Electronic Supplementary Material (ESI) for ChemComm.

SUPPORTING INFORMATION

Transition Structures for the Oxy-Ene Reaction

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Theoretical details

At the beginning of this study, we tested the computational methods used by Fernández and Bickelhaupt,[1] as well as that used by Zhou, Houk, Tang and co-workers[2] in their respective theoretical analysis of the Alder-ene reaction. A slightly better agreement between the calculated and the experimentally determined $\Delta G^{\ddagger}$ reported by Klärner was obtained with the latter (calcd 39.5/40.6 kcal/mol respectively; exp 43.5 kcal/mol).[3] Thus, the geometry optimizations and frequency calculations were carried out at the ωB97XD[4]/ 6-311+G(d,p)[5] level of theory. Single point calculations were then performed at the ωB97XD/def2-QZVPP[6] level. The relevance of this level of theory to study pericyclic reactions has been previously justified.[2] For some computations, solvation correction via PCM computations[7] were obtained at the ωB97XD/def2-QZVPP level.

Why were solvent effects or counterions not always taken into account: it is normal when studying a reaction with parent compounds (Figure 1) to work in the gas phase to analyze the intrinsic features of a mechanism. For instance, no solvation model was used in the study of the Alder-ene reaction[1] and naked anions were used in the study of the oxy-Cope rearrangement.[8] Besides, Klärner's reactions (Scheme 3) were experimentally performed in the gas phase.[3] Borschberg's reactions were performed in benzene (Scheme 3).[9] No strong solvation effect is expected with such a solvent, as confirmed by PCM computations (see Figure S1). The reaction of **1** to give aristone has not been performed experimentally (Scheme 2). The counterion is not known.

Additional computations

Intramolecular reactions corresponding to Klärner's and Borschberg's substrates were studied. The cyclization of **E** requires 40.6 kcal/mol of free energy of activation and is exergonic by 2.2 kcal/mol. The high field NICS(0) value of -22.6 ppm for $\mathbf{TS_{EF}}$ is again consistent with a pericyclic reaction (Table S1). Klärner hypothesized that "metalation of the hydroxy group could lead to the thermolysis already taking place at considerably lower temperatures". The barrier of 23.3 kcal/mol to reach $\mathbf{TS_{GH}}$ is indeed in line with this suggestion. The same lowering of the cyclization barrier was computed with Borschberg's substrate **I**, from 38.3 kcal/mol in the neutral series to 17.5 kcal/mol in the anionic one. It may seem surprising that no strong acceleration was observed when using lithium or potassium salts of the allyl alkoxide **8** (Scheme 3) but these low computed barriers only reflect the gas phase and it is known that the nature of the metal and that of the solvent strongly influence the rate of the oxy-Cope reaction.[10] Metalation is not a guaranty of success, the proper conditions still remain to be found. Since benzene was used as solvent, the dissociation of the OLi bond must be difficult. We computed the oxy-ene reaction with the corresponding lithium alkoxyde and found indeed that the barrier was actually 29.5 kcal/mol ($\mathbf{TS_{K'L'}}$). It is likely that the use of

THF or DMSO,[11] more commonly used in oxy-Cope rearrangements, could facilitate this reaction. In each series, the NICS(0) value is lower for the anionic or metallated transition states than for the neutral ones (Table S1), which means that their ionic character is increased.

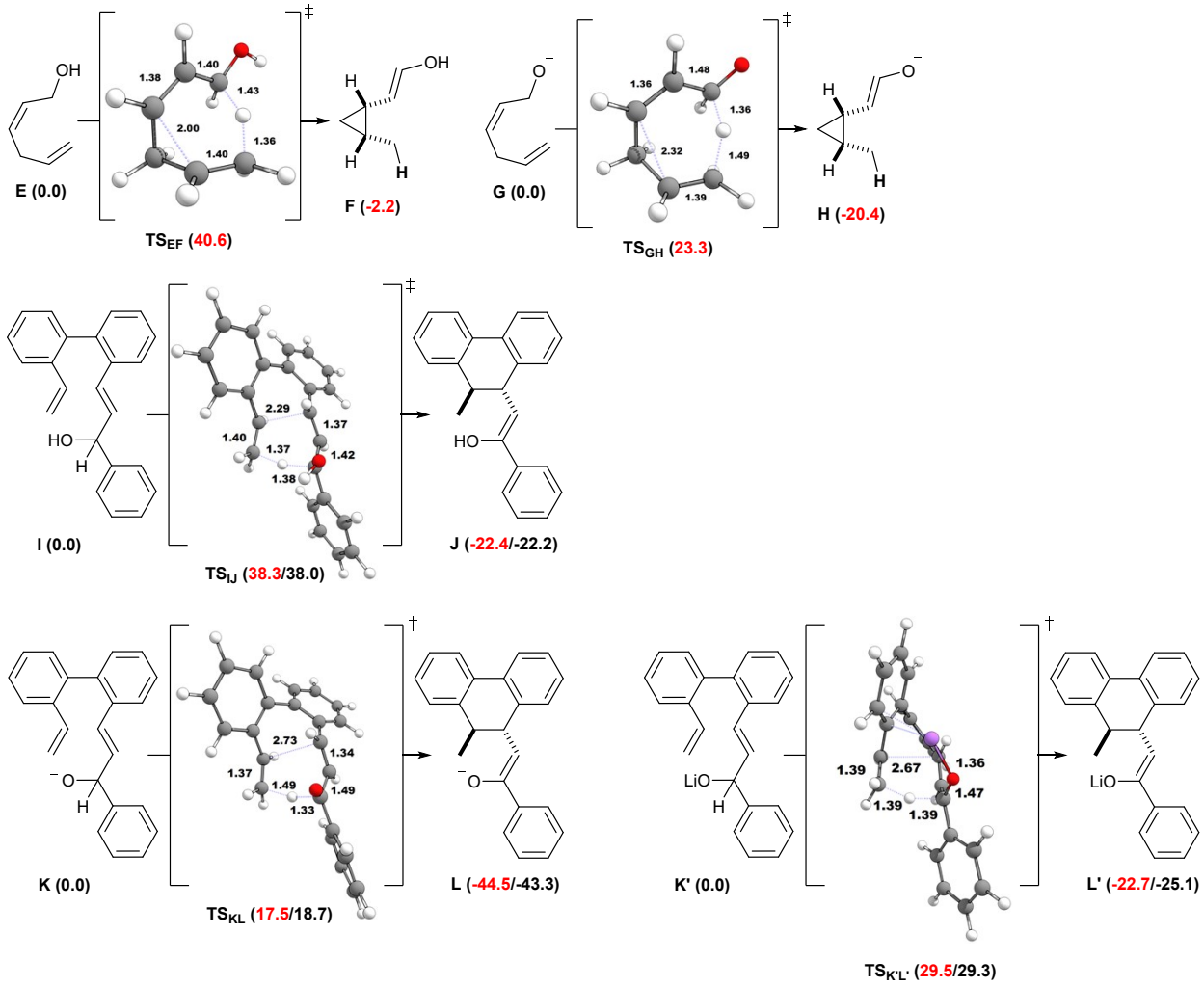

Figure S1. Free energies at 536.45 K (**E** to **H**) and 483.15 K (**I** to **L'**) (Δ*G* kcal/mol) and transition states geometries (selected distances in Å) of the neutral and anionic oxy-ene reactions corresponding to Scheme 3 computed at the ωB97XD/def2-QZVPP//ωB97XD/6-311+G(d,p) level. Values in red are in the gas phase, values in black include solvation correction from PCM calculations (benzene).

Table S1. NICS(0) values of the transition states (ppm)

TS	NICS(0)

TS_{EF}	-22.6
TS_{IJ}	-17.8
TS_{KL}	-8.5
$TS_{K'L'}$	-12.6

Energies and Cartesian coordinates for all the intermediates and transition states

ethene

Zero-point correction= 0.051185 (Hartree/Particle)

Thermal correction to Energy= 0.057211

Thermal correction to Enthalpy= 0.058741

Thermal correction to Gibbs Free Energy= 0.011914

Sum of electronic and zero-point Energies= -78.529499

Sum of electronic and thermal Energies= -78.523473

Sum of electronic and thermal Enthalpies= -78.521943

Sum of electronic and thermal Free Energies= -78.568770

E(RwB97XD) = -78.5955614070

C 0.662828000000 0.000028000000 -0.000072000000

H 1.232089000000 0.923818000000 0.000252000000

H 1.231827000000 -0.923918000000 0.000316000000

C -0.662831000000 0.000029000000 -0.000170000000

H -1.231727000000 -0.923943000000 0.000410000000

H -1.232172000000 0.923703000000 0.000475000000

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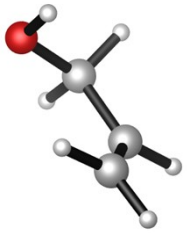
allyl alcohol *s-cis*



Zero-point correction= 0.085802 (Hartree/Particle)

Thermal correction to Energy= 0.096630

Thermal correction to Enthalpy= 0.098160

Thermal correction to Gibbs Free Energy= 0.037031

Sum of electronic and zero-point Energies= -193.026369

Sum of electronic and thermal Energies= -193.015540

Sum of electronic and thermal Enthalpies= -193.014010

Sum of electronic and thermal Free Energies= -193.075139

E(RwB97XD) = -193.147447326

H -1.110861000000 1.240324000000 0.800848000000

C -0.732462000000 0.628851000000 -0.031803000000

C 0.767928000000 0.585322000000 0.039296000000

O -1.358082000000 -0.633376000000 -0.057837000000

C 1.506658000000 -0.514573000000 -0.032754000000

H 1.055907000000 -1.491214000000 -0.176136000000

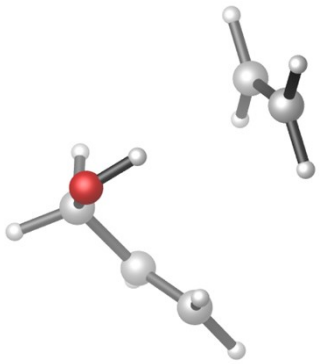
H 1.248507000000 1.554268000000 0.161851000000

H -1.131806000000 -1.099044000000 0.749293000000

H 2.587549000000 -0.470358000000 0.031018000000

H -1.037388000000 1.135434000000 -0.952611000000

A



Zero-point correction= 0.138503 (Hartree/Particle)

Thermal correction to Energy= 0.158493

Thermal correction to Enthalpy= 0.160023

Thermal correction to Gibbs Free Energy= 0.072463

Sum of electronic and zero-point Energies= -271.561296

Sum of electronic and thermal Energies= -271.541305

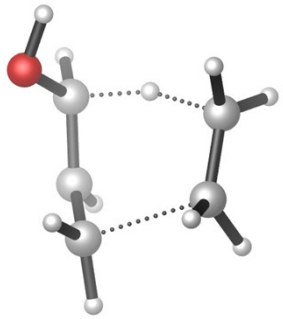
Sum of electronic and thermal Enthalpies= -271.539775

Sum of electronic and thermal Free Energies= -271.627335

E(RwB97XD) = -271.749478503

C	2.385481000000	0.391073000000	-0.421287000000
H	-0.743393000000	-1.302505000000	1.229372000000
H	1.847074000000	1.236530000000	-0.837989000000
C	-1.280862000000	-0.919837000000	0.347725000000
C	-1.514257000000	0.555149000000	0.526169000000
O	-0.618442000000	-1.272045000000	-0.841050000000
H	3.169515000000	-0.044776000000	-1.031994000000
C	-1.216032000000	1.489475000000	-0.367380000000
C	2.099612000000	-0.077516000000	0.787316000000
H	2.636976000000	-0.917772000000	1.214944000000
H	-0.784536000000	1.226812000000	-1.327615000000
H	-1.967868000000	0.836468000000	1.475416000000
H	0.289932000000	-0.961967000000	-0.775102000000
H	-1.414123000000	2.537483000000	-0.174477000000
H	1.316800000000	0.371347000000	1.391063000000
H	-2.246494000000	-1.435325000000	0.329526000000

TS_{AB}



Frequency 122.3394

Zero-point correction= 0.136621 (Hartree/Particle)

Thermal correction to Energy= 0.153366

Thermal correction to Enthalpy= 0.154896

Thermal correction to Gibbs Free Energy= 0.080443

Sum of electronic and zero-point Energies= -271.505121

Sum of electronic and thermal Energies= -271.488376

Sum of electronic and thermal Enthalpies= -271.486846

Sum of electronic and thermal Free Energies= -271.561299

E(RwB97XD) = -271.690374961

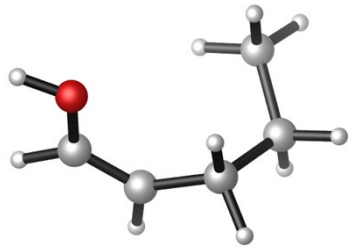
C	1.294394000000	-1.234527000000	0.270166000000
H	-0.059761000000	-0.883061000000	0.664825000000
H	1.095810000000	-2.043768000000	-0.427576000000
C	-1.195554000000	-0.224630000000	0.544740000000
C	-0.591381000000	1.046536000000	0.602207000000
O	-1.647241000000	-0.628074000000	-0.716942000000
H	1.585363000000	-1.551188000000	1.268836000000
C	0.241816000000	1.445646000000	-0.416855000000
C	1.808151000000	-0.036279000000	-0.228219000000
H	2.430351000000	0.578014000000	0.411574000000
H	0.007711000000	1.137058000000	-1.428003000000
H	-0.488325000000	1.488255000000	1.589357000000
H	-1.707592000000	-1.583802000000	-0.732417000000

H 0.803306000000 2.368928000000 -0.323831000000

H 2.017716000000 0.051110000000 -1.286858000000

H -1.851208000000 -0.517433000000 1.367396000000

B



Zero-point correction= 0.142926 (Hartree/Particle)

Thermal correction to Energy= 0.160360

Thermal correction to Enthalpy= 0.161890

Thermal correction to Gibbs Free Energy= 0.083083

Sum of electronic and zero-point Energies= -271.603604

Sum of electronic and thermal Energies= -271.586170

Sum of electronic and thermal Enthalpies= -271.584640

Sum of electronic and thermal Free Energies= -271.663447

E(RwB97XD) = -271.795656981

C 1.738519000000 -1.150734000000 0.294413000000

H 0.999359000000 -1.312427000000 1.083820000000

H 1.441282000000 -1.760255000000 -0.564282000000

C -1.675665000000 0.137969000000 0.471955000000

C -0.588580000000 0.900876000000 0.458746000000

O -1.947273000000 -0.766667000000 -0.515863000000

H 2.703825000000 -1.517954000000 0.652824000000

C 0.476633000000 0.882933000000 -0.597895000000

C 1.814510000000 0.324259000000 -0.089002000000

H 2.147656000000 0.913807000000 0.773601000000

H 0.137402000000 0.290747000000 -1.452647000000

H -0.460451000000 1.576860000000 1.298922000000

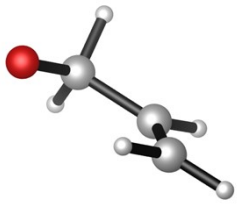
H -2.783615000000 -1.194840000000 -0.340376000000

H 0.634332000000 1.905054000000 -0.960564000000

H 2.571246000000 0.463037000000 -0.868648000000

H -2.405352000000 0.197491000000 1.274951000000

Alkoxide *s-cis*



Zero-point correction= 0.069544 (Hartree/Particle)

Thermal correction to Energy= 0.079484

Thermal correction to Enthalpy= 0.081014

Thermal correction to Gibbs Free Energy= 0.021772

Sum of electronic and zero-point Energies= -192.431411

Sum of electronic and thermal Energies= -192.421471

Sum of electronic and thermal Enthalpies= -192.419941

Sum of electronic and thermal Free Energies= -192.479183

E(RwB97XD) = -192.532638734

H -1.101591000000 1.163576000000 0.881708000000

C -0.819521000000 0.499232000000 -0.000238000000

C 0.706154000000 0.582564000000 0.000157000000

O -1.363734000000 -0.704493000000 0.000160000000

C 1.504868000000 -0.483845000000 -0.000022000000

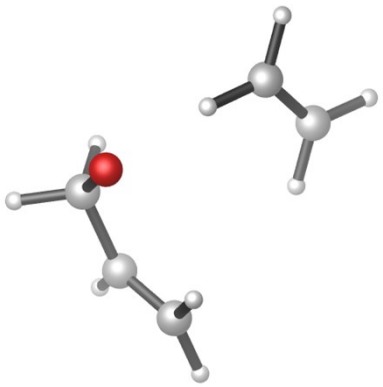
H 1.040458000000 -1.467030000000 -0.000504000000

H 1.133813000000 1.592413000000 0.000210000000

H 2.589978000000 -0.403991000000 -0.000051000000

H -1.101792000000 1.163272000000 -0.882021000000

C



Zero-point correction= 0.122251 (Hartree/Particle)

Thermal correction to Energy= 0.141167

Thermal correction to Enthalpy= 0.142697

Thermal correction to Gibbs Free Energy= 0.057317

Sum of electronic and zero-point Energies= -270.973781

Sum of electronic and thermal Energies= -270.954865

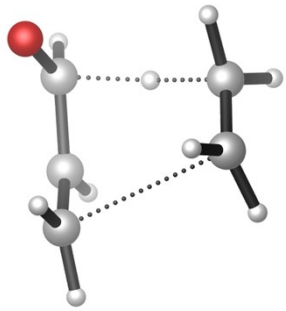
Sum of electronic and thermal Enthalpies= -270.953335

Sum of electronic and thermal Free Energies= -271.038716

E(RwB97XD) = -271.142310491

C	2.260621000000	-0.452292000000	-0.110267000000
H	-0.510506000000	-0.962011000000	1.417023000000
H	1.286273000000	-0.896113000000	-0.387030000000
C	-1.160436000000	-0.904970000000	0.488006000000
C	-1.590488000000	0.558188000000	0.467840000000
O	-0.590990000000	-1.379122000000	-0.616484000000
H	3.149274000000	-1.084650000000	-0.118562000000
C	-1.402638000000	1.368166000000	-0.572334000000
C	2.361216000000	0.827141000000	0.238367000000
H	3.307888000000	1.286586000000	0.520933000000
H	-0.925123000000	0.959630000000	-1.459516000000
H	-2.064696000000	0.935557000000	1.380682000000
H	-1.706700000000	2.412402000000	-0.562432000000
H	1.475574000000	1.457714000000	0.253324000000
H	-2.093710000000	-1.453535000000	0.817779000000

TS_{CD}



Frequency -967.7102

Zero-point correction= 0.119248 (Hartree/Particle)

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Thermal correction to Enthalpy= 0.138022

Thermal correction to Gibbs Free Energy= 0.061097

Sum of electronic and zero-point Energies= -270.940230

Sum of electronic and thermal Energies= -270.922986

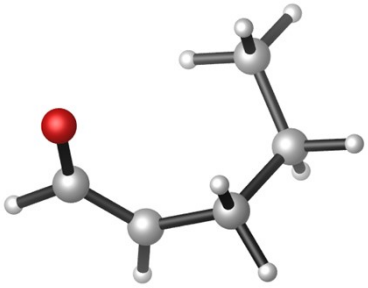
Sum of electronic and thermal Enthalpies= -270.921456

Sum of electronic and thermal Free Energies= -270.998380

E(RwB97XD) = -271.105389419

C	1.628014000000	-0.778795000000	0.377562000000
H	0.269069000000	-0.728801000000	0.727364000000
H	1.481892000000	-1.717512000000	-0.159689000000
C	-1.097808000000	-0.698835000000	0.356815000000
C	-1.003950000000	0.740009000000	0.636260000000
O	-1.228341000000	-1.184414000000	-0.811222000000
H	2.036782000000	-0.887693000000	1.384600000000
C	-0.630239000000	1.640760000000	-0.293501000000
C	1.998913000000	0.335461000000	-0.359841000000
H	2.385031000000	1.230388000000	0.116638000000
H	-0.617314000000	1.355692000000	-1.339046000000
H	-1.013555000000	1.017137000000	1.692533000000
H	-0.415967000000	2.674267000000	-0.036469000000
H	1.829335000000	0.375970000000	-1.428751000000
H	-1.498124000000	-1.275732000000	1.228824000000

D



Zero-point correction= 0.128057 (Hartree/Particle)

Thermal correction to Energy= 0.144374

Thermal correction to Enthalpy= 0.145904

Thermal correction to Gibbs Free Energy= 0.070285

Sum of electronic and zero-point Energies= -271.040919

Sum of electronic and thermal Energies= -271.024603

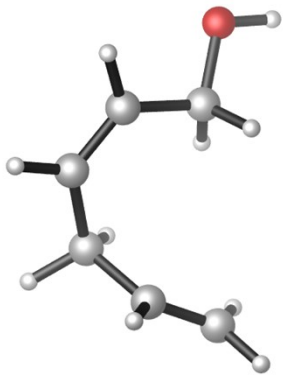
Sum of electronic and thermal Enthalpies= -271.023072

Sum of electronic and thermal Free Energies= -271.098691

E(RwB97XD) = -271.214120556

C	1.548730000000	-1.182638000000	0.259131000000
H	0.697440000000	-1.335671000000	0.927118000000
H	1.312979000000	-1.705397000000	-0.672898000000
C	-1.712751000000	0.024022000000	0.320498000000
C	-0.711177000000	0.971239000000	0.393994000000
O	-1.831692000000	-0.954270000000	-0.473911000000
H	2.442573000000	-1.639660000000	0.702331000000
C	0.466329000000	0.985847000000	-0.538878000000
C	1.741672000000	0.309948000000	0.004549000000
H	2.031151000000	0.804998000000	0.942063000000
H	0.178927000000	0.467853000000	-1.464299000000
H	-0.785301000000	1.741523000000	1.160397000000
H	0.727618000000	2.018510000000	-0.819982000000
H	2.573458000000	0.460885000000	-0.702408000000
H	-2.522121000000	0.170610000000	1.083199000000

E



Zero-point correction= 0.147638 (Hartree/Particle)

Thermal correction to Energy= 0.170903

Thermal correction to Enthalpy= 0.172602

Thermal correction to Gibbs Free Energy= 0.074386

Sum of electronic and zero-point Energies= -309.661532

Sum of electronic and thermal Energies= -309.638266

Sum of electronic and thermal Enthalpies= -309.636567

Sum of electronic and thermal Free Energies= -309.734783

E(RwB97XD) = -309.864309802

C	-2.179299000000	1.426225000000	-0.077307000000
H	1.071513000000	1.182448000000	-0.880361000000
H	-2.714801000000	2.059885000000	-0.775415000000
C	1.387195000000	0.543479000000	-0.042278000000
C	1.042803000000	-0.878554000000	-0.355333000000
O	2.790925000000	0.624449000000	0.151119000000
H	-1.779618000000	1.901455000000	0.814634000000
C	-0.113009000000	-1.476923000000	-0.079683000000
C	-2.022929000000	0.126494000000	-0.297947000000
H	-0.244843000000	-2.507587000000	-0.396877000000
H	3.037861000000	1.545606000000	0.231210000000
H	0.847218000000	0.889494000000	0.848963000000
C	-1.284201000000	-0.817942000000	0.613313000000

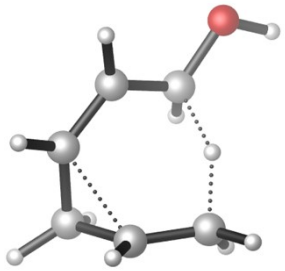
H -0.946176000000 -0.272155000000 1.501202000000

H -1.974963000000 -1.591449000000 0.963579000000

H -2.431149000000 -0.312851000000 -1.206317000000

H 1.824198000000 -1.427118000000 -0.874167000000

TS_{EF}



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Zero-point correction= 0.143743 (Hartree/Particle)

Thermal correction to Energy= 0.164910

Thermal correction to Enthalpy= 0.166609

Thermal correction to Gibbs Free Energy= 0.078576

Sum of electronic and zero-point Energies= -309.604954

Sum of electronic and thermal Energies= -309.583787

Sum of electronic and thermal Enthalpies= -309.582088

Sum of electronic and thermal Free Energies= -309.670121

E(RwB97XD) = -309.803809588

C -0.788326000000 1.639530000000 -0.195867000000

H 0.441228000000 1.056190000000 -0.180037000000

H -0.789018000000 2.376122000000 -0.995577000000

C 1.294775000000 0.016164000000 0.309358000000

C 0.611280000000 -1.024372000000 -0.331802000000

O 2.643406000000 0.137474000000 -0.006120000000

H -0.696871000000 2.074201000000 0.800922000000

C -0.747863000000 -1.233730000000 -0.222822000000

C -1.660187000000 0.548908000000 -0.329308000000

H -1.200290000000 -1.936928000000 -0.913733000000

H 2.965859000000 0.974908000000 0.325290000000

H 1.059740000000 0.237954000000 1.353725000000

C -1.693108000000 -0.529697000000 0.695233000000

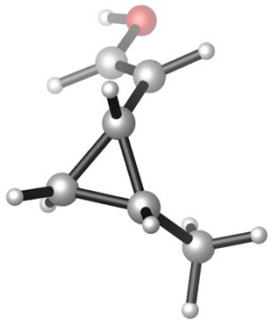
H -1.277384000000 -0.229724000000 1.659102000000

H -2.643476000000 -1.043030000000 0.826045000000

H -2.243631000000 0.405923000000 -1.230305000000

H 1.137167000000 -1.516226000000 -1.145234000000

F



Zero-point correction= 0.148170 (Hartree/Particle)

Thermal correction to Energy= 0.170980

Thermal correction to Enthalpy= 0.172678

Thermal correction to Gibbs Free Energy= 0.078398

Sum of electronic and zero-point Energies= -309.665430

Sum of electronic and thermal Energies= -309.642621

Sum of electronic and thermal Enthalpies= -309.640922

Sum of electronic and thermal Free Energies= -309.735202

E(RwB97XD) = -309.869812390

C -1.777515000000 1.427689000000 0.219374000000

H -0.837787000000 1.658846000000 0.727052000000

H -1.857334000000 2.089526000000 -0.648149000000

C 1.696748000000 -0.198599000000 0.214642000000

C 0.743550000000 -0.080090000000 -0.700896000000

O 2.897531000000 0.439534000000 0.096741000000

H -2.599068000000 1.663972000000 0.901807000000

C -0.574244000000 -0.759931000000 -0.623116000000

C -1.827134000000 -0.021288000000 -0.197121000000

H -0.737846000000 -1.489865000000 -1.412075000000

H 3.450430000000 0.228665000000 0.847549000000

H 1.565515000000 -0.811395000000 1.103419000000

C -1.239611000000 -1.085600000000 0.691821000000

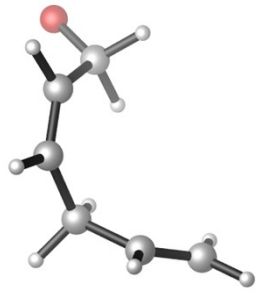
H -0.757777000000 -0.745892000000 1.602575000000

H -1.752767000000 -2.035165000000 0.785814000000

H -2.726324000000 -0.304670000000 -0.735965000000

H 0.941952000000 0.536616000000 -1.574171000000

G



Zero-point correction= 0.132024 (Hartree/Particle)

Thermal correction to Energy= 0.154151

Thermal correction to Enthalpy= 0.155850

Thermal correction to Gibbs Free Energy= 0.058915

Sum of electronic and zero-point Energies= -309.065982

Sum of electronic and thermal Energies= -309.043855

Sum of electronic and thermal Enthalpies= -309.042156

Sum of electronic and thermal Free Energies= -309.139091

E(RwB97XD) = -309.249641153

C -2.642620000000 1.134265000000 -0.183379000000

H 1.711394000000 1.219797000000 -1.195970000000

H -3.478728000000 1.410051000000 -0.818913000000

C 1.749713000000 0.681825000000 -0.196587000000

C 1.171766000000 -0.695573000000 -0.502081000000

O 2.965471000000 0.601881000000 0.354910000000

H -2.146576000000 1.932572000000 0.361769000000

C 0.024226000000 -1.258833000000 -0.108081000000

C -2.212662000000 -0.120880000000 -0.099545000000

H -0.184484000000 -2.293764000000 -0.387163000000

H 0.986218000000 1.245105000000 0.412033000000

C -1.045127000000 -0.587908000000 0.724163000000

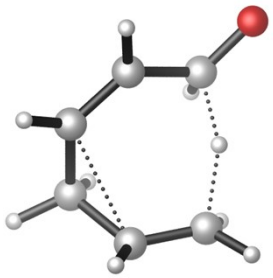
H -0.619931000000 0.260140000000 1.266532000000

H -1.417566000000 -1.303049000000 1.472193000000

H -2.715857000000 -0.889417000000 -0.688084000000

H 1.869990000000 -1.313866000000 -1.068617000000

TS_{GH}



Frequency -1139.9197

Zero-point correction= 0.128638 (Hartree/Particle)

Thermal correction to Energy= 0.148771

Thermal correction to Enthalpy= 0.150470

Thermal correction to Gibbs Free Energy= 0.064201

Sum of electronic and zero-point Energies= -309.037948

Sum of electronic and thermal Energies= -309.017815

Sum of electronic and thermal Enthalpies= -309.016116

Sum of electronic and thermal Free Energies= -309.102385

E(RwB97XD) = -309.217718841

C -0.812158000000 1.637076000000 -0.151921000000

H 0.528334000000 1.003885000000 -0.244460000000

H -0.762803000000 2.429029000000 -0.898215000000

C 1.419659000000 0.115066000000 0.279905000000

C 0.721678000000 -1.051440000000 -0.297603000000

O 2.653128000000 0.351235000000 0.008879000000

H -0.568506000000 1.964480000000 0.862014000000

C -0.589583000000 -1.379191000000 -0.164119000000

C -1.755454000000 0.632758000000 -0.302234000000

H -0.972967000000 -2.187828000000 -0.788643000000

H 1.060124000000 0.337982000000 1.319116000000

C -1.618759000000 -0.583597000000 0.585958000000

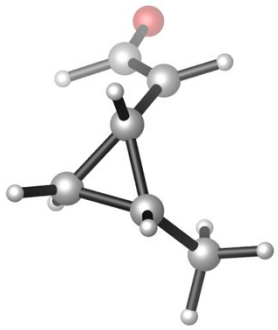
H -1.268901000000 -0.288207000000 1.584799000000

H -2.552885000000 -1.144850000000 0.699220000000

H -2.198668000000 0.457330000000 -1.281283000000

H 1.318953000000 -1.605725000000 -1.023492000000

H



Zero-point correction= 0.133327 (Hartree/Particle)

Thermal correction to Energy= 0.154849

Thermal correction to Enthalpy= 0.156548

Thermal correction to Gibbs Free Energy= 0.065032

Sum of electronic and zero-point Energies= -309.102934

Sum of electronic and thermal Energies= -309.081411

Sum of electronic and thermal Enthalpies= -309.079713

Sum of electronic and thermal Free Energies= -309.171229

E(RwB97XD) = -309.288332385

C -1.858751000000 1.345815000000 0.263415000000

H -0.883930000000 1.646732000000 0.656769000000

H -2.097688000000 2.018915000000 -0.568752000000

C 1.856785000000 -0.130939000000 0.187722000000

C 0.802143000000 0.073690000000 -0.680373000000

O 2.986491000000 0.431245000000 0.234343000000

H -2.617040000000 1.486723000000 1.043905000000

C -0.465818000000 -0.699218000000 -0.651613000000

C -1.793042000000 -0.087115000000 -0.200946000000

H -0.621475000000 -1.433433000000 -1.449247000000

H 1.648704000000 -0.919206000000 0.959772000000

C -1.107053000000 -1.124042000000 0.651575000000

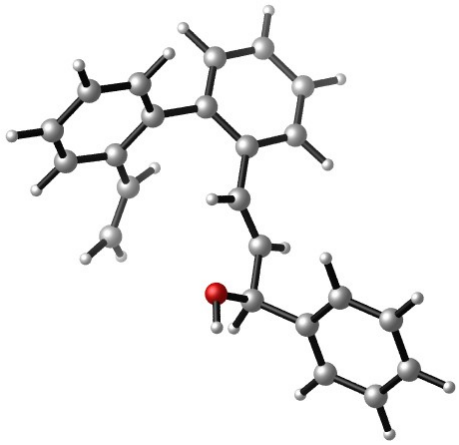
H -0.631254000000 -0.774781000000 1.561608000000

H -1.546657000000 -2.114657000000 0.724891000000

H -2.673243000000 -0.432394000000 -0.740933000000

H 0.925074000000 0.802995000000 -1.481439000000

I



Zero-point correction= 0.363688 (Hartree/Particle)

Thermal correction to Energy= 0.415306

Thermal correction to Enthalpy= 0.416837

Thermal correction to Gibbs Free Energy= 0.257340

Sum of electronic and zero-point Energies= -963.227580

Sum of electronic and thermal Energies= -963.175961

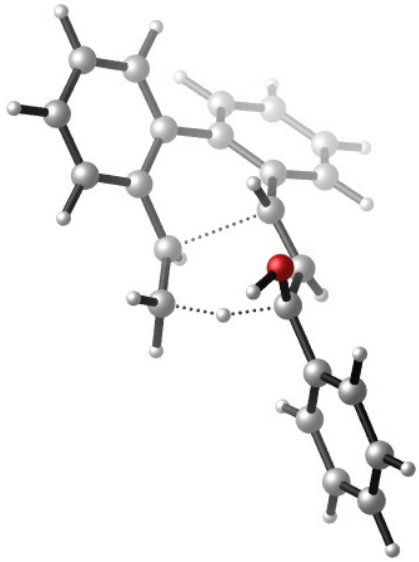
Sum of electronic and thermal Enthalpies= -963.174431

Sum of electronic and thermal Free Energies= -963.333928

E(RwB97XD) = -963.756278032

C	1.695360000000	-1.884590000000	2.618186000000
H	-2.225181000000	-1.488571000000	1.506614000000
H	1.575229000000	-2.903866000000	2.265002000000
C	-2.126720000000	-1.023882000000	0.513189000000
C	-3.506317000000	-0.552467000000	0.080655000000
C	-1.183348000000	0.136500000000	0.643003000000
O	-1.586284000000	-1.963106000000	-0.399760000000
C	-3.672317000000	0.062371000000	-1.161380000000
C	-4.927646000000	0.485933000000	-1.571883000000
H	-2.806350000000	0.205766000000	-1.799179000000
C	-6.031991000000	0.308354000000	-0.741513000000
H	-5.047672000000	0.961562000000	-2.538952000000
H	1.313180000000	-1.657904000000	3.606736000000
C	-4.613656000000	-0.729925000000	0.903487000000
C	-0.055886000000	0.271504000000	-0.048527000000
C	0.863978000000	1.417406000000	0.071401000000
C	2.247320000000	1.240909000000	-0.111064000000
C	2.828587000000	-0.097528000000	-0.419079000000
C	3.100084000000	2.340705000000	-0.012819000000
H	4.165671000000	2.189657000000	-0.150096000000
C	3.391322000000	-0.308941000000	-1.678135000000
H	3.383964000000	0.503870000000	-2.396683000000
C	3.935725000000	-1.537742000000	-2.023590000000
H	4.364266000000	-1.684086000000	-3.008629000000
C	0.382958000000	2.702439000000	0.341999000000
C	1.241276000000	3.786230000000	0.450514000000
H	0.842082000000	4.772704000000	0.658465000000
H	-0.686565000000	2.854064000000	0.439868000000
C	2.821046000000	-1.143578000000	0.520732000000
C	3.385865000000	-2.371027000000	0.161057000000
H	3.420150000000	-3.169440000000	0.893967000000
C	2.258624000000	-0.939323000000	1.870203000000
H	2.300552000000	0.077131000000	2.252622000000
C	3.930504000000	-2.573929000000	-1.097483000000
H	4.363612000000	-3.535253000000	-1.350210000000
C	2.607900000000	3.606963000000	0.271984000000
H	3.286641000000	4.448869000000	0.348536000000
H	0.233399000000	-0.528382000000	-0.722630000000
H	-1.486741000000	0.883655000000	1.372563000000
C	-5.873593000000	-0.298359000000	0.496916000000
H	-7.012192000000	0.643355000000	-1.061772000000
H	-6.729484000000	-0.440523000000	1.147253000000
H	-4.492471000000	-1.209155000000	1.870503000000
H	-2.266258000000	-2.606728000000	-0.603012000000

TS_{IJ}



Frequency -1222.2228

Zero-point correction= 0.360604 (Hartree/Particle)

Thermal correction to Energy= 0.409693

Thermal correction to Enthalpy= 0.411223

Thermal correction to Gibbs Free Energy= 0.264987

Sum of electronic and zero-point Energies= -963.177754

Sum of electronic and thermal Energies= -963.128665

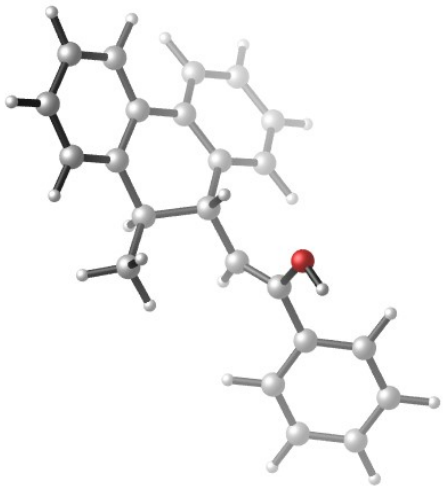
Sum of electronic and thermal Enthalpies= -963.127135

Sum of electronic and thermal Free Energies= -963.273371

E(RwB97XD) = -963.702873943

C	-0.462241000000	-1.580541000000	1.363314000000
H	-1.373440000000	-1.003217000000	0.524814000000
H	-0.482703000000	-2.620256000000	1.043518000000
C	-1.927506000000	-0.333473000000	-0.548243000000
C	-3.369015000000	-0.123909000000	-0.218908000000
C	-1.007793000000	0.735975000000	-0.433437000000
O	-1.661207000000	-1.223012000000	-1.590063000000
C	-4.377016000000	-0.488242000000	-1.111293000000
C	-5.713588000000	-0.291653000000	-0.782585000000
H	-4.109313000000	-0.904216000000	-2.075853000000
C	-6.060851000000	0.268195000000	0.440527000000
H	-6.486394000000	-0.571426000000	-1.490028000000
H	-1.037178000000	-1.383955000000	2.266415000000
C	-3.727260000000	0.427867000000	1.013950000000
C	0.325563000000	0.506691000000	-0.645408000000
C	1.401216000000	1.478849000000	-0.368947000000
C	2.668301000000	0.989873000000	0.005215000000
C	2.920178000000	-0.475135000000	0.044362000000
C	3.676599000000	1.894354000000	0.329445000000
H	4.641901000000	1.518147000000	0.651171000000
C	4.100644000000	-0.986080000000	-0.489618000000
H	4.817998000000	-0.302207000000	-0.930450000000
C	4.359708000000	-2.351743000000	-0.494607000000
H	5.284425000000	-2.726926000000	-0.917885000000
C	1.196677000000	2.854656000000	-0.440484000000
C	2.215566000000	3.746594000000	-0.124300000000
H	2.037215000000	4.814246000000	-0.186717000000
H	0.232315000000	3.229487000000	-0.765872000000
C	1.961374000000	-1.363140000000	0.579972000000
C	2.241147000000	-2.729729000000	0.574047000000
H	1.532412000000	-3.418746000000	1.018445000000
C	0.706967000000	-0.837024000000	1.166600000000
H	0.833396000000	0.054881000000	1.772626000000
C	3.424537000000	-3.225198000000	0.039610000000
H	3.614592000000	-4.292636000000	0.049242000000
C	3.457071000000	3.266084000000	0.266719000000
H	4.254839000000	3.953788000000	0.523388000000
H	0.588013000000	-0.332579000000	-1.279912000000
H	-1.327197000000	1.599726000000	0.142879000000
C	-5.061126000000	0.629012000000	1.338546000000
H	-7.103494000000	0.420104000000	0.695335000000
H	-5.322702000000	1.058929000000	2.299038000000
H	-2.952624000000	0.691635000000	1.727430000000
H	-2.047310000000	-2.074379000000	-1.373942000000

J



Zero-point correction= 0.367170 (Hartree/Particle)

Thermal correction to Energy= 0.416667

Thermal correction to Enthalpy= 0.418197

Thermal correction to Gibbs Free Energy= 0.267912

Sum of electronic and zero-point Energies= -963.270332

Sum of electronic and thermal Energies= -963.220834

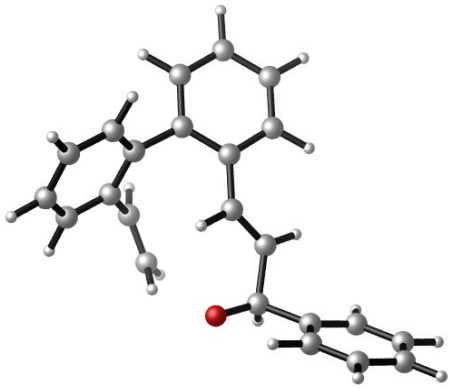
Sum of electronic and thermal Enthalpies= -963.219304

Sum of electronic and thermal Free Energies= -963.369589

E(RwB97XD) = -963.802566326

C	0.435100000000	-2.595778000000	0.632672000000
H	-0.612185000000	-2.516118000000	0.928455000000
H	0.464921000000	-2.996327000000	-0.385534000000
C	-2.105507000000	-0.277009000000	-0.637288000000
C	-3.534510000000	-0.259308000000	-0.243625000000
C	-1.097939000000	-0.128023000000	0.223218000000
O	-1.847742000000	-0.399172000000	-1.977264000000
C	-4.479890000000	0.384242000000	-1.047847000000
C	-5.819147000000	0.411539000000	-0.679901000000
H	-4.160869000000	0.894243000000	-1.951064000000
C	-6.233712000000	-0.205610000000	0.494182000000
H	-6.538790000000	0.924336000000	-1.308054000000
H	0.912531000000	-3.316155000000	1.300640000000
C	-3.963383000000	-0.885246000000	0.929105000000
C	0.357288000000	-0.166628000000	-0.133174000000
C	1.029875000000	1.185227000000	0.055812000000
C	2.429050000000	1.234473000000	0.155234000000
C	3.200977000000	-0.019281000000	0.006799000000
C	3.053073000000	2.463675000000	0.378084000000
H	4.128970000000	2.505442000000	0.504434000000
C	4.530839000000	-0.011610000000	-0.417255000000
H	5.008350000000	0.928204000000	-0.669674000000
C	5.247489000000	-1.191999000000	-0.549688000000
H	6.278708000000	-1.165471000000	-0.883317000000
C	0.300958000000	2.368602000000	0.127807000000
C	0.934183000000	3.589550000000	0.324134000000
H	0.347699000000	4.499781000000	0.381527000000
H	-0.778267000000	2.330207000000	0.030946000000
C	2.568803000000	-1.245957000000	0.273624000000
C	3.300129000000	-2.422902000000	0.134014000000
H	2.831692000000	-3.378600000000	0.333287000000
C	1.112138000000	-1.229709000000	0.703275000000
H	1.082515000000	-0.887618000000	1.749339000000
C	4.630525000000	-2.402485000000	-0.268250000000
H	5.176702000000	-3.333314000000	-0.372978000000
C	2.315190000000	3.635459000000	0.461725000000
H	2.817715000000	4.579789000000	0.638578000000
H	0.449846000000	-0.449864000000	-1.189334000000
H	-1.350170000000	0.061224000000	1.262294000000
C	-5.301176000000	-0.852897000000	1.297650000000
H	-7.278987000000	-0.185424000000	0.780603000000
H	-5.619333000000	-1.346097000000	2.209222000000
H	-3.242480000000	-1.412180000000	1.543992000000
H	-2.598755000000	-0.812628000000	-2.407093000000

K



Zero-point correction= 0.348262 (Hartree/Particle)

Thermal correction to Energy= 0.398669

Thermal correction to Enthalpy= 0.400199

Thermal correction to Gibbs Free Energy= 0.246363

Sum of electronic and zero-point Energies= -962.652951

Sum of electronic and thermal Energies= -962.602543

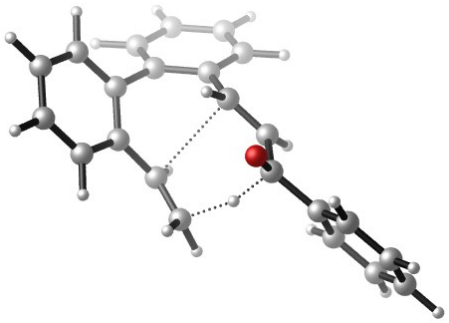
Sum of electronic and thermal Enthalpies= -962.601013

Sum of electronic and thermal Free Energies= -962.754850

E(RwB97XD) = -963.163298602

C	0.953736000000	-1.322267000000	2.489588000000
H	-2.269672000000	-0.646190000000	1.940481000000
H	0.285211000000	-1.961461000000	1.908595000000
C	-2.082030000000	-0.706852000000	0.824232000000
C	-3.471479000000	-0.386767000000	0.211139000000
C	-1.204432000000	0.537385000000	0.585925000000
O	-1.550517000000	-1.851990000000	0.425602000000
C	-3.914751000000	-1.158976000000	-0.858329000000
C	-5.147178000000	-0.909597000000	-1.453511000000
H	-3.251819000000	-1.957542000000	-1.178034000000
C	-5.964352000000	0.114028000000	-0.980505000000
H	-5.478618000000	-1.520709000000	-2.288899000000
H	0.605297000000	-0.986093000000	3.461849000000
C	-4.300643000000	0.630105000000	0.686126000000
C	-0.020609000000	0.425289000000	-0.013992000000
C	1.008477000000	1.466798000000	-0.108190000000
C	2.372185000000	1.121193000000	-0.236727000000
C	2.803631000000	-0.301439000000	-0.369074000000
C	3.342586000000	2.123470000000	-0.300256000000
H	4.384508000000	1.832707000000	-0.396220000000
C	3.361879000000	-0.717146000000	-1.578502000000
H	3.479261000000	0.011271000000	-2.374563000000
C	3.723839000000	-2.041502000000	-1.789542000000
H	4.143479000000	-2.344186000000	-2.743237000000
C	0.686741000000	2.831610000000	-0.062605000000
C	1.659114000000	3.817214000000	-0.115010000000
H	1.369315000000	4.862748000000	-0.076796000000
H	-0.358822000000	3.113780000000	-0.002090000000
C	2.625440000000	-1.239295000000	0.662180000000
C	2.975515000000	-2.570265000000	0.429820000000
H	2.815619000000	-3.290587000000	1.224442000000
C	2.087879000000	-0.844039000000	1.986909000000
H	2.657587000000	-0.090571000000	2.528837000000
C	3.517462000000	-2.975202000000	-0.782877000000
H	3.773483000000	-4.017680000000	-0.940366000000
C	3.001074000000	3.466941000000	-0.231637000000
H	3.770666000000	4.230479000000	-0.275799000000
H	0.222689000000	-0.580809000000	-0.347374000000
H	-1.539812000000	1.483537000000	1.015099000000
C	-5.535776000000	0.883517000000	0.098317000000
H	-6.928630000000	0.306344000000	-1.441556000000
H	-6.168425000000	1.678676000000	0.483414000000
H	-3.977028000000	1.226967000000	1.536529000000

TS_{KL}



Frequency -1058.5494

Zero-point correction= 0.344803 (Hartree/Particle)

Thermal correction to Energy= 0.393749

Thermal correction to Enthalpy= 0.395279

Thermal correction to Gibbs Free Energy= 0.248679

Sum of electronic and zero-point Energies= -962.631081

Sum of electronic and thermal Energies= -962.582135

Sum of electronic and thermal Enthalpies= -962.580605

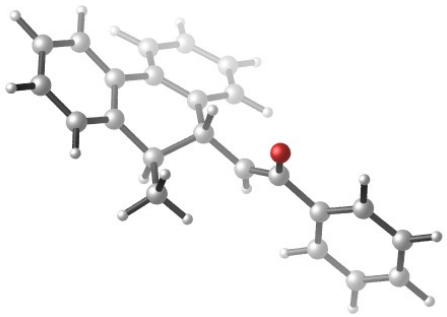
Sum of electronic and thermal Free Energies= -962.727204

E(RwB97XD) = -963.137747138

C	-0.495680000000	-1.344055000000	1.629115000000
H	-1.399990000000	-0.777059000000	0.582607000000
H	-0.691388000000	-2.369438000000	1.320367000000

C	-1.866915000000	-0.412319000000	-0.610709000000
C	-3.320745000000	-0.106820000000	-0.244863000000
C	-0.946333000000	0.760275000000	-0.544488000000
O	-1.658363000000	-1.355038000000	-1.454067000000
C	-4.327129000000	-0.733780000000	-0.978152000000
C	-5.668241000000	-0.514305000000	-0.684075000000
H	-4.008073000000	-1.396957000000	-1.775255000000
C	-6.030578000000	0.330590000000	0.360850000000
H	-6.437667000000	-1.007713000000	-1.271235000000
H	-1.120330000000	-0.979193000000	2.442170000000
C	-3.694632000000	0.728523000000	0.811497000000
C	0.344773000000	0.588064000000	-0.869214000000
C	1.448328000000	1.485409000000	-0.500752000000
C	2.652474000000	0.929600000000	-0.004769000000
C	2.828115000000	-0.549058000000	0.067706000000
C	3.677778000000	1.779124000000	0.402025000000
H	4.586336000000	1.343644000000	0.806851000000
C	3.921004000000	-1.126765000000	-0.573685000000
H	4.627905000000	-0.477652000000	-1.082238000000
C	4.097171000000	-2.505876000000	-0.614848000000
H	4.950458000000	-2.934509000000	-1.129512000000
C	1.339779000000	2.874385000000	-0.585051000000
C	2.374756000000	3.710333000000	-0.176686000000
H	2.261496000000	4.787293000000	-0.253216000000
H	0.427265000000	3.297224000000	-0.992535000000
C	1.871171000000	-1.372600000000	0.716481000000
C	2.064165000000	-2.761297000000	0.649889000000
H	1.347381000000	-3.407850000000	1.144411000000
C	0.754679000000	-0.789881000000	1.452326000000
H	0.930596000000	0.200834000000	1.859833000000
C	3.148841000000	-3.321254000000	-0.006705000000
H	3.258502000000	-4.401084000000	-0.036447000000
C	3.550002000000	3.163955000000	0.318832000000
H	4.362931000000	3.805639000000	0.642903000000
H	0.592582000000	-0.342506000000	-1.372567000000
H	-1.246873000000	1.630216000000	0.038065000000
C	-5.033908000000	0.949203000000	1.111288000000
H	-7.077140000000	0.500290000000	0.594301000000
H	-5.302216000000	1.600501000000	1.938046000000
H	-2.928129000000	1.199917000000	1.419919000000

L



Zero-point correction= 0.352373 (Hartree/Particle)

Thermal correction to Energy= 0.401135

Therma correctilon to Enthalpy= 0.402665

Therma correctilon to Gibbs Free Energy= 0.253482

Sum of electronic and zero-point Energies= -962.727234

Sum of electronic and thermal Energies= -962.678472

Sum of electronic and thermal Enthalpies= -962.676942

Sum of electronic and thermal Free Energies= -962.826124

E(RwB97XD) = -963.241339668

C	0.306438000000	-2.437118000000	0.851531000000
H	-0.735857000000	-2.250809000000	1.112259000000
H	0.311887000000	-2.920988000000	-0.129560000000
C	-2.107373000000	-0.507314000000	-0.575508000000
C	-3.566443000000	-0.292339000000	-0.189701000000
C	-1.140881000000	0.074239000000	0.219472000000
O	-1.902823000000	-1.192229000000	-1.622349000000
C	-4.534891000000	-0.500862000000	-1.174743000000

C -5.887069000000 -0.321301000000 -0.908797000000

H -4.179780000000 -0.818583000000 -2.149068000000

C -6.308804000000 0.055573000000 0.362951000000

H -6.618559000000 -0.482134000000 -1.695915000000

H 0.736870000000 -3.119723000000 1.591793000000

C -4.005639000000 0.072159000000 1.086880000000

C 0.313243000000 -0.078083000000 -0.104362000000

C 1.083645000000 1.233839000000 -0.072476000000

C 2.485918000000 1.229217000000 0.031622000000

C 3.196803000000 -0.068789000000 0.007491000000

C 3.177396000000 2.440729000000 0.124254000000

H 4.254342000000 2.436793000000 0.257017000000

C 4.524539000000 -0.167022000000 -0.414219000000

H 5.046647000000 0.722338000000 -0.750006000000

C 5.181996000000 -1.389348000000 -0.444344000000

H 6.212452000000 -1.443949000000 -0.780123000000

C 0.427773000000 2.462141000000 -0.150672000000

C 1.125116000000 3.661475000000 -0.089079000000

H 0.587150000000 4.602576000000 -0.147758000000

H -0.651245000000 2.449594000000 -0.257973000000

C 2.499980000000 -1.233059000000 0.379346000000

C 3.173139000000 -2.453191000000 0.335942000000

H 2.647830000000 -3.360057000000 0.609002000000

C 1.049266000000 -1.106206000000 0.804765000000

H 1.048298000000 -0.679088000000 1.820953000000

C 4.502207000000 -2.538204000000 -0.064165000000

H 4.997264000000 -3.503614000000 -0.093427000000

C 2.506857000000 3.653775000000 0.066079000000

H 3.059244000000 4.584780000000 0.144143000000

H 0.357973000000 -0.474749000000 -1.130977000000

H -1.406795000000 0.660164000000 1.093083000000

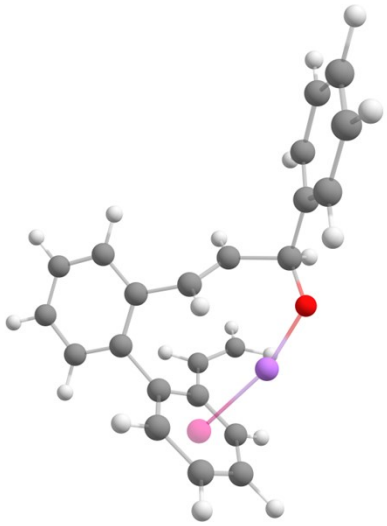
C -5.357820000000 0.245588000000 1.361518000000

H -7.364823000000 0.189986000000 0.576943000000

H -5.672076000000 0.523247000000 2.363711000000

H -3.280612000000 0.206639000000 1.881982000000

K’



Zero-point correction= 0.352903 (Hartree/Particle)

Thermal correction to Energy= 0.406040

Thermal correction to Enthalpy= 0.407570

Thermal correction to Gibbs Free Energy= 0.246663

Sum of electronic and zero-point Energies= -970.211559

Sum of electronic and thermal Energies= -970.158422

Sum of electronic and thermal Enthalpies= -970.156892

Sum of electronic and thermal Free Energies= -970.317800

E(RwB97XD) = -970.728510073

C 1.694872000 -0.921147000 3.007269000

H -1.997721000 -1.105170000 1.795156000

H 1.143281000 -1.854377000 2.942681000

C -1.889898000 -0.840997000 0.722097000

C -3.281818000 -0.382514000 0.267868000

C -0.965801000 0.386564000 0.708627000

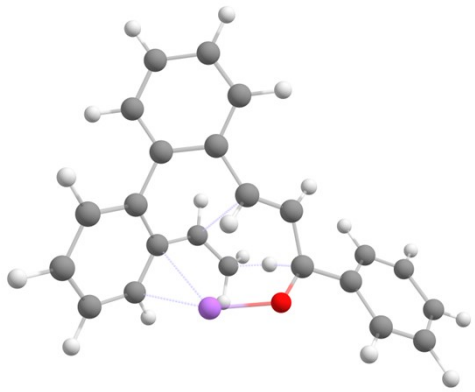
O -1.385052000 -1.874955000 -0.004379000

C -3.787572000 -0.817395000 -0.951483000

C -5.035154000 -0.387320000 -1.391854000

H	-3.185329000	-1.509488000	-1.528636000
C	-5.793397000	0.481211000	-0.614676000
H	-5.421295000	-0.737013000	-2.343967000
H	1.624426000	-0.373756000	3.939598000
C	-4.051176000	0.480091000	1.048266000
C	-0.097642000	0.591970000	-0.276184000
C	0.997199000	1.580022000	-0.309523000
C	2.307815000	1.098597000	-0.476376000
C	2.516411000	-0.380074000	-0.516918000
C	3.378298000	1.983984000	-0.542178000
H	4.385068000	1.598695000	-0.667352000
C	2.592917000	-1.049582000	-1.738766000
H	2.562675000	-0.469129000	-2.654277000
C	2.665930000	-2.438472000	-1.796130000
H	2.714644000	-2.940318000	-2.755380000
C	0.797149000	2.953350000	-0.186254000
C	1.871739000	3.833894000	-0.238119000
H	1.699117000	4.900180000	-0.143714000
H	-0.213980000	3.326545000	-0.066168000
C	2.525660000	-1.123504000	0.680631000
C	2.624606000	-2.519293000	0.610423000
H	2.664260000	-3.091041000	1.530646000
C	2.395370000	-0.442192000	1.983648000
H	2.873296000	0.529153000	2.067445000
C	2.681964000	-3.176485000	-0.615111000
H	2.753236000	-4.257570000	-0.646323000
C	3.161844000	3.352924000	-0.425113000
H	3.999234000	4.039386000	-0.475471000
H	-0.139630000	-0.092353000	-1.123515000
H	-0.986581000	1.059721000	1.564727000
C	-5.297605000	0.912346000	0.612126000
H	-6.767446000	0.813866000	-0.956775000
H	-5.886327000	1.581186000	1.231357000
H	-3.674749000	0.812043000	2.012740000
Li	0.287989000	-2.095599000	-0.353788000

$TS_{K'L'}$



Zero-point correction= 0.349859 (Hartree/Particle)

Thermal correction to Energy= 0.400839

Thermal correction to Enthalpy= 0.402369

Thermal correction to Gibbs Free Energy= 0.252223

Sum of electronic and zero-point Energies= -970.173396

Sum of electronic and thermal Energies= -970.122416

Sum of electronic and thermal Enthalpies= -970.120886

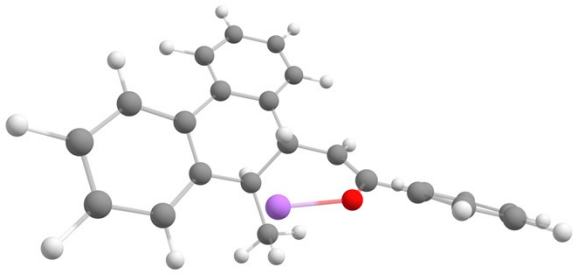
Sum of electronic and thermal Free Energies= -970.271032

E(RwB97XD) = -970.686951899

C	-0.554169000	-0.950040000	1.883456000
H	-1.382493000	-0.430893000	0.900558000
H	-0.853949000	-1.992597000	1.763264000
C	-1.807068000	-0.200713000	-0.404871000
C	-3.281061000	0.043030000	-0.216069000
C	-0.904556000	0.954960000	-0.436930000
O	-1.461107000	-1.289885000	-1.046653000
C	-4.190613000	-0.742493000	-0.920866000
C	-5.558808000	-0.551418000	-0.765687000
H	-3.800462000	-1.498532000	-1.591188000
C	-6.037153000	0.419993000	0.105338000

H	-6.254744000	-1.165271000	-1.327535000
H	-1.040475000	-0.455052000	2.721342000
C	-3.769697000	1.009997000	0.665961000
C	0.387430000	0.740623000	-0.747179000
C	1.581510000	1.545365000	-0.459045000
C	2.740641000	0.847600000	-0.045327000
C	2.723012000	-0.643235000	0.041666000
C	3.887795000	1.563761000	0.276439000
H	4.768623000	1.028554000	0.615810000
C	3.640047000	-1.384986000	-0.689919000
H	4.377324000	-0.855885000	-1.284990000
C	3.610392000	-2.780988000	-0.712795000
H	4.336289000	-3.332625000	-1.297797000
C	1.618640000	2.933051000	-0.545345000
C	2.775234000	3.636346000	-0.221475000
H	2.786838000	4.718029000	-0.295793000
H	0.735513000	3.463018000	-0.885593000
C	1.725075000	-1.314483000	0.809127000
C	1.716679000	-2.722162000	0.776714000
H	1.010805000	-3.257214000	1.406013000
C	0.738442000	-0.552106000	1.558344000
H	1.051111000	0.436057000	1.872616000
C	2.638793000	-3.445287000	0.018256000
H	2.607083000	-4.529594000	0.029116000
C	3.910856000	2.953572000	0.188063000
H	4.814035000	3.496257000	0.442624000
H	0.598359000	-0.168564000	-1.301261000
H	-1.211090000	1.863153000	0.073206000
C	-5.135521000	1.199057000	0.824427000
H	-7.104334000	0.567246000	0.228815000
H	-5.498685000	1.951996000	1.515520000
H	-3.079992000	1.611584000	1.249803000
Li	0.031230000	-2.162419000	-0.785005000

L’



Zero-point correction= 0.356862 (Hartree/Particle)

Thermal correction to Energy= 0.407821

Thermal correction to Enthalpy= 0.409351

Thermal correction to Gibbs Free Energy= 0.257548

Sum of electronic and zero-point Energies= -970.255149

Sum of electronic and thermal Energies= -970.204190

Sum of electronic and thermal Enthalpies= -970.202660

Sum of electronic and thermal Free Energies= -970.354463

E(RwB97XD) = -970.775532751

C	0.042517000	-1.669414000	1.895005000
H	-0.825372000	-1.154670000	2.306320000
H	-0.364193000	-2.440538000	1.230626000
C	-1.995105000	-0.353444000	-0.262815000
C	-3.477318000	-0.150100000	-0.196029000
C	-1.132279000	0.553174000	0.280887000
O	-1.592481000	-1.428802000	-0.888049000
C	-4.287501000	-0.791288000	-1.134318000
C	-5.665854000	-0.618805000	-1.121893000
H	-3.811772000	-1.427034000	-1.871060000
C	-6.262241000	0.186599000	-0.158260000
H	-6.278040000	-1.118200000	-1.865455000
H	0.563619000	-2.183580000	2.706741000
C	-4.088434000	0.645111000	0.776619000
C	0.327711000	0.288132000	0.149591000
C	1.286716000	1.453416000	0.017883000

C	2.654897000	1.132062000	-0.081586000
C	3.034187000	-0.300918000	-0.098753000
C	3.595366000	2.154633000	-0.191125000
H	4.652252000	1.914124000	-0.236012000
C	4.144550000	-0.775458000	-0.791915000
H	4.773865000	-0.079143000	-1.335182000
C	4.440235000	-2.135105000	-0.828271000
H	5.306594000	-2.483777000	-1.378538000
C	0.893814000	2.783492000	-0.040236000
C	1.840849000	3.796119000	-0.157346000
H	1.520250000	4.831395000	-0.191183000
H	-0.160595000	3.029268000	-0.000781000
C	2.202188000	-1.220582000	0.574897000
C	2.503270000	-2.579635000	0.527066000
H	1.887433000	-3.289705000	1.070895000
C	0.967957000	-0.651756000	1.235191000
H	1.302689000	0.014495000	2.041051000
C	3.619399000	-3.039880000	-0.173300000
H	3.844412000	-4.100227000	-0.196378000
C	3.192276000	3.483381000	-0.224810000
H	3.932548000	4.271435000	-0.302765000
H	0.437634000	-0.217575000	-0.828570000
H	-1.490262000	1.443674000	0.778664000
C	-5.466794000	0.814182000	0.794670000
H	-7.338692000	0.317858000	-0.143527000
H	-5.923003000	1.431145000	1.561515000
H	-3.484898000	1.122916000	1.540246000
Li	-0.009017000	-2.158312000	-0.843039000

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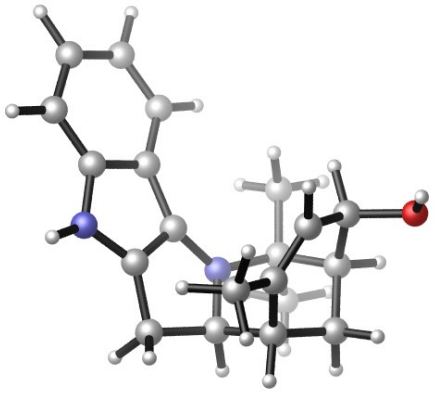


Zero-point correction= 0.408045 (Hartree/Particle)

Thermal correction to Energy= 0.427526

Thermal correction to Enthalpy= 0.428470

Thermal correction to Gibbs Free Energy= 0.362024

Sum of electronic and zero-point Energies= -960.820719

Sum of electronic and thermal Energies= -960.801239

Sum of electronic and thermal Enthalpies= -960.800294

Sum of electronic and thermal Free Energies= -960.866741

E(RwB97XD) = -961.390343578

H	0.260203000000	2.175529000000	-2.719737000000
H	-0.348950000000	3.074688000000	-1.323352000000
H	-0.997141000000	0.642906000000	2.851595000000
C	-0.026489000000	2.087344000000	-1.663794000000
C	2.557636000000	-1.702315000000	0.229448000000
H	1.962796000000	-2.596695000000	0.132037000000
C	4.681226000000	-0.703894000000	0.859048000000
C	4.243753000000	0.546105000000	0.470606000000
C	-0.996522000000	2.895263000000	1.424385000000
H	-2.632666000000	2.303243000000	-0.620575000000
H	-3.938274000000	0.443085000000	0.451109000000
H	-3.659361000000	0.118446000000	-1.256205000000
H	-3.114664000000	-1.889905000000	0.121371000000
H	-1.740633000000	3.670337000000	1.213588000000
H	-0.757987000000	2.928188000000	2.489373000000

H -0.087338000000 3.153391000000 0.874638000000

C -1.299156000000 -1.394440000000 -0.919480000000

C 2.954725000000 0.661313000000 -0.047687000000

C -2.138972000000 1.364748000000 -0.340883000000

C -3.163202000000 0.230036000000 -0.288692000000

C -2.418882000000 -1.045608000000 0.111890000000

C 2.055912000000 -0.443815000000 -0.151258000000

C -1.955471000000 -0.873197000000 1.564432000000

O -3.093627000000 -1.183502000000 2.384042000000

H -1.171422000000 -1.597777000000 1.804366000000

C 1.054270000000 1.440682000000 -0.878215000000

C -1.135769000000 1.030608000000 -1.478908000000

C 0.826579000000 0.115096000000 -0.677869000000

C -1.507929000000 1.538220000000 1.027479000000

C -1.442322000000 0.504899000000 1.866813000000

N -0.429106000000 -0.246758000000 -1.233118000000

N 2.341051000000 1.786456000000 -0.540414000000

H -2.994510000000 -0.732416000000 3.223308000000

H 2.705107000000 2.719195000000 -0.470127000000

C 3.842650000000 -1.820146000000 0.724239000000

H 4.209896000000 -2.799186000000 1.010555000000

H 5.681918000000 -0.825270000000 1.257670000000

H 4.886821000000 1.416409000000 0.548481000000

C -0.484883000000 -2.589928000000 -0.444177000000

H -1.154056000000 -3.437488000000 -0.276501000000

H 0.245726000000 -2.874073000000 -1.205122000000

H 0.040326000000 -2.390916000000 0.486429000000

C -1.967042000000 -1.827735000000 -2.241891000000

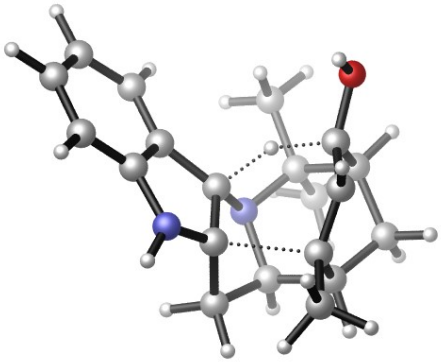
H -1.194350000000 -2.119030000000 -2.956174000000

H -2.629519000000 -2.681191000000 -2.072821000000

H -2.560575000000 -1.035597000000 -2.699622000000

H -1.726620000000 0.944829000000 -2.394808000000

TS_{1-2}



Frequency -1053.4341

Zero-point correction= 0.403835 (Hartree/Particle)

Thermal correction to Energy= 0.421725

Thermal correction to Enthalpy= 0.422669

Thermal correction to Gibbs Free Energy= 0.361301

Sum of electronic and zero-point Energies= -960.759058

Sum of electronic and thermal Energies= -960.741167

Sum of electronic and thermal Enthalpies= -960.740223

Sum of electronic and thermal Free Energies= -960.801592

E(RwB97XD) = -961.322108077

C 0.440918000000 -0.088431000000 -0.467511000000

H -0.046046000000 -0.299176000000 0.847691000000

C 1.872689000000 -0.381992000000 -0.299018000000

C 2.642664000000 -1.538416000000 -0.198466000000

H 2.195263000000 -2.513420000000 -0.334852000000

C 4.004659000000 -1.434967000000 0.056272000000

C 4.605650000000 -0.187487000000 0.237917000000

C 3.863232000000 0.981506000000 0.146078000000

H 5.668659000000 -0.128635000000 0.443472000000

C 2.508592000000 0.873239000000 -0.150445000000

H 4.329586000000 1.952128000000 0.275197000000

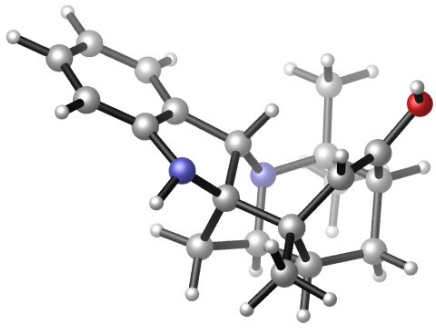
N 1.585896000000 1.887791000000 -0.350350000000

C 0.346959000000 1.323767000000 -0.653186000000

C -0.433282000000 1.519877000000 -1.928814000000

H	0.184244000000	1.256341000000	-2.795072000000
H	-0.870704000000	2.507316000000	-2.084827000000
C	-1.473354000000	0.456754000000	-1.623216000000
C	-2.303791000000	1.056197000000	-0.455699000000
H	-2.982581000000	1.798876000000	-0.889250000000
C	-3.097849000000	-0.026643000000	0.270084000000
H	-3.638186000000	0.408700000000	1.114247000000
H	-3.833459000000	-0.486785000000	-0.392645000000
C	-1.372881000000	1.772255000000	0.551087000000
C	-1.418239000000	3.281988000000	0.577325000000
H	-2.414411000000	3.634355000000	0.867802000000
H	-0.697195000000	3.678583000000	1.296845000000
H	-1.198129000000	3.722330000000	-0.398889000000
C	-2.081303000000	-1.051606000000	0.767141000000
H	-2.555450000000	-1.816920000000	1.387583000000
C	-1.384017000000	-1.738966000000	-0.446422000000
N	-0.630585000000	-0.712405000000	-1.209848000000
C	-0.439115000000	-2.833207000000	0.048975000000
C	-2.389089000000	-2.410461000000	-1.388325000000
C	-1.062820000000	-0.317841000000	1.661496000000
O	-0.744472000000	-1.076575000000	2.786880000000
C	-1.143590000000	1.097683000000	1.744317000000
H	-0.667752000000	1.608219000000	2.578944000000
H	-0.112953000000	-0.588484000000	3.318440000000
H	-2.102490000000	0.185084000000	-2.471063000000
H	1.843334000000	2.828521000000	-0.587753000000
H	4.607112000000	-2.333966000000	0.116229000000
H	-1.026212000000	-3.641541000000	0.492072000000
H	0.130864000000	-3.239424000000	-0.790417000000
H	0.250500000000	-2.480182000000	0.815552000000
H	-1.846700000000	-2.977404000000	-2.148337000000
H	-3.023601000000	-3.101916000000	-0.826736000000
H	-3.041302000000	-1.707189000000	-1.905425000000

2



Zero-point correction= 0.410297 (Hartree/Particle)

Thermal correction to Energy= 0.427852

Thermal correction to Enthalpy= 0.428796

Thermal correction to Gibbs Free Energy= 0.367913

Sum of electronic and zero-point Energies= -960.834599

Sum of electronic and thermal Energies= -960.817044

Sum of electronic and thermal Enthalpies= -960.816100

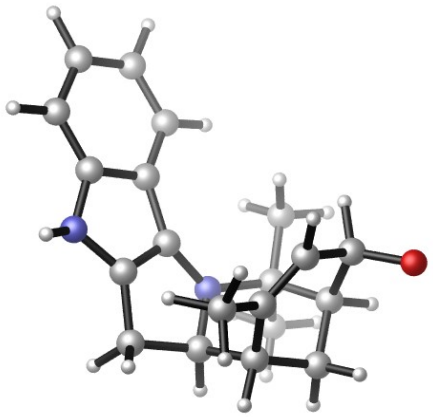
Sum of electronic and thermal Free Energies= -960.876983

E(RwB97XD) = -961.403927865

C	0.527992000000	-0.299304000000	0.075168000000
H	0.186567000000	-0.446597000000	1.096583000000
C	2.015657000000	-0.548034000000	0.078150000000
C	2.769273000000	-1.699180000000	-0.002501000000
H	2.286885000000	-2.653927000000	-0.183659000000
C	4.157782000000	-1.611233000000	0.130658000000
C	4.759887000000	-0.377911000000	0.352425000000
C	4.003895000000	0.792426000000	0.439213000000
H	5.838163000000	-0.318887000000	0.453353000000
C	2.628659000000	0.693923000000	0.297854000000
H	4.483805000000	1.751223000000	0.604238000000
N	1.671374000000	1.732748000000	0.342325000000
C	0.480603000000	1.184109000000	-0.286954000000
C	0.476830000000	1.048174000000	-1.825649000000

H	1.372280000000	0.554065000000	-2.205152000000
H	0.320538000000	1.989981000000	-2.355860000000
C	-0.759343000000	0.168743000000	-1.819782000000
C	-1.777188000000	1.115109000000	-1.153126000000
H	-2.033857000000	1.908182000000	-1.862576000000
C	-3.033371000000	0.378302000000	-0.725578000000
H	-3.765291000000	1.061799000000	-0.287161000000
H	-3.505078000000	-0.086865000000	-1.595154000000
C	-0.947583000000	1.746401000000	0.038958000000
C	-0.962564000000	3.274665000000	-0.007384000000
H	-1.986154000000	3.649655000000	0.080575000000
H	-0.376501000000	3.691205000000	0.817660000000
H	-0.546670000000	3.652618000000	-0.946378000000
C	-2.611055000000	-0.664505000000	0.312734000000
H	-3.466758000000	-1.264283000000	0.636149000000
C	-1.540796000000	-1.644704000000	-0.296525000000
N	-0.383284000000	-0.934430000000	-0.890864000000
C	-1.055093000000	-2.632785000000	0.767625000000
C	-2.192400000000	-2.475866000000	-1.412398000000
C	-2.143229000000	0.131099000000	1.506096000000
O	-2.543383000000	-0.404576000000	2.695176000000
C	-1.451856000000	1.266605000000	1.379124000000
H	-1.146427000000	1.826091000000	2.261219000000
H	-2.210139000000	0.136520000000	3.415157000000
H	-1.082456000000	-0.216937000000	-2.787108000000
H	1.989932000000	2.616512000000	-0.030797000000
H	4.767535000000	-2.504427000000	0.058717000000
H	-1.880451000000	-3.282150000000	1.069657000000
H	-0.256806000000	-3.254552000000	0.353906000000
H	-0.683002000000	-2.147800000000	1.670549000000
H	-1.475706000000	-3.217814000000	-1.770487000000
H	-3.076728000000	-2.996974000000	-1.035130000000
H	-2.499841000000	-1.874463000000	-2.268580000000

M



Zero-point correction= 0.392990 (Hartree/Particle)

Thermal correction to Energy= 0.411686

Thermal correction to Enthalpy= 0.412630

Thermal correction to Gibbs Free Energy= 0.348005

Sum of electronic and zero-point Energies= -960.229449

Sum of electronic and thermal Energies= -960.210753

Sum of electronic and thermal Enthalpies= -960.209809

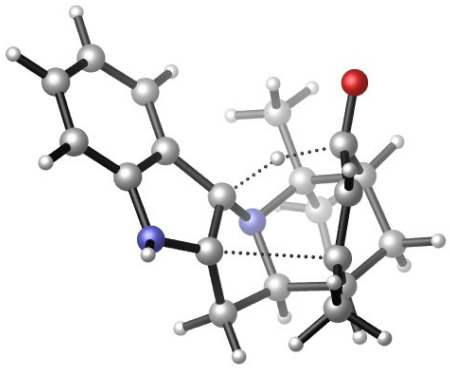
Sum of electronic and thermal Free Energies= -960.274434

E(RwB97XD) = -960.781128602

C	0.836695000000	0.106836000000	-0.644333000000
H	-1.364822000000	-1.603829000000	1.920708000000
C	2.080796000000	-0.430474000000	-0.120559000000
C	2.588982000000	-1.674549000000	0.290330000000
H	1.983619000000	-2.565410000000	0.237393000000
C	3.879790000000	-1.776596000000	0.779661000000
C	4.715322000000	-0.655565000000	0.879991000000
C	4.267564000000	0.583264000000	0.459546000000
H	5.718134000000	-0.760703000000	1.280186000000
C	2.976976000000	0.679802000000	-0.054936000000
H	4.906145000000	1.459735000000	0.511446000000
N	2.361544000000	1.790926000000	-0.584708000000
C	1.056824000000	1.429729000000	-0.868911000000

C	-0.030554000000	2.053932000000	-1.660692000000
H	0.266406000000	2.152098000000	-2.715179000000
H	-0.374389000000	3.033492000000	-1.316674000000
C	-1.127874000000	0.979497000000	-1.480651000000
C	-2.164444000000	1.320524000000	-0.384699000000
H	-2.653996000000	2.253574000000	-0.703597000000
C	-3.184020000000	0.179474000000	-0.361973000000
H	-3.976203000000	0.380367000000	0.363882000000
H	-3.645049000000	0.065472000000	-1.352186000000
C	-1.586001000000	1.519675000000	1.006047000000
C	-1.099227000000	2.895546000000	1.387348000000
H	-1.827864000000	3.670990000000	1.113147000000
H	-0.933886000000	2.955699000000	2.466473000000
H	-0.151839000000	3.154262000000	0.897155000000
C	-2.456575000000	-1.077979000000	0.106629000000
H	-3.145292000000	-1.929175000000	0.082481000000
C	-1.273200000000	-1.436537000000	-0.846793000000
N	-0.404952000000	-0.282335000000	-1.182302000000
C	-0.454991000000	-2.581775000000	-0.267948000000
C	-1.844373000000	-1.946140000000	-2.189359000000
C	-2.173040000000	-0.878713000000	1.644375000000
O	-3.288202000000	-1.029287000000	2.379181000000
C	-1.576962000000	0.504629000000	1.873538000000
H	-1.230376000000	0.678196000000	2.892208000000
H	-1.682738000000	0.854797000000	-2.416990000000
H	2.644936000000	2.728841000000	-0.360043000000
H	4.247494000000	-2.746179000000	1.098339000000
H	-1.126373000000	-3.415909000000	-0.048769000000
H	0.298030000000	-2.919213000000	-0.987916000000
H	0.023505000000	-2.299822000000	0.666739000000
H	-1.024996000000	-2.226193000000	-2.858612000000
H	-2.478882000000	-2.820910000000	-2.018704000000
H	-2.452222000000	-1.193509000000	-2.695549000000

TS_{MN}



Frequency -1032.0515

Zero-point correction= 0.388227 (Hartree/Particle)

Thermal correction to Energy= 0.405948

Thermal correction to Enthalpy= 0.406893

Thermal correction to Gibbs Free Energy= 0.345374

Sum of electronic and zero-point Energies= -960.195544

Sum of electronic and thermal Energies= -960.177823

Sum of electronic and thermal Enthalpies= -960.176879

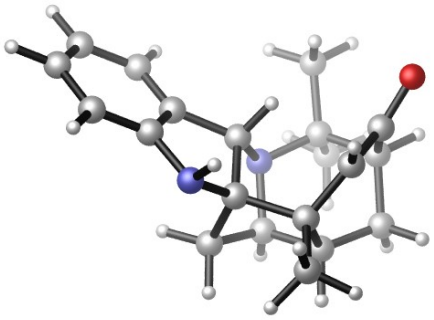
Sum of electronic and thermal Free Energies= -960.238397

E(RwB97XD) = -960.740846921

C	0.490302000000	0.033128000000	-0.401288000000
H	-0.083939000000	-0.242259000000	0.892788000000
C	1.932196000000	-0.285785000000	-0.210817000000
C	2.679092000000	-1.435191000000	0.038003000000
H	2.210018000000	-2.407381000000	0.047656000000
C	4.043190000000	-1.343186000000	0.299574000000
C	4.680524000000	-0.102211000000	0.341450000000
C	3.969408000000	1.061214000000	0.083750000000
H	5.741081000000	-0.045355000000	0.566419000000
C	2.615577000000	0.954928000000	-0.225964000000
H	4.459128000000	2.030366000000	0.090437000000
N	1.756061000000	1.965697000000	-0.611303000000
C	0.456966000000	1.412098000000	-0.705247000000

C	-0.481324000000	1.648979000000	-1.842469000000
H	0.019219000000	1.493227000000	-2.812712000000
H	-0.982015000000	2.623958000000	-1.871646000000
C	-1.458014000000	0.519897000000	-1.544010000000
C	-2.418531000000	0.970569000000	-0.404608000000
H	-3.133485000000	1.664566000000	-0.869460000000
C	-3.153944000000	-0.243840000000	0.165722000000
H	-3.796225000000	0.069626000000	0.993922000000
H	-3.796504000000	-0.708986000000	-0.590368000000
C	-1.740290000000	1.687872000000	0.765318000000
C	-1.863185000000	3.185020000000	0.833319000000
H	-2.917039000000	3.494551000000	0.895762000000
H	-1.345031000000	3.578214000000	1.712571000000
H	-1.445165000000	3.673963000000	-0.054294000000
C	-2.079908000000	-1.206655000000	0.663423000000
H	-2.522846000000	-2.052005000000	1.198157000000
C	-1.262121000000	-1.741886000000	-0.538395000000
N	-0.550327000000	-0.616881000000	-1.188306000000
C	-0.281113000000	-2.799863000000	-0.037633000000
C	-2.136393000000	-2.426348000000	-1.601290000000
C	-1.137543000000	-0.512858000000	1.720787000000
O	-0.775698000000	-1.221267000000	2.729562000000
C	-1.343151000000	0.945093000000	1.823328000000
H	-0.933568000000	1.417875000000	2.714003000000
H	-2.053557000000	0.240283000000	-2.418673000000
H	1.890540000000	2.889890000000	-0.230759000000
H	4.610659000000	-2.247162000000	0.494465000000
H	-0.843929000000	-3.692167000000	0.252735000000
H	0.416539000000	-3.072944000000	-0.835139000000
H	0.251427000000	-2.463807000000	0.852583000000
H	-1.492627000000	-2.913116000000	-2.339846000000
H	-2.764369000000	-3.188314000000	-1.128155000000
H	-2.793289000000	-1.740449000000	-2.137408000000

N



Zero-point correction= 0.394867 (Hartree/Particle)

Thermal correction to Energy= 0.412289

Thermal correction to Enthalpy= 0.413234

Thermal correction to Gibbs Free Energy= 0.352434

Sum of electronic and zero-point Energies= -960.278933

Sum of electronic and thermal Energies= -960.261510

Sum of electronic and thermal Enthalpies= -960.260566

Sum of electronic and thermal Free Energies= -960.321365

E(RwB97XD) = -960.829407883

C	0.499278000000	-0.286785000000	0.023877000000
H	0.167700000000	-0.419828000000	1.053881000000
C	1.986930000000	-0.531702000000	0.004945000000
C	2.741234000000	-1.684190000000	-0.074206000000
H	2.254544000000	-2.637211000000	-0.255085000000
C	4.127822000000	-1.604384000000	0.091616000000
C	4.733440000000	-0.378692000000	0.343900000000
C	3.977276000000	0.794853000000	0.407476000000
H	5.809841000000	-0.327310000000	0.474771000000
C	2.606047000000	0.708249000000	0.231690000000
H	4.451825000000	1.757202000000	0.568735000000
N	1.682215000000	1.792123000000	0.187409000000
C	0.443349000000	1.196961000000	-0.324424000000
C	0.370798000000	1.085760000000	-1.855537000000
H	1.247110000000	0.602261000000	-2.294556000000

H 0.188738000000 2.039808000000 -2.354565000000

C -0.861582000000 0.199209000000 -1.801938000000

C -1.848768000000 1.124435000000 -1.063532000000

H -2.149717000000 1.922658000000 -1.754079000000

C -3.068453000000 0.373251000000 -0.565832000000

H -3.756335000000 1.052861000000 -0.055072000000

H -3.608766000000 -0.064499000000 -1.415643000000

C -0.972798000000 1.747546000000 0.101608000000

C -0.990240000000 3.278957000000 0.028997000000

H -2.021519000000 3.635094000000 0.110063000000

H -0.427258000000 3.713297000000 0.862568000000

H -0.558279000000 3.660446000000 -0.903629000000

C -2.574779000000 -0.681358000000 0.421786000000

H -3.404883000000 -1.296603000000 0.784358000000

C -1.555740000000 -1.644110000000 -0.273716000000

N -0.425143000000 -0.925742000000 -0.923787000000

C -1.003599000000 -2.655124000000 0.736307000000

C -2.258254000000 -2.456068000000 -1.375495000000

C -2.050660000000 0.062762000000 1.685605000000

O -2.290033000000 -0.484862000000 2.799380000000

C -1.419193000000 1.277530000000 1.461190000000

H -1.071312000000 1.837012000000 2.328576000000

H -1.232612000000 -0.171788000000 -2.760020000000

H 1.541853000000 2.214145000000 1.099311000000

H 4.733919000000 -2.502358000000 0.028359000000

H -1.805611000000 -3.328385000000 1.050836000000

H -0.207348000000 -3.246166000000 0.270353000000

H -0.628134000000 -2.180688000000 1.642774000000

H -1.558615000000 -3.186583000000 -1.792452000000

H -3.118833000000 -2.988564000000 -0.959221000000

H -2.618186000000 -1.833182000000 -2.196563000000

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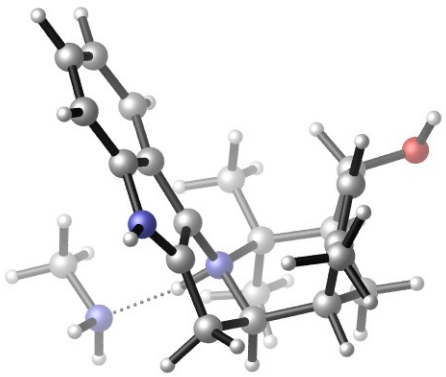
1 ($MeNH_3^+$)



Zero-point correction= 0.490406 (Hartree/Particle)

Thermal correction to Energy= 0.514096

Thermal correction to Enthalpy= 0.515040

Thermal correction to Gibbs Free Energy= 0.438573

Sum of electronic and zero-point Energies= -1057.026219

Sum of electronic and thermal Energies= -1057.002529

Sum of electronic and thermal Enthalpies= -1057.001584

Sum of electronic and thermal Free Energies= -1057.078051

E(RwB97XD) = -1057.69424792

C -0.708934000000 0.003171000000 -0.375757000000

H 1.196121000000 -0.737151000000 2.333835000000

C -1.866642000000 -0.320801000000 0.423612000000

C -2.424371000000 0.019424000000 1.669282000000

H -1.959373000000 0.740989000000 2.322200000000

C -3.609902000000 -0.563746000000 2.069540000000

C -4.280439000000 -1.496497000000 1.265054000000

C -3.779720000000 -1.841565000000 0.027660000000

H -5.204061000000 -1.941320000000 1.614463000000

C -2.593257000000 -1.239037000000 -0.384915000000

H -4.295028000000 -2.549123000000 -0.611686000000

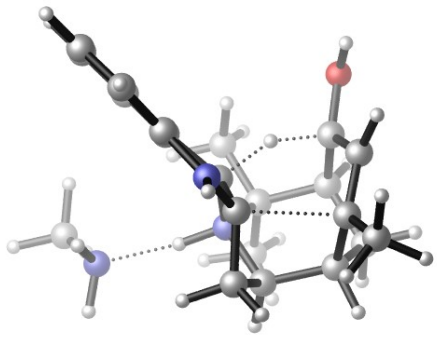
N -1.943032000000 -1.392439000000 -1.596264000000

C -0.823704000000 -0.628458000000 -1.570321000000

C 0.187030000000 -0.216219000000 -2.577278000000

H	-0.237434000000	0.500359000000	-3.288472000000
H	0.634999000000	-1.026227000000	-3.153186000000
C	1.223816000000	0.448392000000	-1.654613000000
C	2.357493000000	-0.497632000000	-1.212718000000
H	2.914440000000	-0.708784000000	-2.132102000000
C	3.262396000000	0.226008000000	-0.218492000000
H	4.107697000000	-0.409461000000	0.048337000000
H	3.671190000000	1.142282000000	-0.649187000000
C	1.912594000000	-1.824806000000	-0.610654000000
C	1.658620000000	-2.992101000000	-1.524165000000
H	2.442063000000	-3.075944000000	-2.283355000000
H	1.629546000000	-3.926242000000	-0.961596000000
H	0.702536000000	-2.902184000000	-2.048478000000
C	2.427340000000	0.503796000000	1.028666000000
H	3.032934000000	1.034986000000	1.767367000000
C	1.253106000000	1.458586000000	0.717037000000
N	0.398687000000	0.975178000000	-0.466586000000
C	0.367674000000	1.690963000000	1.931307000000
C	1.795986000000	2.832330000000	0.282846000000
C	2.079323000000	-0.840100000000	1.693444000000
O	3.203456000000	-1.136283000000	2.517064000000
C	1.820000000000	-1.945868000000	0.711151000000
H	1.548069000000	-2.907297000000	1.142442000000
H	3.146286000000	-2.042042000000	2.826768000000
H	1.671173000000	1.323438000000	-2.127103000000
H	-2.238570000000	-1.997756000000	-2.342866000000
H	-4.031851000000	-0.292173000000	3.029692000000
H	0.961359000000	2.190406000000	2.699300000000
H	-0.476140000000	2.339593000000	1.685195000000
H	-0.009398000000	0.766567000000	2.356690000000
H	0.980494000000	3.553487000000	0.190766000000
H	2.480876000000	3.201712000000	1.047104000000
H	2.339521000000	2.812825000000	-0.661296000000
N	-1.230423000000	3.008692000000	-1.510144000000
H	-1.753308000000	2.549410000000	-2.249396000000
H	-0.086265000000	1.847420000000	-0.834911000000
H	-0.814706000000	3.831989000000	-1.933947000000
C	-2.157545000000	3.409687000000	-0.436706000000
H	-2.583310000000	2.514510000000	0.021137000000
H	-1.604795000000	3.956625000000	0.329777000000
H	-2.974523000000	4.046192000000	-0.786920000000

$TS_{1\text{-}2}$ ($MeNH_3^+$)



Frequency -1111.9482

Zero-point correction= 0.485227 (Hartree/Particle)

Thermal correction to Energy= 0.507815

Thermal correction to Enthalpy= 0.508760

Thermal correction to Gibbs Free Energy= 0.436129

Sum of electronic and zero-point Energies= -1056.970405

Sum of electronic and thermal Energies= -1056.947816

Sum of electronic and thermal Enthalpies= -1056.946872

Sum of electronic and thermal Free Energies= -1057.019503

E(RwB97XD) = -1057.63137841

C	-0.335421000000	-0.233436000000	-0.107903000000
H	0.391428000000	-0.499970000000	1.020996000000
C	-1.749796000000	-0.421245000000	0.253680000000
C	-2.683068000000	0.267023000000	1.029215000000
H	-2.452821000000	1.231370000000	1.460892000000

C	-3.931288000000	-0.297312000000	1.246117000000
C	-4.245748000000	-1.559717000000	0.734091000000
C	-3.329938000000	-2.275231000000	-0.019958000000
H	-5.222566000000	-1.986381000000	0.928192000000
C	-2.096959000000	-1.684199000000	-0.275747000000
H	-3.574151000000	-3.253876000000	-0.416291000000
N	-1.047669000000	-2.170441000000	-1.043670000000
C	-0.022579000000	-1.246132000000	-1.058602000000
C	0.553309000000	-0.597291000000	-2.287478000000
H	-0.245978000000	-0.150996000000	-2.890953000000
H	1.156311000000	-1.234708000000	-2.934050000000
C	1.397435000000	0.438437000000	-1.573610000000
C	2.570586000000	-0.329507000000	-0.929445000000
H	3.275022000000	-0.522898000000	-1.743858000000
C	3.245884000000	0.489512000000	0.166836000000
H	4.053551000000	-0.089271000000	0.616194000000
H	3.685253000000	1.404725000000	-0.231946000000
C	2.108959000000	-1.684107000000	-0.351732000000
C	2.495872000000	-2.931247000000	-1.104053000000
H	3.585762000000	-3.033554000000	-1.142788000000
H	2.092863000000	-3.822353000000	-0.618835000000
H	2.144965000000	-2.921890000000	-2.139269000000
C	2.172519000000	0.790114000000	1.207489000000
H	2.597647000000	1.279051000000	2.086904000000
C	1.095012000000	1.734749000000	0.624466000000
N	0.418433000000	0.982792000000	-0.517569000000
C	0.058885000000	2.097852000000	1.682764000000
C	1.665503000000	3.033393000000	0.051292000000
C	1.565116000000	-0.543604000000	1.686611000000
O	1.330308000000	-0.515577000000	3.047260000000
C	1.940105000000	-1.732826000000	1.017197000000
H	1.804490000000	-2.689112000000	1.516237000000
H	1.054516000000	-1.382102000000	3.354735000000
H	1.729338000000	1.272973000000	-2.188585000000
H	-1.117668000000	-2.957432000000	-1.664411000000
H	-4.666666000000	0.240519000000	1.831842000000
H	0.542702000000	2.724298000000	2.434249000000
H	-0.757927000000	2.675969000000	1.244429000000
H	-0.341376000000	1.227460000000	2.200561000000
H	0.852340000000	3.695882000000	-0.256869000000
H	2.235597000000	3.546583000000	0.827925000000
H	2.327093000000	2.891462000000	-0.801873000000
N	-1.635294000000	2.385625000000	-1.844512000000
H	-2.309102000000	1.632115000000	-1.952329000000
H	-0.267466000000	1.626799000000	-1.013282000000
H	-1.407054000000	2.697208000000	-2.783399000000
C	-2.260201000000	3.488245000000	-1.095267000000
H	-2.597469000000	3.114521000000	-0.127359000000
H	-1.524020000000	4.275452000000	-0.921933000000
H	-3.120490000000	3.926124000000	-1.608721000000

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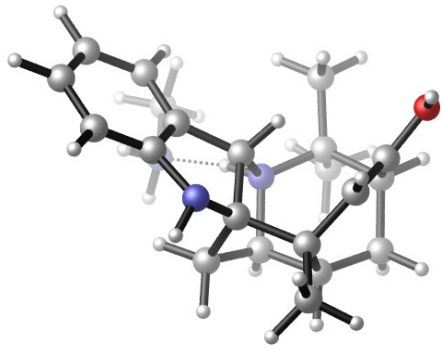
2 ($MeNH_3^+$)



Zero-point correction=	0.492201 (Hartree/Particle)
Thermal correction to Energy=	0.514280
Thermal correction to Enthalpy=	0.515225
Thermal correction to Gibbs Free Energy=	0.444189
Sum of electronic and zero-point Energies=	-1057.047443
Sum of electronic and thermal Energies=	-1057.025364

Sum of electronic and thermal Enthalpies= -1057.024420

Sum of electronic and thermal Free Energies= -1057.095455

E(RwB97XD) = -1057.71506145

C	-0.363109000000	-0.266745000000	0.302831000000
H	0.095033000000	-0.378271000000	1.277440000000
C	-1.851590000000	-0.392590000000	0.442910000000
C	-2.822370000000	0.462391000000	0.932432000000
H	-2.575175000000	1.481211000000	1.213330000000
C	-4.127755000000	-0.006602000000	1.065381000000
C	-4.428141000000	-1.327766000000	0.742619000000
C	-3.447959000000	-2.208391000000	0.292748000000
H	-5.445533000000	-1.684372000000	0.853140000000
C	-2.153178000000	-1.730205000000	0.152151000000
H	-3.692310000000	-3.239425000000	0.064924000000
N	-0.999134000000	-2.439977000000	-0.230303000000
C	-0.024183000000	-1.443450000000	-0.613942000000
C	-0.213008000000	-0.767832000000	-1.991466000000
H	-1.230369000000	-0.406049000000	-2.149721000000
H	0.083913000000	-1.393776000000	-2.832952000000
C	0.809030000000	0.309003000000	-1.705429000000
C	2.063954000000	-0.519477000000	-1.413190000000
H	2.413578000000	-0.910992000000	-2.371261000000
C	3.157309000000	0.301260000000	-0.757490000000
H	4.056798000000	-0.297603000000	-0.608205000000
H	3.434727000000	1.143287000000	-1.395223000000
C	1.520529000000	-1.722939000000	-0.537498000000
C	1.868901000000	-3.076356000000	-1.156701000000
H	2.952812000000	-3.197454000000	-1.222008000000
H	1.476196000000	-3.891708000000	-0.543341000000
H	1.459916000000	-3.179589000000	-2.165919000000
C	2.618461000000	0.758067000000	0.598656000000
H	3.347905000000	1.384682000000	1.117695000000
C	1.343836000000	1.640024000000	0.433277000000
N	0.289154000000	0.903902000000	-0.395851000000
C	0.730578000000	2.023058000000	1.779657000000
C	1.678516000000	2.930455000000	-0.323640000000
C	2.457074000000	-0.502950000000	1.420474000000
O	2.845963000000	-0.328581000000	2.707317000000
C	2.034595000000	-1.649668000000	0.881152000000
H	1.972574000000	-2.552218000000	1.483414000000
H	2.780595000000	-1.154653000000	3.194610000000
H	0.934565000000	1.104839000000	-2.436589000000
H	-1.135028000000	-3.208282000000	-0.871892000000
H	-4.906205000000	0.650189000000	1.433377000000
H	1.411731000000	2.703265000000	2.293575000000
H	-0.218416000000	2.547772000000	1.634805000000
H	0.567301000000	1.174545000000	2.442961000000
H	0.806654000000	3.587053000000	-0.355950000000
H	2.474284000000	3.459892000000	0.202632000000
H	2.015075000000	2.760582000000	-1.345953000000
N	-1.780467000000	2.584316000000	-1.375045000000
H	-2.578786000000	1.959921000000	-1.292787000000
H	-0.456723000000	1.602098000000	-0.678443000000
H	-1.669190000000	2.765728000000	-2.367711000000
C	-2.070550000000	3.846102000000	-0.675205000000
H	-2.156303000000	3.656479000000	0.396884000000
H	-1.246561000000	4.545162000000	-0.827055000000
H	-2.993240000000	4.326312000000	-1.012283000000

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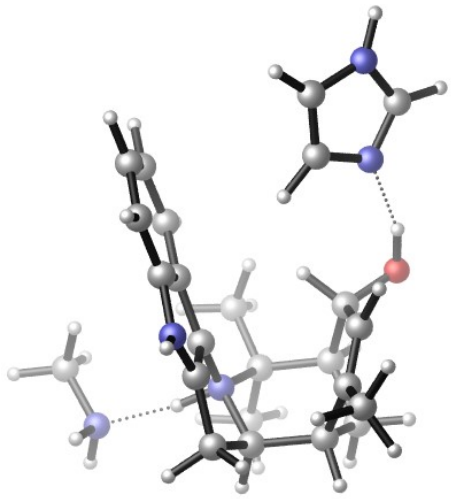
1 (im, $MeNH_3^+$)



Zero-point correction= 0.564847 (Hartree/Particle)

Thermal correction to Energy= 0.593622

Thermal correction to Enthalpy= 0.594566

Thermal correction to Gibbs Free Energy= 0.504649

Sum of electronic and zero-point Energies= -1283.179779

Sum of electronic and thermal Energies= -1283.151004

Sum of electronic and thermal Enthalpies= -1283.150060

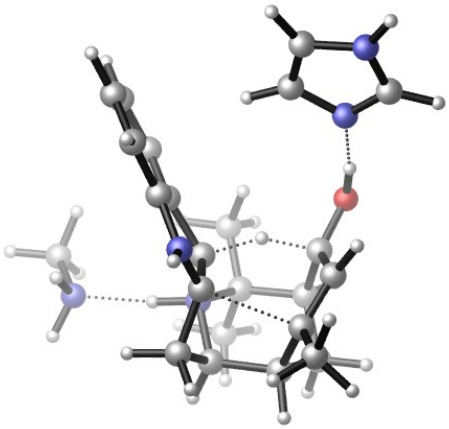
Sum of electronic and thermal Free Energies= -1283.239977

E(RwB97XD) = -1283.96038984

C	-1.014248000000	0.836188000000	0.369861000000
H	0.690022000000	-0.887216000000	-0.871091000000
C	0.074359000000	1.726078000000	0.055132000000
C	0.775840000000	2.177563000000	-1.075973000000
H	0.512307000000	1.853824000000	-2.070266000000
C	1.824406000000	3.061467000000	-0.920079000000
C	2.212265000000	3.526125000000	0.344922000000
C	1.532779000000	3.128263000000	1.478137000000
H	3.042842000000	4.216242000000	0.431936000000
C	0.463365000000	2.249267000000	1.320316000000
H	1.809989000000	3.495059000000	2.459830000000
N	-0.381294000000	1.752367000000	2.296840000000
C	-1.261679000000	0.912676000000	1.699387000000
C	-2.461224000000	0.152467000000	2.134436000000
H	-3.327799000000	0.813872000000	2.239220000000
H	-2.352905000000	-0.400179000000	3.066750000000
C	-2.614952000000	-0.802781000000	0.936618000000
C	-1.912024000000	-2.160948000000	1.159275000000
H	-2.546559000000	-2.672539000000	1.891610000000
C	-1.869467000000	-2.964804000000	-0.141203000000
H	-1.375337000000	-3.919677000000	0.041747000000
H	-2.871471000000	-3.186955000000	-0.513200000000
C	-0.493756000000	-2.104102000000	1.713412000000
C	-0.285743000000	-2.242927000000	3.196050000000
H	-0.840251000000	-3.101008000000	3.589857000000
H	0.770750000000	-2.387411000000	3.426902000000
H	-0.623635000000	-1.362478000000	3.752648000000
C	-1.064198000000	-2.147320000000	-1.146344000000
H	-0.950935000000	-2.703913000000	-2.079343000000
C	-1.820954000000	-0.856998000000	-1.513624000000
N	-2.049450000000	-0.002013000000	-0.258986000000
C	-1.088676000000	-0.058744000000	-2.586599000000
C	-3.226023000000	-1.149220000000	-2.068556000000
C	0.379993000000	-1.914244000000	-0.633047000000
O	1.225375000000	-2.808335000000	-1.317510000000
C	0.523315000000	-2.052460000000	0.858762000000
H	1.548463000000	-2.091951000000	1.217367000000
H	2.132109000000	-2.477259000000	-1.170782000000
H	-3.664453000000	-0.984823000000	0.704951000000
H	-0.309808000000	1.942638000000	3.281508000000
H	2.361654000000	3.400457000000	-1.797489000000
H	-1.246291000000	-0.557802000000	-3.544269000000
H	-1.485865000000	0.955524000000	-2.671927000000
H	-0.016228000000	-0.015422000000	-2.421685000000
H	-3.662193000000	-0.239685000000	-2.489836000000
H	-3.140786000000	-1.881407000000	-2.872934000000

H	-3.924510000000	-1.550199000000	-1.335713000000
N	-3.850030000000	2.114858000000	-0.702993000000
H	-3.928018000000	2.572794000000	0.199687000000
H	-2.813232000000	0.688514000000	-0.516808000000
H	-4.801364000000	1.928152000000	-1.003030000000
C	-3.190496000000	3.024527000000	-1.656237000000
H	-2.154242000000	3.177488000000	-1.346986000000
H	-3.186759000000	2.564857000000	-2.646319000000
H	-3.680377000000	3.998969000000	-1.734657000000
N	3.553253000000	-1.308280000000	-0.671597000000
C	4.818764000000	-1.469874000000	-0.976281000000
C	3.478256000000	-0.105068000000	-0.008398000000
C	4.716605000000	0.457660000000	0.082716000000
N	5.563228000000	-0.426707000000	-0.540512000000
H	5.240482000000	-2.311805000000	-1.503152000000
H	6.558289000000	-0.323419000000	-0.650075000000
H	5.061669000000	1.379115000000	0.519418000000
H	2.542461000000	0.286012000000	0.360846000000

$TS_{1\text{-}2}$ (im, $MeNH_3^+$)



Frequency -1080.5707

Zero-point correction= 0.559005 (Hartree/Particle)

Thermal correction to Energy= 0.586882

Thermal correction to Enthalpy= 0.587827

Thermal correction to Gibbs Free Energy= 0.500192

Sum of electronic and zero-point Energies= -1283.130716

Sum of electronic and thermal Energies= -1283.102839

Sum of electronic and thermal Enthalpies= -1283.101894

Sum of electronic and thermal Free Energies= -1283.189529

E(RwB97XD) = -1283.90370899

C	-0.629195000000	0.383309000000	0.380183000000
H	-0.020967000000	-0.576511000000	-0.395238000000
C	0.189730000000	1.599305000000	0.251681000000
C	0.447041000000	2.530208000000	-0.755007000000
H	-0.089947000000	2.504419000000	-1.692940000000
C	1.413427000000	3.505102000000	-0.550188000000
C	2.155957000000	3.539065000000	0.634309000000
C	1.938020000000	2.613236000000	1.641874000000
H	2.912057000000	4.303690000000	0.768694000000
C	0.936338000000	1.666062000000	1.451190000000
H	2.514515000000	2.637856000000	2.559283000000
N	0.502026000000	0.682427000000	2.321189000000
C	-0.526016000000	-0.033748000000	1.735011000000
C	-1.905777000000	-0.205960000000	2.305575000000
H	-2.340244000000	0.767989000000	2.562264000000
H	-1.991825000000	-0.858370000000	3.174818000000
C	-2.541443000000	-0.824853000000	1.077410000000
C	-1.981857000000	-2.258363000000	0.966040000000
H	-2.537753000000	-2.844109000000	1.704698000000
C	-2.193787000000	-2.834946000000	-0.431035000000
H	-1.767410000000	-3.837330000000	-0.483881000000
H	-3.254788000000	-2.919745000000	-0.671534000000
C	-0.482950000000	-2.315590000000	1.323015000000
C	-0.105043000000	-2.915118000000	2.652617000000
H	-0.416783000000	-3.964247000000	2.705125000000
H	0.975849000000	-2.879319000000	2.802713000000

H	-0.580908000000	-2.405139000000	3.494859000000
C	-1.468987000000	-1.905950000000	-1.398061000000
H	-1.470971000000	-2.307729000000	-2.413807000000
C	-2.156510000000	-0.522102000000	-1.444582000000
N	-2.023095000000	0.085798000000	-0.051180000000
C	-1.481597000000	0.387670000000	-2.465142000000
C	-3.648475000000	-0.587547000000	-1.777883000000
C	0.009944000000	-1.790770000000	-0.973459000000
O	0.843648000000	-1.756608000000	-2.051794000000
C	0.394419000000	-2.377470000000	0.263245000000
H	1.446657000000	-2.585097000000	0.430096000000
H	1.768449000000	-1.568594000000	-1.750024000000
H	-3.629683000000	-0.798546000000	1.055706000000
H	0.795135000000	0.594905000000	3.277765000000
H	1.603909000000	4.239435000000	-1.323263000000
H	-1.691668000000	-0.003265000000	-3.462244000000
H	-1.887505000000	1.401033000000	-2.411874000000
H	-0.398584000000	0.410818000000	-2.355740000000
H	-4.054488000000	0.421983000000	-1.886127000000
H	-3.777506000000	-1.101774000000	-2.732049000000
H	-4.247725000000	-1.115306000000	-1.037452000000
N	-3.213033000000	2.631488000000	0.276938000000
H	-2.560128000000	3.057350000000	0.928713000000
H	-2.570580000000	0.992782000000	-0.005518000000
H	-4.116013000000	2.631187000000	0.740609000000
C	-3.280640000000	3.449235000000	-0.944848000000
H	-2.281692000000	3.523665000000	-1.377099000000
H	-3.934030000000	2.963982000000	-1.672622000000
H	-3.652361000000	4.462388000000	-0.767917000000
N	3.302638000000	-1.041667000000	-1.092910000000
C	4.432559000000	-1.693346000000	-0.945356000000
C	3.554497000000	0.252044000000	-0.700637000000
C	4.854621000000	0.372629000000	-0.310417000000
N	5.401402000000	-0.877906000000	-0.471528000000
H	4.597081000000	-2.735865000000	-1.169358000000
H	6.356166000000	-1.138712000000	-0.288531000000
H	5.426480000000	1.210793000000	0.049185000000
H	2.792851000000	1.014678000000	-0.733714000000

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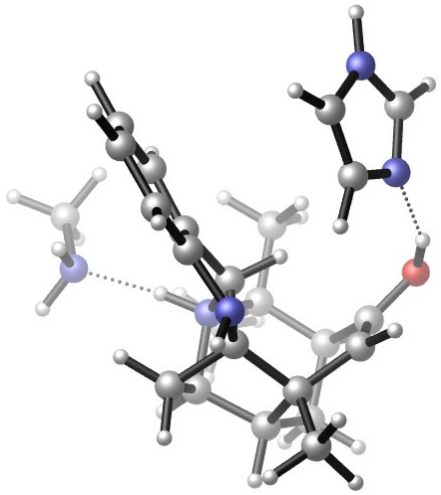
2 (im, $MeNH_3^+$)



Zero-point correction= 0.565959 (Hartree/Particle)

Thermal correction to Energy= 0.592354

Thermal correction to Enthalpy= 0.593298

Thermal correction to Gibbs Free Energy= 0.511464

Sum of electronic and zero-point Energies= -1283.207205

Sum of electronic and thermal Energies= -1283.180811

Sum of electronic and thermal Enthalpies= -1283.179867

Sum of electronic and thermal Free Energies= -1283.261701

E(RwB97XD) = -1283.98609819

C	-0.071148000000	0.363468000000	0.279241000000
H	0.208033000000	-0.532807000000	-0.260294000000
C	1.145630000000	1.228080000000	0.418779000000
C	1.844956000000	2.006610000000	-0.484267000000
H	1.454096000000	2.183850000000	-1.481112000000
C	3.066881000000	2.555557000000	-0.098531000000

C	3.581166000000	2.286653000000	1.167544000000
C	2.905041000000	1.466706000000	2.068048000000
H	4.530921000000	2.719732000000	1.459958000000
C	1.683902000000	0.934232000000	1.679486000000
H	3.325220000000	1.250634000000	3.043694000000
N	0.870922000000	0.026189000000	2.381191000000
C	-0.424478000000	0.051557000000	1.734224000000
C	-1.345088000000	1.251163000000	2.048789000000
H	-0.838600000000	2.213313000000	1.950038000000
H	-1.825968000000	1.192860000000	3.025289000000
C	-2.306941000000	0.920424000000	0.928879000000
C	-2.734358000000	-0.506246000000	1.291127000000
H	-3.411080000000	-0.423749000000	2.145153000000
C	-3.427122000000	-1.213920000000	0.142605000000
H	-3.751138000000	-2.210544000000	0.445829000000
H	-4.320608000000	-0.663625000000	-0.161085000000
C	-1.388943000000	-1.191677000000	1.766619000000
C	-1.509130000000	-1.759361000000	3.180137000000
H	-2.284481000000	-2.528246000000	3.214340000000
H	-0.567625000000	-2.221652000000	3.489024000000
H	-1.769523000000	-0.988205000000	3.911601000000
C	-2.406639000000	-1.338595000000	-0.986321000000
H	-2.847042000000	-1.818781000000	-1.864233000000
C	-1.919343000000	0.062210000000	-1.468634000000
N	-1.377651000000	0.869291000000	-0.284168000000
C	-0.820631000000	-0.034392000000	-2.527425000000
C	-3.081313000000	0.869946000000	-2.056958000000
C	-1.311099000000	-2.258160000000	-0.486281000000
O	-0.786522000000	-3.042537000000	-1.443722000000
C	-0.939306000000	-2.259521000000	0.800518000000
H	-0.190012000000	-2.967342000000	1.140971000000
H	0.168417000000	-3.182365000000	-1.240649000000
H	-3.119774000000	1.615546000000	0.728761000000
H	0.874433000000	0.098652000000	3.388701000000
H	3.620981000000	3.184703000000	-0.784437000000
H	-1.243531000000	-0.481541000000	-3.428451000000
H	-0.454739000000	0.963825000000	-2.787987000000
H	0.021711000000	-0.657347000000	-2.228609000000
H	-2.720744000000	1.819175000000	-2.459677000000
H	-3.527195000000	0.307278000000	-2.878635000000
H	-3.871145000000	1.082810000000	-1.337156000000
N	-1.035437000000	3.644658000000	-0.831875000000
H	-0.178732000000	3.830123000000	-0.317016000000
H	-1.256355000000	1.872293000000	-0.595012000000
H	-1.756963000000	4.201728000000	-0.385230000000
C	-0.874068000000	4.076274000000	-2.228791000000
H	-0.117449000000	3.456956000000	-2.715370000000
H	-1.814652000000	3.936848000000	-2.764162000000
H	-0.575018000000	5.123511000000	-2.328540000000
N	1.902300000000	-2.655219000000	-1.029071000000
C	2.729732000000	-2.571000000000	-2.045409000000
C	2.499161000000	-1.963250000000	0.000635000000
C	3.694694000000	-1.454578000000	-0.410671000000
N	3.828110000000	-1.852034000000	-1.718635000000
H	2.581223000000	-3.009262000000	-3.020224000000
H	4.613909000000	-1.667188000000	-2.319867000000
H	4.435562000000	-0.857458000000	0.093168000000
H	2.032994000000	-1.866714000000	0.968842000000

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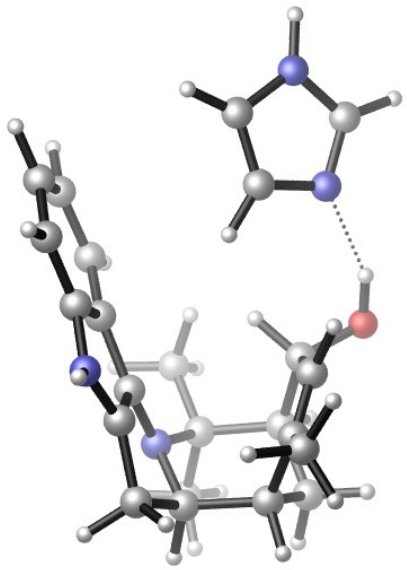
1 (im)



Zero-point correction= 0.482283 (Hartree/Particle)

Thermal correction to Energy= 0.506743

Thermal correction to Enthalpy= 0.507687

Thermal correction to Gibbs Free Energy= 0.428138

Sum of electronic and zero-point Energies= -1186.966654

Sum of electronic and thermal Energies= -1186.942194

Sum of electronic and thermal Enthalpies= -1186.941250

Sum of electronic and thermal Free Energies= -1187.020799

E(RwB97XD) = -1187.64851524

C	-0.816175000000	1.424289000000	-0.323320000000
H	0.163218000000	-1.218858000000	-0.594134000000
C	0.547018000000	1.779486000000	-0.648711000000
C	1.473221000000	1.536713000000	-1.679289000000
H	1.205397000000	0.948657000000	-2.542657000000
C	2.750017000000	2.058763000000	-1.604285000000
C	3.159205000000	2.839785000000	-0.512897000000
C	2.274040000000	3.132794000000	0.506538000000
H	4.168857000000	3.234303000000	-0.478558000000
C	0.977877000000	2.627272000000	0.418671000000
H	2.567839000000	3.756300000000	1.344416000000
N	-0.074130000000	2.833618000000	1.276993000000
C	-1.128644000000	2.077436000000	0.826641000000
C	-2.574919000000	1.976645000000	1.149879000000
H	-3.111465000000	2.867278000000	0.797542000000
H	-2.828892000000	1.827770000000	2.201199000000
C	-2.931135000000	0.742813000000	0.293005000000
C	-2.889265000000	-0.584792000000	1.103498000000
H	-3.732888000000	-0.536845000000	1.803312000000
C	-3.073868000000	-1.765961000000	0.144613000000
H	-3.047840000000	-2.703286000000	0.705604000000
H	-4.041658000000	-1.716589000000	-0.360080000000
C	-1.621713000000	-0.835094000000	1.899074000000
C	-1.569441000000	-0.413968000000	3.341486000000
H	-2.462332000000	-0.746554000000	3.882159000000
H	-0.691661000000	-0.832782000000	3.838311000000
H	-1.518047000000	0.674971000000	3.443665000000
C	-1.922843000000	-1.726376000000	-0.861701000000
H	-1.991833000000	-2.577118000000	-1.544882000000
C	-2.008620000000	-0.423248000000	-1.707796000000
N	-1.967639000000	0.773235000000	-0.842314000000
C	-0.918512000000	-0.396719000000	-2.776546000000
C	-3.338280000000	-0.370258000000	-2.488589000000
C	-0.573089000000	-1.883009000000	-0.124637000000
O	-0.122679000000	-3.220316000000	-0.280293000000
C	-0.615673000000	-1.489691000000	1.325856000000
H	0.276802000000	-1.735197000000	1.897175000000
H	0.809515000000	-3.209338000000	-0.010906000000
H	-3.944475000000	0.841681000000	-0.102352000000
H	-0.011007000000	3.289216000000	2.169188000000
H	3.449620000000	1.858010000000	-2.407865000000
H	-1.154856000000	-1.143734000000	-3.537835000000
H	-0.885316000000	0.583862000000	-3.258228000000
H	0.067637000000	-0.638236000000	-2.388071000000
H	-3.312796000000	0.471483000000	-3.184265000000

H -3.472754000000 -1.292584000000 -3.060659000000

H -4.215187000000 -0.245707000000 -1.854660000000

N 2.594983000000 -2.352884000000 0.394664000000

C 3.790459000000 -2.864225000000 0.235635000000

C 2.781863000000 -0.993951000000 0.508653000000

C 4.107543000000 -0.692411000000 0.416164000000

N 4.743870000000 -1.899147000000 0.242887000000

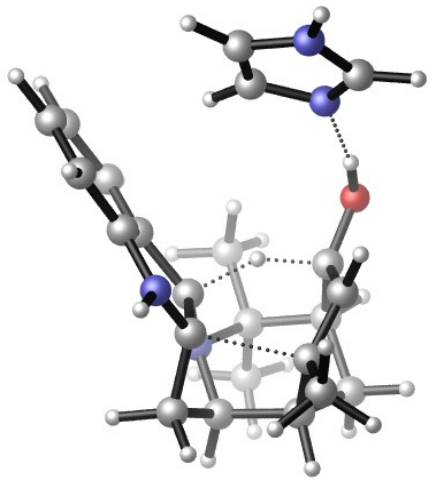
H 4.019922000000 -3.911340000000 0.110566000000

H 5.733457000000 -2.042069000000 0.137921000000

H 4.631213000000 0.247780000000 0.440989000000

H 1.956979000000 -0.310038000000 0.638174000000

$TS_{1\text{-}2}$ (im)



Frequency -1081.1163

Zero-point correction= 0.477385 (Hartree/Particle)

Thermal correction to Energy= 0.500537

Thermal correction to Enthalpy= 0.501481

Thermal correction to Gibbs Free Energy= 0.425942

Sum of electronic and zero-point Energies= -1186.909794

Sum of electronic and thermal Energies= -1186.886642

Sum of electronic and thermal Enthalpies= -1186.885697

Sum of electronic and thermal Free Energies= -1186.961237

E(RwB97XD) = -1187.58464109

C -0.670087000000 0.965426000000 0.276955000000

H -0.403133000000 -0.199898000000 -0.493607000000

C 0.553822000000 1.760442000000 0.085674000000

C 1.071760000000 2.552784000000 -0.936150000000

H 0.488283000000 2.760919000000 -1.822360000000

C 2.345835000000 3.096131000000 -0.808166000000

C 3.120706000000 2.842126000000 0.326033000000

C 2.631736000000 2.054989000000 1.359774000000

H 4.111727000000 3.275523000000 0.406822000000

C 1.344369000000 1.542367000000 1.240651000000

H 3.226598000000 1.861672000000 2.246047000000

N 0.633135000000 0.780467000000 2.148509000000

C -0.636266000000 0.518785000000 1.630042000000

C -1.943673000000 0.939222000000 2.248236000000

H -1.948177000000 2.021040000000 2.427640000000

H -2.238600000000 0.421830000000 3.163073000000

C -2.799702000000 0.555100000000 1.055011000000

C -2.778785000000 -0.997378000000 1.042484000000

H -3.464210000000 -1.334715000000 1.828489000000

C -3.220135000000 -1.539534000000 -0.314265000000

H -3.156876000000 -2.630573000000 -0.319013000000

H -4.255663000000 -1.266941000000 -0.529526000000

C -1.363108000000 -1.525906000000 1.365962000000

C -1.154653000000 -2.157972000000 2.721296000000

H -1.786469000000 -3.046414000000 2.837852000000

H -0.113305000000 -2.466097000000 2.847337000000

H -1.408065000000 -1.480159000000 3.541550000000

C -2.263030000000 -0.952923000000 -1.348317000000

H -2.445067000000 -1.369679000000 -2.342516000000

C -2.429411000000 0.594600000000 -1.408381000000

N -2.054885000000 1.170023000000 -0.092244000000

C -1.541387000000 1.169145000000 -2.511582000000

C -3.868102000000 1.012732000000 -1.731924000000

C -0.824227000000 -1.352808000000 -0.963178000000

O -0.084345000000 -1.706029000000 -2.071457000000

C -0.630691000000 -2.001275000000 0.289554000000

H 0.294104000000 -2.547479000000 0.452387000000

H 0.845493000000 -1.856824000000 -1.802684000000

H -3.817925000000 0.943893000000 1.090691000000

H 0.860444000000 0.725258000000 3.124457000000

H 2.740381000000 3.725170000000 -1.597746000000

H -1.916661000000 0.838438000000 -3.483266000000

H -1.572019000000 2.261524000000 -2.481597000000

H -0.508178000000 0.830310000000 -2.437842000000

H -3.904540000000 2.094361000000 -1.881598000000

H -4.201204000000 0.523308000000 -2.651562000000

H -4.582089000000 0.764561000000 -0.946870000000

N 2.558358000000 -1.837088000000 -1.156736000000

C 3.379990000000 -2.743993000000 -0.689020000000

C 3.124434000000 -0.620564000000 -0.861387000000

C 4.305117000000 -0.804258000000 -0.206185000000

N 4.457604000000 -2.167855000000 -0.102547000000

H 3.243882000000 -3.812910000000 -0.746683000000

H 5.229217000000 -2.651292000000 0.323675000000

H 5.023744000000 -0.107689000000 0.189866000000

H 2.646512000000 0.308821000000 -1.128947000000

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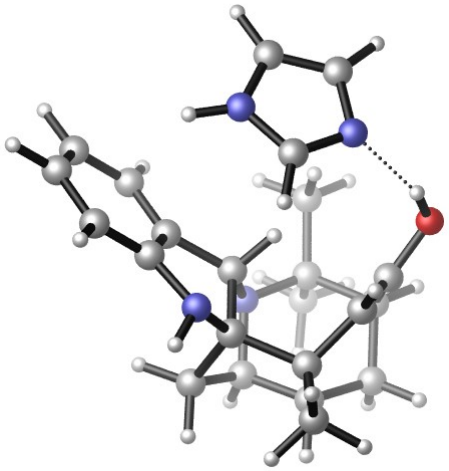
2 (im)



Zero-point correction= 0.484165 (Hartree/Particle)

Thermal correction to Energy= 0.506780

Thermal correction to Enthalpy= 0.507724

Thermal correction to Gibbs Free Energy= 0.434513

Sum of electronic and zero-point Energies= -1186.993957

Sum of electronic and thermal Energies= -1186.971342

Sum of electronic and thermal Enthalpies= -1186.970398

Sum of electronic and thermal Free Energies= -1187.043609

E(RwB97XD) = -1187.67421799

C 0.014474000000 0.568802000000 -0.444064000000

H 0.130105000000 -0.444378000000 -0.069241000000

C 1.408854000000 1.042371000000 -0.762886000000

C 2.243649000000 0.812547000000 -1.834934000000

H 1.862992000000 0.316589000000 -2.721237000000

C 3.578745000000 1.221998000000 -1.758535000000

C 4.052676000000 1.844557000000 -0.607791000000

C 3.213477000000 2.081684000000 0.485223000000

H 5.088225000000 2.163287000000 -0.558045000000

C 1.888492000000 1.678646000000 0.392962000000

H 3.590205000000 2.573170000000 1.376015000000

N 0.888245000000 1.759939000000 1.381563000000

C -0.373153000000 1.506167000000 0.697855000000

C -0.991037000000 2.647948000000 -0.135814000000

H	-0.276182000000	3.102926000000	-0.823965000000
H	-1.477564000000	3.423378000000	0.459464000000
C	-1.984190000000	1.714865000000	-0.807251000000
C	-2.749493000000	1.178826000000	0.419981000000
H	-3.389619000000	1.978384000000	0.806944000000
C	-3.588554000000	-0.039211000000	0.078261000000
H	-4.142817000000	-0.390523000000	0.952494000000
H	-4.323053000000	0.217076000000	-0.690062000000
C	-1.597618000000	0.893548000000	1.466430000000
C	-1.838135000000	1.623154000000	2.788157000000
H	-2.773829000000	1.285845000000	3.242260000000
H	-1.028518000000	1.417521000000	3.495613000000
H	-1.904283000000	2.706943000000	2.648259000000
C	-2.627237000000	-1.130783000000	-0.394082000000
H	-3.171198000000	-2.030919000000	-0.696196000000
C	-1.802907000000	-0.632798000000	-1.639562000000
N	-1.108414000000	0.656313000000	-1.386125000000
C	-0.781743000000	-1.689647000000	-2.071676000000
C	-2.751555000000	-0.415795000000	-2.827771000000
C	-1.787313000000	-1.501595000000	0.807263000000
O	-1.473435000000	-2.815198000000	0.880243000000
C	-1.416920000000	-0.584206000000	1.710009000000
H	-0.849543000000	-0.890483000000	2.584730000000
H	-0.603483000000	-2.904399000000	1.320966000000
H	-2.625065000000	2.160314000000	-1.568588000000
H	0.917164000000	2.588260000000	1.959825000000
H	4.246243000000	1.058732000000	-2.596770000000
H	-1.305095000000	-2.590156000000	-2.402003000000
H	-0.189935000000	-1.305003000000	-2.907211000000
H	-0.102274000000	-1.993245000000	-1.274695000000
H	-2.167466000000	-0.147331000000	-3.710776000000
H	-3.308757000000	-1.332004000000	-3.041784000000
H	-3.475914000000	0.381171000000	-2.655365000000
N	1.286465000000	-2.689046000000	1.342324000000
C	1.907250000000	-1.538507000000	1.479208000000
C	1.983458000000	-3.371895000000	0.372866000000
C	3.028885000000	-2.616847000000	-0.073444000000
N	2.972502000000	-1.453245000000	0.651139000000
H	1.607975000000	-0.724096000000	2.121799000000
H	3.537812000000	-0.628879000000	0.507661000000
H	3.784579000000	-2.793884000000	-0.819517000000
H	1.684560000000	-4.357428000000	0.052748000000

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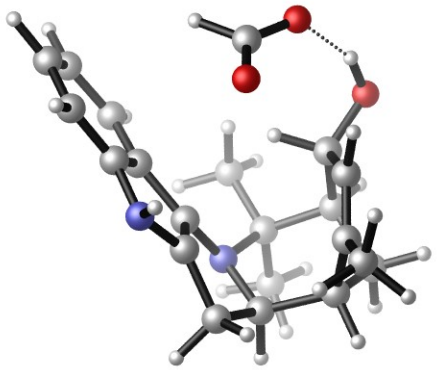
1 (HCO_2^-)



Zero-point correction= 0.431103 (Hartree/Particle)

Thermal correction to Energy= 0.453259

Thermal correction to Enthalpy= 0.454203

Thermal correction to Gibbs Free Energy= 0.381728

Sum of electronic and zero-point Energies= -1150.030491

Sum of electronic and thermal Energies= -1150.008334

Sum of electronic and thermal Enthalpies= -1150.007390

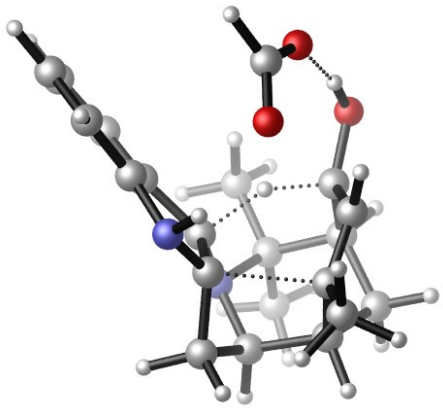
Sum of electronic and thermal Free Energies= -1150.079866

E(RwB97XD) = -1150.65099436

H	0.144786000000	-0.122481000000	1.295870000000
C	1.126961000000	-0.558384000000	1.514911000000
C	-0.294710000000	0.908909000000	-0.890072000000
C	-1.660633000000	1.105207000000	-0.433164000000
C	-0.348581000000	0.038639000000	-1.922001000000

N	1.016559000000	1.443129000000	-0.739256000000
C	-2.345268000000	1.889813000000	0.508380000000
C	-2.437300000000	0.218850000000	-1.226714000000
H	-1.829463000000	2.619775000000	1.112369000000
C	-3.709244000000	1.730113000000	0.680784000000
C	-4.432886000000	0.790957000000	-0.064264000000
H	-4.221869000000	2.334218000000	1.421916000000
C	-3.798943000000	0.029065000000	-1.027682000000
H	-5.494256000000	0.659331000000	0.116217000000
H	-4.339169000000	-0.706720000000	-1.612548000000
N	-1.641964000000	-0.378596000000	-2.193187000000
H	-1.814120000000	-1.352438000000	-2.400139000000
C	0.919248000000	0.044046000000	-2.700653000000
C	1.843564000000	-1.774045000000	-0.538806000000
H	0.828842000000	0.738845000000	-3.547579000000
H	1.256355000000	-0.915139000000	-3.094574000000
C	1.882873000000	0.598707000000	-1.629081000000
C	2.664412000000	-0.557949000000	-0.927751000000
H	2.629944000000	1.254102000000	-2.087354000000
H	3.428032000000	-0.868562000000	-1.653810000000
C	3.332298000000	-0.054315000000	0.355429000000
H	3.831371000000	-0.889264000000	0.853677000000
H	4.092696000000	0.703702000000	0.147809000000
C	2.222300000000	0.509829000000	1.240374000000
C	1.849924000000	-2.988491000000	-1.425713000000
C	1.206914000000	-1.766476000000	0.627061000000
H	2.875924000000	-3.329552000000	-1.618593000000
H	1.292513000000	-3.801444000000	-0.956825000000
H	1.390509000000	-2.798763000000	-2.402115000000
H	2.624701000000	0.797175000000	2.216212000000
C	1.632393000000	1.779359000000	0.564122000000
C	0.646246000000	2.449492000000	1.515082000000
C	2.722699000000	2.833317000000	0.284440000000
H	1.204102000000	2.852263000000	2.364835000000
H	0.140686000000	3.278722000000	1.013284000000
H	-0.093609000000	1.757022000000	1.911730000000
H	2.245723000000	3.775589000000	0.002587000000
H	3.327021000000	3.000563000000	1.181868000000
H	3.396613000000	2.553181000000	-0.525334000000
O	1.143119000000	-0.917530000000	2.884399000000
H	0.307695000000	-1.413459000000	3.001573000000
H	0.598666000000	-2.606680000000	0.946024000000
O	-1.328636000000	-2.089408000000	2.478105000000
C	-2.024500000000	-2.009367000000	1.432157000000
O	-1.883177000000	-2.616317000000	0.354307000000
H	-2.882903000000	-1.289331000000	1.484486000000

$TS_{1\text{-}2}$ (HCO_2^-)



Frequency -950.8931

Zero-point correction=	0.426634 (Hartree/Particle)
Thermal correction to Energy=	0.448234
Thermal correction to Enthalpy=	0.449179
Thermal correction to Gibbs Free Energy=	0.378484
Sum of electronic and zero-point Energies=	-1149.985868
Sum of electronic and thermal Energies=	-1149.964268
Sum of electronic and thermal Enthalpies=	-1149.963323
Sum of electronic and thermal Free Energies=	-1150.034018

E(RwB97XD) = -1150.59968728

H	0.206366000000	0.128525000000	0.648710000000
C	0.923254000000	-0.458553000000	1.535454000000
C	0.077215000000	0.673011000000	-0.677133000000
C	-1.265742000000	1.269650000000	-0.613316000000
C	-0.046794000000	-0.498967000000	-1.462674000000
N	1.407284000000	1.214962000000	-0.841063000000
C	-1.804194000000	2.458794000000	-0.132212000000
C	-2.133340000000	0.271701000000	-1.104766000000
H	-1.163657000000	3.255494000000	0.222162000000
C	-3.186561000000	2.616639000000	-0.097279000000
C	-4.031363000000	1.585923000000	-0.509774000000
H	-3.610073000000	3.543534000000	0.275361000000
C	-3.511936000000	0.399681000000	-1.014324000000
H	-5.107093000000	1.713293000000	-0.443996000000
H	-4.157290000000	-0.406990000000	-1.342397000000
N	-1.419196000000	-0.787205000000	-1.678260000000
H	-1.733583000000	-1.698223000000	-1.341648000000
C	1.012238000000	-0.381938000000	-2.532677000000
C	1.199594000000	-1.893476000000	-0.356472000000
H	0.719596000000	0.367217000000	-3.278893000000
H	1.290485000000	-1.304450000000	-3.045859000000
C	2.105692000000	0.126531000000	-1.606133000000
C	2.471852000000	-1.105670000000	-0.735008000000
H	2.980233000000	0.534673000000	-2.117912000000
H	3.116848000000	-1.750516000000	-1.345178000000
C	3.198169000000	-0.691904000000	0.544880000000
H	3.396978000000	-1.575109000000	1.157727000000
H	4.158620000000	-0.219342000000	0.320174000000
C	2.266790000000	0.264239000000	1.288681000000
C	0.949087000000	-3.216204000000	-1.042573000000
C	0.751296000000	-1.740908000000	0.942615000000
H	1.744232000000	-3.934740000000	-0.804209000000
H	-0.003954000000	-3.629765000000	-0.702837000000
H	0.915828000000	-3.124945000000	-2.132191000000
H	2.670725000000	0.535540000000	2.269095000000
C	2.074174000000	1.558889000000	0.441695000000
C	1.229198000000	2.560598000000	1.228239000000
C	3.404751000000	2.251757000000	0.121828000000
H	1.798478000000	2.903059000000	2.097332000000
H	0.997376000000	3.425703000000	0.600540000000
H	0.304113000000	2.122983000000	1.602605000000
H	3.202641000000	3.219343000000	-0.345403000000
H	3.971117000000	2.420378000000	1.043215000000
H	4.037476000000	1.682363000000	-0.559535000000
O	0.370400000000	-0.198740000000	2.772788000000
H	-0.532849000000	-0.596221000000	2.746351000000
H	-0.055298000000	-2.365814000000	1.307568000000
O	-2.095629000000	-1.271385000000	2.369580000000
C	-2.762142000000	-1.834762000000	1.470725000000
O	-2.364601000000	-2.506305000000	0.495115000000
H	-3.872722000000	-1.719020000000	1.565955000000

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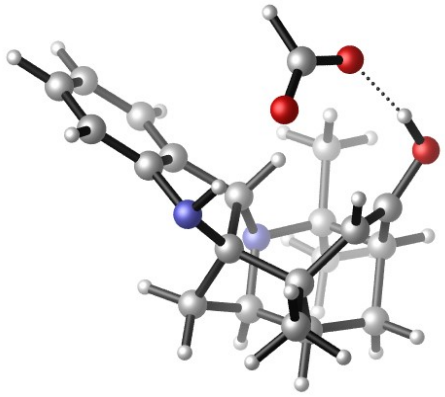
2 (HCO_2^-)



Zero-point correction= 0.432023 (Hartree/Particle)

Thermal correction to Energy= 0.453644

Thermal correction to Enthalpy= 0.454588

Thermal correction to Gibbs Free Energy= 0.383223

Sum of electronic and zero-point Energies= -1150.065016

Sum of electronic and thermal Energies= -1150.043395

Sum of electronic and thermal Enthalpies= -1150.042451

Sum of electronic and thermal Free Energies= -1150.113815

E(RwB97XD) = -1150.68407877

H	-0.155724000000	-0.222973000000	0.806385000000
C	1.960401000000	-1.275525000000	0.652991000000
C	-0.315214000000	0.590729000000	0.101940000000
C	-1.768252000000	0.977576000000	0.227185000000
C	-0.297966000000	0.068587000000	-1.336556000000
N	0.771584000000	1.584506000000	0.151506000000
C	-2.438181000000	1.795938000000	1.112609000000
C	-2.471222000000	0.208076000000	-0.712455000000
H	-1.882757000000	2.387685000000	1.833495000000
C	-3.834877000000	1.838335000000	1.071290000000
C	-4.531133000000	1.050980000000	0.160207000000
H	-4.378945000000	2.478856000000	1.757942000000
C	-3.855354000000	0.230390000000	-0.745290000000
H	-5.616220000000	1.081272000000	0.144534000000
H	-4.394256000000	-0.373111000000	-1.467183000000
N	-1.612262000000	-0.526312000000	-1.582838000000
H	-1.616549000000	-1.509270000000	-1.285998000000
C	-0.033427000000	1.405285000000	-2.057843000000
C	1.025125000000	-0.738451000000	-1.587745000000
H	-0.824890000000	2.139388000000	-1.897304000000
H	0.151526000000	1.293545000000	-3.128098000000
C	1.233642000000	1.676282000000	-1.263448000000
C	2.073947000000	0.443148000000	-1.648094000000
H	1.732269000000	2.628958000000	-1.455503000000
H	2.415128000000	0.564888000000	-2.682782000000
C	3.266706000000	0.251611000000	-0.726201000000
H	3.853792000000	-0.620754000000	-1.027489000000
H	3.926016000000	1.124406000000	-0.780907000000
C	2.718021000000	0.034609000000	0.685122000000
C	0.962902000000	-1.511221000000	-2.906546000000
C	1.306400000000	-1.675350000000	-0.443931000000
H	1.948112000000	-1.929408000000	-3.138362000000
H	0.251912000000	-2.338287000000	-2.830891000000
H	0.652140000000	-0.872158000000	-3.738886000000
H	3.530372000000	-0.073772000000	1.412588000000
C	1.848958000000	1.272182000000	1.121941000000
C	1.238848000000	1.043187000000	2.508769000000
C	2.742511000000	2.518932000000	1.230769000000
H	2.037732000000	0.981862000000	3.253203000000
H	0.587314000000	1.885800000000	2.760966000000
H	0.665309000000	0.119949000000	2.583315000000
H	2.152813000000	3.349759000000	1.626680000000
H	3.580243000000	2.327930000000	1.908789000000
H	3.154728000000	2.832901000000	0.270376000000
O	1.975448000000	-1.975348000000	1.809031000000
H	1.083204000000	-2.413033000000	1.889206000000
H	0.739682000000	-2.599898000000	-0.415999000000
O	-0.548660000000	-2.681460000000	2.059257000000
C	-1.533476000000	-2.828378000000	1.292368000000
O	-1.548063000000	-2.980040000000	0.056159000000
H	-2.528172000000	-2.818640000000	1.803160000000

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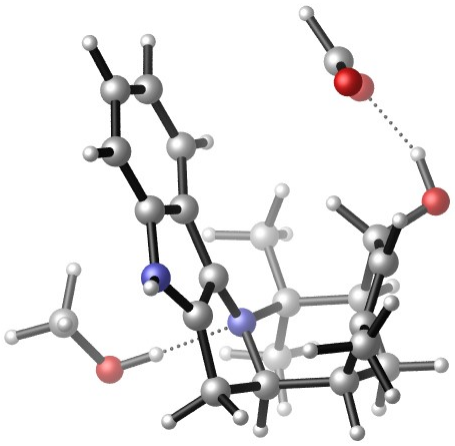
1 (HCO_2^-,MeOH)



Zero-point correction= 0.484610 (Hartree/Particle)

Thermal correction to Energy= 0.512341

Thermal correction to Enthalpy= 0.513285

Thermal correction to Gibbs Free Energy= 0.424872

Sum of electronic and zero-point Energies= -1265.727541

Sum of electronic and thermal Energies= -1265.699810

Sum of electronic and thermal Enthalpies= -1265.698866

Sum of electronic and thermal Free Energies= -1265.787279

E(RwB97XD) = -1266.42199964

H	0.360900000000	-1.733896000000	0.338082000000
C	1.405132000000	-1.868995000000	0.037346000000
C	-0.355317000000	0.947669000000	-0.124425000000
C	-1.703577000000	0.452898000000	0.060391000000
C	-0.347604000000	1.671978000000	-1.269542000000
N	0.879016000000	1.140792000000	0.575597000000
C	-2.397999000000	-0.353809000000	0.974299000000
C	-2.433770000000	0.953114000000	-1.053877000000
H	-1.902908000000	-0.791750000000	1.825782000000
C	-3.732670000000	-0.641947000000	0.763028000000
C	-4.420578000000	-0.149674000000	-0.353388000000
H	-4.245137000000	-1.292665000000	1.462123000000
C	-3.774610000000	0.651461000000	-1.275246000000
H	-5.462495000000	-0.410825000000	-0.503251000000
H	-4.290962000000	1.035807000000	-2.149141000000
N	-1.606924000000	1.750625000000	-1.823057000000
H	-1.787179000000	1.947850000000	-2.791856000000
C	0.921581000000	2.419254000000	-1.460805000000
C	1.861466000000	-0.485098000000	-1.999627000000
H	0.807238000000	3.463406000000	-1.139200000000
H	1.335083000000	2.415056000000	-2.472284000000
C	1.818961000000	1.637586000000	-0.477873000000
C	2.642001000000	0.505452000000	-1.152614000000
H	2.532955000000	2.317506000000	-0.006458000000
H	3.372610000000	1.014868000000	-1.796434000000
C	3.370732000000	-0.282863000000	-0.059568000000
H	3.968622000000	-1.075879000000	-0.516228000000
H	4.054271000000	0.361938000000	0.501441000000
C	2.304562000000	-0.896747000000	0.848322000000
C	1.689318000000	-0.206331000000	-3.468424000000
C	1.387022000000	-1.594708000000	-1.436917000000
H	2.638902000000	0.081433000000	-3.937049000000
H	1.304542000000	-1.089371000000	-3.983481000000
H	0.980192000000	0.610487000000	-3.647129000000
H	2.776454000000	-1.510141000000	1.620254000000
C	1.505184000000	0.221756000000	1.562507000000
C	0.475808000000	-0.372537000000	2.523768000000
C	2.431192000000	1.091405000000	2.439863000000
H	1.000083000000	-0.732200000000	3.412770000000
H	-0.236303000000	0.395325000000	2.840670000000
H	-0.055539000000	-1.229524000000	2.114257000000
H	1.827698000000	1.768324000000	3.050084000000
H	3.013272000000	0.447328000000	3.104992000000
H	3.134266000000	1.700389000000	1.871654000000
O	1.752443000000	-3.205957000000	0.312121000000
H	0.927636000000	-3.594527000000	0.692855000000
H	0.843297000000	-2.339221000000	-2.011846000000

O -0.665714000000 -3.697322000000 1.381519000000

C -1.574754000000 -3.683994000000 0.503099000000

O -1.469853000000 -3.479488000000 -0.711853000000

H -2.607237000000 -3.878698000000 0.899508000000

C -1.348119000000 3.653870000000 1.499068000000

H -1.750174000000 4.575987000000 1.927610000000

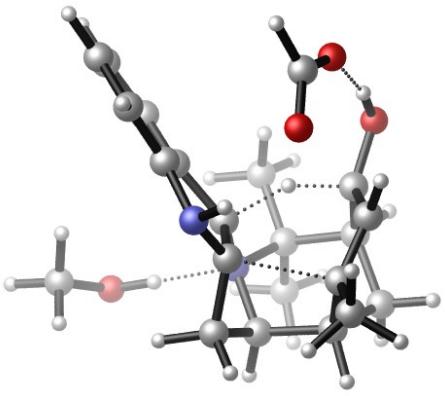
H -1.587643000000 3.634055000000 0.427011000000

H -1.856164000000 2.802125000000 1.968804000000

O 0.042083000000 3.641143000000 1.734381000000

H 0.383624000000 2.781436000000 1.423015000000

$TS_{1\text{-}2}$ (HCO_2^-,MeOH)



Frequency -956.7609

Zero-point correction= 0.480651 (Hartree/Particle)

Thermal correction to Energy= 0.506827

Thermal correction to Enthalpy= 0.507771

Thermal correction to Gibbs Free Energy= 0.425444

Sum of electronic and zero-point Energies= -1265.680385

Sum of electronic and thermal Energies= -1265.654209

Sum of electronic and thermal Enthalpies= -1265.653265

Sum of electronic and thermal Free Energies= -1265.735592

E(RwB97XD) = -1266.36750836

H -0.012070000000 -0.574565000000 0.728100000000

C 0.422736000000 -1.656433000000 1.273726000000

C 0.154749000000 0.488392000000 -0.211654000000

C -0.992710000000 1.353874000000 0.100333000000

C -0.144280000000 -0.140975000000 -1.442693000000

N 1.593481000000 0.662999000000 -0.109501000000

C -1.276558000000 2.323247000000 1.057024000000

C -2.003147000000 0.954277000000 -0.798300000000

H -0.510555000000 2.678086000000 1.733476000000

C -2.565460000000 2.840639000000 1.137749000000

C -3.574842000000 2.373341000000 0.295305000000

H -2.790641000000 3.601392000000 1.877595000000

C -3.304570000000 1.420529000000 -0.679235000000

H -4.581885000000 2.765108000000 0.394830000000

H -4.078513000000 1.054707000000 -1.343981000000

N -1.502115000000 0.087380000000 -1.777218000000

H -2.073532000000 -0.751832000000 -1.886869000000

C 1.042680000000 0.112672000000 -2.339721000000

C 0.584840000000 -2.175350000000 -1.055904000000

H 1.044926000000 1.153728000000 -2.685953000000

H 1.149249000000 -0.544467000000 -3.204502000000

C 2.099834000000 -0.144502000000 -1.277789000000

C 2.044639000000 -1.675713000000 -1.036398000000

H 3.103275000000 0.192479000000 -1.544918000000

H 2.588890000000 -2.146990000000 -1.864092000000

C 2.681557000000 -2.058481000000 0.299659000000

H 2.582742000000 -3.135317000000 0.458552000000

H 3.747464000000 -1.815894000000 0.314641000000

C 1.921150000000 -1.295672000000 1.383378000000

C 0.110359000000 -2.955279000000 -2.259004000000

C 0.020685000000 -2.461087000000 0.171567000000

H 0.667693000000 -3.895976000000 -2.357611000000

H -0.950858000000 -3.191303000000 -2.146491000000

H 0.243111000000 -2.405510000000 -3.195312000000

H 2.250485000000 -1.587887000000 2.385207000000

C	2.158901000000	0.231578000000	1.203494000000
C	1.485382000000	0.999175000000	2.340412000000
C	3.646023000000	0.607140000000	1.227913000000
H	2.004637000000	0.772783000000	3.275882000000
H	1.555316000000	2.074840000000	2.156618000000
H	0.442314000000	0.714099000000	2.475128000000
H	3.746169000000	1.695543000000	1.232996000000
H	4.113753000000	0.209039000000	2.133501000000
H	4.203734000000	0.229720000000	0.370560000000
O	-0.207576000000	-1.800767000000	2.490871000000
H	-1.170088000000	-1.872750000000	2.281056000000
H	-0.951752000000	-2.936853000000	0.216901000000
O	-2.774929000000	-1.843234000000	1.617556000000
C	-3.440834000000	-1.788960000000	0.557779000000
O	-3.088514000000	-2.055436000000	-0.611006000000
H	-4.503278000000	-1.457992000000	0.686165000000
C	1.205377000000	3.923049000000	-1.330050000000
H	1.355653000000	5.004395000000	-1.395717000000
H	1.261910000000	3.513009000000	-2.349836000000
H	0.195377000000	3.735780000000	-0.944743000000
O	2.203383000000	3.396147000000	-0.490197000000
H	2.008921000000	2.443530000000	-0.357487000000

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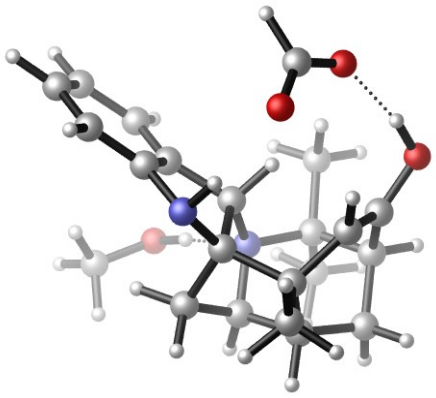
2 (HCO_2^-,MeOH)



Zero-point correction= 0.487239 (Hartree/Particle)

Thermal correction to Energy= 0.512886

Thermal correction to Enthalpy= 0.513830

Thermal correction to Gibbs Free Energy= 0.433336

Sum of electronic and zero-point Energies= -1265.759082

Sum of electronic and thermal Energies= -1265.733434

Sum of electronic and thermal Enthalpies= -1265.732490

Sum of electronic and thermal Free Energies= -1265.812985

E(RwB97XD) = -1266.45262576

H	0.083201000000	-0.589998000000	0.808794000000
C	2.392733000000	-0.999092000000	0.664909000000
C	-0.313743000000	0.122448000000	0.090129000000
C	-1.815255000000	0.071691000000	0.221168000000
C	-0.144603000000	-0.395373000000	-1.341040000000
N	0.438533000000	1.398250000000	0.114968000000
C	-2.689868000000	0.661739000000	1.111295000000
C	-2.265797000000	-0.876735000000	-0.709270000000
H	-2.333362000000	1.402461000000	1.819721000000
C	-4.037991000000	0.296791000000	1.073326000000
C	-4.478637000000	-0.662149000000	0.167049000000
H	-4.742013000000	0.757084000000	1.758547000000
C	-3.596938000000	-1.257328000000	-0.736660000000
H	-5.526102000000	-0.946892000000	0.155004000000
H	-3.938693000000	-1.996663000000	-1.452232000000
N	-1.231992000000	-1.344607000000	-1.573137000000
H	-0.954619000000	-2.283104000000	-1.261281000000
C	-0.275514000000	0.945749000000	-2.088940000000
C	1.354147000000	-0.793127000000	-1.583772000000
H	-1.246697000000	1.421020000000	-1.942455000000
H	-0.065416000000	0.870571000000	-3.157326000000
C	0.860296000000	1.587068000000	-1.309821000000
C	2.019237000000	0.639032000000	-1.667213000000
H	1.062104000000	2.640206000000	-1.515979000000

H	2.313012000000	0.835658000000	-2.704429000000
C	3.213900000000	0.813318000000	-0.745075000000
H	4.024536000000	0.137895000000	-1.032194000000
H	3.597815000000	1.835926000000	-0.816280000000
C	2.744174000000	0.473454000000	0.670140000000
C	1.518272000000	-1.572879000000	-2.889527000000
C	1.889649000000	-1.590238000000	-0.425125000000
H	2.582343000000	-1.694754000000	-3.117242000000
H	1.074434000000	-2.567650000000	-2.797581000000
H	1.038766000000	-1.064405000000	-3.731617000000
H	3.550596000000	0.613868000000	1.398224000000
C	1.568223000000	1.425692000000	1.091558000000
C	1.036993000000	1.066702000000	2.482854000000
C	2.078996000000	2.874602000000	1.167202000000
H	1.818779000000	1.247007000000	3.225587000000
H	0.178584000000	1.702986000000	2.719659000000
H	0.742458000000	0.022239000000	2.579545000000
H	1.296802000000	3.525194000000	1.564459000000
H	2.948756000000	2.926616000000	1.828850000000
H	2.374154000000	3.273755000000	0.195601000000
O	2.598181000000	-1.641060000000	1.834971000000
H	1.860797000000	-2.306896000000	1.927374000000
H	1.612506000000	-2.637929000000	-0.380595000000
O	0.368239000000	-3.003709000000	2.101970000000
C	-0.521623000000	-3.458182000000	1.339519000000
O	-0.481314000000	-3.633426000000	0.106856000000
H	-1.475591000000	-3.737957000000	1.850371000000
C	-2.079318000000	3.772294000000	-0.448583000000
H	-2.682410000000	4.669515000000	-0.281795000000
H	-1.579095000000	3.876977000000	-1.423403000000
H	-2.756491000000	2.908914000000	-0.502339000000
O	-1.162049000000	3.661617000000	0.608395000000
H	-0.633378000000	2.842628000000	0.469941000000

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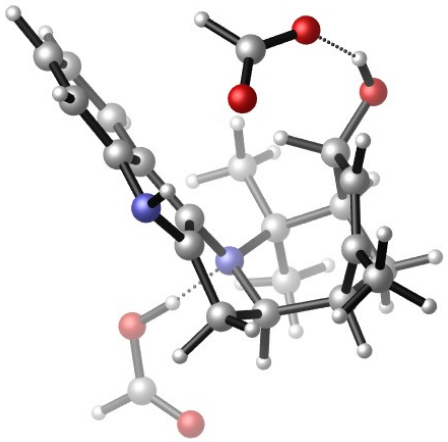
1 (HCO_2^-,HCO_2H)



Zero-point correction= 0.466960 (Hartree/Particle)

Thermal correction to Energy= 0.494143

Thermal correction to Enthalpy= 0.495087

Thermal correction to Gibbs Free Energy= 0.409465

Sum of electronic and zero-point Energies= -1339.787782

Sum of electronic and thermal Energies= -1339.760599

Sum of electronic and thermal Enthalpies= -1339.759655

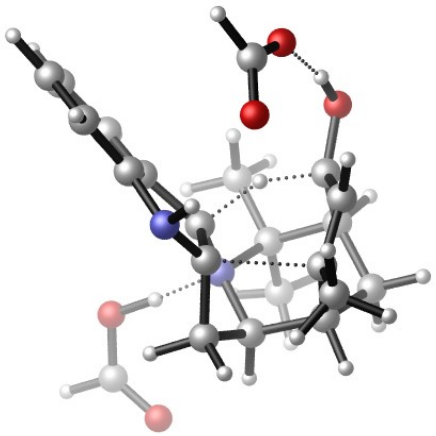
Sum of electronic and thermal Free Energies= -1339.845277

E(RwB97XD) = -1340.47529244

H	-0.822212000000	-0.800668000000	1.118819000000
C	-0.345254000000	-1.773519000000	1.280139000000
C	0.041201000000	0.861122000000	-0.317005000000
C	-1.034802000000	1.750347000000	0.083353000000
C	-0.235536000000	0.435171000000	-1.563591000000
N	1.360018000000	0.446932000000	0.100159000000
C	-1.344390000000	2.604782000000	1.151311000000
C	-1.967085000000	1.667257000000	-0.983014000000
H	-0.651021000000	2.764652000000	1.962904000000
C	-2.560895000000	3.266256000000	1.170813000000
C	-3.499014000000	3.095865000000	0.145924000000
H	-2.792207000000	3.921587000000	2.003941000000

C	-3.205867000000	2.293886000000	-0.942334000000
H	-4.457679000000	3.600060000000	0.202068000000
H	-3.914381000000	2.148034000000	-1.749386000000
N	-1.454803000000	0.899322000000	-2.023808000000
H	-2.103686000000	0.206037000000	-2.395022000000
C	0.964797000000	-0.141262000000	-2.227122000000
C	0.331662000000	-2.655481000000	-0.947046000000
H	1.455059000000	0.638574000000	-2.823418000000
H	0.785201000000	-0.992346000000	-2.881049000000
C	1.820041000000	-0.518372000000	-0.996756000000
C	1.702562000000	-2.049401000000	-0.709506000000
H	2.872854000000	-0.290054000000	-1.169847000000
H	2.415202000000	-2.512569000000	-1.403213000000
C	2.068729000000	-2.397166000000	0.734122000000
H	1.893035000000	-3.462367000000	0.900875000000
H	3.120611000000	-2.200953000000	0.951462000000
C	1.159509000000	-1.551528000000	1.620570000000
C	0.089974000000	-3.465270000000	-2.190151000000
C	-0.577063000000	-2.549841000000	0.014438000000
H	0.749056000000	-4.343651000000	-2.209834000000
H	-0.946234000000	-3.806265000000	-2.228286000000
H	0.293313000000	-2.904930000000	-3.109436000000
H	1.279774000000	-1.836528000000	2.669637000000
C	1.591448000000	-0.067396000000	1.492746000000
C	0.854743000000	0.767701000000	2.533059000000
C	3.095488000000	0.112399000000	1.779871000000
H	1.202227000000	0.459778000000	3.522804000000
H	1.091023000000	1.827148000000	2.408218000000
H	-0.224417000000	0.626680000000	2.505266000000
H	3.307312000000	1.165458000000	1.981481000000
H	3.380265000000	-0.467951000000	2.662252000000
H	3.731064000000	-0.188248000000	0.946929000000
O	-0.992842000000	-2.391907000000	2.380164000000
H	-1.938076000000	-2.357281000000	2.143488000000
H	-1.578508000000	-2.950902000000	-0.096421000000
O	-3.407120000000	-1.900779000000	0.972105000000
C	-3.620079000000	-1.095291000000	0.034886000000
O	-3.332958000000	-1.211232000000	-1.176237000000
H	-4.134685000000	-0.143438000000	0.327176000000
H	2.217641000000	1.767925000000	-0.115741000000
O	2.686735000000	2.689872000000	-0.246769000000
O	4.413983000000	1.572379000000	-1.166802000000
C	3.862897000000	2.586907000000	-0.804881000000
H	4.332184000000	3.578790000000	-0.918778000000

$TS_{1\text{-}2}$ (HCO_2^-,HCO_2H)



Frequency -972.6482

Zero-point correction= 0.461986 (Hartree/Particle)

Thermal correction to Energy= 0.487915

Thermal correction to Enthalpy= 0.488859

Thermal correction to Gibbs Free Energy= 0.407383

Sum of electronic and zero-point Energies= -1339.745570

Sum of electronic and thermal Energies= -1339.719641

Sum of electronic and thermal Enthalpies= -1339.718697

Sum of electronic and thermal Free Energies= -1339.800173

E(RwB97XD) = -1340.42652891

H	-0.453870000000	0.495141000000	0.738304000000
C	-0.406721000000	1.643887000000	1.318113000000
C	0.090421000000	0.458293000000	-0.174060000000
C	-0.783659000000	1.622090000000	0.033877000000
C	-0.257570000000	0.085919000000	-1.431240000000
N	1.510389000000	0.212606000000	0.066519000000
C	-0.872444000000	2.648469000000	0.968596000000
C	-1.782440000000	1.500412000000	-0.954005000000
H	-0.102932000000	2.790220000000	1.715473000000
C	-1.970917000000	3.501149000000	0.938398000000
C	-2.991804000000	3.315534000000	0.005498000000
H	-2.042241000000	4.306697000000	1.661424000000
C	-2.909801000000	2.309257000000	-0.948645000000
H	-3.856913000000	3.970385000000	0.018281000000
H	-3.693408000000	2.158303000000	-1.681960000000
N	-1.457973000000	0.508605000000	-1.887207000000
H	-2.229944000000	0.134354000000	-2.066490000000
C	1.028758000000	0.209203000000	-2.210563000000
C	-0.184002000000	2.243038000000	-0.987462000000
H	1.367061000000	0.776371000000	-2.552663000000
H	1.018476000000	0.889285000000	-3.063567000000
C	1.867736000000	0.739964000000	-1.059826000000
C	1.348847000000	2.179732000000	-0.826124000000
H	2.943400000000	0.695995000000	-1.227557000000
H	1.810258000000	2.804938000000	-1.599817000000
C	1.725029000000	2.697453000000	0.561707000000
H	1.313190000000	3.699341000000	0.705701000000
H	2.809990000000	2.761212000000	0.678410000000
C	1.114149000000	1.727873000000	1.571377000000
C	-0.748780000000	2.880340000000	-2.234461000000
C	-0.919917000000	2.319922000000	0.177193000000
H	-0.477199000000	3.942770000000	-2.285298000000
H	-1.838810000000	2.801553000000	-2.224798000000
H	-0.377716000000	2.412170000000	-3.150691000000
H	1.251313000000	2.079587000000	2.598482000000
C	1.799090000000	0.340548000000	1.432111000000
C	1.266665000000	0.611407000000	2.502201000000
C	3.321275000000	0.418942000000	1.606652000000
H	1.610210000000	0.265686000000	3.481037000000
H	1.656490000000	1.619917000000	2.337871000000
H	0.177823000000	0.638625000000	2.533600000000
H	3.733982000000	0.587308000000	1.712680000000
H	3.556800000000	0.982987000000	2.513993000000
H	3.833073000000	0.889045000000	0.767982000000
O	-1.160736000000	1.572406000000	2.469112000000
H	-2.080693000000	1.370182000000	2.169010000000
H	-1.987725000000	2.496908000000	0.126698000000
O	-3.540053000000	0.900813000000	1.369716000000
C	-4.062822000000	0.689276000000	0.250616000000
O	-3.691096000000	1.071379000000	-0.879137000000
H	-4.997763000000	0.073274000000	0.277486000000
H	2.338812000000	1.523082000000	-0.155298000000
O	2.853297000000	2.430825000000	-0.266633000000
O	4.506237000000	1.254820000000	-1.248457000000
C	4.009966000000	2.285856000000	-0.853544000000
H	4.523884000000	3.257063000000	-0.958742000000

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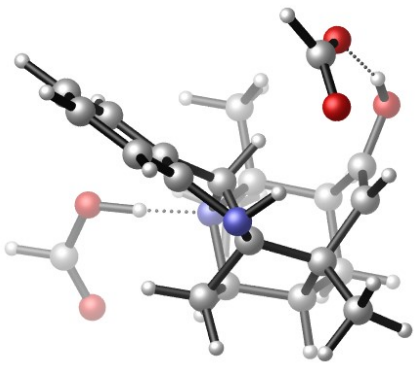
2 (HCO_2^-,HCO_2H)



Zero-point correction= 0.467209 (Hartree/Particle)

Thermal correction to Energy= 0.492988

Thermal correction to Enthalpy= 0.493932

Thermal correction to Gibbs Free Energy= 0.412770

Sum of electronic and zero-point Energies= -1339.826061

Sum of electronic and thermal Energies= -1339.800282

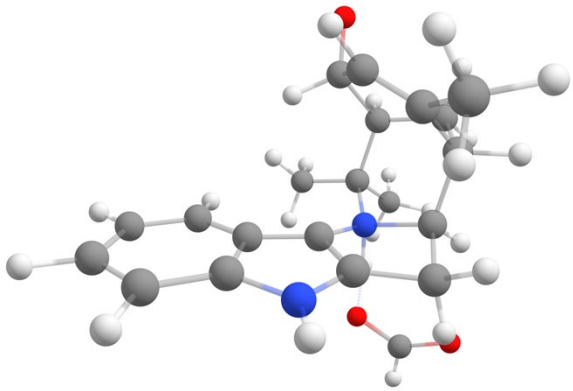
Sum of electronic and thermal Enthalpies= -1339.799338

Sum of electronic and thermal Free Energies= -1339.880500

E(RwB97XD) = -1340.51155505

H	-0.642006000000	-0.388908000000	0.797304000000
C	0.158319000000	-2.591498000000	0.702876000000
C	-0.217929000000	0.305737000000	0.077742000000
C	-1.034320000000	1.571698000000	0.167971000000
C	-0.529678000000	-0.124809000000	-1.359752000000
N	1.271628000000	0.301601000000	0.146825000000
C	-1.022254000000	2.628729000000	1.056652000000
C	-2.050309000000	1.455761000000	-0.792576000000
H	-0.232626000000	2.718444000000	1.793938000000
C	-2.039476000000	3.582744000000	0.984511000000
C	-3.058109000000	3.452713000000	0.046325000000
H	-2.039226000000	4.424362000000	1.669038000000
C	-3.072251000000	2.388127000000	-0.854844000000
H	-3.850256000000	4.193874000000	0.008289000000
H	-3.858930000000	2.285505000000	-1.593624000000
N	-1.891563000000	0.321838000000	-1.640254000000
H	-2.567354000000	-0.392061000000	-1.344647000000
C	0.583984000000	0.656294000000	-2.082618000000
C	-0.112409000000	-1.622933000000	-1.568294000000
H	0.508241000000	1.736832000000	-1.947343000000
H	0.656275000000	0.429037000000	-3.147214000000
C	1.690716000000	0.005478000000	-1.272096000000
C	1.460544000000	-1.476313000000	-1.603062000000
H	2.701245000000	0.372203000000	-1.445328000000
H	1.811418000000	-1.645354000000	-2.626670000000
C	2.186605000000	-2.403666000000	-0.644379000000
H	2.027082000000	-3.449091000000	-0.921773000000
H	3.263514000000	-2.212394000000	-0.680621000000
C	1.606041000000	-2.152222000000	0.746622000000
C	-0.660874000000	-2.174970000000	-2.885287000000
C	-0.570823000000	-2.469434000000	-0.411752000000
H	-0.224190000000	-3.159053000000	-3.084392000000
H	-1.746449000000	-2.290586000000	-2.829048000000
H	-0.433500000000	-1.517019000000	-3.729401000000
H	2.107694000000	-2.766652000000	1.501968000000
C	1.828916000000	-0.657839000000	1.162997000000
C	1.199546000000	-0.361672000000	2.527998000000
C	3.336640000000	-0.378340000000	1.284171000000
H	1.731286000000	-0.929967000000	3.295741000000
H	1.300445000000	0.704104000000	2.755885000000
H	0.148757000000	-0.641798000000	2.594797000000
H	3.501472000000	0.584187000000	1.773060000000
H	3.805278000000	-1.155396000000	1.894459000000
H	3.845626000000	-0.344132000000	0.320940000000
O	-0.328306000000	-3.074319000000	1.866558000000
H	-1.264542000000	-2.735133000000	1.942209000000
H	-1.615998000000	-2.759214000000	-0.396483000000
O	-2.555818000000	-1.714270000000	2.079639000000
C	-3.387238000000	-1.213699000000	1.279262000000
O	-3.527590000000	-1.433096000000	0.061693000000
H	-4.084445000000	-0.469638000000	1.735731000000
H	1.821038000000	1.665314000000	0.443539000000
O	2.173621000000	2.646953000000	0.709332000000
O	3.855304000000	2.404056000000	-0.771585000000
C	3.235811000000	3.029720000000	0.061429000000
H	3.543303000000	4.046237000000	0.365183000000

M (HCO_2H)



Zero-point correction= 0.429061 (Hartree/Particle)

Thermal correction to Energy= 0.452238

Thermal correction to Enthalpy= 0.453183

Thermal correction to Gibbs Free Energy= 0.376914

Sum of electronic and zero-point Energies= -1149.986664

Sum of electronic and thermal Energies= -1149.963487

Sum of electronic and thermal Enthalpies= -1149.962542

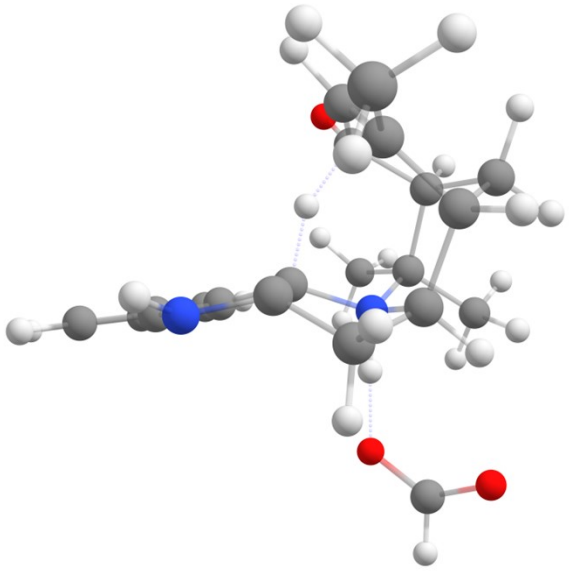
Sum of electronic and thermal Free Energies= -1150.038811

E(RwB97XD) = -1150.60516265

H	-0.064877000	-2.253858000	1.499918000
C	0.863229000	-2.563932000	0.942729000
C	-0.688905000	0.434671000	-0.115735000
C	-2.006544000	0.208259000	0.415308000
C	-0.805328000	0.671037000	-1.441969000
N	0.702213000	0.689792000	0.279091000
C	-2.612238000	-0.039230000	1.656720000
C	-2.864497000	0.280299000	-0.721194000
H	-2.026726000	-0.078153000	2.561281000
C	-3.979320000	-0.230330000	1.732190000
C	-4.792632000	-0.182397000	0.591517000
H	-4.430272000	-0.425097000	2.698931000
C	-4.239673000	0.077046000	-0.647940000
H	-5.860927000	-0.344876000	0.682158000
H	-4.854670000	0.128040000	-1.540500000
N	-2.107309000	0.585667000	-1.833155000
H	-2.445765000	0.628978000	-2.776709000
C	0.469350000	1.045261000	-2.102635000
C	0.876895000	-1.940312000	-1.534512000
H	0.558917000	2.130568000	-2.211570000
H	0.647274000	0.570831000	-3.068817000
C	1.466378000	0.542994000	-1.043306000
C	1.958593000	-0.897671000	-1.287208000
H	2.307695000	1.232142000	-0.981561000
H	2.582597000	-0.820816000	-2.188678000
C	2.814917000	-1.357708000	-0.104941000
H	3.176910000	-2.372662000	-0.283915000
H	3.685099000	-0.705032000	0.023610000
C	1.912531000	-1.390504000	1.123573000
C	0.432170000	-2.196344000	-2.952597000
C	0.411334000	-2.652672000	-0.507992000
H	1.289876000	-2.293835000	-3.631468000
H	-0.147667000	-3.121219000	-3.006705000
H	-0.200445000	-1.393662000	-3.352950000
H	2.484053000	-1.717037000	1.997058000
C	1.417560000	0.031872000	1.460354000
C	0.511810000	0.051169000	2.686525000
C	2.601935000	0.967553000	1.782830000
H	1.132758000	-0.128297000	3.567146000
H	0.028614000	1.026176000	2.801821000
H	-0.228477000	-0.742459000	2.647678000
H	2.240332000	1.915473000	2.186481000
H	3.228686000	0.475212000	2.529524000
H	3.225997000	1.197195000	0.920182000
O	1.371388000	-3.733411000	1.347997000
H	-0.303745000	-3.454184000	-0.686662000
H	0.710633000	1.767071000	0.495714000

O	0.594865000	3.242082000	0.788973000
O	2.000784000	3.687980000	-0.907230000
C	1.279395000	4.005958000	0.044467000
H	1.201735000	5.087967000	0.301445000

TS_{MN} (HCO_2H)



Zero-point correction= 0.425080 (Hartree/Particle)

Thermal correction to Energy= 0.447199

Thermal correction to Enthalpy= 0.448144

Thermal correction to Gibbs Free Energy= 0.375818

Sum of electronic and zero-point Energies= -1149.960312

Sum of electronic and thermal Energies= -1149.938192

Sum of electronic and thermal Enthalpies= -1149.937248

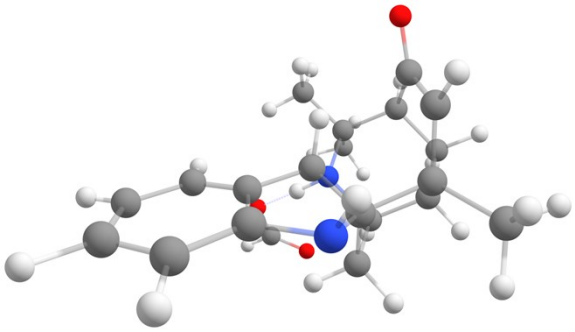
Sum of electronic and thermal Free Energies= -1150.009574

E(RwB97XD) = -1150.57366644

H	-0.187892000	-1.162118000	0.768427000
C	0.705263000	-1.912736000	1.448232000
C	-0.606620000	-0.110524000	-0.129488000
C	-2.031980000	0.126503000	0.199182000
C	-0.581518000	-0.458444000	-1.488469000
N	0.621545000	0.709533000	0.111725000
C	-2.751368000	0.541762000	1.318233000
C	-2.759327000	-0.299274000	-0.938872000
H	-2.245628000	0.885530000	2.207058000
C	-4.139952000	0.508526000	1.303358000
C	-4.834338000	0.036798000	0.186689000
H	-4.688998000	0.838468000	2.178315000
C	-4.150251000	-0.378942000	-0.944013000
H	-5.918965000	0.003776000	0.199742000
H	-4.680060000	-0.730152000	-1.823743000
N	-1.891362000	-0.578681000	-1.972131000
H	-2.141362000	-1.225675000	-2.701461000
C	0.560354000	0.180227000	-2.206001000
C	1.396251000	-2.290667000	-0.898974000
H	0.288306000	1.173474000	-2.588488000
H	0.999813000	-0.391928000	-3.029531000
C	1.538712000	0.301040000	-1.047734000
C	2.270225000	-1.038932000	-0.811306000
H	2.236003000	1.127112000	-1.188306000
H	3.023561000	-1.085538000	-1.607871000
C	2.951060000	-1.041547000	0.558145000
H	3.441573000	-2.004613000	0.719375000
H	3.717310000	-0.263291000	0.621247000
C	1.848273000	-0.832782000	1.589184000
C	1.452424000	-3.099287000	-2.164599000
C	0.834062000	-2.751556000	0.236807000
H	2.474305000	-3.451795000	-2.363428000
H	0.800931000	-3.974507000	-2.097069000
H	1.147957000	-2.515975000	-3.041272000
H	2.227006000	-0.956559000	2.607167000
C	1.279247000	0.591492000	1.472665000
C	0.251706000	0.840374000	2.571056000
C	2.343009000	1.693855000	1.571025000
H	0.791151000	0.962644000	3.513886000

H	-0.301596000	1.762371000	2.372055000
H	-0.415658000	-0.012762000	2.696819000
H	1.859882000	2.666319000	1.684781000
H	2.960936000	1.499573000	2.452338000
H	2.991212000	1.765819000	0.699333000
O	0.205297000	-2.367959000	2.538227000
H	0.270197000	-3.681913000	0.245677000
H	0.393837000	1.761598000	-0.062198000
O	0.125467000	3.247671000	-0.323357000
O	2.096199000	3.412999000	-1.397145000
C	1.028061000	3.862602000	-0.964359000
H	0.809434000	4.941566000	-1.146387000

N (HCO_2H)



Zero-point correction= 0.431687 (Hartree/Particle)

Thermal correction to Energy= 0.453513

Thermal correction to Enthalpy= 0.454457

Thermal correction to Gibbs Free Energy= 0.382692

Sum of electronic and zero-point Energies= -1150.045414

Sum of electronic and thermal Energies= -1150.023589

Sum of electronic and thermal Enthalpies= -1150.022644

Sum of electronic and thermal Free Energies= -1150.094409

E(RwB97XD) = -1150.66347957

H	-0.009731000	-0.819559000	1.238730000
C	2.249484000	-1.356198000	1.418238000
C	-0.427432000	-0.356321000	0.348839000
C	-1.925022000	-0.313278000	0.477052000
C	-0.251853000	-1.274910000	-0.858613000
N	0.388564000	0.847727000	-0.005316000
C	-2.788082000	0.551257000	1.121128000
C	-2.398566000	-1.496543000	-0.110415000
H	-2.423709000	1.489078000	1.523298000
C	-4.140088000	0.210375000	1.201321000
C	-4.601731000	-0.980728000	0.652006000
H	-4.835013000	0.883682000	1.691002000
C	-3.736242000	-1.843836000	-0.021779000
H	-5.654901000	-1.232718000	0.724211000
H	-4.100800000	-2.752381000	-0.488599000
N	-1.382148000	-2.200641000	-0.817358000
H	-1.132706000	-3.075747000	-0.369108000
C	-0.313546000	-0.230742000	-1.984275000
C	1.233324000	-1.801019000	-0.875299000
H	-1.251293000	0.327417000	-2.022281000
H	-0.094452000	-0.641511000	-2.970271000
C	0.850646000	0.567027000	-1.430572000
C	1.960513000	-0.490239000	-1.393415000
H	1.071084000	1.516113000	-1.914245000
H	2.278772000	-0.642982000	-2.430219000
C	3.140344000	-0.076230000	-0.536961000
H	3.915588000	-0.845451000	-0.564336000
H	3.577578000	0.852242000	-0.921507000
C	2.626414000	0.062501000	0.892267000
C	1.382381000	-2.937417000	-1.892985000
C	1.726803000	-2.232028000	0.479728000
H	2.444400000	-3.145336000	-2.051164000
H	0.921220000	-3.856810000	-1.517292000
H	0.922600000	-2.700427000	-2.858904000
H	3.420079000	0.401254000	1.564510000
C	1.519996000	1.148203000	0.975671000

C	0.924089000	1.247551000	2.381306000
C	2.068107000	2.531673000	0.596034000
H	1.674353000	1.688440000	3.041350000
H	0.045145000	1.899686000	2.372508000
H	0.675187000	0.274583000	2.803838000
H	1.315527000	3.299961000	0.782242000
H	2.948023000	2.737417000	1.210441000
H	2.354726000	2.608064000	-0.452296000
O	2.500693000	-1.582502000	2.633624000
H	1.498366000	-3.246533000	0.801194000
H	-0.239451000	1.731363000	-0.039563000
O	-1.127851000	2.998019000	-0.032255000
O	-0.104276000	3.584958000	-1.944727000
C	-0.923369000	3.747852000	-1.035227000
H	-1.571051000	4.655053000	-1.072256000

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