C	-5.77887200	-2.46742200	1.10461800
C	-6.00288600	-3.71333900	0.49325600
C	-5.96478000	-2.37802400	2.49025500
C	-6.41612900	-4.81835900	1.23097200
H	-5.83989700	-3.82080700	-0.57780200
C	-6.38242200	-3.47967100	3.23471700
H	-5.76288200	-1.44316300	3.00505200
C	-6.61266600	-4.69970500	2.60538000
H	-6.58072900	-5.77135100	0.73778000
H	-6.51994600	-3.38690800	4.30759500
H	-6.93405800	-5.55940900	3.18515500
C	0.47001800	3.44335200	2.69483400
C	0.89349700	2.14160100	2.99911000
C	0.59068700	1.58461200	4.22689500
C	-0.12490600	2.34764400	5.15753800
C	-0.53205100	3.64060600	4.84368300
C	-0.24262400	4.21302800	3.60034100
C	1.58817100	2.75592600	0.82437300
C	1.57454300	1.55390100	1.78399100
H	0.89544500	0.56907200	4.46514800
H	-0.36725900	1.92583500	6.12662300
H	-1.08917800	4.21912900	5.57344600
H	-0.57029700	5.21839400	3.35744900
N	0.90106200	3.78789400	1.40502800
O	2.11520400	2.79560300	-0.27263100
C	0.72915900	0.39832700	1.20385100
C	0.82366500	0.30685900	-0.29070200
O	-0.11845000	0.50773100	-1.02916900

H	1.05075600	-0.55581400	1.63297900
H	-0.33068800	0.52737500	1.42678800
C	0.54041400	4.98024300	0.64938800
H	1.34893900	5.13987600	-0.06856500
H	0.50947400	5.83362900	1.33218500
C	-0.78159000	4.78760500	-0.06155900
C	-1.94103400	5.40571100	0.40346900
C	-0.85626500	3.91567300	-1.15564500
C	-3.16767400	5.16055400	-0.21224100
H	-1.88656800	6.08403800	1.25196400
C	-2.08329000	3.66474200	-1.76132300
H	0.04131600	3.41316700	-1.51352300
C	-3.23994600	4.28780200	-1.29291600
H	-4.06589600	5.64225700	0.16070500
H	-2.13351100	2.96876400	-2.59313000
H	-4.19614000	4.08664800	-1.76544100
C	3.72480700	0.43658000	0.85348800
C	2.99713400	1.06466100	2.02873100
H	3.61319600	1.89310200	2.39317800
H	2.96944600	0.32009000	2.83774100
C	5.21082000	0.30937200	1.02367300
C	5.82103000	0.42297900	2.27726100
C	6.01739100	0.05692900	-0.09695100
C	7.20425600	0.30906500	2.40658800
H	5.23029500	0.59369100	3.17110400
C	7.39284200	-0.06404800	0.03775700
H	5.54216500	-0.05154000	-1.06735700
C	7.99483500	0.07048000	1.28957400
H	7.65803100	0.40133600	3.38808600
H	7.99961900	-0.26270300	-0.83998600
H	9.07163900	-0.01939000	1.39109100
N	3.31026800	-0.02348600	-0.26742700
N	2.08036000	-0.01826200	-0.82394200
S	2.13393500	-0.33895800	-2.54474900
O	1.14443100	-1.36167700	-2.83618900
O	3.53433700	-0.55924000	-2.84531600
C	1.62525300	1.20188000	-3.25321900
C	0.38446600	1.29039200	-3.87550400
C	2.48194200	2.29154900	-3.15883900
C	0.00030600	2.50883600	-4.41737000
H	-0.25931200	0.41860300	-3.91289000
C	2.06850700	3.50871600	-3.68986800
H	3.44043300	2.19377700	-2.65958600
C	0.82479900	3.63589700	-4.31427300

H	-0.96276300	2.59725900	-4.91296800
H	2.71856200	4.37483500	-3.60979100
C	0.34581800	4.96912200	-4.82245900
H	-0.36742400	5.40075500	-4.11154600
H	1.17220100	5.67261900	-4.94099600
H	-0.16525200	4.86699200	-5.78300400

PS+NHC

Total energy= -4208.362730

Zero-point correction= 1.033348 (Hartree/Particle)

Thermal correction to Energy= 1.102727

Thermal correction to Enthalpy= 1.103671

Thermal correction to Gibbs Free Energy= 0.925043

Sum of electronic and zero-point Energies= -4207.329383

Sum of electronic and thermal Energies= -4207.260003

Sum of electronic and thermal Enthalpies= -4207.259059

Sum of electronic and thermal Free Energies= -4207.437688

C	1.63351100	5.15934800	0.21381100
C	2.41160700	4.02846900	-0.07312800
C	3.22022900	4.00848200	-1.19637600
C	3.28593100	5.15256000	-2.00038100
C	2.51745900	6.27234800	-1.69515000
C	1.66667100	6.29065700	-0.58569300
C	1.12096800	3.68530800	1.88387900
C	2.00859800	2.93413800	0.88353600
H	3.77156800	3.11134800	-1.46785900
H	3.92274000	5.15777200	-2.87802200
H	2.56568400	7.14674700	-2.33590800
H	1.05279600	7.15781700	-0.36730800
N	0.87559600	4.93980100	1.37675200
O	0.64940500	3.21950600	2.90139700
C	1.04990800	2.00518700	0.10368200
C	0.51620700	0.86499900	0.93050900
O	-0.63295200	0.76186900	1.29217600
H	0.18098500	2.56234700	-0.25764000
H	1.56885700	1.58740400	-0.76135100
C	-0.32692700	5.67751600	1.74926500
H	-0.51564100	5.43985800	2.79891800
H	-0.13210400	6.75029000	1.66856200
C	-1.48882700	5.25228600	0.87311700
C	-2.04323100	6.11847600	-0.06688100
C	-1.96505000	3.93808000	0.96000700
C	-3.06083500	5.68135400	-0.91466800
H	-1.67649500	7.13959400	-0.14012800

C	-2.97106300	3.49519800	0.10642100
H	-1.54024100	3.25150200	1.68844100
C	-3.52044300	4.37023000	-0.83272100
H	-3.48532200	6.36434100	-1.64373000
H	-3.32388400	2.46788200	0.17546000
H	-4.30609500	4.02649200	-1.49944200
C	3.51785000	0.85684800	0.92737300
C	3.06858200	2.11314800	1.63236300
H	3.92354900	2.73405400	1.90182900
H	2.58550800	1.78359500	2.56452700
C	4.93871100	0.69387100	0.53320000
C	5.73374000	1.79623300	0.20652900
C	5.51200300	-0.58560300	0.54840700
C	7.07258500	1.62183100	-0.13167700
H	5.30869500	2.79568700	0.20537800
C	6.85223600	-0.75294300	0.22608600
H	4.89450900	-1.43591700	0.82721300
C	7.63392800	0.34908100	-0.12100700
H	7.67647300	2.48315600	-0.39708600
H	7.28937200	-1.74569700	0.24620100
H	8.68072600	0.21402300	-0.37328100
N	2.75784300	-0.16310600	0.73210400
N	1.47529700	-0.11237900	1.27870300
S	0.86297200	-1.70575900	1.62942600
O	0.04179100	-1.58065500	2.81847400
O	0.32620900	-2.29716500	0.41370100
C	2.38045600	-2.52713200	2.04104400
C	3.08942500	-2.12522100	3.17135000
C	2.82447600	-3.55718600	1.22444100
C	4.28685200	-2.76185900	3.46368700
H	2.70993800	-1.32431600	3.79924000
C	4.02842200	-4.18511400	1.53618500
H	2.23213200	-3.86347300	0.36854400
C	4.77654000	-3.79157700	2.64778500
H	4.85657400	-2.45804800	4.33714300
H	4.38869000	-4.98723200	0.89959200
C	6.09861100	-4.44022400	2.96146600
H	6.92515400	-3.78234300	2.67296300
H	6.21592200	-5.38290400	2.42405000
H	6.19554400	-4.63737400	4.03193900
C	-2.67653000	-1.73350500	-3.59253500
C	-3.36540800	-0.41621200	-3.14135400
C	-2.51009400	0.12463100	-1.97178100
C	-1.26678500	-1.50222700	-3.14707900

C	0.05268400	-0.24550700	-1.80692300
H	-3.09302200	-2.60168500	-3.07069900
H	-2.76078100	-1.91288600	-4.66485900
H	-3.35326300	0.30205100	-3.96506800
H	-2.46729800	1.21658800	-1.93994700
N	-0.10238300	-2.04454900	-3.30398700
N	0.68366200	-1.24585700	-2.47701500
N	-1.19917900	-0.43276500	-2.29000500
C	2.04205000	-1.56434300	-2.32481900
C	2.43227500	-2.86840900	-2.03664100
C	3.03351500	-0.59335500	-2.45439900
C	3.77247300	-3.19946700	-1.90407700
C	4.37626800	-0.91548800	-2.32424500
C	4.74788500	-2.22745300	-2.06460400
F	2.71333200	0.67680100	-2.69700100
F	5.30280900	0.02853800	-2.45989000
F	6.03114800	-2.55298100	-1.94567900
F	4.11989600	-4.45024800	-1.59986400
F	1.52737500	-3.82056600	-1.83900800
H	-4.40255900	-0.57418000	-2.83651200
C	-2.92181100	-0.40908000	-0.60492100
H	-3.07112900	-1.49810400	-0.67984500
H	-2.10727700	-0.23143600	0.10133800
O	-4.09186900	0.25865200	-0.17085200
Si	-5.40482200	-0.58856300	0.43319900
C	-6.57320500	0.74956800	1.07888100
C	-5.94914700	1.32995000	2.36039800
C	-6.73167000	1.89510100	0.06803200
C	-7.93946400	0.13774900	1.41661500
H	-5.84344100	0.57070400	3.14142300
H	-4.95825000	1.75611200	2.16635900
H	-6.58813400	2.13285700	2.75036500
H	-7.17497800	1.57125900	-0.87857300
H	-7.38651500	2.66934500	0.48876800
H	-5.76499900	2.35766400	-0.15427400
H	-8.59729100	0.90209900	1.85008800
H	-8.43913500	-0.27196800	0.53221900
H	-7.84301400	-0.66920100	2.15252700
C	-4.81018900	-1.71993300	1.80275900
C	-5.58731400	-2.81040600	2.22295700
C	-3.59044700	-1.48366600	2.45554900
C	-5.16844300	-3.63169900	3.26602500
H	-6.52671800	-3.02982700	1.71768600
C	-3.15913300	-2.31217300	3.48952300

H	-2.95688200	-0.65158200	2.15381300
C	-3.95163200	-3.38229800	3.89799800
H	-5.78334000	-4.47027900	3.57838600
H	-2.19790700	-2.12485300	3.95620000
H	-3.61739100	-4.02851900	4.70408400
C	-6.08398200	-1.67194300	-0.95491400
C	-7.05882100	-1.23151900	-1.86332000
C	-5.48786500	-2.92141600	-1.19906100
C	-7.41551500	-1.99375300	-2.97332600
H	-7.55000700	-0.27503200	-1.71046000
C	-5.83365500	-3.68625600	-2.31180500
H	-4.74680300	-3.30857600	-0.50258000
C	-6.79595300	-3.21983000	-3.20400700
H	-8.17412700	-1.62975800	-3.65925600
H	-5.35590100	-4.64710300	-2.47800200
H	-7.06837000	-3.81296100	-4.07140500

PR

Total energy= -2098.262597

Zero-point correction= 0.532900 (Hartree/Particle)

Thermal correction to Energy= 0.566467

Thermal correction to Enthalpy= 0.567412

Thermal correction to Gibbs Free Energy= 0.461155

Sum of electronic and zero-point Energies= -2097.729697

Sum of electronic and thermal Energies= -2097.696130

Sum of electronic and thermal Enthalpies= -2097.695186

Sum of electronic and thermal Free Energies= -2097.801442

C	3.50802800	0.68888500	-0.71135000
C	2.57629500	0.96478500	-1.71869700
C	3.00150100	1.42332300	-2.95160200
C	4.37341000	1.59587700	-3.16919800
C	5.28784000	1.30929900	-2.15953400
C	4.87033800	0.84814600	-0.90711400
C	1.48899400	0.14334000	0.21954100
C	1.18878800	0.70422400	-1.18108700
H	2.28618100	1.64405500	-3.73957800
H	4.72600100	1.95049400	-4.13126000
H	6.34871900	1.44128600	-2.34504800
H	5.58583200	0.60941900	-0.12777000
N	2.83947200	0.25230300	0.44410200
O	0.67301400	-0.32583100	0.98857700
C	0.44150100	-0.34360800	-2.00605900
C	-1.00405800	-0.66349400	-1.67877500
O	-1.42531000	-1.78718000	-1.77964900

H	0.41158600	0.00578800	-3.04696500
C	3.48209800	-0.21231700	1.66074800
H	2.68309000	-0.29434200	2.40325700
H	4.18907100	0.55244300	1.99955700
C	4.18167400	-1.54154200	1.47509800
C	5.53699500	-1.68487200	1.76301500
C	3.45710300	-2.64369200	1.01398700
C	6.16803300	-2.91626800	1.59257000
H	6.10323900	-0.82959600	2.12492900
C	4.08569400	-3.87144400	0.84093500
H	2.39562200	-2.53359900	0.80317700
C	5.44350400	-4.00943500	1.12932600
H	7.22472900	-3.01808400	1.81799400
H	3.51619500	-4.72427100	0.48568100
H	5.93231200	-4.96871600	0.99351500
C	-0.78646700	1.93077600	-0.11697800
C	0.37771000	2.01420600	-1.07044500
H	1.03671000	2.83365700	-0.78055700
H	-0.02412000	2.24903800	-2.06496300
C	-0.77421400	2.73538400	1.13187700
C	0.42621300	3.03152000	1.78312100
C	-1.98078200	3.18632100	1.67898800
C	0.42029800	3.76054200	2.96898500
H	1.37259600	2.67900400	1.38070100
C	-1.98253100	3.92397400	2.85561500
H	-2.90594900	2.95926100	1.15913400
C	-0.78230300	4.21052800	3.50529800
H	1.35674200	3.97597000	3.47292400
H	-2.92144100	4.28144100	3.26579200
H	-0.78548200	4.78663200	4.42488500
N	-1.82992500	1.22139400	-0.31117800
N	-1.90235800	0.43878000	-1.47483900
S	-3.57387900	0.12384600	-1.81227200
O	-3.58734200	-0.54036100	-3.10156200
O	-4.21080800	1.41466600	-1.62992100
C	-4.15423400	-0.96851100	-0.54946300
C	-4.21816600	-2.33488600	-0.80381100
C	-4.55462100	-0.42600700	0.66879600
C	-4.70144900	-3.17225600	0.19326300
H	-3.89002800	-2.71870700	-1.76293600
C	-5.02522400	-1.28425300	1.65452300
H	-4.50214900	0.64523000	0.82724000
C	-5.10368200	-2.66255400	1.43211400
H	-4.76737300	-4.24049900	0.00887900

H	-5.34395300	-0.87861600	2.61023900
C	-5.58938600	-3.58515100	2.51853900
H	-6.32589600	-3.09186700	3.15671000
H	-6.04077200	-4.48717000	2.09982300
H	-4.75440900	-3.89586700	3.15496600
H	0.97487000	-1.29663800	-1.99348100

PS

Total energy= -2098.266475
Zero-point correction= 0.533565 (Hartree/Particle)
Thermal correction to Energy= 0.566946
Thermal correction to Enthalpy= 0.567890
Thermal correction to Gibbs Free Energy= 0.464278
Sum of electronic and zero-point Energies= -2097.732910
Sum of electronic and thermal Energies= -2097.699529
Sum of electronic and thermal Enthalpies= -2097.698584
Sum of electronic and thermal Free Energies= -2097.802197

C	-3.27219700	1.43915800	0.29054600
C	-2.00437300	1.51328000	-0.29978000
C	-1.71164100	2.53885000	-1.18212300
C	-2.69017300	3.50478100	-1.44427800
C	-3.94271900	3.41903000	-0.84275800
C	-4.25954600	2.37690400	0.03336200
C	-2.17388500	-0.40122400	1.09317300
C	-1.19432700	0.32036300	0.14898500
H	-0.73767100	2.59839900	-1.66205400
H	-2.47374900	4.31813000	-2.12792500
H	-4.69524000	4.16935900	-1.06228900
H	-5.24497800	2.29657100	0.47886300
N	-3.34357100	0.31541400	1.12633000
O	-1.94508500	-1.42983800	1.69592600
C	-0.88658400	-0.60422200	-1.04605000
C	0.01992600	-1.77367100	-0.72739200
O	-0.29438500	-2.92955200	-0.86497700
H	-1.80940000	-1.02154600	-1.45374600
H	-0.40091700	-0.01038900	-1.82930700
C	-4.53191700	-0.13275300	1.83101700
H	-4.18557900	-0.87755800	2.55300300
H	-4.95702300	0.71158700	2.38379900
C	-5.55596100	-0.72963500	0.88990600
C	-6.84376600	-0.20672200	0.80051200
C	-5.20073600	-1.82216900	0.09371300
C	-7.77213700	-0.76511800	-0.07717700

H	-7.12437900	0.64103500	1.42141600
C	-6.12473900	-2.37845700	-0.78308700
H	-4.19990400	-2.24129600	0.17504500
C	-7.41243600	-1.84907600	-0.87116000
H	-8.77249000	-0.34931800	-0.14253300
H	-5.84297400	-3.22907000	-1.39511700
H	-8.13249100	-2.28307600	-1.55729000
C	1.30820000	0.82197600	0.10022500
C	0.08593000	0.63002400	0.95776200
H	-0.07921300	1.48163000	1.61860400
H	0.28146600	-0.25318200	1.58174200
C	1.98020600	2.14020800	-0.01287900
C	1.30544800	3.32975300	0.27851500
C	3.33060200	2.19291300	-0.38886800
C	1.96333600	4.55336000	0.17986200
H	0.25891000	3.31196600	0.56663400
C	3.98405200	3.41369100	-0.47653500
H	3.85448100	1.26437000	-0.59612400
C	3.30171900	4.59848800	-0.19581300
H	1.42682900	5.47017100	0.40043700
H	5.03130200	3.44312500	-0.76036200
H	3.81499000	5.55208800	-0.26625300
N	1.86870300	-0.15434500	-0.52004200
N	1.32591800	-1.42406100	-0.31586900
S	2.52434600	-2.68241600	-0.52356900
O	2.23140100	-3.69321700	0.47221800
O	2.61422300	-3.01444500	-1.93484800
C	3.98740400	-1.80284600	-0.04941600
C	4.21533200	-1.54696500	1.30017500
C	4.87975700	-1.40339900	-1.03508000
C	5.36358400	-0.85461600	1.65869700
H	3.50665800	-1.89024000	2.04753500
C	6.03110000	-0.72126000	-0.65322000
H	4.66765600	-1.62529400	-2.07531000
C	6.28246000	-0.43024400	0.69025900
H	5.55771500	-0.64339200	2.70636200
H	6.74367100	-0.40745500	-1.41040600
C	7.51125400	0.33753400	1.10004800
H	7.24014300	1.34441200	1.43312100
H	8.21542200	0.43300700	0.27161200
H	8.02162100	-0.15566500	1.93131800