

## SUPPORTING INFORMATION

### Isotope Effects and Mechanism of the Chiral Brønsted Acid Catalyzed Aziridination Reaction

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## 1. Experimental Section

### A. Kinetic isotope effects (KIEs) and transition state (TS) geometry

Kinetic isotope effect measurements are powerful mechanistic probes. Figure S1 is a 2D representation of the vibrational normal modes associated with the reactant and the transition state for a reaction, focusing on as an example the stretching vibration of a C-H bond. Isotopic substitution, in this case by deuterium, affects the zero-point energy (ZPE) of the vibrational normal modes of a molecule. The main origin of KIEs lies in how the ZPE is different at the stage of reactants versus the transition state. When the normal modes are looser at the transition state versus the starting material, as is most common, the ZPE is decreased and lighter isotopes encounter a smaller barrier. As a result, lighter isotopes tend to react faster ( $k_{\text{light}}/k_{\text{heavy}} > 1$ ) and this observation is referred to as a “normal” isotope effect. Sometimes the normal modes are tighter at the transition state versus the starting material; this causes the ZPE to be increased at the transition state and heavier isotopes encounter a lower barrier. The resulting faster rate for the heavier isotope ( $k_{\text{light}}/k_{\text{heavy}} < 1$ ) is an “inverse” isotope effect. Since the KIEs are intimately associated with the normal modes at the transition state, KIEs can be used to experimentally probe the transition state geometry, i.e. the extent of bond formation / bond breaking occurring as the reaction goes over the transition state.

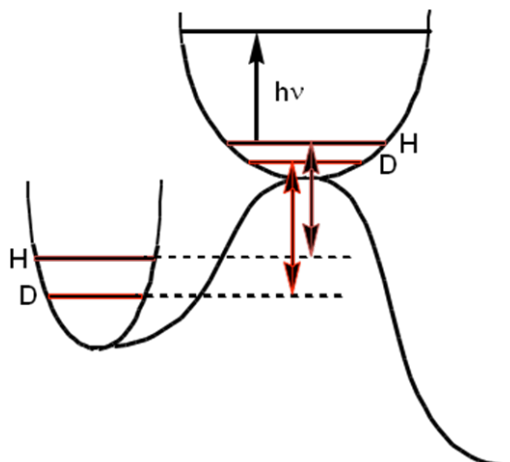


Figure S1. **The origin of a kinetic isotope effect**

### B. The Singleton method for determining KIEs using natural abundance $^{13}\text{C}$ NMR

Each individual carbon and hydrogen in an organic molecule contains at natural abundance approximately 1.1% of  $^{13}\text{C}$  and 0.015% of  $^2\text{H}$ . As a reaction progresses, the starting materials are enriched in the slower reacting isotopomers (isotopically substituted isomers) and the products in the faster reacting ones. If this isotopic enrichment at every position in a molecule can be measured, KIEs can be determined without the use of explicitly labeled substrate. The Singleton method applies this idea to determine  $^{13}\text{C}$  and  $^2\text{H}$  KIEs at natural abundance using carefully acquired NMR as a method to determine these isotopic compositions. There are two main strategies that can be used for the determination of KIEs using this methodology.

- (a) *Intermolecular starting material KIEs* – The original methodology developed in the Singleton group measured KIEs by analysis of starting material recovered from reactions taken to high conversion, typically ~80%. The isotopic composition of this recovered material is determined by NMR at natural abundance and compared to that of unreacted starting material (drawn from the bottle originally used for the reaction). The enrichment (depletion) thus measured can be used to determine the KIEs based on eq 1, where  $F_1$  is the fractional conversion of the lighter isotopomer and  $R/R_0$  is the proportion of minor isotopic component in recovered starting material versus the original material.

$$\frac{\log(1-F_1)}{\log[(1-F_1)(R/R_0)]} \quad (1)$$

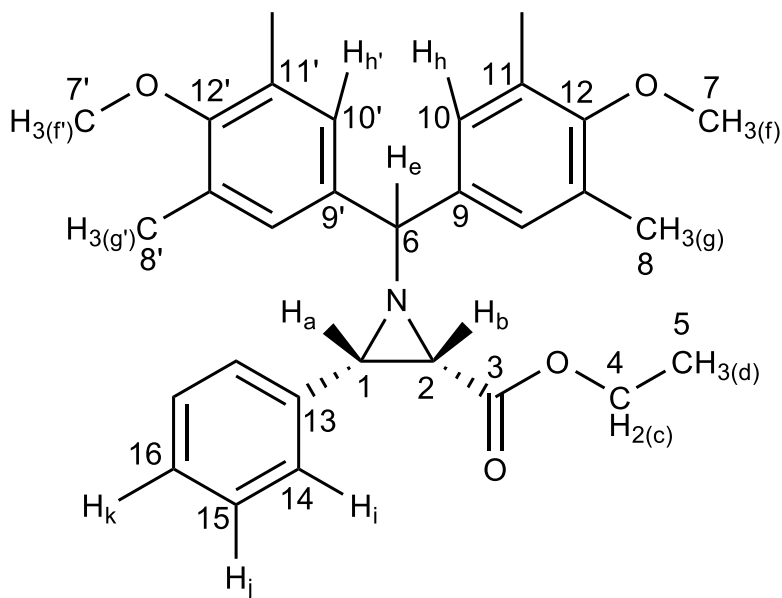
This methodology has some advantages when it can be applied. One advantage is that the precision of the KIEs obtained can exceed the precision of the analysis. Another advantage is that the KIEs are insensitive to further side reactions that the product may undergo. A disadvantage is that the methodology cannot be applied to reactants that must be used in large excess.

- (b) *Intermolecular product KIEs* – An alternative process involves taking reactions to low conversion (typically ~20%) and analyzing the isolated reaction product. The isotopic composition of the product, enriched in the faster reacting isotope, is compared to that of product isolated from a reaction taken to 100% conversion reaction (no isotopic fractionation). Equation 2 is then used to calculate the KIEs. This method is prone to two possible errors.

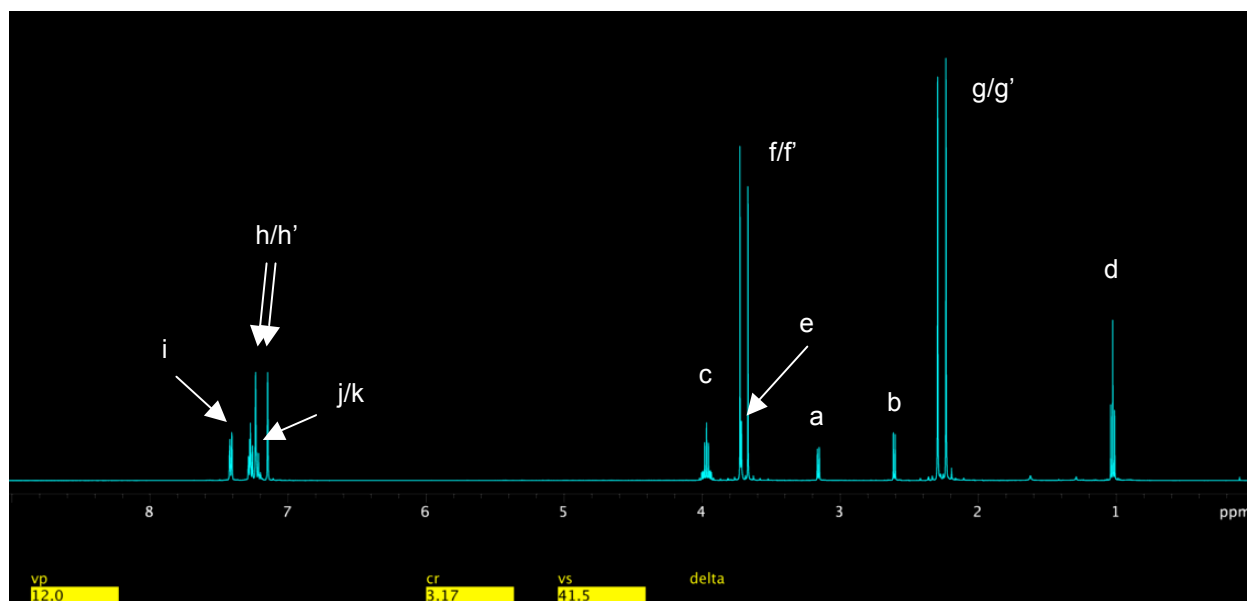
$$\frac{\log(1-F_1)}{\log[1-(F_1R_p/R_o)]} \quad (2)$$

Further conversion of product to form side product will adversely affect the measurement. Also, errors may arise from any inefficiency in the 100% conversion reaction. The subtle modification of this methodology described in this work was originally developed by MJV during his graduate studies in the Singleton group. This modification is time-efficient and accurate, especially for reactions where it is required to determine KIEs for both reactants in a bimolecular reaction. In such cases separate low conversion and 100% conversion reactions are usually performed for each reactant (total 4 reactions for one KIE experiment) in order to ensure accurate determination of fractional conversion, since 1:1 mixtures of starting materials rarely give quantitative yields of product. By using this modified methodology, we eliminate the 100% conversion reactions (thereby getting the same information from 2 reactions instead of 4 reactions) by performing the low conversion reaction for each reactant using limiting amounts (0.2 eq to get to 20% conversion) of the other. Under these conditions, the limiting reagent in both reactions undergo no isotopic fractionation upon going from starting material to product and hence serve as the 100% sample for the complementary reaction.

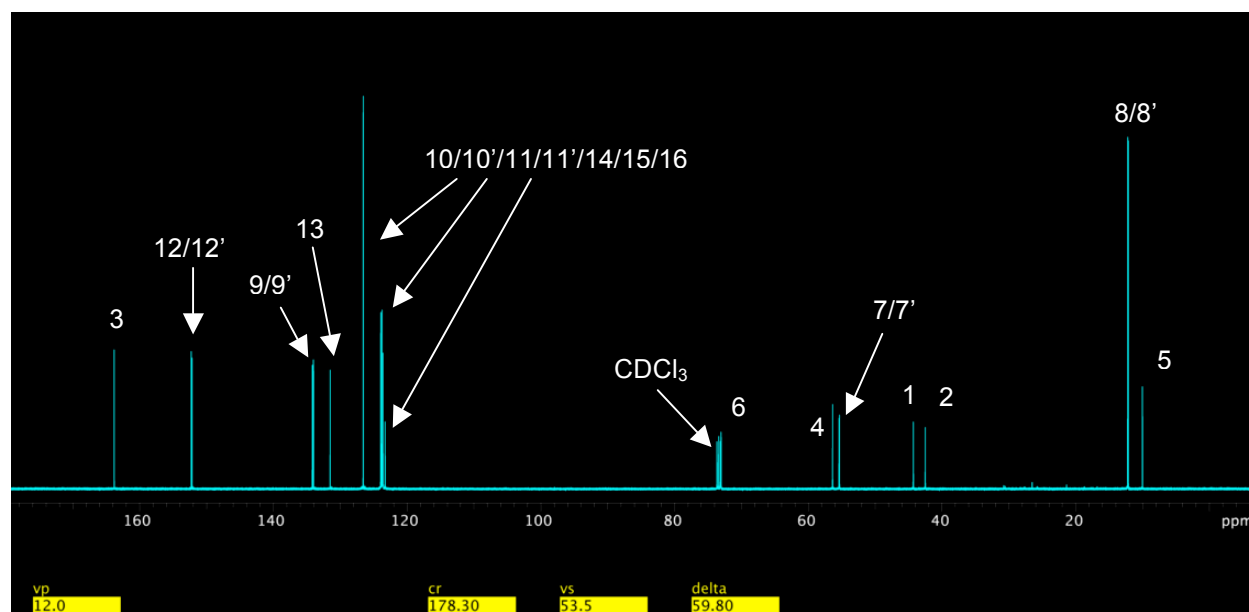
**C. Complete structural assignment of 4a,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra for a representative KIE experiment, and 2D (HMQC and HMBC) NMR spectra**



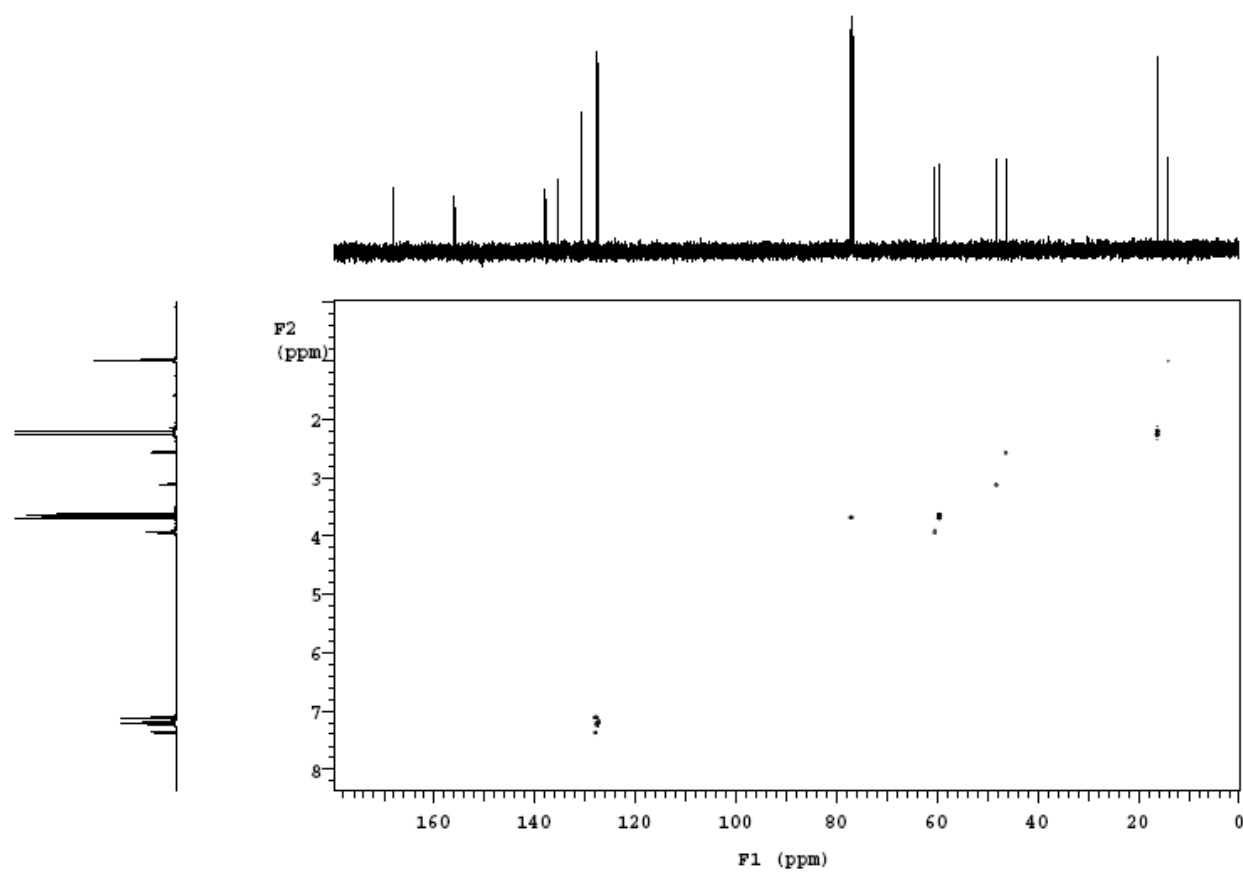
$^1\text{H}$  NMR Spectrum of **4a** from a KIE experiment (500 MHz,  $\text{CDCl}_3$ ):



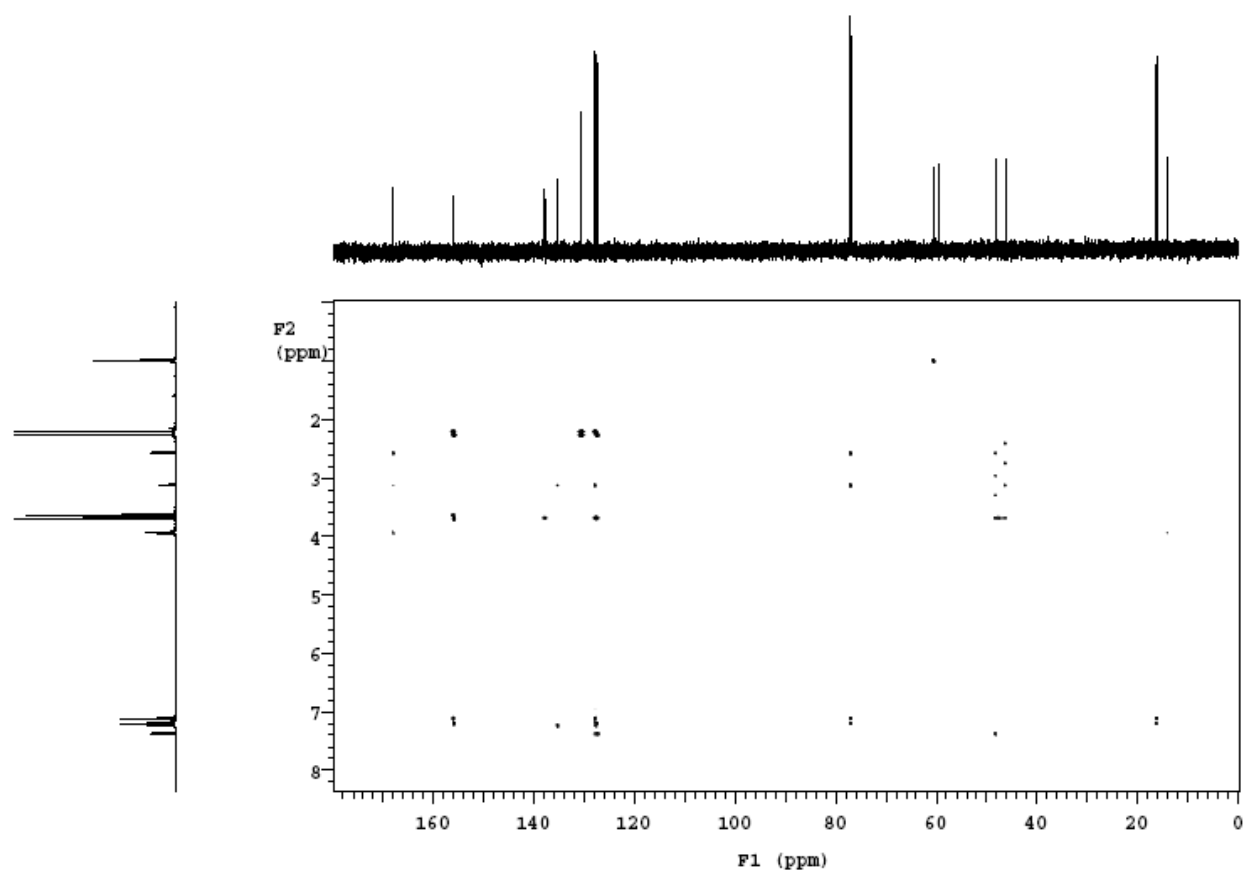
$^{13}\text{C}$  NMR Spectrum of **4a** from a KIE experiment (125 MHz,  $\text{CDCl}_3$ ):



2-D HMQC (Heteronuclear Multiple Quantum Coherence) experiment NMR Spectrum ( $\text{CDCl}_3$ ):



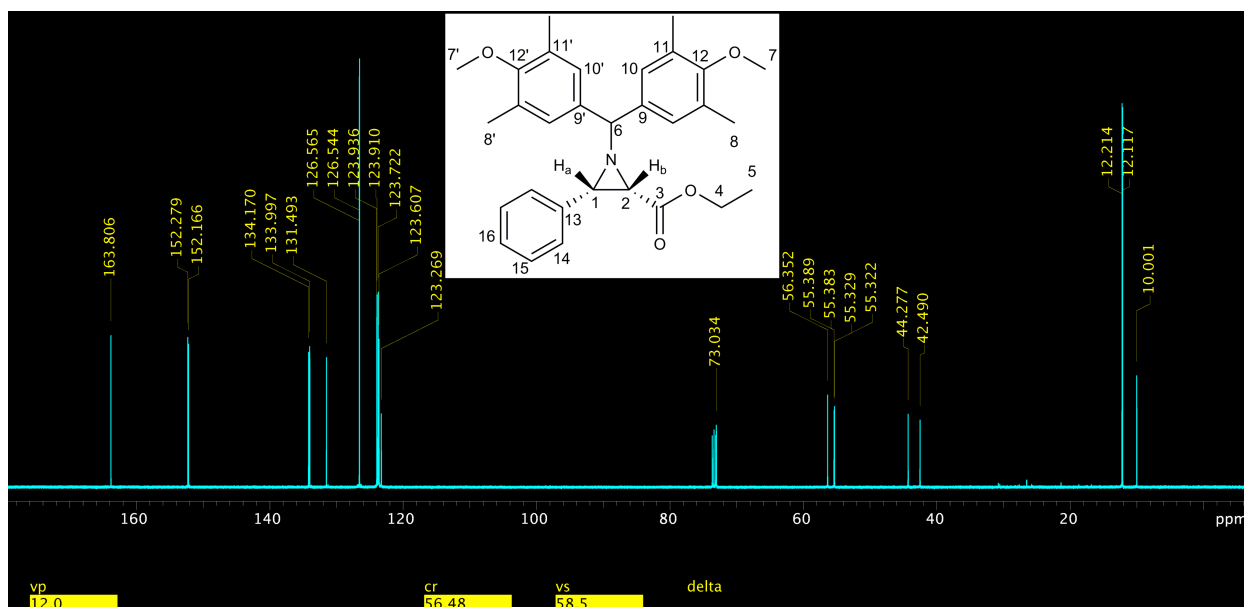
2-D HMBC (Heteronuclear Multiple Bond Correlation) experiment NMR Spectrum (CDCl<sub>3</sub>):





## D. NMR measurements and trivial KIEs

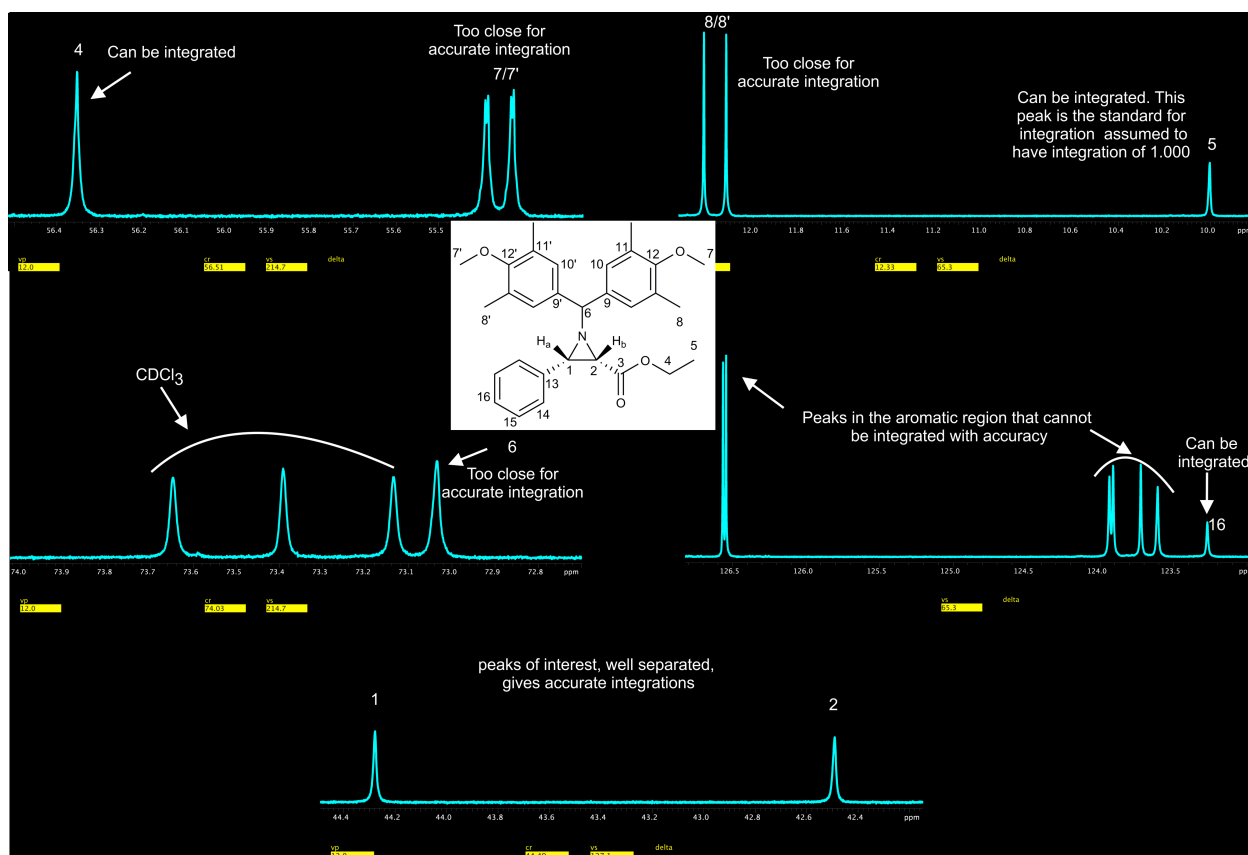
All samples were prepared using a constant 450 mg of **4a** in 5 mm NMR tubes filled with CDCl<sub>3</sub> to a constant height of 5.5 cm. The <sup>13</sup>C spectra were recorded at 125 MHz using inverse gated decoupling, 15 s (5 times T1) delays between calibrated  $\pi/2$  pulses, and a 5.0 s acquisition time. Integrations were determined numerically using a constant integration region for each peak. A zero-order baseline correction was generally applied, but in no case was a first-order (tilt) correction applied. Six spectra each with 512 transients were obtained for each four samples of **4a** (two samples per experiment). The integration of the methyl peak of the ester moiety of **4a** (peak 5, Figure S2) was set to 1.000 since the KIE at this position is expected to be negligible.



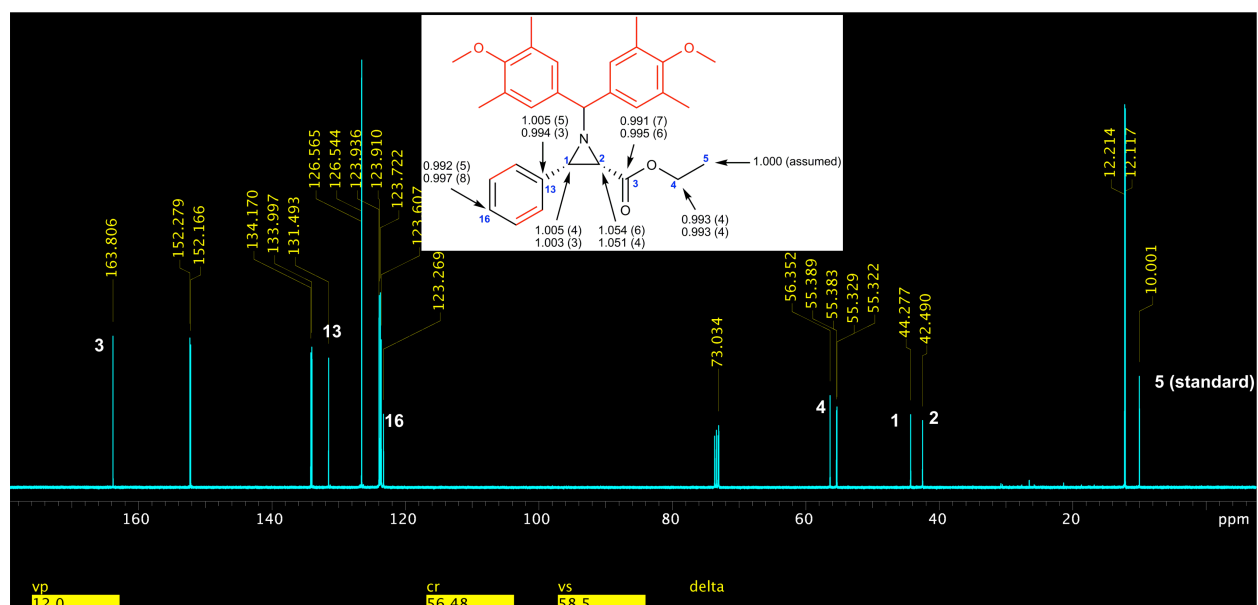
**Figure S2.** Representative NMR spectrum showing accurate chemical shift that illustrates near-overlap of several peaks and the good separation of the peaks of interest. CDCl<sub>3</sub> is at  $\delta$  73.4.

Using the Singleton method, one can measure the KIE for every carbon in a molecule provided the peaks are well separated. We were fortunate that the peaks of interest in **4a**, namely C1, C2, C5 ( $\delta$  44.277, 42.490 and 10.001, Figure S2) were separated from all other peaks by at least 2 ppm. This enables us to use C5 as the standard peak and accurately determine the integrations of C1 and C2 (see Figure S3). This is one of the largest published molecules used for KIE analysis by the Singleton method. The primary goal during acquisition of NMR spectra for KIE measurements was to have the best line shapes and line widths for the peaks of interest including the standard peak.

Due to the diastereotopic nature of the aromatic groups on the MEDAM moiety, there were several pairs of peaks that were too close for accurate reproducible integrations (Figure S3).



**Figure S3.** Peaks that are easily integrated versus ones that are too close for reproducible integrations.



**Figure S4.** Spectrum highlighting the well-separated peaks and the corresponding KIEs from two experiments. The carbon atoms shown in red are the ones that were too close for meaningful integrations. Nevertheless, the spectrum was acquired with a delay time of 5 times the T1 relaxation time of the peak with the largest T1 relaxation time.

## 2. Theoretical Section

### A. Methods and general comments

The ONIOM calculations were setup using GaussView 5.0 (the interface between Gaussian and Windows). Intermediates were located by performing IRC calculations from the relevant transition structures and optimizing the geometry of the resulting structures. A thorough conformational search was also performed for locating the lowest energy starting materials used for the calculation of theoretical KIEs.

**TS<sub>conf</sub>** was located after a careful conformational search performed by fixing the dihedral angle (between the C2-N<sub>2</sub><sup>+</sup> (diazonium) and the C1-N (imine) bond along the C1-C2 bond) at a series of values between -100° and -130° and locating the energy maxima. A transition state search was then performed on this geometry to arrive at the unrestricted **TS<sub>conf</sub>** with one imaginary frequency of ~ -6, which corresponds to bond rotation about the C1-C2 bond. The KIE for this transition state was computed as an equilibrium isotope effect between **TS<sub>conf</sub>** and free starting material, since imaginary frequencies below -50 cannot be used by ISOEFF98 for the prediction of KIEs. This is expected to make little or no difference to the actual value of the KIEs since there is no bond formation/breaking occurring at this transition state.

A very detailed search was performed for locating the lowest energy carbon-carbon bond forming (**TS1** in main text and **TS1a-d** in Supporting Information) and ring-closing (**TS2** in main text and **TS2a – TS2f** in Supporting Information) transition states. Finally, Single-point energies were performed on TS1, TS2, TS3 and TS4 using M062x/6-31+G\*\* method and a PCM model for toluene (reaction solvent) to further support that the trends in the relative energies of the transition structures reported in the paper. The relative energies of the addition and ring-closing transition structure from these single-point energy calculations for the *cis*- and *trans*- aziridination pathway are shown below.

	Relative Gibbs Free Energies (from Figure 9) (kcal/mol)	Relative Potential Energies (kcal/mol) M062x/6-31+G** (toluene)
<b>TS1</b>	0.0	0.0
<b>TS2</b>	4.0	8.2
<b>TS3</b>	0.0	0.0
<b>TS4</b>	0.6	1.4

### 3. References

- Zhang, Y.; Lu, Z.; Desai, A.; Wulff, W. D. *Org. Lett.* **2008**, *10*, 5429-5432.

### 4. Coordinates of calculated structures

#### A. Coordinates of Stationary Points in Figure 2 (Lowest energy structures)

##### catalyst-1a complex

cat-imine-complex-ONIOM-M062x-BB

E(RAM1) = -0.731982597510

E(RM062X) = -969.291063700

E(RAM1) = -1.08399419095

Zero-point correction= 1.174664  
(Hartree/Particle)  
Thermal correction to Energy= 1.246902  
Thermal correction to Enthalpy= 1.247847  
Thermal correction to Gibbs Free Energy= 1.052209  
Sum of electronic and zero-point Energies= -967.764388  
Sum of electronic and thermal Energies= -967.692150  
Sum of electronic and thermal Enthalpies= -967.691206  
Sum of electronic and thermal Free Energies= -967.886843

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	782.443	274.729	411.754

C,0,3.5965674711,2.4256351177,-0.7383548768  
C,0,4.2837656741,1.9756187675,0.3979546934  
C,0,5.5430014475,2.5235931916,0.6895532367  
C,0,6.0998154051,3.4957573005,-0.1386370396  
C,0,5.4107050122,3.9332236166,-1.2692795263  
C,0,4.1601429406,3.3934126061,-1.5678313  
C,0,3.6803280618,0.9949582727,1.307359738  
C,0,2.9478650538,-0.1365228474,0.8306839287  
C,0,2.1941913918,-0.8744791138,1.7479985534  
C,0,2.3383594289,-0.6723310752,3.1626118428  
C,0,3.1670306763,0.3809422019,3.6154687009  
C,0,3.7848676916,1.231305071,2.6657206926  
C,0,3.3399506446,0.5693813279,5.0147255275  
C,0,2.7139568242,-0.2601044121,5.9128648902  
C,0,1.881513305,-1.3101979057,5.4575387701  
C,0,1.6970338631,-1.513057747,4.110633566  
H,0,1.3969195137,-1.9673929783,6.1938282857  
C,0,2.9621937068,-0.5201468737,-0.5830715254  
C,0,1.7635498545,-0.693616731,-1.2741473391  
C,0,1.7342241737,-0.9222407893,-2.6869596597  
C,0,2.9638589133,-1.0005339161,-3.3837214088  
C,0,4.1752062705,-0.9612445115,-2.6496363491  
C,0,4.1866697837,-0.7695472062,-1.2809289481  
C,0,0.5181551683,-1.0769350487,-3.4038690299  
C,0,0.5295211595,-1.2528173713,-4.7660940823  
C,0,1.7568780844,-1.2902195576,-5.4701974159  
C,0,2.947362211,-1.1736927556,-4.7954748873  
H,0,-0.4221876696,-1.0750097188,-2.8293268767  
O,0,0.5511246005,-0.6022364027,-0.6325039438  
B,0,0.2552158254,-1.6749225179,0.3696547659  
O,0,1.3421113144,-1.8716035075,1.3815698377

C,0,5.4640276734,-0.9332727991,-0.5791198235  
C,0,6.6364416134,-0.3594772968,-1.0926436657  
C,0,7.8617312144,-0.5819275814,-0.4675311519  
C,0,7.9328362943,-1.3837083537,0.6712052694  
C,0,6.7720729739,-1.9606724121,1.1856734388  
C,0,5.54371519,-1.7388145785,0.5663661027  
O,0,-0.9861342209,-1.182074457,1.0432332234  
B,0,-1.9786568626,-2.0390414456,1.4159100696  
O,0,-1.9719606007,-3.3497549845,1.0391688466  
B,0,-0.9836919999,-3.7910188789,0.1547529838  
O,0,-1.1788591232,-5.1005199337,-0.2695181606  
C,0,-0.3764201255,-5.8337368263,-1.1175021514  
C,0,-0.9047024319,-7.0935383678,-1.4555413038  
C,0,-0.1658989658,-7.9260833108,-2.2903424401  
C,0,1.0740943485,-7.5178870265,-2.7844778502  
C,0,1.5841563011,-6.2662106127,-2.4420358207  
C,0,0.8656125401,-5.4124215963,-1.6063206718  
O,0,-2.9852213333,-1.4518932404,2.1922428273  
C,0,-4.1502642529,-2.0322288607,2.6476860109  
C,0,-4.5704248924,-3.3315364125,2.3387829468  
C,0,-5.7825510795,-3.7878508168,2.8545770527  
C,0,-6.5637751811,-2.9653244512,3.6655811601  
C,0,-6.1330516076,-1.6732122225,3.9691103661  
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O,0,0.0098549009,-2.9738587448,-0.2276569115  
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C,0,-2.2859080073,2.9314581453,3.9856365018  
C,0,-2.2082015103,2.7411864777,5.3594961102  
C,0,-1.6004784628,1.5897873528,5.8597616058  
C,0,-1.0761980532,0.6294960604,4.9915672006  
C,0,-1.1613193285,0.8048534476,3.6172398902  
C,0,-1.6615274699,1.7687022346,-0.7419949663  
C,0,-1.4951862998,3.2348447908,-0.9578404273  
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C,0,-1.0970263923,5.9664690623,-1.3783862581  
C,0,0.0118948621,5.1382285793,-1.118310823  
C,0,-0.2019265624,3.7729348716,-0.9170767309  
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H,0,3.6204958626,3.7223014977,-2.4682063192  
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H,0,4.3494556003,2.1011313726,3.0348984489  
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H,0,-6.72364482,-0.1467117637,-0.1380813804  
H,0,-7.6413716559,-0.335161544,-4.6979109334  
H,0,-6.0724078034,0.5244824349,-5.133679769  
H,0,-7.2183934016,1.2754679719,-3.9138173007  
H,0,-2.6817808335,-1.0602413,-4.7023306176  
H,0,-3.7265160527,0.2217854792,-5.4477459208  
H,0,-4.4780040274,-1.30948852,-4.8222762172  
H,0,-1.7526276249,0.5526871002,-3.1185786328  
H,0,-0.4108151763,-1.3781318317,-5.3222802988  
H,0,1.0650130697,-2.3331771941,3.7320061595

## Ethyldiazoacetate 2

ethyldiazoacetate-M06-BB  
E(RM062X) = -415.788118424

Zero-point correction= 0.105956  
(Hartree/Particle)  
Thermal correction to Energy= 0.114528  
Thermal correction to Enthalpy= 0.115473  
Thermal correction to Gibbs Free Energy= 0.071736  
Sum of electronic and zero-point Energies= -415.682162  
Sum of electronic and thermal Energies= -415.673590  
Sum of electronic and thermal Enthalpies= -415.672646  
Sum of electronic and thermal Free Energies= -415.716383

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.868	28.600	92.052

C,0,-1.6288194483,-1.4132412007,0.  
O,0,-0.2394915023,-1.0449329006,0.  
C,0,0.0040450833,0.2773044876,0.  
C,0,1.4364865414,0.5312134596,0.  
N,0,1.8009014801,1.7887270843,0.  
N,0,2.087666021,2.8773062038,0.  
O,0,-0.8581915604,1.1311056544,0.  
C,0,-1.6905435388,-2.9246498456,0.  
H,0,-2.1054366772,-0.980174042,0.8844388213  
H,0,-2.1054366772,-0.980174042,-0.8844388213  
H,0,2.2099681753,-0.2196289796,0.  
H,0,-2.7335775479,-3.2516650893,0.  
H,0,-1.1993626741,-3.3314343908,-0.887292435  
H,0,-1.1993626741,-3.3314343908,0.887292435

## TS 1

E(RM062X) = -1385.07842391

E(RAM1) = -1.09790935653

Zero-point correction= 1.282225  
(Hartree/Particle)  
Thermal correction to Energy= 1.363503  
Thermal correction to Enthalpy= 1.364447  
Thermal correction to Gibbs Free Energy= 1.148463  
Sum of electronic and zero-point Energies= -1383.441898  
Sum of electronic and thermal Energies= -1383.360620  
Sum of electronic and thermal Enthalpies= -1383.359675  
Sum of electronic and thermal Free Energies= -1383.575660

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	855.611	306.574	454.577

C,0,5.8810084179,-1.2659556592,-2.2797804306  
C,0,6.0982305608,-1.5466174022,-0.9229712494  
C,0,7.0371147736,-2.5271160138,-0.5701267366  
C,0,7.7385675389,-3.217482444,-1.556508322  
C,0,7.5171588907,-2.933035306,-2.903626932  
C,0,6.5878928304,-1.9568315666,-3.2620170613  
C,0,5.4180098531,-0.7638253977,0.114381625  
C,0,4.019602527,-0.4684284377,0.0492859227  
C,0,3.5101270902,0.5154476218,0.8968231505  
C,0,4.3011437823,1.0755763142,1.9524913193  
C,0,5.6471294123,0.6581317804,2.0855802235  
C,0,6.1915622552,-0.2338042686,1.1291824421  
C,0,6.4305057454,1.180434236,3.1519072969  
C,0,5.8946228853,2.087014654,4.0332290917  
C,0,4.5546490034,2.5183962509,3.8870729281  
C,0,3.7766181855,2.0247780038,2.8683911311  
C,0,3.1472930671,-1.1383445913,-0.9185096374  
C,0,2.3923275685,-0.3703216223,-1.8084706388  
C,0,1.7060020041,-0.9701720304,-2.914928243  
C,0,1.708518234,-2.3811468688,-3.0260252082  
C,0,2.3374551642,-3.1533998327,-2.0180490518  
C,0,3.0313200485,-2.5612056949,-0.9787425652  
C,0,1.0458550902,-0.1931692507,-3.9035015026  
C,0,0.4204669603,-0.8035094568,-0.4570611003  
C,0,0.4258263869,-2.2138708084,-5.0798255507  
C,0,1.0525064887,-2.9868369703,-4.1330331154  
O,0,2.318807332,0.9894653217,-1.6954303052  
B,0,1.7049284914,1.5668664045,-0.4570611003  
O,0,2.2096653532,0.9458415981,0.816836395  
C,0,3.5533132762,-3.4341369667,0.0781355163  
C,0,3.3880692777,-3.1013844795,1.4303366396

C,0,3.8184630915,-3.971605869,2.4296245548  
 C,0,4.4198247471,-5.1841342004,2.0940352284  
 C,0,4.5943246539,-5.5209510517,0.7521245055  
 C,0,4.16388193,-4.6543895963,-0.2504464926  
 O,0,0.2356471812,1.3081198909,-0.4340860937  
 B,0,-0.5554670397,2.1408079548,-1.1391621712  
 O,0,-0.1361038507,3.3668041381,-1.5839806097  
 B,0,1.1084872702,3.8215810682,-1.1414502999  
 O,0,1.3131863298,5.1790191397,-1.3913712812  
 C,0,2.4636059503,5.9015755891,-1.1594670814  
 C,0,3.6762204238,5.3554827586,-0.7216137836  
 C,0,4.7693747082,6.201522143,-0.5416546446  
 C,0,4.6572972818,7.5685161436,-0.7933375741  
 C,0,3.4438548098,8.1005784134,-1.2319674892  
 C,0,2.3366651956,7.2789225861,-1.4192875921  
 O,0,-1.8875249206,1.6995712797,-1.3578995988  
 C,0,-2.7770890147,2.3375584115,-2.2020723128  
 C,0,-3.5876799981,1.4978817822,-2.9833158296  
 C,0,-4.5836330285,2.0695662919,-3.7715468833  
 C,0,-4.7592433493,3.4536070821,-3.7986923156  
 C,0,-3.9320096704,4.2784784699,-3.0360820166  
 C,0,-2.9343428226,3.7293729539,-2.2329452894  
 O,0,1.9574609199,2.9991344285,-0.5050354937  
 N,0,-0.7657972502,-0.8550914638,0.7791025163  
 N,0,-1.3182682685,-1.2269643654,-0.1066104936  
 C,0,-0.3164115934,-0.2480979415,1.9154944231  
 C,0,-1.8070541292,1.0804998645,2.2288889432  
 C,0,-1.1442250781,2.4093517336,2.0677753225  
 C,0,0.0517121337,2.67899206,2.7410366297  
 C,0,0.6499226491,3.9269768934,2.6268750175  
 C,0,0.0616672841,4.9185076209,1.8418344495  
 C,0,-1.1442599695,4.6652282634,1.1961925679  
 C,0,-1.7563901687,3.4197954611,1.3224374578  
 C,0,-0.3697838596,-1.1823928697,3.0746590224  
 O,0,-1.0033765372,-2.2128589004,3.1159406583  
 O,0,0.3082426541,-0.6543470623,4.0911376442  
 C,0,0.2978265146,-1.4104214244,5.323135684  
 N,0,-2.8522786472,0.7594283446,1.4507044914  
 C,0,-3.7999107689,-0.3283505712,1.8725122976  
 C,0,-4.5994176194,0.049330014,3.0787560578  
 C,0,-4.7643869974,-0.9029396664,4.0914944847  
 C,0,-5.5270614127,-0.6172215601,5.2264172278  
 C,0,-6.1217641333,0.6531479916,5.3405121514  
 C,0,-5.9585389035,1.6248915764,4.3374946678  
 C,0,-5.1952562466,1.3061887914,3.2099009916  
 C,0,-5.6814818225,-1.629736714,6.295718575  
 O,0,-6.788041445,0.9701039709,6.519475557  
 C,0,-8.2099969043,0.8972296021,6.4080715896  
 C,0,-6.5742916285,2.9665447871,4.4570624056  
 C,0,-4.6941406297,-0.7322065735,0.7493101878  
 C,0,-5.5112363083,0.1986348087,0.1028561333  
 C,0,-6.3657839692,-0.1929059071,-0.9321215137  
 C,0,-6.3873545537,-1.5460349488,-1.3147814882  
 C,0,-5.5774277279,-2.4987789299,-0.6690547235  
 C,0,-4.7336839061,-2.0760708158,0.3613163189  
 C,0,-7.2216147222,0.8128283135,-1.6020293542  
 O,0,-7.2925950128,-1.9841506562,-2.2755532105  
 C,0,-6.8538466494,-1.7555240982,-3.6155559567  
 C,0,-5.626012396,-3.92813399,-1.0523913392  
 H,0,0.6120506446,0.2984115905,1.7122384173  
 H,0,-0.0853593603,-0.2045740923,-5.7349053883  
 H,0,2.7335183255,2.3512122046,2.7257755287  
 H,0,-3.4265227738,0.4113186604,-2.9658749373  
 H,0,-5.2256778524,1.4213319227,-4.3868275164  
 H,0,-5.5421956902,3.8951719815,-4.4317096687  
 H,0,-4.0591034553,5.370655792,-3.0735007613  
 H,0,-2.2484645074,4.3695703057,-1.6550882174  
 H,0,1.3774187421,7.6809378871,-1.7714869534  
 H,0,3.3581129181,9.1782049213,-1.4347901371  
 H,0,5.5250081371,8.2274364463,-0.6498512809

H,0,5.726968523,5.7808299282,-0.2002338619  
 H,0,3.758937149,4.2731207411,-0.5274066708  
 H,0,6.4997794301,2.4926235634,4.8570201823  
 H,0,7.4733125262,0.8444845525,3.2507619528  
 H,0,7.2640452015,-0.4757061517,1.1887354707  
 H,0,7.2129744364,-2.7554885384,0.4916972208  
 H,0,8.469426137,-3.9871736577,-1.2696174924  
 H,0,8.0740709469,-3.4759550271,-3.6804683827  
 H,0,6.410074854,-1.7284237209,-4.3230710485  
 H,0,5.1433439619,-0.4973936953,-2.5623564478  
 H,0,4.3150459155,-4.9200562215,-1.3078294469  
 H,0,5.0757118609,-6.472128965,0.4820184289  
 H,0,4.7589526782,-5.869507342,2.8837097408  
 H,0,3.6878070547,-3.696766965,3.4861657306  
 H,0,2.9316715951,-2.1355944948,1.6973562032  
 H,0,2.2516161876,-4.2495851364,-2.0716862522  
 H,0,1.065852877,-4.0833520293,-4.2167140776  
 H,0,-0.0754492083,-2.6807922245,-5.9402713404  
 H,0,-3.1819059894,-1.2042248484,-2.1429892237  
 H,0,-2.8569540098,1.0703053262,0.4784621796  
 H,0,-1.9332687474,0.7624447545,3.2671232374  
 H,0,0.5285569939,1.9024339436,3.3352327195  
 H,0,1.5882151178,4.124444851,3.1355030586  
 H,0,0.5459253975,5.8835174611,1.7293328997  
 H,0,-1.6050841105,5.4300714926,0.5799630237  
 H,0,-2.7079725971,3.2412181983,0.8321856256  
 H,0,-5.4961385159,1.2553562485,0.4129528369  
 H,0,-6.628163991,1.3552373195,-2.3843491201  
 H,0,-7.5998484558,1.5639282272,-0.865639301  
 H,0,-8.0984006325,0.3231297304,-2.0944757222  
 H,0,-7.7135330738,-2.1065126665,-4.2389788742  
 H,0,-5.9361265771,-2.3553630081,-3.8288762806  
 H,0,-6.6556441615,-0.6685565251,-3.7840663706  
 H,0,-4.6283788065,-4.413465263,-0.9180097898  
 H,0,-5.9418700721,-4.0397376755,-2.1198412069  
 H,0,-6.3713427352,-4.4658416555,-0.4130618558  
 H,0,-4.1016651426,-2.820063085,0.8717033216  
 H,0,-4.2958751309,-1.8959111055,3.9975593138  
 H,0,-6.6492292862,-1.4844516665,6.8380581471  
 H,0,-4.8506633432,-1.5260269396,7.038786144  
 H,0,-5.6541598136,-2.6647231625,5.8752616362  
 H,0,-8.5707251712,1.2065032606,7.4206317101  
 H,0,-8.5276171685,-0.1476156889,6.1742239908  
 H,0,-8.5770957072,1.6007558503,5.6217503948  
 H,0,-6.7558290462,3.2235364548,5.5307394821  
 H,0,-7.5548333422,2.9880347535,3.9172784408  
 H,0,-5.9114399,3.7483226741,4.0107368381  
 H,0,-5.0690097151,2.0667574465,2.4234655279  
 H,0,1.0610239297,0.9037933159,-3.7959497898  
 H,0,4.1503290435,3.2559911543,4.5946790673  
 C,0,1.1289076896,-0.6384707736,6.3222053333  
 H,0,-0.740883619,-1.529107968,5.6451317032  
 H,0,0.7079664369,-2.4027676982,5.1170864791  
 H,0,1.1545677346,-1.178828952,7.2717109228  
 H,0,2.1531429932,-0.5196737226,5.9613247878  
 H,0,0.7024647112,0.3520199349,6.4982960925

### Gauche 3a

E(RM062X) = -1385.08307588

E(RAM1) = -1.09980699019

Zero-point correction=	1.284209
(Hartree/Particle)	
Thermal correction to Energy=	1.365603
Thermal correction to Enthalpy=	1.366547
Thermal correction to Gibbs Free Energy=	1.150146
Sum of electronic and zero-point Energies=	-1383.444832

Sum of electronic and thermal Energies= -1383.363437  
 Sum of electronic and thermal Enthalpies= -1383.362493  
 Sum of electronic and thermal Free Energies= -1383.578895

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.929	307.310	455.455

C,0,-6.4855151673,-1.5609868348,1.173463165  
 C,0,-6.2817338201,-1.8610972771,-0.1813241561  
 C,0,-7.0438061498,-2.8762223881,-0.7780317967  
 C,0,-7.9848912358,-3.5816646819,-0.0307783585  
 C,0,-8.1815178638,-3.2780395866,1.3160127481  
 C,0,-7.4304658363,-2.2671488256,1.9151754972  
 C,0,-5.3496213188,-1.0628253966,-0.9847063941  
 C,0,-4.0414718228,-0.7208414882,-0.5174869175  
 C,0,-3.325415593,0.2718032237,-1.1942175348  
 C,0,-3.810265676,0.8282572347,-2.425132486  
 C,0,-5.0395065732,0.3575227878,-2.9466396728  
 C,0,-5.8053446049,-0.5628796443,-2.1892642526  
 C,0,-5.50062979,0.86155426,-4.1943549737  
 C,0,-4.7778277734,1.8112142367,-4.8735151674  
 C,0,-3.5691672505,2.3101458585,-4.3320537743  
 C,0,-3.0985268827,1.8325718352,-3.1331008405  
 C,0,-3.4754440488,-1.3448738138,0.6810004174  
 C,0,-3.0367215336,-0.534478563,1.7311735612  
 C,0,-2.6883755534,-1.0888806496,3.0063654601  
 C,0,-2.6884056758,-2.4965510883,3.153547502  
 C,0,-2.9751826151,-3.3094433116,2.0287068859  
 C,0,-3.3476511037,-2.7618769832,0.8147703226  
 C,0,-2.3654361783,-0.2702107489,4.1210805587  
 C,0,-2.0608266987,-0.8376952501,5.3349120507  
 C,0,-2.0647571916,-2.2448488355,5.4856513274  
 C,0,-2.3692985275,-3.0574357308,4.4208674538  
 O,0,-2.9679813558,0.8256523083,1.6071832276  
 B,0,-2.0191807213,1.3916359484,0.6038900752  
 O,0,-2.111731386,0.7136302544,-0.7503315  
 C,0,-3.5130103271,-3.6727111772,-0.3229300134  
 C,0,-2.9660671736,-3.3613400667,-1.5759126907  
 C,0,-3.0561065052,-4.2661420828,-2.6314240154  
 C,0,-3.6962416926,-5.4919464097,-2.4526904204  
 C,0,-4.2507518603,-5.8073748943,-1.2125722712  
 C,0,-4.1596481093,-4.906728768,-0.1532786452  
 O,0,-0.6085267426,1.1493104523,1.0134451324  
 B,0,0.0723000279,2.0809621999,1.7161292484  
 O,0,-0.37793397,3.3647768394,1.8440886459  
 B,0,-1.5307528595,3.7315623259,1.1455953204  
 O,0,-1.7756804412,5.1032667025,1.1750104144  
 C,0,-2.8674728996,5.765586246,0.6554692769  
 C,0,-3.99937815,5.1423249487,0.1168993133  
 C,0,-5.0431625012,5.9360117704,-0.3565950594  
 C,0,-4.961136129,7.3265911829,-0.2945380135  
 C,0,-3.8277912843,7.9359866592,0.2461718286  
 C,0,-2.7709489617,7.1679197481,0.7248709842  
 O,0,1.2909668083,1.6325809643,2.2819787294  
 C,0,2.0605906827,3.2120172486,3.2039846172  
 C,0,3.3389311921,1.7665392123,3.4179217618  
 C,0,4.1646995815,2.3463739982,4.3774136778  
 C,0,3.7373704826,3.4554677527,5.1071964979  
 C,0,2.470926796,3.9933474218,4.8781205457  
 C,0,1.6224962492,3.4283798741,3.9280408176  
 O,0,-2.2848758215,2.813869005,0.5177924426  
 N,0,0.6811147666,-0.9369696463,0.4217468988  
 N,0,0.7823983982,-1.3745285926,1.4226704084  
 C,0,0.6987571556,-0.4061508308,-0.9125926009  
 C,0,1.989434856,0.5788085145,-1.0662521412  
 C,0,1.5601839951,2.0405909578,-1.055846233  
 C,0,0.4126444212,2.4475232315,-1.7393358057  
 C,0,0.0300288782,3.7853699672,-1.7458669464  
 C,0,0.8018860326,4.7386432279,-1.0835901735

C,0,1.9679217546,4.3448764848,-0.4345513411  
 C,0,2.3491407756,3.0043015937,-0.4230988547  
 C,0,0.7257544073,-1.6174069725,-1.8426311612  
 O,0,0.8970487925,-2.7574490205,-1.4942664781  
 O,0,0.5316415666,-1.1842684099,-3.0753109727  
 C,0,0.4964236797,-2.2008133011,-4.110728161  
 N,0,3.0440884609,0.3066783148,-0.1538331406  
 C,0,3.7675877344,-0.9947243771,-0.2984882596  
 C,0,4.5330565446,-1.0886260866,-1.5828794164  
 C,0,4.5569523658,-2.3149612591,-2.2579283275  
 C,0,5.2796719267,-2.4678192425,-3.4431741236  
 C,0,5.9798067218,-1.3601886056,-3.9562954838  
 C,0,5.9628809479,-0.1200494,-3.2946818693  
 C,0,5.2366948022,-0.0006055375,-2.1049087496  
 C,0,5.2835900248,-3.7684173656,-4.1509984669  
 O,0,6.6054102425,-1.485696219,-5.1926752897  
 C,0,8.0180349146,-1.6717970549,-5.0996769919  
 C,0,6.6929648835,1.0505405291,-3.8334559755  
 C,0,4.6878822399,-1.2198949093,0.8588071401  
 C,0,5.6021367753,-0.2391725269,1.2525750717  
 C,0,6.4776776622,-0.4615142069,2.3200089225  
 C,0,6.4168570833,-1.6912182688,2.9990734225  
 C,0,5.5069565912,-2.6926475515,2.6118618616  
 C,0,4.6486351208,-2.4421846282,1.538242291  
 C,0,7.4495035633,0.5866370662,2.7078843698  
 O,0,7.3333085649,-1.979784965,4.0050309817  
 C,0,6.9862131159,-1.4120720107,5.2687681776  
 C,0,5.4699871428,-3.9987616483,3.3081842982  
 H,0,-0.2661346596,0.1173632324,-1.0134267843  
 H,0,-1.8158361681,-0.2069501065,6.2016743868  
 H,0,-2.1742334584,2.2269769254,-2.6812394817  
 H,0,3.6762675173,0.8955581096,2.8386645669  
 H,0,5.1638111797,1.9216348272,4.5573374545  
 H,0,4.3985178989,3.9056210921,5.8610525338  
 H,0,2.1338304033,4.8707694773,5.4503243098  
 H,0,0.625114131,3.8573025974,3.7379400515  
 H,0,-1.8745556743,7.6317883767,1.1576299926  
 H,0,-3.7655596549,9.0329617973,0.26962318533  
 H,0,-5.7892942895,7.9439762622,-0.6966819862  
 H,0,-5.9371724904,5.4551208884,-0.7808418541  
 H,0,-4.058588999,4.042235577,0.07100592  
 H,0,-5.1331990955,2.2025804716,-5.8379340736  
 H,0,-6.4498582954,0.4782794606,-4.5970936191  
 H,0,-6.8017993297,-0.8468840267,-2.5621250403  
 H,0,-6.8907987242,-3.1192393596,-1.8401238928  
 H,0,-8.5746494925,-4.3781884196,-0.5069003068  
 H,0,-8.9272624351,-3.8327480565,1.9030806365  
 H,0,-7.5828252908,-2.0228885208,2.9766894217  
 H,0,-5.8896549608,-0.764075143,1.6471761036  
 H,0,-4.6091957959,-5.1566338305,0.8199110885  
 H,0,-4.7644204562,-6.7691733927,-1.0686339535  
 H,0,-3.7673235608,-6.2048306734,-3.286464226  
 H,0,-2.6238267954,-4.0082733506,-3.6091182431  
 H,0,-2.4779923705,-2.3859685356,-1.7254364819  
 H,0,-2.8836268825,-4.4011885237,2.1378738321  
 H,0,-2.3806306543,-4.1518216677,4.5298718599  
 H,0,-1.8240510759,-2.6770804329,6.4681123331  
 H,0,3.045387478,-1.8383244065,-0.3014272112  
 H,0,2.828569769,0.5632781747,0.8084136305  
 H,0,2.3408708611,0.3263347996,-2.0777605314  
 H,0,-0.2142696657,1.7232434356,-2.2522535172  
 H,0,-0.8862674959,4.0766095665,-2.2500978937  
 H,0,0.4872085878,5.7769357033,-1.0634018881  
 H,0,2.5779326369,5.0787411885,0.0827854662  
 H,0,3.2589669918,2.7041288013,0.0844423969  
 H,0,5.6472765481,0.718452947,0.7091170266  
 H,0,6.9571145099,1.339372807,3.3751482285  
 H,0,7.8358319561,1.1202543424,1.8046154611  
 H,0,8.3161338594,0.1394927503,3.2560734906  
 H,0,7.8442754392,-1.6912516078,5.9295534705

H,0,6.0332676279,-1.8576372114,5.6440244548  
H,0,6.890082488,-0.3017880851,5.1870301901  
H,0,4.4408363195,-4.4337153739,3.292389797  
H,0,5.7998484176,-3.8875030219,4.3714741251  
H,0,6.166304195,-4.7157617907,2.8037396166  
H,0,3.9441151119,-3.2286397513,1.2252561198  
H,0,4.0069754208,-3.1791265093,-1.851998893  
H,0,6.2176658115,-3.8852546291,-4.7555291625  
H,0,4.4110024674,-3.823156219,-4.8499408906  
H,0,5.2119930077,-4.617877559,-3.4283694551  
H,0,8.3496059886,-1.7225174154,-6.1666489662  
H,0,8.2495495945,-2.6247891848,-4.5653107908  
H,0,8.4926353582,-0.8069987307,-4.575324807  
H,0,6.8374161391,0.9520572128,-4.9384405855  
H,0,7.6998158083,1.1299524551,-3.3505827342  
H,0,6.1314029398,1.9955636607,-3.6298642822  
H,0,5.2242467886,0.9691934591,-1.5820427141  
H,0,-2.3781218891,0.8230714519,3.9815863413  
H,0,-3.0200549081,3.0897015863,-4.879313028  
C,0,0.2714924644,-1.4865941141,-5.4225549917  
H,0,1.4447328987,-2.744398857,-4.0840545191  
H,0,-0.3119171868,-2.8960876031,-3.8658751346  
H,0,0.232405834,-2.219722654,-6.2318653323  
H,0,-0.6714089987,-0.9356696181,-5.4060759356  
H,0,1.085224513,-0.7872050267,-5.6276110466

### TS<sub>conf</sub>

E(RM062X) = -1385.08063867

E(RAM1) = -1.11442946535

Zero-point correction= 1.284438  
(Hartree/Particle)  
Thermal correction to Energy= 1.365075  
Thermal correction to Enthalpy= 1.366019  
Thermal correction to Gibbs Free Energy= 1.152010  
Sum of electronic and zero-point Energies= -1383.442529  
Sum of electronic and thermal Energies= -1383.361892  
Sum of electronic and thermal Enthalpies= -1383.360948  
Sum of electronic and thermal Free Energies= -1383.574957

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	856.597	305.156	450.419

C,0,-5.9784719904,-0.8522724152,1.1744461245  
C,0,-5.6654201532,-1.6811243915,0.0870925871  
C,0,-6.4655785348,-2.8046213817,-0.1675879504  
C,0,-7.5520607903,-3.0961944508,0.6546639477  
C,0,-7.8566749352,-2.2678700626,1.7343929937  
C,0,-7.0680978891,-1.1467434622,1.9915835564  
C,0,-4.5723910319,-1.3247687857,-0.8235377183  
C,0,-3.302762444,-0.8707103972,-0.3460614858  
C,0,-2.4339602615,-0.2601566903,-1.2511020417  
C,0,-2.7058112999,-0.2421216376,-2.6561120375  
C,0,-3.9009777865,-0.8411745483,-3.1216507961  
C,0,-4.8332480383,-1.3434691187,-2.1806978771  
C,0,-4.1604217786,-0.8684060962,-4.5201070064  
C,0,-3.2795826196,-0.2956370582,-5.4041079013  
C,0,-2.1047353158,0.3382697055,-4.9331322142  
C,0,-1.8237326673,0.3647300551,-3.588798553  
C,0,-2.9272785821,-0.9754533852,1.0666450687  
C,0,-2.539698881,0.1799436521,1.752047904  
C,0,-2.3191213234,0.1698724669,3.1683439791  
C,0,-2.4015443334,-1.0640923502,3.8563526628  
C,0,-2.6648020797,-2.2480186468,3.1248853908  
C,0,-2.9205494463,-2.2209027415,1.7656048382

C,0,-2.039395295,1.3572188735,3.8962251668  
C,0,-1.8482862183,1.31071948,5.2560039595  
C,0,-1.9287140396,0.0773725249,5.9458356968  
C,0,-2.1974875173,-1.0841098161,5.264052047  
O,0,-2.4048117596,1.379945153,1.113655095  
B,0,-1.3551843451,1.5228556476,0.0505940747  
O,0,-1.250769992,0.3081675873,-0.8390681237  
C,0,-3.1229176473,-3.5065908039,1.0883641647  
C,0,-2.4985076779,-3.7917129567,-0.1338298115  
C,0,-2.6752412432,-5.0332272121,-0.7424410027  
C,0,-3.4615124778,-6.010533168,-0.1337094059  
C,0,-4.0789358811,-5.7390462438,1.0868452448  
C,0,-3.9139674197,-4.496131061,1.6939282834  
O,0,-0.0098687254,1.6399353438,0.6744199273  
B,0,0.3314176745,2.8520200088,1.1914625574  
O,0,-0.2437062624,4.0073984185,0.7328701813  
B,0,-1.1991808793,3.9251256946,-0.2819189444  
O,0,-1.546684797,5.1629700742,-0.8122455828  
C,0,-2.489958278,5.4167296522,-1.7854716075  
C,0,-3.4017726606,4.4754253642,-2.2772388717  
C,0,-4.3258820374,4.8744695021,-3.2417850382  
C,0,-4.3408768924,6.1884019727,-3.7082811829  
C,0,-3.4260572664,7.1173787723,-3.2098542282  
C,0,-2.4919466129,6.7456769427,-2.2478782258  
O,0,1.3093230317,2.829164736,2.1945455451  
C,0,1.8350043639,3.892010497,2.899765733  
C,0,2.6847423873,3.5174382309,3.9568741717  
C,0,3.2860239883,4.5136261938,4.7202064635  
C,0,3.0468027476,5.8605923597,4.4446481382  
C,0,2.1964869682,6.2177486535,3.3988697506  
C,0,1.582495522,5.2397138946,2.617562325  
O,0,-1.6670200767,2.7312541799,-0.6892819431  
N,0,1.5401803674,-0.1832969402,1.5492212004  
N,0,1.7692952386,0.1514567291,2.568851592  
C,0,1.339047493,-0.7366789479,0.2279460375  
C,0,2.0352299467,0.1421786301,-0.9196268201  
C,0,2.9758960589,1.2015347239,-0.3962134199  
C,0,2.7824040327,2.5328912937,-0.7668191234  
C,0,3.688544956,3.5115492135,-0.365776696  
C,0,4.7902580279,3.1645028009,0.4139564645  
C,0,4.9879512322,1.8355949184,0.7880457774  
C,0,4.0875052433,0.8542878056,0.379960393  
C,0,1.9455592786,-2.1420307481,0.2936802072  
O,0,2.9316026358,-2.4017260277,0.9383084281  
O,0,1.2378594979,-2.9682883684,-0.4442632632  
C,0,1.8196468621,-4.2802997174,-0.6386839525  
N,0,2.6955960223,-0.791092647,-1.8194464489  
C,0,2.1801274485,-0.8261583789,-3.2256126701  
C,0,2.61236984,0.3387595627,-4.065535334  
C,0,1.6499484594,1.079714235,-4.7571580569  
C,0,2.0143711561,2.1672109534,-5.5565921128  
C,0,3.3754318168,2.5062843196,-5.6569461834  
C,0,4.3591529686,1.7725054159,-4.9700713598  
C,0,3.9604615999,0.6917122793,-4.1789477565  
C,0,0.9761386884,2.9566295209,-6.2574053194  
O,0,3.7289182839,3.6496115475,-6.367166449  
C,0,4.2173070693,3.3737409371,-7.6799002493  
C,0,5.7937299922,2.1256894404,-5.0732660438  
C,0,2.5391924385,-2.1040552764,-3.9160662665  
C,0,3.8472233744,-2.5946616623,-3.9286911037  
C,0,4.1687070328,-3.7716474276,-4.6127203229  
C,0,3.1478484754,-4.4574453118,-5.2924095891  
C,0,1.8217663674,-3.9873679454,-5.279541911  
C,0,1.5319192864,-2.8109969798,-4.5841251097  
C,0,5.5630993216,-4.2705787118,-4.6164328082  
O,0,3.4598606443,-5.5598754677,-6.0834571796  
C,0,3.5095703785,-6.7841194423,-5.3524124189  
C,0,0.7533734245,-4.7238936101,-5.9929710442  
H,0,0.2502900861,-0.7231020872,0.0673311284  
H,0,-1.6373731295,2.2290592195,5.8230322404



H,0,-0.9291356859,0.8704998553,-3.1904358054  
H,0,2.8595891565,2.4551501543,4.1702442285  
H,0,3.9513999727,4.2321886255,5.5497740583  
H,0,3.5252446648,6.6389649586,5.055753132  
H,0,2.0017187428,7.2796179403,3.1859304535  
H,0,0.9010484241,5.5203470369,1.7978216364  
H,0,-1.7675351733,7.464974692,-1.8430229316  
H,0,-3.440155884,8.1538136557,-3.5777991455  
H,0,-5.0739022276,6.4942717149,-4.4677693643  
H,0,-5.0477204563,4.1423333865,-3.6332533695  
H,0,-3.3831526888,3.4381458889,-1.9044906368  
H,0,-3.4803733726,-0.3120298223,-6.4853348588  
H,0,-5.0839850383,-1.3500562597,-4.873981196  
H,0,-5.8013424361,-1.7158255899,-2.5505566723  
H,0,-6.2276101407,-3.4619610432,-1.0171596381  
H,0,-8.1708234106,-3.9814459538,0.4486906854  
H,0,-8.7166267079,-2.4971186637,2.3797208942  
H,0,-7.3051947235,-0.4892506054,2.8408347906  
H,0,-5.3539252126,0.0327874392,1.3783733142  
H,0,-4.420357007,-4.2801153188,2.6472027645  
H,0,-4.7041259119,-6.5042475888,1.569657073  
H,0,-3.5989234104,-6.9887443162,-0.6161106594  
H,0,-2.2025216728,-5.2369437543,-1.7145507271  
H,0,-1.8770689707,-3.02271885,-0.6197264109  
H,0,-2.6585173649,-3.2067273851,3.6662761316  
H,0,-2.2705230215,-2.0460247679,5.792411823  
H,0,-1.7783394756,0.0645527239,7.0354757977  
H,0,1.0814984643,-0.7959871246,-3.1311770962  
H,0,3.7002188184,-0.6455561147,-1.8017319834  
H,0,1.1806752464,0.6204170141,-1.4044040782  
H,0,1.9182949485,2.8015623973,-1.3690846201  
H,0,3.5266048752,4.5446643945,-0.6563009574  
H,0,5.4925717631,3.9283464004,0.7330831735  
H,0,5.8443104896,1.5624243598,1.3967716789  
H,0,4.2500847483,-0.184519925,0.6680422705  
H,0,4.6498866624,-2.0525024546,-3.4060560415  
H,0,5.7560161301,-4.8769667237,-3.6955363246  
H,0,6.2887875029,-3.4206294336,-4.6352275996  
H,0,5.748267521,-4.9178287133,-5.5100182742  
H,0,3.7866469065,-7.54505942,-6.1237745062  
H,0,2.5094897617,-7.012549723,-4.9103088349  
H,0,4.2864797954,-6.7278623942,-4.5513318789  
H,0,-0.1440524767,-4.0788441726,-6.1564852399  
H,0,0.4439517093,-5.6184934251,-5.3953061077  
H,0,1.1264194036,-5.0820831217,-6.9852326561  
H,0,0.4958987474,-2.435853005,-4.5722077419  
H,0,0.5840648729,0.8064468366,-4.6809821287  
H,0,1.395738727,3.431171689,-7.1792977899  
H,0,0.6041228015,3.7723791397,-5.5864589549  
H,0,0.1083887252,2.3126024352,-6.5438670927  
H,0,4.4638517187,4.3848282305,-8.0894904606  
H,0,3.4265214533,2.878258318,-8.2934467377  
H,0,5.1295386928,2.7306139503,-7.6293961095  
H,0,5.9161636671,3.2037103677,-5.3463313761  
H,0,6.2859114777,1.5028918244,-5.8626158554  
H,0,6.3184710416,1.9417068377,-4.1036309544  
H,0,4.7326268418,0.1126339176,-3.6493898374  
H,0,-1.9919385506,2.3073828232,3.339096671  
H,0,-1.43145091,0.8182248453,-5.6589248477  
C,0,0.9328840282,-5.0137302757,-1.6162404165  
H,0,2.8358998723,-4.1377801454,-1.0170934397  
H,0,1.8743500462,-4.7751562203,0.3348080716  
H,0,1.3226011148,-6.0216260409,-1.7779082199  
H,0,-0.0865203438,-5.0906174256,-1.2266625116  
H,0,0.906033098,-4.4897897863,-2.5770290264

E(RAM1) = -0.766607128196

E(RM062X) = -1385.08572471

E(RAM1) = -1.12012104302

Zero-point correction= 1.285025  
(Hartree/Particle)  
Thermal correction to Energy= 1.366090  
Thermal correction to Enthalpy= 1.367034  
Thermal correction to Gibbs Free Energy= 1.155075  
Sum of electronic and zero-point Energies= -1383.447186  
Sum of electronic and thermal Energies= -1383.366121  
Sum of electronic and thermal Enthalpies= -1383.365177  
Sum of electronic and thermal Free Energies= -1383.577135

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	857.234	307.129	446.105

C,0,-5.8820607497,-1.43222248,1.4730279191  
C,0,-5.7283918074,-0.0393609831,1.5289363805  
C,0,-6.8687936594,0.775937276,1.4817890467  
C,0,-8.1363337096,0.2076359558,1.3721432612  
C,0,-8.28116132,-1.178233391,1.3160095408  
C,0,-7.1522129048,-1.9954388331,1.3668679916  
C,0,-4.4013636583,0.5526376521,1.7285428514  
C,0,-3.2549483239,0.125626004,0.98571434  
C,0,-1.9950268073,0.5247954022,1.4280444766  
C,0,-1.8313200421,1.4542738885,2.503471828  
C,0,-2.9905345657,1.9786439009,3.123844374  
C,0,-4.2619114,1.4869608295,2.736970069  
C,0,-2.8437682473,2.9433792872,4.1586833263  
C,0,-1.5948825965,3.3399756338,4.5698443625  
C,0,-0.4361404123,2.7827708211,3.977410283  
C,0,-0.5514832225,1.8561119097,2.9696243683  
C,0,-3.3845024832,-0.759624087,-0.1740235209  
C,0,-2.6740538474,-1.9634240496,-0.2115936346  
C,0,-2.9770467456,-2.9732986691,-1.1875570417  
C,0,-3.9218177729,-2.6768506367,-2.1985927095  
C,0,-4.4884790532,-1.3796085116,-2.2551912062  
C,0,-4.2272896572,-0.4329286125,-1.2815419125  
C,0,-2.3877603379,-4.2648203093,-1.1391757249  
C,0,-2.7301913974,-5.2200887215,-2.0659528973  
C,0,-3.6735150585,-4.9253674673,-3.0788642019  
C,0,-4.2554633546,-3.6828901828,-3.1468084533  
O,0,-1.703219771,-2.2832090605,0.6872547259  
B,0,-0.5278520173,-1.3839200931,0.9653742725  
O,0,-0.8497572136,0.0751334122,0.8116321075  
C,0,-4.7675067308,0.916451227,-1.4796396194  
C,0,-3.9689023942,2.0478997072,-1.2591669569  
C,0,-4.462152544,3.3235867615,-1.5253280234  
C,0,-5.7587697909,3.4869636298,-2.0120285074  
C,0,-6.5631702128,2.3682220158,-2.2270247483  
C,0,-6.0728066052,1.0906243947,-1.9649338843  
O,0,0.5401816462,-1.6091753632,-0.0438029364  
B,0,1.5074154386,-2.5263225565,0.1912187054  
O,0,1.7189025436,-3.0635200146,1.4314893466  
B,0,0.938755189,-2.6085526734,2.4970786135  
O,0,1.3400352645,-3.1184822352,3.7264052168  
C,0,0.7407588152,-2.9183988376,4.9526496697  
C,0,-0.4548992519,-2.2193559127,5.1530950551  
C,0,-0.9581312889,-2.1058679674,6.4484411436  
C,0,-0.2816969158,-2.6793218975,7.5243479784  
C,0,0.9094975897,-3.3748791179,7.3104548796  
C,0,1.4345818128,-3.5028623725,6.0282923436  
O,0,2.2886420904,-2.8726616824,-0.9292061784  
C,0,3.3756432447,-3.7251859597,-0.9152941436  
C,0,3.6690922575,-4.3332645311,-2.1479575215  
C,0,4.7974705613,-5.1432203427,-2.2458876326

## Anti 3a

anti-3a-ONIOM-M06-BB

C,0,5.6161575384,-5.3558666492,-1.1363721243  
 C,0,5.3066954751,-4.7563613756,0.0845106589  
 C,0,4.1859997123,-3.937139482,0.2071649841  
 O,0,-0.0571976527,-1.7301376569,2.2912790077  
 N,0,-0.2793051965,-1.0988954108,-2.4209676453  
 N,0,-0.5045492917,-2.1233964676,-2.7481794854  
 C,0,0.1078704768,0.2554909694,-2.1351552103  
 C,0,1.73419064,0.3696477462,-2.3064283992  
 C,0,2.0686030888,0.0200698972,-3.7410109506  
 C,0,2.3249142215,-1.3139582229,-4.0687552692  
 C,0,2.5486884021,-1.6834543476,-5.3949518195  
 C,0,2.52161011,-0.7220280455,-6.402170311  
 C,0,2.2860185416,0.6143691216,-6.0771840666  
 C,0,2.0626425501,0.9854817117,-4.7536466874  
 C,0,-0.5685576352,1.1749063036,-3.1425602879  
 O,0,-0.4929752997,2.3697662994,-3.0169896883  
 O,0,-1.1184259111,0.5222720086,-4.1540959847  
 C,0,-1.6224244014,1.3368123811,-5.2421316267  
 N,0,2.1863299841,1.6480105871,-1.8963840885  
 C,0,2.2408860595,1.9075175748,-0.4141480323  
 C,0,3.4265144492,1.2510556722,0.2195048912  
 C,0,3.2414446931,0.5008536325,1.3851910475  
 C,0,4.3207110652,-0.1266534764,2.015656926  
 C,0,5.6038273921,0.0160224601,1.4589365223  
 C,0,5.8094194457,0.7682783257,0.2887492541  
 C,0,4.709581129,1.3782423267,-0.320721824  
 C,0,4.0905843069,-0.9265994136,3.2403865017  
 O,0,6.6939332381,-0.524667309,2.1361704939  
 C,0,7.1238192607,-1.7762983328,1.6017815087  
 C,0,7.159842139,0.9178638853,-0.3007416335  
 C,0,2.2589261585,3.3810047956,-0.1515696098  
 C,0,3.1447112578,4.2301724645,-0.8220760035  
 C,0,3.1630414459,5.6032326677,-0.5601318597  
 C,0,2.2693247288,6.1215927858,0.3933089989  
 C,0,1.3658080336,5.2847808456,1.0724696148  
 C,0,1.3696405625,3.9169426771,0.7852809157  
 C,0,4.1133627123,6.4811117349,-1.2810012105  
 O,0,2.1940836113,7.4954834456,0.6050177767  
 C,0,3.1949958718,7.9863614139,1.4963962782  
 C,0,0.407580209,5.8363712702,2.0572216701  
 H,0,-0.1975534355,0.4386703975,-1.0927140603  
 H,0,-2.2840817015,-6.2244754792,-2.024863811  
 H,0,0.3351561477,1.3871812033,2.5117382718  
 H,0,3.0146455033,-4.1673850915,-3.0136213519  
 H,0,5.0386930096,-5.622277307,-3.2062626319  
 H,0,6.5019976272,-6.0009104024,-1.2237880401  
 H,0,5.9470794442,-4.9312368073,0.9621540015  
 H,0,3.923981253,-3.4753901762,1.1733850515  
 H,0,2.3689265,-4.0492815082,5.8424698819  
 H,0,1.4412986867,-3.8276917256,8.1601520024  
 H,0,-0.6859727867,-2.5848219104,8.5419146737  
 H,0,-1.8973591936,-1.5581677388,6.6164583923  
 H,0,-0.9847467927,-1.7683175881,4.2981790984  
 H,0,-1.4789943156,4.0854714593,5.3702332175  
 H,0,-3.7504986471,3.3578404285,4.6236546213  
 H,0,-5.1482097117,1.8359722001,3.2898756205  
 H,0,-6.7583321627,1.8698288767,1.525292589  
 H,0,-9.0238373136,0.8556024624,1.3327506759  
 H,0,-9.2822407895,-1.6251191107,1.2343027835  
 H,0,-7.2613160287,-3.0890930134,1.3255622655  
 H,0,-4.989971171,-2.077769477,1.5119118742  
 H,0,-6.7174183238,0.2125250353,-2.122830107  
 H,0,-7.5901515555,2.4926182087,-2.6005019287  
 H,0,-6.1472051292,4.4943685126,-2.2197258639  
 H,0,-3.8254628474,4.2025304648,-1.3453854232  
 H,0,-2.951395921,1.9252674797,-0.855658157  
 H,0,-5.1475744894,-1.1348057025,-3.1022415885  
 H,0,-4.9980770507,-3.4479134548,-3.9234605792  
 H,0,-3.9389335598,-5.7078099484,-3.8052941278  
 H,0,1.3316479377,1.4938436129,0.0682415556

H,0,1.7409299805,2.4187088023,-2.3840712547  
 H,0,2.1186852913,-0.3974832774,-1.6265856948  
 H,0,2.3665784037,-2.057293576,-3.273847359  
 H,0,2.7517169281,-2.7220450457,-5.6363968056  
 H,0,2.6984417664,-1.0079414802,-7.4342628397  
 H,0,2.2858337392,1.3715180869,-6.8555444421  
 H,0,1.8978650504,2.0330287084,-4.5143879702  
 H,0,3.8475699092,3.8209609518,-1.5645455991  
 H,0,3.7347910021,7.5333660091,-1.3103060947  
 H,0,4.263375782,6.1262277264,-2.3302591224  
 H,0,5.1064818324,6.4768719752,-0.7643534363  
 H,0,3.0000538927,9.0868640411,1.5358124318  
 H,0,4.2149346945,7.7765287833,1.0913242962  
 H,0,3.0767176296,7.5253992343,2.5067810181  
 H,0,0.1143300998,5.0615678559,2.8104315964  
 H,0,-0.5164914966,6.1854930045,1.5306315901  
 H,0,0.8532170291,6.7130402858,2.5900694359  
 H,0,0.6600735348,3.2591471022,1.3164462881  
 H,0,2.2318840147,0.3834592834,1.8145441168  
 H,0,5.0289539611,-1.4387941391,3.5675425432  
 H,0,3.3025156309,-1.7042871901,3.0560290514  
 H,0,3.7417449246,-0.2650552424,4.0723062988  
 H,0,7.9439862201,-2.0938532665,2.2922875717  
 H,0,7.5091442409,-1.6384288374,0.5617910074  
 H,0,6.2865330319,-2.5178053834,1.6077694704  
 H,0,7.3197058988,0.1446763865,-1.09427491  
 H,0,7.948452023,0.7885060919,0.4820582186  
 H,0,7.2801160637,1.9272133948,-0.7655675356  
 H,0,4.8649474954,1.9625790806,-1.2406396848  
 H,0,-1.6698440354,-4.4778825709,-0.3297892243  
 H,0,0.5539779336,3.0938922242,4.3415152682  
 C,0,-1.9631411567,0.3945519225,-6.3723770646  
 H,0,-2.4890254467,1.8927724225,-4.8742166662  
 H,0,-0.8386335544,2.048634317,-5.5151505224  
 H,0,-2.3528656816,0.9658535193,-7.2182802596  
 H,0,-1.0713754263,-0.1472023899,-6.6976862513  
 H,0,-2.7234580945,-0.3264976813,-6.0630236757

## TS 2

cis-RC-TS7-ONIOM-M06-BB  
 E(RM062X) = -1385.06957582

E(RAM1) = -1.08984926175

Zero-point correction=	1.282303
(Hartree/Particle)	
Thermal correction to Energy=	1.364231
Thermal correction to Enthalpy=	1.365175
Thermal correction to Gibbs Free Energy=	1.147260
Sum of electronic and zero-point Energies=	-1383.434314
Sum of electronic and thermal Energies=	-1383.352386
Sum of electronic and thermal Enthalpies=	-1383.351442
Sum of electronic and thermal Free Energies=	-1383.569357

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.068	307.376	458.640

C,0,-5.3619236834,-2.4856089182,1.9257238108  
 C,0,-5.5696094276,-1.0994337583,1.979666176  
 C,0,-6.8480166752,-0.6124167657,2.2895239963  
 C,0,-7.8979541466,-1.4954066016,2.5334568433  
 C,0,-7.6837507446,-2.8722368526,2.4778174354  
 C,0,-6.4147078035,-3.3641386727,2.1736502934  
 C,0,-4.4447411423,-0.1756878713,1.8017143968  
 C,0,-3.4653608816,-0.3635496739,0.7745717266  
 C,0,-2.2653493464,0.3397615642,0.8741871476  
 C,0,-2.0931543057,1.4040788246,1.8165125785  
 C,0,-3.1499026138,1.6822252603,2.7169680284

C,0,-4.292589064,0.8438646424,2.721427994  
 C,0,-3.0181952344,2.7704100883,3.6229923434  
 C,0,-1.8781348698,3.5359947719,3.6325151006  
 C,0,-0.8125781384,3.2416350175,2.7488438246  
 C,0,-0.9145732574,2.194478021,1.8651920933  
 C,0,-3.6908854394,-1.290372759,-0.337560619  
 C,0,-2.7599736017,-2.2975112824,-0.6038431139  
 C,0,-3.0285715867,-3.3309748585,-1.562185299  
 C,0,-4.223911915,-3.2596277285,-2.3156933153  
 C,0,-5.0900455573,-2.1528782302,-2.1352711876  
 C,0,-4.8381417208,-1.1820046205,-1.1836463694  
 C,0,-2.1427294337,-4.4231454658,-1.7604366112  
 C,0,-2.4436655242,-5.4055290118,-2.6730818635  
 C,0,-3.6400774316,-5.3376727246,-3.425636241  
 C,0,-4.5107368569,-4.2892050871,-3.2538903022  
 O,0,-1.5816802412,-2.3961343284,0.0750855886  
 B,0,-0.5876107206,-1.2762824239,0.0792651139  
 O,0,-1.2111129827,0.0872253704,0.0278051879  
 C,0,-5.7463728698,-0.0307132122,-1.1341092702  
 C,0,-5.2517603882,1.2776493786,-1.0394388314  
 C,0,-6.1240084417,2.3647785939,-1.0509877384  
 C,0,-7.4988384435,2.162278636,-1.1644476754  
 C,0,-8.0000930206,0.864496362,-1.2611628659  
 C,0,-7.1323074523,-0.2252902641,-1.2459428202  
 O,0,0.2591461925,-1.3254097625,-1.1444456083  
 B,0,1.2562078692,-2.2420032399,-1.1722409671  
 O,0,1.7516471037,-2.8049156601,-0.0251307232  
 B,0,1.2765297118,-2.3401389988,1.2044788116  
 O,0,2.015487809,-2.8048850156,2.2878202052  
 C,0,1.7792354889,-2.5583975366,3.6238668633  
 C,0,0.64481039,-1.9112422318,4.127473971  
 C,0,0.5204626825,-1.7475258443,5.5063647495  
 C,0,1.5094825649,-2.2200167468,6.36827612  
 C,0,2.6355031957,-2.8644222503,5.8533923663  
 C,0,2.7854645832,-3.0403462487,4.481255402  
 O,0,1.793322564,-2.5118328427,-2.4449735535  
 C,0,2.7933305044,-3.4060815347,-2.7654532564  
 C,0,2.9590935833,-3.6123686812,-4.1479386107  
 C,0,3.9605499369,-4.4735962549,-4.5851449764  
 C,0,4.7855444939,-5.1265318058,-3.6681470022  
 C,0,4.6075088042,-4.9188427855,-2.3011016492  
 C,0,3.6115271181,-4.0604170008,-1.8367167076  
 O,0,0.2441821979,-1.4816439402,1.2576064288  
 N,0,-1.0121621001,0.1343375153,-3.0746276678  
 N,0,-1.5309849718,-0.6900363424,-3.5773519022  
 C,0,0.0781035792,1.3441462078,-2.3593116251  
 C,0,1.4739590983,0.9901093277,-2.8246520247  
 C,0,1.7233720575,1.0425180458,-4.3151138715  
 C,0,1.6490089603,-0.1659287256,-5.017057453  
 C,0,1.83191096,-0.1908126389,-6.3978180764  
 C,0,2.1003279716,0.9902484717,-7.0875108718  
 C,0,2.187211194,2.194220169,-6.3907288816  
 C,0,1.9958718519,2.2240244888,-5.0105205278  
 C,0,-0.5419720835,2.6467393816,-2.8740773919  
 O,0,0.1060493928,3.6410574316,-3.0776063872  
 O,0,-1.8487154801,2.5331803829,-3.0486556745  
 C,0,-2.5313369393,3.7260448652,-3.5128363639  
 N,0,2.0626505144,1.9785645353,-1.9475033629  
 C,0,2.9759643052,1.4983144369,-0.8675978735  
 C,0,4.2848159844,0.9600917259,-1.3576989698  
 C,0,4.7628380658,-0.2381385248,-0.8182047867  
 C,0,5.9921262156,-0.769506315,-1.2216724001  
 C,0,6.7439891802,-0.0750889698,-2.1848601888  
 C,0,6.275567325,1.1273158293,-2.7451548762  
 C,0,5.0460755204,1.6343111497,-2.316953294  
 C,0,6.4662997233,-2.0436461636,-0.6347303688  
 O,0,8.0171554371,-0.5314573198,-2.5149837178  
 C,0,8.031636947,-1.3724803544,-3.6684634083  
 C,0,7.0621040026,1.8501304572,-3.7709220519  
 C,0,3.203858732,2.5626756597,0.1556883003  
 C,0,3.7305033281,3.8097052552,-0.1932262883  
 C,0,3.9674069533,4.7863741267,0.777427256  
 C,0,3.6673547537,4.4918997343,2.1200041975  
 C,0,3.1350553828,3.2443206751,2.4896654425  
 C,0,2.8971844711,2.2921872853,1.4928364806  
 C,0,4.5285812614,6.0999021512,0.3863080192  
 O,0,3.7996441845,5.4819364862,3.0895320754  
 C,0,5.1267367613,5.5965966831,3.603186132  
 C,0,2.8074626634,2.9270437977,3.8986389797  
 H,0,-0.163742682,1.0713292881,-1.3270842244  
 H,0,-1.7625273225,-6.25521178,-2.8251028268  
 H,0,-0.0866460215,1.9382927799,1.1852044845  
 H,0,2.3003442709,-3.0989277535,-4.8609701704  
 H,0,4.0966050186,-4.6426975024,-5.6635341681  
 H,0,5.5706056775,-5.8083201054,-4.0243803642  
 H,0,5.2529280005,-5.4377429705,-1.5764427692  
 H,0,3.4621698693,-3.9089298826,-0.7551318596  
 H,0,3.6629525292,-3.5492503265,4.0605069478  
 H,0,3.4134264213,-3.2390553704,6.5347959312  
 H,0,1.4022641129,-2.0875772585,7.453981368  
 H,0,-0.3687547383,-1.2422465191,5.911891177  
 H,0,-0.1339160906,-1.5414382321,3.4402748096  
 H,0,-1.7760058982,4.3812118413,4.3288738045  
 H,0,-3.8478390636,2.9827247905,4.3134570309  
 H,0,-5.053753924,1.0014751889,3.501398204  
 H,0,-7.0222954384,0.4731199969,2.3318750692  
 H,0,-8.8970840916,-1.103272551,2.7720082167  
 H,0,-8.5123091851,-3.5674999253,2.6742107827  
 H,0,-6.2402647014,-4.4491898037,2.1294060643  
 H,0,-4.3595458104,-2.8740053579,1.6819920128  
 H,0,-7.5348808705,-1.2481012611,-1.3060249584  
 H,0,-9.0841046239,0.6983418145,-1.3441549602  
 H,0,-8.1850380605,3.0210740188,-1.1716012315  
 H,0,-5.7248966614,3.3854710152,-0.9585838793  
 H,0,-4.1673634533,1.4407327926,-0.9359210347  
 H,0,-5.9755189374,-2.0738713405,-2.7846972987  
 H,0,-5.4452960205,-4.2300301577,-3.8306556417  
 H,0,-3.8634609277,-6.1377653108,-4.146627997  
 H,0,2.4265521497,0.6766372897,-0.3775829968  
 H,0,2.302048904,2.8601865771,-2.3847510939  
 H,0,1.7007616365,-0.0141432605,-2.4643285977  
 H,0,1.4730329419,-1.0880195756,-4.4653910285  
 H,0,1.7761717478,-1.1351144232,-6.9302052314  
 H,0,2.2482816373,0.9721168785,-8.1627476795  
 H,0,2.4034628277,3.1159948315,-6.9215983694  
 H,0,2.0518570489,3.173262635,-4.4871292736  
 H,0,3.9771871645,4.0324805955,-1.2425190043  
 H,0,4.2647763045,6.882632327,1.1408344542  
 H,0,4.1358113708,6.4183610424,-0.6104976151  
 H,0,5.644207063,6.0350211965,0.320078607  
 H,0,5.0542349588,6.4314091815,4.3438007766  
 H,0,5.8403671721,5.852460224,2.7824022892  
 H,0,5.4333498595,4.6463476796,4.1034561209  
 H,0,3.2206127097,1.9269228438,4.1810888242  
 H,0,1.6956943318,2.8963422457,4.0332103959  
 H,0,3.2252470033,3.6991159781,4.5910765711  
 H,0,2.4642845377,1.3191777561,1.7784359184  
 H,0,4.1711042289,-0.7819056813,-0.0633337891  
 H,0,7.506091,-2.2785876538,-0.9716448566  
 H,0,5.7890585594,-2.8823455813,-0.9457093183  
 H,0,6.4586503102,-1.9830489282,0.4820381573  
 H,0,9.1093094458,-1.6476600365,-3.7843701232  
 H,0,7.6659038289,-0.8091012403,-4.5613852986  
 H,0,7.4045203045,-2.2803296331,-3.495569623  
 H,0,6.712222332,1.5608069286,-4.7941202909  
 H,0,8.1484142595,1.5963505435,-3.6859983332  
 H,0,6.9434239986,2.9556350741,-3.6578600091  
 H,0,4.687150745,2.5822021798,-2.7458547987  
 H,0,-1.2211248913,-4.4600179666,-1.156966001  
 H,0,0.0968414553,3.8603584246,2.7815318125

C,0,-3.9525085335,3.3265749718,-3.8324229063  
 H,0,-2.4714855953,4.4730544702,-2.716734247  
 H,0,-1.9941172406,4.1054593029,-4.3853622602  
 H,0,-4.5107404128,4.2048761362,-4.1654875856  
 H,0,-3.974975513,2.5807104267,-4.6304377229  
 H,0,-4.4499853439,2.9114027862,-2.94969836

### cis-aziridine 4a

medam-cis-aziridine-ONIOM-M06-BB  
 E(RAM1) = -0.909651454324E-01

E(RM062X) = -671.228041599

E(RAM1) = -0.235241149350E-01

Zero-point correction= 0.596774  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.632768  
 Thermal correction to Enthalpy= 0.633712  
 Thermal correction to Gibbs Free Energy= 0.521890  
 Sum of electronic and zero-point Energies= -670.698709  
 Sum of electronic and thermal Energies= -670.662715  
 Sum of electronic and thermal Enthalpies= -670.661771  
 Sum of electronic and thermal Free Energies= -670.773593

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	397.068	130.190	235.349

C,0,2.054689426,-0.6019212885,-0.8855257236  
 C,0,3.2781106733,-0.6446542641,-0.0258279345  
 O,0,4.3782798757,-0.5154974896,-0.7873382668  
 C,0,5.63072755,-0.5998654447,-0.0880307054  
 C,0,6.7307588787,-0.4337346059,-1.1131342159  
 C,0,1.1408229779,-1.8053989078,-0.9894678876  
 H,0,0.6904400632,-1.9091565177,-1.9804409191  
 N,0,0.7748091072,-0.640188251,-0.2278237587  
 C,0,-0.2856865048,0.2395193132,-0.8260737236  
 C,0,-1.6589359505,-0.2728445936,-0.5312452395  
 C,0,-2.5998636586,-0.3199189822,-1.5659692452  
 C,0,-3.9019243661,-0.7693624441,-1.3328873758  
 C,0,-4.2509461151,-1.1844453491,-0.0351314812  
 C,0,-3.164135072,-1.1522105887,1.0146518853  
 C,0,-2.0224827607,-0.6912401222,0.7512509394  
 C,0,-4.8824092212,-0.8060022563,-2.4422420518  
 O,0,-5.5073680825,-1.7347075323,0.2046468561  
 C,0,-6.5247502424,-0.7546347261,0.4072578139  
 C,0,-3.6761797114,-1.6174468732,2.3735453415  
 C,0,-0.1543598414,1.6561882275,-0.3659262251  
 C,0,0.0570555965,1.9702361954,0.978962932  
 C,0,0.1663779288,3.3010840763,1.3953563007  
 C,0,0.0540956295,4.3225507253,0.4361049208  
 C,0,-0.1629034905,4.025127758,-0.9214271487  
 C,0,-0.262818744,2.6861380935,-1.3071097796  
 C,0,-0.2865669366,5.0987371705,-1.9340804809  
 O,0,0.0577628275,5.6471683741,0.8655361325  
 C,0,1.3134306057,6.2989564096,0.6792035517  
 C,0,0.3733663728,3.6145257426,2.8276673234  
 O,0,3.3021246158,-0.797371767,1.1700237242  
 H,0,-0.1539705203,0.2309592225,-1.9302601057  
 C,0,1.3858354413,-3.0992681415,-0.2888462855  
 H,0,2.1652859724,-0.0160732813,-1.7983347337  
 H,0,-2.3202748766,0.0025468421,-2.580794499  
 H,0,-1.2850662483,-0.6618606315,1.5695316705  
 H,0,-0.4375500219,2.4477150624,-2.3676373882  
 H,0,0.1444960739,1.1645824695,1.7258205799  
 H,0,-5.6808611598,-1.5626454306,-2.2386194781  
 H,0,-5.3668036848,0.1963482415,-2.5595302608  
 H,0,-4.3808727959,-1.0675510305,-3.4063493045

H,0,-3.3966324364,-2.6951212386,2.4904546167  
 H,0,-3.1370411138,-1.026029864,3.1536156994  
 H,0,-4.7775402686,-1.5243248503,2.5451757421  
 H,0,-7.4519346985,-1.3605957049,0.5615484853  
 H,0,-6.2975945661,-0.1387619848,1.3108660473  
 H,0,-6.6217532116,-0.1005655594,-0.4934039399  
 H,0,-0.6218998831,6.0538026579,-1.4577291627  
 H,0,0.7023672333,5.2779079124,-2.4269606982  
 H,0,-1.025413365,4.8156239742,-2.7236615775  
 H,0,1.013676344,2.8396226775,3.3163609417  
 H,0,0.8594804968,4.6146633914,2.9479878058  
 H,0,-0.6133932708,3.6429561576,3.3554051868  
 H,0,1.1331221052,7.3374510386,1.0529803363  
 H,0,2.1078377601,5.7930170237,1.2795116042  
 H,0,1.5916884147,6.3080583132,-0.4029021715  
 H,0,5.6576839606,0.181327876,0.6775786231  
 H,0,5.6805784094,-1.5680649325,0.4192500254  
 H,0,7.7062166812,-0.4983127369,-0.6239124781  
 H,0,6.6707265814,-1.2167138797,-1.8730111852  
 H,0,6.6541942855,0.5376485465,-1.6079908597  
 C,0,1.611963873,-4.2487709655,-1.051232827  
 C,0,1.8456461826,-5.4731978799,-0.4304577787  
 C,0,1.8516845172,-5.5566362748,0.9612726051  
 C,0,1.6219500948,-4.4125339692,1.7240957214  
 C,0,1.3889039067,-3.1864279658,1.1053304611  
 H,0,1.6001925721,-4.1838716156,-2.1369693504  
 H,0,2.0172270901,-6.3607634321,-1.0318199406  
 H,0,2.0316692051,-6.5101791086,1.4481618257  
 H,0,1.6238329351,-4.4738743372,2.8079473257  
 H,0,1.2162589895,-2.2858366733,1.684323163

### (S)-VANOL-BOROX catalyst neutral

protonated-catalyst-ONIOM-M06-BB  
 E(RAM1) = -0.726377884039

E(RM062X) = -604.415384573

E(RAM1) = -1.17017353123

Zero-point correction= 0.675393  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.717372  
 Thermal correction to Enthalpy= 0.718316  
 Thermal correction to Gibbs Free Energy= 0.593103  
 Sum of electronic and zero-point Energies= -603.296196  
 Sum of electronic and thermal Energies= -603.254217  
 Sum of electronic and thermal Enthalpies= -603.253273  
 Sum of electronic and thermal Free Energies= -603.378486

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	450.158	165.131	263.534

C,0,-5.3617414969,-3.9941262054,1.3742594562  
 C,0,-5.1221047739,-2.7250641605,0.8209478701  
 C,0,-6.0762027298,-2.0717487293,0.0357032288  
 C,0,-7.2967193906,-2.7063504306,-0.1968616654  
 C,0,-7.5535910171,-3.9652207071,0.3444730688  
 C,0,-6.5885025522,-4.6036316308,1.1258542427  
 O,0,-3.8768669169,-2.2015181749,1.1310756405  
 B,0,-3.3408833254,-1.0093688984,0.7191112737  
 O,0,-3.8893714802,-0.080702823,-0.0876518631  
 B,0,-3.2774503836,1.147744387,-0.3800337838  
 O,0,-2.0164220316,1.3984635806,0.0229081634  
 B,0,-1.0363253444,0.4539096727,0.4099825881  
 O,0,-2.0639120013,-0.7249338929,1.2287454486  
 O,0,-0.1925767738,0.7730751587,1.5305143742  
 C,0,1.0480527124,1.3094409675,1.2423047916

C,0,1.9861212233,0.6122056023,0.486828108  
 C,0,3.1798104932,1.3012939655,0.0975211742  
 C,0,3.4624095228,2.5430668209,0.6330110277  
 C,0,2.5708876875,3.1932889223,1.5234343496  
 C,0,1.3200706347,2.5940659422,1.8081000295  
 C,0,2.8792014644,4.4536541649,2.104987651  
 C,0,1.9725963112,5.0842602392,2.9218598477  
 C,0,0.7166247384,4.4899338397,3.191529311  
 C,0,0.394123064,3.2709968543,2.6457004038  
 C,0,1.7308629559,-0.7719003348,0.07938291  
 C,0,2.6657894296,-1.818722894,0.3667771756  
 C,0,2.4850509022,-3.0733418742,-0.181897536  
 C,0,1.3659955781,-3.3759609259,-0.9983168219  
 C,0,0.3596751875,-2.3972586173,-1.1805054737  
 C,0,0.5514604769,-1.112973269,-0.5773237922  
 C,0,1.208650131,-4.6498623997,-1.6098170417  
 C,0,0.0958996943,-4.927219654,-2.3660186101  
 C,0,-0.9097863493,-3.9477273701,-2.5450718822  
 C,0,-0.7828359826,-2.7088809768,-1.9644418885  
 C,0,3.7709602756,-1.6369825319,1.3131119563  
 C,0,3.5542314708,-1.0104498891,2.5488028536  
 C,0,4.5874667963,-0.9116782769,3.4784685938  
 C,0,5.8466654646,-1.4355148748,3.1870588781  
 C,0,6.0706405318,-2.0587019824,1.9596879561  
 C,0,5.0399590412,-2.1627118296,1.0278020457  
 O,0,-0.4935089308,-0.2250207918,-0.7334119015  
 C,0,4.0790951015,0.7788668337,-0.9359267224  
 C,0,5.4696899612,0.8458416369,-0.7642313225  
 C,0,6.3251379211,0.4201096914,-1.7783913607  
 C,0,5.804485858,-0.0700798387,-2.9757161716  
 C,0,4.423044081,-0.136569166,-3.1548835807  
 C,0,3.5630994939,0.2849166644,-2.14268862  
 O,0,-4.1084489414,2.0182327251,-1.0504329264  
 C,0,-3.8119765131,3.2904515303,-1.5051151436  
 C,0,-4.829303863,3.8601872345,-2.2913019509  
 C,0,-4.6476878154,5.1508465926,-2.7790700864  
 C,0,-3.4787822045,5.8599279255,-2.4954246615  
 C,0,-2.4790660549,5.2784226912,-1.717183774  
 C,0,-2.6354893855,3.9869979148,-1.213258534  
 H,0,-1.7907078773,-4.1906766102,-3.157307961  
 H,0,-0.5778187373,2.7915269958,2.8428147541  
 H,0,-5.8666227871,-1.0773547896,-0.3901003225  
 H,0,-8.0580656495,-2.2044972101,-0.8127189206  
 H,0,-8.5186001246,-4.4578172346,0.1560958469  
 H,0,-6.7942445381,-5.5973766691,1.5512232443  
 H,0,-4.591059726,-4.4824074864,1.9861371104  
 H,0,-5.7420278686,3.2874578846,-2.5049489594  
 H,0,-5.4344978369,5.6116962425,-3.3946828532  
 H,0,-3.3472249539,6.8782972849,-2.8883589047  
 H,0,-1.5570052818,5.8364892088,-1.4957655977  
 H,0,-1.8465998336,3.5215115702,-0.6014169284  
 H,0,2.2102769236,6.0585430186,3.3741633556  
 H,0,3.8562325143,4.9094139484,1.8858980809  
 H,0,4.3881662777,3.0670776398,0.34614444  
 H,0,5.8844612754,1.2286691523,0.1804202065  
 H,0,7.413864372,0.4730839508,-1.6325640177  
 H,0,6.4810511739,-0.4019949127,-3.7763143393  
 H,0,4.0075880603,-0.5212078291,-4.097890887  
 H,0,2.4721891876,0.2303172742,-2.284975726  
 H,0,5.2228555259,-2.6499624092,0.0581315241  
 H,0,7.0629763006,-2.4703735122,1.7245014496  
 H,0,6.6603111762,-1.3571812635,3.9224357542  
 H,0,4.4062425462,-0.4179738665,4.4445050476  
 H,0,2.5622151405,-0.5907467545,2.7785365203  
 H,0,3.2091763803,-3.8762478858,0.0297067324  
 H,0,1.9972815415,-5.4034524299,-1.4661087019  
 H,0,-0.0261908277,-5.9113900731,-2.8423152336  
 H,0,0.0043448521,5.0170161111,3.8430258895  
 H,0,-1.5491577335,-1.9305330926,-2.1051683655  
 H,0,-1.6343764179,-1.3803246392,1.794980458

## Nitrogen (N<sub>2</sub>)

n2-M06-BB  
 E(RM062X) = -109.492028295

Zero-point correction=	0.005761
(Hartree/Particle)	
Thermal correction to Energy=	0.008122
Thermal correction to Enthalpy=	0.009066
Thermal correction to Gibbs Free Energy=	-0.012676
Sum of electronic and zero-point Energies=	-109.486267
Sum of electronic and thermal Energies=	-109.483906
Sum of electronic and thermal Enthalpies=	-109.482962
Sum of electronic and thermal Free Energies=	-109.504704

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	5.097	4.969	45.760

N,0,0.,0.,0.1598154916  
 N,0,0.,0.,1.2581845084

## B. Alternative Carbon-Carbon Bond Forming Transition Structures (major enantiomer)

### TS1a

E(RAM1) = -0.749167104996

E(RM062X) = -1385.07070620

E(RAM1) = -1.10467003059

Zero-point correction=	1.282301
(Hartree/Particle)	
Thermal correction to Energy=	1.363798
Thermal correction to Enthalpy=	1.364742
Thermal correction to Gibbs Free Energy=	1.147243
Sum of electronic and zero-point Energies=	-1383.432902
Sum of electronic and thermal Energies=	-1383.351406
Sum of electronic and thermal Enthalpies=	-1383.350462
Sum of electronic and thermal Free Energies=	-1383.567960

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	855.796	306.404	457.764

C,0,-5.9957798336,-0.7016780034,0.9677747753  
 C,0,-5.5770704274,0.5862791213,1.3327699343  
 C,0,-6.531138426,1.6085201949,1.4434468198  
 C,0,-7.8757916814,1.3472385279,1.1879200985  
 C,0,-8.2845867733,0.0640028275,0.826205995  
 C,0,-7.3421850177,-0.9581349304,0.7165725777  
 C,0,-4.1756550776,0.8353394698,1.6869584718  
 C,0,-3.088910498,0.3236524609,0.9076804926  
 C,0,-1.8149934031,0.3304037518,1.4743036763  
 C,0,-1.5492495229,0.9619223972,2.7305877992  
 C,0,-2.6140943756,1.6161554277,3.3957400756  
 C,0,-3.924239538,1.5060495293,2.8692822045  
 C,0,-2.3488569168,2.3115524519,4.6082273829  
 C,0,-1.0857387194,2.3191614723,5.1465201799  
 C,0,-0.0343154604,1.6154944709,4.5108673681  
 C,0,-0.2635828524,0.9449852519,3.3343520401  
 C,0,-3.3069359789,-0.2397829354,-0.4264272463  
 C,0,-2.8468841491,-1.5252704259,-0.7303777031  
 C,0,-3.2562930554,-2.1958330057,-1.9345029812

C,0,-4.0532720048,-1.4900116444,-2.8660624573  
 C,0,-4.3632649481,-0.1287027102,-2.6197301021  
 C,0,-3.9891228209,0.49639477,-1.4450527829  
 C,0,-2.9009112588,-3.5441153062,-2.2003887698  
 C,0,-3.3367682149,-4.1652920311,-3.3468976249  
 C,0,-4.1433201334,-3.4651388511,-4.274047916  
 C,0,-4.4929360935,-2.1566498079,-4.0423131263  
 O,0,-2.0582305233,-2.2514015041,0.1041903327  
 B,0,-0.7821282395,-1.740539317,0.7161825469  
 O,0,-0.7447444552,-0.2433932983,0.8237584873  
 C,0,-4.2324518521,1.9391615744,-1.334641209  
 C,0,-3.2297952293,2.7983157415,-0.8619887786  
 C,0,-3.4359762357,4.176020073,-0.8336388457  
 C,0,-4.6443314895,4.7137916355,-1.275793876  
 C,0,-5.6485540032,3.867050967,-1.7440115843  
 C,0,-5.4457400316,2.4888958555,-1.7760456936  
 O,0,0.3721129994,-2.1022381968,-0.1443222963  
 B,0,0.8709542749,-3.3564315497,-0.0142752532  
 O,0,0.5921814317,-4.1568541374,1.0592123332  
 B,0,-0.1309868842,-3.6128769251,2.1224955601  
 O,0,-0.160360548,-4.4332144091,3.2447099827  
 C,0,-0.8086714702,-4.195766266,4.4379000087  
 C,0,-1.6812653151,-3.1270178556,4.6734726267  
 C,0,-2.2886105937,-3.0176376428,5.9235249183  
 C,0,-2.0306993585,-3.9567909887,6.9214435553  
 C,0,-1.1590556485,-5.0183981347,6.6735013682  
 C,0,-0.5385064265,-5.1510368466,5.4352021609  
 O,0,1.7554810296,-3.7584924486,-1.0351908147  
 C,0,2.4491693008,-4.9479225495,-1.1270889428  
 C,0,2.9723731296,-5.2148462699,-2.4054920877  
 C,0,3.7505667888,-6.3541481384,-2.5878147898  
 C,0,3.9986034334,-7.2214905162,-1.5229645127  
 C,0,3.459204735,-6.9541289571,-0.2651952073  
 C,0,2.6793222248,-5.8176535605,-0.0546931417  
 O,0,-0.6711217525,-2.3876417999,2.0146625405  
 N,0,3.2489974923,-1.3331084665,-1.0359432822  
 N,0,3.8183847812,-1.4505381791,-0.091860377  
 C,0,2.4546355327,-1.0129878166,-2.0946141521  
 C,0,1.9524293463,0.8492234278,-1.690463214  
 C,0,0.9944693334,0.9959896084,-2.823935224  
 C,0,1.4444215943,1.6405165594,-3.979545171  
 C,0,0.5941997553,1.7900638301,-5.0719473558  
 C,0,-0.7044731268,-1.2874068569,-5.0111924885  
 C,0,-1.1501797999,0.6385495103,-3.8585102594  
 C,0,-0.3057314418,0.4891695756,-2.762131648  
 C,0,3.2016806009,-0.9839904589,-3.384293528  
 O,0,4.348233741,-0.6102600977,-3.490265639  
 O,0,2.3980845477,-1.3309559006,-4.3794672643  
 C,0,2.9075627876,-1.1180857877,-5.7125927351  
 N,0,1.5567180177,0.946488296,-0.4121671825  
 C,0,2.2312206839,1.7410263174,0.6642051124  
 C,0,3.7153101019,1.5774961964,0.7247748438  
 C,0,4.2609975568,0.7928263554,1.748351458  
 C,0,5.6447626963,0.6572223977,1.8939918719  
 C,0,6.4883435312,1.3207511158,0.9847487561  
 C,0,5.9597230937,2.1177467793,-0.0474152597  
 C,0,4.5718920365,2.2409258984,-0.1582950588  
 C,0,6.1946596495,-0.1641999584,2.9969525443  
 O,0,7.8671650778,1.2944923986,1.1618745715  
 C,0,8.4851643783,0.1069513087,0.6646670535  
 C,0,6.8485073829,2.8434681605,-0.9831577051  
 C,0,1.8537618587,3.1896420984,0.6390670165  
 C,0,1.8452088444,3.9435824253,-0.5372796846  
 C,0,1.5140302973,5.3012499698,-0.5199365456  
 C,0,1.1812338644,5.9009543488,0.7082656962  
 C,0,1.1606124723,5.1537524478,1.8993147974  
 C,0,1.4935676349,3.7972084587,1.8475141719  
 C,0,1.4874645657,6.0786742625,-1.7797812598  
 O,0,0.7585485323,7.2265867703,0.704372463  
 C,0,1.7567046767,8.1433231514,1.1527316767  
 C,0,0.7803634208,5.7705117784,3.1910233762  
 H,0,1.5201427641,-1.5672544703,-2.0194375888  
 H,0,-3.0679926057,-5.2112975974,-3.5526005376  
 H,0,0.5240708821,0.3502057205,2.8461530656  
 H,0,2.7528206004,-4.5349351423,-3.2393953161  
 H,0,4.1652062077,-6.5731957185,-3.5829160236  
 H,0,4.6122052718,-8.1201249964,-1.679050678  
 H,0,3.6429106044,-7.6455325517,0.5708963374  
 H,0,2.2307288082,-5.6165563365,0.9318547652  
 H,0,0.146431616,-5.9826064785,5.2223784658  
 H,0,-0.9585753013,-5.7596949574,7.4609051903  
 H,0,-2.5148642562,-3.8630868553,7.9035085576  
 H,0,-2.9772372609,-2.1819258069,6.1177331911  
 H,0,-1.8803786724,-2.3889777718,3.879240925  
 H,0,-0.878850526,2.8557973297,6.08382109  
 H,0,-3.1786685172,2.8354069496,5.1055203277  
 H,0,-4.7583225939,1.9320789969,3.4486316091  
 H,0,-6.2124106479,2.6233214832,1.7249332657  
 H,0,-8.61516243,2.156500255,1.2736859642  
 H,0,-9.3463462118,-0.1413169565,0.6288641984  
 H,0,-7.6592900642,-1.971999897,0.43316011395  
 H,0,-5.2504421692,-1.5083559664,0.877144977  
 H,0,-6.2455096835,1.8242708821,-2.1365055075  
 H,0,-6.6055082963,4.2859840747,-2.0875040735  
 H,0,-4.8054736199,5.8009650736,-1.2522546295  
 H,0,-2.6428018402,4.8389643433,-0.4577405455  
 H,0,-2.2791041597,2.3741409339,-0.5027457538  
 H,0,-4.9036007532,0.4324274941,-3.3972238147  
 H,0,-5.1235616972,-1.6055082706,-4.7550069265  
 H,0,-4.488422447,-3.9836257664,-5.1806224532  
 H,0,1.8140991259,1.3088358447,1.5874705989  
 H,0,0.6114072181,0.6450324074,-0.1513530169  
 H,0,2.9316311192,1.2995035554,-1.8823120685  
 H,0,2.4604923355,2.0273736706,-4.0205431757  
 H,0,0.9440273099,2.2994880183,-5.9645561737  
 H,0,-1.3722790509,1.4027118518,-5.8592538777  
 H,0,-2.1653225649,0.24840837,-3.8058740085  
 H,0,-0.6570151885,-0.0226248017,-1.8669988786  
 H,0,2.0861925463,3.4734452386,-1.5039294868  
 H,0,1.6673942688,7.1641036431,-1.5769759129  
 H,0,0.4831308522,5.9787755667,-2.264452774  
 H,0,2.2634405435,5.7110642132,-2.4947311522  
 H,0,1.2376212292,9.1337502581,1.1278691053  
 H,0,2.6303523139,8.1347936111,0.4569137064  
 H,0,2.0839534506,7.8909260438,2.1906298373  
 H,0,0.2037166158,5.0465060127,3.8189053404  
 H,0,0.1492437876,6.6790428555,3.0244445888  
 H,0,1.6975799948,6.0739522473,3.7563484911  
 H,0,1.4481613645,3.1994341622,2.7743782108  
 H,0,3.5971975729,0.2808122326,2.4644269877  
 H,0,7.2307276975,0.1681895108,3.2575549938  
 H,0,6.2338510052,-1.2408493086,2.6927723985  
 H,0,5.55373026,-0.0819148315,3.9093941083  
 H,0,9.5655468972,0.2451368526,0.9195621514  
 H,0,8.3440166407,0.0303730712,-0.4405766145  
 H,0,8.0677566418,-0.7948963149,1.1749690911  
 H,0,7.0247416757,3.8831757293,-0.6070710204  
 H,0,6.391445812,2.907533221,-2.000882407  
 H,0,7.8400228055,2.3314860846,-1.0633845198  
 H,0,4.1578699133,2.8992034638,-0.9391164597  
 H,0,-2.2782168549,-4.0727936769,-1.4603230526  
 H,0,0.9588919952,1.6002645638,4.9817877383  
 C,0,1.7930513877,-1.479124402,-6.6670014043  
 H,0,3.2036105688,-0.0672209791,-5.7980244726  
 H,0,3.7980078923,-1.7386207174,-5.8456962935  
 H,0,2.1204624284,-1.3149557923,-7.6967387088  
 H,0,1.5114002837,-2.5283277934,-6.5528421044  
 H,0,0.9149124758,-0.8580973257,-6.4709508412

**TS1b**

E(RAM1) = -0.749165201903

E(RM062X) = -1385.07070346

E(RAM1) = -1.10466549511

Zero-point correction= 1.282299  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.363796  
 Thermal correction to Enthalpy= 1.364740  
 Thermal correction to Gibbs Free Energy= 1.147240  
 Sum of electronic and zero-point Energies= -1383.432904  
 Sum of electronic and thermal Energies= -1383.351407  
 Sum of electronic and thermal Enthalpies= -1383.350463  
 Sum of electronic and thermal Free Energies= -1383.567963

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	855.795	306.405	457.768

C,0,-6.0673685761,-0.5825290531,0.4945018814  
 C,0,-5.6501922118,0.6840114041,0.9294867454  
 C,0,-6.5883685563,1.7242436949,1.0016958696  
 C,0,-7.9154978697,1.5017545663,0.6399213695  
 C,0,-8.3229341529,0.2396062417,0.2090831224  
 C,0,-7.3964650943,-0.8002850574,0.137060364  
 C,0,-4.2740459348,0.8900452462,1.3934032426  
 C,0,-3.1433483901,0.3768149429,0.6804963968  
 C,0,-1.9151414071,0.3373083327,1.3392125502  
 C,0,-1.7302770339,0.9249141869,2.6308148504  
 C,0,-2.8276971615,1.5834936597,3.2360295064  
 C,0,-4.0971663848,1.5193380174,2.6114560437  
 C,0,-2.6387582789,2.2362563603,4.4859315932  
 C,0,-1.4191875215,2.1987251615,5.1156326035  
 C,0,-0.3383672687,1.4901778085,4.537290551  
 C,0,-0.4935955747,0.860386634,3.3266693261  
 C,0,-3.2734672953,-0.1414956585,-0.683047787  
 C,0,-2.8189907587,-1.4276384662,-0.9925640763  
 C,0,-3.1518763846,-2.0524498856,-2.2439635964  
 C,0,-3.8627435448,-1.3010245918,-3.2089461754  
 C,0,-4.161739252,0.0591445469,-2.9434632449  
 C,0,-3.8627681009,0.6402133611,-1.7254472163  
 C,0,-2.8059018693,-3.400064248,-2.5251964935  
 C,0,-3.1684040102,-3.976633074,-3.7195486616  
 C,0,-3.8892586324,-3.230782137,-4.6810169877  
 C,0,-4.2277802008,-1.9220482564,-4.4346512462  
 O,0,-2.109647145,-2.196302589,-0.1255463269  
 B,0,-0.872229403,-1.7334791307,0.5945601759  
 O,0,-0.8117396449,-0.2414619254,0.7514981458  
 C,0,-4.0834758636,2.0842966376,-1.5880120916  
 C,0,-3.1009181237,2.9056078907,-1.0162644862  
 C,0,-3.279849999,4.2862581242,-0.9599476783  
 C,0,-4.440616625,4.8647302838,-1.4726002178  
 C,0,-5.4248048099,4.0557282909,-2.0396537051  
 C,0,-5.2489662619,2.6748147649,-2.0999044341  
 O,0,0.3350120788,-2.0960190547,-0.1894651278  
 B,0,0.796699941,-3.3646485253,-0.062278381  
 O,0,0.4223209632,-4.1899376558,0.962173513  
 B,0,-0.3665314362,-3.6612694251,1.9857331853  
 O,0,-0.496347891,-4.5136638222,3.0764909214  
 C,0,-1.2265583449,-4.2968816866,4.2254854589  
 C,0,-2.0917553811,-3.2157032188,4.4295049579  
 C,0,-2.7880082985,-3.1295304985,5.6341915913  
 C,0,-2.6247257966,-4.1036734611,6.6184438304  
 C,0,-1.7594075867,-5.177327028,6.4022478745  
 C,0,-1.0513516096,-5.2873979424,5.2095200577  
 O,0,1.7461801239,-3.7564969817,-1.0272955179  
 C,0,2.4199604393,-4.9583225477,-1.1049458362

C,0,3.0310345786,-5.1992781033,-2.3490646835  
 C,0,3.7968380914,-6.3502717363,-2.5090516302  
 C,0,3.947055228,-7.2541960987,-1.4564047719  
 C,0,3.3213729721,-7.0118228549,-0.2340320602  
 C,0,2.5517365937,-5.8644475718,-0.0461686544  
 O,0,-0.871615485,-2.4212752132,1.8767648376  
 N,0,3.2856862748,-1.3672066112,-0.8430752991  
 N,0,3.7811330495,-1.5257478233,0.1360460586  
 C,0,2.5785566824,-0.9976990655,-1.9465825638  
 C,0,2.0865972033,0.8627873638,-1.5225417023  
 C,0,1.2186262917,1.0650480456,-2.7182433128  
 C,0,1.7663031541,1.7329917383,-3.8169711687  
 C,0,1.0027206855,1.9342845139,-4.9637115605  
 C,0,-0.3070178812,1.4600121217,-5.0143003773  
 C,0,-0.8503279775,0.7877342303,-3.9183102783  
 C,0,-0.0927893901,0.5866160331,-2.7680331451  
 C,0,3.4193608053,-0.9478665015,-3.1765262687  
 O,0,4.5781434514,-0.5977036104,-3.1864843328  
 O,0,2.684528493,-1.2466869389,-4.2382438993  
 C,0,3.2955820834,-1.0064198158,-5.5231545292  
 N,0,1.5991771714,0.9312781923,-0.2744211558  
 C,0,2.2083417459,1.6775974948,0.8730659794  
 C,0,3.6800922621,1.4780279255,1.0375498154  
 C,0,4.1317259129,0.6510014652,2.0735260984  
 C,0,5.4977134523,0.479156991,2.3163312952  
 C,0,6.420182058,1.1495841033,1.4928029592  
 C,0,5.9864601351,1.988783437,0.4499046379  
 C,0,4.6135780744,2.147281407,0.2410645377  
 C,0,5.9468725482,-0.3870344302,3.4306077397  
 O,0,7.781188683,1.0861976978,1.7700282896  
 C,0,8.4094599919,-0.1001253615,1.2828894115  
 C,0,6.9572834941,2.7210999355,-0.3947468656  
 C,0,1.8641348946,3.134669936,0.8657120489  
 C,0,1.9588329207,3.923311502,-0.2837971123  
 C,0,1.6557174879,5.2871630439,-0.2482488964  
 C,0,1.2451131563,5.857562076,0.9703308299  
 C,0,1.1203642847,5.075890598,2.1325505384  
 C,0,1.4278417095,3.7141439775,2.0628232468  
 C,0,1.7391333093,6.1022182733,-1.4815480587  
 O,0,0.8516941953,7.1921616507,0.9769385521  
 C,0,1.8326504584,8.0717541015,1.5262918906  
 C,0,0.6580656651,5.6625266369,3.411468205  
 H,0,1.6297431893,-1.5322863596,-1.9573363367  
 H,0,-2.9069509304,-5.0219790281,-3.9376669137  
 H,0,0.3155711872,0.2623594493,2.8793305126  
 H,0,2.888172261,-4.4901429649,-3.175256908  
 H,0,4.279621025,-6.5492659284,-3.4772748601  
 H,0,4.5517949967,-8.1616855754,-1.5948491298  
 H,0,3.42808932,-7.7316902985,0.5913396163  
 H,0,2.035358771,-5.6823580333,0.9104661127  
 H,0,-0.3699908416,-6.1279004005,5.0217828065  
 H,0,-1.6335908396,-5.9461629696,7.1786366739  
 H,0,-3.1785550668,-4.028044627,7.5645945228  
 H,0,-3.4715766308,-2.2842505417,5.8032297998  
 H,0,-2.2157760871,-2.4499532215,3.646307111  
 H,0,-1.2713040645,2.7023620763,6.0819627948  
 H,0,-3.4921055293,2.7641106092,4.9370406485  
 H,0,-4.9628978526,1.9470871275,3.1409663369  
 H,0,-6.2703634973,2.7226095374,1.3375264535  
 H,0,-8.6421974728,2.3249471877,0.6964107739  
 H,0,-9.3711640893,0.064785442,-0.0721370634  
 H,0,-7.7125743312,-1.7976490587,-0.2020952173  
 H,0,-5.3343057085,-1.4031331411,0.43368444596  
 H,0,-6.033498554,2.039869141,-2.5388146641  
 H,0,-6.3447101643,4.5067009881,-2.4392176116  
 H,0,-4.5803465028,5.9541578356,-1.4268820635  
 H,0,-2.5030712768,4.9192186215,-0.5061900968  
 H,0,-2.1885331793,2.4490742011,-0.6016278319  
 H,0,-4.6311376344,0.6554820159,-3.7405654843  
 H,0,-4.7922298911,-1.3355418976,-5.174100443

H,0,-4.1769244458,-3.7139654974,-5.626312666  
H,0,1.7148587221,1.2278908772,1.7490999124  
H,0,0.6310743461,0.6440436916,-0.0933816186  
H,0,3.0864753423,1.2958883313,-1.6277123208  
H,0,2.7904156127,2.0974453022,-3.7710875864  
H,0,1.4282676466,2.4617313127,-5.8118585329  
H,0,-0.9075525912,1.6156725315,-5.9051401752  
H,0,-1.874441948,0.4196164987,-3.9525649977  
H,0,-0.5200568284,0.0567597745,-1.9175695921  
H,0,2.2611575073,3.4767135119,-1.2443493112  
H,0,1.9271302776,7.1764872745,-1.2320135991  
H,0,0.7713772644,6.0409492603,-2.0412518359  
H,0,2.5575945167,5.7376061896,-2.1490833302  
H,0,1.3376675675,9.074243146,1.4943658067  
H,0,2.7552930105,8.0637279193,0.8968776565  
H,0,2.0764011885,7.7810218013,2.5770481769  
H,0,0.0213138944,4.9336820519,3.972072584  
H,0,0.0602060377,6.5899948197,3.2274700228  
H,0,1.5368332258,5.9276536801,4.0521163229  
H,0,1.3011586546,3.0902348608,2.9645811404  
H,0,3.4060148438,0.1335276355,2.7224622669  
H,0,6.9674541588,-0.0865955159,3.7769931126  
H,0,5.9860036449,-1.4548409702,3.0967015021  
H,0,5.2418140082,-0.3169235014,4.2955287328  
H,0,9.470569033,0.0054131869,1.6208281808  
H,0,8.3492560416,-0.1407206958,0.1684037692  
H,0,7.9365277425,-1.0067525269,1.7326988952  
H,0,7.9409437773,2.1886213823,-0.4180979701  
H,0,7.1271775971,3.744676639,0.0258709271  
H,0,6.5783269719,2.8262680039,-1.4407402692  
H,0,4.2725483339,2.8377822687,-0.5471814  
H,0,-2.2509216643,-3.9647555105,-1.7583410486  
H,0,0.6166191556,1.4380483506,5.0792708079  
C,0,2.2474923432,-1.3133858631,-6.5675003  
H,0,3.6189529441,0.0394020452,-5.5539298148  
H,0,4.1803234967,-1.6431247673,-5.6098238728  
H,0,2.6536052501,-1.1266221971,-7.5648469342  
H,0,1.9363191491,-2.3587032867,-6.5069210417  
H,0,1.3704051908,-0.6782641928,-6.4172446828

## TS1c

E(RAM1) = -0.743583391008

E(RM062X) = -1385.07714767

E(RAM1) = -1.09600395298

Zero-point correction= 1.283134  
(Hartree/Particle)  
Thermal correction to Energy= 1.364154  
Thermal correction to Enthalpy= 1.365098  
Thermal correction to Gibbs Free Energy= 1.151306  
Sum of electronic and zero-point Energies= -1383.441593  
Sum of electronic and thermal Energies= -1383.360573  
Sum of electronic and thermal Enthalpies= -1383.359629  
Sum of electronic and thermal Free Energies= -1383.573421

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.020	306.163	449.963

C,0,6.2025136968,-1.1320308725,-2.1922992634  
C,0,6.3601587315,-1.4477865095,-0.83493502  
C,0,7.3567894662,-2.359494235,-0.4570502052  
C,0,8.173985212,-2.9482652579,-1.4199468275  
C,0,8.011366406,-2.62940852,-2.7677343789  
C,0,7.0248637849,-1.7210579231,-3.1507079354  
C,0,5.5527673915,-0.7670764953,0.1830379467

C,0,4.1410057596,-0.5868599492,0.0375517387  
C,0,3.4973070825,0.3157371873,0.8841885617  
C,0,4.1710149404,0.8993219148,2.0060338038  
C,0,5.5371012966,0.5905741795,2.2119878822  
C,0,6.2137909827,-0.2152227308,1.263736867  
C,0,6.2059399997,1.1356696308,3.3430259961  
C,0,5.5417697784,1.961335632,4.2164060061  
C,0,4.1816335677,2.2857871377,3.9976170744  
C,0,3.5125723477,1.7675021924,2.915838736  
C,0,3.3903872744,-1.2850689322,-1.0090090828  
C,0,2.6317653788,-0.5439332785,-1.9181301561  
C,0,2.0663912355,-1.1506159667,-3.0874017747  
C,0,2.1921377932,-2.5510992327,-3.248556894  
C,0,2.8205014832,-3.3113974927,-2.2307988158  
C,0,3.3968389381,-2.708968409,-1.1278386817  
C,0,1.4040725247,-0.3894702788,-4.0867048397  
C,0,0.895259719,-1.0043618675,-5.2053820096  
C,0,1.0235520569,-2.4038693374,-5.3707608202  
C,0,1.6550227516,-3.1619536153,-4.4150782724  
O,0,2.4416385074,0.8003077075,-1.7610705967  
B,0,1.7071950301,1.2769098622,-0.5452770641  
O,0,2.1708485351,0.6361089179,0.7336458826  
C,0,3.9226833475,-3.5790544254,-0.0706276789  
C,0,3.6441510991,-3.317153995,1.2786010973  
C,0,4.0831298649,-4.1889593738,2.2727370603  
C,0,4.8059329056,-5.3326105822,1.9349035882  
C,0,5.0928624731,-5.5985448042,0.5964110485  
C,0,4.654325884,-4.7302217246,-0.4011213285  
O,0,0.2610051361,0.9237183745,-0.6396485241  
B,0,-0.5187656019,1.7231438179,-1.3948335446  
O,0,-0.1343649432,2.9765509606,-1.7922838156  
B,0,1.0284942915,3.5035718917,-1.2240186814  
O,0,1.1637020905,4.8766694637,-1.4340488127  
C,0,2.2336278726,5.6694817169,-1.0794791412  
C,0,3.4372151324,5.1945583275,-0.5444084366  
C,0,4.4479523771,6.1071950515,-0.2468804587  
C,0,4.263546381,7.4700287959,-0.477944276  
C,0,3.0601299939,7.9309075261,-1.0139026617  
C,0,2.0343362482,7.0418083655,-1.3194961592  
O,0,-1.8080583929,1.2151681439,-1.7093670024  
C,0,-2.7139839829,1.799942848,-2.57195602  
C,0,-3.5832785986,0.903370324,-3.2176172255  
C,0,-4.5946788198,1.4120795764,-4.0280489328  
C,0,-4.7341436396,2.7884965242,-4.208615962  
C,0,-3.8520631008,3.6670718667,-3.5797021599  
C,0,-2.8359981777,3.1830375351,-2.7574265421  
O,0,1.862369661,2.7252577543,-0.5171847968  
N,0,-0.5804770219,-1.3326740539,0.5697489045  
N,0,-0.9933961673,-1.73676135,-0.3753358695  
C,0,-0.29328591,-0.7004007607,1.7438244499  
C,0,-1.9028164723,0.5396770909,1.879110984  
C,0,-1.2976283934,1.9030890134,1.7991404037  
C,0,-0.1975169345,2.2244918024,2.6012804374  
C,0,0.3371792602,3.5053035203,2.5727372774  
C,0,-0.2191841171,4.479276507,1.7433743231  
C,0,-1.3356969194,4.1751908895,0.9712428344  
C,0,-1.8859173415,2.8951609452,1.0113552001  
C,0,-0.4761447807,-1.6124399607,2.9013763177  
O,0,-1.1378205681,-2.6272527363,2.8946678811  
O,0,0.0973487525,-1.0793021531,3.9803612646  
C,0,-0.0625286111,-1.8155130257,5.2127477991  
N,0,-2.8269983824,0.1567929214,0.9877411632  
C,0,-3.8734397433,-0.8637143223,1.322300262  
C,0,-5.2175678485,-0.250876122,1.5497418222  
C,0,-6.0039908306,-0.753455143,2.5930612271  
C,0,-7.2753683791,-0.2340323163,2.8484295845  
C,0,-7.7526496246,0.8131405386,2.0392764081  
C,0,-6.9759420184,1.3309602494,0.9874632906  
C,0,-5.7091500529,0.7862112983,0.7532714819  
C,0,-8.0933036051,-0.7885698394,3.9515903972



O,0,-9.052187478,1.2822802602,2.2010764395  
 C,0,-9.1877190518,2.2312195798,3.2592459307  
 C,0,-7.4904045684,2.415277445,0.12025244  
 C,0,-3.9475837764,-1.9600966059,0.3133888202  
 C,0,-4.4106666073,-1.7188881321,-0.9827161016  
 C,0,-4.5168443433,-2.7590943378,-1.9094200514  
 C,0,-4.1595204892,-4.0606422318,-1.509700906  
 C,0,-3.6813590688,-4.3193920188,-0.2124082267  
 C,0,-3.5726337944,-3.2554324008,0.6876420523  
 C,0,-4.9708851953,-2.4949181141,-3.2933792399  
 O,0,-4.1827258485,-5.0721453041,-2.4634714317  
 C,0,-5.3161824062,-5.933787919,-2.3540385871  
 C,0,-3.2859488015,-5.6839669245,0.2058363213  
 H,0,0.6252747444,-0.1121292643,1.6396486335  
 H,0,0.386546829,-0.417390527,-5.9835174997  
 H,0,2.456686227,2.0129955504,2.715713466  
 H,0,-3.450903415,-0.1813098344,-3.0879758983  
 H,0,-5.2805759418,0.7173550782,-4.5358536483  
 H,0,-5.5322130551,3.179256569,-4.8558555058  
 H,0,-3.9507265009,4.7516599347,-3.7367463388  
 H,0,-2.1167879742,3.8696635102,-2.2819265641  
 H,0,1.0849679789,7.3877319092,-1.7494162439  
 H,0,2.9178462886,9.0055012125,-1.2003751472  
 H,0,5.0668067294,8.1818310308,-0.2417593084  
 H,0,5.3982706066,5.7428493043,0.1710598187  
 H,0,3.5770072202,4.115114029,-0.3672908866  
 H,0,6.0583433164,2.3846776687,5.0900329862  
 H,0,7.2654505265,0.883743511,3.4981374097  
 H,0,7.297213387,-0.3695985874,1.3847509358  
 H,0,7.4865165898,-2.6150757271,0.6051908941  
 H,0,8.9495678245,-3.6649553772,-1.1138762209  
 H,0,8.6591994314,-3.0920839558,-3.5257806051  
 H,0,6.8926643152,-1.4661300585,-4.2123980191  
 H,0,5.4194936502,-0.4177177817,-2.4946767305  
 H,0,4.893438175,-4.9390293831,-1.4550319816  
 H,0,5.6696387517,-6.494750085,0.3252058012  
 H,0,5.1520191407,-6.0191636034,2.7204755792  
 H,0,3.862958685,-3.9694269917,3.3273511209  
 H,0,3.0907853169,-2.4044150284,1.5487471984  
 H,0,2.8280261402,-4.4078369235,-2.3291715575  
 H,0,1.7608729956,-4.2499914515,-4.5355529305  
 H,0,0.6117063566,-2.8746294092,-6.2754559265  
 H,0,-3.5393045952,-1.3115286045,2.2718955123  
 H,0,-2.7471565652,0.494216042,0.0272790907  
 H,0,-2.1227709747,0.21117083251,2.8963415634  
 H,0,0.2538781211,1.4644448551,3.2349563953  
 H,0,1.2042910859,3.7417866191,3.181464732  
 H,0,0.2204131583,5.470713763,1.6958848644  
 H,0,-1.7725550636,4.9275220281,0.3230995654  
 H,0,-2.7735170523,2.6764291643,0.4257510179  
 H,0,-4.7038855489,-0.6974801974,-1.2779609219  
 H,0,-4.0890628563,-2.4945859706,-3.9841861384  
 H,0,-5.4846118867,-1.505262461,-3.3722129929  
 H,0,-5.6722809833,-3.2981670783,-3.6321378612  
 H,0,-5.1529548485,-6.6886428101,-3.1632027968  
 H,0,-6.2578831333,-5.3595085614,-2.5294733049  
 H,0,-5.3401819119,-6.4238373776,-1.3504245386  
 H,0,-2.4250170468,-5.6466628581,0.9182319331  
 H,0,-2.98947648,-6.2978941454,-0.6813329011  
 H,0,-4.1425119991,-6.19140497,0.717719076  
 H,0,-3.1789910521,-3.4488094968,1.7006843426  
 H,0,-5.6277288767,-1.577582642,3.2192529949  
 H,0,-9.1819399103,-0.6133060516,3.7618358324  
 H,0,-7.8190129863,-0.2956766877,4.918521673  
 H,0,-7.9225650835,-1.8882389435,4.0576234417  
 H,0,-10.2795264515,2.4741699335,3.2589061211  
 H,0,-8.5775834998,3.1418011644,3.045103503  
 H,0,-8.8807042872,1.7772361506,4.2327951561  
 H,0,-8.2424009544,3.0361313681,0.6684623381  
 H,0,-7.9941123016,1.9743567264,-0.7771687844

H,0,-6.6604940456,3.0767873157,-0.2297999491  
 H,0,-5.1062033578,1.1933709162,-0.0739293707  
 H,0,1.3208171553,0.6996118045,-3.9386921303  
 H,0,3.673446321,2.9612805889,4.7001942558  
 C,0,0.6549874299,-1.0364013305,6.2912215165  
 H,0,-1.1322792733,-1.9216713911,5.4153293594  
 H,0,0.3579328159,-2.8148673086,5.0705452566  
 H,0,0.5633295651,-1.5618747077,7.2449661285  
 H,0,1.7157615663,-0.9329348171,6.0513608725  
 H,0,0.222926433,-0.0388313793,6.4019255215

## TS1d

E(RAM1) = -0.745459055666

E(RM062X) = -1385.07484967

E(RAM1) = -1.09781905791

Zero-point correction= 1.283321  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.364180  
 Thermal correction to Enthalpy= 1.365124  
 Thermal correction to Gibbs Free Energy= 1.152675  
 Sum of electronic and zero-point Energies= -1383.439169  
 Sum of electronic and thermal Energies= -1383.358310  
 Sum of electronic and thermal Enthalpies= -1383.357366  
 Sum of electronic and thermal Free Energies= -1383.569815

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.036	306.058	447.137

C,0,6.3901373384,-1.165012477,-1.7854408004  
 C,0,6.47518845,-1.3511699562,-0.3979601801  
 C,0,7.4665731348,-2.1987592134,0.1178563039  
 C,0,8.3498995397,-2.8521266614,-0.7391696738  
 C,0,8.2591780756,-2.6621778936,-2.1176850674  
 C,0,7.2783433421,-1.8180711799,-2.6376970892  
 C,0,5.5962869969,-0.6015454073,0.5059430546  
 C,0,4.1915575452,-0.4731809478,0.2663576979  
 C,0,3.4815812811,0.485021102,0.9895974759  
 C,0,4.0750896333,1.1843359976,2.0902189071  
 C,0,5.4337261648,0.9330640088,2.3981089339  
 C,0,6.1816192053,0.064286275,1.5656670763  
 C,0,6.0236516419,1.5936771936,3.5111539184  
 C,0,5.2907130751,2.4724597203,4.2703487201  
 C,0,3.9378679983,2.7369715812,3.9497210208  
 C,0,3.344334157,2.1082328719,2.8824374417  
 C,0,3.5172994591,-1.2844809285,-0.7502603116  
 C,0,2.7945748655,-0.6517272567,-1.7646380423  
 C,0,2.3129985463,-1.3786496233,-2.9026327222  
 C,0,2.4819414062,-2.7835834704,-2.9267519576  
 C,0,3.0669341244,-3.4294062818,-1.8090506439  
 C,0,3.5631529528,-2.7126250978,-0.7358106901  
 C,0,1.6915692861,-0.731087547,-4.0031109069  
 C,0,1.2643501377,-1.4594800357,-5.0872686148  
 C,0,1.4368699128,-2.8636708965,-5.115926798  
 C,0,2.0296810549,-3.5130693777,-4.0606138972  
 O,0,2.5620992306,0.6944837052,-1.7450848518  
 B,0,1.7561145711,1.2647870568,-0.6173146446  
 O,0,2.1596185185,0.755548034,0.7357069119  
 C,0,4.0444395114,-3.4677637932,0.425898836  
 C,0,3.6870358806,-3.0871731883,1.7274896791  
 C,0,4.0850360563,-3.8519001271,2.8219982955  
 C,0,4.8446275815,-5.005923034,2.6331845489  
 C,0,5.2101336662,-5.3894532257,1.3432275324  
 C,0,4.8133980762,-4.6280168679,0.2458842979  
 O,0,0.3225933109,0.8737686542,-0.7525636842

B,0,-0.4280629636,1.5821947286,-1.6187363184  
 O,0,-0.0417628137,2.7993656225,-2.1134406649  
 B,0,1.0778389806,3.4040044622,-1.5350595517  
 O,0,1.1964922176,4.7555012795,-1.8623979994  
 C,0,2.2219935725,5.6065120803,-1.5107478553  
 C,0,3.3984258617,5.2140248562,-0.8607614302  
 C,0,4.3652653435,6.1777533634,-0.5788421669  
 C,0,4.1643574704,7.5101900403,-0.9379567939  
 C,0,2.9886344567,7.8885942411,-1.5878067596  
 C,0,2.0066945213,6.9471595439,-1.8805989504  
 O,0,-1.6929208331,1.0215696544,-1.9476629948  
 C,0,-2.566262437,1.4958020438,-2.9056831445  
 C,0,-3.4557798398,0.5323820831,-3.4145999194  
 C,0,-4.4277687611,0.9289204884,-4.328618517  
 C,0,-4.5140258783,2.2593587697,-4.7401477538  
 C,0,-3.6170932722,3.2026310243,-4.2397230529  
 C,0,-2.6367404406,2.8316680381,-3.320692815  
 O,0,1.886307323,2.7129699634,-0.7179847675  
 N,0,-0.4646235696,-1.3114501044,0.654424404  
 N,0,-0.7971585238,-1.8021673771,-0.2836669509  
 C,0,-0.2834706662,-0.5591525355,1.7727824923  
 C,0,-1.9752499161,0.6342400928,1.679646064  
 C,0,-1.4026442017,2.000461049,1.5144680524  
 C,0,-0.3703497482,2.432243883,2.354669712  
 C,0,0.135750702,3.7189384901,2.2289549981  
 C,0,-0.3855114847,4.5884384211,1.2699478351  
 C,0,-1.4421854107,4.1780206519,0.4635672144  
 C,0,-1.9619082405,2.8923074223,0.5957922192  
 C,0,-0.4260505912,-1.2940431814,3.0500179654  
 O,0,-0.1850306643,-0.7700095284,4.1115489305  
 O,0,-0.9363751397,-2.5270623936,2.9081806757  
 C,0,-1.0983657413,-3.2749080136,4.1339481452  
 N,0,-2.8033970233,0.1260383066,0.7618489557  
 C,0,-3.8366808059,-0.8959799275,1.1253121526  
 C,0,-5.1911615238,-0.2964531808,1.3269050152  
 C,0,-5.9825637436,-0.7872252929,2.3719016222  
 C,0,-7.2617825098,-0.2764900998,2.6050063533  
 C,0,-7.7419882591,0.7500923124,1.7714916796  
 C,0,-6.9602460024,1.2561096155,0.7174988471  
 C,0,-5.6858795113,0.7201179868,0.5058337995  
 C,0,-8.0844018955,-0.8178979917,3.7111870536  
 O,0,-9.0475468389,1.2085090252,1.9117327961  
 C,0,-9.2037121848,2.1761207158,2.9503401486  
 C,0,-7.4765972043,2.3194983065,-0.1741874036  
 C,0,-3.8869267468,-2.0329348003,0.1608764204  
 C,0,-4.5142466319,-1.9082468229,-1.0799845587  
 C,0,-4.6145511583,-3.0016398461,-1.9476397775  
 C,0,-4.0651907429,-4.2322128774,-1.5487699132  
 C,0,-3.4110664158,-4.3709964529,-0.3088605533  
 C,0,-3.326861419,-3.2615774246,0.5335224685  
 C,0,-5.2896984846,-2.847531518,-3.2565926902  
 O,0,-4.0578755173,-5.316350182,-2.41886364  
 C,0,-5.2983385499,-6.0225187136,-2.4632504628  
 C,0,-2.8054591771,-5.6647196354,0.0799368189  
 H,0,0.5870639066,0.0940932996,1.6493958247  
 H,0,0.7870399272,-0.9608168744,-5.9430200888  
 H,0,2.2949512765,2.3035357968,2.6065805171  
 H,0,-3.3647831419,-0.5162602327,-3.0954218545  
 H,0,-5.1254275991,0.1822673954,-4.7366778723  
 H,0,-5.2819543529,2.5607941169,-5.4666555492  
 H,0,-3.674864682,4.2489488599,-4.5755279718  
 H,0,-1.9094746819,3.5699944596,-2.9450646065  
 H,0,1.0798517374,7.2277439367,-2.3982732381  
 H,0,2.8335048295,8.938990662,-1.8747791416  
 H,0,4.9329035898,8.2626843348,-0.7126133199  
 H,0,5.2939132042,5.8780398403,-0.07055139  
 H,0,3.5519148829,4.158146464,-0.581982461  
 H,0,5.7454527719,2.9833262183,5.1314996941  
 H,0,7.0778685582,1.386002406,3.7467307986  
 H,0,7.2594969928,-0.0486212951,1.7599516551

H,0,7.5398387076,-2.3524322557,1.2048521233  
 H,0,9.1209027288,-3.5176707567,-0.3251112338  
 H,0,8.9591048313,-3.1754878288,-2.7921952374  
 H,0,7.2028305791,-1.6646506477,-3.7241489401  
 H,0,5.6117056037,-0.5014727787,-2.1959232925  
 H,0,5.1160227851,-4.928302602,-0.7688898852  
 H,0,5.817223498,-6.293450314,1.1894881403  
 H,0,5.1594564821,-5.6073534459,3.4977717994  
 H,0,3.8053454087,-3.5373804212,3.8379166832  
 H,0,3.1054942095,-2.1647281012,1.8804871451  
 H,0,3.1063690663,-4.5294888131,-1.8053325792  
 H,0,2.1698722839,-4.6037382728,-4.0748580299  
 H,0,1.0904993274,-3.4262748941,-5.9952392451  
 H,0,-3.5019738612,-1.3005680495,2.0954830164  
 H,0,-2.6773605919,0.390731852,-0.2172359032  
 H,0,-2.2364781244,0.3765465143,2.7071426825  
 H,0,0.0487462839,1.7539155222,3.0950513918  
 H,0,0.9526242093,4.0413309071,2.8668107661  
 H,0,0.0334811338,5.5827150581,1.1496974454  
 H,0,-1.8543597843,4.850022907,-0.2816520779  
 H,0,-2.8033832978,2.5897877738,-0.019593354  
 H,0,-4.9466852499,-0.9394407563,-1.380836114  
 H,0,-4.9197356508,-3.6127885621,-3.9842079423  
 H,0,-5.0999872726,-1.8299149283,-3.6823394824  
 H,0,-6.3951131383,-2.9766354001,-3.1357629291  
 H,0,-5.1217753852,-6.8175152244,-3.2301401505  
 H,0,-6.126569845,-5.3419794036,-2.7774751937  
 H,0,-5.5222616095,-6.4738320972,-1.4664505541  
 H,0,-2.517884849,-5.6715561478,1.1603879369  
 H,0,-1.890075783,-5.8541385788,-0.5366225254  
 H,0,-3.524607998,-6.5005960391,-0.110841183  
 H,0,-2.8137971158,-3.363206651,1.5056383176  
 H,0,-5.6038835641,-1.5941321033,3.0184688128  
 H,0,-9.1729089808,-0.6566750483,3.5085085673  
 H,0,-7.8234565273,-0.304060288,4.6709238722  
 H,0,-7.9043786664,-1.9136543684,3.8397102553  
 H,0,-10.2979340499,2.4074517641,2.9339122866  
 H,0,-8.6006758544,3.0886727735,2.7248910972  
 H,0,-8.9022626174,1.7437565415,3.9353714899  
 H,0,-8.2389090344,2.9435049547,0.3559740744  
 H,0,-7.9684801155,1.8578352024,-1.0677169475  
 H,0,-6.6495301074,2.9820852858,-0.5289860809  
 H,0,-5.0783709786,1.1185624399,-0.3225178276  
 H,0,1.5727624748,0.3639087404,-3.9606319117  
 H,0,3.3728274175,3.4523746832,4.5639242909  
 C,0,-1.6599960437,-4.6296311872,3.7663382826  
 H,0,-0.1204100544,-3.3511228026,4.6167382846  
 H,0,-1.7612961086,-2.7123599295,4.7975155931  
 H,0,-1.7508217144,-5.2425991573,4.6665989151  
 H,0,-2.6507456022,-4.5370616444,3.3130108861  
 H,0,-0.9998493678,-5.1436259138,3.0631159581

### C. Alternative Ring Closing Transition Structures (major enantiomer)

#### TS2a

cis-RC-TS1-ONIOM-M06-BB  
 E(RAM1) = -0.728770402400

E(RM062X) = -1385.06430300

E(RAM1) = -1.08316478035

Zero-point correction= 1.283065  
 (Hartree/Particle)

Thermal correction to Energy= 1.364861

Thermal correction to Enthalpy= 1.365805  
 Thermal correction to Gibbs Free Energy= 1.148392  
 Sum of electronic and zero-point Energies= -1383.426843  
 Sum of electronic and thermal Energies= -1383.345047  
 Sum of electronic and thermal Enthalpies= -1383.344103  
 Sum of electronic and thermal Free Energies= -1383.561517

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	856.463	306.902	457.586

C,0,2.8510415847,6.261263955,-3.0276176408  
 C,0,2.8513700967,4.9609700646,-2.4893351675  
 C,0,3.9852382766,4.4374032743,-1.8573149206  
 C,0,5.1296422578,5.2282668765,-1.7656807467  
 C,0,5.1442064284,6.5182554095,-2.2947684595  
 C,0,4.0070152497,7.0285069509,-2.9230275279  
 O,0,1.6630166971,4.2841456739,-2.6622344859  
 B,0,1.3286937935,3.0248693588,-2.1758706962  
 O,0,0.0496314998,2.612213112,-2.5580415845  
 B,0,-0.4310372788,1.4411028083,-2.0439276805  
 O,0,-1.7639518527,1.0222803411,-2.2853383265  
 C,0,-2.6380766891,1.6740476411,-3.1343704844  
 C,0,-2.6819878716,3.067119911,-3.2777016828  
 C,0,-3.6628153959,3.6317337396,-4.0905867347  
 C,0,-4.5839740309,2.8217541573,-4.7551425602  
 C,0,-4.5227649289,1.4351716314,-4.6157385235  
 C,0,-3.5513318975,0.8467380568,-3.8092524396  
 O,0,0.301307696,0.6300185318,-1.2537185885  
 B,0,1.7486592082,0.8859509056,-1.0275936344  
 O,0,2.0913530398,2.2489423963,-1.3913925647  
 O,0,1.9313902345,0.615394665,0.4529588093  
 C,0,3.2282268811,0.7056896623,0.9019896013  
 C,0,4.2019883716,-0.1995407645,0.4774856867  
 C,0,5.5673793179,0.0741027312,0.8068614506  
 C,0,5.8708354559,1.0735814251,1.7115017821  
 C,0,4.8618434783,1.8868447974,2.2858272786  
 C,0,3.5231008761,1.7369817131,1.8499336928  
 C,0,2.5223774456,2.6038283418,2.3640321308  
 C,0,2.8442570311,3.5645274369,3.2920534341  
 C,0,4.1780818845,3.7023778016,3.7446471983  
 C,0,5.1657327735,2.884955806,3.2522844519  
 C,0,3.8130483094,-1.3754622876,-0.3052213663  
 C,0,3.0406533674,-1.2202701061,-1.4606313969  
 C,0,2.7478229946,-2.3313848149,-2.3216695653  
 C,0,3.1937699032,-3.6181283929,-1.9410023867  
 C,0,3.8747227674,-3.7772167446,-0.7090725695  
 C,0,4.1776465954,-2.6973907067,0.1007695667  
 C,0,2.9246212444,-4.7225246928,-2.7958201138  
 C,0,2.241360207,-4.5413467031,-3.9736329866  
 C,0,1.7924839765,-3.253384145,-4.3503508818  
 C,0,2.0396913516,-2.1696990206,-3.5420344619  
 C,0,6.6779286032,-0.6048150901,0.1317040894  
 C,0,6.6590485984,-0.7769663971,-1.2603167614  
 C,0,7.7483749009,-1.3515185647,-1.9121235758  
 C,0,8.8665532191,-1.7600475955,-1.1856622863  
 C,0,8.8927756349,-1.5918674746,0.1984174758  
 C,0,7.8076477497,-1.0147847991,0.8549354454  
 O,0,2.5765307546,-0.0127342363,-1.8829486906  
 C,0,4.817180955,-2.9884253989,1.3900472465  
 C,0,4.4046718449,-2.3598664295,2.5731270156  
 C,0,4.9650829916,-2.715195975,3.7986087548  
 C,0,5.949915538,-3.6999096594,3.8612971603  
 C,0,6.3792653252,-4.3214715979,2.6890137448  
 C,0,5.8190618837,-3.9704444604,1.462918393  
 N,0,0.6084712396,-1.6379915787,1.489172251  
 N,0,1.2242219124,-2.5448351151,1.549292664  
 C,0,-0.7481493631,-0.5865263001,1.1757660523  
 C,0,-1.1991232315,-0.2327797445,2.5934715164  
 O,0,-0.9428031962,1.0406639647,2.8149248996

C,0,-1.3542942932,1.5638930649,4.1003833877  
 C,0,-0.9486362088,3.0188572928,4.1309210146  
 C,0,-1.637796778,-1.310525234,0.1833419809  
 H,0,-1.1601971744,-1.1393255775,-0.7849380994  
 N,0,-2.6825160128,-0.3024553315,0.3265169894  
 C,0,-3.9522242813,-0.5983933558,1.0508351703  
 C,0,-4.5427454063,0.6555955797,1.6154512416  
 C,0,-4.7413124573,0.7503780841,2.9966120569  
 C,0,-5.3101406228,1.8950915977,3.5618950395  
 C,0,-5.6648880299,2.9621969816,2.7170507659  
 C,0,-5.4606815477,2.8887306719,1.3272451192  
 C,0,-4.8993097489,1.7258313297,0.7910890116  
 C,0,-5.5055665796,1.9736330626,5.0277727365  
 O,0,-6.1244839795,4.1426430817,3.2930201981  
 C,0,-7.5418898083,4.2974306244,3.2183935953  
 C,0,-5.8249008492,4.0125502565,0.4341968891  
 C,0,-4.988798593,-1.3324447188,0.2558187979  
 C,0,-5.2572683958,-1.033359338,-1.0825064804  
 C,0,-6.2554341854,-1.7188111898,-1.7819803667  
 C,0,-6.9902252436,-2.7167586474,-1.116756878  
 C,0,-6.7386954005,-3.0273881947,0.2307639845  
 C,0,-5.7337071185,-2.3262879032,0.9018031288  
 C,0,-7.5167650373,-4.0685992376,0.9404416527  
 O,0,-8.0505861715,-3.3175836464,-1.7889537945  
 C,0,-7.7419915145,-4.6174067596,-2.2907208184  
 C,0,-6.5581794687,-1.3824546734,-3.1914386837  
 O,0,-1.6858177076,-1.0036358341,3.3862427282  
 H,0,1.2516984381,-3.1311654633,-5.2998030159  
 H,0,1.4916887425,2.4860916103,1.991886084  
 H,0,-1.927896419,3.6965748179,-2.7784422914  
 H,0,-3.7017868304,4.7245247781,-4.2131238037  
 H,0,-5.352207234,3.2752339405,-5.3976060657  
 H,0,-5.2398429058,0.7981227464,-5.1549940138  
 H,0,-3.4824611103,-0.2445783985,-3.7038302586  
 H,0,1.9487323955,6.646585384,-3.5208921983  
 H,0,4.0203765066,8.0457930114,-3.3408781599  
 H,0,6.0510584495,7.1341396564,-2.2182560786  
 H,0,6.0257644589,4.8254179039,-1.2707824569  
 H,0,3.9662326345,3.4170844552,-1.4404207124  
 H,0,4.4121867996,4.477757229,4.4886855923  
 H,0,6.2072554282,2.9898592423,3.5903484417  
 H,0,6.92003839,1.2772190739,1.976569849  
 H,0,7.8318756871,-0.8864454855,-1.9473897509  
 H,0,9.7719592947,-1.9133900216,0.7751330515  
 H,0,9.7251273958,-2.2119628338,-1.7024846618  
 H,0,7.7233835429,-1.480433309,-3.0041283358  
 H,0,5.7739073138,-0.4562032715,-1.833700857  
 H,0,6.1745747362,-4.4548695047,0.5405160477  
 H,0,7.1655647021,-5.0894472059,2.7299875524  
 H,0,6.3905884046,-3.9800284701,4.8286690943  
 H,0,4.6329776127,-2.2100788878,4.7172972909  
 H,0,3.6531775917,-1.5574338892,2.530583852  
 H,0,4.1521882626,-4.7966683941,-0.39889645  
 H,0,3.2820915261,-5.7187264055,-2.4968130249  
 H,0,2.0394562817,-5.3932338886,-4.6395280398  
 H,0,-3.6709557302,-1.2448604275,1.8975149039  
 C,0,-1.9589975739,-2.7831382119,0.3007233447  
 H,0,1.7081670972,-1.1551391412,-3.8181564582  
 H,0,2.0750834818,4.2447327067,3.6854184909  
 H,0,-0.184379828,0.2175044491,0.7079309788  
 H,0,-4.4516754973,-0.0848246263,3.6545620972  
 H,0,-4.7440137889,1.6581657519,-0.2975557429  
 H,0,-5.5352570453,-2.5607771703,1.9594462048  
 H,0,-4.6889961985,-0.2475048124,-1.6083901734  
 H,0,-4.5239079623,2.1583987115,5.5329417038  
 H,0,-6.1981284407,2.8107672812,5.2934895544  
 H,0,-5.9289503869,1.016768153,5.4214698521  
 H,0,-5.8437298526,4.9775386727,0.9997504662  
 H,0,-5.0915064819,4.1048227934,-0.4046750237  
 H,0,-6.8398521773,3.8390252306,-0.005151592

H,0,-7.7243752746,5.298681004,3.6821740891  
H,0,-7.8818816566,4.2830432792,2.1543228413  
H,0,-8.0500465015,3.4907190705,3.8001024911  
H,0,-8.5171542124,-4.2096598422,0.4598213945  
H,0,-6.9691898785,-5.0444396793,0.9109074229  
H,0,-7.6721435813,-3.7862651991,2.0108461646  
H,0,-5.7239292402,-0.8026174524,-3.6591659933  
H,0,-6.7324483256,-2.3146991056,-3.7850813011  
H,0,-7.4916501726,-0.7661735621,-3.2396412251  
H,0,-8.69680744,-4.9521997177,-2.7673860078  
H,0,-6.9208251379,-4.5583326391,-3.0454695319  
H,0,-7.4527833858,-5.3006977263,-1.4554074795  
H,0,-2.7575789134,0.2777424569,-0.5059914525  
H,0,-2.4385935692,1.4250800827,4.187281178  
H,0,-0.8643764191,0.9728971638,4.8793050761  
H,0,-1.2227843487,3.4535904022,5.0953877053  
H,0,0.1315894467,3.1190755849,3.9929037013  
H,0,-1.4552065629,3.5771431624,3.340667417  
C,0,-2.1225532171,-3.4845059498,-0.8995141587  
C,0,-2.4136304553,-4.8459603232,-0.8947174198  
C,0,-2.5313584064,-5.5276996721,0.3148381759  
C,0,-2.3599121076,-4.8396229071,1.5139219176  
C,0,-2.078920267,-3.4739845089,1.5112333394  
H,0,-2.0116111138,-2.9590164685,-1.8443295928  
H,0,-2.5333103137,-5.3738102966,-1.8351541527  
H,0,-2.7470582452,-6.5913173377,0.3226971039  
H,0,-2.4430792766,-5.3648974961,2.4601569822  
H,0,-1.9489702311,-2.9521224351,2.4533418578

## TS2b

E(RAM1) = -0.738595660514

E(RM062X) = -1385.06876159

E(RAM1) = -1.09045901661

Zero-point correction= 1.283027  
(Hartree/Particle)  
Thermal correction to Energy= 1.364452  
Thermal correction to Enthalpy= 1.365396  
Thermal correction to Gibbs Free Energy= 1.150569  
Sum of electronic and zero-point Energies= -1383.433871  
Sum of electronic and thermal Energies= -1383.352446  
Sum of electronic and thermal Enthalpies= -1383.351502  
Sum of electronic and thermal Free Energies= -1383.566329

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	856.207	306.809	452.141

C,0,-5.3801685877,-1.9817941032,1.317264025  
C,0,-5.2348052127,-0.5965934796,1.4820977849  
C,0,-6.3823389796,0.20734051,1.5475996724  
C,0,-7.6490120513,-0.3636635099,1.4422388314  
C,0,-7.7855961436,-1.7417387621,1.2779241628  
C,0,-6.649383903,-2.5480020751,1.2157269503  
C,0,-3.9049780152,-0.0105564209,1.6821670765  
C,0,-2.7802884844,-0.3719208468,0.8738976549  
C,0,-1.5088938647,-0.0027566867,1.3120891273  
C,0,-1.3173549486,0.82377664,2.464123816  
C,0,-2.458282804,1.2939694597,3.1574249884  
C,0,-3.7395319524,0.8402850975,2.7591438454  
C,0,-2.2802956635,2.1522589388,4.2781202017  
C,0,-1.0194908628,2.489670469,4.7049657454  
C,0,0.1213824183,1.9752109616,4.0427052556  
C,0,-0.0242015131,1.1572636897,2.9489999616  
C,0,-2.9382398552,-1.1720407245,-0.3431113936  
C,0,-2.2132699234,-2.360138673,-0.4883823778

C,0,-2.5137100514,-3.2897992455,-1.5420729637  
C,0,-3.4869408397,-2.9325522486,-2.5046322562  
C,0,-4.0931530874,-1.6541659732,-2.4334732873  
C,0,-3.8229553194,-0.7819297168,-1.395112426  
C,0,-1.8846750043,-4.5602657585,-1.6242833453  
C,0,-2.2144393782,-5.436509958,-2.6304674497  
C,0,-3.1870170905,-5.0809588189,-3.5947417029  
C,0,-3.8094939587,-3.8578793787,-3.5354494982  
O,0,-1.238487261,-2.7447392886,0.3768807835  
B,0,-0.0681280342,-1.8657367419,0.7577169059  
O,0,-0.3780902666,-0.4030792641,0.632505872  
C,0,-4.4074534645,0.5618622157,-1.4694133485  
C,0,-3.628382224,1.6982891419,-1.2094388023  
C,0,-4.1696729917,2.9743759627,-1.3541763906  
C,0,-5.4937706945,3.1328984327,-1.7619270458  
C,0,-6.2775099115,2.0084443832,-2.0196740882  
C,0,-5.7400902494,0.7309682473,-1.8764684506  
O,0,1.0523903177,-2.1130121978,-0.1845046435  
B,0,1.7874572307,-3.2361224626,0.0309294481  
O,0,1.8040951396,-3.875681209,1.2393615204  
B,0,1.1126839586,-3.3063554177,2.3096302972  
O,0,1.387539735,-3.9125055905,3.5295449742  
C,0,0.8383028432,-3.6097779944,4.7571444148  
C,0,-0.2355923463,-2.7346454216,4.9568874971  
C,0,-0.713508407,-2.5411034308,6.2521281106  
C,0,-0.1310020864,-3.2076700291,7.3294487027  
C,0,0.9399910192,-4.0772501892,7.1168393635  
C,0,1.4376484458,-4.2879134283,5.8346836885  
O,0,2.5513170909,-3.6768474912,-1.0637509132  
C,0,3.3645804697,-4.7889268011,-1.1384552202  
C,0,4.1366879183,-4.8570592595,-2.3127658938  
C,0,4.963859812,-5.9584805032,-2.5107961986  
C,0,5.0309794652,-6.9750014399,-1.557244292  
C,0,4.2653188318,-6.8919515185,-0.3946682055  
C,0,3.4258556677,-5.8009808756,-0.1733499672  
O,0,0.3045242746,-2.250464576,2.1069267735  
N,0,0.7305351075,-1.6272245851,-2.7664784651  
N,0,0.8894113043,-2.613591213,-3.218954539  
C,0,0.6307480577,0.0278136377,-2.2495295239  
C,0,1.9844164904,0.4795094839,-1.7417173984  
C,0,3.1893791075,0.2252628168,-2.6269418597  
C,0,3.8552696318,-0.9939048588,-2.4694863191  
C,0,4.9667551437,-1.2990854888,-3.2516407411  
C,0,5.4316893081,-0.382385916,-4.1922224359  
C,0,4.7755203878,0.8369959019,-4.3487583268  
C,0,3.6572307687,1.1397516741,-3.5736885941  
C,0,0.1016238801,0.644481369,-3.5513034705  
O,0,0.6966840879,1.4705281769,-4.1952098176  
O,0,-1.0738034815,0.1192721001,-3.8502714599  
C,0,-1.7420073474,0.6474255763,-5.0256834515  
N,0,1.5098354502,1.8307890213,-1.5358843791  
C,0,1.6041817603,2.450160393,-0.1790268131  
C,0,2.995034151,2.645834285,0.3410187433  
C,0,3.2080092759,2.5048570868,1.7173981199  
C,0,4.4746046656,2.6936048113,2.2756404907  
C,0,5.5431570359,3.0312575323,1.426055766  
C,0,5.3494481115,3.180917991,0.0413011739  
C,0,4.0687634362,2.9865187885,-0.4853644574  
C,0,4.6682292458,2.5373550728,3.735607443  
O,0,6.7944990583,3.3272579336,1.9581582689  
C,0,7.5718600931,2.1687484749,2.2608962977  
C,0,6.4707460844,3.5623614969,-0.8474206715  
C,0,0.8624862031,3.7487434465,-0.1864165567  
C,0,1.3752606842,4.8602674753,-0.8616568393  
C,0,0.6813566877,6.0724821455,-0.8796127782  
C,0,-0.553192926,6.1523710209,-0.2093342124  
C,0,-1.0874765012,5.0424145084,0.4686900174  
C,0,-0.3676701753,3.8431608811,0.4701367053  
C,0,1.2315205205,7.2371449634,-1.6096074848  
O,0,-1.2917851136,7.3272371427,-0.3178883628

C,0,-1.2082485442,8.1591623466,0.8392339659  
 C,0,-2.3912699596,5.121552368,1.1666141335  
 H,0,-0.0972844779,-0.1077914972,-1.4424891926  
 H,0,-1.7345110083,-6.4239640224,-2.6920733757  
 H,0,0.8442773137,0.7066753042,2.4409752818  
 H,0,4.0759807621,-4.0485591625,-3.053591864  
 H,0,5.5684957557,-6.0241314328,-3.4273259639  
 H,0,5.6883133905,-7.8402455725,-1.7230315786  
 H,0,4.320162119,-7.6922153256,0.3586637383  
 H,0,2.8250154875,-5.7312002873,0.7482566037  
 H,0,2.277885083,-4.9704451055,5.6495513186  
 H,0,1.3977683219,-4.6029194527,7.9676409495  
 H,0,-0.5150747069,-3.0498161828,8.3468991085  
 H,0,-1.5580667305,-1.856240644,6.4191661217  
 H,0,-0.6891038511,-2.2100398571,4.100151841  
 H,0,-0.8797490926,3.1503156277,5.573142787  
 H,0,-3.1732599213,2.5280527528,4.7991807743  
 H,0,-4.6112456112,1.1403100335,3.361770016  
 H,0,-6.2789831708,1.29514109,1.6759425492  
 H,0,-8.5421788107,0.2757264043,1.4915607075  
 H,0,-8.7857901562,-2.1912155668,1.1997073718  
 H,0,-6.7516886708,-3.6356651677,1.0881270745  
 H,0,-4.4821892181,-2.6185930365,1.2663256242  
 H,0,-6.3671611034,-0.1532462957,-2.0676713672  
 H,0,-7.3249949084,2.1281002883,-2.332842934  
 H,0,-5.9191562193,4.140383222,-1.8751652423  
 H,0,-3.5494301534,3.8582430481,-1.1377987706  
 H,0,-2.5871746681,-1.5755075958,-0.8718113381  
 H,0,-4.7846501567,-1.3595036042,-3.2374294898  
 H,0,-4.5745024461,-3.5768401066,-4.2739764737  
 H,0,-3.4414672739,-5.800496177,-4.38696331  
 H,0,1.0779867088,1.7499889068,0.4928187595  
 H,0,1.6979516061,2.4578172568,-2.3096318285  
 H,0,2.1264360855,-0.0086037036,-0.7740607111  
 H,0,3.5024978922,-1.7136639827,-1.7356478805  
 H,0,5.473636886,-2.2495587893,-3.1122751095  
 H,0,6.302590061,-0.6145564374,-4.7971942835  
 H,0,5.1310206177,1.5563430721,-5.0798599881  
 H,0,3.1515115253,2.0875457785,-3.7276484848  
 H,0,2.3487423504,4.7883444989,-1.3719981398  
 H,0,0.8523262428,8.1931835596,-1.1694015193  
 H,0,0.9116874626,7.1994172086,-2.6815874242  
 H,0,2.3484269268,7.2407623401,-1.5727696097  
 H,0,-1.8757340318,9.0225632729,0.5947948052  
 H,0,-0.1566180556,8.5013639435,0.9955062195  
 H,0,-1.5771342219,7.6131905979,1.7414469727  
 H,0,-2.9420480817,4.1509865279,1.0870041758  
 H,0,-3.0267946901,5.9303459805,0.7270895587  
 H,0,-2.2322041678,5.3450954404,2.2518727203  
 H,0,-0.779063348,2.9657307163,1.0009376659  
 H,0,2.3632029975,2.2487441031,2.3795782516  
 H,0,5.5346523676,3.1515103534,4.0867440901  
 H,0,4.8708884378,1.4642771209,3.9828082998  
 H,0,3.7527556513,2.8565311615,4.2929370006  
 H,0,8.5116710503,2.5867245552,2.7000654072  
 H,0,7.7901513221,1.593689146,1.3286618845  
 H,0,7.0397844679,1.5221884329,3.0004238996  
 H,0,7.4473409473,3.2307514791,-0.4138540083  
 H,0,6.5029799224,4.6756104981,-0.9601140851  
 H,0,6.35235778,3.1065761958,-1.8606727868  
 H,0,3.9253497348,3.0986826722,-1.5717846659  
 H,0,-1.1437454406,-4.8237630305,-0.8516056351  
 H,0,1.1215089096,2.2304624977,4.4232751302  
 C,0,-2.3757566204,1.9892237174,-4.7189754754  
 H,0,-1.0100145574,0.7138170268,-5.8338272192  
 H,0,-2.4869816636,-0.1132138404,-5.2596233999  
 H,0,-2.9725520392,2.31234658,-5.5757664092  
 H,0,-3.0334850612,1.9106914987,-3.8469740222  
 H,0,-1.6124757489,2.7456510746,-4.52574358

## TS2c

E(RAM1) = -0.733664460149

E(RM062X) = -1385.06890407

E(RAM1) = -1.08536024914

Zero-point correction=	1.282379
(Hartree/Particle)	
Thermal correction to Energy=	1.364081
Thermal correction to Enthalpy=	1.365025
Thermal correction to Gibbs Free Energy=	1.149478
Sum of electronic and zero-point Energies=	-1383.434866
Sum of electronic and thermal Energies=	-1383.353164
Sum of electronic and thermal Enthalpies=	-1383.352220
Sum of electronic and thermal Free Energies=	-1383.567767

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	855.974	307.254	453.658

C,0,-5.460252218,-2.5420562791,0.6375715932  
 C,0,-5.506354685,-1.2025504933,1.0500691004  
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 H,0,-2.3443525055,2.1008773703,-4.5021049366  
 H,0,-2.77166237,4.5788816452,-4.3165721772  
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 H,0,-1.4008582729,4.7314522363,-3.199263756

## TS2d

E(RAM1) = -0.728447014753

E(RM062X) = -1385.06964320

E(RAM1) = -1.08230502754

Zero-point correction= 1.282222  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.363782  
 Thermal correction to Enthalpy= 1.364726  
 Thermal correction to Gibbs Free Energy= 1.151317  
 Sum of electronic and zero-point Energies= -1383.433563  
 Sum of electronic and thermal Energies= -1383.352003  
 Sum of electronic and thermal Enthalpies= -1383.351059  
 Sum of electronic and thermal Free Energies= -1383.564468

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	855.786	307.556	449.156

C,0,-5.8360921689,-1.3725855392,1.5848711934  
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 C,0,-7.1170162192,-1.9164564292,1.5123246184

C,0,-4.3194929386,0.5895429469,1.8045695651  
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 H,0,3.4597031612,3.889272254,-1.8334295384  
 H,0,3.2920763706,7.5971938161,-1.6200064728  
 H,0,3.686311396,6.1839429292,-2.6906364903  
 H,0,4.7586650996,6.5813049877,-1.2839390902  
 H,0,2.970410114,9.1888164813,1.2806092783  
 H,0,4.1349272143,7.9000215366,0.669213882  
 H,0,3.2416418575,7.6485825153,2.2508656279  
 H,0,0.3112977852,5.1000731734,-2.9918994054  
 H,0,-0.3732301229,6.3330028559,1.8459298001  
 H,0,1.1364302678,6.7101925365,2.7694915618  
 H,0,0.7710668894,3.3071091335,1.5180147857  
 H,0,2.2953240317,0.2662798653,1.6895126948  
 H,0,5.2208982265,-1.6679343237,3.0267096675  
 H,0,3.4151179225,-1.7254254944,2.8054361251  
 H,0,4.1684138972,-0.4376179298,3.8415572069  
 H,0,8.1409842325,-1.9446114683,1.6293042244  
 H,0,7.5521856965,-1.3888602484,-0.0245212307  
 H,0,6.4586668153,-2.4096663467,1.0374471053  
 H,0,7.2044002945,0.5229814721,-1.5099412051

H,0,7.9005863239,1.0556356076,0.079501265  
 H,0,7.1113061912,2.2664798738,-1.0207778597  
 H,0,4.6692022121,2.2211893505,-1.3601224423  
 H,0,-1.6891836811,-4.4693018754,-0.3100167825  
 H,0,0.7358508533,2.9844749067,4.3575670143  
 C,0,-3.1473149924,-0.0531468954,-5.5748362661  
 H,0,-2.7095135112,1.8182084646,-4.5472925002  
 H,0,-1.4908988596,1.3549743037,-5.7538141987  
 H,0,-3.7607696383,0.4117436926,-6.3501967958  
 H,0,-2.601467411,-0.8888749055,-6.0183258794  
 H,0,-3.8073742954,-0.4373695577,-4.7919644067

## TS2e

E(RAM1) = -0.740870058300

E(RM062X) = -1385.06837739

E(RAM1) = -1.09351061405

Zero-point correction= 1.282578  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.364022  
 Thermal correction to Enthalpy= 1.364966  
 Thermal correction to Gibbs Free Energy= 1.150954  
 Sum of electronic and zero-point Energies= -1383.433158  
 Sum of electronic and thermal Energies= -1383.351715  
 Sum of electronic and thermal Enthalpies= -1383.350771  
 Sum of electronic and thermal Free Energies= -1383.564783

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	855.937	307.232	450.427

C,0,-5.9051544113,-1.6597255608,1.4862897537  
 C,0,-5.8302380125,-0.2600916018,1.5386459664  
 C,0,-7.0174869123,0.4859800792,1.5753943151  
 C,0,-8.2538135349,-0.1563264292,1.5522092703  
 C,0,-8.3202027789,-1.5482633494,1.4993644997  
 C,0,-7.1441428153,-2.2970679398,1.4664566572  
 C,0,-4.5289212402,0.4073177184,1.6511927  
 C,0,-3.4054852448,0.0295138275,0.8490966082  
 C,0,-2.1422008418,0.4874830744,1.2227726238  
 C,0,-1.9669120234,1.4244519744,2.29008198  
 C,0,-3.1157601174,1.9092943232,2.960321001  
 C,0,-4.3821063588,1.3607376263,2.6409278249  
 C,0,-2.9590648289,2.8828736106,3.9856443059  
 C,0,-1.7081830878,3.3158268496,4.3507358266  
 C,0,-0.5567348597,2.787659734,3.7188522286  
 C,0,-0.6834086393,1.8610205687,2.7124713071  
 C,0,-3.5524138201,-0.866672657,-0.3004274704  
 C,0,-2.7774758866,-2.0285830586,-0.3737477939  
 C,0,-3.037973385,-3.0354401234,-1.363726335  
 C,0,-4.0265841701,-2.7821762451,-2.3438255356  
 C,0,-4.692486287,-1.5321072128,-2.3476977487  
 C,0,-4.4652689707,-0.5873112621,-1.3635732307  
 C,0,-2.3560017914,-4.2814240846,-1.3661228893  
 C,0,-2.6500026995,-5.233627187,-2.3122846164  
 C,0,-3.6363758169,-4.9813456327,-3.29527882  
 C,0,-4.3089986521,-3.7839913874,-3.3133783442  
 O,0,-1.7864981758,-2.3127763862,0.5159301196  
 B,0,-0.6446980909,-1.3697515607,0.774368195  
 O,0,-1.0094491987,0.0716454032,0.5581766088  
 C,0,-5.1337792331,0.7115238651,-1.5009928392  
 C,0,-4.4337637607,1.9076631943,-1.2884703629  
 C,0,-5.0599634612,3.137300138,-1.4853487285  
 C,0,-6.3912914667,3.1897752477,-1.8966620706  
 C,0,-7.0964443691,2.0052902086,-2.1083514512  
 C,0,-6.47416224,0.7740444069,-1.9135994691  
 O,0,0.4514890311,-1.626724284,-0.1943378382

B,0,1.3717395381,-2.5739197362,0.1043670209  
 O,0,1.5526890073,-3.051086866,1.3746555078  
 B,0,0.7843491034,-2.5057338323,2.4045318043  
 O,0,1.1866761743,-2.9256119837,3.6683001791  
 C,0,0.596917576,-2.6236582486,4.8777899126  
 C,0,-0.6072209584,-1.9258211261,5.0257730095  
 C,0,-1.1035069321,-1.7061538609,6.3099405614  
 C,0,-0.411945409,-2.1741958994,7.4266294565  
 C,0,0.7873136376,-2.8698672291,7.265104297  
 C,0,1.3058812565,-3.1022856252,5.9949520847  
 O,0,2.1595971857,-3.0165363538,-0.9755335425  
 C,0,3.2038195649,-3.9168364087,-0.9008654995  
 C,0,3.4899534326,-4.588584907,-2.1025061827  
 C,0,4.5769593165,-5.4572553806,-2.1446061223  
 C,0,5.364615238,-5.6628178254,-1.0112857967  
 C,0,5.0652317303,-4.9964772008,0.1768759242  
 C,0,3.9845865804,-4.1186322786,0.2440456265  
 O,0,-0.1950753355,-1.6290385169,2.1330733819  
 N,0,-0.1352634944,-1.1782986258,-2.7772580056  
 N,0,-0.2256004217,-2.2124478599,-3.1302288106  
 C,0,0.325373539,0.432643896,-2.3013810945  
 C,0,1.8371232892,0.4490061543,-2.1662226086  
 C,0,2.6398200006,0.1245555624,-3.4130603224  
 C,0,2.9849833675,-1.2142369024,-3.6299281821  
 C,0,3.7113171152,-1.5839997175,-4.7599342555  
 C,0,4.1150182,-0.6182403126,-5.6789701738  
 C,0,3.7854314775,0.7180653481,-5.4616352129  
 C,0,3.048107231,1.088672199,-4.3391581613  
 C,0,-0.2930772025,1.2508025843,-3.4425667685  
 O,0,0.2891374622,2.1374170619,-4.0106480558  
 O,0,-1.5231162995,0.8374672778,-3.7027008069  
 C,0,-2.2218887411,1.5299875077,-4.7716262146  
 N,0,1.8345304628,1.8060128551,-1.672966511  
 C,0,2.1994617695,2.0640425443,-0.2438896351  
 C,0,3.4246363864,1.334832136,0.2136841008  
 C,0,3.3144734851,0.4741124607,1.3115010793  
 C,0,4.4159189374,-0.2538233322,1.7719863141  
 C,0,5.6494468223,-0.096290185,1.115543878  
 C,0,5.7829497918,0.7722830452,0.0170427408  
 C,0,4.6601912368,1.4787636988,-0.4226052582  
 C,0,4.2610502551,-1.1689808405,2.9259033412  
 O,0,6.7703411718,-0.7439628157,1.6264068254  
 C,0,7.0919178974,-1.9485864482,0.9303771592  
 C,0,7.0820002959,0.9415900918,-0.6738262724  
 C,0,2.3182744342,3.5345650034,0.0011181325  
 C,0,3.1489851518,4.3473980903,-0.7761755995  
 C,0,3.2581431882,5.7185392084,-0.525035136  
 C,0,2.5094452986,6.2740477044,0.526692371  
 C,0,1.6572374211,5.4761380459,1.3114074552  
 C,0,1.5692021161,4.109816535,1.0333525932  
 C,0,4.1497418452,6.554934732,-1.3604777164  
 O,0,2.5167799762,7.6491340779,0.7408193011  
 C,0,3.636972004,8.0976697507,1.5037024137  
 C,0,0.8475913694,6.0762969683,2.3959974117  
 H,0,-0.2123242993,0.441884712,-1.3444988573  
 H,0,-2.1302716509,-6.2026351713,-2.3111949115  
 H,0,0.1975875273,1.4104916424,2.2267112996  
 H,0,2.8586812267,-4.4241865389,-2.9857682593  
 H,0,4.8091856075,-5.9899223469,-3.0786359477  
 H,0,6.2168904128,-6.3557962302,-1.0539366905  
 H,0,5.6801439426,-5.1665466701,1.0734665143  
 H,0,3.7299403305,-3.6043108068,1.1856781254  
 H,0,2.2457456537,-3.651602029,5.8505153831  
 H,0,1.3306112064,-3.240037944,8.1469148359  
 H,0,-0.8110507043,-1.9968122329,8.4350922201  
 H,0,-2.0494039132,-1.1588238223,6.4367015408  
 H,0,-1.1479657655,-1.5586199248,4.1380810782  
 H,0,-1.584079497,4.0659422064,5.1454050439  
 H,0,-3.8597538947,3.2717195695,4.4833358951  
 H,0,-5.2536476644,1.6755305397,3.2360541223



	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
H,0,-6.9697285048,1.584486365,1.6154734125			
H,0,-9.1785461697,0.4379710248,1.5780709104			
H,0,-9.2963857672,-2.0535915239,1.4856362803			
H,0,-7.1909545096,-3.3952179702,1.4266749937			
H,0,-4.9757251796,-2.251322381,1.458719455			
H,0,-7.0407473896,-0.157140982,-2.0670909031			
H,0,-8.1491558048,2.0410059808,-2.4247548576			
H,0,-6.8846289852,4.1605429355,-2.0479042236			
H,0,-4.5014583585,4.0678864239,-1.3068740789			
H,0,-3.3867096567,1.8690667802,-0.9484768603			
H,0,-5.4003989898,-1.3215192226,-3.1638287065			
H,0,-5.0842981525,-3.5825045967,-4.0670520315			
H,0,-3.8604387392,-5.7602677454,-4.0389918062			
H,0,1.348067833,1.686994236,0.3503443905			
H,0,2.1258558969,2.5060126506,-2.3433081182			
H,0,2.1047226657,-0.2484460983,-1.3668545041			
H,0,2.7048974989,-1.9639839406,-2.8929853838			
H,0,3.9748765187,-2.6265510469,-4.909018537			
H,0,4.688898356,-0.9018966101,-6.555537682			
H,0,4.0982169749,1.4786289535,-6.1699787824			
H,0,2.7854173872,2.1329636668,-4.2093859905			
H,0,3.740568947,3.9187695412,-1.5994457965			
H,0,3.8190126619,7.6241239994,-1.3425705855			
H,0,4.1497639923,6.2002787164,-2.4202828573			
H,0,5.1986613047,6.5035204032,-0.972848736			
H,0,3.4931202865,9.2052588392,1.5612633751			
H,0,4.5912880444,7.8462095474,0.9798773533			
H,0,3.6217680477,7.6412966521,2.5229227199			
H,0,0.4328664841,5.2903773434,3.0754997664			
H,0,-0.004887247,6.653129305,1.9558166759			
H,0,1.4691723195,6.7870132169,2.9961710472			
H,0,0.8946828539,3.4834613346,1.6431568384			
H,0,2.3441035094,0.3501438812,1.8220587716			
H,0,5.1488707597,-1.8415976647,3.0239882621			
H,0,3.3413713061,-1.8015041483,2.8087542917			
H,0,4.162240528,-0.5782805435,3.8711469151			
H,0,7.9788607805,-2.3460020746,1.4834196598			
H,0,7.3536094998,-1.7219390133,-0.1320886129			
H,0,6.2375810955,-2.6700045694,0.9740060597			
H,0,7.1343158294,0.2643560716,-1.5635879497			
H,0,7.9290413636,0.6889745052,0.0120155582			
H,0,7.209863405,1.9946514129,-1.0259549895			
H,0,4.7633549582,2.155596049,-1.2838930029			
H,0,-1.6032627867,-4.4621548537,-0.5811323727			
H,0,0.4368669764,3.1186907081,4.0551068886			
C,0,-2.7306598466,2.8791983285,-4.3078532036			
H,0,-1.5365236292,1.6207678421,-5.6178301996			
H,0,-3.0365096876,0.8516129388,-5.0250956696			
H,0,-3.3241428922,3.3320573001,-5.106478688			
H,0,-3.3696126027,2.7659614452,-3.4251594284			
H,0,-1.9022100989,3.5491157843,-4.0714225598			
Total	855.839	307.257	454.970
C,0,-5.4575606847,-2.6614074667,0.0542858013			
C,0,-5.534247772,-1.4229737629,0.7078667696			
C,0,-6.7908770273,-0.8317349579,0.9050650955			
C,0,-7.9459038449,-1.4642403401,0.449621477			
C,0,-7.861586475,-2.6952596892,-0.2001743912			
C,0,-6.616085177,-3.291221692,-0.3962720577			
C,0,-4.327147439,-0.8005285467,1.2621178421			
C,0,-3.1053761062,-0.7084876047,0.5229578807			
C,0,-1.940594191,-0.3695485891,1.2098408311			
C,0,-1.9637599173,0.0300084799,2.5837657152			
C,0,-3.2088468203,0.0596203043,3.2570371655			
C,0,-4.3704730431,-0.3859464328,2.5797334072			
C,0,-3.2512485361,0.4789028014,4.6157674627			
C,0,-2.0976585289,0.8254018329,5.2749835048			
C,0,-0.8492820686,0.7664883903,4.6100879023			
C,0,-0.7838867534,0.3783224978,3.2941731293			
C,0,-3.0527225245,-1.025504712,-0.9057927418			
C,0,-2.1627459126,-1.9975333263,-1.3738779686			
C,0,-2.2797018593,-2.5274599558,-2.7052051637			
C,0,-3.2207246535,-1.9447884064,-3.586466262			
C,0,-3.97904987,-0.8300272237,-3.1507192168			
C,0,-3.9002439837,-0.3683066814,-1.8500944415			
C,0,-1.5092964776,-3.6378205566,-3.1417262571			
C,0,-1.6716743644,-4.1418279723,-4.4099777715			
C,0,-2.6064746338,-3.5555025835,-5.2959023845			
C,0,-3.3630969718,-2.4810524772,-4.8960323888			
O,0,-1.1841225445,-2.5515168399,-0.610825732			
B,0,-0.2104447411,-1.7595023063,0.2256195345			
O,0,-0.7182037333,-0.3872927531,0.5745899514			
C,0,-4.6448338895,0.8502503619,-1.5133345477			
C,0,-4.0354224232,1.8877766458,-0.7930372619			
C,0,-4.7234649045,3.0746724022,-0.5473693869			
C,0,-6.0281958433,3.2395365047,-1.0111488741			
C,0,-6.6444969616,2.2103731945,-1.7224314269			
C,0,-5.958574406,1.0242580738,-1.9755586192			
O,0,1.02109622,-1.502040132,-0.5580003415			
B,0,2.0463063935,-2.3833660881,-0.4982087771			
O,0,2.1333034052,-3.3456082739,0.4698220279			
B,0,1.147271601,-3.3860674946,1.4574291449			
O,0,1.4224604719,-4.2979920301,2.4703821245			
C,0,0.6376408788,-4.5994090452,3.5631153585			
C,0,-0.6555697375,-4.1093333782,3.7781214652			
C,0,-1.3462617841,-4.5126119298,4.9200612736			
C,0,-0.758573898,-5.3891051281,5.8314248994			
C,0,0.531597557,-5.8712372254,5.6048675776			
C,0,1.2439367285,-5.4842404828,4.4740375767			
O,0,3.0315553406,-2.2281779128,-1.4948459118			
C,0,4.1687684606,-2.99959067,-1.6333338449			
C,0,4.7100046812,-3.027252538,-2.930617593			
C,0,5.9036733411,-3.7105800725,-3.1470085509			
C,0,6.5460651415,-4.365909115,-2.0962127973			
C,0,5.9903387481,-4.3445624369,-0.817028509			
C,0,4.7989957998,-3.663563415,-0.5734741461			
O,0,0.0827127019,-2.5696164468,1.3935437846			
N,0,0.5512250019,-0.6870116106,-3.0702982797			
N,0,0.8089984317,-1.5682763173,-3.6691639154			
C,0,0.5533536032,0.8699627991,-2.1478840421			
C,0,2.0178315288,1.1199362281,-1.8646412876			
C,0,2.8584267657,1.4477895022,-3.0739415296			
C,0,3.7718496795,0.4973424795,-3.5333145353			
C,0,4.5476431885,0.7583348513,-4.6612675205			
C,0,4.4189474933,1.9708427632,-5.3345310882			
C,0,3.50620103,2.9222893507,-4.8815686708			
C,0,2.7254484567,2.6605088052,-3.7592054089			
C,0,-0.1611983351,1.7284258699,-3.2019168107			
O,0,-0.303973839,1.3701841496,-4.342780862			

## TS2f

E(RAM1) = -0.733425710501

E(RM062X) = -1385.06880864

E(RAM1) = -1.08586518483

Zero-point correction=	1.282144
(Hartree/Particle)	
Thermal correction to Energy=	1.363866
Thermal correction to Enthalpy=	1.364810
Thermal correction to Gibbs Free Energy=	1.148639
Sum of electronic and zero-point Energies=	-1383.434225
Sum of electronic and thermal Energies=	-1383.352503
Sum of electronic and thermal Enthalpies=	-1383.351559
Sum of electronic and thermal Free Energies=	-1383.567730

O,0,-0.563298809,2.8789263518,-2.6914475069  
 C,0,-1.2514460101,3.7716902174,-3.6068398983  
 N,0,1.6760446563,2.237920534,-1.0069906321  
 C,0,1.7415562762,2.0524137966,0.4791504988  
 C,0,3.1157038104,1.7798471894,1.0063821684  
 C,0,3.252375516,0.8610343258,2.0532147843  
 C,0,4.5060042632,0.5666906614,2.5968732573  
 C,0,5.639366165,1.2071662653,2.065581106  
 C,0,5.5232201489,2.1338151378,1.0137653586  
 C,0,4.254221257,2.4121381636,0.4981508994  
 C,0,4.6172674699,-0.4053540033,3.708684619  
 O,0,6.8909265307,1.0123158947,2.6416618573  
 C,0,7.5268951805,-0.1958790006,2.2239167896  
 C,0,6.716099086,2.8249204658,0.4733736205  
 C,0,1.1200840494,3.2456990298,1.1300161559  
 C,0,1.8400204615,4.4270663297,1.3254647903  
 C,0,1.237208399,5.5482932934,1.9017577925  
 C,0,-0.1186411572,5.4722618985,2.2687195621  
 C,0,-0.8609349441,4.2937876229,2.0738777329  
 C,0,-0.2260937975,3.185186801,1.5054737773  
 C,0,2.0127865209,6.7945530523,2.0957385104  
 O,0,-0.7445761624,6.6245693668,2.7355344637  
 C,0,-0.9126537866,6.6449608612,4.1531006971  
 C,0,-2.2908306194,4.2131797329,2.4505168515  
 H,0,-0.024188866,0.5152048584,-1.2880434809  
 H,0,-1.0847896722,-5.0086212267,-4.7469268667  
 H,0,0.177351522,0.3139221141,2.7596384187  
 H,0,4.1904063465,-2.5212870964,-3.7550365588  
 H,0,6.3362566033,-3.7383086909,-4.1580264162  
 H,0,7.4860107496,-4.905821696,-2.2789665229  
 H,0,6.490056531,-4.8729494834,0.0086648924  
 H,0,4.3415158468,-3.6642103631,0.4289247115  
 H,0,2.2583127346,-5.8570244603,4.2790442479  
 H,0,0.9931565674,-6.5638689059,6.323870257  
 H,0,-1.3108956234,-5.7019667535,6.7284997729  
 H,0,-2.3633818797,-4.1328673588,5.0977826989  
 H,0,-1.1136271184,-3.4160226733,3.0538185323  
 H,0,-2.1273573308,1.1430273254,6.3275388338  
 H,0,-4.2253521653,0.5097005476,5.1259174731  
 H,0,-5.3160253258,-0.4387033562,3.1420061291  
 H,0,-6.8613118826,0.1397520958,1.4167387403  
 H,0,-8.925884661,-0.9908951402,0.6064042052  
 H,0,-8.7741718056,-3.195135667,-0.5548873844  
 H,0,-6.5443276661,-4.2629361552,-0.9065140176  
 H,0,-4.4732122509,-3.1312818191,-0.1024771586  
 H,0,-6.452768543,0.2109394925,-2.5287571758  
 H,0,-7.6763999542,2.3319945637,-2.0829932438  
 H,0,-6.5703261572,4.1752073475,-0.8128308167  
 H,0,-4.2347735301,3.8809449862,0.0201132318  
 H,0,-3.0119389148,1.7540769155,-0.4076723603  
 H,0,-4.6358276658,-0.3286300311,-3.8779028577  
 H,0,-4.0977652096,-2.0230260371,-5.5746069053  
 H,0,-2.7220910632,-3.9764330192,-6.3056425005  
 H,0,1.1076528125,1.1754085666,0.6996527719  
 H,0,2.0263776108,3.1318658445,-1.3319430981  
 H,0,2.4352089374,0.2731119754,-1.3137293403  
 H,0,3.8685545766,-0.4443214489,-2.9964903973  
 H,0,5.2573280371,0.0142207645,-5.008640366  
 H,0,5.0262117168,2.1753741749,-6.210587087  
 H,0,3.398698086,3.8671235278,-5.4048997055  
 H,0,2.0069200002,3.4096966604,-3.4290771945  
 H,0,2.9026322204,4.4768768131,1.0395835499  
 H,0,1.5874438395,7.3962511576,2.937537309  
 H,0,1.9683054277,7.4189391834,1.1679157312  
 H,0,3.0840110046,6.5678355688,2.3193349842  
 H,0,-1.4544061403,7.6047629506,4.342871607  
 H,0,0.0820768396,6.6428353339,4.6610297809  
 H,0,-1.5217819895,5.7704091973,4.4880990017  
 H,0,-2.851669584,3.5603336106,1.7353105085  
 H,0,-2.7581018166,5.229308682,2.4510821154

H,0,-2.3935837494,3.7740873714,3.4752686525  
 H,0,-0.7955546073,2.2482310992,1.3618599768  
 H,0,2.3606847895,0.3565595757,2.46102951  
 H,0,5.5504035363,-0.2266627745,4.2989449913  
 H,0,4.6461743142,-1.4490231536,3.3041916627  
 H,0,3.7388215269,-0.3226269666,4.3954174635  
 H,0,8.4802032296,-0.2098766077,2.8085404984  
 H,0,7.7336145395,-0.1648984185,1.126746375  
 H,0,6.8924512733,-1.0805386889,2.4746473925  
 H,0,7.6284496384,2.1892878318,0.5973188192  
 H,0,6.8840911314,3.7818305182,1.0294020835  
 H,0,6.5860260283,3.0626960499,-0.6106073066  
 H,0,4.1711596416,3.142462821,-0.321296249  
 H,0,-0.8010352228,-4.0911633102,-2.4287653472  
 H,0,0.0638736352,1.0305914108,5.162652509  
 C,0,-2.6925958587,3.3482403356,-3.8002939237  
 H,0,-1.1745318224,4.7430621414,-3.1174322225  
 H,0,-0.7000595311,3.7851846035,-4.550580559  
 H,0,-3.2130194463,4.0981055919,-4.4018326771  
 H,0,-2.7509715724,2.3894707374,-4.3192081006  
 H,0,-3.2003691458,3.2649742995,-2.8331872414

## D. Side-products

### TS2-H-migration

E(RAM1) = -0.728076640075

E(RM062X) = -1385.05609651

E(RAM1) = -1.08032946431

Zero-point correction=	1.278967
(Hartree/Particle)	
Thermal correction to Energy=	1.360993
Thermal correction to Enthalpy=	1.361938
Thermal correction to Gibbs Free Energy=	1.146744
Sum of electronic and zero-point Energies=	-1383.424877
Sum of electronic and thermal Energies=	-1383.342850
Sum of electronic and thermal Enthalpies=	-1383.341906
Sum of electronic and thermal Free Energies=	-1383.557100

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	854.036	308.644	452.913

C,0,5.0778449818,-0.7880735526,0.3181626721  
 C,0,4.7671415872,-0.8408910185,-1.0437650872  
 C,0,5.6705282515,-1.4274891452,-1.9367985719  
 C,0,6.8781636193,-1.9696127158,-1.4890548428  
 C,0,7.1694432914,-1.9173185166,-0.1151688079  
 C,0,6.2764113235,-1.3255568683,0.797362918  
 C,0,3.5041214756,-0.246244902,-1.5876181624  
 C,0,3.668509139,1.23299402,-1.7385042583  
 C,0,4.221496135,1.709609602,-2.9343643796  
 C,0,4.416052706,3.0758442068,-3.1403932763  
 C,0,4.0322783105,3.974317563,-2.1266825924  
 C,0,3.4640156606,3.5161425232,-0.9262749253  
 C,0,3.2962250868,2.1377504107,-0.7431603445  
 C,0,4.9897752036,3.5672991783,-4.4138169838  
 O,0,4.1311258866,5.338243583,-2.3857312764  
 C,0,5.2449085237,5.9592337853,-1.7451047267  
 C,0,3.0347977045,4.4561690963,0.1347742772  
 C,0,7.8228733997,-2.5743584738,-2.4559729921  
 O,0,8.4060603461,-2.3500203238,0.355396006  
 C,0,8.4847967851,-3.7632957665,0.5323620951  
 C,0,6.6226579002,-1.2460861612,2.2341015525  
 N,0,2.2613065674,-0.6111377616,-0.8511372211  
 C,0,1.48926757,-1.6855110534,-1.3713903889  
 C,0,2.1058404143,-3.0740391028,-1.5314665394

C,0,1.7747249077,-3.883754071,-2.6205754363  
 C,0,2.2991352535,-5.1713023137,-2.7175152771  
 C,0,3.1589330554,-5.6508244794,-1.7312964293  
 C,0,3.5015585473,-4.8369247481,-0.6523262013  
 C,0,2.9779531736,-3.5496899337,-0.5518316247  
 C,0,0.13084007,-1.6901330645,-0.8488814121  
 C,0,-0.810917881,-2.7874956668,-1.2535833831  
 O,0,-1.2260528886,-2.6996706875,-2.3835661901  
 N,0,0.5695184773,-2.2639141843,1.2477831338  
 N,0,0.6923213918,-2.5763017559,2.2923455199  
 O,0,-1.0748504601,-3.6989395139,-0.3561253968  
 C,0,-2.0138858775,-4.7366113345,-0.7664138167  
 O,0,-1.8252939173,0.5228754698,-0.4760410816  
 C,0,-3.0904265269,0.7419157991,-0.9648159984  
 C,0,-4.2083362574,0.1733096804,-0.35498872  
 C,0,-5.5032394117,0.574894636,-0.813380177  
 C,0,-5.6242640878,1.3278419857,-1.9657240745  
 C,0,-4.4873868396,1.7833464296,-2.679216276  
 C,0,-3.1974036548,1.5340127891,-2.1523008794  
 C,0,-4.6083901132,2.5303895801,-3.8832839604  
 C,0,-3.4915445975,3.0201443016,-4.5150521409  
 C,0,-2.2047386758,2.7957663422,-3.9700325144  
 C,0,-2.0600022786,2.0708631067,-2.8120247628  
 C,0,-4.0395907514,-0.7746022556,0.7494541352  
 C,0,-3.2521657503,-0.4313630562,1.8526941488  
 C,0,-3.2116896563,-1.2549837888,3.0276222437  
 C,0,-3.914766329,-2.4825065002,3.0197465269  
 C,0,-4.5880915541,-2.8843574722,1.8399984449  
 C,0,-4.6455334216,-2.068584424,0.7246341172  
 C,0,-2.5054203265,-0.8628477522,4.1958555754  
 C,0,-2.5090306985,-1.6641483019,5.3123174883  
 C,0,-3.216990706,-2.8893629066,5.3086319678  
 C,0,-3.9030661454,-3.2921756202,4.1889156834  
 O,0,-2.5390164321,0.7286006592,1.9157467482  
 B,0,-1.5077784393,1.0705022383,0.8939587397  
 O,0,-0.2051483719,0.4182972563,1.2077695243  
 B,0,0.8029981571,1.1099057234,1.7694291696  
 O,0,1.9425000469,0.3465471616,2.1378645279  
 C,0,2.9164064959,0.7756581934,3.0196553603  
 C,0,3.4039514765,2.0883078175,3.0534698342  
 C,0,4.4357676805,2.402664671,3.9360736284  
 C,0,4.9723992055,1.4257533866,4.7748617939  
 C,0,4.4752912741,0.1225973191,4.7369719338  
 C,0,3.4422714958,-0.2153622589,3.8658565565  
 C,0,-5.2770697411,-2.6196608733,-0.4802881358  
 C,0,-4.6516752582,-2.5233885474,-1.7316201181  
 C,0,-5.2260089624,-3.1145620939,-2.8555588413  
 C,0,-6.4290800064,-3.8108886028,-2.7455925682  
 C,0,-7.0594628008,-3.9103044348,-1.50535582  
 C,0,-6.4887855884,-3.3210464924,-0.3793113365  
 C,0,-6.720254671,0.3049594344,-0.04101836  
 C,0,-6.7440030674,0.5301646242,1.3433049277  
 C,0,-7.9230691988,0.3527369175,2.0643473362  
 C,0,-9.0900209293,-0.04960547,1.415263901  
 C,0,-9.0745310069,-0.2749989238,0.0391993055  
 C,0,-7.8988618504,-0.0963704508,-0.6870981504  
 O,0,-1.3749619475,2.5156009598,0.910015742  
 B,0,-0.3388046487,3.1659637381,1.4559163061  
 O,0,0.7741646352,2.4674879632,1.9364259194  
 O,0,-0.2080399589,4.5455414937,1.5860767102  
 C,0,-1.1357599448,5.5093422013,1.2508480659  
 C,0,-2.4098775523,5.2475148778,0.7340742687  
 C,0,-3.2507060078,6.3207506124,0.4426746272  
 C,0,-2.8297636467,7.631637435,0.6631296297  
 C,0,-1.5572302339,7.8790661891,1.1803868226  
 C,0,-0.6975154489,6.8268002281,1.4797922036  
 H,0,-1.9684143656,-1.3607705458,6.2204098666  
 H,0,-1.0701751551,1.9021360805,-2.3600148698  
 H,0,2.9552095438,2.8608735449,2.4060149428  
 H,0,4.8224183307,3.4321469079,3.9726775559

H,0,5.7825915405,1.6839199812,5.4717666692  
 H,0,4.892374024,-0.6446506347,5.4059550225  
 H,0,3.0317818835,-1.2335038862,3.8399753953  
 H,0,0.3057438614,7.0045883638,1.8890999836  
 H,0,-1.2268317671,8.9135187941,1.3546718316  
 H,0,-3.4994904054,8.4711601077,0.4301285903  
 H,0,-4.2537221532,6.1250889727,0.035216989  
 H,0,-2.737342408,4.2088244219,0.5625762895  
 H,0,-3.5834729846,3.5995019209,-5.4453884449  
 H,0,-5.6137002552,2.7100552696,-4.2918476376  
 H,0,-6.6212098919,1.6206883121,-2.3303540055  
 H,0,-7.8907690828,-0.2770503189,-1.7724044584  
 H,0,-9.992258493,-0.5921999881,-0.4766219412  
 H,0,-10.0194267334,-0.1866826446,1.9860521651  
 H,0,-7.9303192861,0.533596826,3.1492027285  
 H,0,-5.8211560529,0.8466302613,1.8561882111  
 H,0,-6.9972842761,-3.3897271374,0.5945818208  
 H,0,-8.0133746833,-4.4502197998,-1.4150497392  
 H,0,-6.8822168366,-4.2737289883,-3.6338692816  
 H,0,-4.7291766773,-3.0223690417,-3.8326012795  
 H,0,-3.7094091813,-1.9596341436,-1.8288875739  
 H,0,-5.0670535185,-3.875396318,1.8247697463  
 H,0,-4.4621419847,-4.2391052531,4.1790028519  
 H,0,-3.2128479606,-3.5111646965,6.2159520607  
 H,0,3.3632479476,-0.6568917036,-2.6030621987  
 H,0,1.1005575022,-1.379671829,-2.3899210618  
 H,0,-1.9694258301,0.1003438124,4.1783206816  
 H,0,-1.3266804944,3.2173479753,-4.4801757172  
 H,0,-0.3231801576,-0.7530622908,-0.5034805026  
 H,0,1.1070628478,-3.5110246418,-3.3938048688  
 H,0,2.0423021009,-5.793573709,-3.5687722382  
 H,0,3.5718432786,-6.6512950117,-1.8097025455  
 H,0,4.1829418015,-5.2005359069,0.1098646096  
 H,0,3.2673705537,-2.9015208781,0.2733088127  
 H,0,4.5174841477,1.0010128912,-3.7232231293  
 H,0,2.8544623223,1.7859219513,0.2061879115  
 H,0,5.4399245392,-1.4551536972,-3.0133546421  
 H,0,4.3871861452,-0.2991850631,1.0281423162  
 H,0,5.5564878216,4.5175252903,-4.2473709054  
 H,0,5.6772069609,2.8104103443,-4.8641725003  
 H,0,4.1674108208,3.7797839462,-5.142933353  
 H,0,2.0919752212,4.1001803421,0.6289656142  
 H,0,3.8300716246,4.5389754098,0.9182774173  
 H,0,2.8470438479,5.4736309989,-0.2902574449  
 H,0,5.1370078072,7.0397914134,-2.0127116409  
 H,0,5.1929304729,5.8162916695,-0.6383665831  
 H,0,6.2017202844,5.5442553284,-2.1452151839  
 H,0,8.8669821359,-2.5507078839,-2.0546789407  
 H,0,7.5431432949,-3.6402102096,-2.6523941695  
 H,0,7.8023968111,-2.0219799944,-3.4276588397  
 H,0,5.7198937615,-1.0384918717,2.8625425636  
 H,0,7.0936295212,-2.2020861738,2.5746098537  
 H,0,7.3641406234,-0.4226736684,2.3957899639  
 H,0,9.5354868544,-3.9304436972,0.8776353058  
 H,0,7.7546111389,-4.0998337808,1.3077050842  
 H,0,8.2948885648,-4.2906593771,-0.4341842012  
 H,0,2.3136174315,-0.5586982098,0.1635542087  
 C,0,-2.3232553534,-5.5549713293,0.4640158847  
 H,0,-2.899723108,-4.2414712464,-1.1787685343  
 H,0,-1.5292091383,-5.3183064679,-1.5551959353  
 H,0,-3.0077307784,-6.3630458073,0.1946707747  
 H,0,-1.4134276186,-5.9923083783,0.880685322  
 H,0,-2.8038113988,-4.9332796827,1.2251776865

## TS2-phenyl-migration

enamine-TS1-ONIOM-M06-BB  
 E(RAM1) = -0.727321374470

E(RM062X) = -1385.06497071

E(RAM1) = -1.08143022017

Zero-point correction= 1.281644  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.363640  
 Thermal correction to Enthalpy= 1.364584  
 Thermal correction to Gibbs Free Energy= 1.147408  
 Sum of electronic and zero-point Energies= -1383.429218  
 Sum of electronic and thermal Energies= -1383.347222  
 Sum of electronic and thermal Enthalpies= -1383.346278  
 Sum of electronic and thermal Free Energies= -1383.563454

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	855.697	307.331	457.086

C,0,5.9815961316,0.7792536049,0.0960795821  
 C,0,5.6053029074,-0.4732599085,0.6027798524  
 C,0,6.5536893808,-1.50552660539,0.6457999966  
 C,0,7.8509936295,-1.2891687634,0.185540284  
 C,0,8.2182019235,-0.0409092518,-0.3161009639  
 C,0,7.2811523439,0.9910463524,-0.3599494173  
 C,0,4.2652897204,-0.6709260669,1.1660674872  
 C,0,3.0866533025,-0.1843256534,0.5162916801  
 C,0,1.9051403114,-0.1295940985,1.2553798621  
 C,0,1.8007511331,-0.7122050738,2.5583538042  
 C,0,2.9467401073,-1.3290390289,3.115204816  
 C,0,4.17506938,-1.2606507934,2.4131456404  
 C,0,2.8450897237,-1.9514159914,4.3904391122  
 C,0,1.6588699244,-1.9359819669,5.0818938856  
 C,0,0.5223316856,-1.2906844914,4.5376368192  
 C,0,0.5925279258,-0.6884517427,3.3051474733  
 C,0,3.115499287,0.2916921675,-0.8689823492  
 C,0,2.6395257854,1.569169885,-1.1816868347  
 C,0,2.8460611436,2.1447576794,-2.4815690303  
 C,0,3.4601819492,1.3556348802,-3.4823348917  
 C,0,3.7915817454,0.0086483402,-3.1933319656  
 C,0,3.6127466571,-0.5261278103,-1.9305386829  
 C,0,2.4699607986,3.4809830238,-2.7797946525  
 C,0,2.7089778097,4.0093098053,-4.026054574  
 C,0,3.3322082664,3.2252001653,-5.0251170009  
 C,0,3.6982944354,1.9274502031,-4.7623840429  
 O,0,2.0250962741,2.3726324093,-0.2719147207  
 B,0,0.8354487952,1.9406210363,0.5324355972  
 O,0,0.770143494,0.4555543916,0.7425204294  
 C,0,3.8649294308,-1.9624190322,-1.7651408401  
 C,0,2.927824989,-2.7833374238,-1.1218234611  
 C,0,3.1256086076,-4.1611830569,-1.0523600422  
 C,0,4.2657481282,-4.7339174474,-1.6153762403  
 C,0,5.2082291607,-3.9240921056,-2.2484835218  
 C,0,5.0092505045,-2.5474054398,-2.3283428271  
 O,0,-0.4224051023,2.2621290329,-0.1890909074  
 B,0,-0.9571817264,3.4965903906,-0.0509216745  
 O,0,-0.5515305811,4.3740271161,0.9135901473  
 B,0,0.3460177742,3.9126821609,1.884310105  
 O,0,0.5254096676,4.8113436535,2.9297731672  
 C,0,1.3510842478,4.6664662567,4.0244693464  
 C,0,2.2495520849,3.6101144548,4.2138251032  
 C,0,3.0390696204,3.5967902499,5.3627923875  
 C,0,2.9349776075,4.618097195,6.306397228  
 C,0,2.0355218823,5.6663072058,6.1052076433  
 C,0,1.2348750678,5.7041174567,4.9678706703  
 O,0,-2.0233245922,3.7693494666,-0.9369190257  
 C,0,-2.751257973,4.9346848724,-1.0503033711  
 C,0,-3.5221538754,5.021287574,-2.2241575901  
 C,0,-4.3444778053,6.128855399,-2.407682456  
 C,0,-4.3950089124,7.1405370795,-1.4478137942  
 C,0,-3.6126894347,7.0504558202,-0.2967043305

C,0,-2.7831986362,5.9497752474,-0.0866940916  
 O,0,0.8982177723,2.6938091043,1.7766241028  
 N,0,-3.5763585901,1.5446023079,-0.0425737712  
 N,0,-4.1890285084,1.8484885274,0.8143355504  
 C,0,-2.6257798394,0.7502111557,-1.4487948457  
 C,0,-2.5254028985,-0.659135917,-1.0070607865  
 C,0,-1.7145970845,-1.0375646696,-2.2771549757  
 C,0,-2.3720418054,-1.6059929922,-3.3786228025  
 C,0,-1.6632330684,-1.8825158347,-4.5406620783  
 C,0,-0.3011596438,-1.5759438002,-4.6139370603  
 C,0,0.3497246331,-0.9997622555,-3.5251239722  
 C,0,-0.3534739925,-0.7197055368,-2.3544453796  
 C,0,-3.5554179357,1.0899917816,-2.6063577208  
 O,0,-4.7182346609,0.7709118897,-2.618117928  
 O,0,-2.8978500562,1.7356965145,-3.5459399019  
 C,0,-3.6340133081,2.021647194,-4.7582591599  
 N,0,-1.9556948172,-0.7669112076,0.2969886557  
 C,0,-2.1649063809,-1.9834473851,1.131611821  
 C,0,-3.6186717543,-2.2237449465,1.4086747338  
 C,0,-4.1795118558,-1.6416263555,2.5524196468  
 C,0,-5.5249432828,-1.8344107007,2.87686281  
 C,0,-6.3179559556,-2.6251245116,2.0259912715  
 C,0,-5.774290138,-3.2187831181,0.8731038556  
 C,0,-4.4236851578,-3.0070235852,0.5789338453  
 C,0,-6.0868477889,-1.2184036942,4.1009426707  
 O,0,-7.631621747,-2.9262152567,2.372253745  
 C,0,-8.5576377651,-1.8890997221,2.0501581784  
 C,0,-6.6017709659,-4.0790306874,-0.0030354467  
 C,0,-1.4588538828,-3.2400008373,0.7262416711  
 C,0,-1.5408102919,-3.7865969977,-0.5558310792  
 C,0,-0.8773148534,-4.9736416509,-0.8810399214  
 C,0,-0.1073034049,-5.6116097895,0.1072833644  
 C,0,-0.0042583362,-5.0768155389,1.4035454926  
 C,0,-0.6836773789,-3.8915393327,1.69523282  
 C,0,-0.9618788098,-5.5284713681,-2.2511895463  
 O,0,0.6453519923,-6.7256044569,-0.2533545214  
 C,0,0.0679415658,-7.9622649884,0.1640199626  
 C,0,0.8158152715,-5.7350397334,2.4465050101  
 H,0,-1.7405200931,1.3767770361,-1.3061779635  
 H,0,2.4254173086,5.0458788736,-4.2577314773  
 H,0,-0.2699024562,-0.1576545647,2.8712843313  
 H,0,-3.4546936717,4.224943007,-2.9706335345  
 H,0,-4.9527853836,6.2078632876,-3.320714709  
 H,0,-5.0462007934,8.0123957811,-1.6037374429  
 H,0,-3.64331683,7.85481934,0.4537554417  
 H,0,-2.146676347,5.8848015255,0.8112990531  
 H,0,0.5247537203,6.5232297031,4.79268735  
 H,0,1.9560129988,6.4722256762,6.8494267017  
 H,0,3.5620291549,4.5995425047,7.208677069  
 H,0,3.7491084643,2.7712651016,5.5200033595  
 H,0,2.3271258814,2.8064287994,3.4632209258  
 H,0,1.5795445274,-2.4132855451,6.0694864437  
 H,0,3.7380674365,-2.437707592,4.8103035232  
 H,0,5.0792490167,-1.6566820683,2.9012757492  
 H,0,6.2667883323,-2.4931094535,1.0370865157  
 H,0,8.586008637,-2.1061529632,0.2200751667  
 H,0,9.2431723886,0.1292483776,-0.675082616  
 H,0,7.5656811694,1.9774390617,-0.7545331173  
 H,0,5.2398580835,1.5934904298,0.058178953  
 H,0,5.7576693017,-1.9109994315,-2.8242649094  
 H,0,6.1122070391,-4.3711153896,-2.6868249692  
 H,0,4.4203104004,-5.820885069,-1.5588071048  
 H,0,2.3752178531,-4.7992982413,-0.5562081153  
 H,0,2.0349844809,-2.3285917964,-0.6647132161  
 H,0,4.1922775657,-0.6171376037,-4.0053427782  
 H,0,4.1882796008,1.3117007325,-5.5306091461  
 H,0,3.5227440929,3.6708031992,-6.0124548096  
 H,0,-1.7167512384,-1.6786158988,2.0942974873  
 H,0,-1.0002853245,-0.4104357443,0.3819084379  
 H,0,-3.501231557,-1.1598631498,-1.0473834202

H,0,-3.4338767431,-1.8335356119,-3.3151679752  
H,0,-2.1659271753,-2.3400860704,-5.3867694161  
H,0,0.2522902923,-1.7911153699,-5.5228758726  
H,0,1.4111184127,-0.7602123989,-3.5793387081  
H,0,0.1564266503,-0.2686077282,-1.5027657753  
H,0,-2.1220079848,-3.2754656111,-1.3402706363  
H,0,-0.8628029785,-6.6427145529,-2.2303595273  
H,0,-0.1281447279,-5.1198204854,-2.8767022471  
H,0,-1.9329144837,-5.2610618931,-2.734461873  
H,0,0.8107802353,-8.7289464456,-0.169511588  
H,0,-0.9174411328,-8.1190717761,-0.33789955534  
H,0,-0.054551008,-7.9829153035,1.2742963343  
H,0,1.2962447799,-4.974215448,3.1102930729  
H,0,1.6190502169,-6.3590755759,1.9806979694  
H,0,0.1727695193,-6.3978233229,3.0790550617  
H,0,-0.5877078481,-3.4597648023,2.7056040602  
H,0,-3.552400581,-1.0288182882,3.2196948776  
H,0,-6.9760696967,-1.7946400508,4.4600487702  
H,0,-6.4080756106,-0.1669425422,3.8905414541  
H,0,-5.3241451095,-1.1943066101,4.9180098957  
H,0,-9.5366724748,-2.2823841804,2.4215064159  
H,0,-8.588653402,-1.7254204232,0.9457422242  
H,0,-8.2840267907,-0.9420483516,2.5758808924  
H,0,-7.6779609896,-3.7783563802,0.0511144097  
H,0,-6.5232685771,-5.1445778035,0.3315891727  
H,0,-6.2611504188,-4.0162846306,-1.0653297694  
H,0,-3.9939041588,-3.490823764,-0.3122514563  
H,0,1.99372026,4.0758186312,-1.9834011808  
H,0,-0.4089117506,-1.2682942805,5.121302143  
C,0,-2.6830541558,2.7317203705,-5.6926096204  
H,0,-3.9955793713,1.0713844579,-5.1634822036  
H,0,-4.4993221031,2.634750928,-4.4905178901  
H,0,-3.2008214751,2.9786657906,-6.6227714756  
H,0,-2.3185571468,3.6557732827,-5.2380009339  
H,0,-1.8259086136,2.0961683353,-5.9269123609

C,0,-3.6787092284,0.6943866087,1.4485680236  
C,0,-3.3747770965,1.398146879,2.6205848005  
C,0,-3.1958399839,2.7823864282,2.5951402664  
C,0,-3.3039532561,3.4581969916,1.3646465666  
C,0,-3.559058261,2.7606780128,0.1711614453  
C,0,-3.7516991843,1.3758612901,0.2325164752  
C,0,-2.8697542857,3.5196568913,3.8369948135  
O,0,-3.0425709313,4.8244029597,1.341860484  
C,0,-4.2199040991,5.6262100999,1.2477832125  
C,0,-3.608091725,3.4503253198,-1.1385924569  
C,0,-8.4729669475,-1.5750612534,3.4953252738  
O,0,-9.5275059068,-1.6161825572,0.8170143032  
C,0,-9.9981571762,-2.9581379911,0.9372461849  
C,0,-7.9194263253,-1.3764989892,-1.4961923139  
N,0,-3.1002630345,-1.6220054261,0.6814695687  
C,0,-2.2289988417,-2.4827165432,1.222433225  
C,0,-1.6669631443,-3.6177027679,0.4467900323  
C,0,-1.2677952498,-4.7508278245,1.1650462506  
C,0,-0.7092727331,-5.8420103799,0.5055344552  
C,0,-0.5373714982,-5.8013507625,-0.8771452793  
C,0,-0.9207874026,-4.6679969994,-1.5931687978  
C,0,-1.4799797681,-3.573389361,-0.9380724898  
C,0,-0.5759626893,-1.4636631026,1.769671183  
C,0,-0.4909728771,-1.6450597445,3.2404363997  
O,0,-1.3399725878,-1.2025371739,3.9808521633  
N,0,0.4895207377,-2.0007780331,1.0884492744  
N,0,1.2245093529,-2.5863071962,0.5037899013  
O,0,0.5347433836,-2.4086533966,3.6206178369  
C,0,0.6428389772,-2.667905128,5.0373406568  
O,0,1.1973785867,0.530199942,0.5142915085  
C,0,2.4297366685,1.0539762,0.8350515457  
C,0,3.6066160958,0.4713344048,0.3675187471  
C,0,4.8387067171,1.1620200053,0.6046076313  
C,0,4.8690897302,2.247909569,1.4582128356  
C,0,3.689954929,2.7528537383,2.061055222  
C,0,2.4411797226,2.1849483628,1.7120466832  
C,0,3.7216551394,3.8486490984,2.9667869168  
C,0,2.555854443,4.3618176784,3.4805696  
C,0,1.3065440775,3.8112232258,3.1077482176  
C,0,1.2487238045,2.7473016013,2.2404158387  
C,0,3.5739155892,-0.7922370586,-0.3727512143  
C,0,2.7441041011,-0.9419657357,-1.488819654  
C,0,2.8815420149,-2.068833753,-2.3722085028  
C,0,3.7930791848,-3.0935502496,-2.0269842828  
C,0,4.494919286,-3.0094590406,-0.798501232  
C,0,4.3854015256,-1.9026183217,0.0219177388  
C,0,2.148313553,-2.1655415267,-3.5838603425  
C,0,2.3259035134,-3.2422987415,-4.4200871383  
C,0,3.2403263692,-4.2662147554,-4.0791475704  
C,0,3.9568326509,-4.196790848,-2.9088362439  
O,0,1.8043225038,-0.0338069918,-1.8554802415  
B,0,0.8077040342,0.6003213898,-0.9225067985  
O,0,-0.4843538754,-0.1542167402,-0.9971501774  
B,0,-1.3656510718,0.2039071054,-1.9519235151  
O,0,-2.4820906619,-0.6648920047,-2.1185397764  
C,0,-3.4508378971,-0.6232767099,-3.0993262756  
C,0,-3.633483827,0.4260097607,-4.0076480764  
C,0,-4.6662687468,0.337442278,-4.9403282726  
C,0,-5.5043513266,-0.7766549215,-4.9699033225  
C,0,-5.3135177459,-1.8169680477,-4.0595312514  
C,0,-4.2902209869,-1.7534960275,-3.1184349644  
C,0,5.0548168076,-1.9591372143,1.326826231  
C,0,4.391959174,-1.5536412051,2.4941113196  
C,0,5.0045263995,-1.6877381291,3.7383848731  
C,0,6.2871222163,-2.226254912,3.8353529682  
C,0,6.9572457363,-2.6266862846,2.6798271912  
C,0,6.3472820252,-2.4962196974,1.4339243077  
C,0,6.072314893,0.8226348657,-0.1123604983  
C,0,6.0509108814,0.6149653566,-1.4993615643  
C,0,7.2354873821,0.3742101822,-2.1925171516

## E. Trans-Aziridine Reaction Coordinate

### TS3

E(RAM1) = -0.758027203980

E(RM062X) = -1385.07281933

E(RAM1) = -1.11171428998

Zero-point correction=	1.282965
(Hartree/Particle)	
Thermal correction to Energy=	1.364164
Thermal correction to Enthalpy=	1.365108
Thermal correction to Gibbs Free Energy=	1.151006
Sum of electronic and zero-point Energies=	-1383.436167
Sum of electronic and thermal Energies=	-1383.354968
Sum of electronic and thermal Enthalpies=	-1383.354024
Sum of electronic and thermal Free Energies=	-1383.568126

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.026	306.610	450.616

C,0,-5.9703403519,-1.1025228457,0.0432577721  
C,0,-5.4196764141,-1.0313691979,1.3253200619  
C,0,-6.2457698299,-1.1922038536,2.4434596107  
C,0,-7.616533765,-1.4200700445,2.2970475402  
C,0,-8.153400835,-1.4922198197,0.9994457038  
C,0,-7.3379758159,-1.3324392208,-0.1355145441  
C,0,-3.9653434195,-0.7669480526,1.5514467848

C,0,8.452686697,0.3383632016,-1.5127494343  
 C,0,8.4821971688,0.544489665,-0.1339015855  
 C,0,7.3009307173,0.7887295788,0.563634743  
 O,0,0.6333046031,1.9644509006,-1.3981582549  
 B,0,-0.2608836151,2.2666525361,-2.3487561307  
 O,0,-1.2550773923,1.3445467743,-2.6949005425  
 O,0,-0.3640743908,3.4630185573,-3.049566843  
 C,0,0.4733670092,4.5554211471,-2.9679991141  
 C,0,1.5532266435,4.6703198657,-2.0850205276  
 C,0,2.3128295244,5.8392157329,-2.1005431942  
 C,0,2.0017720167,6.8752858651,-2.9804277055  
 C,0,0.9230872736,6.7474652098,-3.8568832358  
 C,0,0.1487798209,5.5913896245,-3.8632547662  
 H,0,1.768141228,-3.3145839588,-5.3647500335  
 H,0,0.286118402,2.3155005915,1.9235280544  
 H,0,-2.9662208195,1.3039052834,-3.9911929601  
 H,0,-4.8146465507,1.1566894593,-5.6601081774  
 H,0,-6.3130963125,-0.8380418868,-5.7119208691  
 H,0,-5.9703637941,-2.6993290618,-4.0866998058  
 H,0,-4.123100477,-2.5694330323,-2.402139399  
 H,0,-0.7014469329,5.4740224155,-4.548115353  
 H,0,0.6801621383,7.5647154656,-4.5516470799  
 H,0,2.6063721423,7.7929029049,-2.985508992  
 H,0,3.1638333693,5.9388083612,-1.4104700717  
 H,0,1.795135921,3.8463278054,-1.3938581605  
 H,0,2.5780958946,5.2108465547,4.1792930997  
 H,0,4.6971883967,4.2766112092,3.2405614311  
 H,0,5.8202144935,2.7665925843,1.6559417467  
 H,0,7.3285224392,0.9492866162,1.6517656555  
 H,0,9.4395746289,0.5169857416,0.4060728749  
 H,0,9.38594278,0.1499306596,-2.0622097613  
 H,0,7.2068591074,0.2137951857,-3.2802221558  
 H,0,5.0886463616,0.6407750126,-2.0358749312  
 H,0,6.8865012561,-2.8020045253,0.5242687645  
 H,0,7.9725670728,-3.0436156405,2.7495257986  
 H,0,6.7704100887,-2.3288791334,4.8173391144  
 H,0,4.4767109633,-1.3568483769,4.6447556343  
 H,0,3.3875272815,-1.1089614711,2.420872497  
 H,0,5.125793191,-3.860552521,-0.4998150966  
 H,0,4.6743649644,-4.9849541237,-2.637671755  
 H,0,3.3734460498,-5.1144736931,-4.7665773704  
 H,0,-3.7193278948,-1.078000089,2.5794769029  
 H,0,-2.471763711,-2.7373444675,2.2544962178  
 H,0,1.4499556353,-1.3504176842,-3.8346947525  
 H,0,0.3841375282,4.2531619115,3.5122827285  
 H,0,-0.7709583682,-0.4586733354,1.4017703414  
 H,0,-1.3981481914,-4.778081087,2.245196237  
 H,0,-0.4076384209,-6.7189773031,1.0691637445  
 H,0,-0.0955109491,-6.6469624266,-1.3945805905  
 H,0,-0.7696248336,-4.6259020552,-2.6668656611  
 H,0,-1.7501518861,-2.6860921056,-1.5014746953  
 H,0,-3.2701843054,0.8596208434,3.5767833367  
 H,0,-3.9538973396,0.8240787248,-0.7011016204  
 H,0,-5.8205271892,-1.1269354678,3.4572988568  
 H,0,-5.3322047603,-0.9745561295,-0.8482286027  
 H,0,-3.3241114809,4.5418557828,3.8154414076  
 H,0,-3.2411168254,2.9759350891,4.7393995181  
 H,0,-1.7591201229,3.6377489773,3.9239424483  
 H,0,-2.9919463526,2.8940877393,-1.8938731051  
 H,0,-4.6619709784,3.5028435267,-1.5095776713  
 H,0,-3.2029333975,4.4899092277,-1.0590803113  
 H,0,-3.8240316456,6.6680982497,1.1542956301  
 H,0,-4.8195503643,5.3456542253,0.3480149143  
 H,0,-4.8351748388,5.5156721258,-2.1736322299  
 H,0,-9.5336752415,-1.3091163245,3.2588801087  
 H,0,-8.4453698429,-2.6352413993,3.8534323541  
 H,0,-8.1167810483,-0.9154361406,4.3246316273  
 H,0,-7.1427864907,-1.6318522044,-2.2605127552  
 H,0,-8.7430425727,-2.1319101842,-1.5456015153  
 H,0,-8.3537505952,-0.3767685188,-1.7522063521

H,0,-11.1031292699,-2.866445693,0.7902851772  
 H,0,-9.5442653001,-3.6020506322,0.1455494286  
 H,0,-9.7636335617,-3.3656941065,1.9507471688  
 H,0,-3.0123825433,-1.3750168341,-0.3041006207  
 C,0,1.8900563959,-3.4978246165,5.2400589575  
 H,0,0.6921605515,-1.7073414974,5.556549231  
 H,0,-0.2642340593,-3.1855372737,5.3628416778  
 H,0,2.0240322582,-3.7061310965,6.3042802626  
 H,0,1.8150590399,-4.4485081003,4.7065955751  
 H,0,2.7717507452,-2.9623913203,4.8752595854

### Trans-anti-3a

trans-diazonium-intermediate-M06-BB

E(RAM1) = -0.755355440067

E(RM062X) = -1385.08624318

E(RAM1) = -1.11052977986

Zero-point correction=	1.285070
(Hartree/Particle)	
Thermal correction to Energy=	1.366017
Thermal correction to Enthalpy=	1.366962
Thermal correction to Gibbs Free Energy=	1.154706
Sum of electronic and zero-point Energies=	-1383.445999
Sum of electronic and thermal Energies=	-1383.365051
Sum of electronic and thermal Enthalpies=	-1383.364107
Sum of electronic and thermal Free Energies=	-1383.576363

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	857.189	306.822	446.730

C,0,5.1051748151,-1.5943859928,0.2331623862  
 C,0,4.9365783877,-1.3838788085,-1.1383843675  
 C,0,5.4991540117,-2.2831908223,-2.0492714369  
 C,0,6.2224036817,-3.3957493187,-1.6096860453  
 C,0,6.3743619945,-3.5958737385,-0.2269136429  
 C,0,5.8218573857,-2.6973907934,0.7046063827  
 C,0,4.1912327835,-0.190912487,-1.6519601382  
 C,0,4.9944856287,1.0497275505,-1.4195796359  
 C,0,5.8745088099,1.4577371232,-2.4293491181  
 C,0,6.6624019731,2.601484541,-2.280439481  
 C,0,6.545829328,3.3485408988,-1.095534166  
 C,0,5.6606962224,2.9598939138,-0.0739698065  
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 C,0,6.5051013561,-5.8926423723,0.2845922692  
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 H,0,1.6867129975,3.6884786248,-1.9656542443  
 H,0,-0.2512699786,5.3498958548,-1.7736226535  
 H,0,-0.6482233521,3.9483341134,-2.7878228864  
 H,0,-1.2494408603,4.0374618083,-1.1102647077

## TS4

E(RAM1) = -0.737583544491

E(RM062X) = -1385.06799008

E(RAM1) = -1.08771404902

Zero-point correction= 1.283115  
(Hartree/Particle)

Thermal correction to Energy= 1.364494

Thermal correction to Enthalpy= 1.365438

Thermal correction to Gibbs Free Energy= 1.150638

Sum of electronic and zero-point Energies= -1383.434744

Sum of electronic and thermal Energies= -1383.353365

Sum of electronic and thermal Enthalpies= -1383.352421  
 Sum of electronic and thermal Free Energies= -1383.567222

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.233	306.610	452.086

C,0,5.4525072191,-1.4293288488,0.3703927724  
 C,0,5.1274361252,-1.3998941335,-0.9883244475  
 C,0,5.7570925111,-2.2829594754,-1.8706504289  
 C,0,6.7078403533,-3.1995198754,-1.4124512727  
 C,0,7.0174519952,-3.2205050373,-0.0411433021  
 C,0,6.3960301431,-2.3364745938,0.8601498344  
 C,0,4.1233871738,-0.4240437342,-1.5172395524  
 C,0,4.6509151856,0.9710057118,-1.4195187755  
 C,0,5.4109613425,1.4511343462,-2.494180201  
 C,0,5.9491242289,2.7393341015,-2.477286189  
 C,0,5.6999938564,3.5585317665,-1.3617177316  
 C,0,4.9325425996,3.0974415382,-0.2775612618  
 C,0,4.4203897334,1.7956540498,-0.3159628025  
 C,0,6.7596499698,3.2198642604,-3.6198033249  
 O,0,6.1225802625,4.8845843326,-1.3629404559  
 C,0,7.4874730589,5.0451690772,-0.976983584  
 C,0,4.6500179048,3.9846696792,0.8733642009  
 C,0,7.3704448492,-4.118779311,-2.3659441628  
 O,0,8.0308203264,-4.0476461873,0.4340486878  
 C,0,7.610002737,-5.3936759043,0.6532742077  
 C,0,6.7536641352,-2.3470358699,2.2964891264  
 N,0,2.7656144393,-0.5717593927,-0.9126193961  
 C,0,1.9249622839,-1.6641354154,-1.3838530974  
 C,0,1.6167381721,-2.8102778634,-0.4548525618  
 C,0,2.0785223423,-4.0877286405,-0.7831056867  
 C,0,1.8145222869,-5.168830744,0.0559881464  
 C,0,1.0795403087,-4.9764669685,1.2237158304  
 C,0,0.6130520187,-3.7034916401,1.5510533951  
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 C,0,0.8090879136,-0.6895717915,-1.6939406734  
 C,0,1.1098805379,0.1636620122,-2.9277512093  
 O,0,1.649748299,-0.3045602957,-3.9024458595  
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 N,0,-1.2366234209,-2.4229480753,-2.4013006401  
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 H,0,5.5647665711,4.5666438867,1.1493689295  
 H,0,7.6547336176,6.1489159188,-1.0446477547  
 H,0,7.642459839,4.6830257703,0.0680443689  
 H,0,8.1586320246,4.4961842823,-1.6816577774  
 H,0,8.3653863762,-4.4453869447,-1.9719486081  
 H,0,6.7381704027,-5.0284314089,-2.5263299877  
 H,0,7.5249585282,-3.6205455141,-3.3546288189  
 H,0,5.9449734511,-1.8850625984,2.9162565803  
 H,0,6.9300639284,-3.3943279193,2.6480278739  
 H,0,7.6982945924,-1.7671824739,2.4543054243  
 H,0,8.5379217554,-5.9078934797,1.0075682467  
 H,0,6.8125402787,-5.4301622078,1.4343589276  
 H,0,7.2419299213,-5.847819098,-0.2988910524  
 H,0,2.7034341453,-0.4185718153,0.0950250703  
 C,0,0.0825319332,2.204312218,-4.9709963106  
 H,0,0.9937569382,3.3122052224,-3.3385856144  
 H,0,2.0895061633,2.1462173201,-4.1327372619  
 H,0,0.2994284794,2.9714284071,-5.7193030757  
 H,0,0.1708218041,1.2257506434,-5.4471693612  
 H,0,-0.9426476438,2.347891105,-4.6146472986

## Trans-aziridine 4a

trans-aziridine-ONIOM-M06-BB  
 E(RAM1) = -0.965580499603E-01

E(RM062X) = -671.229054554

E(RAM1) = -0.297404776099E-01

Zero-point correction= 0.597254  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.633167  
 Thermal correction to Enthalpy= 0.634112  
 Thermal correction to Gibbs Free Energy= 0.522647  
 Sum of electronic and zero-point Energies= -670.698618  
 Sum of electronic and thermal Energies= -670.662705  
 Sum of electronic and thermal Enthalpies= -670.661761  
 Sum of electronic and thermal Free Energies= -670.773225

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	397.319	130.134	234.596

C,0,4.845998321,-0.0852986338,0.364001546  
 C,0,4.7676206902,-0.191489957,-1.0268418733  
 C,0,5.866253737,-0.6779725999,-1.7444185903  
 C,0,7.0411138192,-1.0571215684,-1.0899853572  
 C,0,7.0999163708,-0.9470023531,0.3108022327  
 C,0,6.0058467631,-0.4618145455,1.0484623145  
 C,0,3.5392383082,0.2159102833,-1.7778162  
 C,0,3.4359035983,1.7077960047,-1.819430656  
 C,0,3.8398039109,2.3754532277,-2.9815914152  
 C,0,3.790993261,3.7692675673,-3.0638257451  
 C,0,3.3162796454,4.4952292951,-1.9567976694  
 C,0,2.8964633844,3.8416454543,-0.7852003826  
 C,0,2.9640708457,2.4457640225,-0.730862522  
 C,0,4.2306577113,4.4534862252,-4.3015422355  
 O,0,3.1570875023,5.8758388044,-2.0454025951  
 C,0,4.3647037996,6.6001576325,-1.8139889304  
 C,0,2.3693292397,4.6051794034,0.3688230937  
 C,0,8.1930595432,-1.5628752335,-1.8714473521  
 O,0,8.2883752134,-1.2234167085,0.9819701553  
 C,0,8.4878307525,-2.6145782501,1.2292785712  
 C,0,6.0765351309,-0.3249701719,2.5211513516

N,0,2.3121505884,-0.4052431475,-1.1562660263  
 C,0,1.9943983195,-1.7686168035,-1.4818929121  
 C,0,1.5531092401,-2.6839860226,-0.3893430879  
 C,0,1.4700551562,-4.0576106772,-0.6279185777  
 C,0,1.0335916726,-4.9222529257,0.3738050123  
 C,0,0.6764355726,-4.4189827868,1.6234253508  
 C,0,0.7625978599,-3.0481134054,1.86664163  
 C,0,1.2005039972,-2.1839898919,0.8666901393  
 C,0,1.1132080741,-0.6386243877,-1.9500958427  
 C,0,1.0608344236,-0.3811977391,-3.4226108665  
 O,0,1.9309187478,-0.6572138974,-4.2204753069  
 O,0,-0.1011703872,0.1892005636,-3.7639334463  
 C,0,-0.2747621189,0.4660280259,-5.1645123892  
 H,0,3.6411128613,-0.1461101759,-2.8167671638  
 H,0,2.5690715459,-2.2311399813,-2.2876098143  
 H,0,0.1826268869,-0.4370914754,-1.4259764778  
 H,0,1.750935572,-4.4507232891,-1.6020685964  
 H,0,0.9762481223,-5.9888284157,0.1791459758  
 H,0,0.3369599711,-5.0918694691,2.404783595  
 H,0,0.4924631491,-2.6521095059,2.8408856942  
 H,0,1.288707356,-1.1164837139,1.0464136374  
 H,0,4.2009679651,1.7999194332,-3.8486122684  
 H,0,2.6387196451,1.9307061572,0.1866905123  
 H,0,5.8145966426,-0.7613761558,-2.8413790878  
 H,0,3.9851189703,0.2966732386,0.9351324688  
 H,0,3.7375418466,5.4530262238,-4.3968521522  
 H,0,5.3393938071,4.6067429053,-4.2817111664  
 H,0,3.9779724198,3.8429383405,-5.2031528064  
 H,0,1.2545241808,4.6771873253,0.2978885089  
 H,0,2.6304064347,4.1034219903,1.3326479465  
 H,0,2.7835787643,5.6441838306,0.3780034523  
 H,0,4.0636241362,7.6694103174,-1.9431057285  
 H,0,4.737255972,6.4147223258,-0.7775221175  
 H,0,5.1424259084,6.3122094339,-2.5627306504  
 H,0,9.1490434524,-1.4063667287,-1.3120030286  
 H,0,8.0731343974,-2.6584751683,-2.0672217526  
 H,0,8.2654142029,-1.0373429664,-2.8553975465  
 H,0,5.0806334619,-0.5223565188,2.9882464999  
 H,0,6.8245530511,-1.0379527358,2.9493042432  
 H,0,6.3944722207,0.713977278,2.7903379681  
 H,0,9.4792971898,-2.6546229302,1.7450674124  
 H,0,7.6799074222,-3.0123034297,1.8899863839  
 H,0,8.5163622418,-3.1822044392,0.26729503  
 C,0,-1.628102255,1.1210083953,-5.3282321582  
 H,0,0.5421606421,1.1143908889,-5.4942832616  
 H,0,-0.1997027662,-0.4754282149,-5.7167124409  
 H,0,-1.8021928209,1.3509066429,-6.3826396566  
 H,0,-2.4238773452,0.4574276437,-4.9815663634  
 H,0,-1.6775759466,2.0513661401,-4.7572485082

## F. SN1 mechanism

### TS2-SN1

E(RAM1) = -0.706049386828

E(RM062X) = -1385.05563475

E(RAM1) = -1.06115789833

Zero-point correction= 1.280465  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.362316  
 Thermal correction to Enthalpy= 1.363260  
 Thermal correction to Gibbs Free Energy= 1.147460  
 Sum of electronic and zero-point Energies= -1383.420061  
 Sum of electronic and thermal Energies= -1383.338210  
 Sum of electronic and thermal Enthalpies= -1383.337266

Sum of electronic and thermal Free Energies= -1383.553066

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	854.866	307.885	454.190

C,0,-6.3127424142,-0.8494910708,2.3033845022  
 C,0,-6.1867177041,-1.7606973699,1.2447945707  
 C,0,-6.9466283724,-2.9395387658,1.2644406678  
 C,0,-7.8087864008,-3.2038846285,2.3266822494  
 C,0,-7.9281932965,-2.2933934068,3.3761801212  
 C,0,-7.1790248116,-1.117178428,3.3615596014  
 C,0,-5.3413553696,-1.4430217157,0.0889670186  
 C,0,-4.0171705146,-0.9208706315,0.2321544848  
 C,0,-3.3895662755,-0.3835393512,-0.8915452105  
 C,0,-3.9735978813,-0.4787362437,-2.1959875314  
 C,0,-5.2199457167,-1.1370609023,-2.3307218908  
 C,0,-5.8970375352,-1.5811643497,-1.1683478018  
 C,0,-5.7869831142,-1.2887953324,-3.6264634454  
 C,0,-5.1496812435,-0.7801180583,-4.7312007145  
 C,0,-3.9250275402,-0.0847615232,-4.5907535382  
 C,0,-3.3529747219,0.0659357886,-3.3511041667  
 C,0,-3.3510782965,-0.8859639398,1.5362399819  
 C,0,-2.8688362966,0.329954192,2.0285784924  
 C,0,-2.4431737246,0.4635836596,3.391661818  
 C,0,-2.4044929773,-0.6944989688,4.2043082147  
 C,0,-2.7246691777,-1.9516850992,3.6331667265  
 C,0,-3.1734198119,-2.0610077669,2.3301139183  
 C,0,-2.0824649751,1.7192971541,3.9480538971  
 C,0,-1.7081787149,-1.8131831255,5.2670899031  
 C,0,-1.6756020407,0.6578105737,6.0832867563  
 C,0,-2.0131282542,-0.569056664,5.5655615847  
 O,0,-2.8349863111,1.459053549,1.2596017149  
 B,0,-1.9937001501,1.4623768548,0.0247902311  
 O,0,-2.1517251586,0.2046577206,-0.8051121917  
 C,0,-3.3671105664,-3.4081551085,1.7829058465  
 C,0,-2.9155462251,-3.7311353283,0.4948673363  
 C,0,-3.0356252397,-5.0309389971,0.0071142571  
 C,0,-3.60799471,-6.0269605333,0.7976798645  
 C,0,-4.0650074404,-5.715076782,2.0778073413  
 C,0,-3.9463643822,-4.4165591177,2.5690356925  
 O,0,-0.545522246,1.466872593,0.3657494212  
 B,0,0.1378976275,2.6291661935,0.4369944603  
 O,0,-0.3708520025,3.8050420614,-0.0447050536  
 B,0,-1.5936863326,3.7652484102,-0.7168410049  
 O,0,-1.9100871285,4.9663278669,-1.3507105403  
 C,0,-3.0735966677,5.2719117942,-2.0235008717  
 C,0,-4.206489625,4.4512134098,-2.0766857898  
 C,0,-5.3260259644,4.8943340888,-2.7793927575  
 C,0,-5.3178157246,6.1339468768,-3.4178346825  
 C,0,-4.1828319494,6.9439507436,-3.3558091676  
 C,0,-3.0513355746,6.5257259935,-2.6624905839  
 O,0,1.4284331278,2.5446811459,1.015667903  
 C,0,2.2249359253,3.6199863792,1.3535174783  
 C,0,3.5845474048,3.3168173726,1.543002198  
 C,0,4.4454484052,4.3267348477,1.9649676381  
 C,0,3.9717330094,5.6197625474,2.1856400746  
 C,0,2.6226081851,5.9107729936,1.9828689997  
 C,0,1.7392890679,4.9171158674,1.5665967205  
 O,0,-2.3444688521,2.651975635,-0.7269905737  
 N,0,0.9143194608,-0.5479108649,1.3480310846  
 N,0,0.9900805559,-0.4183821645,2.4353438256  
 C,0,0.7172372353,-0.7889322938,-0.8281978554  
 C,0,1.8823013983,-0.0239796312,-1.4387178805  
 C,0,1.4121376529,1.254907235,-2.1156027545  
 C,0,0.1984290458,1.2593147204,-2.8038900287  
 C,0,-0.2593420663,2.4238946997,-3.4134242447  
 C,0,0.5101655661,3.584710402,-3.3659340443  
 C,0,1.7411616215,3.5707228116,-2.7145477834  
 C,0,2.1938746935,2.4105951705,-2.089708456

C,0,0.6728634665,-2.271906305,-0.8798868124  
 O,0,0.4161386346,-2.6131051229,-2.0119907815  
 O,0,0.8394241616,-3.0054069436,0.185443652  
 C,0,0.6351054944,-4.4407272965,0.0130966017  
 N,0,2.9762120682,0.2029912035,-0.5198266198  
 C,0,3.728293287,-1.0002093624,-0.0447453751  
 C,0,4.3882430918,-1.7439448984,-1.1658527958  
 C,0,4.4337076375,-3.1421238997,-1.1052734104  
 C,0,5.0685962518,-3.8842271544,-2.1031535156  
 C,0,5.6593161923,-3.2005354948,-3.1826074252  
 C,0,5.6182438296,-1.7979754769,-3.2635934826  
 C,0,4.9820776444,-1.0822208199,-2.2435327362  
 C,0,5.0972265157,-5.3629784476,-2.0342110929  
 O,0,6.1939727084,-3.9487105844,-4.2261322514  
 C,0,7.6191578418,-4.0331388888,-4.1956749508  
 C,0,6.230137197,-1.0732511539,-4.4011220288  
 C,0,4.7533411527,-0.6113709165,0.9727950725  
 C,0,5.6855964371,0.3955117437,0.708808624  
 C,0,6.663706901,0.7320910362,1.6498916632  
 C,0,6.6881766545,0.0435045246,2.875646379  
 C,0,5.7569991991,-0.9730810736,3.1582228923  
 C,0,4.7950464517,-1.2894937208,2.1956750207  
 C,0,7.6520829878,1.7911207069,1.3416172414  
 O,0,7.7054351392,0.2859513694,3.7929197563  
 C,0,7.4770142186,1.4400703496,4.6028004076  
 C,0,5.8013733826,-1.7141737302,4.4392954002  
 H,0,-0.27907225,-0.3324507357,-0.7478523415  
 H,0,-1.4332050685,2.7845478727,5.7027712854  
 H,0,-2.4161709479,0.6293504408,-3.2167161096  
 H,0,3.9568122101,2.297518653,1.3653483513  
 H,0,5.5099785796,4.097752484,2.1227357076  
 H,0,4.6611954327,6.4088803373,2.5171376092  
 H,0,2.2482535593,6.9315595327,2.151875055  
 H,0,0.675616914,5.1450991741,1.3907183322  
 H,0,-2.1525497389,7.1535513329,-2.5993641992  
 H,0,-4.1788334199,7.9229671497,-3.8571014728  
 H,0,-6.2054576037,6.4751820223,-3.9686107365  
 H,0,-6.2212643514,4.2564603769,-2.8259233871  
 H,0,-4.2075802547,3.4727499925,-1.5682978011  
 H,0,-5.5859761553,-0.897132296,-5.7339255787  
 H,0,-6.747615371,-1.8164235098,-3.7207969058  
 H,0,-6.9057911259,-2.0082405318,-1.2810453908  
 H,0,-6.8548878406,-3.6602813253,0.4382145708  
 H,0,-8.3977740763,-4.1323074758,2.3341149702  
 H,0,-8.6120824801,-2.5013349609,4.2113467319  
 H,0,-7.2707651279,-0.3951567493,4.1861598336  
 H,0,-5.7181791041,0.0783283376,2.292884067  
 H,0,-4.3244076017,-4.173614444,3.5740131856  
 H,0,-4.5275489045,-6.4943141902,2.7012456208  
 H,0,-3.7074097642,-7.050878952,0.4100468817  
 H,0,-2.6932655692,-5.2657543738,-1.0115258167  
 H,0,-2.4872769871,-2.9402680031,-0.1409703552  
 H,0,-2.5953993674,-2.852319438,4.2526232844  
 H,0,-1.9940559919,-1.4718991151,6.1931984714  
 H,0,-1.3780980725,0.7571141845,7.1375615412  
 H,0,3.038422461,-1.7131746463,0.45521507  
 H,0,2.6879395037,0.8193094162,0.2414345866  
 H,0,2.2546955468,-0.7183738283,-2.2167091203  
 H,0,-0.4167559154,0.36237275,-2.8460489619  
 H,0,-1.2248862976,2.4267726452,-3.909634253  
 H,0,0.143064236,4.4991872947,-3.8204451903  
 H,0,2.3427889451,4.4730412155,-2.6685199619  
 H,0,3.142225699,2.402010585,-1.563735325  
 H,0,5.6603338129,0.9253419434,-0.2570653499  
 H,0,7.2194262982,2.7984841158,1.5702351554  
 H,0,7.9316804789,1.7680269916,0.2594727393  
 H,0,8.579263806,1.6567672466,1.9530344589  
 H,0,8.3928444403,1.5005684689,5.2419036038  
 H,0,6.5629359057,1.2994953448,5.228905694  
 H,0,7.3747271121,2.3514582943,3.9646922918

H,0,4.7757730619,-2.0192066731,4.7615857403  
H,0,6.2604786332,-1.0853144624,5.2427371505  
H,0,6.426048582,-2.6357164553,4.3222463195  
H,0,4.0695495259,-2.0889127259,2.4119374186  
H,0,3.9745920976,-3.6712290664,-0.2549757422  
H,0,6.0174631158,-5.760836467,-2.5311898453  
H,0,4.2085847913,-5.7850440291,-2.5683740498  
H,0,5.0777804985,-5.7169645636,-0.9746731023  
H,0,7.8683574614,-4.629960642,-5.1082356759  
H,0,7.9565834604,-4.560403182,-3.2707582833  
H,0,8.0731191706,-3.0138417322,-4.2496067013  
H,0,6.2910059901,-1.7325923941,-5.3029268166  
H,0,7.265668296,-0.742982414,-4.1330547009  
H,0,5.6301081568,-0.1667041173,-4.6620131993  
H,0,4.9564868281,0.0180782479,-2.3007583698  
H,0,-2.1218641262,2.6059169882,3.2945131661  
H,0,-3.4449574472,0.3379960317,-5.4849307942  
C,0,1.2050174995,-5.1122531352,1.2392715709  
H,0,-0.4446771649,-4.5982246617,-0.0925727914  
H,0,1.1353277765,-4.7453787263,-0.908946843  
H,0,1.052166058,-6.1913499027,1.1627972576  
H,0,2.2770670876,-4.9177257358,1.3228606421  
H,0,0.7070740627,-4.7559368929,2.1437223422

## G. Cis-Aziridine minor enantiomer transition structures

### TS1-ent

E(RAM1) = -0.756470051791

E(RM062X) = -1385.07265592

E(RAM1) = -1.11033819608

Zero-point correction= 1.282662  
(Hartree/Particle)  
Thermal correction to Energy= 1.364045  
Thermal correction to Enthalpy= 1.364989  
Thermal correction to Gibbs Free Energy= 1.149285  
Sum of electronic and zero-point Energies= -1383.436126  
Sum of electronic and thermal Energies= -1383.354743  
Sum of electronic and thermal Enthalpies= -1383.353798  
Sum of electronic and thermal Free Energies= -1383.569503

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	855.951	306.642	453.988

C,0,-5.825767901,-2.1145408966,2.0470916837  
C,0,-5.0914876559,-1.4548292775,1.0562592064  
C,0,-5.5308332608,-1.4856340224,-0.2697006749  
C,0,-6.7003286912,-2.1674194265,-0.6182673503  
C,0,-7.4269804009,-2.8267148012,0.3902886504  
C,0,-6.9992181494,-2.8040700769,1.7298115755  
C,0,-3.8535652186,-0.7130777387,1.4450055066  
C,0,-4.0696052125,0.7602660559,1.3565343045  
C,0,-4.4714283907,1.433950004,2.5180483566  
C,0,-4.722009361,2.8067481583,2.4998791734  
C,0,-4.5471004022,3.5120435693,1.2934591627  
C,0,-4.1325443476,2.8556073878,0.1219944261  
C,0,-3.9124870044,1.4738347766,0.1672751003  
C,0,-5.1370561549,3.5088503494,3.735663193  
O,0,-4.6886586405,4.8950382952,1.3163486769  
C,0,-5.9109534246,5.3547098486,0.7388860789

C,0,-3.9114322306,3.5925868225,-1.1435429732  
C,0,-7.1774737341,-2.1691382028,-2.0194113971  
O,0,-8.6426003837,-3.4143542747,0.055098974  
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## TS2-ent

cis-RC-TS7-ent-ONIOM-M06  
E(RAM1) = -0.734088648194

E(RM062X) = -1385.07065561

E(RAM1) = -1.09110689097

Zero-point correction= 1.282629  
(Hartree/Particle)  
Thermal correction to Energy= 1.364141  
Thermal correction to Enthalpy= 1.365085  
Thermal correction to Gibbs Free Energy= 1.150521  
Sum of electronic and zero-point Energies= -1383.431009  
Sum of electronic and thermal Energies= -1383.349497  
Sum of electronic and thermal Enthalpies= -1383.348553  
Sum of electronic and thermal Free Energies= -1383.563117

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	856.011	307.149	451.588

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C,0,4.1194950973,0.6557201148,-0.2005295034  
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C,0,6.4491157539,0.1129501523,0.2481731459  
C,0,6.5965029935,-0.2829624027,-1.093299425  
C,0,5.5159439231,-0.2225724759,-1.990973334  
C,0,2.7901837059,1.2024533215,0.2253698917  
C,0,2.8451054978,2.6967471551,0.2608734316  
C,0,2.1307336186,3.4331143398,-0.6893330985  
C,0,2.2077801558,4.8295356376,-0.7162418093  
C,0,2.9975206829,5.4858345499,0.2444085028  
C,0,3.7004738531,4.7625999953,1.2240673395  
C,0,3.6143182199,3.3682399033,1.2166292034  
C,0,1.4469489704,5.6006173438,-1.7257260015  
O,0,2.9903637589,6.8774396256,0.2766504038  
C,0,4.1450887466,7.4636567147,-0.3235590779  
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C,0,7.5927906868,0.0681463221,1.1875422611  
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C,0,8.0555126411,-2.0497101591,-1.6478000635  
C,0,5.6642907394,-0.64184028,-3.4038489201  
N,0,2.2867561081,0.667996992,1.5284113287  
C,0,2.0280088277,-0.7514615691,1.6424222255  
C,0,2.9313611106,-1.628105856,2.4858781896  
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O,0,-2.038678064,-0.9696314442,-1.6831855253

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 H,0,9.0910201396,-2.1485815719,-2.0586394589  
 H,0,7.9803865289,-2.5250007335,-0.6398328734  
 H,0,7.3059083624,-2.4990460552,-2.3446432283  
 H,0,2.6965730893,1.0866814739,2.3554915136  
 O,0,-0.6777319891,-0.3815220814,4.1306133088  
 O,0,1.2398812685,0.7902846678,4.1046922928  
 C,0,-1.0061999737,0.1532548682,5.4378507654  
 C,0,-2.1925426393,-0.6306835893,5.9481868842  
 H,0,-0.1263377867,0.0555351209,6.0785291276  
 H,0,-1.2285350591,1.2163579003,5.3101045235  
 N,0,-0.3666193541,-3.1853405287,2.5442282546  
 H,0,-2.5280916561,-0.2073509487,6.8980548332  
 H,0,-3.0203253106,-0.590819442,5.2325101156  
 H,0,-1.9242044649,-1.676906283,6.1120319286