Supporting Information

A mechanistic investigation into N-heterocyclic carbene (NHC) catalyzed umpolung of ketones and benzonitriles: Is cyano group better than a classical carbonyl group for the addition of NHC?

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1. The geometry structures of two isomers of NHC catalyst

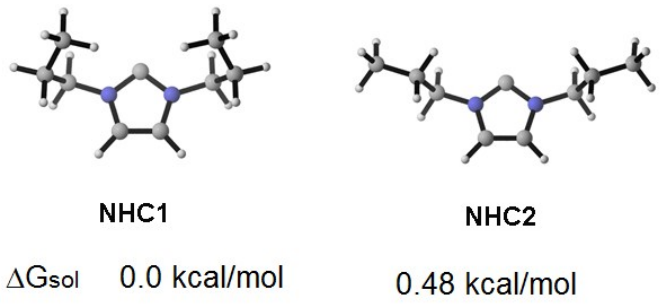

Fig. S1 The structures and relative free energies of two NHC isomers.

2. NHC-catalyzed previous activiton Mode I

Shi and Li et al. proposed that NHC firstly attacks the carbonyl carbon of **1** to form the umpolung of cyclohexanone, then followed by nuclephilic addition, cyclisation and subsequent Dimroth rearrangement. We calculated this mechanism and found that it is impossible under the title reaction conditions (Scheme 3). As depicted in Fig. S2, the nucleophilic attack of C1 of NHC to the carbonyl carbon C2 of **1** via **TS1a** with the energy barrier of 13.4 kcal/mol, leads to the zwitterionic intermediate **4a**. This is the widely accepted umpolung type of computational studies. And the generation of complex **4a** is endothermic by 6.0 kcal/mol in solution.

Then followed by the nucleophilic addition of oxygen of **4a** to cyano carbon C3 of **2**, two isomers transition states can be developed when the free rotation of the C-C single bond between phenyl and cyano group, denoted as **TS2a*1*** and **TS2a*2*,** respectively. The addition of **4a** to the cyano carbon C3 of **2** from the same side of amidogen via **TS2a*1*** is found to be a preferred C-O bond formation step, the activation energy barrier is 18.1 kcal/mol, leading to a five-membered ring intermediate **6a*1***. In addition, the addition of **4a** to cyano carbon C3 of **2** from the opposite side of amidogen via **TS2a*2*** (21.1 kcal/mol) generates the isomeric intermediate **6a*2***, which is 3.0 kcal/mol higher in energy than that of transition state **TS2a*1***. It is responsible for the strong hydrogen-bond interaction between $-NH_2$ of **2** and the O atom of **1** (1.74 Å) in **TS2a*1***, while absence in the **TS2a*2***.

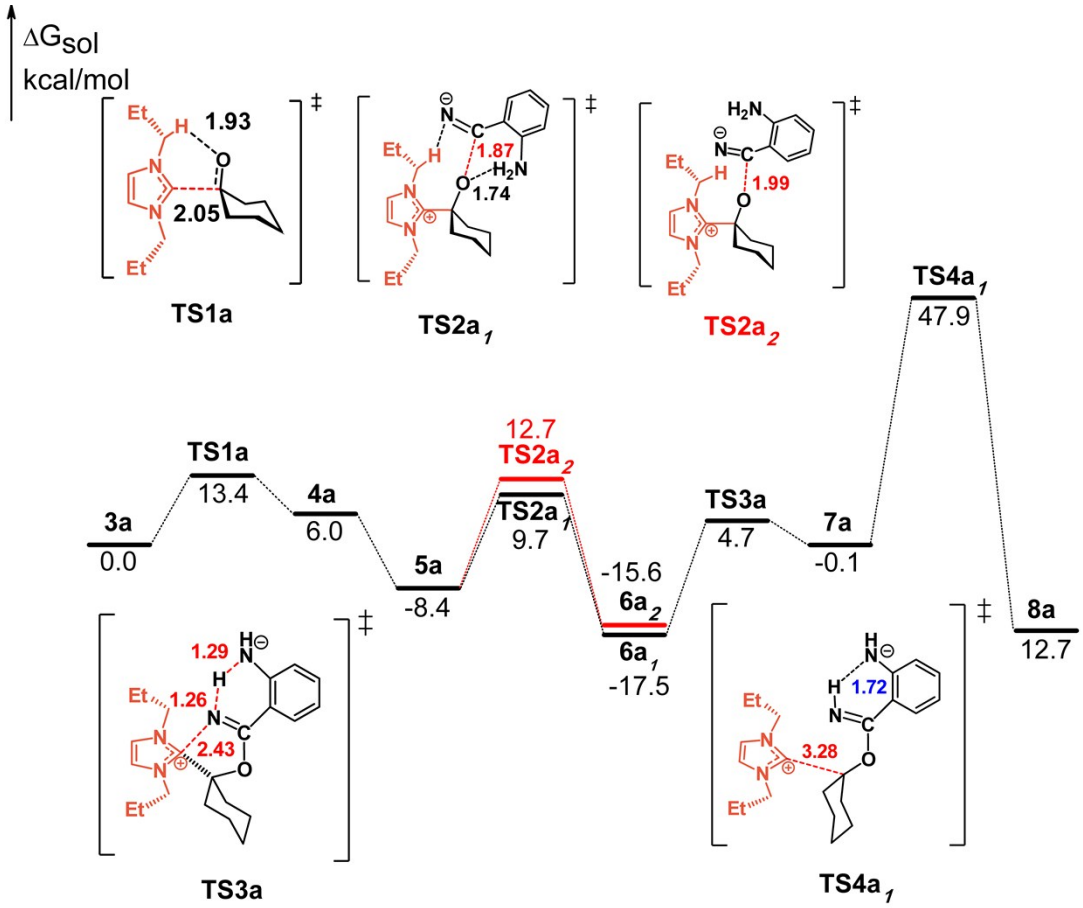

Fig. S2 Gibbs free energy profile (in kcal/mol) for previous mechanism of NHC catalyzed activation Mode I obtained at the PBE0-D3/6-311+G(2d, 2p) level in solvent cyclohexanone.

However, these two types of nucleophilic addition of **2** to zwitterionic intermediate **4a** lead to two five-member ring intermediates **6a*1*** and **6a*2***, rather than the zwitterionic intermediate **X** proposed by Shi et al (Scheme 3). This is due to 1) the unstable geometric structures of intermediate **4a** and transition states **TS2a*1*** and **TS2a*2***, 2) the strong electronic interactions between positive charge of C1 on NHC and negative charge of N1 on cyano group (Fig. S4), and strong C–H···N⁻ interactions between the NHC and **2** extensively promote the five-membered ring formation.

Afterwards, the hydrogen migration from the amino group to *N*-atom on cyano group (**TS3a**, 22.2 kcal/mol) occurs to promote the ring opening of $\mathbf{6a_1}$ (or the $\mathbf{6a_1}$ obtained by conversion of intermediate $\mathbf{6a_2}$) to afford **7a**. Subsequently, the elimination of NHC occurs, herein we explored the NHC elimination transition states $\mathbf{TS4a_1}$, wherein the NHC removal occurs before C3-C(aryl) rotation with the energy barrier of 32.0 kcal/mol. Then the transition states $\mathbf{TS4a_1}$ can lead to the formation of

zwitterionic intermediate **8a**, but the energy barriers of **TS4a$_1$** is too high to proceed under this reaction conditions, so these NHC catalyzed pathways in the Mode **I** could be excluded.

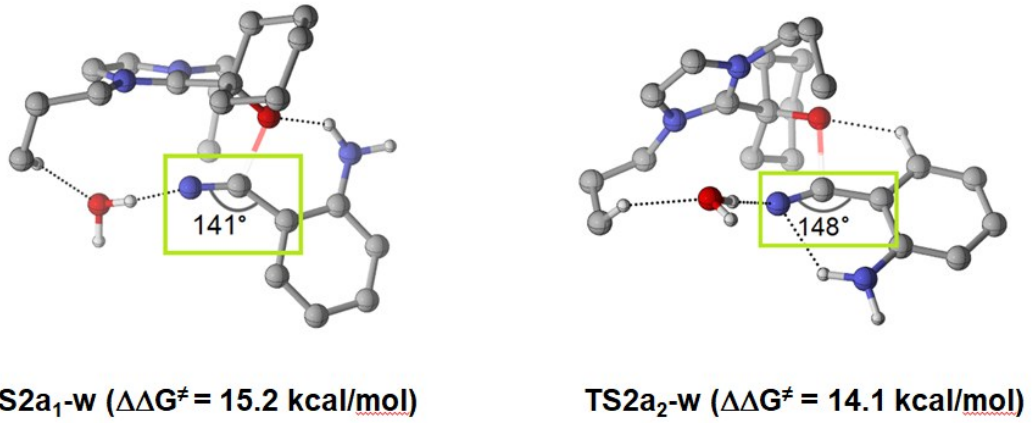

Fig. S3 Optimized structures and ΔΔG$^{\neq}$ values of **TS2a$_1$–w** and **TS2a$_2$–w**.

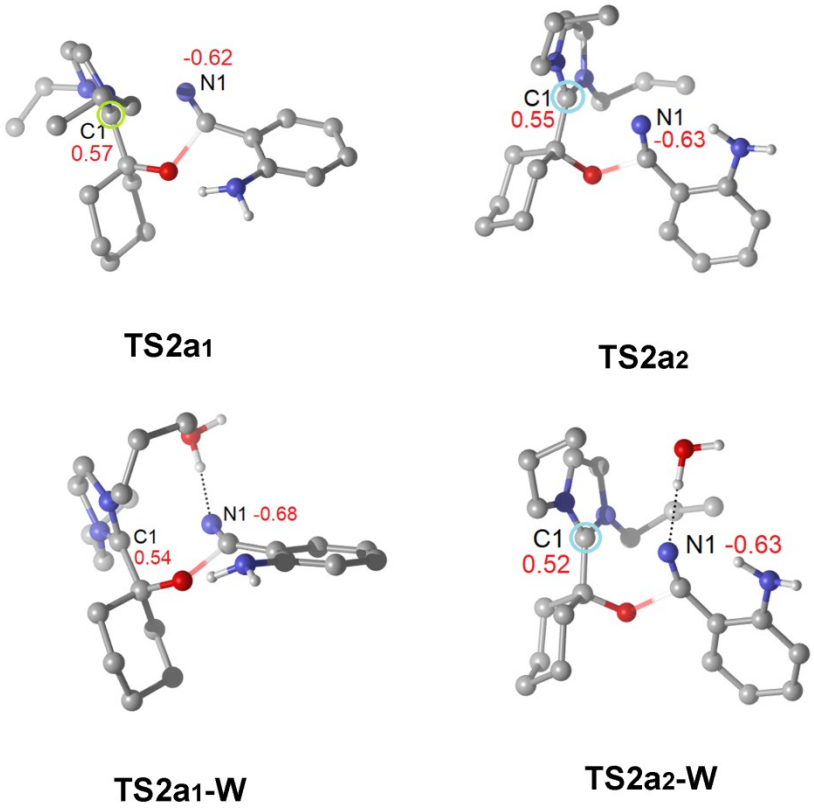

Fig. S4 Optimized structures of transition states **TS2a$_1$/TS2a$_1$-W** and **TS2a$_2$/TS2a$_2$-W**. The values in red are corresponding NPA charge of C1 and N1 atoms.

3. The effect of water on the activation barrier of the rate-determining step

Table S1 The comparation of the activation barriers of the (direct or 1-3 W assisted) rate-determining step of C-N bond formation. ($\Delta\Delta G_{sol}$, in kcal/mol).

TSs	Water-assisted			direct
number	1	2	3	
ΔΔG (kcal/mol)	14.6	15.3	14.9	16.5

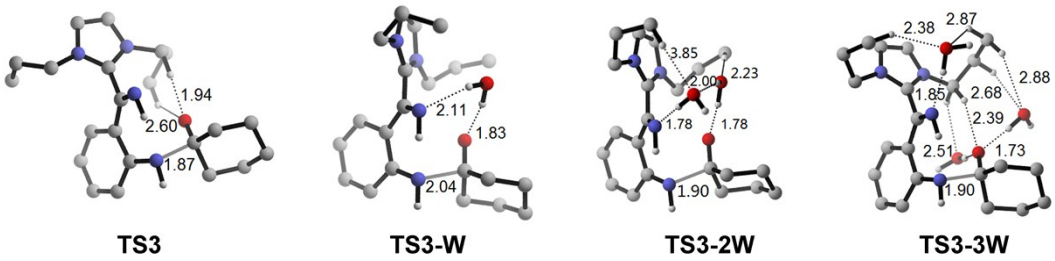

Fig. S5 Optimized geometries of key transition states assisted by 1-3 molecules of water assisted for C-N bond formation process. Distances are in Å.

We have investigated the effect of 1-3 water molecules on the activation barrier of the rate-determining step transition state for C-N bond formation. The inclusion of a larger number of water molecules should obviously have to bear higher entropic costs and hence we have not considered systems beyond three water molecules. The calculation results shown that activation barriers of 1-3 water molecules assisted transition states are favorable than only NHC-catalyzed case by 1.9, 1.2, and 1.6 kcal/mol, and single water-assisted transition state **TS3-W** is the most favorable one. Therefore, we only present the most favorable Path 1-W and the feasible Path 1 to illustrate the role of water in the reaction Mode II (Table S1 and Fig. S5).

4. The optimized geometries of key transition states in Path 1 and Path 1-W

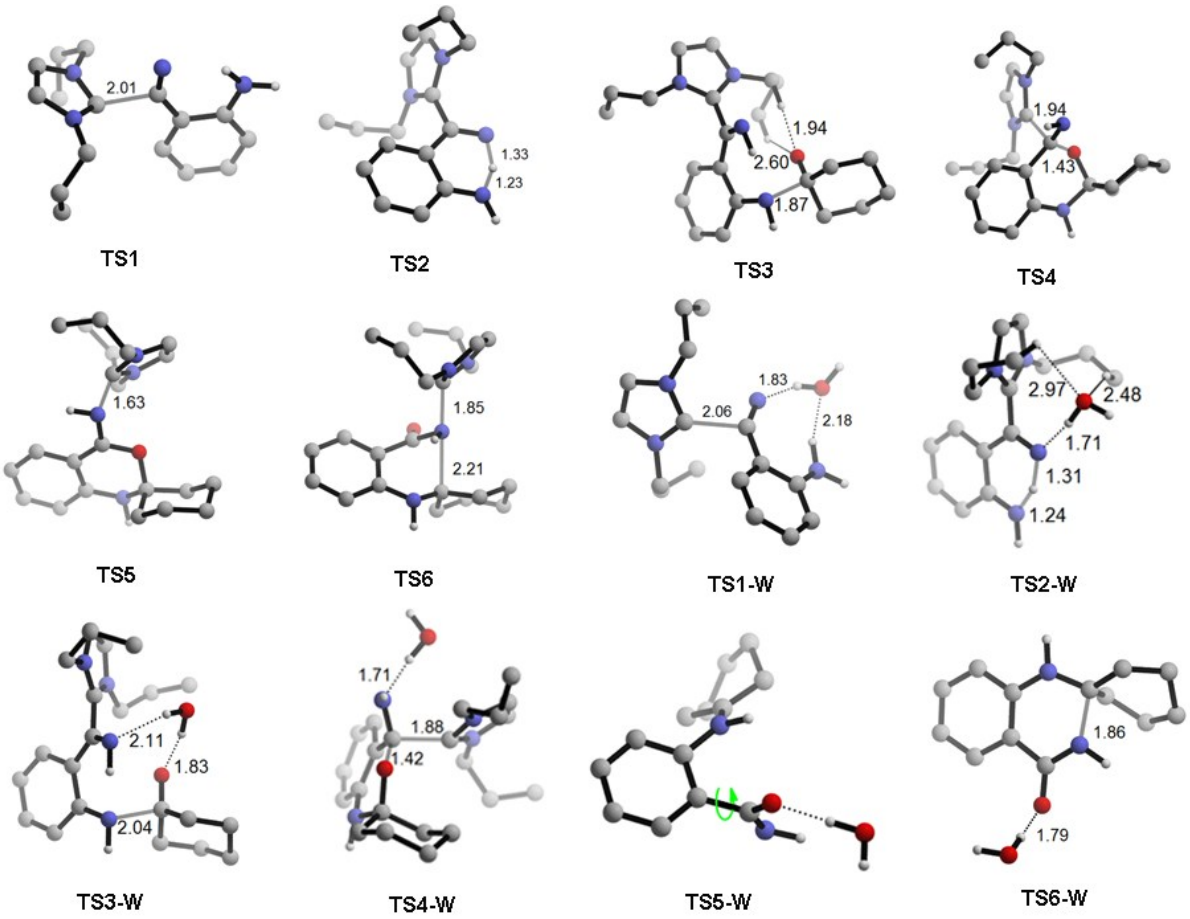

Fig. S6 Optimized geometries of key transition states in Path 1 and Path 1-W. Distances are in Å.

5. Overlay of the free energy profiles for the most favorble pathway 1-W in solvent phase with B3LYP-D3, M06-2X, and PBE0-D3 used

DFT methods B3LYP-D3 and M06-2X with the same basis set 6-311+G(2d, 2p) were employed to calculate the solvation single point energies of the most favored Path 1-W for comparison (Fig. S7). Our computational results indicated that B3LYP-D3, M06-2X, and PBE0-D3 functionals provide the same trend in the relative energies of transition states and intermediates. Additionally, the relative energies of transition states and intermediates on the potential energy surfaces in Path 1-W at the PBE0-

D3/6-311+G** level are much lower than those at the B3LYP-D3 (M06-2X)/6-311+G** cases except the regeneration of NHC.

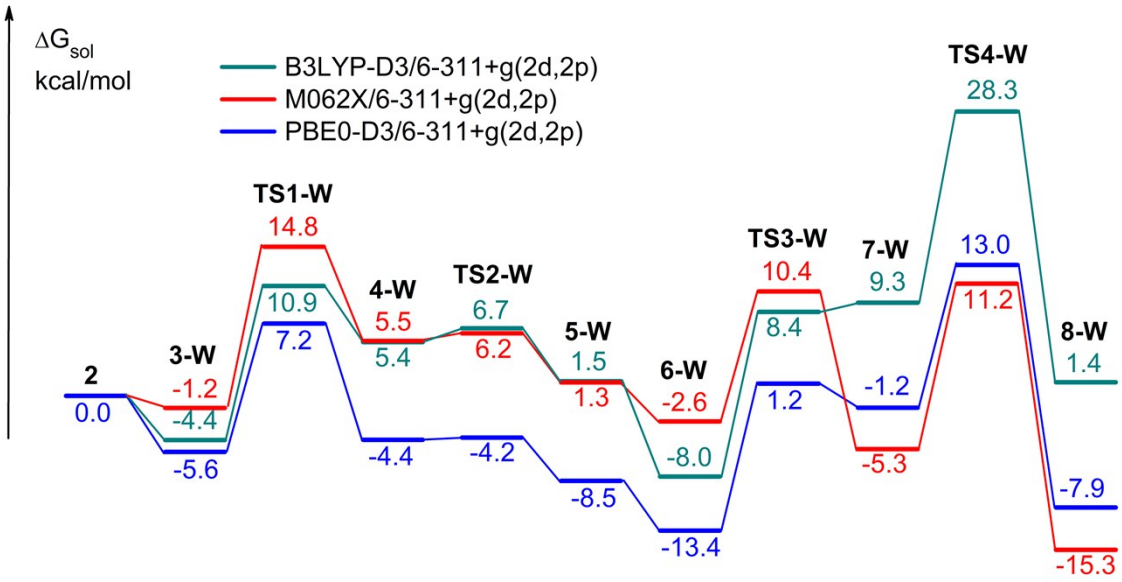

Fig. S7 Free energy profile of the most favorable pathway 1-W in the solution phase with B3LYP-D3, M06-2X and PBE0-D3 used, free energies are given in kcal/mol.

6. Electrostaic potential maps of transition states TS3 and TS3-W

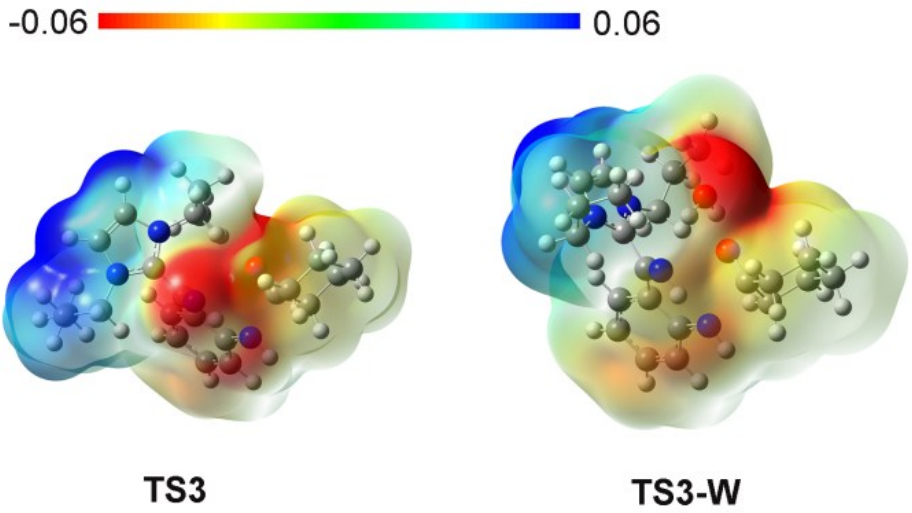

Fig. S8 Electrostatic potential (ESP) maps of **TS3** and **TS3-W**.

The electrostatic potentials on the structures of **TS3** and **TS3-W** are illustrated in Fig. S8. The NHC portion of the two structures are both completely positive, and the

negatively charge is located on the –NH group of substrates **2** in **TS3**, while in the **TS3-W**, the negatively charge is located on the water. Therefore, water is predicted to transfer and capture the negative charge of substrates **2** and **1** and stablize the structure of transition state **TS3-W**.

7. The effect of substituents on NHC catalytic activity of two types of carbons (carbonyl and cyano)

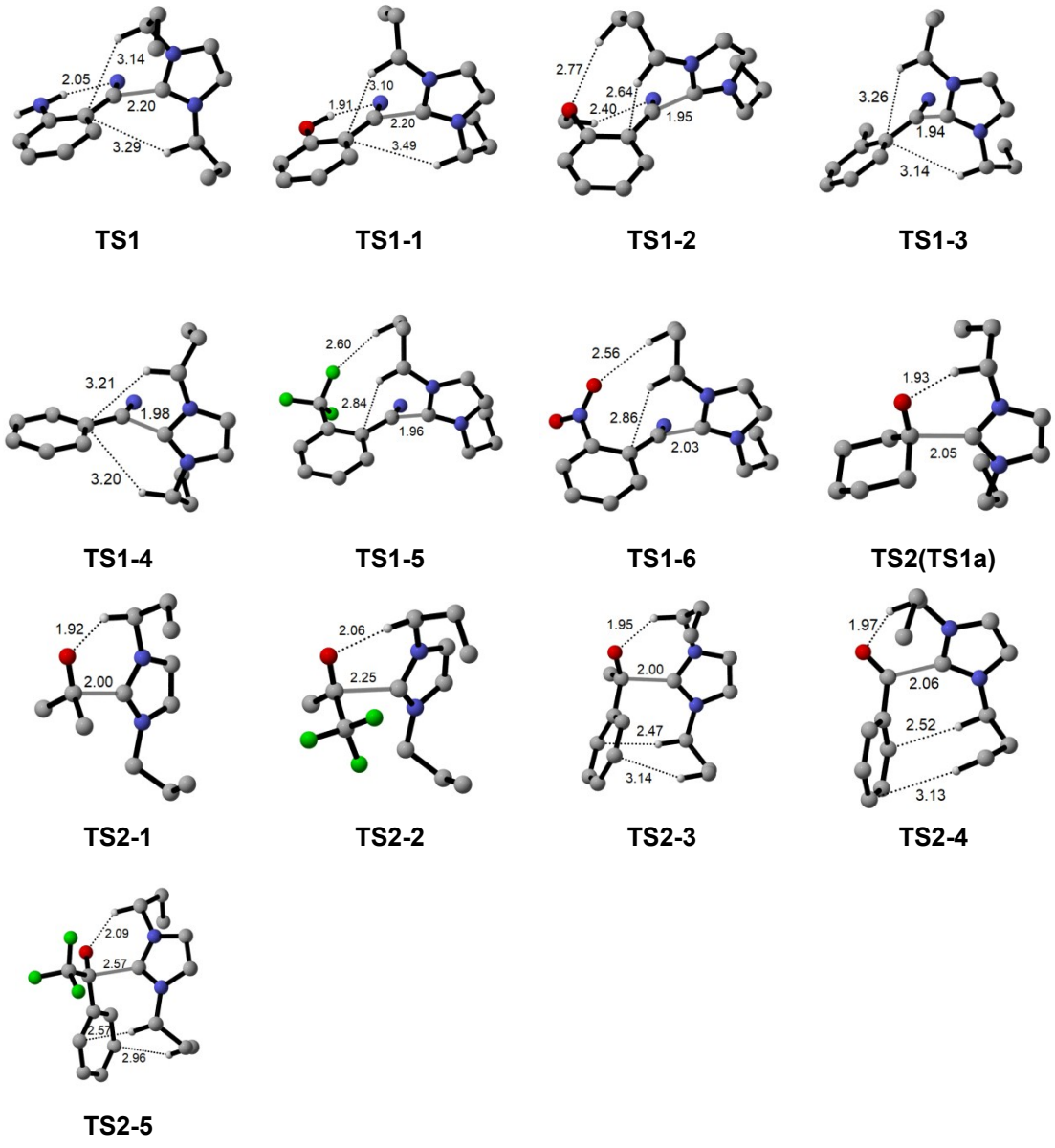

Fig. S9 The corresponding geometry structures of transition states for the NHC activation

different derivatives of nitriles and ketones with various substituents.

8. Cartesian coordination and Gibbs free energies for all the calculated species were performed at the pbe1pbe/6-311+g(2d,2p)//SMD_{CYC} level in the solvent phase.

3a:

Zero-point correction=0.392505 (Hartree/Particle)
Thermal correction to Energy=0.413634
Thermal correction to Enthalpy=0.414609
Thermal correction to Gibbs Free Energy=0.338429
Sum of electronic and zero-point Energies=-770.934287
Sum of electronic and thermal Energies=-770.913159
Sum of electronic and thermal Enthalpies=-770.912183
Sum of electronic and thermal Free Energies=-770.988364

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C	-3.24246400	1.45978600	-0.62248000
H	-3.73389800	2.42097200	-0.58621200
N	-2.67536600	-0.65022500	-0.74128200
N	-1.86805800	1.30925200	-0.60093800
C	-0.93498700	2.42179100	-0.50111600
H	-1.15710700	3.13240800	-1.30669800
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H	-0.31124500	3.99102700	0.79156600
H	-1.99175100	3.53296100	1.02311400
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H	-2.98444700	-2.96306200	2.56562400

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C	4.78051200	-0.75562300	0.59961100
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C	2.98972000	0.66072300	-0.49409500
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H	2.06625000	-2.67202600	-0.40836200
H	2.49614700	-0.79668600	-1.93358800
H	1.13993400	-0.35997000	-0.87326800
H	4.44751700	-0.55514300	1.62723700
H	5.86449400	-0.91092400	0.64896200
H	4.88994600	1.39020300	0.14126800
H	4.92790000	0.31740500	-1.26701100
H	4.47067700	-2.25745400	-0.91809100
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TS1a:

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4a:

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H	-3.90559100	-0.56916100	-1.97139500
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5a:

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C	1.97926600	1.69666600	1.11560300
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N	-1.31573300	-1.53498900	-1.52659200
N	-2.75032200	0.48840100	1.21378100
H	-1.71438000	0.42831700	1.01408800
H	-2.97304300	1.07675400	2.00081700
C	-5.09622100	0.58273000	0.70139600
H	-5.25494400	1.17359800	1.60042400

TS2a$_1$:

Zero-point correction=0.514518 (Hartree/Particle)
Thermal correction to Energy=0.541519
Thermal correction to Enthalpy=0.542495
Thermal correction to Gibbs Free Energy=0.458755
Sum of electronic and zero-point Energies=-1150.350193
Sum of electronic and thermal Energies=-1150.323192
Sum of electronic and thermal Enthalpies=-1150.322216
Sum of electronic and thermal Free Energies=-1150.405956

C	-1.28549500	0.25175900	-0.50130400
C	-2.79833500	0.92787800	-2.00725400
H	-3.56834500	0.82123000	-2.75405400
C	-2.14027300	2.02116900	-1.57618400
H	-2.23673900	3.05353000	-1.86815600
N	-2.29821800	-0.15935800	-1.31279100
N	-1.24482700	1.60855600	-0.61144400
C	-0.20962900	2.50622000	-0.08364900
H	0.57442800	2.57565400	-0.84643200
H	0.24200700	2.01279200	0.77395000

C	-2.56624200	-1.50399200	-1.82741000
H	-1.96217800	-2.21341300	-1.27407700
H	-2.20306800	-1.52230300	-2.86084600
C	-0.73399100	3.89035300	0.27608800
H	0.14042400	4.46666600	0.60092500
H	-1.10528600	4.40984200	-0.61653700
C	-1.79592600	3.90636200	1.36898900
H	-2.12951500	4.92838900	1.57357600
H	-2.67638900	3.31919500	1.08657300
H	-1.40599800	3.49205300	2.30486000
C	-4.04330200	-1.87821700	-1.76032000
H	-4.63478400	-1.18239900	-2.36897600
H	-4.14496400	-2.85602000	-2.24670000
C	-4.61161900	-1.93630800	-0.34795600
H	-4.50183400	-0.97494500	0.16487100
H	-5.67721800	-2.18400300	-0.36623800
H	-4.10502700	-2.69691800	0.25545900
C	-1.36810500	0.02179400	1.95917600
C	-0.78969800	-0.58329300	3.23681800
C	-0.77971100	-2.10828400	3.18746500
C	-0.07764300	-2.60345600	1.92628500
C	-0.72054300	-2.01350000	0.67201800
C	-0.60616800	-0.47217300	0.69672700
H	-0.29515100	-2.51423900	4.08372700
H	0.23643700	-0.21768400	3.36353100
H	-1.36785000	-0.22936600	4.09982000
H	-2.42864300	-0.25578400	1.86197800
H	-1.32909300	1.11353300	2.01390900
H	0.97888100	-2.31420800	1.94836900
H	-0.11559100	-3.69824300	1.87189000
H	-0.21587700	-2.39236800	-0.22235100
H	-1.77193500	-2.32908500	0.65163600
H	-1.81632400	-2.47882300	3.19611400
O	0.71351900	-0.11135800	0.77071200
C	5.66474400	-0.49577400	-0.76826800
C	4.93728900	-1.09727600	-1.79692000
C	3.55480900	-0.98799200	-1.78535200
C	2.86444600	-0.30640600	-0.76912200
C	3.60441700	0.30151800	0.27486900
H	2.95986600	-1.43253900	-2.57742300
H	6.74957800	-0.56168500	-0.75071000
H	5.43896000	-1.63829700	-2.59312100
C	1.41282500	-0.25293900	-0.95841000
N	0.57771400	-0.33022900	-1.81076300

N	3.01067300	1.04158900	1.27623200
H	2.05140000	0.75612300	1.47644900
H	3.59202400	1.18491500	2.08807900
C	5.00820300	0.18966500	0.24048500
H	5.58193700	0.66270500	1.03494800

6a$_{1}$:

Zero-point correction=0.515857 (Hartree/Particle)
Thermal correction to Energy=0.542726
Thermal correction to Enthalpy=0.543702
Thermal correction to Gibbs Free Energy=0.459983
Sum of electronic and zero-point Energies=-1150.395220
Sum of electronic and thermal Energies=-1150.368352
Sum of electronic and thermal Enthalpies=-1150.367376
Sum of electronic and thermal Free Energies=-1150.451095

C	-0.95923100	0.15186300	-0.53426000
C	-2.94316500	0.18787700	-1.73835200
H	-3.82674800	-0.19760400	-2.22568700
C	-2.61727500	1.46174100	-1.49885900
H	-3.17626500	2.35247500	-1.74724500
N	-2.01462700	-0.68424700	-1.13556200
N	-1.46897200	1.53076300	-0.70058800
C	-0.50495200	2.60087200	-0.93183000
H	-0.00198400	2.47887400	-1.90321000
H	0.27150500	2.52351000	-0.16124500
C	-1.58673300	-1.82177900	-1.95155400
H	-0.80180700	-2.35471700	-1.40766100
H	-1.13255300	-1.47372000	-2.89188500
C	-1.13213100	3.99025600	-0.85533400
H	-0.32816800	4.71279700	-1.04296700
H	-1.84227500	4.12405200	-1.68117800
C	-1.81187000	4.30761800	0.47111100
H	-2.23663600	5.31666300	0.46344900
H	-2.61911200	3.60001800	0.68338400
H	-1.09847300	4.25528100	1.30179400
C	-2.72748800	-2.78807100	-2.25913200
H	-3.47266200	-2.29638200	-2.89753600
H	-2.30536800	-3.59467000	-2.87189000
C	-3.41000400	-3.37516200	-1.02997900
H	-3.86032300	-2.58858900	-0.41682900
H	-4.20032200	-4.07655700	-1.31664000
H	-2.69476300	-3.91795700	-0.40149500

C	-1.25701300	0.78333300	1.98117600
C	-0.92569800	0.43830300	3.43222800
C	-1.32391600	-0.99381500	3.77644500
C	-0.67509400	-1.97574500	2.80575700
C	-1.01348000	-1.63747700	1.35441900
C	-0.66293700	-0.19841200	0.98373600
H	-1.04423100	-1.23327600	4.80943100
H	0.15253100	0.56890200	3.59972300
H	-1.42893800	1.14945200	4.09810000
H	-2.34431400	0.77154400	1.83021700
H	-0.92683600	1.79568200	1.73867400
H	0.41513900	-1.95770800	2.94228700
H	-0.99580200	-3.00173000	3.02228000
H	-0.49228600	-2.32518000	0.67994300
H	-2.08571300	-1.76876400	1.17257600
H	-2.41764100	-1.09158700	3.71547800
O	0.79229600	-0.08669100	1.02938700
C	5.37578900	-0.39084000	-1.17799700
C	4.41374000	-0.32695000	-2.19228300
C	3.08143800	-0.22211200	-1.83774000
C	2.66868500	-0.17895100	-0.49464200
C	3.64530900	-0.23103700	0.53238200
H	2.30409200	-0.17409100	-2.59396900
H	6.42989400	-0.47606300	-1.42841000
H	4.70471600	-0.36105000	-3.23707400
C	1.22422900	-0.09187900	-0.25890000
N	0.33580700	-0.01738000	-1.17882400
N	3.34576000	-0.12950600	1.86733700
H	2.38406800	-0.24251500	2.14731900
H	4.05104300	-0.42414900	2.52176500
C	4.99868500	-0.34242400	0.15108500
H	5.75476100	-0.38006100	0.93199700

TS2a$_2$:

Zero-point correction=0.514228 (Hartree/Particle)
Thermal correction to Energy=0.541383
Thermal correction to Enthalpy=0.542359
Thermal correction to Gibbs Free Energy=0.458226
Sum of electronic and zero-point Energies=-1150.354754
Sum of electronic and thermal Energies=-1150.327599
Sum of electronic and thermal Enthalpies=-1150.326623
Sum of electronic and thermal Free Energies=-1150.410756

C	-1.61901200	-0.00276100	0.47794700
C	-3.07846900	-1.66977400	0.76339300
H	-3.87388300	-2.34923100	0.50899900
C	-2.31556000	-1.59795000	1.87650500
H	-2.33018200	-2.19483600	2.77331900
N	-2.64017200	-0.68414100	-0.09597700
N	-1.41980600	-0.57054500	1.69064600
C	-0.41953900	-0.19073200	2.70161900
H	-0.93450300	0.38672000	3.47857300
H	0.28894500	0.45945600	2.17776200
C	-3.10146500	-0.56194400	-1.48455700
H	-2.22515900	-0.29642500	-2.07309700
H	-3.82977800	0.25382400	-1.54155700
C	0.28360500	-1.39116600	3.32531100
H	0.95095200	-0.97771400	4.09174400
H	-0.43139600	-2.01970600	3.87361800
C	1.08734100	-2.23317800	2.34281700
H	1.57290300	-3.06778900	2.85817900
H	0.45747100	-2.64678900	1.54926600
H	1.86473700	-1.63618600	1.85730800
C	-3.70128000	-1.84024800	-2.05727500
H	-4.59083600	-2.14695200	-1.49188500
H	-4.07770100	-1.56139400	-3.04916800
C	-2.71338100	-2.99315900	-2.20039000
H	-2.33125000	-3.33347600	-1.23379100
H	-3.18722300	-3.84558300	-2.69710700
H	-1.84392700	-2.68625000	-2.78894500
C	-1.20152000	1.82402500	-1.35054600
C	-0.55796600	3.19324400	-1.56546400
C	-1.12023200	4.23596200	-0.60442600
C	-0.96914200	3.76945800	0.83982500
C	-1.57929300	2.38602600	1.04688500
C	-0.92363000	1.33478400	0.09394400
H	-0.62018900	5.20171800	-0.74835500
H	0.52300800	3.09585000	-1.41386100
H	-0.71423200	3.50610400	-2.60523800
H	-2.27997100	1.91325000	-1.54019400
H	-0.77667000	1.10866700	-2.05887600
H	0.09486600	3.71590100	1.09884400
H	-1.43912700	4.48292400	1.52864500
H	-1.44644600	2.08300600	2.08976400
H	-2.66333600	2.42276000	0.85531400
H	-2.18664400	4.39875700	-0.82532600
O	0.41369600	1.24129200	0.32848500

C	5.29862900	0.06528800	-0.39603000
C	4.49809000	1.12899300	0.02781200
C	3.11670500	1.01211300	-0.05185800
C	2.51670400	-0.15056300	-0.54844500
C	3.32989900	-1.23434700	-0.98019500
H	2.45553300	1.81111700	0.26129900
H	6.38167800	0.14181600	-0.34143800
H	4.94801500	2.03914000	0.41221500
C	1.08477100	-0.32856900	-0.69462100
N	0.23610500	-1.03665800	-1.13734500
N	2.76748300	-2.40248300	-1.42927700
H	1.78025900	-2.35400500	-1.66230400
H	3.34198300	-3.00290500	-1.99738300
C	4.72644400	-1.09742100	-0.88911000
H	5.35706100	-1.92380300	-1.20937600

6a$_2$:

Zero-point correction=0.515046 (Hartree/Particle)
Thermal correction to Energy=0.542105
Thermal correction to Enthalpy=0.543081
Thermal correction to Gibbs Free Energy=0.459329
Sum of electronic and zero-point Energies=-1150.398411
Sum of electronic and thermal Energies=-1150.371353
Sum of electronic and thermal Enthalpies=-1150.370377
Sum of electronic and thermal Free Energies=-1150.454128

C	-1.12019700	-0.18008500	0.05440000
C	-3.14159600	-1.33147700	-0.15608400
H	-4.04271800	-1.67620000	-0.64036800
C	-2.81999500	-1.35292700	1.14630200
H	-3.39432200	-1.71662300	1.98581000
N	-2.13482100	-0.66897500	-0.87243000
N	-1.59400900	-0.71562100	1.32585300
C	-0.80877400	-0.80173600	2.53401500
H	-1.26931400	-0.18526000	3.32444200
H	0.17137700	-0.35961000	2.32700300
C	-1.84295300	-0.96779900	-2.26410900
H	-0.79528900	-0.70120800	-2.43700800
H	-2.45182200	-0.32406000	-2.91829200
C	-0.61327000	-2.21805100	3.08153200
H	-0.09959700	-2.12588700	4.04767500
H	-1.59441600	-2.65736100	3.30404000
C	0.16678700	-3.14302100	2.15950500

H	0.26369200	-4.14253900	2.59619200
H	-0.33571600	-3.24097400	1.19292800
H	1.17350600	-2.75486800	1.97034600
C	-2.05176000	-2.42453800	-2.67998800
H	-3.10063800	-2.70703600	-2.52448200
H	-1.88711300	-2.47555100	-3.76447900
C	-1.14059600	-3.41397500	-1.96760200
H	-1.30348700	-3.38275200	-0.88619700
H	-1.32912600	-4.43756200	-2.30817000
H	-0.08707700	-3.18191600	-2.15765300
C	-1.31731100	2.02737600	-1.29985300
C	-1.11628100	3.54170800	-1.31761400
C	-1.89611600	4.21862200	-0.19456100
C	-1.50770700	3.62590400	1.15669600
C	-1.68784400	2.10797600	1.18422700
C	-0.96088400	1.40339000	0.04930700
H	-1.71794600	5.30060200	-0.20252200
H	-0.04754400	3.76820400	-1.20760300
H	-1.42235700	3.93757000	-2.29338800
H	-2.36648200	1.78360600	-1.50711600
H	-0.71826600	1.55810100	-2.08812600
H	-0.45726700	3.86553100	1.36934000
H	-2.10094600	4.07708400	1.96105900
H	-1.35029000	1.70631900	2.14304100
H	-2.75125600	1.84969400	1.09164700
H	-2.97408500	4.07551000	-0.36077000
O	0.47268500	1.56591300	0.23446500
C	5.28097700	0.34942500	-0.21931500
C	4.59750600	1.53773800	0.06618700
C	3.21404200	1.51894300	0.09664600
C	2.48681700	0.34304200	-0.15090500
C	3.18133400	-0.86089900	-0.45289500
H	2.65747900	2.42318500	0.32031000
H	6.36751600	0.34062300	-0.24575200
H	5.14084700	2.45624200	0.26207000
C	1.03204400	0.37552900	-0.07488100
N	0.23849000	-0.62598000	-0.25486000
N	2.51972900	-2.01288100	-0.74583900
H	1.51349700	-2.02357000	-0.59287200
H	3.03399700	-2.87685800	-0.76459700
C	4.59141300	-0.82178800	-0.47394800
H	5.13413300	-1.73568200	-0.70366300

TS3a

Zero-point correction=	0.511777 (Hartree/Particle)
Thermal correction to Energy=	0.538284
Thermal correction to Enthalpy=	0.539260
Thermal correction to Gibbs Free Energy=	0.456126
Sum of electronic and zero-point Energies=	-1150.363147
Sum of electronic and thermal Energies=	-1150.336640
Sum of electronic and thermal Enthalpies=	-1150.335664
Sum of electronic and thermal Free Energies=	-1150.418798

C	-1.54980900	0.05973000	0.44800100
C	-3.21173600	-1.39895100	0.76953200
H	-4.08811500	-1.97614800	0.52884200
C	-2.44921600	-1.40089700	1.88267100
H	-2.54086100	-1.97199600	2.79167900
N	-2.66329900	-0.48816200	-0.11268900
N	-1.43292200	-0.48851400	1.68695500
C	-0.35557800	-0.29068300	2.66737000
H	-0.76068400	0.29310600	3.50290600
H	0.42057100	0.29699500	2.17744100
C	-2.98340600	-0.45575100	-1.54616200
H	-2.01534500	-0.38151000	-2.04775900
H	-3.57953900	0.43566900	-1.76219900
C	0.22900700	-1.60363500	3.18409100
H	0.98657100	-1.32013900	3.92531600
H	-0.53298100	-2.16152600	3.74419900
C	0.85392000	-2.48282000	2.10939200
H	1.24883900	-3.40255000	2.55166400
H	0.12869300	-2.76031100	1.33911500
H	1.67608800	-1.97069200	1.60074200
C	-3.70055800	-1.69925300	-2.05742000
H	-4.65621000	-1.84876200	-1.53794400
H	-3.97445400	-1.46623600	-3.09369100
C	-2.85416800	-2.96806000	-2.03845600
H	-2.56657800	-3.26058400	-1.02447700
H	-3.40133900	-3.80277500	-2.48734400
H	-1.92736000	-2.82150700	-2.60103400
C	-1.15531400	1.94150100	-1.30896200
C	-0.43189600	3.26890600	-1.53864200
C	-0.80316900	4.31127300	-0.49037600
C	-0.53379400	3.77149700	0.90947300
C	-1.22691800	2.42939000	1.13607600
C	-0.83418000	1.36939400	0.08391800
H	-0.24403700	5.23944300	-0.65616500

H	0.65011100	3.09359600	-1.52048700
H	-0.67618100	3.62966100	-2.54451000
H	-2.23672800	2.10604000	-1.39471200
H	-0.84854700	1.22489800	-2.07202800
H	0.54560500	3.64187000	1.05236900
H	-0.87491600	4.48167200	1.67238100
H	-1.00409100	2.06903200	2.14304900
H	-2.31684200	2.56043400	1.07845400
H	-1.86988200	4.56429000	-0.58634500
O	0.56179600	1.16834300	0.19646800
C	5.23932100	-0.48353300	-0.47223000
C	4.70146200	0.67692800	0.11091800
C	3.32505300	0.84675700	0.10278300
C	2.47283200	-0.10676100	-0.47002000
C	3.01166500	-1.29566500	-1.07832300
H	2.88323900	1.73566700	0.54469400
H	6.31712300	-0.63313700	-0.47433000
H	5.35024100	1.42503200	0.55600600
C	1.02063000	0.01490100	-0.48579000
N	0.20122500	-0.80843900	-0.99081200
N	2.15763900	-2.17403800	-1.61948200
H	0.97863700	-1.69550900	-1.42790200
H	2.57605400	-3.00143600	-2.02469300
C	4.42823900	-1.44157400	-1.04735400
H	4.86572200	-2.33142400	-1.49572700

7a

Zero-point correction=	0.516833 (Hartree/Particle)
Thermal correction to Energy=	0.543473
Thermal correction to Enthalpy=	0.544449
Thermal correction to Gibbs Free Energy=	0.459264
Sum of electronic and zero-point Energies=	-1150.368718
Sum of electronic and thermal Energies=	-1150.342079
Sum of electronic and thermal Enthalpies=	-1150.341103
Sum of electronic and thermal Free Energies=	-1150.426288

C	-1.53926300	0.02872000	0.46984600
C	-3.15271600	-1.47150900	0.82742300
H	-4.02505400	-2.06349500	0.60945100
C	-2.34154200	-1.48204500	1.90567400
H	-2.37621600	-2.07961100	2.80146600
N	-2.66267300	-0.52787700	-0.05402200

N	-1.35617900	-0.54221700	1.68782200
C	-0.24365300	-0.34212100	2.63108700
H	-0.62686100	0.22559200	3.48752800
H	0.50721600	0.26179100	2.12304400
C	-3.08110800	-0.44261600	-1.46019900
H	-2.16045900	-0.29131700	-2.02619800
H	-3.73470800	0.42580900	-1.58720400
C	0.37595400	-1.65365000	3.10903200
H	1.17287400	-1.36533500	3.80572900
H	-0.34899500	-2.21617100	3.71227800
C	0.94450400	-2.52756600	1.99943400
H	1.38367700	-3.43729900	2.41971100
H	0.17539500	-2.82619100	1.28128600
H	1.72220000	-2.00674900	1.43329300
C	-3.76905100	-1.69750200	-1.98403100
H	-4.68647300	-1.91104700	-1.42031100
H	-4.11073300	-1.43695600	-2.99321200
C	-2.86801900	-2.92552300	-2.06126900
H	-2.50453300	-3.23728800	-1.07778400
H	-3.40598300	-3.76964700	-2.50321700
H	-1.98633500	-2.72268300	-2.67656500
C	-1.23022100	1.94789000	-1.27535200
C	-0.53045300	3.28885100	-1.50228300
C	-0.87788500	4.30707300	-0.42281800
C	-0.55472600	3.74415100	0.95620200
C	-1.22626800	2.39081100	1.18040400
C	-0.85858100	1.35512300	0.09613200
H	-0.33448400	5.24410800	-0.58994000
H	0.55347600	3.12690300	-1.52475300
H	-0.81319000	3.66420000	-2.49244700
H	-2.31555900	2.09965400	-1.32417300
H	-0.93749200	1.25014700	-2.06095800
H	0.53022000	3.62465300	1.06049900
H	-0.87715500	4.43485700	1.74438600
H	-0.96684300	2.01344600	2.17223400
H	-2.31857600	2.51041900	1.16043800
H	-1.94978000	4.54999200	-0.47782700
O	0.54625700	1.17305100	0.15879800
C	5.22879900	-0.38433700	-0.48630500
C	4.64736800	0.77099400	0.08679100
C	3.27375400	0.89338100	0.05974400
C	2.44514700	-0.09131000	-0.51788400
C	3.01840600	-1.28374100	-1.12263800
H	2.80273600	1.77326200	0.48987400

H	6.31109100	-0.50057600	-0.47521900
H	5.26740000	1.54219600	0.53303400
C	1.01316500	0.04765100	-0.52074900
N	0.13290400	-0.74408000	-1.01465300
N	2.24357300	-2.20758800	-1.67182300
H	0.65691900	-1.55720000	-1.42385700
H	2.80728600	-2.97319800	-2.03471800
C	4.45748600	-1.36315000	-1.05992700
H	4.92893000	-2.24178400	-1.49739600

TS4a*1*

Zero-point correction=	0.510589 (Hartree/Particle)
Thermal correction to Energy=	0.538571
Thermal correction to Enthalpy=	0.539546
Thermal correction to Gibbs Free Energy=	0.450705
Sum of electronic and zero-point Energies=	-1150.289992
Sum of electronic and thermal Energies=	-1150.262011
Sum of electronic and thermal Enthalpies=	-1150.261035
Sum of electronic and thermal Free Energies=	-1150.349876

C	2.24535800	-0.58908000	0.37367100
C	3.05907700	-2.53649500	1.24591700
H	3.09228600	-3.38680300	1.91022000
C	3.89398000	-2.17063300	0.24272000
H	4.79144200	-2.63968700	-0.13295300
N	2.07251400	-1.57118400	1.30268100
N	3.38251500	-0.99183200	-0.26807800
C	3.96329700	-0.30372300	-1.40638300
H	5.03474700	-0.16192200	-1.21982400
H	3.49778800	0.68455100	-1.44198900
C	0.96120400	-1.62334000	2.24562600
H	0.33279600	-0.75150700	2.05003400
H	1.36219200	-1.53166700	3.26301300
C	3.74940200	-1.03706500	-2.72922600
H	4.30691400	-0.49358200	-3.50286700
H	4.20714200	-2.03283500	-2.66608500
C	2.28496900	-1.16181800	-3.12761200
H	2.18067300	-1.70433400	-4.07208000
H	1.70687900	-1.69388400	-2.36630300
H	1.82505700	-0.17547300	-3.25576800
C	0.12997600	-2.89787700	2.12150400
H	0.74131900	-3.76961200	2.39289300

H	-0.66309400	-2.83393700	2.87599000
C	-0.48722500	-3.09852800	0.74364600
H	0.28148600	-3.15174100	-0.03505000
H	-1.06261200	-4.02873400	0.70914000
H	-1.16852500	-2.27981600	0.49402100
C	0.49044800	2.27241900	1.60765100
C	0.48555300	3.81066900	1.76241700
C	1.35740100	4.50333200	0.72058600
C	0.94738800	4.09977400	-0.69226100
C	0.98046800	2.56736300	-0.85904400
C	0.15266300	1.93217600	0.20264100
H	1.28528900	5.59104200	0.83440100
H	-0.54757900	4.17337800	1.68740300
H	0.82472800	4.04459500	2.77667600
H	1.50874400	1.88950000	1.75931600
H	-0.19158900	1.78167400	2.29891900
H	-0.06469800	4.46664300	-0.90708100
H	1.61001900	4.54679500	-1.44093400
H	0.63165700	2.24939400	-1.84402700
H	2.00448400	2.20510300	-0.71284700
H	2.41037400	4.23685000	0.88624200
O	-0.84378500	1.27847100	-0.21763200
C	-4.88956900	-0.96391300	-2.01938200
C	-3.81863500	-0.22498900	-2.58067700
C	-2.84239900	0.26833600	-1.74602700
C	-2.88126100	0.05837000	-0.34860600
C	-3.97221400	-0.70228300	0.25240900
H	-2.01734300	0.83264500	-2.16788400
H	-5.66661300	-1.35765100	-2.67126700
H	-3.76869700	-0.05285700	-3.65107000
C	-1.89577100	0.55459200	0.56092100
N	-1.76324300	0.47211300	1.81177200
N	-4.00622700	-0.90593600	1.55708800
H	-2.60719500	-0.07897000	2.12152500
H	-4.82722000	-1.44939100	1.81384300
C	-4.96494600	-1.19306300	-0.67224700
H	-5.79447600	-1.76299900	-0.25825900

8a

Zero-point correction= 0.514995 (Hartree/Particle)
Thermal correction to Energy= 0.542662
Thermal correction to Enthalpy= 0.543637
Thermal correction to Gibbs Free Energy= 0.454498

Sum of electronic and zero-point Energies= -1150.392308
Sum of electronic and thermal Energies= -1150.364641
Sum of electronic and thermal Enthalpies= -1150.363665
Sum of electronic and thermal Free Energies= -1150.452805

C	2.13673600	0.61838200	-0.06103400
C	4.23904000	1.26781700	0.53414000
H	5.03592200	1.55750100	1.20289400
C	4.21552000	1.16541300	-0.81874300
H	4.98840000	1.34982000	-1.55004400
N	2.97034600	0.93151100	0.96762600
N	2.93389600	0.77149600	-1.15302600
C	2.48252000	0.52677600	-2.51526900
H	2.66838100	1.42836500	-3.11086100
H	1.40053500	0.38128400	-2.45492300
C	2.56827600	0.89929400	2.36502900
H	1.48504200	0.75094400	2.36325800
H	2.77303000	1.88011400	2.81043900
C	3.15061800	-0.68374200	-3.16187300
H	2.78821600	-0.74151900	-4.19566300
H	4.23341600	-0.51358300	-3.22801400
C	2.87122600	-1.99379800	-2.43725100
H	3.35441300	-2.83294500	-2.94695000
H	3.24664600	-1.96637400	-1.40900900
H	1.79644300	-2.20000000	-2.39267900
C	3.25698600	-0.20166800	3.16728100
H	4.34169200	-0.03158300	3.16589400
H	2.93429000	-0.09514100	4.21044600
C	2.94788000	-1.60583500	2.66568600
H	3.28627200	-1.74198600	1.63334700
H	3.44568800	-2.35975600	3.28308400
H	1.87129700	-1.80640700	2.69004400
C	-2.02504600	1.30588100	1.22764400
C	-2.98010500	2.48358500	1.40784600
C	-2.48628300	3.71024700	0.64338200
C	-2.27340800	3.38487700	-0.83398700
C	-1.33003100	2.19799300	-1.02006100
C	-1.79660400	0.96459200	-0.25510700
H	-3.19945200	4.53652300	0.74885200
H	-3.97438500	2.19856300	1.04224500
H	-3.08639700	2.71257600	2.47512400
H	-1.04299100	1.55059500	1.65599500
H	-2.39096600	0.41661900	1.75411200
H	-3.23855400	3.14539900	-1.29614200

H	-1.87203000	4.25609300	-1.36532100
H	-1.24340200	1.92410700	-2.07709200
H	-0.32324500	2.44864000	-0.65928900
H	-1.53788600	4.05552900	1.08270600
O	-3.04037700	0.58870800	-0.85433200
C	-0.80538200	-3.65713300	0.55311900
C	-2.17611400	-3.93782300	0.60754800
C	-3.08063400	-2.93575800	0.28998200
C	-2.65306100	-1.65484500	-0.07702700
C	-1.26893500	-1.36886400	-0.09455700
H	-4.14524800	-3.15356700	0.32479200
H	-0.08409800	-4.43467700	0.79178000
H	-2.52741500	-4.92531500	0.88894200
C	-3.59760200	-0.60659800	-0.52064300
N	-4.85517200	-0.69425300	-0.70564600
N	-0.84877900	-0.11098900	-0.43309400
H	-5.17391400	-1.64260000	-0.52437900
H	0.14245800	0.12221000	-0.25211800
C	-0.35247000	-2.39428900	0.21048200
H	0.71006600	-2.17047500	0.18263400

3a-w

Zero-point correction=	0.416570 (Hartree/Particle)
Thermal correction to Energy=	0.440368
Thermal correction to Enthalpy=	0.441343
Thermal correction to Gibbs Free Energy=	0.359924
Sum of electronic and zero-point Energies=	-847.303514
Sum of electronic and thermal Energies=	-847.279716
Sum of electronic and thermal Enthalpies=	-847.278740
Sum of electronic and thermal Free Energies=	-847.360159

C	-1.62941600	0.25880300	-0.73335600
C	-3.70457200	1.14243000	-0.33968300
H	-4.78216700	1.15062200	-0.26578600
C	-2.79956600	2.13620400	-0.15558700
H	-2.94027800	3.17330900	0.11153800
N	-2.97289000	0.02065900	-0.68708300
N	-1.55859700	1.57861500	-0.39947400
C	-0.30765600	2.31738500	-0.30977700
H	-0.38570700	3.20887100	-0.94393700
H	0.45992400	1.67200700	-0.74180600
C	-3.56284400	-1.27390800	-0.97355800

H	-2.74974700	-1.89129400	-1.36501800
H	-4.30804300	-1.15400400	-1.76986600
C	0.06224500	2.72141600	1.11491500
H	1.00411000	3.27998400	1.05649400
H	-0.69426100	3.41290600	1.51080900
C	0.22548000	1.53928300	2.06096700
H	0.49502000	1.87781000	3.06638700
H	-0.69678800	0.95347500	2.13491900
H	1.01776600	0.86849800	1.71149600
C	-4.19948200	-1.93349200	0.24750700
H	-5.00612000	-1.29339600	0.62858500
H	-4.68065700	-2.86029500	-0.09024900
C	-3.20598800	-2.23503100	1.36166400
H	-2.71761900	-1.32104100	1.71339000
H	-3.70358700	-2.70428800	2.21619400
H	-2.41896300	-2.91323200	1.01394000
C	1.69030900	-1.50758400	-1.29302300
C	1.38120000	-2.40661500	-0.08914300
C	2.64741400	-2.90953600	0.59852700
C	3.53168200	-1.74305900	1.03017600
C	3.90363400	-0.85064500	-0.15998800
C	2.69778800	-0.43570400	-0.96825000
H	2.38523400	-3.52372800	1.46796900
H	0.77182400	-1.83472100	0.62238000
H	0.75815000	-3.24487100	-0.42040900
H	2.13178200	-2.11474000	-2.09905700
H	0.78094200	-1.03132300	-1.67208300
H	3.00053400	-1.14056700	1.77904300
H	4.44699000	-2.10262500	1.51350400
H	4.45042300	0.04521600	0.14809500
H	4.55345600	-1.41978000	-0.84279100
H	3.20943100	-3.56044100	-0.08747200
O	2.55662900	0.71451200	-1.36173800
O	3.63714900	2.86983500	0.09126900
H	3.32627900	2.16673300	-0.50656000
H	4.08089200	3.51153800	-0.46841100

TS1a-w

Zero-point correction=	0.416813 (Hartree/Particle)
Thermal correction to Energy=	0.437480
Thermal correction to Enthalpy=	0.438456
Thermal correction to Gibbs Free Energy=	0.367657
Sum of electronic and zero-point Energies=	-847.274565
Sum of electronic and thermal Energies=	-847.253897

Sum of electronic and thermal Enthalpies= -847.252921
Sum of electronic and thermal Free Energies= -847.323721

C	0.63038900	0.01818400	-0.48606200
C	2.41605300	1.22937800	-1.18518100
H	2.97054900	2.11522800	-1.45491700
C	2.77554100	-0.07639400	-1.19452800
H	3.70380600	-0.55166600	-1.47383900
N	1.10540900	1.26615000	-0.74747100
N	1.67589100	-0.79442100	-0.77014600
C	1.70532600	-2.25106300	-0.61630300
H	2.18215700	-2.65790300	-1.51492600
H	0.66223900	-2.57820800	-0.57787500
C	0.37391400	2.51456900	-0.57599900
H	-0.64005600	2.25187400	-0.27371300
H	0.31036300	3.01370100	-1.55018300
C	2.46071100	-2.68899100	0.63534300
H	2.49889900	-3.78534200	0.61328900
H	3.50336700	-2.34398400	0.58811100
C	1.80818100	-2.22243600	1.93036800
H	2.33672300	-2.62224500	2.80169300
H	1.81720200	-1.12984500	2.00923400
H	0.76345100	-2.54607300	1.97197200
C	1.01237500	3.44272000	0.45490100
H	2.01624800	3.73114900	0.11774100
H	0.42166700	4.36709600	0.46616500
C	1.08548000	2.84992500	1.85587600
H	1.67201600	1.92565800	1.86768200
H	1.55479800	3.55238600	2.55116800
H	0.08815000	2.61269400	2.24042500
C	-1.66541800	-0.06687300	1.12571700
C	-3.17141500	-0.29615200	1.30338600
C	-3.95355400	0.22185600	0.09478600
C	-3.45618600	-0.40123400	-1.21081000
C	-1.95072900	-0.17201200	-1.39683500
C	-1.23869300	-0.76157600	-0.17088300
H	-5.02499200	0.02390300	0.22380700
H	-3.34840600	-1.37246000	1.42100000
H	-3.52216000	0.19090500	2.22213500
H	-1.46465400	1.01156500	1.09987200
H	-1.09946100	-0.49747100	1.95751100
H	-3.64248800	-1.48223700	-1.19548900
H	-4.00863900	0.01031600	-2.06506600
H	-1.58600400	-0.68128400	-2.29464100

H	-1.75942000	0.90328300	-1.51015800
H	-3.84541300	1.31642800	0.03685800
O	-1.12761300	-2.01487200	-0.12964900
O	-0.00541524	-4.34856762	-0.50615965
H	-0.07985570	-5.30543709	-0.52759384
H	-0.88181404	-3.96001627	-0.45563247

4a-w

Zero-point correction= 0.420543 (Hartree/Particle)
Thermal correction to Energy= 0.442480
Thermal correction to Enthalpy= 0.443455
Thermal correction to Gibbs Free Energy= 0.368776
Sum of electronic and zero-point Energies= -847.310227
Sum of electronic and thermal Energies= -847.288290
Sum of electronic and thermal Enthalpies= -847.287314
Sum of electronic and thermal Free Energies= -847.361993

C	0.50434200	0.26863100	-0.58278600
C	2.20044600	1.69795200	-0.91633500
H	2.69589700	2.65303100	-0.98481300
C	2.66526500	0.44539400	-1.12088000
H	3.64631800	0.09309400	-1.39673800
N	0.87023400	1.58018200	-0.57650100
N	1.61838200	-0.42161800	-0.90994300
C	1.81747600	-1.88093700	-1.02693000
H	2.16556000	-2.06214900	-2.05003000
H	0.81994200	-2.31003300	-0.89684600
C	0.06231700	2.76960900	-0.29317600
H	-0.93049700	2.44010300	0.00059600
H	-0.03929800	3.33321700	-1.22740000
C	2.82857900	-2.39754100	-0.00907700
H	2.92404900	-3.47352700	-0.19986500
H	3.82302700	-1.96873800	-0.20172200
C	2.42388100	-2.16898600	1.44193700
H	3.17443100	-2.59021200	2.11877800
H	2.34656700	-1.09902800	1.67064000
H	1.45779900	-2.63803100	1.65773300
C	0.66928100	3.64905300	0.79778600
H	1.62812600	4.06061300	0.45872100
H	0.00059300	4.51144400	0.90749200
C	0.84662500	2.95001700	2.13959200
H	1.50926000	2.08235400	2.05728900

H	1.28421300	3.63272500	2.87371900
H	-0.10997200	2.59808500	2.53775200
C	-1.48878500	0.02950700	0.99516900
C	-2.93745400	-0.43986100	1.11277200
C	-3.81018100	0.13721900	-0.00031600
C	-3.24421100	-0.20365800	-1.37770900
C	-1.81006700	0.29489200	-1.52392300
C	-0.92356600	-0.34624300	-0.40804100
H	-4.83658300	-0.23929900	0.09168600
H	-2.95172900	-1.53349400	1.06379500
H	-3.33265900	-0.15812000	2.09681800
H	-1.44983600	1.10795500	1.19926100
H	-0.87060800	-0.46778000	1.75145100
H	-3.23889100	-1.29099600	-1.51272700
H	-3.86985600	0.22774600	-2.16947400
H	-1.39559400	-0.01811100	-2.48981400
H	-1.80625900	1.39419800	-1.50224200
H	-3.87138800	1.23232900	0.10965300
O	-0.89982800	-1.67952900	-0.57010400
O	-0.71138800	-3.29029900	1.45778000
H	-1.29058200	-4.03735300	1.29203800
H	-0.83629800	-2.66164200	0.67944900

5a-w

Zero-point correction=	0.536597 (Hartree/Particle)
Thermal correction to Energy=	0.568498
Thermal correction to Enthalpy=	0.569473
Thermal correction to Gibbs Free Energy=	0.473116
Sum of electronic and zero-point Energies=	-1226.742212
Sum of electronic and thermal Energies=	-1226.710312
Sum of electronic and thermal Enthalpies=	-1226.709336
Sum of electronic and thermal Free Energies=	-1226.805693

C	1.77052300	0.39807700	0.16080600
C	2.96636600	-1.02086300	1.39705600
H	3.34600500	-1.47706900	2.29595100
C	3.12519000	-1.37817300	0.10356700
H	3.65176700	-2.21538900	-0.31850800
N	2.13456800	0.07121000	1.42001300
N	2.38731200	-0.49402000	-0.65407500
C	2.33653300	-0.52919200	-2.12402800
H	2.76441400	0.40997700	-2.48658400
H	1.28688900	-0.56289200	-2.41847800

C	1.80005300	0.78592200	2.66390900
H	1.00879900	1.48875400	2.38070500
H	2.70115900	1.32707300	2.97594600
C	3.07254500	-1.69997900	-2.76379500
H	3.16666600	-1.43407200	-3.82373800
H	4.10292600	-1.75444100	-2.39078000
C	2.36779400	-3.04937500	-2.65526500
H	2.93552500	-3.81765000	-3.18993100
H	2.23154600	-3.38933600	-1.62424500
H	1.37283800	-2.99605700	-3.11067600
C	1.32377700	-0.14714000	3.77110300
H	2.11702400	-0.84794500	4.06501600
H	1.15698200	0.49107200	4.64798700
C	0.04820600	-0.90670400	3.42965200
H	0.19881400	-1.58059900	2.58109100
H	-0.28150600	-1.50954900	4.28185800
H	-0.75753800	-0.21861800	3.15704800
C	1.82341200	2.86700000	-0.07183000
C	1.03256500	4.15411400	-0.28998800
C	0.29082700	4.13669800	-1.62444900
C	-0.58753600	2.89319900	-1.74750100
C	0.23778600	1.62221500	-1.55180600
C	0.86779300	1.63198900	-0.13346100
H	-0.31435500	5.04518500	-1.73490700
H	0.30851600	4.24622000	0.52813300
H	1.70533700	5.01933000	-0.23456100
H	2.61539800	2.77472400	-0.83271200
H	2.31631800	2.89500300	0.90731200
H	-1.37747500	2.92164200	-0.98943100
H	-1.07465000	2.86489400	-2.73027400
H	-0.39876000	0.73594400	-1.65972400
H	0.99822400	1.59799600	-2.34175200
H	1.02184700	4.14653700	-2.44812100
O	-0.09588200	1.69575700	0.81515700
C	-5.70904300	-0.43350300	-0.30328400
C	-5.27195500	-1.62233800	-0.91047100
C	-3.92682900	-1.92782100	-0.85998800
C	-3.00632300	-1.07081500	-0.22298700
C	-3.43121100	0.15070900	0.37838200
H	-3.55194000	-2.84456900	-1.30612100
H	-6.76452700	-0.17431800	-0.32491000
H	-5.97305900	-2.28831700	-1.40163400
C	-1.65501300	-1.49729900	-0.15832300
N	-0.56571100	-1.90968800	-0.12415100

N	-2.58635500	0.99484100	0.99842200
H	-1.53503700	1.09167300	0.82206100
H	-3.00123300	1.85097100	1.33415700
C	-4.82384700	0.42226800	0.31761100
H	-5.18610200	1.34080100	0.77295300
O	1.36472300	-3.99322000	0.58433000
H	0.72541400	-3.28454500	0.39155400
H	0.83466300	-4.78307400	0.71850100

TS2a$_1$-w

Zero-point correction=	0.538483 (Hartree/Particle)
Thermal correction to Energy=	0.568119
Thermal correction to Enthalpy=	0.569095
Thermal correction to Gibbs Free Energy=	0.479092
Sum of electronic and zero-point Energies=	-1226.722056
Sum of electronic and thermal Energies=	-1226.692420
Sum of electronic and thermal Enthalpies=	-1226.691444
Sum of electronic and thermal Free Energies=	-1226.781448

C	1.51154400	0.35923900	0.50315000
C	2.60905700	-1.08904400	1.79876800
H	2.76800100	-1.75257800	2.63161700
C	3.37024900	-0.86113800	0.70799200
H	4.30733700	-1.30066700	0.41581300
N	1.47198600	-0.32657000	1.67051100
N	2.69338500	0.04304500	-0.08286300
C	3.17153900	0.47481700	-1.40458000
H	3.47552100	1.52294800	-1.32774500
H	2.32382600	0.40617200	-2.08678600
C	0.41834400	-0.30053800	2.69639700
H	-0.46637300	0.10950100	2.20907800
H	0.74074400	0.38992500	3.48517000
C	4.32654100	-0.34611100	-1.96532700
H	4.70081800	0.23153400	-2.81955800
H	5.16307800	-0.37075400	-1.25552200
C	3.94676200	-1.74696300	-2.43420500
H	4.82920200	-2.27951600	-2.80323900
H	3.47512900	-2.35385100	-1.65512500
H	3.22647800	-1.68732400	-3.25716400
C	0.11611100	-1.66791000	3.29955000
H	0.99161600	-2.05709700	3.83606700
H	-0.63835300	-1.48175800	4.07411200

C	-0.40482200	-2.70014600	2.30774000
H	0.32208400	-2.91863900	1.51908300
H	-0.63498400	-3.63806000	2.82359000
H	-1.32106300	-2.34609200	1.82546800
C	0.78828300	2.62033700	1.17784600
C	-0.17033800	3.79653500	1.00242700
C	-0.15276900	4.33156900	-0.42601300
C	-0.40253600	3.20765000	-1.42709500
C	0.60798700	2.07506600	-1.25146800
C	0.48564400	1.47523500	0.16942300
H	-0.89977400	5.12598900	-0.54316300
H	-1.18424300	3.46192500	1.25268200
H	0.09310900	4.58779800	1.71540000
H	1.82460100	2.95906800	1.02607600
H	0.72229700	2.24331500	2.20305700
H	-1.41232800	2.80407800	-1.29282700
H	-0.33884300	3.58917100	-2.45335900
H	0.41865800	1.29023800	-1.98833800
H	1.60994300	2.48505200	-1.42427100
H	0.82691800	4.79010500	-0.63075600
O	-0.79364100	1.01040100	0.36111200
C	-5.23046700	-1.16368800	-1.23114200
C	-4.27623800	-1.61836000	-2.14336500
C	-2.93768800	-1.36623700	-1.88499600
C	-2.51094500	-0.65813300	-0.74816200
C	-3.48232200	-0.18964900	0.17144300
H	-2.16999400	-1.71732100	-2.56790300
H	-6.28759900	-1.34906100	-1.40284900
H	-4.57099500	-2.16068100	-3.03621600
C	-1.05321700	-0.55567700	-0.62338800
N	-0.05153700	-1.09613400	-0.98101600
N	-3.15164300	0.46638500	1.33819500
H	-2.27502800	0.98602800	1.27588200
H	-3.91673700	0.96299500	1.76900400
C	-4.83645700	-0.46851600	-0.10029200
H	-5.58522400	-0.12142800	0.60878800
O	1.51820700	-3.37968100	-0.72570900
H	0.94854800	-2.59327600	-0.89004200
H	1.03619600	-4.12061300	-1.10126700

6a$_1$-w

Zero-point correction= 0.540076 (Hartree/Particle)
Thermal correction to Energy= 0.570401

Thermal correction to Enthalpy= 0.571377
Thermal correction to Gibbs Free Energy= 0.480208
Sum of electronic and zero-point Energies= -1226.757079
Sum of electronic and thermal Energies= -1226.726754
Sum of electronic and thermal Enthalpies= -1226.725779
Sum of electronic and thermal Free Energies= -1226.816947

C	1.06664300	0.24932300	0.11990600
C	2.98260700	0.02490100	1.42929000
H	3.56952000	0.01366200	2.33555900
C	3.39101900	0.11513100	0.15416100
H	4.39566700	0.18477700	-0.23216000
N	1.58794800	0.00207700	1.45790500
N	2.27515300	0.16804600	-0.69008900
C	2.26783800	-0.27628700	-2.07544500
H	2.21168200	0.58887500	-2.75383600
H	1.35426000	-0.86347900	-2.23177200
C	0.79956100	-0.32965800	2.61777100
H	-0.22969300	-0.49579500	2.28377100
H	0.76931100	0.51550300	3.32758100
C	3.47616700	-1.11331400	-2.49171400
H	3.37742500	-1.26802400	-3.57394300
H	4.39601500	-0.52656100	-2.36645200
C	3.60455500	-2.46406400	-1.79738900
H	4.45441700	-3.02471600	-2.20165100
H	3.76311000	-2.34718200	-0.72016300
H	2.69637700	-3.05938600	-1.93305400
C	1.27913100	-1.57430900	3.36853300
H	2.28747400	-1.39798900	3.76454900
H	0.62979700	-1.69697800	4.24493100
C	1.27166100	-2.84090300	2.52490700
H	1.94174500	-2.73462400	1.66567400
H	1.60288300	-3.70521100	3.10966100
H	0.26418800	-3.05123100	2.14821400
C	0.65005400	2.64829600	1.06680300
C	-0.09927600	3.97233100	0.91125500
C	0.07440000	4.56587300	-0.48363800
C	-0.34017400	3.55711300	-1.55055200
C	0.43848800	2.25039400	-1.40743600
C	0.30793500	1.63663400	-0.01491700
H	-0.50773800	5.48993700	-0.58074900
H	-1.16874100	3.80900900	1.10527900
H	0.24657100	4.67713400	1.67656500
H	1.73323400	2.81845800	1.00839300

H	0.45383000	2.21554200	2.05082000
H	-1.41644900	3.35394300	-1.46640700
H	-0.17951800	3.96816800	-2.55413200
H	0.10891100	1.52227000	-2.15715300
H	1.50536300	2.43324800	-1.58302900
H	1.12871500	4.84041200	-0.63361200
O	-1.07863800	1.22102400	0.14167400
C	-4.90818700	-2.00481700	-0.63775700
C	-3.72370100	-2.66731900	-0.97390800
C	-2.51621300	-2.02022800	-0.78395300
C	-2.44651700	-0.71319100	-0.26637400
C	-3.65136300	-0.04338000	0.08123000
H	-1.59436600	-2.53035100	-1.04433300
H	-5.86905400	-2.49215900	-0.78056300
H	-3.74332700	-3.67230600	-1.38224800
C	-1.11883400	-0.10795600	-0.12613500
N	0.01588200	-0.71016200	-0.23606000
N	-3.69284300	1.20157300	0.65962000
H	-2.87410200	1.78368100	0.58191200
H	-4.58231000	1.67294500	0.65402900
C	-4.86930500	-0.72395700	-0.12004800
H	-5.79370700	-0.21838200	0.14983900
O	0.45597700	-3.44210600	-0.97423200
H	0.40770500	-2.52454000	-0.63150100
H	0.72017000	-3.98442000	-0.22672500

TS2a$_2$-w

Zero-point correction=	0.538335 (Hartree/Particle)
Thermal correction to Energy=	0.568976
Thermal correction to Enthalpy=	0.569952
Thermal correction to Gibbs Free Energy=	0.477859
Sum of electronic and zero-point Energies=	-1226.722705
Sum of electronic and thermal Energies=	-1226.692063
Sum of electronic and thermal Enthalpies=	-1226.691087
Sum of electronic and thermal Free Energies=	-1226.783180

C	-1.60731300	0.37793200	0.51901400
C	-3.26782100	-1.09579600	0.76306600
H	-4.11387400	-1.69636400	0.47945900
C	-2.53131200	-1.11534900	1.89527300
H	-2.62851500	-1.72501300	2.77757600
N	-2.69097300	-0.17163300	-0.08193200
N	-1.51286700	-0.20747400	1.73489600
C	-0.52464100	0.08603800	2.78610500

H	-0.99482700	0.77761600	3.49530800
H	0.29254500	0.59888900	2.26642400
C	-3.20127600	0.12386100	-1.42937200
H	-2.34372600	0.13985500	-2.10141900
H	-3.64195900	1.12545800	-1.40769500
C	-0.03396200	-1.15646800	3.51928700
H	0.65338600	-0.78745100	4.29084100
H	-0.85437400	-1.63667200	4.06973300
C	0.67787800	-2.17404800	2.63669200
H	1.05330400	-3.00668800	3.24039000
H	0.01190200	-2.58708900	1.87223200
H	1.52959600	-1.71746800	2.12317700
C	-4.22509500	-0.87481300	-1.95336300
H	-5.06870700	-0.96472500	-1.25738900
H	-4.64886000	-0.40827500	-2.85116300
C	-3.65633700	-2.24207200	-2.32014300
H	-3.15811100	-2.74423000	-1.48546700
H	-4.44979600	-2.89921800	-2.69023800
H	-2.91014800	-2.14269800	-3.11575700
C	-0.77170400	1.96648700	-1.38238100
C	0.14387000	3.16203400	-1.63974200
C	-0.26698500	4.36385700	-0.79330200
C	-0.30645000	3.99746000	0.68755400
C	-1.18041300	2.77187000	0.94147800
C	-0.66962300	1.55006300	0.10899300
H	0.41920600	5.20367000	-0.95889200
H	1.17258900	2.87125800	-1.39978000
H	0.11516100	3.41851700	-2.70614400
H	-1.79478300	2.26020400	-1.65097000
H	-0.47115800	1.12600500	-2.01408500
H	0.70792200	3.76723000	1.03388700
H	-0.67375900	4.84182200	1.28464800
H	-1.16567600	2.52697200	2.00873900
H	-2.22631400	2.99109500	0.67344100
H	-1.26413200	4.70736000	-1.11021600
O	0.61245000	1.24289400	0.43487300
C	5.43237800	-0.24850900	-0.34788200
C	4.66338000	0.76185600	0.23583000
C	3.27990600	0.69141800	0.16311300
C	2.64795500	-0.37966200	-0.48106400
C	3.42722700	-1.41147700	-1.07293300
H	2.63689500	1.45462600	0.58522700
H	6.51746700	-0.20336700	-0.30207300
H	5.14089200	1.59827700	0.73641300

C	1.21726300	-0.52209800	-0.61128800
N	0.30411700	-1.15635400	-1.01438100
N	2.83784300	-2.49732400	-1.67429300
H	1.85643300	-2.39966900	-1.90495300
H	3.39806500	-3.00962300	-2.33609100
C	4.82725900	-1.31666600	-0.99100500
H	5.43363700	-2.10177400	-1.43668100
O	-1.15701600	-3.50855600	-0.35147600
H	-0.67417600	-2.70146900	-0.62244800
H	-0.51152300	-4.21779100	-0.40682700

6a$_2$-w

Zero-point correction=	0.539245 (Hartree/Particle)
Thermal correction to Energy=	0.569977
Thermal correction to Enthalpy=	0.570953
Thermal correction to Gibbs Free Energy=	0.478843
Sum of electronic and zero-point Energies=	-1226.763164
Sum of electronic and thermal Energies=	-1226.732432
Sum of electronic and thermal Enthalpies=	-1226.731456
Sum of electronic and thermal Free Energies=	-1226.823567

C	1.17908000	-0.16600100	0.10047800
C	2.87668100	-1.34064400	1.19433200
H	3.44348800	-1.71525000	2.03328300
C	3.20993300	-1.29308800	-0.10369500
H	4.11453600	-1.62513600	-0.59017700
N	1.63071800	-0.73824500	1.36397600
N	2.19660500	-0.64354800	-0.82007700
C	1.97998500	-0.90052200	-2.23335100
H	2.71326000	-0.32557800	-2.82026800
H	0.99814100	-0.50838500	-2.50585400
C	0.85865600	-0.79858000	2.58143600
H	-0.16345600	-0.48431900	2.34716100
H	1.24452000	-0.07944300	3.32459000
C	2.07202500	-2.37119500	-2.64731300
H	1.98918900	-2.40352700	-3.74130300
H	3.07266000	-2.75228700	-2.40688600
C	1.01712500	-3.27206100	-2.02049400
H	1.17231300	-4.31581800	-2.31334800
H	1.05727400	-3.21889900	-0.92805400
H	0.01178900	-2.98023900	-2.34184000
C	0.81171400	-2.18385400	3.23082400
H	1.82534000	-2.48415800	3.52600100

H	0.24724600	-2.08333800	4.16695800
C	0.18897800	-3.26108700	2.35447300
H	0.74715300	-3.37203400	1.41960600
H	0.18934200	-4.22997600	2.86447900
H	-0.84681300	-3.01232400	2.09981700
C	1.87421800	2.09521100	1.20181900
C	1.71430400	3.61573600	1.20937600
C	1.97726500	4.22107700	-0.16629500
C	1.08209700	3.56967200	-1.21600800
C	1.26331700	2.05257900	-1.23859800
C	1.03744600	1.41445500	0.13168900
H	1.81474200	5.30525900	-0.14332900
H	0.69339000	3.86666900	1.52720100
H	2.38970600	4.04807200	1.95719800
H	2.92023300	1.82425100	1.00526500
H	1.62257700	1.68435000	2.18249500
H	0.03241500	3.80803600	-0.99865100
H	1.29532800	3.97474600	-2.21220000
H	0.58403600	1.60124400	-1.97070900
H	2.28450400	1.80334400	-1.55153700
H	3.03158900	4.06631800	-0.43891600
O	-0.37448200	1.57605300	0.45616800
C	-5.21934800	0.46731300	0.15123800
C	-4.50320400	1.66548900	0.26292300
C	-3.12048600	1.61696000	0.25560200
C	-2.42604800	0.40127600	0.13521400
C	-3.15405000	-0.81732100	0.03474300
H	-2.53735400	2.52843600	0.33682400
H	-6.30603800	0.48220000	0.15156300
H	-5.02124800	2.61464400	0.35092600
C	-0.96817000	0.41680300	0.11366100
N	-0.20305500	-0.57733200	-0.20409100
N	-2.52945400	-2.02464400	-0.03221700
H	-1.52345700	-2.03096800	-0.17289900
H	-3.06647400	-2.83716800	-0.28300600
C	-4.56299900	-0.74514900	0.04255200
H	-5.13203000	-1.66856100	-0.03291200
O	-1.41751100	-0.67980500	-3.09130500
H	-1.07494400	-0.80946300	-2.19438100
H	-2.28181700	-0.27671900	-2.96678100

TS3a-w

Zero-point correction= 0.540332 (Hartree/Particle)

Thermal correction to Energy=	0.569443
Thermal correction to Enthalpy=	0.570419
Thermal correction to Gibbs Free Energy=	0.482234
Sum of electronic and zero-point Energies=	-1226.731985
Sum of electronic and thermal Energies=	-1226.702875
Sum of electronic and thermal Enthalpies=	-1226.701899
Sum of electronic and thermal Free Energies=	-1226.790083

C	-1.54714900	0.20488300	-0.38249400
C	-2.89659700	-0.75323800	-1.90818600
H	-3.24310900	-1.03572100	-2.88864500
C	-3.38693200	-1.04734200	-0.69019600
H	-4.23984500	-1.64277000	-0.41271200
N	-1.78827000	0.05848100	-1.72386000
N	-2.58560900	-0.42592900	0.25781600
C	-2.59584700	-0.80353200	1.68045700
H	-3.13301100	-0.03842800	2.25069100
H	-1.55461500	-0.83066300	2.01086400
C	-0.92164600	0.47511800	-2.82824200
H	-0.01532000	0.89633500	-2.39233500
H	-1.42988100	1.27343700	-3.38427700
C	-3.20192300	-2.17411100	1.96187600
H	-3.23202900	-2.25266000	3.05531000
H	-4.25053900	-2.22051600	1.63921400
C	-2.39205800	-3.33892700	1.40359900
H	-2.85249300	-4.29428700	1.67523500
H	-2.31954700	-3.30287600	0.31166500
H	-1.37645000	-3.31579000	1.81126500
C	-0.55966700	-0.65756700	-3.78742100
H	-1.46533200	-1.03235400	-4.28132000
H	0.03800300	-0.19682500	-4.58409500
C	0.21256500	-1.80920600	-3.15904100
H	-0.36573600	-2.30077300	-2.37148100
H	0.45837700	-2.56079500	-3.91557100
H	1.14809800	-1.46589500	-2.70712000
C	-1.35457000	2.71067300	-0.53805400
C	-0.63902500	3.98728800	-0.09814700
C	-0.65615500	4.14894100	1.41739800
C	-0.08464200	2.90497100	2.08761600
C	-0.82348300	1.63678600	1.65930800
C	-0.78934600	1.45034100	0.13369000
H	-0.08922600	5.03964000	1.71212300
H	0.39897400	3.95399000	-0.45120100
H	-1.11328100	4.84657100	-0.58687200

H	-2.41855500	2.76818100	-0.27066600
H	-1.30710300	2.61907300	-1.62512900
H	0.97844000	2.80423100	1.83868300
H	-0.14450100	2.99087900	3.17852500
H	-0.37455700	0.76847400	2.14806700
H	-1.86876200	1.70728100	1.98220300
H	-1.69064900	4.30699600	1.75722400
O	0.58267900	1.32789300	-0.25903500
C	5.24640700	-0.47132600	-0.07222000
C	4.70795700	0.79823300	-0.37471600
C	3.33831100	0.95476500	-0.33437400
C	2.48196800	-0.11320600	0.00065200
C	3.01236900	-1.40957400	0.36349000
H	2.89111500	1.91544400	-0.57468900
H	6.32386000	-0.61863200	-0.11072600
H	5.35648200	1.62746100	-0.63841000
C	1.05512800	0.05523800	-0.03181900
N	0.15241900	-0.84422100	0.11134800
N	2.20311200	-2.39950500	0.75554200
H	0.58756300	-1.77650700	0.26465300
H	2.74167700	-3.24669200	0.92170700
C	4.43973500	-1.52832100	0.27659800
H	4.88132600	-2.49422300	0.51508500
O	0.51272900	-1.92694400	2.96638200
H	1.14301800	-2.08744200	2.21476200
H	1.03039200	-2.05883000	3.76463500

7a-w

Zero-point correction= 0.541340 (Hartree/Particle)
Thermal correction to Energy= 0.571092
Thermal correction to Enthalpy= 0.572068
Thermal correction to Gibbs Free Energy= 0.481984
Sum of electronic and zero-point Energies= -1226.737563
Sum of electronic and thermal Energies= -1226.707811
Sum of electronic and thermal Enthalpies= -1226.706835
Sum of electronic and thermal Free Energies= -1226.796919

C	1.70973200	0.49929900	0.11882000
C	3.31781600	0.10079200	1.61012000
H	3.83122100	0.15088000	2.55583800
C	3.62915100	-0.56591100	0.47775200
H	4.46334900	-1.21011000	0.25962500

N	2.13711500	0.77181300	1.37578000
N	2.63950000	-0.30779300	-0.44764400
C	2.49527300	-1.07129500	-1.70305100
H	2.82907900	-0.44040800	-2.53251000
H	1.43351600	-1.29735200	-1.81973800
C	1.43370000	1.52877200	2.42154000
H	0.42438400	1.71581300	2.05480500
H	1.94614400	2.48990600	2.54697400
C	3.24875700	-2.39502400	-1.71474600
H	3.14511300	-2.76556700	-2.74150000
H	4.32744300	-2.24834900	-1.56941200
C	2.68395400	-3.43772700	-0.75591900
H	3.22507700	-4.38415000	-0.85345600
H	2.74967500	-3.12028800	0.28960100
H	1.62803300	-3.61527200	-0.98152400
C	1.36991500	0.79425800	3.75825900
H	2.38083600	0.63957300	4.15654100
H	0.88697400	1.49000000	4.45577200
C	0.60318200	-0.52065200	3.72046400
H	1.04437600	-1.22768200	3.01230600
H	0.59489100	-0.98614500	4.71068800
H	-0.43411400	-0.36636600	3.40883400
C	0.99619700	2.80117800	-0.50307200
C	-0.06341400	3.72003900	-1.10921100
C	-0.39216200	3.32671300	-2.54425400
C	-0.78149100	1.85506500	-2.61208400
C	0.29616700	0.94517700	-2.02054500
C	0.59461600	1.31189500	-0.55512400
H	-1.19857800	3.95718000	-2.93627900
H	-0.97154500	3.66952400	-0.49690500
H	0.29733900	4.75447400	-1.06067800
H	1.93712600	2.90085200	-1.06164900
H	1.20468500	3.11164800	0.52316200
H	-1.72324900	1.69116500	-2.07572800
H	-0.95603100	1.54896100	-3.64976300
H	-0.03503500	-0.09393000	-2.09148400
H	1.21596700	1.05546300	-2.60807600
H	0.48629500	3.50505900	-3.18271700
O	-0.60524600	1.17429100	0.20177100
C	-5.22130800	-0.67374300	0.61622700
C	-4.67974200	0.62536700	0.69871100
C	-3.31148100	0.77172200	0.57546200
C	-2.45929700	-0.33043200	0.37452400
C	-2.99701500	-1.66733900	0.24036000

H	-2.86373400	1.75913400	0.64892600
H	-6.29525800	-0.81563100	0.72090400
H	-5.32036400	1.48638500	0.86111200
C	-1.02483500	-0.15181900	0.32248000
N	-0.10652700	-1.03685500	0.36172000
N	-2.20141500	-2.70975500	-0.02886000
H	-0.55461600	-1.96705900	0.40830700
H	-2.75226400	-3.56506500	-0.05609000
C	-4.41922000	-1.77010100	0.39853000
H	-4.86266600	-2.76190100	0.32753800
O	-0.55672400	-2.52629600	-2.26125700
H	-1.16050500	-2.59935600	-1.46419500
H	-1.07948000	-2.84460300	-3.00176500

TS4a$_1$-w

Zero-point correction=	0.536444 (Hartree/Particle)
Thermal correction to Energy=	0.568148
Thermal correction to Enthalpy=	0.569124
Thermal correction to Gibbs Free Energy=	0.471060
Sum of electronic and zero-point Energies=	-1226.663302
Sum of electronic and thermal Energies=	-1226.631598
Sum of electronic and thermal Enthalpies=	-1226.630622
Sum of electronic and thermal Free Energies=	-1226.728685

C	2.57610800	-0.04455900	0.29656000
C	4.76964100	0.34457700	0.81397700
H	5.82651600	0.13265300	0.88170700
C	4.05905500	1.43101600	1.20635300
H	4.38197300	2.34490400	1.68177900
N	3.85200300	-0.53333900	0.26673100
N	2.74210300	1.17495000	0.87922600
C	1.65573500	2.12727800	1.09028000
H	1.48628000	2.24731600	2.16666900
H	0.76265400	1.68421000	0.64758900
C	4.22414400	-1.79310500	-0.35136500
H	3.28956700	-2.31693400	-0.56754600
H	4.78988700	-2.39145300	0.37369800
C	1.91545500	3.48088100	0.43646800
H	1.03403500	4.09824300	0.64642400
H	2.76330000	3.98442900	0.92160700
C	2.14251900	3.38938400	-1.06751400
H	2.25807700	4.38572900	-1.50632000
H	3.04750100	2.81664300	-1.29897400

H	1.29711100	2.89077400	-1.55124300
C	5.03222000	-1.61565000	-1.63554800
H	5.96537100	-1.08542100	-1.40500200
H	5.32714000	-2.61473200	-1.98118100
C	4.27344000	-0.88155300	-2.73287900
H	3.96815700	0.11711700	-2.40635500
H	4.89155400	-0.77090200	-3.62902900
H	3.36411000	-1.42301500	-3.01587000
C	0.30758200	-2.58901500	-0.02620800
C	-0.61752000	-3.61953900	0.66443300
C	-0.93389100	-3.19736700	2.09648100
C	-1.54189100	-1.79882100	2.13895200
C	-0.63569000	-0.75122000	1.44024000
C	-0.34725100	-1.26169700	0.08196800
H	-1.62359500	-3.91742200	2.55139900
H	-1.54742900	-3.71941000	0.09030200
H	-0.12181900	-4.59568500	0.63695900
H	1.25943300	-2.53236100	0.50826300
H	0.49184000	-2.83622600	-1.07393200
H	-2.52641200	-1.79560800	1.65590700
H	-1.69387200	-1.46261600	3.16926600
H	-1.09478500	0.24237300	1.45298800
H	0.32716200	-0.70266700	1.96132300
H	-0.01285600	-3.21905300	2.69532900
O	-0.82440000	-0.78253400	-0.98764600
C	-5.81893800	-0.32365500	-0.84282800
C	-4.93030800	-1.39438200	-1.08481800
C	-3.57588700	-1.13422800	-1.08992700
C	-3.06493200	0.15829800	-0.84727400
C	-3.95791600	1.27013800	-0.58226900
H	-2.88354200	-1.93921300	-1.32191100
H	-6.89131400	-0.50679500	-0.84636800
H	-5.30493700	-2.39285500	-1.28534000
C	-1.66306700	0.45988300	-0.93338700
N	-0.98695200	1.51465300	-0.99007400
N	-3.46918500	2.48173600	-0.32119000
H	-1.67694300	2.28807100	-0.93966500
H	-4.23115700	3.14463300	-0.19618000
C	-5.35755100	0.94798600	-0.60734200
H	-6.06152800	1.75747500	-0.42425100
O	-1.91710200	2.22823900	1.97653200
H	-2.45829100	2.39879700	1.15741400
H	-2.50330900	2.42944800	2.71048400

8a-w

Zero-point correction=	0.536445 (Hartree/Particle)
Thermal correction to Energy=	0.568149
Thermal correction to Enthalpy=	0.569124
Thermal correction to Gibbs Free Energy=	0.471049
Sum of electronic and zero-point Energies=	-1226.663301
Sum of electronic and thermal Energies=	-1226.631597
Sum of electronic and thermal Enthalpies=	-1226.630621
Sum of electronic and thermal Free Energies=	-1226.728696

C	2.57618200	-0.04454300	0.29655900
C	4.76968900	0.34448600	0.81415000
H	5.82653500	0.13247200	0.88205700
C	4.05916800	1.43107600	1.20621400
H	4.38211800	2.34502400	1.68150100
N	3.85203400	-0.53344900	0.26696100
N	2.74223600	1.17507400	0.87896600
C	1.65589800	2.12747500	1.08984300
H	1.48645400	2.24769100	2.16621600
H	0.76278800	1.68438800	0.64722000
C	4.22415100	-1.79329600	-0.35099500
H	3.28956800	-2.31704600	-0.56733900
H	4.78969000	-2.39166200	0.37421300
C	1.91567300	3.48096000	0.43581200
H	1.03423000	4.09835700	0.64556600
H	2.76346700	3.98460800	0.92093500
C	2.14287900	3.38917600	-1.06813000
H	2.25863500	4.38543000	-1.50709300
H	3.04779900	2.81626100	-1.29940200
H	1.29745100	2.89060500	-1.55186400
C	5.03254000	-1.61599900	-1.63500300
H	5.96564400	-1.08576800	-1.40427500
H	5.32752800	-2.61512300	-1.98045500
C	4.27405300	-0.88199700	-2.73259600
H	3.96891300	0.11680100	-2.40632800
H	4.89231100	-0.77166100	-3.62868400
H	3.36466100	-1.42335200	-3.01559700
C	0.30743300	-2.58883700	-0.02659200
C	-0.61780400	-3.61950400	0.66364500
C	-0.93446100	-3.19762900	2.09571600
C	-1.54242000	-1.79906700	2.13840400
C	-0.63609700	-0.75133600	1.44004500
C	-0.34743200	-1.26154100	0.08170200

H	-1.62427700	-3.91776400	2.55033800
H	-1.54759200	-3.71925900	0.08930100
H	-0.12209600	-4.59564400	0.63607800
H	1.25917500	-2.53230200	0.50808900
H	0.49192300	-2.83583900	-1.07432500
H	-2.52689100	-1.79569900	1.65526000
H	-1.69449400	-1.46308000	3.16877600
H	-1.09520900	0.24224500	1.45289300
H	0.32665500	-0.70284600	1.96131800
H	-0.01354900	-3.21948100	2.69474700
O	-0.82435800	-0.78216800	-0.98791200
C	-5.81891300	-0.32376000	-0.84206600
C	-4.93024200	-1.39437100	-1.08441500
C	-3.57584500	-1.13409500	-1.08978400
C	-3.06494500	0.15844000	-0.84704700
C	-3.95797500	1.27016300	-0.58169800
H	-2.88348800	-1.93898900	-1.32205700
H	-6.89127300	-0.50699700	-0.84538800
H	-5.30482600	-2.39284700	-1.28500300
C	-1.66312100	0.46016000	-0.93341100
N	-0.98707700	1.51496800	-0.99012300
N	-3.46929800	2.48177700	-0.32059500
H	-1.67711900	2.28831900	-0.93946400
H	-4.23131500	3.14459200	-0.19541400
C	-5.35758500	0.94788900	-0.60650400
H	-6.06159400	1.75729000	-0.42314300
O	-1.91702400	2.22838100	1.97702200
H	-2.45826900	2.39877700	1.15790200
H	-2.50271500	2.43110800	2.71096900

3:

Zero-point correction=0.357497 (Hartree/Particle)
Thermal correction to Energy=0.379785
Thermal correction to Enthalpy=0.380761
Thermal correction to Gibbs Free Energy=0.302640
Sum of electronic and zero-point Energies=-840.869050
Sum of electronic and thermal Energies=-840.846762
Sum of electronic and thermal Enthalpies=-840.845786
Sum of electronic and thermal Free Energies=-840.923907

C	-1.64136600	-0.07195600	-0.66229700

C	-3.90264700	-0.39469700	-0.79361400
H	-4.82334100	-0.95711500	-0.84546100
C	-3.68230300	0.94322000	-0.82590800
H	-4.37567700	1.76687900	-0.91113700
N	-2.65519200	-0.98448100	-0.69522000
N	-2.31225600	1.11093800	-0.74483000
C	-1.65822300	2.41075300	-0.73846700
H	-1.96814800	2.96025000	-1.63563100
H	-0.58623500	2.21824700	-0.81627700
C	-2.44319400	-2.41805700	-0.61207800
H	-1.37001600	-2.57215700	-0.75399000
H	-2.96471800	-2.89905100	-1.44859300
C	-1.95968800	3.22999900	0.51354300
H	-1.48004700	4.20783400	0.38351100
H	-3.03947300	3.42224200	0.57700400
C	-1.46550500	2.57869000	1.79830300
H	-1.70367900	3.19925000	2.66812400
H	-1.92531200	1.59643100	1.94925400
H	-0.38022200	2.43900000	1.76739800
C	-2.90060200	-3.02286300	0.71345700
H	-3.97839500	-2.85319800	0.83721300
H	-2.76973600	-4.11031000	0.64241600
C	-2.14700400	-2.48234100	1.92138700
H	-2.27354000	-1.39954700	2.01578800
H	-2.50388500	-2.94683200	2.84594500
H	-1.07238700	-2.67821100	1.83753100
C	3.70563400	-2.34641400	-0.21542200
C	2.33667100	-2.10090900	-0.35821900
C	1.86941600	-0.79555300	-0.32441700
C	2.77530900	0.26197800	-0.14988600
C	4.16440100	0.02498000	-0.00938700
H	0.80461700	-0.57614700	-0.42956600
H	4.07822200	-3.36707600	-0.23940100
H	1.64193800	-2.92349000	-0.49474500
C	2.31270700	1.60870400	-0.09484200
N	1.99386800	2.72700600	-0.03161200
N	5.05087300	1.06550600	0.11055000
H	4.68715900	1.97795900	0.34127600
H	5.96618100	0.86291600	0.47680600
C	4.60739300	-1.30662800	-0.04475400
H	5.66964700	-1.51410600	0.05591800

TS1:

Zero-point correction=0.357507 (Hartree/Particle)
Thermal correction to Energy=0.378359
Thermal correction to Enthalpy=0.379335
Thermal correction to Gibbs Free Energy=0.306969
Sum of electronic and zero-point Energies=-840.853679
Sum of electronic and thermal Energies=-840.832828
Sum of electronic and thermal Enthalpies=-840.831852
Sum of electronic and thermal Free Energies=-840.904217

C	1.00117300	-0.00106700	-0.39127700
C	3.03103800	0.79862700	-0.99373500
H	3.77014800	1.54595500	-1.24018900
C	3.11566500	-0.55552500	-0.97607500
H	3.94324100	-1.21104000	-1.20205800
N	1.73789600	1.11382000	-0.62267800
N	1.87198300	-1.02039800	-0.59507800
C	1.51301600	-2.42495500	-0.49087400
H	1.78209500	-2.91766700	-1.43183700
H	0.42400900	-2.45923900	-0.40329400
C	1.20413200	2.46466800	-0.55532000
H	0.12254600	2.36265700	-0.43457200
H	1.38301700	2.95296400	-1.51992200
C	2.17177800	-3.12514400	0.69438800
H	1.90640800	-4.18801300	0.63532800
H	3.26351700	-3.07695300	0.58703000
C	1.75420800	-2.55698400	2.04435500
H	2.23985900	-3.09517900	2.86413100
H	2.02531000	-1.49967400	2.13140600
H	0.67048300	-2.63349800	2.18562900
C	1.79701800	3.28737500	0.58509600
H	2.88167000	3.38277900	0.44311600
H	1.38895600	4.30228100	0.50172200
C	1.49922000	2.71611200	1.96505500
H	1.91289500	1.70824000	2.07491700
H	1.93214000	3.34253200	2.75099200
H	0.41982500	2.65200200	2.14045500
C	-3.93015300	-0.05254100	1.60871000
C	-2.60741400	-0.04408300	2.05881600
C	-1.58172500	-0.05660900	1.12231000
C	-1.84127600	-0.07565100	-0.24845000
C	-3.18864500	-0.07595200	-0.70853400
H	-0.53869900	-0.05749000	1.42633500
H	-4.74904200	-0.04559300	2.32345600
H	-2.38325500	-0.03103200	3.12087700

C	-0.80371100	-0.12318400	-1.27171000
N	-0.65096000	-0.20377500	-2.45496000
N	-3.46774800	-0.05056400	-2.04314500
H	-2.68890100	-0.20630800	-2.67762500
H	-4.39529100	-0.28865700	-2.34943200
C	-4.21736100	-0.06661400	0.25236700
H	-5.25089800	-0.06348100	-0.08616500

4:

Zero-point correction=0.358954 (Hartree/Particle)
Thermal correction to Energy=0.379903
Thermal correction to Enthalpy=0.380878
Thermal correction to Gibbs Free Energy=0.308369
Sum of electronic and zero-point Energies=-840.869405
Sum of electronic and thermal Energies=-840.848456
Sum of electronic and thermal Enthalpies=-840.847481
Sum of electronic and thermal Free Energies=-840.919990

C	0.94489200	0.01132100	-0.60155600
C	3.03148300	0.79630100	-0.45451200
H	3.81442200	1.53707800	-0.41322600
C	3.09922300	-0.55824900	-0.44732400
H	3.95254900	-1.21612500	-0.39794900
N	1.69439800	1.13450800	-0.52187700
N	1.80345100	-1.02993100	-0.51025900
C	1.41667900	-2.42976300	-0.62581700
H	1.80335100	-2.81045300	-1.57798900
H	0.32644100	-2.44348200	-0.69239100
C	1.16758900	2.48716300	-0.65031000
H	0.08047100	2.39109400	-0.69948500
H	1.50205500	2.89139600	-1.61257300
C	1.89981100	-3.27870900	0.54454100
H	1.59932400	-4.31204100	0.33344100
H	2.99743000	-3.28637400	0.57330600
C	1.34248300	-2.83641000	1.89138200
H	1.68787200	-3.49606600	2.69299500
H	1.66102800	-1.81830200	2.13905700
H	0.24745000	-2.84937000	1.89027000
C	1.57852500	3.39772800	0.50118200
H	2.66939100	3.52252600	0.50866400
H	1.16583800	4.39016400	0.28377000
C	1.09578700	2.91717700	1.86366500
H	1.53158300	1.94582600	2.12047700

H	1.37747900	3.62467000	2.64924400
H	0.00648600	2.80659400	1.88122500
C	-3.81045700	-0.09153000	1.50616600
C	-2.51529500	-0.05724600	2.03106700
C	-1.44115100	-0.03956000	1.14670800
C	-1.61893100	-0.05040400	-0.23904600
C	-2.94069700	-0.07493800	-0.76749100
H	-0.42395600	-0.02214200	1.53643000
H	-4.66703200	-0.11017700	2.17539200
H	-2.35097400	-0.04822100	3.10432500
C	-0.46899700	-0.05967700	-1.17337700
N	-0.41795400	-0.11250100	-2.42840000
N	-3.11276200	-0.05217100	-2.11415300
H	-2.24207300	-0.12711500	-2.66761300
H	-4.02235500	-0.22316800	-2.50721100
C	-4.02269800	-0.10050400	0.13517100
H	-5.03618800	-0.12185100	-0.26001300

TS2:

Zero-point correction=0.355758 (Hartree/Particle)
Thermal correction to Energy=0.375842
Thermal correction to Enthalpy=0.376818
Thermal correction to Gibbs Free Energy=0.306130
Sum of electronic and zero-point Energies=-840.869462
Sum of electronic and thermal Energies=-840.849378
Sum of electronic and thermal Enthalpies=-840.848402
Sum of electronic and thermal Free Energies=-840.919090

C	0.98842900	-0.09134500	-0.60581500
C	2.89767600	1.03996300	-0.43392200
H	3.54748800	1.90021700	-0.42856800
C	3.17933100	-0.27861000	-0.27669100
H	4.11818600	-0.78035000	-0.10211700
N	1.53448100	1.14044600	-0.62192500
N	1.98820600	-0.96301600	-0.37828700
C	1.84064400	-2.41549400	-0.33119000
H	2.49190800	-2.83490500	-1.10484100
H	0.81126300	-2.62573900	-0.62847100
C	0.80349900	2.36201800	-0.96324600
H	-0.25843300	2.11483000	-0.89095000
H	1.01969500	2.59748700	-2.01126400
C	2.16331300	-3.00067800	1.03892100
H	2.06536400	-4.08903400	0.94630100

H	3.21661200	-2.81245000	1.28652900
C	1.26208500	-2.48734900	2.15405500
H	1.49296400	-2.98525700	3.10040200
H	1.38923600	-1.41088300	2.30912400
H	0.20560000	-2.66326600	1.92707100
C	1.14687600	3.53902500	-0.05956900
H	2.20442400	3.80956000	-0.17702600
H	0.58056300	4.39618000	-0.44233100
C	0.81713200	3.31463800	1.41065800
H	1.39306300	2.48286300	1.83058200
H	1.04951400	4.20685600	1.99961400
H	-0.24461400	3.08529200	1.54592400
C	-3.81554000	0.19007100	1.37850300
C	-2.54488400	0.44184600	1.92340500
C	-1.42985100	0.22940600	1.12352100
C	-1.54501600	-0.22155500	-0.19596100
C	-2.84047700	-0.49781300	-0.75255300
H	-0.43538300	0.41097500	1.53148000
H	-4.70121000	0.35220000	1.98888500
H	-2.43902500	0.78758700	2.94714500
C	-0.39746100	-0.45148000	-1.07745000
N	-0.41139100	-0.90081600	-2.27000300
N	-2.87950600	-0.95398800	-2.01178700
H	-1.72482200	-1.03932900	-2.42303400
H	-3.79204800	-1.14436100	-2.40354900
C	-3.96775800	-0.26547400	0.08241100
H	-4.96086200	-0.45985800	-0.31736300

5:

Zero-point correction=0.360748 (Hartree/Particle)
Thermal correction to Energy=0.381078
Thermal correction to Enthalpy=0.382054
Thermal correction to Gibbs Free Energy=0.310798
Sum of electronic and zero-point Energies=-840.879940
Sum of electronic and thermal Energies=-840.859609
Sum of electronic and thermal Enthalpies=-840.858633
Sum of electronic and thermal Free Energies=-840.929889

C	0.96431400	-0.00006000	-0.69447300
C	3.01270700	0.68007400	-0.19512600
H	3.80878000	1.38127400	-0.00213300
C	3.01312400	-0.67877000	-0.19490500
H	3.80962300	-1.37942100	-0.00167500

N	1.73119700	1.08254400	-0.50170700
N	1.73186400	-1.08212600	-0.50136000
C	1.28186900	-2.46267700	-0.69825400
H	1.72326100	-2.82257300	-1.63328500
H	0.20005400	-2.41083700	-0.84165800
C	1.28037000	2.46274700	-0.69917500
H	0.19855900	2.41021500	-0.84236900
H	1.72140600	2.82245600	-1.63444700
C	1.63505700	-3.37631400	0.46778800
H	1.28481300	-4.37729500	0.18964400
H	2.72556000	-3.46119800	0.56398100
C	1.01593900	-2.95756800	1.79492400
H	1.24867500	-3.68676700	2.57639800
H	1.39522600	-1.98565000	2.12825700
H	-0.07289600	-2.87526800	1.71867500
C	1.63322700	3.37716200	0.46635400
H	2.72369800	3.46267500	0.56235600
H	1.28242500	4.37781400	0.18772700
C	1.01450600	2.95881300	1.79380000
H	1.39444300	1.98734000	2.12769200
H	1.24685100	3.68863600	2.57480800
H	-0.07428400	2.87577500	1.71770500
C	-3.62919900	0.00005600	1.57307400
C	-2.29012100	0.00048900	2.03970600
C	-1.27699800	0.00026800	1.10582900
C	-1.52347300	-0.00036500	-0.28582300
C	-2.89234100	-0.00084600	-0.78545700
H	-0.24407300	0.00058700	1.45493900
H	-4.44481200	0.00022200	2.29355800
H	-2.07148200	0.00097100	3.10291800
C	-0.43448900	-0.00059700	-1.22709100
N	-0.43397000	-0.00120000	-2.51986500
N	-3.12346400	-0.00147900	-2.08358800
H	-1.43208900	-0.00149900	-2.80965100
H	-4.12692800	-0.00175600	-2.26034900
C	-3.91817200	-0.00057400	0.23436100
H	-4.95411300	-0.00090300	-0.10064200

6:

Zero-point correction=0.512754 (Hartree/Particle)
Thermal correction to Energy=0.541708
Thermal correction to Enthalpy=0.542684
Thermal correction to Gibbs Free Energy=0.450705

Sum of electronic and zero-point Energies=-1150.381606
Sum of electronic and thermal Energies=-1150.352652
Sum of electronic and thermal Enthalpies=-1150.351676
Sum of electronic and thermal Free Energies=-1150.443655

C	2.02705500	0.39927900	-0.71797900
C	3.10295300	2.31560800	-0.44743100
H	3.22892300	3.36105800	-0.21683100
C	4.00648200	1.38434600	-0.85090500
H	5.06678100	1.46436500	-1.03139700
N	1.88180400	1.68593000	-0.36401100
N	3.32098100	0.20213100	-1.01474400
C	3.90418900	-1.05827800	-1.47719900
H	4.33209000	-0.87332100	-2.46747300
H	3.07026600	-1.74998500	-1.60938500
C	0.58757200	2.33311900	-0.09615500
H	-0.11412400	1.53985400	0.16234300
H	0.24012900	2.78137900	-1.03144400
C	4.94977400	-1.61257800	-0.51678100
H	5.33870800	-2.52887800	-0.97682200
H	5.80225000	-0.92340600	-0.45238200
C	4.40985500	-1.91343100	0.87508200
H	5.18058500	-2.37786300	1.49702400
H	4.08158400	-1.00204100	1.38520500
H	3.55149200	-2.59163800	0.83473500
C	0.64223400	3.36820700	1.01506500
H	1.28756700	4.20941100	0.72791800
H	-0.37352500	3.77344100	1.07433600
C	1.05806500	2.81295800	2.37157100
H	2.07720200	2.40959900	2.35596900
H	1.02746900	3.59635800	3.13478500
H	0.38626500	2.00786200	2.68602200
C	-0.86871000	-2.38505200	2.48330000
C	0.19312300	-1.46528700	2.65242700
C	0.74694900	-0.89616600	1.52479900
C	0.28873600	-1.18379600	0.22067700
C	-0.80767300	-2.12140700	0.02700600
H	1.57714300	-0.20131100	1.64701000
H	-1.31429600	-2.85491700	3.35791500
H	0.56877200	-1.22411100	3.64168000
C	0.92882100	-0.59588000	-0.93434100
N	0.71480600	-0.79151800	-2.19317100
N	-1.25220100	-2.38796900	-1.19097400
H	-0.06886100	-1.46917600	-2.25659600

H	-1.99920400	-3.08006500	-1.14316700
C	-1.34418000	-2.70097800	1.23602200
H	-2.15545000	-3.41949600	1.12750000
C	-3.22897600	0.54775300	-1.56605300
C	-4.68161200	0.16564700	-1.88335900
C	-5.28985400	-0.67647500	-0.76445000
C	-5.22212700	0.05796900	0.57219800
C	-3.78300900	0.45694300	0.92534600
C	-3.09886000	1.18396300	-0.20822600
H	-6.33047300	-0.92757700	-1.00278300
H	-5.28302300	1.07528900	-2.02219600
H	-4.71141400	-0.37758200	-2.83454200
H	-2.62032500	-0.37293300	-1.54887400
H	-2.80244100	1.22017800	-2.31565900
H	-5.84556000	0.96163100	0.52087300
H	-5.63681500	-0.56050500	1.37657000
H	-3.73430300	1.08150500	1.82193200
H	-3.19106000	-0.45102400	1.11760300
H	-4.74306800	-1.62684800	-0.68826700
O	-2.45948200	2.20899100	-0.02187500

TS3:

Zero-point correction=0.514229 (Hartree/Particle)
Thermal correction to Energy=0.541153
Thermal correction to Enthalpy=0.542128
Thermal correction to Gibbs Free Energy=0.457962
Sum of electronic and zero-point Energies=-1150.361171
Sum of electronic and thermal Energies=-1150.334247
Sum of electronic and thermal Enthalpies=-1150.333271
Sum of electronic and thermal Free Energies=-1150.417437

C	-1.73089600	-0.86355400	-0.51602500
C	-2.75949700	-2.68714700	0.17939000
H	-2.85578400	-3.65882700	0.63725300
C	-3.69067100	-1.88483600	-0.40054300
H	-4.74963300	-2.02754000	-0.54248500
N	-1.54934200	-2.03817900	0.09666500
N	-3.03362100	-0.74950600	-0.82192200
C	-3.61031000	0.35012000	-1.60232900
H	-3.65051100	0.02813200	-2.64815000
H	-2.90083000	1.17876100	-1.53836400
C	-0.25440300	-2.58917600	0.53039200
H	0.52964100	-1.87347600	0.23399100

H	-0.11469200	-3.52078400	-0.02793400
C	-4.98549800	0.78098500	-1.11105400
H	-5.32371300	1.56174900	-1.80226500
H	-5.70340100	-0.04117900	-1.22697200
C	-5.00727300	1.31070300	0.31720800
H	-6.01322800	1.64291300	0.58955700
H	-4.70735600	0.54390800	1.03949300
H	-4.32732500	2.16070800	0.43307700
C	-0.19653100	-2.82925000	2.03309600
H	-0.97252300	-3.54316400	2.34525600
H	0.76456800	-3.32297400	2.21824200
C	-0.27651200	-1.54564200	2.84883500
H	-1.25029000	-1.05557800	2.73535300
H	-0.13792400	-1.75319000	3.91448300
H	0.49563400	-0.84269800	2.51988400
C	-0.07450000	3.61721700	1.35652400
C	-1.13784400	2.75481800	1.66228900
C	-1.25354800	1.56832100	0.95693300
C	-0.33586400	1.20290300	-0.04342200
C	0.79890400	2.03645600	-0.29622900
H	-2.09020700	0.90826600	1.17741000
H	0.02417500	4.56302900	1.88379800
H	-1.85855400	3.01308800	2.43213300
C	-0.63949000	0.07727500	-0.92851600
N	-0.17144400	-0.22368900	-2.08225200
N	1.76270200	1.59816800	-1.14475900
H	0.60755300	0.42399400	-2.27602200
H	2.45943400	2.32716000	-1.27789800
C	0.86843900	3.26414300	0.40961800
H	1.70935200	3.92431600	0.20700000
C	3.26834900	-0.49941500	-1.62639300
C	4.36324900	-1.48382400	-1.19881600
C	5.45377200	-0.79223900	-0.37844800
C	4.86895500	-0.04960300	0.82381500
C	3.79474400	0.94655400	0.37709500
C	2.69985700	0.17077400	-0.37237700
H	6.20077800	-1.52518500	-0.04717100
H	3.90175400	-2.27435200	-0.59188900
H	4.80117900	-1.97069700	-2.07986000
H	3.68812000	0.25177200	-2.30921700
H	2.46015200	-1.01953800	-2.15009300
H	4.40970000	-0.76876300	1.51447600
H	5.66367400	0.46806800	1.37660100
H	3.34063000	1.45322200	1.23556500

H	4.26436800	1.70432100	-0.26719900
H	5.98594500	-0.07323900	-1.02018800
O	1.91383000	-0.51541200	0.35647000

7:

Zero-point correction=0.515222 (Hartree/Particle)
Thermal correction to Energy=0.542297
Thermal correction to Enthalpy=0.543273
Thermal correction to Gibbs Free Energy=0.459259
Sum of electronic and zero-point Energies=-1150.360888
Sum of electronic and thermal Energies=-1150.333813
Sum of electronic and thermal Enthalpies=-1150.332837
Sum of electronic and thermal Free Energies=-1150.416850

C	-1.60308400	-0.90003800	-0.43186100
C	-2.55984200	-2.71675300	0.37346500
H	-2.61862400	-3.65282500	0.90606600
C	-3.50707000	-2.02506600	-0.31193200
H	-4.54822000	-2.24303200	-0.48538600
N	-1.38486900	-2.00746000	0.28666800
N	-2.89641100	-0.89357600	-0.80307300
C	-3.50716800	0.09590400	-1.69768300
H	-3.45742600	-0.30419500	-2.71544700
H	-2.86912800	0.98145400	-1.66452500
C	-0.08743800	-2.48034800	0.80304900
H	0.69010700	-1.78430700	0.43161200
H	0.06662800	-3.47035900	0.36053300
C	-4.93736900	0.44995000	-1.31509800
H	-5.29255000	1.14678700	-2.08321000
H	-5.58459900	-0.43215400	-1.40200300
C	-5.08040000	1.08378800	0.06304300
H	-6.12216800	1.35433800	0.25775300
H	-4.76323100	0.40175800	0.85923500
H	-4.47540500	1.99270500	0.14277700
C	-0.05219800	-2.54597100	2.32410900
H	-0.83207700	-3.22066500	2.70755800
H	0.90674500	-3.01393400	2.57605500
C	-0.13946300	-1.17801900	2.98777200
H	-1.11994300	-0.71389100	2.83128200
H	0.01271600	-1.26002600	4.06874100
H	0.62039800	-0.51151100	2.56620300
C	-0.17974500	3.73398200	1.30699300
C	-1.25380600	2.88040200	1.56963900
C	-1.31184800	1.65704600	0.91383100

C	-0.32248400	1.25750600	0.00392500
C	0.81687100	2.08582000	-0.19173600
H	-2.16317900	1.00455700	1.09665300
H	-0.12213800	4.70358100	1.79474600
H	-2.03502200	3.16876700	2.26640400
C	-0.59541000	0.11593600	-0.88557000
N	-0.25148900	-0.06751600	-2.10450400
N	1.84827900	1.64172600	-0.98384000
H	0.44743400	0.64172800	-2.35421900
H	2.53352800	2.37871800	-1.11688000
C	0.83958000	3.33559100	0.45376100
H	1.70024300	3.98254200	0.29815600
C	3.07869800	-0.40380100	-1.73310900
C	4.01072100	-1.55663400	-1.36489000
C	5.21131600	-1.07062300	-0.55376800
C	4.76544700	-0.28912200	0.68214200
C	3.84655300	0.86783000	0.29615900
C	2.60323100	0.32532900	-0.45714600
H	5.84403700	-1.91882700	-0.26098900
H	3.44107200	-2.28059600	-0.76728400
H	4.34834300	-2.07903400	-2.26967300
H	3.60129400	0.29832000	-2.40098200
H	2.20291900	-0.78258800	-2.27040100
H	4.20937400	-0.95353100	1.35564000
H	5.63796600	0.08263900	1.23553200
H	3.49369200	1.40330000	1.18594000
H	4.40970500	1.57836200	-0.33201300
H	5.83463200	-0.41983200	-1.18678500
O	1.82297000	-0.39084000	0.32394700

TS4:

Zero-point correction=0.514660 (Hartree/Particle)
Thermal correction to Energy=0.540898
Thermal correction to Enthalpy=0.541874
Thermal correction to Gibbs Free Energy=0.459369
Sum of electronic and zero-point Energies=-1150.349849
Sum of electronic and thermal Energies=-1150.323611
Sum of electronic and thermal Enthalpies=-1150.322635
Sum of electronic and thermal Free Energies=-1150.405140

C	-1.21512000	-0.77222500	0.45438500
C	-2.45306600	-1.04667200	2.31719300
H	-2.81642000	-0.82550900	3.30902100

C	-2.77032200	-2.04991200	1.46352500
H	-3.45826200	-2.87524000	1.56656800
N	-1.50066000	-0.27587100	1.68073500
N	-2.00061900	-1.86431700	0.33166300
C	-2.01299400	-2.79357500	-0.80010000
H	-1.84511300	-3.79688900	-0.39233500
H	-1.14528100	-2.52088100	-1.41706200
C	-0.84527700	0.86358400	2.31526900
H	-0.09063800	1.22975100	1.62037700
H	-0.31496100	0.48966200	3.19888400
C	-3.32230000	-2.75544100	-1.58095000
H	-3.26880700	-3.55246600	-2.33288900
H	-4.16196100	-3.01618100	-0.92157000
C	-3.59746600	-1.42116200	-2.26160100
H	-4.54269400	-1.44803000	-2.81280400
H	-3.66272900	-0.60783300	-1.53080800
H	-2.80038900	-1.17352700	-2.97054500
C	-1.81823800	1.97032500	2.70790700
H	-2.53146200	1.59328600	3.45334000
H	-1.22964500	2.74144500	3.22024700
C	-2.56521700	2.58211500	1.53063400
H	-3.16909400	1.83229000	1.00857600
H	-3.23924800	3.37570100	1.86850300
H	-1.87247700	3.01084200	0.79981200
C	-0.10496600	3.86648600	-1.57079400
C	-1.08290400	2.98942100	-2.04483600
C	-0.97675700	1.63495500	-1.74497400
C	0.08019300	1.13376300	-0.98647300
C	1.06246500	2.02302100	-0.50993800
H	-1.73399800	0.93945500	-2.09911800
H	-0.16651900	4.92773600	-1.79643700
H	-1.91574000	3.35806200	-2.63592800
C	0.24977000	-0.34458400	-0.74375300
N	0.33108700	-1.17348700	-1.76643400
N	2.08425000	1.54517300	0.29728400
H	-0.05043800	-0.71969800	-2.59459800
H	2.89362300	2.14874900	0.35180500
C	0.95431000	3.39100700	-0.80914200
H	1.71390800	4.07745800	-0.44040200
C	3.21170500	-0.21920400	-1.04542100
C	3.62027600	-1.68871100	-1.08349500
C	4.40241900	-2.07993500	0.16892700
C	3.61688000	-1.74266800	1.43500300
C	3.20311700	-0.27287800	1.46304100

C	2.40738000	0.12001000	0.22009400
H	4.64388600	-3.14976900	0.15002000
H	2.70725000	-2.28853300	-1.17345700
H	4.21977800	-1.87862000	-1.98226100
H	4.10882500	0.41902500	-1.03723500
H	2.62733900	0.03772200	-1.93260400
H	2.71262400	-2.36175500	1.47740100
H	4.20752000	-1.97403500	2.32994900
H	2.59234600	-0.04667400	2.34396800
H	4.09773600	0.36509600	1.51024900
H	5.36323000	-1.54262500	0.18432600
O	1.18326000	-0.58935100	0.31340900

8:

Zero-point correction=0.515228 (Hartree/Particle)
Thermal correction to Energy=0.543006
Thermal correction to Enthalpy=0.543982
Thermal correction to Gibbs Free Energy=0.454437
Sum of electronic and zero-point Energies=-1150.385910
Sum of electronic and thermal Energies=-1150.358132
Sum of electronic and thermal Enthalpies=-1150.357156
Sum of electronic and thermal Free Energies=-1150.446702

C	2.94864300	-0.40279600	-0.67159400
C	5.23287700	-0.50600500	-0.63866900
H	6.24255300	-0.12410600	-0.60482700
C	4.77172600	-1.77620100	-0.75122200
H	5.30376800	-2.71261300	-0.83267100
N	4.11263000	0.30412500	-0.59361600
N	3.39252800	-1.68740800	-0.77089700
C	2.51908600	-2.84928900	-0.86950600
H	2.87073300	-3.46698300	-1.70440800
H	1.52154300	-2.48029900	-1.11903900
C	4.17304200	1.74939800	-0.46514700
H	3.16493800	2.11697800	-0.67296400
H	4.83573500	2.14157200	-1.24605600
C	2.47279700	-3.67341900	0.41499700
H	1.86422300	-4.56235700	0.20627900
H	3.47993400	-4.03995000	0.65650200
C	1.89032000	-2.91421300	1.60004900
H	1.84032700	-3.55245600	2.48822600
H	2.49911600	-2.03885000	1.84922600
H	0.88013300	-2.55814000	1.37229800

C	4.64621600	2.21447100	0.91050700
H	5.66110500	1.83617000	1.09063300
H	4.73068700	3.30831100	0.87800400
C	3.72525400	1.79306400	2.04798200
H	3.63034500	0.70393200	2.09815200
H	4.10733400	2.14381400	3.01175500
H	2.71778200	2.20276100	1.91630500
C	-1.09368100	4.12115500	0.08560600
C	0.08692400	3.37211100	0.08581400
C	0.02657200	2.00371700	-0.14102500
C	-1.19666700	1.36511300	-0.36728200
C	-2.38480800	2.12241900	-0.34189800
H	0.93819000	1.40886100	-0.15676500
H	-1.05813500	5.19358100	0.25749200
H	1.04278000	3.85793000	0.25763700
C	-1.26941400	-0.08046500	-0.67942400
N	-0.31639400	-0.90274400	-0.83113900
N	-3.58191200	1.47542000	-0.56901600
H	0.60347200	-0.45737200	-0.74297900
H	-4.41476500	1.99222800	-0.32490100
C	-2.31924000	3.50657900	-0.12258600
H	-3.23665000	4.09057600	-0.11498600
C	-3.58246400	-0.22335600	1.25181900
C	-3.69212600	-1.71657500	1.55487400
C	-4.95376800	-2.31333800	0.93419300
C	-5.00558900	-2.04549600	-0.56887900
C	-4.88219500	-0.55527500	-0.87885800
C	-3.63143700	0.05710500	-0.25920400
H	-4.99762400	-3.39183900	1.12649200
H	-2.80820400	-2.22764100	1.15380100
H	-3.68667700	-1.87233100	2.64014200
H	-4.42016300	0.31512100	1.71748700
H	-2.66147700	0.19601500	1.67296900
H	-4.18378900	-2.57645500	-1.06387100
H	-5.93869900	-2.42998700	-0.99692100
H	-4.84847700	-0.37342800	-1.95796500
H	-5.75404400	-0.01813400	-0.47810800
H	-5.83987100	-1.87298100	1.41609500
O	-2.52831200	-0.57123700	-0.90295400

TS5:

Zero-point correction=0.513474 (Hartree/Particle)
Thermal correction to Energy=0.539351

Thermal correction to Enthalpy=0.540326
Thermal correction to Gibbs Free Energy=0.457991
Sum of electronic and zero-point Energies=-1150.329772
Sum of electronic and thermal Energies=-1150.303895
Sum of electronic and thermal Enthalpies=-1150.302919
Sum of electronic and thermal Free Energies=-1150.385255

C	-1.95250900	-0.06103900	-0.06303000
C	-2.25542000	-1.01930200	1.97363600
H	-2.15454700	-1.13609800	3.04196800
C	-2.91078000	-1.78516100	1.06760700
H	-3.48141500	-2.69253800	1.19917800
N	-1.68736800	0.03303200	1.28025900
N	-2.73756000	-1.19398500	-0.16956400
C	-3.15655600	-1.75572300	-1.43217500
H	-3.31975700	-2.82694900	-1.27408000
H	-2.30847000	-1.65192100	-2.12390500
C	-1.01387300	1.16641300	1.88832000
H	-0.65081100	1.79390900	1.07061100
H	-0.13558900	0.80388300	2.43390200
C	-4.41485100	-1.11891800	-2.02224500
H	-4.72610300	-1.73493500	-2.87627400
H	-5.22255200	-1.18144000	-1.28181400
C	-4.22546000	0.32466300	-2.46968900
H	-5.15853000	0.74139100	-2.86224400
H	-3.89254600	0.95488900	-1.63859600
H	-3.47314900	0.39203400	-3.26487500
C	-1.92863700	1.97983300	2.80158400
H	-2.27401300	1.34861400	3.63124900
H	-1.31764000	2.77057800	3.25435600
C	-3.12389000	2.58752500	2.07956300
H	-3.74316600	1.81137100	1.61842700
H	-3.75427700	3.15531900	2.77129600
H	-2.79895200	3.26649900	1.28375700
C	2.81223300	3.81099300	-0.90138100
C	1.56852500	3.75320100	-1.53063100
C	0.79923500	2.59780100	-1.44859000
C	1.24473500	1.46448800	-0.73491900
C	2.50622000	1.54986800	-0.07773800
H	-0.17014000	2.57374200	-1.94144300
H	3.42299000	4.70641300	-0.96690400
H	1.19522700	4.60929600	-2.08550000
C	0.52199200	0.23305400	-0.65185300
N	-0.70790600	-0.01706100	-1.11967300

N	2.89825000	0.47090900	0.71646700
H	-0.98444600	0.63210100	-1.84359900
H	3.88679400	0.45653700	0.93151700
C	3.27204600	2.70753100	-0.17878300
H	4.23275700	2.75228800	0.33116200
C	2.95942200	-1.36476300	-0.96594600
C	2.45512100	-2.76728400	-1.29844700
C	2.73629200	-3.74001900	-0.15495900
C	2.14208600	-3.22978400	1.15654800
C	2.63531500	-1.82229900	1.48746000
C	2.37147700	-0.83972600	0.35233000
H	2.33433800	-4.73294300	-0.39035400
H	1.37459600	-2.71972900	-1.48352100
H	2.92285100	-3.11901500	-2.22596800
H	4.05359000	-1.37627300	-0.86022900
H	2.72271500	-0.66041700	-1.77085200
H	1.04815300	-3.20962200	1.07765100
H	2.39067000	-3.90809500	1.98161300
H	2.15544300	-1.43189400	2.39121700
H	3.71877800	-1.84193900	1.67334100
H	3.82406100	-3.86210800	-0.04044900
O	0.95861100	-0.72016600	0.25337200

9:

Zero-point correction=0.514724 (Hartree/Particle)
Thermal correction to Energy=0.539071
Thermal correction to Enthalpy=0.540047
Thermal correction to Gibbs Free Energy=0.462518
Sum of electronic and zero-point Energies=-1150.360472
Sum of electronic and thermal Energies=-1150.336125
Sum of electronic and thermal Enthalpies=-1150.335149
Sum of electronic and thermal Free Energies=-1150.412678

C	-1.79896800	-0.36873400	0.13848500
C	-3.36918200	-1.23125600	1.46634300
H	-3.84228800	-1.48532200	2.40161400
C	-3.74854300	-1.47163800	0.19504300
H	-4.61233100	-1.98036100	-0.20242400
N	-2.16318500	-0.54770300	1.43731400
N	-2.76946200	-0.94234900	-0.63584100
C	-2.77527100	-1.06067600	-2.08375200
H	-3.12565800	-2.07143400	-2.32279600
H	-1.73685700	-0.99642800	-2.42828600

C	-1.50525400	-0.02996800	2.63607000
H	-0.45963900	0.15197600	2.35300600
H	-1.56046300	-0.82238300	3.39157300
C	-3.64902900	-0.02242900	-2.78481900
H	-3.65336800	-0.27046100	-3.85367700
H	-4.68343000	-0.14062500	-2.43726800
C	-3.19483500	1.41703600	-2.58390000
H	-3.86191200	2.11014100	-3.10460000
H	-3.19489200	1.69662000	-1.52505900
H	-2.18371000	1.57945500	-2.97434900
C	-2.13966300	1.25706800	3.15397700
H	-3.18652000	1.07379200	3.43429100
H	-1.61299700	1.51210700	4.08241800
C	-2.05130200	2.42017200	2.17385000
H	-2.63344600	2.22135000	1.26668700
H	-2.44762900	3.33693400	2.62132200
H	-1.01549500	2.59967600	1.86936300
C	2.96574200	3.66430500	-0.83648300
C	1.58673800	3.76010300	-1.00512500
C	0.75293700	2.71161000	-0.61683700
C	1.27031800	1.53582200	-0.02323100
C	2.69046200	1.43276100	0.08085700
H	-0.32510400	2.82237500	-0.71315900
H	3.62010300	4.48154000	-1.12473900
H	1.15006700	4.66018000	-1.43094300
C	0.46613800	0.45629300	0.43012300
N	-0.70398400	0.22554200	-0.33458800
N	3.19564800	0.22930700	0.59217600
H	-0.70745500	0.43989400	-1.33929200
H	4.18263900	0.09958100	0.40962300
C	3.50725200	2.48498200	-0.30776800
H	4.58722100	2.37749300	-0.21295900
C	2.32953200	-1.25869300	-1.21710300
C	1.57772400	-2.55454400	-1.51335900
C	2.18537100	-3.73254500	-0.75377800
C	2.24196800	-3.44498800	0.74558700
C	2.99314900	-2.14889400	1.04057400
C	2.40569800	-0.95902200	0.28960800
H	1.61299100	-4.64893000	-0.94508200
H	0.52836000	-2.43550500	-1.21167100
H	1.58279100	-2.75176800	-2.59331900
H	3.35873800	-1.33742000	-1.59782400
H	1.87600700	-0.40545700	-1.73344200
H	1.22117800	-3.35708500	1.13850600

H	2.71788500	-4.27783300	1.27758400
H	2.97398000	-1.91127300	2.10914600
H	4.04738500	-2.25793000	0.74588200
H	3.20384000	-3.91549900	-1.12830200
O	1.10262600	-0.74894600	0.82732300

TS6:

Zero-point correction=0.512099 (Hartree/Particle)
Thermal correction to Energy=0.539389
Thermal correction to Enthalpy=0.540365
Thermal correction to Gibbs Free Energy=0.454232
Sum of electronic and zero-point Energies=-1150.293135
Sum of electronic and thermal Energies=-1150.265845
Sum of electronic and thermal Enthalpies=-1150.264869
Sum of electronic and thermal Free Energies=-1150.351002

C	-1.66247200	-0.33623700	-0.30904900
C	-3.34919700	-1.73081300	-0.85971500
H	-3.98932200	-2.59584600	-0.77071200
C	-3.35285700	-0.72127400	-1.76681400
H	-3.99608200	-0.53868100	-2.61450600
N	-2.31376700	-1.48194600	0.01614100
N	-2.31508800	0.12358300	-1.41197700
C	-2.03275700	1.39388700	-2.06209300
H	-1.86696200	1.21093900	-3.13042000
H	-1.09813600	1.76841800	-1.63396300
C	-1.94424900	-2.34474300	1.13053300
H	-0.94141400	-2.03363400	1.44119000
H	-1.89367500	-3.37250800	0.75292300
C	-3.13720000	2.42910900	-1.86043700
H	-2.85907100	3.31678700	-2.44207200
H	-4.07167800	2.05604200	-2.29946700
C	-3.35475400	2.80500800	-0.40102000
H	-4.13727400	3.56404400	-0.30689300
H	-3.65659900	1.93662700	0.19284900
H	-2.43789600	3.20556400	0.04460500
C	-2.92011100	-2.24979100	2.30070500
H	-3.92431000	-2.55615800	1.97604000
H	-2.59935400	-2.98926700	3.04502700
C	-2.96992500	-0.86528200	2.93432100
H	-3.32240600	-0.11388600	2.21993400
H	-3.64694800	-0.85248300	3.79446400
H	-1.97461600	-0.55726900	3.26985400

C	2.23178300	4.03871500	0.73782700
C	1.33256500	3.65926300	1.73568300
C	0.86514100	2.34577100	1.76654900
C	1.27322600	1.42716500	0.80446500
C	2.19231500	1.80938500	-0.18787600
H	0.17975900	2.01124600	2.54049100
H	2.61276100	5.05637300	0.71053200
H	1.01251700	4.37435200	2.48742800
C	0.75682200	0.01892900	0.80063200
N	0.18247000	-0.47412300	-0.38550300
N	2.55269800	0.83663200	-1.10570900
H	0.30680100	0.22770500	-1.11678200
H	3.37800100	1.04253700	-1.66287700
C	2.67029900	3.12498500	-0.21674000
H	3.39195000	3.42379800	-0.97369700
C	2.27868400	-1.44796300	-1.91103900
C	2.00076800	-2.90025800	-1.52788100
C	3.00917100	-3.40548800	-0.49941200
C	3.03595400	-2.49785700	0.72727300
C	3.32592400	-1.04768800	0.34027700
C	2.36804600	-0.53444900	-0.71517600
H	2.76821200	-4.43502200	-0.20650700
H	0.98936500	-2.95580500	-1.10755800
H	2.01797300	-3.52977300	-2.42625400
H	3.24932400	-1.40562600	-2.44759700
H	1.52516100	-1.07933700	-2.61741700
H	2.06840500	-2.53290900	1.24220100
H	3.79089600	-2.84280700	1.44411600
H	3.31278100	-0.40471200	1.22773400
H	4.34996400	-0.98232300	-0.07984200
H	4.01074100	-3.43589100	-0.95542800
O	0.62548500	-0.60397100	1.85573300

3-W:

Zero-point correction=0.381237 (Hartree/Particle)
Thermal correction to Energy=0.406581
Thermal correction to Enthalpy=0.407557
Thermal correction to Gibbs Free Energy=0.321429
Sum of electronic and zero-point Energies=-917.235285
Sum of electronic and thermal Energies=-917.209941
Sum of electronic and thermal Enthalpies=-917.208965
Sum of electronic and thermal Free Energies=-917.295093

C	-1.68811300	-0.25874300	-0.62936800
C	-3.95466800	-0.48171700	-0.84444300
H	-4.89388500	-1.00201800	-0.96224300
C	-3.68235100	0.84511500	-0.77097100
H	-4.34064200	1.70022200	-0.81252200
N	-2.73393100	-1.12644100	-0.75739900
N	-2.31066700	0.95236000	-0.64141400
C	-1.61000800	2.22377900	-0.51600100
H	-1.86077300	2.85029400	-1.37937300
H	-0.54486700	1.99194000	-0.57575400
C	-2.58115800	-2.56950400	-0.77035000
H	-1.51440900	-2.75961100	-0.91772800
H	-3.11588000	-2.97088000	-1.63982800
C	-1.92325600	2.96436900	0.77988800
H	-1.38940500	3.92000300	0.73114800
H	-2.99565500	3.20046600	0.81803800
C	-1.51534500	2.19580900	2.03010100
H	-1.75692200	2.76362700	2.93431400
H	-2.02521300	1.22849300	2.09230000
H	-0.43709000	2.00248400	2.03402400
C	-3.07417300	-3.24213700	0.50914500
H	-4.14263700	-3.02689700	0.64209900
H	-2.99754200	-4.32741200	0.36363500
C	-2.30121100	-2.82436800	1.75302200
H	-2.36303700	-1.74381100	1.91379500
H	-2.69341800	-3.32337300	2.64471600
H	-1.23934700	-3.07902600	1.66332500
C	3.41419000	-2.87691800	-0.12317700
C	2.07702000	-2.49296100	-0.26527900
C	1.74995300	-1.14610400	-0.27317400
C	2.76699100	-0.18660000	-0.13924200
C	4.12485600	-0.56304900	0.00410800
H	0.71211500	-0.81955300	-0.38116400
H	3.67631300	-3.93159000	-0.11544800
H	1.29783100	-3.24117200	-0.36868700
C	2.44713100	1.19958400	-0.13653700
N	2.24386100	2.34503800	-0.12093900
N	5.11869100	0.37872000	0.08799000
H	4.86246600	1.32987400	0.30514100
H	6.01321600	0.08550400	0.44445400
C	4.42298500	-1.93479000	0.00895000
H	5.45770000	-2.25133100	0.11157600
O	0.69707900	4.85788200	-0.27477500
H	1.28042100	4.08472600	-0.21422600

H	1.17129200	5.49765800	-0.81107900

TS1-W:

Zero-point correction=0.382537 (Hartree/Particle)
Thermal correction to Energy=0.406570
Thermal correction to Enthalpy=0.407546
Thermal correction to Gibbs Free Energy=0.326878
Sum of electronic and zero-point Energies=-917.219044
Sum of electronic and thermal Energies=-917.195011
Sum of electronic and thermal Enthalpies=-917.194035
Sum of electronic and thermal Free Energies=-917.274703

C	-0.98578800	0.74248200	-0.56501500
C	-3.18982900	1.22775600	-0.43712300
H	-4.24389600	1.12316200	-0.64219900
C	-2.52959100	2.13681600	0.32283700
H	-2.90037400	2.96325900	0.90999400
N	-2.23008300	0.38428400	-0.96191300
N	-1.18649400	1.82158800	0.22995200
C	-0.12636200	2.56239400	0.90412500
H	-0.17689500	3.60596000	0.57120700
H	0.81862400	2.14510500	0.54865600
C	-2.49404100	-0.73005300	-1.86676900
H	-1.58072200	-1.32866100	-1.87662500
H	-2.65212500	-0.33089300	-2.87625700
C	-0.21096100	2.48448800	2.42571500
H	0.56358900	3.15200000	2.82390000
H	-1.17003800	2.90170400	2.76077800
C	-0.02655200	1.07812000	2.98087700
H	-0.09817400	1.07972600	4.07282700
H	-0.78235900	0.38742500	2.59502500
H	0.95193900	0.66876200	2.70884700
C	-3.68360000	-1.58713700	-1.44872200
H	-4.61056800	-1.00182000	-1.51510400
H	-3.78063500	-2.37388400	-2.20719400
C	-3.54838000	-2.21101500	-0.06537800
H	-3.50480800	-1.44712000	0.71703900
H	-4.40029100	-2.86404300	0.14863200
H	-2.62816700	-2.79617700	0.01519300
C	4.17022400	0.73336000	-1.55953300
C	2.99626900	1.22744100	-2.13615700
C	1.77773200	0.76048600	-1.66597600
C	1.69366400	-0.19335600	-0.64744300

C	2.88747700	-0.71416200	-0.07319000
H	0.84206900	1.12881900	-2.07671000
H	5.13844200	1.08841900	-1.90289900
H	3.03459700	1.96226200	-2.93393800
C	0.41897800	-0.71497800	-0.16805300
N	-0.08912300	-1.62748500	0.40639900
N	2.87144600	-1.62520700	0.93917200
H	2.04226700	-2.17077100	1.14158900
H	3.74365700	-2.05156800	1.20256900
C	4.11688200	-0.21252400	-0.55016900
H	5.03714200	-0.58812900	-0.10858200
O	0.78184100	-3.72762400	1.99059200
H	0.26139300	-3.07945100	1.47049600
H	0.68364600	-4.56606500	1.53258800

4-W:

Zero-point correction=0.383599 (Hartree/Particle)
Thermal correction to Energy=0.405754
Thermal correction to Enthalpy=0.406729
Thermal correction to Gibbs Free Energy=0.332192
Sum of electronic and zero-point Energies=-917.241768
Sum of electronic and thermal Energies=-917.219614
Sum of electronic and thermal Enthalpies=-917.218638
Sum of electronic and thermal Free Energies=-917.293176

C	0.55593900	0.00409000	-0.51115200
C	2.29976100	0.71794500	-1.69022200
H	2.97469400	1.43057900	-2.13588100
C	2.33743600	-0.63794900	-1.67484600
H	3.05130400	-1.32125900	-2.10525100
N	1.18803400	1.10040200	-0.97017900
N	1.24889800	-1.06558900	-0.94505300
C	0.82180300	-2.45649900	-0.77837900
H	0.39148300	-2.78500000	-1.73166700
H	0.02136300	-2.44371200	-0.03447300
C	0.68941700	2.47004800	-0.83118300
H	-0.14057700	2.42373000	-0.12173200
H	0.28366500	2.77203000	-1.80378700
C	1.94000000	-3.39495000	-0.34277500
H	1.53819500	-4.41218400	-0.43048500
H	2.76804100	-3.34566400	-1.06223100
C	2.44461000	-3.14560900	1.07227700
H	3.26472500	-3.82989100	1.31239200

H	2.79334000	-2.11691900	1.21480300
H	1.64392800	-3.31336400	1.80089700
C	1.74417000	3.46224400	-0.35770200
H	2.59836200	3.45314600	-1.04777300
H	1.29607700	4.45858300	-0.46033300
C	2.21155700	3.23659300	1.07387900
H	2.61750000	2.23034000	1.22511500
H	2.98076800	3.96712500	1.34435200
H	1.37741800	3.35314600	1.77439000
C	-4.59056900	-0.09450500	-0.83548600
C	-3.54822100	-0.08401800	-1.76774100
C	-2.24001700	-0.05322400	-1.29901400
C	-1.93590200	-0.03010000	0.06679800
C	-3.00360300	-0.03464000	1.01017600
H	-1.41898300	-0.04996700	-2.01601400
H	-5.62267100	-0.12076900	-1.17577500
H	-3.75538400	-0.10131700	-2.83319500
C	-0.53523200	-0.01382400	0.54948200
N	-0.09394200	-0.01376700	1.73403300
N	-2.71752300	0.00715400	2.33417200
H	-1.71055200	-0.02140000	2.56953800
H	-3.45158700	-0.08184000	3.01508600
C	-4.32731400	-0.07058100	0.52500000
H	-5.14731400	-0.07598000	1.23994300
O	2.58896500	0.04928300	2.02536700
H	1.57751400	0.02181000	1.97031900
H	2.79570800	0.06701200	2.96333300

TS2-W:

Zero-point correction=0.380724 (Hartree/Particle)
Thermal correction to Energy=0.403726
Thermal correction to Enthalpy=0.404702
Thermal correction to Gibbs Free Energy=0.327660
Sum of electronic and zero-point Energies=-917.239746
Sum of electronic and thermal Energies=-917.216744
Sum of electronic and thermal Enthalpies=-917.215769
Sum of electronic and thermal Free Energies=-917.292811

C	0.53175400	-0.09211500	-0.43601400
C	2.41588000	0.04537900	-1.59263200
H	3.30279100	0.50063300	-2.00031900
C	1.95597400	-1.22803300	-1.69861700
H	2.36676300	-2.08249800	-2.21231200

N	1.52326400	0.73480100	-0.80526300
N	0.78469200	-1.29440700	-0.97760700
C	-0.04675900	-2.49003900	-0.82603100
H	-0.37589700	-2.78797600	-1.82726500
H	-0.93219500	-2.18514200	-0.26316000
C	1.57184000	2.15857400	-0.44080200
H	1.20783700	2.21883600	0.58802800
H	0.86111900	2.68539500	-1.08662300
C	0.68187300	-3.63079500	-0.12460900
H	0.01555000	-4.50102300	-0.17259900
H	1.57579200	-3.90518600	-0.70049400
C	1.05411400	-3.32527500	1.32027800
H	1.56483800	-4.18180900	1.77140600
H	1.71301900	-2.45397800	1.40356500
H	0.16038500	-3.11371300	1.91686300
C	2.95658900	2.77613700	-0.55986000
H	3.32223700	2.69013700	-1.59208300
H	2.81515800	3.85139600	-0.39781100
C	3.98229200	2.24186200	0.43334400
H	3.65494300	2.41956600	1.46125900
H	4.12490400	1.16129200	0.34776800
H	4.94839900	2.73490300	0.28637600
C	-4.55208200	0.74320400	-0.87220900
C	-3.53517800	0.48696000	-1.80991700
C	-2.23814200	0.32291100	-1.35006300
C	-1.92298200	0.40256200	0.01449700
C	-2.95672500	0.67659100	0.97603300
H	-1.43901100	0.13367000	-2.06750900
H	-5.57577300	0.87335800	-1.21588100
H	-3.76200000	0.42359800	-2.86948800
C	-0.56724600	0.24002900	0.53595600
N	-0.21137000	0.34413300	1.76131200
N	-2.59504300	0.76152700	2.26204900
H	-1.36973900	0.59282600	2.32311700
H	-3.32911800	0.96670100	2.92686000
C	-4.28004400	0.83755300	0.47764900
H	-5.08024900	1.04184700	1.18587500
O	2.41933900	-0.19586700	2.13368000
H	1.43687900	0.01816200	2.09939700
H	2.62090200	-0.34946300	3.06013200

TS2-W1:

Zero-point correction=0.381154 (Hartree/Particle)

Thermal correction to Energy=0.403284
Thermal correction to Enthalpy=0.404260
Thermal correction to Gibbs Free Energy=0.328710
Sum of electronic and zero-point Energies=-917.237194
Sum of electronic and thermal Energies=-917.215064
Sum of electronic and thermal Enthalpies=-917.214088
Sum of electronic and thermal Free Energies=-917.289638

C	0.87803100	0.41601300	-0.37401700
C	2.00292400	2.32871600	-0.24868600
H	2.18235600	3.35880900	0.01681600
C	2.78601100	1.42850100	-0.89562100
H	3.77497900	1.52828600	-1.31362700
N	0.82381800	1.68895700	0.06310600
N	2.07818800	0.24953300	-0.96056800
C	2.56868100	-0.98590900	-1.57780400
H	2.65078000	-0.80962600	-2.65604000
H	1.80276300	-1.74008700	-1.39477800
C	-0.26237600	2.30110800	0.83451000
H	-1.15560600	1.69602600	0.66684500
H	-0.44082100	3.28845100	0.39713400
C	3.90306200	-1.44123500	-0.99603200
H	4.15898200	-2.37157700	-1.51736200
H	4.69396000	-0.72596400	-1.26029700
C	3.87399300	-1.67455200	0.50938500
H	4.81849500	-2.11194400	0.84662300
H	3.72852600	-0.73721000	1.05674900
H	3.05077400	-2.33665800	0.79088300
C	0.05768600	2.40447900	2.32239000
H	0.96034500	3.01463000	2.46230400
H	-0.76580200	2.96933800	2.77658300
C	0.20931100	1.05547900	3.01416600
H	1.04345900	0.47627800	2.60549400
H	0.39352100	1.19279700	4.08388000
H	-0.69122100	0.44352500	2.89741300
C	-3.96312800	0.58275500	-1.59421500
C	-2.79562100	0.82362600	-2.32949500
C	-1.59409100	0.36749600	-1.81109800
C	-1.50453500	-0.34742600	-0.60353500
C	-2.70052400	-0.63966300	0.12336600
H	-0.67583800	0.56938900	-2.36217300
H	-4.92206600	0.94119000	-1.96038100
H	-2.82776700	1.35680600	-3.27430400
C	-0.13795800	-0.66613200	-0.10548600

N	0.35454700	-1.63659500	0.54156500
N	-2.68864200	-1.31789000	1.29959100
H	-2.08676600	-2.24011300	1.36943000
H	-3.61332800	-1.43573800	1.69314700
C	-3.91197500	-0.12151700	-0.40683200
H	-4.82969200	-0.31283700	0.14569800
O	-1.22569600	-3.41410800	1.32846300
H	-0.35224900	-2.50800400	0.83682100
H	-1.52454500	-4.07137700	0.69360600

5-W:

Zero-point correction=0.385469 (Hartree/Particle)
Thermal correction to Energy=0.407939
Thermal correction to Enthalpy=0.408915
Thermal correction to Gibbs Free Energy=0.333559
Sum of electronic and zero-point Energies=-917.247782
Sum of electronic and thermal Energies=-917.225311
Sum of electronic and thermal Enthalpies=-917.224335
Sum of electronic and thermal Free Energies=-917.299691

C	-0.51804500	0.08999400	-0.38153300
C	-2.33223300	-0.08643200	-1.63283800
H	-3.19563700	-0.55531500	-2.07413500
C	-1.85942600	1.18106300	-1.76063800
H	-2.23383900	2.01656800	-2.33028100
N	-1.49050900	-0.74751900	-0.77005100
N	-0.73206600	1.27187400	-0.97739400
C	0.09805200	2.46978700	-0.82485500
H	0.46549600	2.73749800	-1.82092100
H	0.96109200	2.17442500	-0.22315200
C	-1.55848000	-2.16156000	-0.36653300
H	-1.24795600	-2.19260300	0.68071600
H	-0.81435300	-2.70313500	-0.96012400
C	-0.65318700	3.62979100	-0.18201000
H	0.02057900	4.49446600	-0.22226200
H	-1.52064300	3.89578900	-0.80073500
C	-1.08653800	3.36121700	1.25309000
H	-1.60495900	4.23311500	1.66392700
H	-1.75960600	2.50026800	1.32824800
H	-0.22027500	3.15336900	1.89000300
C	-2.93553700	-2.78262600	-0.54025700
H	-3.24354300	-2.73413600	-1.59347200

H	-2.80382100	-3.85107900	-0.33218400
C	-4.01387100	-2.21479800	0.37555000
H	-3.73671400	-2.34019400	1.42566800
H	-4.16471700	-1.14161400	0.23051900
H	-4.96670200	-2.72521900	0.20424700
C	4.49479600	-0.75171600	-0.93181000
C	3.41933900	-0.51766200	-1.82809500
C	2.15759400	-0.35377900	-1.30649700
C	1.89596800	-0.40930000	0.08529400
C	2.98461700	-0.67309500	1.01923800
H	1.32770300	-0.18512100	-1.99316800
H	5.50030600	-0.87907800	-1.32746600
H	3.59016400	-0.47450300	-2.89896700
C	0.56638300	-0.23168700	0.59494600
N	0.14156400	-0.31225200	1.81930900
N	2.74387700	-0.75930900	2.31253400
H	0.96657300	-0.53104400	2.41453300
H	3.60771400	-0.94264600	2.82025300
C	4.29171700	-0.82486600	0.41888900
H	5.12914600	-1.01165400	1.08881900
O	-2.51308400	0.25388300	2.12597800
H	-1.53872500	0.04324400	2.15150800
H	-2.75956100	0.47199100	3.02818100

6-W:

Zero-point correction=0.536825 (Hartree/Particle)
Thermal correction to Energy=0.569203
Thermal correction to Enthalpy=0.570179
Thermal correction to Gibbs Free Energy=0.470094
Sum of electronic and zero-point Energies=-1226.751441
Sum of electronic and thermal Energies=-1226.719064
Sum of electronic and thermal Enthalpies=-1226.718088
Sum of electronic and thermal Free Energies=-1226.818172

C	-1.83658900	-0.01550400	0.41841600
C	-3.84344000	-0.30047300	1.29953800
H	-4.89102700	-0.11794100	1.47110900
C	-3.01894000	-1.24800800	1.81870900
H	-3.21473600	-2.04153300	2.52192800
N	-3.09371100	0.45379000	0.42891000
N	-1.77696300	-1.05472100	1.26071300
C	-0.58257600	-1.85467300	1.55780500
H	-0.36095600	-1.72505300	2.62192600

H	0.24537800	-1.42362700	0.99415200
C	-3.53214700	1.63273700	-0.33453200
H	-3.00869000	1.58663900	-1.29267800
H	-3.17955800	2.51830800	0.20493500
C	-0.75341300	-3.32588100	1.20442100
H	0.16806300	-3.81865000	1.53281500
H	-1.57052100	-3.76082200	1.79613500
C	-0.97559300	-3.57168800	-0.28163400
H	-1.08913300	-4.64217800	-0.47923600
H	-1.86794500	-3.06028700	-0.65872200
H	-0.11678600	-3.21145000	-0.85673100
C	-5.03646000	1.69970500	-0.54820400
H	-5.55484200	1.73714200	0.41936000
H	-5.22441200	2.67666600	-1.00921500
C	-5.60605800	0.59881200	-1.43549800
H	-5.13816900	0.61312500	-2.42346800
H	-5.42356500	-0.40075300	-1.03182300
H	-6.68550700	0.73010600	-1.55925200
C	1.93344000	3.30048800	1.36497100
C	0.94953900	2.65827000	2.15636800
C	0.11044500	1.75182500	1.54778600
C	0.20850500	1.42638700	0.17398200
C	1.23256700	2.05596900	-0.64877000
H	-0.66109200	1.27168400	2.14921600
H	2.59518700	4.03184200	1.82442300
H	0.85289000	2.88487500	3.21311300
C	-0.73365700	0.52497500	-0.43731600
N	-0.81251000	0.14801700	-1.67417600
N	1.35777200	1.73008400	-1.92455700
H	-0.03346000	0.60549600	-2.18756900
H	2.09302600	2.28671700	-2.35816300
C	2.06618700	3.02040800	0.03006900
H	2.82510700	3.52909600	-0.56226200
O	-3.02267600	-1.36797100	-2.28597800
H	-2.17564900	-0.85827000	-2.18542600
H	-2.90119900	-1.93046600	-3.05475900
C	3.16296300	-1.25634700	-1.29048300
C	4.56739200	-0.93299800	-1.81419300
C	5.19648700	0.22407100	-1.04286800
C	5.26687500	-0.09436100	0.44812000
C	3.87852700	-0.40145700	1.02085700
C	3.11418700	-1.41859500	0.20625000
H	6.19976100	0.43669500	-1.43113700
H	5.20970700	-1.82037900	-1.72322300

H	4.50767000	-0.69830800	-2.88291600
H	2.49292900	-0.41309600	-1.53491400
H	2.74328000	-2.15565900	-1.75103200
H	5.92574100	-0.96037200	0.60287600
H	5.71228000	0.73933400	1.00294000
H	3.92170700	-0.75014900	2.05680900
H	3.27425200	0.51866700	1.00728100
H	4.59491000	1.13120100	-1.19307200
O	2.44815100	-2.29337600	0.74067700

TS3-W:

Zero-point correction=0.539809 (Hartree/Particle)
Thermal correction to Energy=0.569451
Thermal correction to Enthalpy=0.570427
Thermal correction to Gibbs Free Energy=0.480771
Sum of electronic and zero-point Energies=-1226.735814
Sum of electronic and thermal Energies=-1226.706172
Sum of electronic and thermal Enthalpies=-1226.705196
Sum of electronic and thermal Free Energies=-1226.794852

C	-1.96028100	0.32919300	0.13449400
C	-3.98251000	-0.22597300	0.83949800
H	-5.03476300	-0.44945900	0.76805200
C	-3.15294600	-0.20774900	1.91489700
H	-3.34989500	-0.43127400	2.94999500
N	-3.22760800	0.10551500	-0.25875100
N	-1.90272700	0.13640100	1.46428400
C	-0.70068200	0.27052500	2.31307600
H	-0.66807800	1.30860900	2.66027900
H	0.16864900	0.09282100	1.66989400
C	-3.76878100	0.24996000	-1.61556700
H	-2.92100700	0.47573800	-2.26259900
H	-4.45151000	1.10659600	-1.60305800
C	-0.69093000	-0.69355000	3.49104800
H	0.18291000	-0.40721500	4.08851700
H	-1.55463000	-0.52004100	4.14766000
C	-0.58280300	-2.16271700	3.10138700
H	-0.59232700	-2.79864600	3.99219500
H	-1.39603700	-2.48125300	2.44240100
H	0.34747300	-2.34489400	2.55683300
C	-4.48462000	-1.00691600	-2.09805600
H	-5.35316300	-1.21332200	-1.45846000

H	-4.89618700	-0.76253100	-3.08501200
C	-3.59011500	-2.23587500	-2.19181200
H	-2.73847400	-2.04938100	-2.85238800
H	-3.18813000	-2.52486600	-1.21549500
H	-4.15161500	-3.08810500	-2.58582200
C	1.34399300	4.25579900	0.03068900
C	0.06698300	4.07177300	0.58668900
C	-0.58594400	2.87390500	0.35578200
C	-0.01029000	1.84115800	-0.40728900
C	1.30010300	2.01254600	-0.96721600
H	-1.59466500	2.74461100	0.74667800
H	1.87295400	5.19226300	0.19147100
H	-0.40496700	4.85702600	1.16865700
C	-0.81496900	0.67320300	-0.76133400
N	-0.69495400	-0.10105800	-1.78055400
N	1.86775800	1.00864500	-1.66973800
H	0.17325200	0.16656000	-2.26835500
H	2.75914800	1.32623100	-2.04479900
C	1.93920900	3.26066000	-0.71651100
H	2.93019800	3.41756800	-1.13796400
O	-0.49905900	-2.57272000	-0.26229700
H	-0.77579100	-2.08041500	-1.04857500
H	0.27439800	-2.04020700	0.02442700
C	2.78144400	-1.51846400	-1.49523900
C	3.63488800	-2.61852800	-0.84625300
C	4.88280100	-2.03864300	-0.17747100
C	4.52987400	-0.93873800	0.82592900
C	3.69653900	0.16388100	0.15697800
C	2.44839300	-0.49292500	-0.42231200
H	5.45106900	-2.83579300	0.31796300
H	3.02530400	-3.14192400	-0.09816400
H	3.91770600	-3.36346300	-1.60015600
H	3.34154600	-1.04916800	-2.31321000
H	1.85648300	-1.93150500	-1.90713400
H	3.94888600	-1.36671400	1.65335800
H	5.44125000	-0.50962800	1.26101300
H	3.40025300	0.93427700	0.87590900
H	4.30177200	0.63559200	-0.62766800
H	5.54399000	-1.61847800	-0.95062000
O	1.50412900	-0.73619000	0.38092700

7-W:

Zero-point correction=0.541268 (Hartree/Particle)

Thermal correction to Energy=0.570692
Thermal correction to Enthalpy=0.571668
Thermal correction to Gibbs Free Energy=0.483177
Sum of electronic and zero-point Energies=-1226.740568
Sum of electronic and thermal Energies=-1226.711143
Sum of electronic and thermal Enthalpies=-1226.710167
Sum of electronic and thermal Free Energies=-1226.798658

C	-1.78723100	0.36957400	0.14784000
C	-3.74981500	-0.18286800	1.00939700
H	-4.79629500	-0.44110700	1.01734400
C	-2.86213900	-0.05976000	2.02930300
H	-2.99061300	-0.21203300	3.08780400
N	-3.07362400	0.08801600	-0.15207900
N	-1.65499200	0.29134700	1.48549300
C	-0.42631200	0.52699000	2.27257200
H	-0.42955400	1.58361600	2.56094700
H	0.41563200	0.32760800	1.59109700
C	-3.73696300	0.15720000	-1.46257700
H	-2.95147000	0.33038500	-2.19731600
H	-4.40968500	1.02186900	-1.43541800
C	-0.32224400	-0.37367200	3.49529800
H	0.58264700	-0.03913500	4.01743200
H	-1.14374400	-0.19044100	4.20264300
C	-0.20035700	-1.85682800	3.16551800
H	-0.07708500	-2.44626100	4.07964800
H	-1.07434900	-2.23732300	2.62796100
H	0.66165800	-2.02945100	2.51523900
C	-4.50989300	-1.11298300	-1.79997200
H	-5.31111400	-1.27604300	-1.06706600
H	-5.01810600	-0.91415900	-2.75158300
C	-3.64019500	-2.35731400	-1.91782100
H	-2.87405800	-2.22329500	-2.68812300
H	-3.12830000	-2.58421500	-0.97748100
H	-4.24732700	-3.22573000	-2.19023700
C	1.53423300	4.30830800	-0.17481100
C	0.21564100	4.22673900	0.27417000
C	-0.47110800	3.02855100	0.11372500
C	0.12493200	1.91220600	-0.48471600
C	1.47732900	1.97748600	-0.90243300
H	-1.51223000	2.96834900	0.42772200
H	2.09109000	5.23534400	-0.06702000
H	-0.27208400	5.08434900	0.72704700
C	-0.73340300	0.75674900	-0.83569400

N	-0.78874500	0.16842700	-1.97214900
N	2.08642600	0.88245300	-1.48568900
H	-0.01645400	0.50387000	-2.55305000
H	2.98807300	1.14932400	-1.86687700
C	2.15270600	3.20092000	-0.73949300
H	3.19261100	3.26409900	-1.05253700
O	-0.63431500	-2.40179100	-0.14438800
H	-0.84318300	-2.28600200	-1.07644800
H	0.14085700	-1.77556900	-0.01890100
C	2.48599900	-1.53455100	-1.65573100
C	2.90416100	-2.83276100	-0.96755900
C	4.16185400	-2.63816300	-0.12050500
C	3.98445900	-1.49593000	0.87906100
C	3.59358700	-0.20478700	0.16548100
C	2.27895800	-0.40118200	-0.63122600
H	4.41363700	-3.56886000	0.40372700
H	2.07967900	-3.17250600	-0.32896500
H	3.06831900	-3.61787600	-1.71684500
H	3.25603400	-1.23798900	-2.38496800
H	1.55040900	-1.66969400	-2.21110300
H	3.18810900	-1.75224600	1.58924000
H	4.90408800	-1.34795000	1.46016100
H	3.43731500	0.61123500	0.88208700
H	4.41317800	0.09329200	-0.50905600
H	5.01396900	-2.40990200	-0.77961500
O	1.24302600	-0.59955700	0.19370300

TS4-W:

Zero-point correction=0.539048 (Hartree/Particle)
Thermal correction to Energy=0.568686
Thermal correction to Enthalpy=0.569662
Thermal correction to Gibbs Free Energy=0.478240
Sum of electronic and zero-point Energies=-1226.715190
Sum of electronic and thermal Energies=-1226.685552
Sum of electronic and thermal Enthalpies=-1226.684576
Sum of electronic and thermal Free Energies=-1226.775998

C	-0.43993300	0.88096400	0.05137800
C	-0.83380600	2.91732000	0.94901600
H	-0.59040000	3.84395900	1.44380600
C	-1.98293800	2.49723900	0.37497900
H	-2.93471300	2.99228900	0.26492500
N	0.09564600	1.90958300	0.76679100

N	-1.73301100	1.24438400	-0.13914800
C	-2.72255000	0.49131800	-0.89950500
H	-2.30041400	-0.49972600	-1.06383900
H	-2.82563400	0.98135900	-1.87546000
C	1.40258200	1.94530600	1.41935800
H	1.83075600	2.93798400	1.23828900
H	2.04156400	1.22288200	0.91618600
C	-4.08579600	0.39743000	-0.18712100
H	-4.29975400	-0.65244500	0.04334800
H	-4.02988800	0.90530400	0.78236200
C	-5.23166100	0.97845500	-1.00887100
H	-6.18534900	0.88787700	-0.47958600
H	-5.06730000	2.03952300	-1.22834200
H	-5.33388700	0.45952200	-1.96809200
C	1.37054600	1.64326600	2.91799800
H	0.93043600	0.65127200	3.07475600
H	2.41968600	1.56288900	3.22981600
C	0.66344300	2.66662800	3.79871300
H	1.06875000	3.67396000	3.64442200
H	-0.41277000	2.70007800	3.60472600
H	0.79634700	2.41858400	4.85649100
C	4.58067700	0.21906000	-0.74194200
C	3.85474500	1.23654300	-1.36741600
C	2.48164000	1.08901600	-1.52830900
C	1.81982800	-0.04541000	-1.05839300
C	2.55592900	-1.08722200	-0.47574600
H	1.89165900	1.86234900	-2.01205900
H	5.65434300	0.31783300	-0.60514500
H	4.35611000	2.12875200	-1.72983100
C	0.34249000	-0.21029400	-1.26443700
N	-0.09564600	0.25150800	-2.43661500
N	1.92958400	-2.27500800	-0.15306000
H	-0.95787400	-0.22308000	-2.68943800
H	2.44896200	-2.89489900	0.45117700
C	3.94304100	-0.93417700	-0.30633200
H	4.51629300	-1.73981100	0.14776400
O	-0.56353500	2.90171500	-2.71351100
H	-0.33809700	1.92516900	-2.66612200
H	-0.35074200	3.16676400	-3.61188700
C	0.02249800	-3.75201100	-0.28416300
C	-1.46824400	-3.95177400	-0.02765100
C	-1.84024300	-3.58104100	1.40580800
C	-1.40637400	-2.15321000	1.73197800
C	0.08148800	-1.94570300	1.45901300

C	0.48890700	-2.32747800	0.02537200
H	-2.91964100	-3.69569000	1.56297200
H	-2.03612800	-3.32882800	-0.73021700
H	-1.74116000	-4.99241100	-0.23874200
H	0.59921800	-4.44004900	0.35130700
H	0.28523900	-3.96685800	-1.32446300
H	-1.98419500	-1.44691700	1.12408900
H	-1.62561600	-1.91505700	2.78009900
H	0.37762100	-0.91135000	1.65135900
H	0.66712900	-2.57974300	2.14106800
H	-1.34799200	-4.27778100	2.10060400
O	-0.13098800	-1.51075500	-0.95580000

8-W:

Zero-point correction=0.298137 (Hartree/Particle)
Thermal correction to Energy=0.315776
Thermal correction to Enthalpy=0.316752
Thermal correction to Gibbs Free Energy=0.250687
Sum of electronic and zero-point Energies= -765.299807
Sum of electronic and thermal Energies=-765.282167
Sum of electronic and thermal Enthalpies=-765.281191
Sum of electronic and thermal Free Energies=-765.347256

C	-3.86372400	-1.29269700	-0.06894500
C	-4.07914000	-0.02709500	0.47933100
C	-3.03109300	0.87043900	0.53948300
C	-1.76785400	0.52128500	0.06402500
C	-1.55167100	-0.75871000	-0.46749200
H	-3.17224900	1.86247700	0.94851800
H	-4.67998700	-2.00335800	-0.12168400
H	-5.05767400	0.24928400	0.84971300
C	-0.66978200	1.49099300	0.04358400
N	-0.82418300	2.71452200	0.34359400
N	-0.30006200	-1.06178200	-0.94899900
H	2.52806100	3.49174700	-1.43501400
H	-0.12974300	-2.04038200	-1.13020000
C	3.38949200	-1.50073900	0.82939000
C	2.87144600	-1.79600700	-0.58420300
C	2.08493700	-0.61269700	-1.12645400
C	0.81142300	-0.38437800	-0.31988700
C	1.00626300	-0.78361300	1.15095100
C	2.44397000	-0.56340200	1.59079600
H	3.50379600	-2.43879700	1.37766300

H	3.69930200	-2.02825600	-1.25552100
H	2.69913900	0.28751900	-1.05570800
H	0.30605700	-0.23273900	1.78037000
H	2.53549000	-0.71933600	2.66676700
O	0.53736500	1.03472800	-0.39931600
H	0.75187400	-1.84243300	1.24754500
H	2.71769900	0.47970700	1.40888300
H	4.38243500	-1.04867300	0.77335600
H	2.22919600	-2.68210400	-0.57600000
H	1.81694800	-0.74115800	-2.17574800
O	2.46858700	3.19664600	-0.52325900
H	0.05674600	3.21951000	0.26811900
H	1.92515300	2.39916200	-0.55837800
C	-2.61756800	-1.66089800	-0.53732300
H	-2.45035400	-2.64723200	-0.95378600

TS5-W:

Zero-point correction=0.296554 (Hartree/Particle)
Thermal correction to Energy=0.314334
Thermal correction to Enthalpy=0.315309
Thermal correction to Gibbs Free Energy=0.247252
Sum of electronic and zero-point Energies=-765.276755
Sum of electronic and thermal Energies=-765.258975
Sum of electronic and thermal Enthalpies=-765.258000
Sum of electronic and thermal Free Energies=-765.326057

C	1.01627500	3.35430900	-0.37864800
C	2.26848500	3.05960200	0.14668300
C	2.63737300	1.74326100	0.38334400
C	1.75883800	0.69964400	0.11531600
C	0.50659800	1.01972400	-0.39932500
H	3.61678800	1.51703200	0.78722100
H	0.73279700	4.37972200	-0.57818600
H	2.96335400	3.86059300	0.36735700
C	2.14529300	-0.74277400	0.34126700
N	1.69209000	-1.26929000	1.44323400
N	-0.37137200	-0.06319400	-0.70833500
H	4.51162200	-3.68829800	0.27361200
H	0.03316700	-0.80390600	-1.27491100
C	-4.43634700	-0.61964900	0.38153700
C	-3.79077900	-1.16233000	-0.90298700
C	-2.30827900	-1.46894700	-0.71147100
C	-1.58293500	-0.24451800	-0.30375600

C	-2.29143700	0.71121900	0.57760200
C	-3.41195900	0.00694500	1.33135300
H	-5.19182200	0.12122100	0.11335500
H	-4.29618600	-2.06807700	-1.23665100
H	-2.17974000	-2.18541800	0.11054800
H	-1.58053900	1.20716700	1.24053100
H	-3.89525200	0.72278700	1.99583300
O	2.84022000	-1.26049100	-0.58519400
H	-2.70925100	1.49361500	-0.06791600
H	-2.97011300	-0.76125700	1.96955500
H	-4.95764500	-1.42162000	0.90681500
H	-3.88795900	-0.43509300	-1.71192200
H	-1.84965400	-1.91054500	-1.59634900
O	3.66532100	-3.77323300	-0.16832400
H	2.00616000	-2.23927600	1.48585900
H	3.36452100	-2.84148200	-0.31751400
C	0.12877800	2.32861400	-0.66183100
H	-0.83903300	2.53941900	-1.09788400

9-W:

Zero-point correction=0.296331 (Hartree/Particle)
Thermal correction to Energy=0.314960
Thermal correction to Enthalpy=0.315936
Thermal correction to Gibbs Free Energy=0.245485
Sum of electronic and zero-point Energies=-765.278053
Sum of electronic and thermal Energies=-765.259424
Sum of electronic and thermal Enthalpies=-765.258448
Sum of electronic and thermal Free Energies=-765.328899

C	1.54357600	-3.33912100	-0.09917300
C	2.65244400	-2.65050800	-0.57357900
C	2.70288700	-1.26830200	-0.48869300
C	1.64690800	-0.52831000	0.04148000
C	0.54752100	-1.24688100	0.51102100
H	3.57239800	-0.72607000	-0.83607100
H	1.50077600	-4.41957900	-0.15174000
H	3.48413500	-3.19360800	-1.00550300
C	1.76672600	0.98080700	0.06620200
N	0.66240100	1.65190900	-0.13663800
N	-0.55309200	-0.55973200	1.11959100
H	0.90413700	2.64249700	-0.13357700
H	-0.44140000	-0.28540500	2.09050900
C	-4.11791400	0.68629800	-0.82238800

C	-4.00867200	0.39618100	0.68181000
C	-2.60771800	0.67087700	1.21672700
C	-1.60443500	-0.14909700	0.50371900
C	-1.86149700	-0.46863400	-0.91783300
C	-2.76928700	0.58292900	-1.54173200
H	-4.82956000	-0.01232300	-1.26649800
H	-4.72437900	0.99711900	1.24228800
H	-2.32295900	1.71119600	1.00733200
H	-0.92215000	-0.58450000	-1.45633700
H	-2.91566000	0.34610800	-2.59537100
O	2.94150100	1.42251500	0.24807100
H	-2.35566800	-1.44979800	-0.92663500
H	-2.24827300	1.54214100	-1.50615900
H	-4.52378300	1.68697100	-0.98018800
H	-4.25587800	-0.64836000	0.88404200
H	-2.52830300	0.52968800	2.29518500
O	3.22636800	4.06078600	0.02551100
H	3.47172700	4.20815900	-0.88914800
H	3.12378100	3.07648500	0.10463600
C	0.48984100	-2.63132200	0.45610600
H	-0.37932800	-3.14185800	0.85190800

TS6-W:

Zero-point correction=0.295529 (Hartree/Particle)
Thermal correction to Energy=0.312334
Thermal correction to Enthalpy=0.313309
Thermal correction to Gibbs Free Energy=0.250082
Sum of electronic and zero-point Energies=-765.299567
Sum of electronic and thermal Energies=-765.282762
Sum of electronic and thermal Enthalpies=-765.281787
Sum of electronic and thermal Free Energies=-765.345014

C	-3.05030700	-2.42014800	0.04130000
C	-3.54909500	-1.26451100	0.63801600
C	-2.74643700	-0.13985700	0.69668500
C	-1.45182900	-0.14315800	0.18280300
C	-0.94594400	-1.32182900	-0.39589500
H	-3.11027800	0.78118000	1.13369700
H	-3.66630100	-3.30948100	-0.01908600
H	-4.55235800	-1.24467600	1.04349800
C	-0.68023100	1.12878400	0.19153200
N	0.53261400	1.08740300	-0.36256300
N	0.31806000	-1.34639600	-0.94375900

H	-3.37617200	3.60958900	-1.08912800
H	0.59724600	-2.18767000	-1.42439500
C	3.66442000	0.77525400	0.55263100
C	3.85968300	-0.20648700	-0.59341700
C	2.54788200	-0.45584100	-1.33455000
C	1.36336300	-0.57211600	-0.40507300
C	1.73748400	-0.83017700	1.02819500
C	2.68551600	0.22414000	1.60086300
H	4.62257500	1.00587700	1.02145800
H	4.60565600	0.16381600	-1.29846900
H	2.34547600	0.33506200	-2.05756100
H	0.84531100	-0.93682300	1.64495800
H	3.23775800	-0.23110200	2.42505200
O	-1.18301300	2.17397100	0.63576800
H	2.22969500	-1.81035700	1.01709200
H	2.10340300	1.04042900	2.03166800
H	3.29179500	1.72038300	0.14582600
H	4.24571900	-1.15130400	-0.19953700
H	2.60721300	-1.38792800	-1.90513800
O	-2.52829600	4.02225700	-0.91452100
H	1.12466400	1.89378400	-0.21826500
H	-2.05179900	3.37576600	-0.36330200
C	-1.76584200	-2.45204700	-0.46825100
H	-1.37581400	-3.35546500	-0.92311500

Pr:

Zero-point correction=0.274022 (Hartree/Particle)
Thermal correction to Energy=0.287401
Thermal correction to Enthalpy=0.288376
Thermal correction to Gibbs Free Energy=0.234232
Sum of electronic and zero-point Energies=-688.975220
Sum of electronic and thermal Energies=-688.961842
Sum of electronic and thermal Enthalpies=-688.960866
Sum of electronic and thermal Free Energies=-689.015010

C	3.69621700	-1.27522000	0.25217800
C	3.94721000	0.08297600	0.47157600
C	2.91640200	0.99621200	0.29731700
C	1.64367900	0.56750500	-0.08105900
C	1.38927600	-0.80064000	-0.29210700
H	3.06655300	2.06265400	0.43793600
H	4.49489400	-2.00078200	0.38171700
H	4.93611900	0.41755900	0.76802400

C	0.56822900	1.55354200	-0.32685200
N	-0.64963200	1.00090800	-0.62228700
N	0.12992400	-1.19411800	-0.71030400
H	-1.39168400	1.67474700	-0.74461300
H	-0.04625600	-2.18706600	-0.64111100
C	2.43584400	-1.71910500	-0.12572100
H	2.25475600	-2.77823300	-0.29387300
C	-2.21887100	-0.78044400	-1.17426100
C	-3.50626900	-0.06340700	-0.76562000
C	-3.80679000	-0.23926800	0.72203300
C	-2.61907400	0.19056700	1.58075700
C	-1.35033200	-0.55649300	1.17554300
C	-1.01238700	-0.37734100	-0.32120600
H	-4.70405400	0.32758000	0.99590400
H	-3.43576000	1.00841500	-1.00162900
H	-4.33605200	-0.44145700	-1.37350200
H	-2.36315500	-1.86308300	-1.05084100
H	-1.97375100	-0.60258400	-2.22654900
H	-2.45751600	1.27263700	1.47942300
H	-2.82904900	0.01279500	2.64157500
H	-0.49201700	-0.23243600	1.77516800
H	-1.48759400	-1.63143200	1.36338100
H	-4.03161500	-1.29720600	0.92137000
O	0.74191700	2.76713300	-0.32246300

Gas:
TS1-1

Zero-point correction=0.348445 (Hartree/Particle)
Thermal correction to Energy=0.368105
Thermal correction to Enthalpy=0.369049
Thermal correction to Gibbs Free Energy=0.297562
Sum of electronic and zero-point Energies=-860.461333
Sum of electronic and thermal Energies=-860.441673
Sum of electronic and thermal Enthalpies=-860.440729
Sum of electronic and thermal Free Energies=-860.512216

C	3.29400700	0.02177400	-1.97902600
C	2.03569500	-0.05545900	-1.39688600
C	1.89446200	-0.34153000	-0.03856500
C	3.04796900	-0.56635000	0.75455100
C	4.31178100	-0.48145100	0.16247900
C	4.42827700	-0.18971000	-1.19007400
H	3.39355700	0.24273000	-3.03713700
H	1.12699400	0.09763900	-1.97145300

H	5.18508600	-0.65180600	0.78390000
H	5.41733500	-0.12935700	-1.63613100
C	0.64544500	-0.45235800	0.68682200
N	0.18846200	-0.71540700	1.75134500
C	-0.94157100	0.13953800	-0.71010100
C	-3.18093500	0.02393100	-1.03014900
H	-4.13839800	-0.44687000	-1.19221700
C	-2.85427100	1.33617100	-0.92259000
H	-3.47380700	2.21882600	-0.97030300
N	-2.00249400	-0.68432400	-0.89123300
N	-1.48649100	1.38123000	-0.72563700
C	-0.71937500	2.61026600	-0.56740200
H	-0.81186100	3.19700300	-1.48951300
H	0.32624400	2.30675400	-0.46955300
C	-1.88983400	-2.13627300	-0.97000700
H	-0.86788300	-2.37381500	-0.66552900
H	-2.00808700	-2.44036400	-2.01744100
C	-1.15399900	3.44222800	0.63549800
H	-0.57276200	4.37252000	0.61002300
H	-2.20342800	3.74147300	0.51282000
C	-0.96158900	2.73879600	1.97232300
H	-1.30577100	3.37138100	2.79630100
H	-1.51236600	1.79466200	2.01607900
H	0.09232700	2.50073400	2.14742400
C	-2.89410400	-2.87419800	-0.09078600
H	-3.91393400	-2.68437600	-0.45155300
H	-2.72123200	-3.94603900	-0.24884500
C	-2.78796000	-2.53940200	1.39146400
H	-2.99494800	-1.48148800	1.57961300
H	-3.50213500	-3.13146600	1.97228400
H	-1.78219200	-2.73455300	1.77403800
O	2.96451300	-0.85718700	2.05863100
H	2.01084100	-0.89242500	2.30150500

TS1-2

Zero-point correction=0.375833 (Hartree/Particle)
Thermal correction to Energy=0.397398
Thermal correction to Enthalpy=0.398342
Thermal correction to Gibbs Free Energy=0.322886
Sum of electronic and zero-point Energies=-899.664678
Sum of electronic and thermal Energies=-899.643113
Sum of electronic and thermal Enthalpies=-899.642168
Sum of electronic and thermal Free Energies=-899.717624

C	3.42204700	0.47283500	2.10180100
C	2.08986700	0.29677600	2.47266000
C	1.16485400	-0.13032800	1.52627700
C	1.54220000	-0.41912600	0.21124500
C	2.89383400	-0.24851500	-0.15181200
H	0.11478000	-0.23560600	1.78452800
H	4.15273700	0.82305700	2.82571900
H	1.77097200	0.50073500	3.49090200
C	0.55817200	-0.90621600	-0.76926400
N	0.47211900	-1.62954400	-1.72063800
C	3.81465000	0.20745900	0.79368700
H	4.84104000	0.35780000	0.47169000
O	3.32723400	-0.42212200	-1.43259000
C	3.64057600	-1.76416000	-1.79724600
H	4.01349900	-1.71734200	-2.82200700
H	4.42482400	-2.16602400	-1.14183200
H	2.74441200	-2.39091800	-1.76448700
C	-1.11543100	-0.05758300	-0.40872400
C	-3.23059100	-0.11274500	-1.19980900
H	-4.20529600	-0.53265200	-1.39750700
C	-2.70378100	1.09129700	-1.53665100
H	-3.12886700	1.91571900	-2.08879300
N	-2.25241000	-0.79118000	-0.50199500
N	-1.41599800	1.10838600	-1.03411200
C	-0.48536500	2.21530600	-1.19828300
H	-0.39857000	2.43365100	-2.26860100
H	0.48879500	1.85911100	-0.85537900
C	-2.38391000	-2.15519400	-0.01690700
H	-1.38144800	-2.47842000	0.27214900
H	-2.69408000	-2.78617900	-0.85694000
C	-0.90017700	3.46446600	-0.42613300
H	-0.17096200	4.24884200	-0.66345600
H	-1.86719300	3.82458900	-0.80160200
C	-0.97049700	3.25422600	1.08066500
H	-1.24842300	4.18100100	1.59197900
H	-1.71388000	2.49349000	1.34085600
H	-0.00525300	2.92325900	1.47855100
C	-3.36019700	-2.27993500	1.14913500
H	-4.35739300	-1.94948800	0.82948100
H	-3.45462000	-3.34708200	1.38493700
C	-2.92930700	-1.50719000	2.38880500
H	-2.83170900	-0.43751600	2.17577600
H	-3.65792800	-1.62167400	3.19719100

H	-1.96096200	-1.86326700	2.75810000

TS1-3

Zero-point correction=0.371327 (Hartree/Particle)
Thermal correction to Energy=0.391604
Thermal correction to Enthalpy=0.392548
Thermal correction to Gibbs Free Energy=0.320304
Sum of electronic and zero-point Energies=-824.542740
Sum of electronic and thermal Energies=-824.522463
Sum of electronic and thermal Enthalpies=-824.521519
Sum of electronic and thermal Free Energies=-824.593763

C	-4.35065000	-0.20311100	-1.24013700
C	-3.20297600	-0.18254000	-2.02651900
C	-1.95558500	-0.14947100	-1.41200200
C	-1.82915700	-0.13904400	-0.02137500
C	-2.99160200	-0.16243400	0.78735900
H	-1.04327300	-0.13069000	-2.00152500
H	-5.33427800	-0.22751800	-1.70139700
H	-3.27570100	-0.19177500	-3.11052600
C	-0.51313900	-0.10935800	0.63806600
N	-0.01487600	-0.13407100	1.72695000
C	-4.23411500	-0.19249300	0.14799300
H	-5.13271100	-0.20841100	0.76036900
C	-2.92495100	-0.15614200	2.28523500
H	-3.93184400	-0.15933800	2.71260100
H	-2.37242600	-1.02258000	2.66186500
H	-2.38003300	0.71754400	2.65620600
C	0.88530400	0.03205100	-0.70308400
C	2.95338900	0.90796100	-0.95696200
H	3.70092400	1.68003900	-1.05549700
C	3.08001800	-0.44250900	-0.95653800
H	3.95829700	-1.06146700	-1.05603600
N	1.60587600	1.17659300	-0.80584700
N	1.80698900	-0.95770200	-0.80453800
C	1.47568600	-2.37743200	-0.79901900
H	1.59259100	-2.76517300	-1.81892400
H	0.41593500	-2.44125400	-0.53854200
C	1.01990400	2.51126900	-0.80565100
H	-0.04868700	2.37618600	-0.61839000
H	1.12954000	2.93643700	-1.81128300
C	2.31598700	-3.19665700	0.17501100
H	2.04077300	-4.24823500	0.02467700

H	3.37552700	-3.12701700	-0.10531200
C	2.12929700	-2.80748500	1.63540200
H	2.77873900	-3.40729600	2.28094900
H	2.35265900	-1.75033900	1.80473100
H	1.09418100	-2.95898500	1.95577800
C	1.63413300	3.44564500	0.23178700
H	2.70902200	3.55367100	0.03473600
H	1.20119800	4.43978000	0.06284500
C	1.40363500	3.00839800	1.67213300
H	1.77367400	1.99520800	1.85370000
H	1.90249800	3.69022400	2.36810500
H	0.33641200	2.99735700	1.91471700

TS1-4

Zero-point correction=0.343486 (Hartree/Particle)
Thermal correction to Energy=0.362317
Thermal correction to Enthalpy=0.363261
Thermal correction to Gibbs Free Energy=0.293127
Sum of electronic and zero-point Energies=-785.299262
Sum of electronic and thermal Energies=-785.280432
Sum of electronic and thermal Enthalpies=-785.279488
Sum of electronic and thermal Free Energies=-785.349622

C	3.59074000	0.01598900	-1.52464000
C	2.27119100	0.01222200	-1.07623100
C	1.98846300	0.01388000	0.28961100
C	3.05099400	0.01949500	1.20711400
C	4.36572200	0.02318400	0.75791500
C	4.64170200	0.02142400	-0.61084200
H	3.79702500	0.01471000	-2.59162700
H	1.43869100	0.00806500	-1.77415100
H	2.81902300	0.02085800	2.26793300
H	5.18014500	0.02745800	1.47724600
H	5.67044800	0.02432100	-0.96059600
C	0.62737800	0.01032900	0.84490200
N	0.04772200	0.01212400	1.88880300
C	-0.67289800	-0.00253000	-0.64720000
C	-2.77900900	-0.69810500	-1.08517500
H	-3.57825000	-1.40310900	-1.25438900
C	-2.79008900	0.65832300	-1.08531800
H	-3.60079000	1.35012500	-1.25457200
N	-1.47809000	-1.08033000	-0.81846800

N	-1.49567900	1.06183000	-0.81866100
C	-1.04979200	2.44890400	-0.76841500
H	-1.07472400	2.85809200	-1.78628800
H	-0.00533900	2.42099200	-0.44697900
C	-1.00971000	-2.45997000	-0.76867200
H	0.03646200	-2.41471400	-0.45485600
H	-1.03531600	-2.87141400	-1.78560900
C	-1.87614400	3.32148400	0.17077500
H	-1.51069700	4.34951600	0.05310000
H	-2.92038900	3.33898800	-0.16878800
C	-1.80324300	2.90111700	1.63262000
H	-2.43617700	3.54486100	2.25162400
H	-2.12196600	1.86433400	1.77326500
H	-0.77873800	2.96353600	2.01175600
C	-1.81531700	-3.34377700	0.17807500
H	-2.86219300	-3.37588400	-0.15218700
H	-1.43656200	-4.36666900	0.05765200
C	-1.73523200	-2.92147000	1.63896000
H	-2.06587000	-1.88872700	1.78184200
H	-2.35432400	-3.57284800	2.26393600
H	-0.70667800	-2.97085900	2.00909300

TS1-5

Zero-point correction=0.348227 (Hartree/Particle)
Thermal correction to Energy=0.370594
Thermal correction to Enthalpy=0.371538
Thermal correction to Gibbs Free Energy=0.293658
Sum of electronic and zero-point Energies=-1122.032087
Sum of electronic and thermal Energies=-1122.009719
Sum of electronic and thermal Enthalpies=-1122.008775
Sum of electronic and thermal Free Energies=-1122.086655

C	-3.41940300	-0.88631800	2.38237400
C	-2.11814500	-1.05620400	2.84034200
C	-1.05168800	-0.90374600	1.96081000
C	-1.24812700	-0.60116800	0.61165400
C	-2.57327600	-0.42986200	0.15469000
H	-0.02798300	-1.01557700	2.30434200
H	-4.26345800	-0.99470000	3.05679500
H	-1.92918200	-1.30623600	3.88059400
C	-0.09211800	-0.53321100	-0.30307800
N	0.19854400	-0.71525600	-1.44711500
C	-3.63783400	-0.56872100	1.04473400

H	-4.64903800	-0.42157000	0.68345900
C	-2.90138500	-0.08701300	-1.28122400
F	-2.65686700	-1.09639100	-2.12560500
F	-2.23194300	0.99559100	-1.71628700
F	-4.21636900	0.21069800	-1.41900800
C	1.46313500	0.01552100	0.75788700
C	3.70953700	0.22464300	0.68390400
H	4.73519200	-0.09784200	0.59435300
C	3.19376400	1.46288200	0.88469600
H	3.68518800	2.41746700	0.99348200
N	2.63805300	-0.64219400	0.60480000
N	1.81949100	1.31172300	0.92651800
C	0.87546400	2.40473800	1.12497500
H	1.01864100	2.80822600	2.13486400
H	-0.12239400	1.96145400	1.08351500
C	2.73567000	-2.08406000	0.39982600
H	1.73137200	-2.41682800	0.12888100
H	3.00919000	-2.55573400	1.35192300
C	1.01543500	3.51175900	0.08422800
H	0.29820200	4.29691900	0.35418200
H	2.00858700	3.97221000	0.17133900
C	0.77396700	3.04622500	-1.34570400
H	0.89529100	3.87692600	-2.04763000
H	1.47133000	2.25437600	-1.63602100
H	-0.23528400	2.64318500	-1.46890300
C	3.72840800	-2.47943900	-0.68828900
H	4.74940000	-2.21905600	-0.37764100
H	3.70944000	-3.57518700	-0.73957700
C	3.42124600	-1.88733700	-2.05813400
H	3.49193200	-0.79540500	-2.04813500
H	4.12588400	-2.26431700	-2.80611100
H	2.40378500	-2.12945100	-2.37717600

TS1-6

Zero-point correction=0.345972 (Hartree/Particle)
Thermal correction to Energy=0.367588
Thermal correction to Enthalpy=0.368532
Thermal correction to Gibbs Free Energy=0.291683
Sum of electronic and zero-point Energies=-989.592793
Sum of electronic and thermal Energies=-989.571177
Sum of electronic and thermal Enthalpies=-989.570233
Sum of electronic and thermal Free Energies=-989.647083

C	-3.82508400	1.62557500	-1.48410600
C	-2.56977000	2.06041700	-1.90393400
C	-1.42215300	1.63519100	-1.24178500
C	-1.49211300	0.76893700	-0.14877300
C	-2.76598000	0.33098100	0.23382900
H	-0.43949300	1.96985800	-1.55825000
H	-4.72375500	1.95557500	-1.99583100
H	-2.48312200	2.73993900	-2.74674300
C	-0.30291000	0.45949700	0.65158100
N	0.05799300	0.36426900	1.78103000
C	-3.92440000	0.75539700	-0.40370200
H	-4.88432500	0.39071500	-0.05353100
N	-2.93485100	-0.66663200	1.29448600
O	-3.78462600	-0.44393500	2.14032300
O	-2.25796800	-1.67840100	1.21813100
C	1.19630900	0.19330300	-0.69587200
C	3.43158600	0.01595500	-0.96930000
H	4.46420000	0.32779600	-0.94127900
C	2.87675800	-1.14934100	-1.38721700
H	3.33726700	-2.04177600	-1.78223500
N	2.38930600	0.81657300	-0.54424800
N	1.51220200	-1.02009500	-1.20661700
C	0.53685100	-2.06641300	-1.49487600
H	0.48626800	-2.20817200	-2.58129700
H	-0.43068700	-1.68666100	-1.15885900
C	2.53229400	2.16452800	-0.00509800
H	1.55990200	2.42005900	0.42240500
H	2.73603400	2.85558500	-0.83272700
C	0.85615100	-3.38519700	-0.79664700
H	0.07309600	-4.09568000	-1.08880700
H	1.79466900	-3.79522700	-1.19347300
C	0.92585500	-3.27514600	0.72111200
H	1.14703900	-4.24939600	1.16777500
H	1.70722900	-2.57652200	1.03672800
H	-0.01886000	-2.91414300	1.13671400
C	3.61749300	2.28165500	1.06026900
H	4.60492600	2.11522200	0.60888700
H	3.61778300	3.32843700	1.38878900
C	3.41686700	1.35793700	2.25538400
H	3.48929900	0.30533600	1.96467600
H	4.17677900	1.54768800	3.01981200
H	2.42742700	1.49160200	2.70187300

TS2-1

Zero-point correction=0.329146 (Hartree/Particle)
Thermal correction to Energy=0.346254
Thermal correction to Enthalpy=0.347198
Thermal correction to Gibbs Free Energy=0.283818
Sum of electronic and zero-point Energies=-654.140259
Sum of electronic and thermal Energies=-654.123151
Sum of electronic and thermal Enthalpies=-654.122207
Sum of electronic and thermal Free Energies=-654.185587

C	0.57218600	1.97705400	-0.08874800
O	1.83199900	2.00103200	-0.02269200
C	-0.05507000	2.63754900	-1.32163300
H	0.11490600	3.71754700	-1.22922200
H	0.45837600	2.29641800	-2.22408500
H	-1.13187200	2.46906000	-1.42818200
C	-0.17206100	2.25712300	1.21790400
H	0.05300500	3.29435100	1.49502000
H	-1.25978800	2.15211200	1.15345300
H	0.20933500	1.60855100	2.00977500
C	0.00758400	0.09819200	-0.46955400
C	0.31297800	-2.00540600	-1.23183300
H	0.87760200	-2.87393200	-1.53561800
C	-1.02192700	-1.77895600	-1.21030800
H	-1.84927800	-2.41224300	-1.49149200
N	0.92052700	-0.85108200	-0.78166900
N	-1.18838000	-0.49016600	-0.73959600
C	-2.50406200	0.10818900	-0.55486700
H	-3.00585200	0.14231600	-1.52904100
H	-2.34542300	1.13627100	-0.23042200
C	2.37590100	-0.73960500	-0.64265200
H	2.59595300	0.33000600	-0.57611800
H	2.81509400	-1.14983000	-1.55864700
C	-3.36376500	-0.64383500	0.45856800
H	-4.33940500	-0.14307300	0.48745700
H	-3.55842100	-1.66030000	0.09304500
C	-2.76167700	-0.70100300	1.85634500
H	-3.41541700	-1.25300700	2.53822900
H	-1.78730300	-1.20009400	1.85066900
H	-2.61582200	0.30233500	2.26917600
C	2.90150300	-1.47964100	0.58374100
H	2.67094600	-2.55192600	0.50912500
H	3.99529000	-1.39811300	0.55434700
C	2.37808700	-0.91558500	1.89847300

H	1.29591800	-1.06062300	1.98954000
H	2.85090200	-1.40982200	2.75317900
H	2.57216500	0.16001900	1.95758800

TS2-2

Zero-point correction=0.306325 (Hartree/Particle)
Thermal correction to Energy=0.325607
Thermal correction to Enthalpy=0.326551
Thermal correction to Gibbs Free Energy=0.257433
Sum of electronic and zero-point Energies=-951.642510
Sum of electronic and thermal Energies=-951.623228
Sum of electronic and thermal Enthalpies=-951.622284
Sum of electronic and thermal Free Energies=-951.691402

C	-1.80040300	0.11809900	-0.90048700
O	-2.07954400	1.28896700	-1.15370400
C	-1.84673400	-0.93635400	-1.98671900
H	-2.90097500	-1.08490000	-2.24933800
H	-1.33029200	-0.55334400	-2.86838200
H	-1.42464800	-1.89703900	-1.69156600
C	-2.16634400	-0.37884100	0.51700500
C	0.42283100	0.06527400	-0.56268100
C	2.41284200	1.00611900	-1.09739900
H	3.10592400	1.80817000	-1.30114700
C	2.58885200	-0.33744200	-1.10591600
H	3.46420600	-0.93157900	-1.31977000
N	1.09239200	1.22761500	-0.76157800
N	1.36713200	-0.89083200	-0.77306100
C	1.16946800	-2.32433400	-0.60063800
H	1.36279000	-2.82215800	-1.55838100
H	0.11975800	-2.46598000	-0.34619400
C	0.53936800	2.56712300	-0.56746000
H	-0.53676100	2.44857100	-0.43413600
H	0.69902400	3.13282400	-1.49236600
C	2.05170700	-2.91679300	0.49601400
H	1.85537600	-3.99593900	0.51688000
H	3.10910700	-2.80793100	0.22214100
C	1.80304300	-2.31277700	1.87199200
H	2.43736300	-2.78897200	2.62571100
H	2.02159300	-1.24003900	1.88175300
H	0.75950100	-2.43883700	2.17743800
C	1.17355400	3.29287700	0.61636700
H	2.24894500	3.43057000	0.43901100

H	0.73949100	4.30008900	0.64024900
C	0.95120200	2.60013000	1.95428000
H	1.39519000	1.59910000	1.96490100
H	1.40294700	3.17344000	2.76982200
H	-0.11619900	2.48672200	2.16643500
F	-1.83744000	0.49155500	1.47348000
F	-1.63120100	-1.57571600	0.84824700
F	-3.50791100	-0.54700200	0.56970600

TS2-3

Zero-point correction=0.383111 (Hartree/Particle)
Thermal correction to Energy=0.403147
Thermal correction to Enthalpy=0.404091
Thermal correction to Gibbs Free Energy=0.333362
Sum of electronic and zero-point Energies=-845.610636
Sum of electronic and thermal Energies=-845.590600
Sum of electronic and thermal Enthalpies=-845.589656
Sum of electronic and thermal Free Energies=-845.660385

C	-2.64232200	-1.28601900	-1.69273000
C	-1.45252300	-1.38957900	-0.98167600
C	-1.40671400	-1.11527900	0.38908000
C	-2.59507300	-0.76768900	1.03736600
C	-3.79584500	-0.67177900	0.32951000
C	-3.82260500	-0.92304800	-1.03901600
H	-2.65621200	-1.49955300	-2.75859800
H	-0.53580000	-1.70743300	-1.46909000
H	-2.59889800	-0.58333900	2.10827300
H	-4.71148600	-0.41056700	0.85403100
H	-4.75576500	-0.85155300	-1.59122700
C	-0.08277600	-1.32988100	1.12186500
O	0.59001500	-2.32385000	0.72932300
C	-0.11139600	-1.06704800	2.62957600
H	-0.51819400	-0.08973500	2.91136100
H	-0.71413600	-1.85201300	3.10293100
H	0.90682300	-1.15336200	3.01548400
C	0.91666200	0.32175700	0.61250500
C	2.75366000	1.53855900	0.13348900
H	3.79507100	1.71136500	-0.09158500
C	1.72360500	2.40612500	0.27772100
H	1.69385100	3.48183200	0.19948200
N	2.24156200	0.27410600	0.34357000
N	0.60900800	1.64256800	0.56709300

C	-0.70438400	2.21973500	0.83508600
H	-0.65257500	2.76341700	1.78621600
H	-1.39470700	1.38463400	0.95740200
C	3.07929600	-0.92924400	0.29898700
H	2.45001400	-1.75327300	0.64938500
H	3.90622600	-0.77301700	1.00118200
C	-1.19387000	3.14125800	-0.27781600
H	-2.16251100	3.54046700	0.04712700
H	-0.52804900	4.00964700	-0.36664800
C	-1.34134900	2.44909100	-1.62635900
H	-1.71458100	3.14739100	-2.38183300
H	-0.38245100	2.05614900	-1.98029400
H	-2.03883500	1.60792000	-1.56419400
C	3.61288000	-1.21568800	-1.10105600
H	4.24871000	-0.38750800	-1.44446700
H	4.27185200	-2.08840600	-1.01400800
C	2.51599500	-1.49540600	-2.12014700
H	1.88063100	-0.61559500	-2.27029900
H	2.94316600	-1.76566500	-3.09104700
H	1.87429400	-2.31291800	-1.77712000

TS2-4

Zero-point correction=0.354822 (Hartree/Particle)
Thermal correction to Energy=0.373658
Thermal correction to Enthalpy=0.374602
Thermal correction to Gibbs Free Energy=0.305860
Sum of electronic and zero-point Energies=-806.366968
Sum of electronic and thermal Energies=-806.348132
Sum of electronic and thermal Enthalpies=-806.347188
Sum of electronic and thermal Free Energies=-806.415929

C	-2.62525600	2.09457100	-0.82603700
C	-1.56404000	1.72270300	-0.00719100
C	-1.68121400	0.63517200	0.86033700
C	-2.88725400	-0.06288100	0.91465400
C	-3.95377100	0.30350300	0.09388200
C	-3.82488400	1.38035100	-0.78098700
H	-2.52149700	2.93980500	-1.50157400
H	-0.62481400	2.27090700	-0.05105600
H	-2.96956000	-0.88321300	1.62321700
H	-4.89047100	-0.24572300	0.14506700
H	-4.65533400	1.66961800	-1.41934400
C	-0.56624000	0.23827800	1.80473500

O	-0.70741800	-0.73470400	2.56824900
H	0.03040200	1.11688600	2.13132500
C	0.94278100	-0.31973700	0.50792600
C	2.33692600	-1.99336400	-0.08953300
H	2.61329400	-2.99502800	-0.38266600
C	3.10058800	-0.89549200	0.13585200
H	4.16964000	-0.75763100	0.08007900
N	1.02972600	-1.61823900	0.14361400
N	2.22708500	0.11492400	0.49776200
C	2.64696600	1.47016500	0.82229200
H	3.33079800	1.42581600	1.67793700
H	1.75036900	2.00589600	1.14301400
C	-0.11343500	-2.51359500	0.01577100
H	-0.93278700	-2.05076900	0.56793200
H	0.13675200	-3.44601800	0.53303100
C	3.30871900	2.18881800	-0.35062500
H	3.64812500	3.16542200	0.01591800
H	4.21547200	1.64545900	-0.64627200
C	2.39526300	2.36912100	-1.55542900
H	2.91909300	2.87838900	-2.36989900
H	2.04058300	1.40591500	-1.93560900
H	1.51459000	2.96825200	-1.29974600
C	-0.48832700	-2.78840800	-1.43834000
H	0.33950300	-3.31023100	-1.93788600
H	-1.32915300	-3.49315400	-1.42513700
C	-0.86638100	-1.53960100	-2.22402300
H	-0.02728300	-0.83870800	-2.28191500
H	-1.15649500	-1.79743400	-3.24745300
H	-1.70220800	-1.01123900	-1.75427900

TS2-5

Zero-point correction=0.360254 (Hartree/Particle)
Thermal correction to Energy=0.382475
Thermal correction to Enthalpy=0.383419
Thermal correction to Gibbs Free Energy=0.307564
Sum of electronic and zero-point Energies=-1143.110075
Sum of electronic and thermal Energies=-1143.087854
Sum of electronic and thermal Enthalpies=-1143.086909
Sum of electronic and thermal Free Energies=-1143.162764

C	-3.83743500	-0.16902000	0.25602000
C	-2.65666300	-0.76622600	-0.18683800
C	-1.51363600	-0.75081300	0.61864300

C	-1.58101800	-0.14741900	1.87865900
C	-2.75432100	0.45552800	2.31500000
C	-3.88944600	0.44858100	1.50246000
H	-4.72134900	-0.19851900	-0.37525500
H	-2.64610700	-1.25371100	-1.15590200
H	-0.69872200	-0.17444600	2.51049300
H	-2.78877400	0.92423300	3.29475300
H	-4.81069700	0.91155800	1.84516300
C	-0.22102100	-1.44987500	0.27548600
O	0.44862000	-1.95970300	1.17724700
C	-0.12743400	-2.15301700	-1.10233600
F	-0.89954300	-3.26130300	-1.08195600
F	-0.54602900	-1.41977200	-2.15686900
F	1.12336800	-2.54560700	-1.36379400
C	0.97962100	0.28943500	-0.48213500
C	1.86828000	2.16828500	-1.37828600
H	1.87962200	3.09644900	-1.92835900
C	2.86931600	1.49995200	-0.75576100
H	3.91920800	1.73246200	-0.66184400
N	0.72465000	1.41557300	-1.19434900
N	2.30621500	0.36065300	-0.21674300
C	3.08616400	-0.63581400	0.51750300
H	3.90154000	-0.96373600	-0.13708600
H	2.42530300	-1.48417200	0.70017100
C	-0.57359700	1.78120400	-1.75004300
H	-1.28639200	1.04066000	-1.38689400
H	-0.52000000	1.68793900	-2.84112800
C	3.63908400	-0.09531600	1.83288000
H	4.25360000	-0.89172000	2.27038700
H	4.32160000	0.74348200	1.63890400
C	2.55674100	0.32536400	2.81865800
H	2.99665400	0.66169600	3.76275400
H	1.95572200	1.14954500	2.41920200
H	1.87979000	-0.50903300	3.02741800
C	-1.02033800	3.18509400	-1.35530100
H	-0.32914600	3.93030600	-1.77043300
H	-1.98213000	3.36285600	-1.85200800
C	-1.16554300	3.38313300	0.14762500
H	-0.21241400	3.22760600	0.66389900
H	-1.50630000	4.39790900	0.37530400
H	-1.88871900	2.67836200	0.57029300