SUPPORTING INFORMATION

Dynamics and a Unified Understanding of Competitive [2,3]- and [1,2]-Sigmatropic Rearrangements

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Papers Observing Mixtures of [2,3] and [1,2] Rearrangements

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Experimental Procedures

Synthesis and Rearrangement of 1.

Synthesis of ammonium salt ***1***. The ammonium salt **1** was prepared from the reaction of *N*,*N*-dimethylglycine methyl ester[1] with allyl bromide by methods previously described.[2,3]

General procedures for DBU-induced rearrangements. All glassware, magnetic stirring bars, and molecular sieves used in these reactions were oven-dried overnight. Solvent was dried using 4 Å molecular sieves.

DBU-Induced Rearrangement of **1** - Sample.[4] *Trans*-stilbene (1.81 g, 10.0 mmol, internal standard) and **1** (20.18 g, 84.8 mmol) were dissolved in 25 mL of DMF, then DBU (1.98 g, 14.8 mmol) and 24 g of 4 Å powdered molecular sieves were added and the mixture was left stirring for 30 min at 25 °C, allowing the reaction to proceed to 11.7% conversion. The reaction mixture was diluted with 40 mL of $CHCl_3$ and 70 mL of water, and then the aqueous layer was extracted twice with 70 mL of $CHCl_3$. The organics were washed with 50 mL of water, dried with Na_2SO_4,

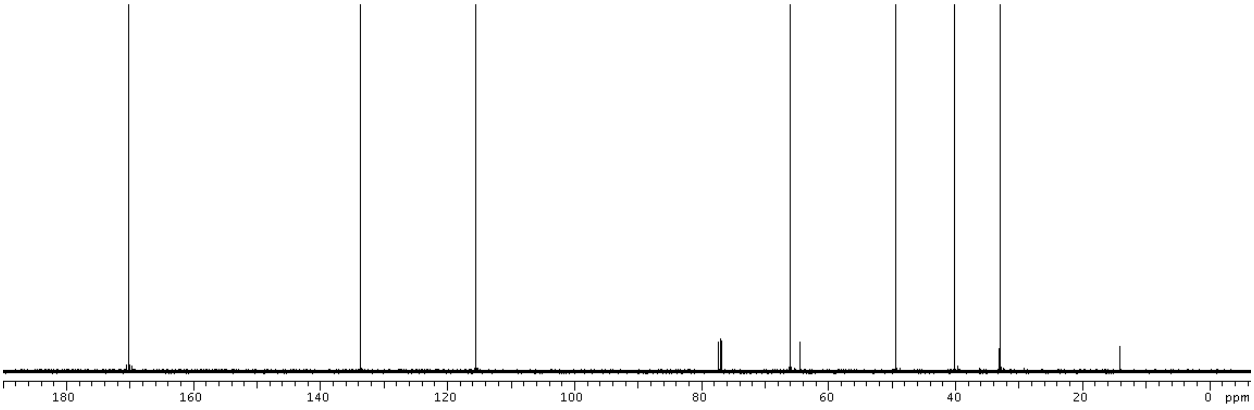
and concentrated under reduced pressure. The residual organics were dissolved in 150 mL of Et_2O, washed twice with 50 mL of water, then dried with Na_2SO_4 and concentrated under reduced pressure. The resulting crude mixture was purified by flash chromatography using 1% MeOH in DCM to afford 0.50 g (4%) of **3**. ^{1}H NMR ($CDCl_3$): δ 2.26 (s, 6 H), 2.35 (m, 2 H), 3.1 (dd, 1 H), 3.6 (s, 3 H), 5.0 (m, 2 H), 5.7 (m, 1 H). ^{13}C NMR ($CDCl_3$): δ 33.7, 41.3, 50.6, 67.2, 116.8, 134.0, 171.7.

DBU-Induced Rearrangement of **1** - Standard.[4] *Trans*-stilbene (0.92 g, 5.1 mmol, internal standard) and **1** (3.57 g, 15 mmol) were dissolved in 15 mL of DMF, then 9.13 g (60 mmol, 4 eq.) of DBU and 12 g of 4 Å powdered molecular sieves were added and the mixture left stirring for 3h at r.t., allowing the reaction to proceed to 100% conversion. The reaction mixture was diluted with 50 mL of $CHCl_3$ and 70 mL of water, and then the aqueous layer was extracted twice with 70 mL of $CHCl_3$. The organics were washed with 50 mL of water, dried with Na_2SO_4, and concentrated under reduced pressure. The residual organics were dissolved in 150 mL of Et_2O, washed twice with 50 mL of water, then dried with Na_2SO_4 and concentrated under reduced pressure. The resulting crude mixture was purified by flash chromatography using 1% MeOH in DCM to afford 0.64 g (27%) of **3**.

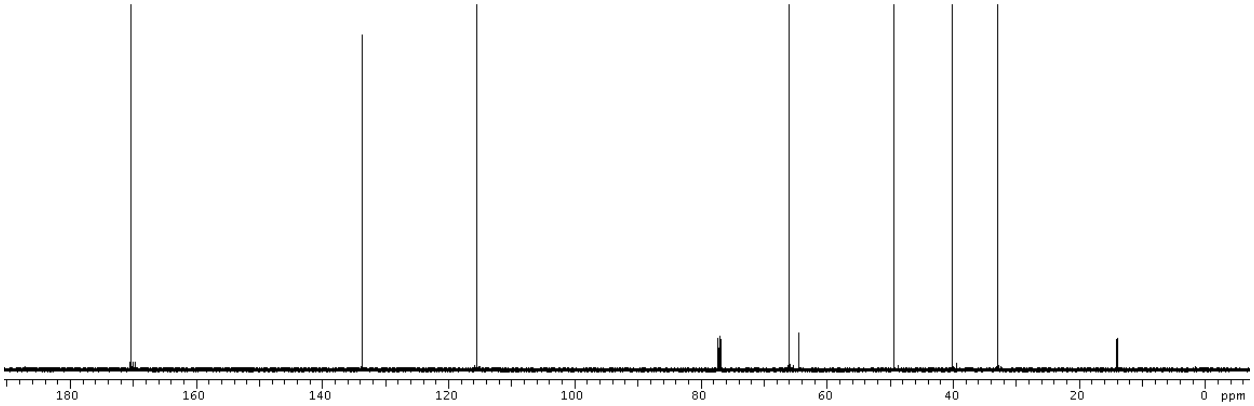
In each case closely analogous reactions were carried out for duplicate measurements of the KIEs. In the duplicate samples the conversion of the sample was 21.3%.

^{13}C NMR Spectrum of Sample

A note on spectra: we certify that all spectra presented are unaltered screen dumps or pdf printouts of the original spectra. Please note that scales are typically increased by a factor of 5 from normal to show impurities clearly. The raw electronic files are saved and always available on request.



^{13}C NMR Spectrum of Standard



NMR Measurements

All NMR samples consisted of approximately 400 mg of **3** in 5 mm NMR tubes filled to a constant height of 5 cm with $CDCl_3$. The ^{13}C spectra were recorded at 125.7 MHz using inverse gated decoupling, 75.5 s delays between calibrated $\pi/2$ pulses, and a 12 s acquisition time to collect 600,000 points. The integrations were obtained numerically by a procedure given in a macro provided in a later section. A zero-order baseline correction was generally applied, but to avoid any qualitative manipulation no first-order or higher-order baseline correction was ever applied. Six spectra were recorded for each sample and standard.

NMR Results and Calculation of KIEs

The raw integrations are shown in Table S1, along with average values and standard deviations. The integration of peak 5, the methyl-ester carbon, was in each case set to 1000.

Table S1.

	macro used: macrokie2samp						
SAMPLE2	File: SEAN-KIE2-SAMPLE-ERIK-CUT-OME					average	stdev
1054.8	1052.3	1055.2	1053.6	1053.4	1054.6	1054.0	1.1
1020.7	1021.2	1022.5	1021.3	1020.8	1021.6	1021.4	0.7
950.5	950.9	952.6	949.1	950.7	949.6	950.6	1.2
992.0	991.6	991.1	992.7	991.8	992.3	991.9	0.6
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
1942.9	1942.8	1943.6	1941.3	1943.7	1943.8	1943.0	1.0
989.5	989.6	990.0	990.0	987.4	990.0	989.4	1.0

	macro used: macrokie2						
Standard2	File: SEAN-KIE2-STANDARD-ERIK-CUT-OME					average	stdev
1063.2	1062.8	1063.1	1063.6	1064.4	1065.0	1063.7	0.9
1022.9	1021.5	1022.5	1022.9	1024.2	1026.2	1023.4	1.6
989.2	992.7	992.1	995.0	992.9	995.0	992.8	2.1
998.7	1000.0	998.0	999.4	1000.5	1000.5	999.5	1.0
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
1943.1	1945.9	1945.1	1946.9	1948.4	1948.9	1946.4	2.2
996.9	999.2	996.7	1000.3	998.5	1000.6	998.7	1.6

macro used: seankiesamp

SAMPLE1	File: SEAN-KIE-SAMPLE-ERIK-CUT					average	stdev
1020.9	1022.4	1024.0	1025.4	1022.5	1026.4	1023.6	2.0
1022.7	1020.9	1021.3	1021.3	1022.2	1022.3	1021.8	0.7
947.7	944.9	949.0	947.4	951.8	948.1	948.2	2.2
985.5	983.3	980.4	986.6	984.9	986.5	984.5	2.4
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
1921.3	1922.3	1922.9	1923.9	1921.5	1922.5	1922.4	1.0
969.8	968.4	966.8	967.1	968.4	968.4	968.1	1.1

macro used: seankiestd

Standard1	File: SEAN-KIE-STANDARD-ERIK-CUT					average	stdev
1033.5	1029.5	1033.8	1032.3	1033.0	1035.1	1032.9	1.9
1021.6	1018.5	1019.3	1018.4	1022.5	1025.2	1020.9	2.7
991.5	988.7	990.2	991.5	992.2	991.3	990.9	1.3
992.8	987.9	987.1	992.9	990.1	996.9	991.3	3.6
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
1927.1	1922.0	1920.3	1926.8	1928.5	1933.6	1926.4	4.8
978.1	978.6	973.6	978.7	977.3	980.9	977.9	2.4

The isotope effects in the main text were then calculated as:

KIE = ln(1-F)/ln(1-(F*IntSample/IntStandard))

where F is the fractional conversion (0.117 for reaction 1, 0.213 for reaction 2), IntSample is the average integration for the sample for the carbon peak of interest in the table above, and IntStandard is the average integration for standard for the carbon peak of interest in the table above. For example, the KIE for carbon 1 of sample 2 /standard 2 was calculated as ln(1-0.213)/ln(1-0.213*1054.0/1063.7).

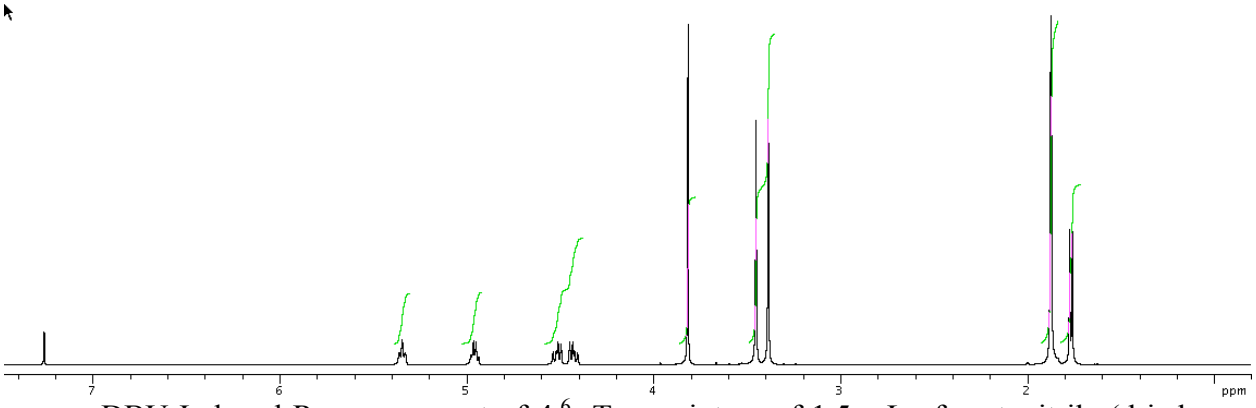
The uncertainties arising from uncertainties in F were negligible, and the major source of uncertainty is random variation in the integrations due to noise. For six measurements, the 95% confidence ranges in the average raw integrations are approximately the standard deviations shown in the table above, and the 95% confidence ranges for the KIEs were approximated as the square-root of the sum of the squares of the fraction uncertainties in the integrations. For example, the uncertainty for carbon 1 of sample 2 /standard 2 was calculated as $[(1.1/1054)^2 + (0.9/1063.7)^2]^{1/2}$

Synthesis and Rearrangement of 4.

N,N-Dimethylalanine Methyl Ester.[5] A mixture of 4.50 g (39.55 mmol) of 40% aqueous solution of dimethylamine and 4 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling, 3.31 g (19.82 mmol) of methyl 2-bromopropanoate was added and the mixture was stirred at 0 °C for 12 h. The stirring was continued further for 12 h at room temperature. The reaction mixture was then poured into 20 mL of water and the organics extracted with three 50-mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous sodium sulfate. The ether was then removed on a rotatory evaporator to afford 1.00 g (38%) crude N,N-dimethylalanine methyl ester (**1**), judged to be more than 95% pure by NMR analysis. ^{1}H NMR (399.53 MHz, $CDCl_3$): δ 1.27 (d, J = 7.0 Hz, 3 H), 2.31 (s, 6 H), 3.22 (q, J =7.0 Hz 1 H), 3.70 (s, 3 H). ^{13}C NMR (75.42 MHz, $CDCl_3$): δ 14.7, 41.9, 51.6, 63.0, 173.9.

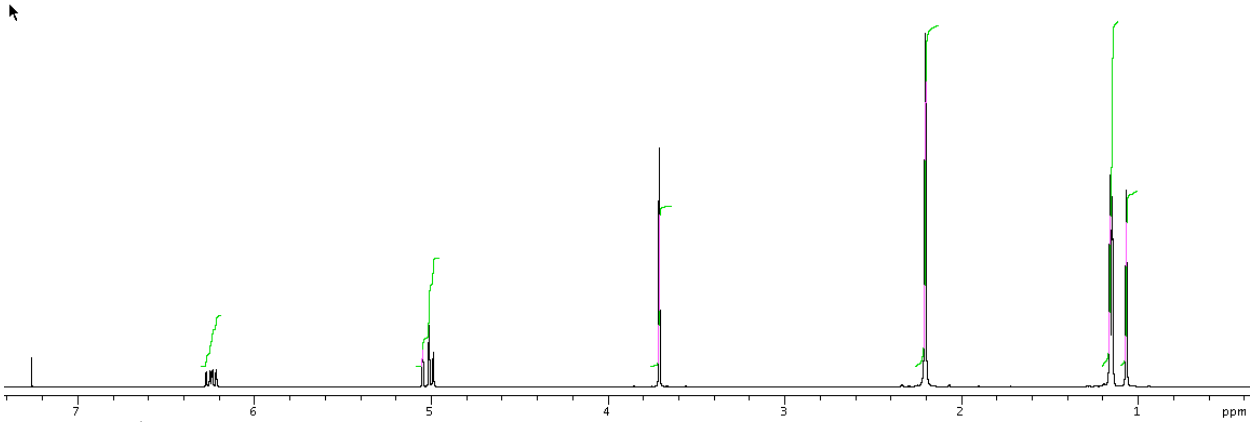
Ammonium salt **4**.[6] To a mixture of 1.00 g (7.62 mmol) of N,N-dimethylalanine methyl ester and 4 mL of hexanes (dried over 4 Å molecular sieves) under nitrogen at room temperature

was added 1.14 g (7.65 mmol) of 1-bromo-3-methylbut-2-ene. The resulting mixture was stirred for 16 h. During the stirring some solid precipitated out from the solution. After the solid was dissolved in minimum amount of dichloromethane, approximately 2 mL of THF was added followed by 10 mL of hexanes, and the mixture was again stirred overnight to precipitate out the solid. This precipitation process was repeated twice to afford 1.14 g (53%) of **4**. ^{1}H NMR ($CDCl_3$): δ 1.76 (d, J=7.2 Hz, 3 H), 1.86 (s, 6 H), 3.37 (s, 3 H), 3.44 (s, 3 H), 3.80 (s, 3 H), 4.43 (q, J = 8.1 Hz, 13.5 Hz, 1 H), 4.49 (q, J = 8.06 Hz, 13.48 Hz, 1 H), 4.92 (q, J = 7.2 Hz, 1 H), 5.34 (t, J = 8.1 Hz, 1H). ^{13}C NMR (100.47 MHz, $CDCl_3$): δ 13.6, 19.4, 26.7, 47.5, 48.6, 53.5, 61.7, 67.0, 110.3, 150.0, and 168.8.



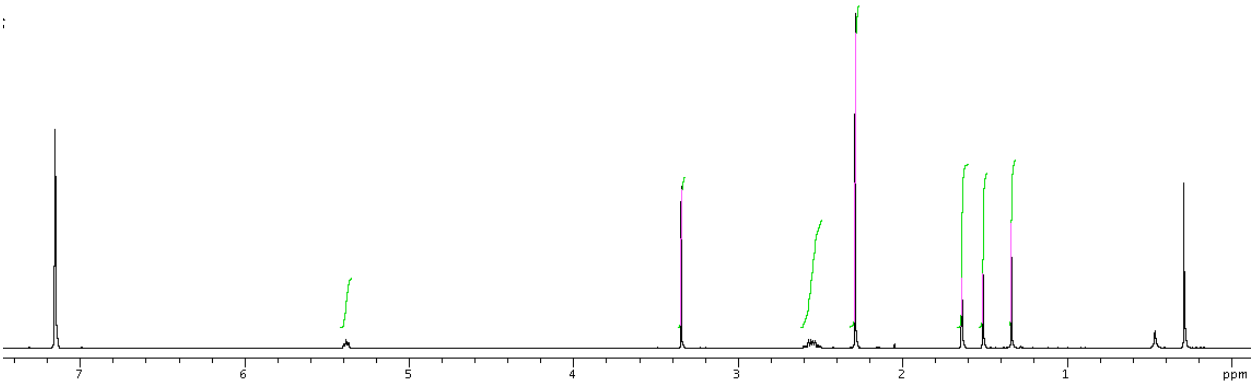
DBU-Induced Rearrangement of **4**.[6] To a mixture of 1.5 mL of acetonitrile (dried over calcium hydride followed by distillation under nitrogen) and 1.58 g (5.63 mmol) of **4** under nitrogen at 90 °C was added 1.53 g (10.0 mmol) of DBU dropwise. The mixture was stirred for 2 h at 90 °C. After cooling the reaction mixture to room temperature, it was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with five 25-mL portions of water, dried (Na_2SO_4), and the volatiles were removed on a rotatory evaporator to afford 779 mg (69%) of mixture of **6** and **7**. The ratio of the [2,3] product **6** and the [1,2] product **7** was determined to be approximately 80:20 by ^{1}H-NMR analysis. The isomers were separated by flash chromatography on silica gel using 20% ethyl acetate in hexanes as eluent.

6: ^{1}H NMR ($CDCl_3$): δ 1.06 (s, 3 H), 1.14 (s, 3 H), 1.16 (s, 3 H), 2.20 (s, 6 H), 3.70 (s, 3 H), 5.01 (t, J = 6.8 Hz, J= 11.3 2 H), 6.24 (q, J = 6.8 Hz, J= 11.3 2 H, 1 H). ^{13}C NMR ($CDCl_3$): 9.1, 24.5, 25.0, 41.3, 42.7, 51.6, 72.8, 111.8, 145.6 and 175.4.



7: ^{1}H NMR (C_6D_6) δ 1.34 (s, 3 H), 1.51 (s, 3 H), 1.64 (s, 3 H), 2.29 (s, 6 H), 2.55 (m, 2 H), 3.34 (s, 3 H), 5.38 (t, J = 7.2 Hz, 1 H). ^{13}C NMR (75 MHz, $CDCl_3$): 18.6, 20.4, 26.6, 36.4,

40.2, 51.1 66.6, 120.9, 134.1, 174.4. The nonintegrated peaks in the ^{1}H NMR spectrum shown below are C_6D_5H (7.15), water (0.46) and silicone grease (0.28).



Product Ratio versus Temperature. To a mixture of 1.5 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 300 mg (1.07 mmol) of **4** under nitrogen at 90 °C was added 305 mg (2.00 mmol) of DBU dropwise. From the reaction mixture 0.30-mL aliquots were withdrawn at 30-min, 60-min and 120-min. The aliquots were diluted with 10 mL of diethyl ether and the mixture was washed with three 5-mL portions of water and dried (Na_2SO_4), and the volatiles were removed on a rotatory evaporator. The ratio of the [2,3] product **6** and the [1,2] product **7** was then evaluated by ^{1}H-NMR analysis.

In closely analogous reactions (identical concentrations), the product ratio was determined at 70 °C, 50 °C, and room temperature. The resulting product ratios, determined by ^{1}H NMR analysis, are shown in Table S2.

In a control experiment, 210 mg of a 95:5 mixture of **6** and **7** was heated at 90 °C for 20 h in 1 mL of acetonitrile in in presence of 0.3 mL of DBU. The proportion of **3a** to **3b** was unaltered based on NMR analysis.

Table S2. Product ratios versus temperature for the rearrangement of **4**.

Temperature	% of **6** ([2,3])	% of **7** ([1,2])
90 °C	80.6	19.4
70 °C	85.3	14.7
50 °C	88.9	11.1
Room temperature	94.9	5.1

Rearrangement of **4** using Potassium Hydride. A 50% suspension of potassium hydride in paraffin oil (800 mg, 10 mmol) was rinsed with pentane, and 5 mL dichloromethane was added, followed by the slow addition of 1.00 g (3.57 mmol) of **4**. The reaction mixture was allowed to stir overnight at room temperature then quenched by the slow addition of 1 mL of water at 0 °C. The reaction mixture was partitioned between 25 mL of ether and 25 mL of water, and the ether layer was dried over anhydrous potassium carbonate. The volatiles were removed on a rotary evaporator, and the ratio of **6** and **7** by ^{1}H-NMR analysis was 95:5.

Synthesis and Rearrangement of 4-d_8.

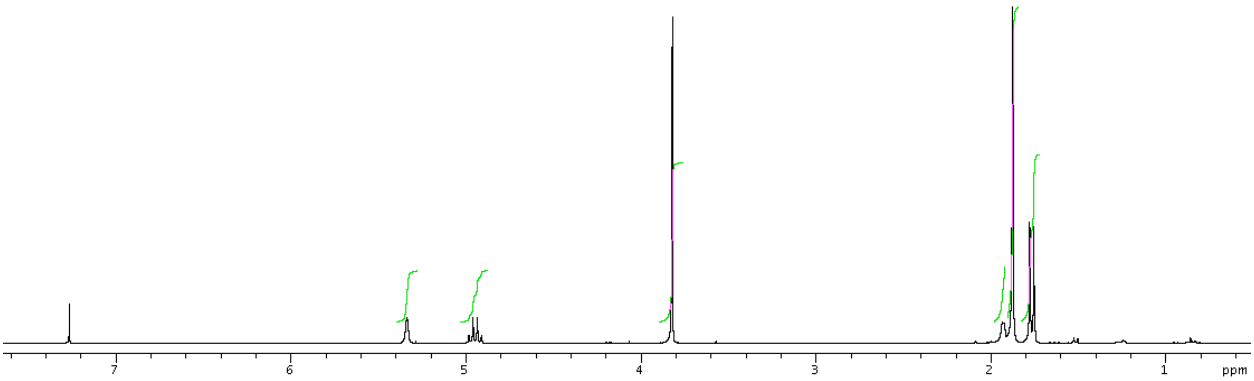
3-Methyl-2-buten-1,1-d_2-1-ol.[7] To a mixture of 40 mL of diethyl ether (dried over sodium followed by distillation under nitrogen) and 476 mg (11.33 mmol) of $LiAlD_4$ under

nitrogen at 0 °C was added dropwise 1.92 g (14.98 mmol) of ethyl 3-methylcrotonate. The mixture was heated to reflux for 1 h then cooled to 0 °C and quenched by the sequential dropwise addition of 0.5 mL of water, 0.5 mL of 15% aqueous sodium hydroxide, and 1.5 mL of water. The resulting mixture was filtered and filtrate was dried over anhydrous magnesium sulfate. The ether was carefully removed on a rotatory evaporator to afford 957 mg (66%) of crude 3-methyl-2-buten-1,1-d_2-1-ol, contaminated with ether but judged to be approximately 90% pure by NMR analysis. This material was used in the next step without further purification. ^{1}H NMR ($CDCl_3$): δ1.68 (d, J = 1.2 Hz, 3 H), 1.74 (d, J = 1.2 Hz, 3 H), 5.40 (br s, 1 H).

1-Bromo-3-methyl-2-butene-1,1-d_2.[8] To a mixture of 957 mg (10.8 mmol) of 3-methyl-2-buten-1,1-d_2-1-ol and 15 mL of pentane under nitrogen at 0 °C was added 1.14 g (4.21 mmol) of phosphorus tribromide over a 20-min period. Stirring of the reaction mixture was continued for additional 2 min before addition of 1 mL (24.7 mmol) of ice-cold methanol. To that mixture 10 mL of 5% aqueous ice-cold sodium bicarbonate solution was added followed by washing the organic layer with 5 mL of ice-cold water and 5 mL of ice-cold brine. The pentane layer was dried over anhydrous magnesium sulfate. The solvent was removed on a rotatory evaporator, keeping the temperature at 0 °C, to afford 635 mg of crude 1-bromo-3-methyl-2-butene-1,1-d_2 (62%), judged to be approximately 90% pure by NMR analysis. The crude material was used in the next step without further purification. ^{1}H NMR (399.53 MHz, $CDCl_3$): δ1.73 (d, J = 1.3 Hz, 3 H), 1.78 (d, J = 1.3 Hz, 3 H), 5.52 (br s, 1 H).

N,*N*-Bis(methyl-d_3)alanine, methyl ester. To a mixture of 1.00 g (11.55 mmol) of bis(methyl-d_3)amine hydrogen chloride, 1 mL water and 600 mg (15 mmol) of sodium hydroxide at 0 °C was added a solution of 831 mg (4.98 mmol) of methyl 2-bromopropanoate in 2 mL of dichloromethane. After stirring overnight the reaction mixture was poured into 20 mL of water and extracted with three 25-mL portions of diethyl ether. The ether layers were combined and dried over anhydrous potassium carbonate, and the volatiles were removed on a rotatory evaporator to afford 459 mg (68%) of crude *N*,*N*-bis(methyl-d_3)alanine, methyl ester, which was used in the next step without further purification. ^{1}H NMR ($CDCl_3$): δ 1.27 (d, J = 7.0 Hz, 3 H), 3.22 (q, J =7.0 Hz 1 H), 3.70 (s, 3 H).

Ammonium salt **4**-d_8. To a mixture of 459 mg (3.35 mmol) of *N*,*N*-bis(methyl-d_3)alanine, methyl ester and 2 mL of hexanes under nitrogen at room temperature was added 525 mg (3.48 mmol) of 1-bromo-3-methyl-2-butene-1,1-d_2. The resulting mixture was stirred for 16 h. During the stirring some solid precipitated out from the solution. After the solid was dissolved in minimum amount of dichloromethane, approximately 1 mL of THF was added followed by 5 mL of hexanes. Then mixture was again stirred overnight to precipitate out the solid. This process was repeated twice to afford 596 mg (62%) of the ammonium salt (**4**-d_8), contaminated with approximately 5% hexanes and a small amount of water: ^{1}H-NMR ($CDCl_3$): δ 1.76 (d, J=7.1 Hz, 3 H), 1.89 (s, 6 H), 3.83 (s, 3 H), 4.92 (q, J = 7.1 Hz, 1 H), 5.01 (br s, 1 H).

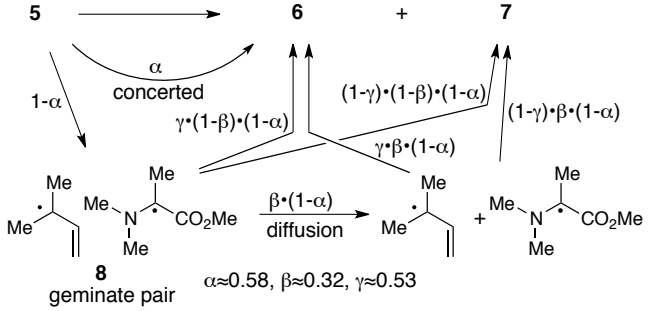


Crossover rearrangement of **4** / **4**-d_8. To a mixture of 280 mg (1.00 mmol) of **4**, 288 mg (1.00 mmol) of **4**-d_8, and 2.8 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) under nitrogen at 90 °C was added 570 mg (3.74 mmol) of DBU dropwise. The stirring of the reaction mixture continued for additional 1 h at 90 °C. After cooling to room temperature the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with five 25-mL portions of water and dried (Na_2SO_4), and the volatiles were removed on a rotary evaporator. The residue was flash chromatographed on silica gel using 20% ethyl acetate in hexanes as eluent, and the separated components **6** and **7** were characterized by ^{1}H-NMR and ESI-MS. In each case the extent of crossover was based on the relative intensities of the M=206 and M=208 peaks, averaging two measurements for **6** and three measurements for **7**, to obtain 4.9% and 17.9% for **6** and **7**, respectively.

Roughly similar results had initially been obtained for an alternatively labeled reactant, **4**-d_5 with the methyl ester labeled with d_3 instead of the methyls of the amine. However, the results with **4**-d_5 were compromised by a slow transesterification, while **4**-d_8 is not susceptible to this problem.

Simulation of the Crossover Results with a Kinetic Model, and Error Analysis.

As described in the main test, the crossover results were interpreted with a kinetic model. There are three experimental observables, the fraction of [2,3]-product **6** (0.804), the crossover in the [2,3]-product (0.049) and the crossover in the [1,2]-product **7** (0.1794). These values were predicted on an Excel™ spreadsheet using as variables α, β, and γ as defined in the main text, along with the ratio of **4** versus **4**-d_8 in the starting mixture (0.56:0.44).



The following equations governed the simulation:

6-d_0: = A6*A4 + A4*B6*B8*A10 + A4*B6*A8*A10*A4

6-d_2: = B4*B6*A8*A10*A4

6-d_6: = B4*B6*A8*A10*A4

6-d_8: = A6*B4 + B4*B6*B8*A10 + B4*B6*A8*A10*B4

7-d_0: = A4*B6*B8*B10 + A4*B6*A8*B10*A4

7-d_2: = B4*B6*A8*B10*A4

7-d_6: = B4*B6*A8*B10*A4

7-d_8: = B4*B6*B8*B10 + B4*B6*A8*B10*B4

where

A4 is the proportion of **4** versus **4**-d_8 (0.56), B4 = 1-A4

A6 = α, B6 = 1-α

A8 = β, B8 = 1-β,

A10 = γ, B10 = 1-γ

The fraction of [2,3]-product **6** was then just calculated as **6**-d_6 (**6**-d_6 + **6**-d_8)

(**6**-d_0 + **6**-d_2 + **6**-d_6 + **6**-d_8) / (**6**-d_0 + **6**-d_2 + **6**-d_6 + **6**-$d_{8\,+}$ **7**-d_0 + **7**-d_2 + **7**-d_6 + **7**-d_8)

The fraction of crossover in **6** was calculated as **6**-d_6 / (**6**-d_6 + **6**-d_8).

The fraction of crossover in **7** was calculated as **7**-d_6 / (**7**-d_6 + **7**-d_8).

The solver function in Excel™ was then used to minimize the difference between the experimental and model-predicted values (although this could also be done analytically, as the simulation is in effect three equations in three unknowns to fit three experimental values).

It is of interest to consider the possible sources of error and their effect on the results. One source of error is that some portion of the radicals that separate diffusionally will undergo side reactions and not lead to observed **6** or **7**. In this way, the amount of diffusional separation is underestimated. Although we have observed small amounts of side products that arise in this way in related reactions, we did not do so for the rearrangement of **5**. Due to the "persistent radical effect", side reactions from radical-radical recombination are sometimes much less prevalent than might otherwise have been expected. Still, we assume that we have simply missed some small amount of side products.

To investigate the effect of the presumed missed side reactions, we redid the simulation assuming that only 50% of the diffusionally separated radicals end up as either **6** or **7**. With this assumption, the values of α, β, and γ change to 0.516, 0.485, and 0.528, respectively. This is a decrease in the amount of concerted rearrangement and an increase in the amount of diffusional separation, but the change would have no effect on the conclusions.

A second possible source of error is related to the assumption in the model that a constant portion γ of recombining radicals afford **6**, regardless of whether recombination occurs from the initial geminate pair or from diffusion together in solution. It is quite plausible that the geminate pair **8** would be created in a geometry that would favor formation of **6** over **7**, relative to **8** that arises from diffusion together in solution. To the extent that this is the case, the simulation will overestimate the amount of concerted rearrangement. It is notable then that both sources of error lead to an overestimate of the value of α, resulting in our view that the α value of 0.58 in the text is likely an upper limit.

Synthesis and Rearrangement of 1-d_5**.**

2-Propen-1,1-d_2-1-ol and allyl bromide-d_2.[9] To a mixture of 250 mL of diethyl ether (dried over sodium followed by distillation under nitrogen) and 2.50 g (60 mmol) of $LiAlD_4$ at 0 °C under nitrogen was added dropwise 9.05 g (100 mmol) of acryloyl chloride in 110 mL of dry

ether. The mixture was allowed to stir overnight at room temperature then quenched by the successive addition of 2.5 mL of 15% aqueous sodium hydroxide, 7.5 mL of water and 2.5 mL of 15% aqueous sodium hydroxide at 0 °C. The reaction mixture was filtered and the filtrate was dried over anhydrous magnesium sulfate, and the volatiles were removed on a rotatory evaporator using an ice-water bath to afford 1.8 g (30%) of crude propen-1,1-d_2-1-ol.

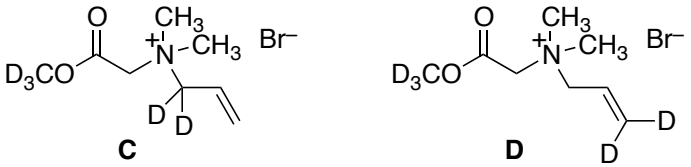
The crude material was used in the next step without further purification. The deuterated alcohol was used to synthesize d_2-allyl bromide using a reported procedure.[9] The resulting ratio of **A** to **B** was found to be 9:1 by NMR analysis.

A **B**

Methyl-d_3 bromoacetate.[10] To a mixture of 3.20 g (88.0 mmol) of d_4-methanol, 4.50 g (44.0 mmol) of triethylamine and 10 mL of dichloromethane (dried over 3Å molecular sieves) under nitrogen at 0° C was added dropwise slowly 8.80 g (43.96 mmol) of bromoacetyl bromide. The mixture was allowed to stir for 2 h, then quenched by the addition of 50 mL of 15% aqueous sulfuric acid at 0 °C. The organic layer was washed with two 25-mL portions of water and two 25-mL portions of saturated aqueous sodium bicarbonate solution. After drying over anhydrous magnesium sulfate the volatiles were removed on a rotatory evaporator to afford 6.1 g (90%) of crude methyl-d_3 bromoacetate contaminated with 6% CH_2Cl_2. ^{1}H NMR ($CDCl_3$): δ 3.84 (s).

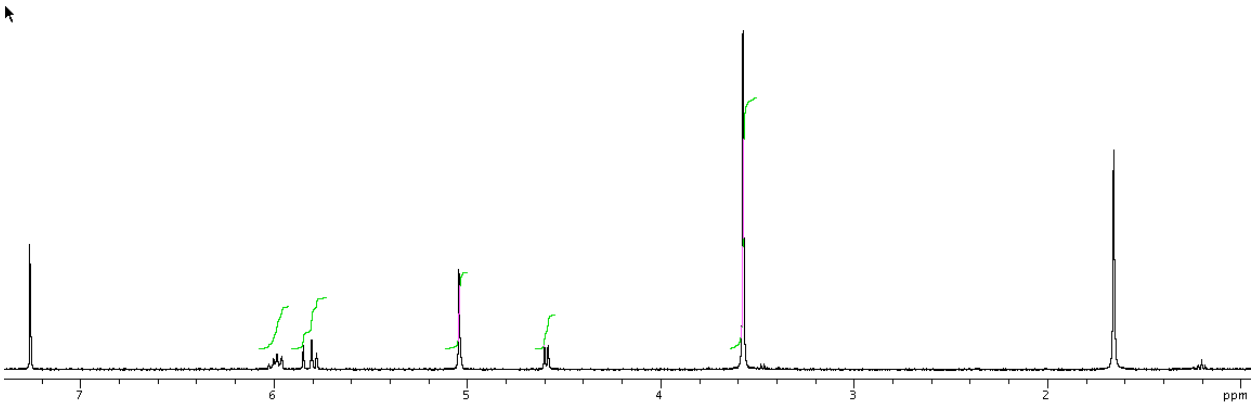
N,*N*-dimethylglycine methyl-d_3 ester. A mixture of 10.00 g (88.89 mmol) of 40% aqueous solution of dimethylamine and 4 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling 6.00 g (38.5 mmol) of methyl-d_3 bromoacetate was added and the mixture was stirred at 0 °C for 12 h. The reaction mixture was then poured into 20 mL of water and the organics were extracted with three 50-mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous sodium sulfate. The volatiles were then removed on a rotatory evaporator to afford 3.77 g (84%) of *N*,*N*-dimethylglycine methyl-d_3 ester contaminated with 8% acetonitrile based on NMR analysis. ^{1}H NMR (399.53 MHz, $CDCl_3$): δ 2.33 (s, 6 H), 3.16 (s, 2 H),

Ammonium salt **1**-d_5. To a mixture of 292 mg (2.43 mmol) of N,N-dimethylglycine methyl-d_3 ester and 2 mL of ether (dried over sodium followed by distillation under nitrogen) under nitrogen at room temperature was added 300 mg (2.43 mmol) of d_2-allyl bromide. The resulting mixture was stirred overnight. During the stirring solid precipitated out from the solution. The volatiles were removed under vacuum to afford 459 mg (78%) of crude ammonium salt **1**-d_5 (**C** and **D**), judged to be more than 95% pure by comparing NMR of the unlabeled **1**. The ratio of **C** to **D** was found to be (10:7) by NMR analysis.



C **D**

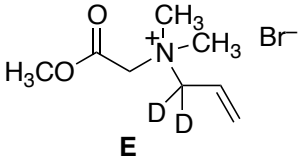
In the ^{1}H NMR spectrum of **C / D** below, the non-integrated peaks are $CHCl_3$ (7.26) and water (1.65). Traces of diethyl ether can be seen in the baseline.



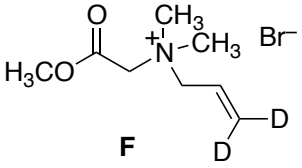
Crossover rearrangement of **1** / **1**-d_5. To a mixture of 249 mg (1.05 mmol) of **1**, 252 mg (1.05 mmol) of **1**-d_5 and 3.0 mL of N,N-dimethylformamide (dried over 3Å molecular sieves) under nitrogen at room temperature was added 600 mg (3.94 mmol) of DBU dropwise. The stirring of the reaction mixture continued for additional 1 h at room temperature before the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with three 25-mL portions of water. Then the ether layer was dried over sodium sulfate. After removing the volatiles on a rotatory evaporator residue was analyzed by ^{1}H-NMR and ESI-MS. The M+3 peak that would be associated with crossover was not detectable in the ESI-MS.

Synthesis and Rearrangement of 1-d_2.

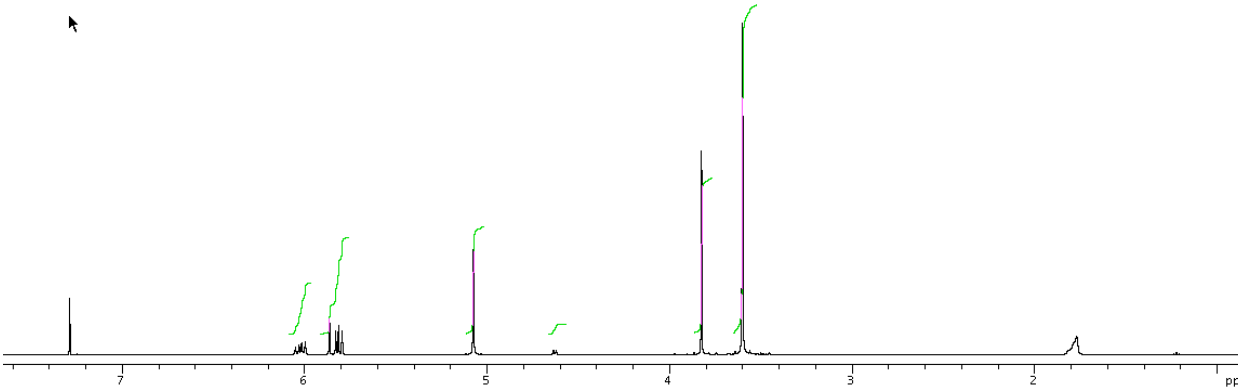
Ammonium salt **1**-d_2. To a mixture of 680 mg (5.81 mmol) of N,N-dimethylglycine methyl ester and 5 mL of ether (dried over sodium followed by distillation under nitrogen) under nitrogen at room temperature was added 685 mg (5.57 mmol) of d_2 -allyl bromide. The resulting mixture was stirred overnight. During the stirring solid precipitated out from the solution. The volatiles were removed under vacuum to afford 748 mg (55%) of crude ammonium salt **1**-d_2 (**E** and **F**), judged to be more than 95% pure by comparing NMR of the unlabeled **1**. The ratio of **E** to **F** was found to be (10:1) by NMR analysis.



E

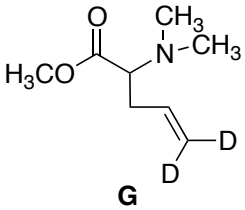


F

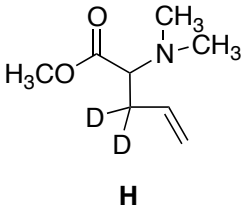


DBU mediated rearrangement **1**-d_2. To a mixture of 1.0 mL of N,N-dimethylformamide (dried over 3Å molecular sieves) and 238 mg (1.00 mmol) of **1**-d_2 (ratio of **E** to **F** is 10:1) under

nitrogen at room temperature, was added 1.52 g (10.0 mmol) of DBU. The stirring of the reaction mixture continued for additional 1 h at room temperature before the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with three 25-mL portions of water. Then the ether layer was dried over sodium sulfate. After removing the volatiles on a rotatory evaporator the ratio of **G** to **H** was judged to be 10:1 from ^{1}H-NMR analysis.



G



H

Computational Procedures and Supporting Computational Results

General

Calculations of structures, energies, and frequencies employed standard procedures in Gaussian09[11,12,13] unless otherwise noted. Structures used in POLYRATE calculations were optimized using the int(grid=ultrafine) and nosymm options. Complete structures and energetics are provided in a section below.

All absolute energies are in Hartrees. All relative energies are presented in kcal/mol.

The program suite PROGDYN used for dynamics is a series of component programs written as either Unix shell scripts or awk programs. Gaussian09 was used to calculate the forces at each point in trajectories. A full description of PROGDYN including listings of the subprograms can be found in a later section. The latest version of this program can be obtained by emailing Daniel Singleton at singleton@mail.chem.tamu.edu. The original version of this program was published in the Supporting Information of a previous paper.[14]

On the Need for Variational Transition State Theory in These Reactions

For reactions not involving hydrogen transfer, it is often sufficient to employ conventional transition state theory (TST) for adequate comparisons with experiment. For example, we have previously observed many times that conventional TST in combination with a one-dimensional tunneling correction[15] was sufficient for the prediction of heavy-atom isotope effects.[16] Two factors associated with the current study lead to the requirements for more careful theory. The first factor is that the transition structures for the rearrangement of **2** involve considerably greater bond breaking than bond making, so that the entropy is increasing significantly in the area of the saddle point. As a result, the maximum in free energy, the variational transition state, is earlier than the potential energy saddle point by an amount that affects isotope effect predictions. The second factor is that the simple C-N bond cleavage of **5** (associated with **10**‡) occurs in an area of the potential energy surface in which the potential energy is relatively flat, while entropy is changing rapidly. In order to compare the rates associated with **9**‡ and **10**‡, it was therefore necessary to compare variational TST calculations.

GAUSSRATE / POLYRATE Calculations

The variational TST calculations in the manuscript made use of the programs GAUSSRATE (reference 5a in the main text) and POLYRATE (reference 5b in the main text, see the last section for the complete reference).[17] These programs were modified in minor ways.

In particular, the subroutine *mepout* was modified to output frequencies with higher precision, and the utility program *shuttle* was modified to save copies of all frequency calculations so that data could be extracted from them later.

To show the complete set of options selected for these calculations, a sample set of input files for GAUSSRATE / POLYRATE are given in a later section. For the sake of simplicity, the starting material in these calculations was generally taken to be the conformer of **2** obtained from a steepest-descent path in mass-weighted coordinates starting at the transition structure. This conformer is not the lowest-energy conformer of the starting material and it is in any case not an appropriate starting material for the calculation of the experimental isotope effect (where **1** is the appropriate starting material), but this does not matter for the purpose at hand of calculating canonical variational transition state theory (CVT) transition structures and CVT / small-curvature tunneling (CVT/SCT) corrections to the conventional TST isotope effects.

The starting materials for variational TST calculations for the [2,3]-rearrangement of **5** and cleavage of **5** were also different. In figuring out the relative rate constants for [2,3]-rearrangement versus cleavage, the difference in starting materials was allowed for in a normal way based on the calculated free energies for the differing starting materials.

KIE Predictions

For the various transition structures (the potential-energy saddle points) versus the appropriate lowest-energy conformation of **1**, we first calculated conventional TST isotope effects by the method of Bigeleisen and Mayer[18] using the program QUIVER.[19] Due to the diversity of computational methods and basis sets employed, along with the questionable applicability of any particular literature scaling factor to carbon isotope effects, we opted to use a single scaling factor of 0.9614 in all cases. The choice of scaling factor has a negligible effect on all of the predicted isotope effects except those at C^3, and for C^3 the choice of scaling factor within a reasonable range affected the predicted KIE by no more than 0.002.

The isotope effects obtained from conventional transition state theory were then corrected for tunneling and variational transition state effects based on results from GAUSSRATE. It was not practical to carry out GAUSSRATE calculations with more than a few of the computational methods employed, so we employed a composite method of correcting the conventional TST KIEs calculated at the various methods by corrections calculated in B3LYP-D2/6-31G*/PCM calculations. The rate constants obtained from GAUSSRATE were used to calculate both "gaussrate-TST" and "gaussrate-CVT/SCT" isotope effects, then the ratio of the gaussrate-CVT/SCT and gaussrate-TST isotope effects was used as the correction factor to turn the conventional TST isotope effects obtained from QUIVER into CVT-SCT isotope effects based appropriately on the starting **1**.

Table S3. KIE Predictions (25 °C, k_{12C}/k_{13C})versus C^3-N and C^1-C^5 Distances.

Method	Basis Set	Solvent Model	C^3-N distance	C^1-C^5 distance	C^5 KIE	C^3 KIE	C^1 KIE	C^6 KIE
wB97	6-31G*	PCM	1.90	2.28	1.023	1.042	1.021	1.008
M11	6-31G*	PCM	1.96	2.36	1.017	1.040	1.019	1.009
wB97X	6-31G*	PCM	1.99	2.40	1.018	1.044	1.018	1.008
lc-B97D	6-31G*	PCM	2.07	2.42	1.019	1.043	1.020	1.010
wB97X	6-31+G**	PCM	2.04	2.43	1.017	1.045	1.018	1.011
M11	6-31G*	gas phase	1.948	2.435	1.015	1.040	1.017	1.007
M06-2X	6-31+G**	PCM	2.03	2.46	1.015	1.045	1.017	1.011
SOGGA11X	6-31G*	PCM	2.04	2.51	1.016	1.046	1.017	1.009
wB97XD	6-31G*	PCM	2.04	2.51	1.015	1.045	1.017	1.009
wB97XD	6-31+G**	PCM	2.09	2.53	1.015	1.045	1.018	1.011
M06-2X	6-31+G**	GAS	1.999	2.534	1.014	1.045	1.016	1.008
N12SX	6-31G*	PCM	2.032	2.55	1.013	1.047	1.016	1.009
PBE0-D3	6-31G*	PCM	2.028	2.57	1.013	1.046	1.016	1.009
SOGGA11X	6-31G*	gas phase	2.014	2.578	1.014	1.047	1.015	1.007
PBE0	6-31+G**	PCM	2.073	2.593	1.012	1.049	1.015	1.011
WB97XD	6-31+G**	gas phase	2.048	2.6	1.012	1.048	1.014	1.008
M06-D3	6-31G*	PCM	2.098	2.609	1.012	1.047	1.015	1.010
N12SX	6-31G*	gas phase	1.997	2.617	1.012	1.047	1.014	1.007
MN12SX	6-31G*	PCM	2.111	2.623	1.012	1.049	1.016	1.010
APFD	6-31G*	PCM	2.045	2.625	1.015	1.044	1.016	1.007
PBE0-D3	6-31G*	gas phase	1.991	2.642	1.012	1.047	1.014	1.007
M06	6-31+G**	PCM	2.14	2.65	1.010	1.050	1.014	1.011
M06-D3	6-31G*	gas phase	2.064	2.66	1.011	1.047	1.014	1.007
PBE0	6-31+G**	GAS	2.029	2.665	1.01	1.049	1.014	1.008
APFD	6-31G*	gas phase	2.001	2.684	1.011	1.053	1.010	1.005
MN12SX	6-31G*	gas phase	2.076	2.684	1.012	1.049	1.014	1.008
B971	6-31G*	PCM	2.08	2.70	1.011	1.046	1.015	1.010
B98	6-31G*	PCM	2.09	2.70	1.011	1.046	1.015	1.010
B3LYP-D2	6-31G*	PCM	2.115	2.708	1.011	1.046	1.015	1.009
M06	6-31+G**	GAS	2.084	2.708	1.009	1.051	1.012	1.008
B972	6-31G*	PCM	2.08	2.71	1.011	1.048	1.014	1.010
B3LYP-D2	6-31+G**	SMD	2.14	2.72	1.012	1.049	1.015	1.012
MN12L	6-31G*	PCM	2.182	2.723	1.012	1.051	1.015	1.010
B3LYP-D2	6-31+G**	PCM	2.15	2.73	1.010	1.047	1.015	1.011
B971	6-31+G**	PCM	2.128	2.729	1.011	1.047	1.016	1.011
B98	6-31+G**	PCM	2.13	2.73	1.011	1.046	1.016	1.012
B972	6-31+G**	PCM	2.112	2.74	1.009	1.050	1.014	1.012
M11L	6-31G*	PCM	2.127	2.756	1.010	1.052	1.017	1.011
BP86-D2	6-31G*	PCM	2.077	2.769	1.010	1.045	1.014	1.008
B3LYP-D3	6-31G*	PCM	2.102	2.77	1.011	1.046	1.014	1.010
PBEPBE-D2	6-31G*	PCM	2.06	2.776	1.009	1.046	1.013	1.008
MN12L	6-31G*	gas phase	2.125	2.777	1.011	1.051	1.013	1.008
B3LYP-D2	6-31G*	gas phase	2.062	2.789	1.010	1.047	1.013	1.007
B3LYP	6-31G*	PCM	2.103	2.791	1.010	1.048	1.013	1.010
N12	6-31G*	PCM	2.035	2.806	1.009	1.050	1.011	1.009
B971	6-31+G**	gas phase	2.067	2.816	1.009	1.049	1.012	1.008
B3LYP	6-31+G**	PCM	2.14	2.82	1.009	1.049	1.013	1.012
B972	6-31+G**	gas phase	2.045	2.822	1.009	1.050	1.012	1.009
M11L	6-31G*	gas phase	2.092	2.823	1.009	1.052	1.016	1.009
N12	6-31+G**	PCM	2.07	2.836	1.007	1.051	1.011	1.011

B3LYP-D3	6-31G*	gas phase	2.038	2.864	1.010	1.046	1.012	1.007
N12	6-31G*	gas phase	1.977	2.869	1.008	1.050	1.0091	1.007
BP86-D2	6-31G*	gas phase	1.985	2.88	1.008	1.046	1.010	1.006
PBEPBE-D2	6-31G*	gas phase	1.978	2.88	1.008	1.047	1.010	1.006
B3LYP	6-31+G**	gas phase	2.058	2.911	1.008	1.049	1.011	1.009
BLYP-D2	6-31G*	PCM	2.061	2.953	1.008	1.047	1.009	1.008
B97D	6-31G*	PCM	2.04	2.96	1.008	1.048	1.0087	1.009
B97D	6-31+G**	PCM	2.063	2.965	1.007	1.049	1.009	1.010
SOGGA11	6-31G*	PCM	2.04	2.97	1.007	1.045	1.013	1.009
B97D	6-31+G**	PCM	2.06	2.97	1.007	1.049	1.0089	1.011
B97D3	6-31G*	PCM	1.953	3.001	1.008	1.050	1.005	1.009
B97D	6-31+G**	gas phase	1.911	3.056	1.007	1.049	1.006	1.007
BLYP-D2	6-31G*	gas phase	1.862	3.062	1.008	1.046	1.005	1.006
SOGGA11	6-31G*	gas phase	1.951	3.135	1.007	1.046	1.008	1.007

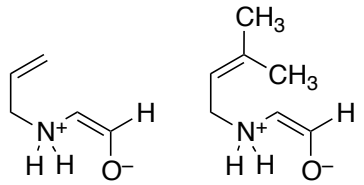
Exploration of DFT and ab initio Methods

The applicability of computational methods to the reactions of interest was explored in detail by a series of studies with varying goals. One goal was to gauge the direction of and magnitude of systematic errors in the energies of **9**‡ versus **10**‡. Another goal was to determine the best practical choice of method for trajectory calculations, and, with the expectation that no method would be entirely satisfactory for what is a difficult computational problem, minimize and gauge the direction of systematic errors.

In general terms we used two methods to evaluate computational methods. From an experimental perspective we considered whether the computational methods led to predictions of kinetic isotope effects for the rearrangement of **2** that were reasonably consistent with experimental observations. This was true of approximately half of the methods explored, as may be discerned from the table in the previous section. M06-2X calculations *did not* lead to a reasonable prediction of the isotope effects, but we explored these calculations in detail because the direction of their error was clear (too tight of transition state, too high of a barrier for bond cleavage) and it was viewed as significant that despite the direction of the error, M06-2X trajectories through **9**‡ still gave a mixture of rearrangement and bond cleavage.

The second method for the evaluation of computational methods was based on a comparison of energetics versus (U)BD(T)[20] single-point energies performed with the largest feasible basis set. Although (U)BD(T) calculations are still incomplete in their description of systems having diradical character, we have previously noted their reasonable accuracy, as have others.[21,22] As a check for the current work, we explored that use of (U)BD(T) calculations for the dissociation of the C-H bond in ethane and the central carbon-carbon bond of 1,5-hexadiene. When the basis set is too small (e.g. 6-31G*, cc-pvdz) the (U)BD(T) calculations unsurprisingly underestimate the barriers for these dissociations, but medium-sized basis sets (6-311+G**, aug-cc-pvdz) perform well and cc-pvtz or larger performs very well versus known experimental data. Further, the (U)BD(T) calculations provide a smooth energy curve with no apparent anomalies.

It was not practical to carry out (U)BD(T) calculations with a good basis set on the reactions of either **2** or **5**, so we employed the model reactions of **A** and **B**.



A **B**

Energetics of [2,3]-Rearrangement versus Bond Cleavage in Structures A and B.

To gauge the direction of and magnitude of systematic errors in the energies of $\mathbf{9}^{\ddagger}$ versus $\mathbf{10}^{\ddagger}$, we explored the barriers for the [2,3]-rearrangement versus C-N bond cleavage in the models **A** and **B**. This was done using single-point calculations on a set of three structures in each system obtained in (U)M06/631+G** (gas phase) calculations: the starting **A** or **B**, the exo s-cis transition structure for the [2,3]-rearrangement of **A** or **B**, and the lowest-energy transition structure for the C-N bond cleavage of **A** or **B**.

Table S4 below summarizes the results. For each system, the table first presents the absolute energies and calculated barriers in the UBD(T) calculations with a series of basis sets. (The closed-shell starting structures **A** and **B** were in each case calculated using RBD(T)). The table then presents the corresponding energies, calculated on the same geometries, for DFT methods. The "Bias favoring cleavage" was defined by comparing the relative barrier for cleavage versus rearrangement as calculated by the DFT methods versus those calculation by the UBD(T) calculations with a cc-pvtz basis set for system **A** and an aug-cc-pvdz basis set for system **B**. It can be noted that in each case the DFT calculations appear to overestimate the facility of the cleavage process.

Table S4. UBD(T) versus DFT methods for [2,3]-rearrangement versus bond cleavage

Structure	Method	P.E. Barrier	Relative Cleavage Barrier	Bias favoring cleavage
	UBD(T)/6-31+G**			
A	-324.968154			
[2,3]-TS	-324.944803	14.7		
cleavage ts	-324.927008	25.8	11.2	
	UBD(T)/6-311+G**			
A	-325.086484			
[2,3]-TS	-325.063202	14.6		
cleavage ts	-325.044343	26.4	11.8	
	UBD(T)/aug-cc-pvdz			
A	-325.029883			
[2,3]-TS	-325.008653	13.3		
cleavage ts	-324.988515	26.0	12.6	
	UBD(T)/cc-pvtz			
A	-325.291245			
[2,3]-TS	-325.267234	15.1		
cleavage ts	-325.247319	27.6	12.5	
	DFT methods			

	(U)M06/6-31+G**			
A	-325.637319			
[2,3]-TS	-325.616474	13.1		
cleavage ts	-325.603027	21.5	8.4	4.1
	(U)M062X/6-31+G**			
A	-325.706939			
[2,3]-TS	-325.681698	15.8		
cleavage ts	-325.664881	26.4	10.6	1.9
	(U)B3LYP/6-31+G**			
A	-325.868930			
[2,3]-TS	-325.851119	11.2		
cleavage ts	-325.842746	16.4	5.3	7.2
	(U)B3LYP/6-31+G**/D2			
A	-325.882674			
[2,3]-TS	-325.869143	8.5		
cleavage ts	-325.856733	16.3	7.8	4.7

Structure	Method	P.E. Barrier	Relative Cleavage Barrier	Bias favoring cleavage
	UBD(T)/6-31+G**			
B	-403.377433			
[2,3]-TS	-403.352115	15.9		
cleavage ts	-403.335068	26.6	10.7	
	UBD(T)/6-311+G**			
B	-403.522106			
[2,3]-TS	-403.496345	16.2		
cleavage ts	-403.478526	27.3	11.2	
	UBD(T)/aug-cc-pvdz			
B	-403.450655			
[2,3]-TS	-403.427451	14.6		
cleavage ts	-403.407668	27.0	12.4	
	DFT methods			
	(U)M06/6-31+G**			
B	-404.216812			
[2,3]-TS	-404.194027	14.3		
cleavage ts	-404.181690	22.0	7.7	4.7
	(U)M062X/6-31+G**			
B	-404.308210			
[2,3]-TS	-404.279571	18.0		
cleavage ts	-404.264754	27.3	9.3	3.1
	(U)B3LYP/6-31+G**			
B	-404.512971			
[2,3]-TS	-404.491524	13.5		
cleavage ts	-404.486286	16.7	3.3	9.1

	(U)B3LYP/6-31+G**/D2			
B	-404.536481			
[2,3]-TS	-404.521091	9.7		
cleavage ts	-404.509314	17.0	7.4	5.0

The Energy Surface for Cleavage During Trajectory Calculations

To be practical, trajectory calculations were limited to DFT surfaces with a moderate or small basis set. In gauging the appropriateness of energy surfaces for the purpose at hand, it was not considered to be critically important that the surface correctly calculate the absolute barrier for the rearrangement. B3LYP calculations in particular underestimate the barrier for the rearrangement since they underestimate the strength of σ bonds relative to π bonds.

Of much greater importance in our view was the shape of the energy surface in the area of the [2,3]-rearrangement transition structure and the energy change as bond cleavage proceeds from the rearrangement transition structure versus that for consummation of the rearrangement. To assess this issue, we developed a representative grid of geometries by fixing the C^3-N and C^1-C^5 distances and optimizing the structure in UB3LYP/6-31G* calculations. Single-point energies were then carried out on these structures at a variety of levels.

Tables S5 and S6 present the results of those calculations, first as absolute energies and then as relative energies. We will then present the results graphically and discuss them.

Table S5. Absolute energies for single points for a grid of representative geometries

C3-N distance	C1-C5 distance	UB3LYP 6-31G*	D2 corrected UB3LYP 6-31G*	UB3LYP 6-31+G**	D2 corrected UB3LYP 6-31+G**	RB3LYP 6-31G*	UM06 6-31G*
2	3.0	-325.81406	-325.83106	-325.85154	-325.86854	-325.81406	-325.58320
2.1	3.0	-325.81324	-325.83041	-325.85104	-325.86821	-325.81324	-325.58134
2.2	3.0	-325.81269	-325.82987	-325.85092	-325.86810	-325.81269	-325.58016
2.3	3.0	-325.81222	-325.82929	-325.85095	-325.86801	-325.81222	-325.57997
2.4	3.0	-325.81197	-325.82880	-325.85106	-325.86789	-325.81175	-325.58053
2.6	3.0	-325.81258	-325.82892	-325.85200	-325.86834	-325.81055	-325.58205
2.8	3.0	-325.81259	-325.82986	-325.85202	-325.86757	-325.80934	-325.58298
3	3.0	-325.81547	-325.83057	-325.85323	-325.86833	-325.80857	-325.58399
2.8	2.8	-325.81643	-325.83303	-325.85368	-325.87027		-325.58537
2.8	2.6	-325.82121	-325.83832	-325.85783	-325.87493		-325.58905
2.8	2.4	-325.82771	-325.84527	-325.86373	-325.88129		-325.59641
2.8	2.2	-325.83569	-325.85355	-325.87097	-325.88883		-325.60666

C3-N distance	C1-C5 distance	UM062X 6-31G*	UB97D 6-31G*	UwB97XD 6-31G*	UPBE1PBE 6-31G*	UBD(T) 6-31+G**	UBD(T) 6-311+G**
2.0	3.0	-325.64996	-325.60470	-325.69903	-325.42580	-324.94459	-325.06263
2.1	3.0	-325.64733	-325.60522	-325.69651	-325.42402	-324.94388	-325.06187

2.2	3.0	-325.64519	-325.60559	-325.69494	-325.42264	-324.94357	-325.06139
2.3	3.0	-325.64355	-325.60569	-325.69506	-325.42176	-324.94118	-325.05891
2.4	3.0	-325.64304	-325.60559	-325.69603	-325.42171	-324.93995	-325.05767
2.6	3.0	-325.64412	-325.60487	-325.69830	-325.42253	-324.93999	-325.05768
2.8	3.0	-325.64499	-325.60456	-325.69982	-325.42385	-324.93916	-325.05745
3.0	3.0	-325.64645	-325.60378	-325.70150	-325.42515	-324.94061	-325.05875
2.8	2.8	-325.64671	-325.60961			-324.94146	-325.06028
2.8	2.6	-325.65231	-325.61429			-324.94887	-325.06821
2.8	2.4	-325.66238	-325.61919			-324.95847	
2.8	2.2	-325.67411	-325.62488			-324.96777	

Table S6. Relative energies for single points for a grid of representative geometries

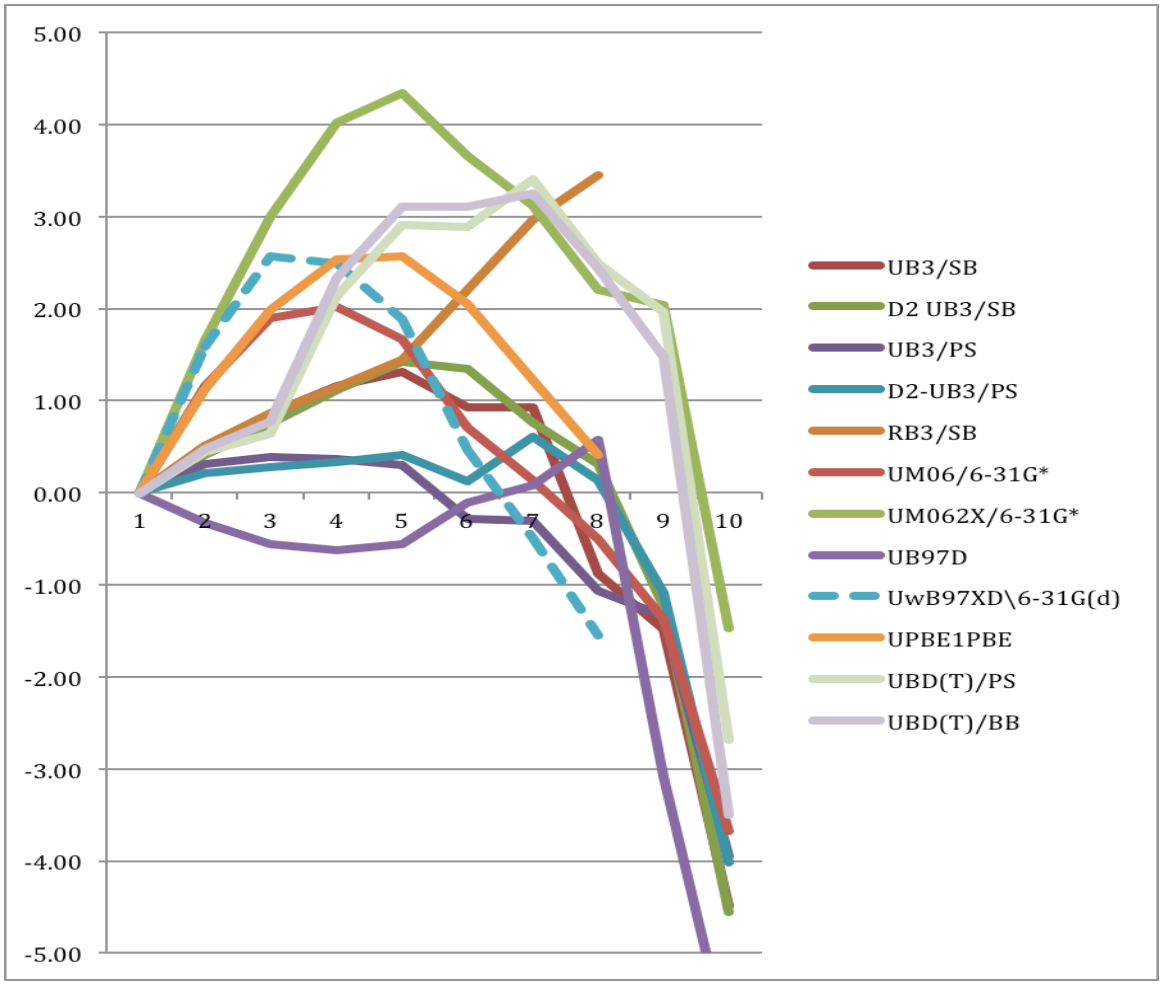
C3-N distance	C1-C5 distance	UB3LYP 6-31G*	D2 corrected UB3LYP 6-31G*	UB3LYP 6-31+G**	D2 corrected UB3LYP 6-31+G**	RESTRICTED B3LYP 6-31G*	UM06 6-31G*
2	3.0	0.00	0.00	0.00	0.00	0.00	0.00
2.1	3.0	0.51	0.41	0.31	0.21	0.51	1.16
2.2	3.0	0.86	0.75	0.39	0.28	0.86	1.90
2.3	3.0	1.15	1.12	0.37	0.33	1.15	2.02
2.4	3.0	1.31	1.42	0.30	0.41	1.45	1.67
2.6	3.0	0.93	1.35	-0.29	0.13	2.20	0.72
2.8	3.0	0.93	0.76	-0.30	0.61	2.96	0.14
3	3.0	-0.88	0.31	-1.06	0.13	3.45	-0.50
2.8	2.8	-1.49	-1.23	-1.34	-1.09		-1.37
2.8	2.6	-4.49	-4.55	-3.95	-4.01		-3.68
2.8	2.4	-8.56	-8.91	-7.65	-8.00		-8.29
2.8	2.2	-13.57	-14.11	-12.19	-12.73		-14.73
	Graph legend:	UB3/SB	D2 UB3/SB	UB3/PS	D2-UB3/PS	RB3/SB	UM06/6-31G*

C3-N distance	C1-C5 distance	UM062X 6-31G*	UB97D 6-31G*	UwB97XD 6-31G*	UPBE1PBE 6-31G*	UBD(T) 6-31+G**	UBD(T) 6-311+G**
2	3.0	0.00	0.00	0.00	0.00	0.00	0.00
2.1	3.0	1.65	-0.33	1.59	1.12	0.44	0.48
2.2	3.0	3.00	-0.56	2.57	1.98	0.64	0.78
2.3	3.0	4.02	-0.62	2.49	2.53	2.14	2.34
2.4	3.0	4.34	-0.56	1.89	2.56	2.91	3.11
2.6	3.0	3.66	-0.11	0.46	2.05	2.89	3.11
2.8	3.0	3.12	0.09	-0.49	1.22	3.41	3.25
3	3.0	2.20	0.58	-1.55	0.41	2.50	2.44
2.8	2.8	2.04	-3.08			1.96	1.48
2.8	2.6	-1.47	-6.02			-2.69	-3.50
2.8	2.4	-7.79	-9.09			-8.71	

2.8	2.2	-15.16	-12.66			-14.54	
	Graph legend:	UM062X/6-31G*	UB97D	UwB97XD\6-31G(d)	UPBE1PBE	UBD(T)/PS	UBD(T)/BB

For the graph below, the relative energies of the single points are plotted versus the first point in the series. The legend can be understood with reference to the table above, where the graph legends are listed in the column containing the data. As observations, we note that UM06-2X has too large of a barrier to dissociation in the grid of representative geometries, yet UM06-2X trajectories still lead to substantial amounts of dissociation. None of the DFT methods are entirely satisfactory matched for the UBD(T)/6-311+G** results. However, the UB3LYP-D2/6-31G* results exhibit a feature in common with the UBD(T) results but not present in the other DFT methods, namely a relatively distant maximum in energy (at grid points 5 and 6 in UB3LYP-D2/6-31G*, grid points 6 and 7 in UBD(T)/6-311+G**, but earlier in most other methods.

For this reason, along with relatively good predictions of the experimental kinetic isotope effects, we considered the UB3LYP-D2/6-31G* as the best choice for trajectories. Even so, the UB3LYP-D2/6-31G* surface underestimates the energy-maximum for dissociation (relative to the saddle point) in the model by about 1.5 kcal/mol, so it is not surprising that the trajectories afford too much dissociation versus that suggested by the crossover experiments.



Wave Function Stability and Spin Contamination.

All trajectories were calculated using unrestricted calculations and employing the "guess=mix" option in Gaussian09. The use of guess=mix is interestingly not completely reliable, and there is a sporadic complication with wave function instability that requires some discussion. In trajectories that have completed bond cleavage, that is, after the C^3-N distance is greater than 2.9 Å and with the C^1-C^5 distance > 3.2 Å, guess=mix occasionally fails to lead to the broken-symmetry solution. This is recognizable by the presence of trajectory points with S**2=0 in the midst of those with high S**2 values. When these "bad points" are checked with the "stable=opt" option in Gaussian09, it is found that a lower-energy broken-symmetry solution is present. It should be noted that if such bad points affected the results, the direction of their error would be to cause the fragments to recombine, but this never happens; [2,3]-rearrangement trajectories never show any bad points at all. Bond-cleavage trajectories never show any bad points until their outcome is decided. Overall, the error does not affect the results.

To gauge approximately the range of geometries subject to spin contamination, exploratory studies of grids of geometries associated with bond cleavage in **2** were carried out in M06-2X/6-31G* and M06/6-31G* calculations. It was found that S**2=0 when C^3-N < 2.3 and C^1-C^5 < 3.4, and when C^3-N < 2.4 and C^1-C^5 < 3.0, and when C^3-N < 2.5 and C^1-C^5 < 3.9, and when C^3-N < 2.6 and C^1-C^5 < 2.8, and when C^3-N < 2.7 and C^1-C^5 < 2.7. Outside of this range there is significant spin contamination.

All of the 2,3-rearrangement transition structures were within the range in which no spin contamination occurs. All of the B3LYP, M06-2X, and M06 2,3-rearrangement transition structures were checked with the "stable=opt" option in Gaussian09, and many of the 2,3-rearrangement transition structure were checked with the guess=mix option. In each case the 2,3-rearrangement transition structures had a stable S**2=0 wavefunction. The cleavage transition states $\mathbf{10}^{\ddagger}$ exhibited spin contamination with S**2 values before annihilation of 0.37 to 0.54. As shown by the comparison of model DFT versus UBD(T) energetics described above, the error in these structures likely underestimates their energy.

We note that the surfaces for cleavage via the [2,3]-rearrangement transition state $\mathbf{9}^{\ddagger}$ and direct cleavage via $\mathbf{10}^{\ddagger}$ are both subject to the same spin contamination error, and it seems fair to expect some cancellation of error in the comparison of bond cleavage via $\mathbf{9}^{\ddagger}$ with that via $\mathbf{10}^{\ddagger}$.

Variational TST Rates for C-N Bond Cleavage versus [2,3]-Rearrangement

As described in the main text, variational TST calculations were carried out for the [2,3]-rearrangement via $\mathbf{9}^{\ddagger}$ and C^3-N bond cleavage via $\mathbf{10}^{\ddagger}$ in order to make a prediction of the relative rates of the two processes if they were to occur by these separate transition states. These calculations were carried out on UB3LYP-D2, UM06, and UM06-2X energy surfaces, each employing a 6-31+G** basis set and each including a PCM solvent model for acetonitrile. A complication in these calculations is that the GAUSSRATE calculations for rearrangement and cleavage used differing starting materials. To compare rate constants fairly, it was necessary to allow for the difference in starting materials based on the difference in free energies between the starting structures at the temperature of interest, 90 °C.

Table S7 summarizes these calculations and their results. Two things should be noted. First, due to the bias suggested by calculations described in a previous section, the rearrangement

/ cleavage ratio would be expected to be 1-4 orders of magnitude greater than those calculated here. Second, on these energy surfaces without any adjustment, the preponderance of cleavage would occur by way of the [2,3]-rearrangement transition state.

Table S7. Relative rate constants for C-N bond cleavage versus [2,3]-rearrangement

(U)M06/6-31+G**	
90 °C, CVT/SCT	
rate constants (s-1)	starting material energetics
[2,3]-rearrangement	free energy 363
3.69E+05	-636.301632
cleavage	
5.02E+03	-636.302376
raw ratio of rate constants	difference (kcal/mol)
73.5	0.467
corrected ratio at 363	
38.5	(rearrangement / cleavage)

(U)B3LYP-D2/6-31+G**	
90 °C, CVT/SCT	
rate constants (s-1)	
[2,3]-rearrangement	free energy 363
8.18E+06	-636.803383
cleavage	
5.78E+05	-636.802746
raw ratio of rate constants	difference (kcal/mol)
14.2	-0.400
corrected ratio at 363	
24.6	(rearrangement / cleavage)

(U)M062X/6-31+G**	
90 °C, CVT/SCT	
rate constants (s-1)	
[2,3]-rearrangement	free energy 363
2.56E+01	-636.443701
cleavage	
1.49E+00	-636.442537
raw ratio of rate constants	difference (kcal/mol)
17.2	-0.731
corrected ratio at 363	
47.3	(rearrangement / cleavage)

Initialization of Trajectories and Additional Details on Trajectories

Most of the trajectories employed in the manuscript are quasiclassical, i. e. including

zero-point energy plus a Boltzmann distribution of quantized vibrational energies for each mode. As denoted in the main text in Table 1, some sets of trajectories were carried out in fully classical mode, i. e. including only a classical Boltzmann distribution of energy. For the trajectories, the desired energy in each of the normal modes was mapped from a random number generator to a Boltzmann distribution set at 25 °C. The phase of each of the normal modes was mapped from a Gaussian distribution of random numbers. This distribution is not correct for a classical oscillator but would be approximately correct for a quantum oscillator in its ground state (only ignoring mode displacements outside of the classical limit), and has the advantage that a larger portion of the trajectories start with an energy approximating the initially desired energy. The sign on the velocity of the normal modes was randomized. After an energy/force calculation on the initial geometry, the total initial energy was calculated and the trajectory was thrown out if the energy did not agree satisfactorily (within 1 kcal/mol) with the desired energy. (This is a variation of the conventional practice of scaling energies.[23]) The mode corresponding to the transition vector was treated classically.

The trajectories were initiated from the area of the potential energy saddle points (these geometries are given in a later section) and not the somewhat earlier CVT transition structure **9**‡. The trajectories were integrated both forward and backward in time to obtain complete trajectories connecting the starting **5** to either **6** or **8**. A relatively large proportion of the trajectories, 10-30%, were not productive, connecting either **6** with **8** or **8** with **8** or **6** with **6**. These are formally "recrossing" trajectories but in the current case they were not considered to be significant because the use of the potential energy saddle points instead of the CVT transition structures as the starting areas for the trajectories. In other words, since the trajectories did not start at the best choice of transition state, it is not surprising that some portion connect products with products and do not actually cross the variational transition state. The non-productive trajectories were ignored.

A 500 fs time limit was set for the trajectories to avoid the effect of nonphysical intramolecular redistribution of the zero-point energy. Only a very small proportion of trajectories, approximately 1%, did not complete within this time limit. The median times for formation of the 2,3 product **6**, the geminate pair **8**, and reformation of starting material **5** starting from the initial point in the area of the saddle point were 114 fs, 150 fs, and 60 fs, respectively.

To carry out the fully classical trajectories in the presence of acetonitrile solvent molecules, a combination of B3LYP-D2/6-31G*/PCM variational transition state structure (the 6-31G* analog of **9**‡) and 24 acetonitrile molecules placed arbitrarily (but roughly surrounding the transition structure) was subjected to two cycles of simulated annealing on a PM3 surface, starting the velocities as would be appropriate for 2363 K (in random directions) then cooling slowly (removing 0.1% of the energy per fs) to 363.15 K. In these cycles, the positions of the C^1, C^3, C^5, and N atoms were fixed but all other atoms were freely variable. The atoms were nudged into a cubic box with an edge dimension of 13.42 Å by an algorithm that reverses the momentum of atoms moving away from the boundary of the box. A final annealing cycle was then carried out on an ONIOM surface (using UB3LYP-D2/6-31G* for the atoms of **9**‡ and PM3 for the CH_3CN molecules) using an initial temperature of 1363 K and (removing 0.2% of the energy per fs) to 363.15 K. After reaching 363 K, the temperature was maintained at 363 with an algorithm that adjusts the energy toward the target temperature by 0.5% per fs, and the simulation was continued in this way for 15 ps. At intervals of 125 fs, the simulation was used

as a starter for production ONIOM trajectories by giving the C^1, C^3, C^5, and N atoms a Boltzmann-random direction and velocity while all other atoms continued their current velocity, and the trajectories were integrated both forward and backward in time until **5**, **6**, or **8** were formed.

Programs for Calculations and NMR Integrations, and Sample Input Files

Program Suite PROGDYN

A full listing of the subprograms of PROGDYN is given below. To allow the reader to understand or make use of PROGDYN, we describe here first the overall structure of the program.

The master control program for dynamics, in the form of a Unix Shell Script, is called *progdynstarterHP*. For a user to start to use *progdynstarterHP*, some early lines in it that assign the scratch space and the location of the program files and input files would have to be modified for the local environment. These lines are between lines 29 and 40 and should be apparent. The location of the scratch space is usually passed to *progdynstarterHP* as a parameter.

progdynstarterHP takes as necessary input files:
freqinHP - This is the standard output from a Gaussian 98, 03, or 09 frequency calculation using freq=hpmodes. For isotopically labeled compounds, use freq=(hpmodes,readisotopes).
progdyn.conf – This is a file giving a variety of configuration options, called on by many of the subprograms. progdyn.conf is listed below and contains explanations of the program options.

progdynstarterHP takes optional input the files listed below. These are not needed for basic runs.
isomernumber - A number in file isomernumber provides a start for numbering runs. The default is 1.
detour – A signal file that, by existing, signals the program to do a side calculations
nogo – A signal file that, by existing, signals the program to stop between points
bypassproggen - A signal file that, by existing, signals the program to use a supplied input file *geoPlusVel* instead of generating one for itself.
methodfile – A file that contains lines to be added to the end of each g09.com input file, such as lines that call for an NMR calculation
ZMAT – An input file for the CFOUR (http://www.cfour.de) suite of programs. When ZMAT is supplied, *progdynstarterHP* will automatically run call CFOUR (which must be set up independently by the user) by making use of the script *progcfour*.
cannontraj – A file containing a vector for each atom, used to fire an initial geometry in a particular direction.

progdynstarterHP calls the following programs:
proggenHP - An awk program that starts a trajectory, giving each mode its zero point energy (if a quasiclassical calculation) plus random additional excitations depending on the temperature.
prog1stpoint – Awk program that creates the first Gaussian input file for each run
prog2ndpoint – Awk program that creates the second Gaussian input file for each run. prog2ndpoint also checks the energy of the first point to see if it fits with the desired energy, and aborts the run if it does not by creating appropriate output in file Echeck
progdynb – Creates subsequent Gaussian input files until run is completed, used the awk
proganal – A program to analyze the latest point and see if a run is done. This program must be redone for each new system. Elaborate changes are often programmed into proganal, such as the automatic changing of configuration variables. proganal creates the output to dynfollowfile and NMRlist or NMRlistdis
randgen – A program that generates random numbers between 0 and 1. These are generated all at once and stored in a file for use by proggenHP.
progcfour – A control script to run CFOUR calculations (not needed for most kinds of runs).

progdynstarterHP has the following output files:
isomernumber – A running tab of the trajectory number
runpointnumber – a running tab of the point in the trajectory
Echeck – output form where prog2ndpoint checks the energy of the trajectory to see if it fits with the desired energy
geoRecord – A record of all of the geoPlusVel files.

geoPlusVel – Created by proggen, this gives the starting positions, velocities, isotopic masses, excitations of the normal modes, and initial displacements of the normal modes for current run.
g09.com – Created by prog1stpoint, prog2ndpoint, and progdynb, this is the latest input file for Gaussian09 for current run and latest point.
olddynrun and *olderdynrun* – files containing the last two outputs from Gaussian, for creation of the next point
traj, traj1, traj2, traj3, etc. – files containing the geometries and energies for each trajectory, numbered by the isomernumber, in a format suitable for reading by Molden.
dyn - A record of the Gaussian outputs.
dynfollowfile – A short record of the runs and their results. The data desired for *dynfollowfile* must be programed into the script *proganal* as needed for each system studied.
NMRlist or *NMRlistdis* – output of NMR predictions at each point in a trajectory
skipstart - A signal file that, by existing, tells progdynstarterHP that we are in the middle of a run. For trajectories that are propagated forward and backward in time, skipstart keeps track of whether one is in the forward or reverse part.
diagnostics – optional output that follows which subprograms are running and configuration variables, decided by variable in progdyn.conf
vellist – optional output that lists the velocities of each atom, decided by variable in progdyn.conf, or lists the total kinetic energy in the system and the classical temperature.
A number of files starting with *'temp'* are created then later erased.

Program progdynstarterHP

```
#!/bin/bash
#progdynstarterHP, made to use high-precision modes from Gaussian output with freq=hpmodes
#updated to create a random number file temp811 that is used by proggenHP
#version September 16, 2005, made for workstations
#version August 2007 to allow periodic copying of g09.log to dyn putting it under control of progdynb
#version Feb 2008 moves variables like the scratch directory and location of randgen to the beginning
#version March 2008 added proganal reporting to points 1 and 2
#version Jan 2009 fixed bug generator of having proganal run twice in checking for complete runs
#version May 2009 Echeck catches bad energies after only one point, other lines written simpler, triple while loop, revised comments
#version Aug 2010 isomernumber adds words to ease parsing, increased elements up to bromine, runpointnumber checked for more appropriate restarts
#
#LIMITATIONS - standard version only handles elements up to bromine, must change program to do higher atomic numbers
#   only handles up to 4000th excited state for modes - this could start to affect the initialization of classical modes or transition vectors at
#    extremely high temperatures
#   The routine that checks whether the actual energy approximately equals the desired energy checks for lines containing "SCF Done" or "EUMP2 =" or " Energy="
#   This should handle ordinary calculations HF, DFT, ONIOM, and MP2 calculatons but the routine in prog2ndpoint would have to be changed for other calcs.
#
#                                   OUTLINE
# A. initilize to perform Gaussian jobs and know where we are
#    start loop
# B. if no file named "skipstart" then generate a new isomer.  Instructions: Get rid of skipstart to start new isomer.
#    the B loop generates geoPlusVel, adds it to geoRecord, generates and runs first and second points, and sets up for continuous loop
# C. loop over propagation steps
#
#  AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#origdir, randdir, scratchdir, g09root, logfile all may need varied from system to system and assigned here or by program calling this one
export LC_ALL=C
echo $1
scratchdir=$1
export g09root=/apps/lms/g09_A02_XEON
. $g09root/g09/bsd/g09.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
cp /data/d-singleton/binall700/* /tmp/$PBS_JOBID
cp /data/d-singleton/binall700/GENBAS $scratchdir
cp /data/d-singleton/binall700/progcfour $scratchdir
proggramdir=/tmp/$PBS_JOBID
```

```
freqfile=/data/d-singleton/binall700/freqinHP
echo ORIGDIR:
echo $origdir
echo SCRATCHDIR:
echo $scratchdir
ls $scratchdir
echo PROGGRAMDIR:
echo $proggramdir
ls $proggramdir

rm -f nogo    # assume that if someone is starting a job, they want it to go.
rm -f diagnostics goingwell tempdone # diagnostics contains extra info from previous runs, other two files are from older
versions of progdyn

#### Triple 'while' loop - will have to break multiple times to get out, but advantage is ability to control starting over
while (true)
do

# As long as there is a file "goingwell" the program will not exit entirely by itself
rm -f $scratchdir/goingwell
while (true)
do
#  BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
  if (test -f skipstart) then
    echo "skipping start and continuing from previous runs"
  else
#  B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1 generate geoPlusVel and first input file
    if [ `cat runpointnumber` = "1" ]; then
      echo "X did not complete first point so new isomer started" >> dynfollowfile
    fi
    if [ `cat runpointnumber` = "2" ]; then
      echo "X did not complete second point so new isomer started" >> dynfollowfile
    fi
    if [ `cat runpointnumber` = "3" ]; then
      echo "X did not complete third point so new isomer started" >> dynfollowfile
    fi
    cd $origdir
    if (test -f bypassproggen) then
      echo "taking starting conditions from pre-generated geoPlusVel"
    else
      $randdir/randgen > temp811
# the next 8 lines would have to be changed to use low-precision modes
      awk '/        1          2/,/Harmonic frequencies/ {print}' $freqfile > temp401
      awk '/Frequencies --/ {print $3;print $4;print $5;print $6;print $7}' temp401 > tempfreqs
      awk '/Reduced masses/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempredmass
      awk '/Force constants/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempfrc
      awk '/0/ && ((length($1) < 2) && ($1 < 4)) {print}' temp401 > tempmodes
      awk '/has atomic number/ {print}' $freqfile > tempmasses
      awk '/Standard orientation:/,/tional const/ {if ($3==0) print}' $freqfile > tempstangeos
      awk '/Input orientation:/,/Stoichiometry/ {if ($3==0) print}' $freqfile > tempinputgeos
      awk -f $proggramdir/proggenHP $freqfile > geoPlusVel
    fi
    if (test -f isomernumber) then
      cp isomernumber temp533
      awk 'BEGIN {getline;i=$1+1;print i,"----trajectory isomer number----"}' temp533 > isomernumber
      rm temp533
    else
      echo "1 ----trajectory isomer number----" > isomernumber
    fi
    echo 1 > runpointnumber
    rm g09.com
    awk -f $proggramdir/prog1stpoint isomernumber > g09.com
#  B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2  if first part successfule then
clean up and run the first input file, otherwise die
    if (test -s g09.com) then
      rm tempfreqs tempredmass tempfrc tempmodes tempstangeos tempmasses temp401 temp811 tempinputgeos
      cat isomernumber >> geoRecord
      cat geoPlusVel >> geoRecord
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
```

```
        cd $origdir
        grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
        if (test -s $scratchdir/goingwell) then
          cat $scratchdir/g09.log >> dyn
          cp $scratchdir/g09.log olderdynrun
        else
          cp $scratchdir/g09.log $origdir/g09.log
          break
        fi
      else
        break
      fi
#  B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3 if B2 worked then you are here.
create 2nd point, run it, and set up for propagation loop
      rm g09.com
      echo 2 > runpointnumber
      awk -f $proggramdir/prog2ndpoint $scratchdir/g09.log > g09.com
# before we decide to run this, check the energy
      awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
      rm -f $scratchdir/tempdone
      tail -1 dynfollowfile | awk '/XXXX/ {print}' > $scratchdir/tempdone
      if (test  -s $scratchdir/tempdone) then
        rm -f dyn
        rm -f traj
        echo 0 > runpointnumber
        break
      fi
      if (test -s g09.com) then
        rm -f $scratchdir/goingwell
        cd $scratchdir
        cp $origdir/g09.com $scratchdir/g09.com
        $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
        cd $origdir
        grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
        if (test -s $scratchdir/goingwell) then
          cp $scratchdir/g09.log olddynrun
          cat $scratchdir/g09.log >> dyn
          awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
          awk '/Input orientation/,/Distance matrix/ {print}' olddynrun | awk '/   0   / {print}' > old
          awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun | awk '/   0   / {print}' > older
          echo 3 > runpointnumber
          awk -f $proggramdir/progdynb olddynrun > g09.com
          rm -f old older
        else
          cp $scratchdir/g09.log $origdir/g09.log
          break
        fi
      else
        break
      fi
# we've just completed a start, so lets skipstart until instructed otherwise
      echo "forward" > skipstart
    fi
# Reverse trajectories starter routine
    if [ `cat skipstart` = "reverserestart" ]; then
      cd $origdir
      rm g09.com
      echo 1 > runpointnumber
      awk -f $proggramdir/prog1stpoint isomernumber > g09.com
      if (test -s g09.com) then
        rm -f $scratchdir/goingwell
        cd $scratchdir
        cp $origdir/g09.com $scratchdir/g09.com
        $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
        cd $origdir
        grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
        if (test -s $scratchdir/goingwell) then
          cp $scratchdir/g09.log olderdynrun
        else
          cp $scratchdir/g09.log $origdir/g09.log
          break
        fi
```

```
    else
      break
    fi
    rm g09.com
    echo 2 > runpointnumber
    awk -f $proggramdir/prog2ndpoint $scratchdir/g09.log > g09.com
    awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
    rm -f $scratchdir/tempdone
    if (test -s g09.com) then
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cp $scratchdir/g09.log olddynrun
        cat $scratchdir/g09.log >> dyn
        awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
        awk '/Input orientation/,/Distance matrix/ {print}' olddynrun | awk '/   0   / {print}' > old
        awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun | awk '/   0   / {print}' > older
        echo 3 > runpointnumber
        awk -f $proggramdir/progdynb olddynrun > g09.com
        rm -f old older
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
# we've just completed a reversestart, so lets skipstart until instructed otherwise
    echo "reverse" > skipstart
  fi

#  END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___

#  CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC  propagation loop
  while (true)
  do
#increment runpointnumber
    cp runpointnumber $scratchdir/temp533
    awk 'BEGIN {getline;i=$1+1;print i}' $scratchdir/temp533 > runpointnumber
    rm $scratchdir/temp533
    rm -f $scratchdir/goingwell
    cd $scratchdir
    cp $origdir/g09.com $scratchdir/g09.com
    $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
    cd $origdir
    grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
    if (test -s $scratchdir/goingwell) then
      awk -f $proggramdir/proganal $scratchdir/g09.log >> $origdir/dynfollowfile
      mv olddynrun olderdynrun
      awk '/Input orientation/,/Distance matrix/ {print}' $scratchdir/g09.log | awk '/   0   / {print}' > old
      cp $scratchdir/g09.log olddynrun
      awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun | awk '/   0   / {print}' > older
      awk -f $proggramdir/progdynb $scratchdir/g09.log > g09.com
      rm -f old older
    else
      cp $scratchdir/g09.log $origdir/g09.log
      break
    fi
# kludge to do a side calculation of NMR using progcfour.  If ZMAT is there then it gets ran and renamed.
# creation of ZMAT is under the control of progdynb, which is controlled by keyword NMRcc in progdyn.conf
# decisions to be made: erase ZMAT at beginning?  what to do if cfour calc dies?
    if (test  -f ZMAT) then
      cp ZMAT $scratchdir
      cd $scratchdir
      $scratchdir/progcfour $origdir $scratchdir
      cd $origdir
      mv ZMAT temp.ZMAT
      echo "generic one two three" `cat runpointnumber`  "runisomer" `cat isomernumber` >> NMRlistcc
```

```
        awk '/Nuclear Magnetic Resonance/,/HF-SCF/ {if ($2=="C") print $1,$2,"Isotropic =",$3; if ($2=="H") print
$1,$2,"Isotropic =",$3}' x.log >> NMRlistcc
      fi

# here is a cool link that lets you interupt the dynamics with a short job, then
# it automatically goes back to the dynamics  just make the file 'detour' and it
# will delete detour, run run.com, then go back to dynamics
      if (test  -f detour) then
        rm detour
        date >> $logfile
        cat run.com >> $logfile
        cp run.log temp.log
        cd $scratchdir
        $g09root/g09/g09 $origdir/run.com > $origdir/run.log
        cd $origdir
      fi

#stop it all nicely by creating a nogo file
      if (test  -f nogo) then
        break
      fi

#figure out if this isomer is done - change in april 2013 is to move proganal call up from here
      rm -f $scratchdir/tempdone
      tail -2 dynfollowfile | awk '/XXXX/ {print}' > $scratchdir/tempdone
      if (test  -s $scratchdir/tempdone) then
        if [ `awk '/reversetraj/ {if ($1=="reversetraj") print $2}' progdyn.conf` = "true" ]; then
          if [ `cat skipstart` = "reverse" ]; then
            rm -f skipstart
            rm -f geoPlusVel
            rm -f olddynrun
            rm -f olderdynrun
            a=`awk '{print $1}' isomernumber`
            mv traj traj$a
            mv dyn dyn$a
          fi
          if [ `cat skipstart` = "forward" ]; then
            echo reverserestart > skipstart
          fi
        else
          rm -f skipstart
          rm -f geoPlusVel
          rm -f olddynrun
          rm -f olderdynrun
          a=`awk '{print $1}' isomernumber`
          mv traj traj$a
          mv dyn dyn$a
        fi
        break
      fi
    done
#
END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_L
oop____

# We've got to break a second time to get out of this loop
# if we really want to quit.  Otherwise, it will start over
# at the top
    if (test  -f nogo) then
      break
    fi
    if (test  -s $scratchdir/goingwell) then
      echo "starting a new point or a new direction"
    else
      break
    fi
done

    if (test  -f nogo) then
      break
    fi
    if (test  -s $scratchdir/goingwell) then
```

```
    echo "starting a new point or a new direction2"
  else
    break
  fi
done
exit 0
```

Program proggenHP

```
BEGIN {
# Aut 2010 changes classicalSpacing to 2 and upped possible excited states to 4000
# Jan 2009 - a number of little changes to improve reporting, precision, etc, specification of displacement on particular modes
# Jan 2009 cannonball trajectories.  adds desired energy to initial velocities based on file cannontraj, so one can shoot toward a ts
# updated Nov 2008 to incorporate running DRPs
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
# updated Aug 2008 added to atom list to handle a large number of atoms without changes needed
# updated June 2008 to incorportate new method for choosing displacements with initialdis 2
# updated Jan 17 2008 - bug fix for > 99 atoms, 300 excitations of low modes possible
# version August 2007 - incorporates classical trajectory calculation option
#also allows listing of number of imaginary frequencies
# version Sept 16, 2005 - incorportates searchdir but not yet rotation
# now reads random numbers from temp811, starting at a random place
# The input files are generated before this and are tempfreqs, tempredmass,
# tempfrc, tempmodes, and tempstangeos.
# It will count the number of atoms.

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
geometry="nonlinear";rotationmode=0

#initialization and constants
for (i=1;i<=10000;i++) {disMode[i]=-1}
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0; classicalSpacing=2
zpeGauss=0; zpeGaussK=0; zpePlusE=0; potentialE=0

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="initialdis") initialDis=$2
  if ($1=="timestep") timestep=$2
  if ($1=="scaling") scaling=$2
  if ($1=="temperature") temp=$2
  if ($1=="searchdir") searchdir=$2
  if ($1=="classical") classical=$2
  if ($1=="numimag") numimag=$2
  if ($1=="geometry") geometry=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="DRP") DRP=$2; if (DRP==1) classical=2 #this lets one start a DRP from a point that is not a freq calc
  if ($1=="maxAtomMove") maxAtomMove=$2
  if ($1=="cannonball") cannonball=$2
  if ($1=="displacements") disMode[$2]=$3
```

```
  if ($1=="controlphase") controlPhase[$2]=$3
  if ($1=="rotationmode") rotationmode=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag>=1) print "***************** starting proggen *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title,initialdis,timestep,scaling,temperature" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4,initialDis,timestep,scaling,temp >> "diagnostics"
if (diag>=1) print "classical,numimag,highlevel,boxon,boxsize,DRP,maxAtomMove,cannonball" >> "diagnostics"
if (diag>=1) print classical,numimag,highlevel,boxon,boxsize,DRP,maxAtomMove,cannonball >> "diagnostics"

# put geometries into array, also figure out number of atoms
# note that this picks out the last geometry in a file, assuming
# that if there is an optimization followed by a freq, nothing else follows
# kludgy - repeats last line twice - must be a better way
do {
  getline < "tempstangeos"
  if (oldline==$0) $0=""
  oldline=$0
  atom = $1
  if (atom>numAtoms) numAtoms=atom
  atNum[atom]=$2
  geoArr[atom,1]=$4; geoArr[atom,2]=$5; geoArr[atom,3]=$6
  geoArrOrig[atom,1]=$4; geoArrOrig[atom,2]=$5; geoArrOrig[atom,3]=$6
  velArr[atom,1]=0; velArr[atom,2]=0; velArr[atom,3]=0
  }
while (length($0) > 0)

#output the number of atoms, used in many routines
print numAtoms

# put in atomic symbols and atomic weights - assigns a default mass but then reads it from tempmasses when possible
for (i=1;i<=numAtoms;i++) {
  getline < "tempmasses"
  if (atNum[i]==1) {atSym[i]="H";atWeight[i]=1.00783}
  if (atNum[i]==2) {atSym[i]="He";atWeight[i]=4.0026}
  if (atNum[i]==3) {atSym[i]="Li";atWeight[i]=6.941}
  if (atNum[i]==4) {atSym[i]="Be";atWeight[i]=9.012}
  if (atNum[i]==5) {atSym[i]="B";atWeight[i]=10.811}
  if (atNum[i]==6) {atSym[i]="C";atWeight[i]=12.}
  if (atNum[i]==7) {atSym[i]="N";atWeight[i]=14.007}
  if (atNum[i]==8) {atSym[i]="O";atWeight[i]=15.9994}
  if (atNum[i]==9) {atSym[i]="F";atWeight[i]=18.9984}
  if (atNum[i]==10) {atSym[i]="Ne";atWeight[i]=20.1797}
  if (atNum[i]==11) {atSym[i]="Na";atWeight[i]=22.989}
  if (atNum[i]==12) {atSym[i]="Mg";atWeight[i]=24.305}
  if (atNum[i]==13) {atSym[i]="Al";atWeight[i]=26.98154}
  if (atNum[i]==14) {atSym[i]="Si";atWeight[i]=28.0855}
  if (atNum[i]==15) {atSym[i]="P";atWeight[i]=30.9738}
  if (atNum[i]==16) {atSym[i]="S";atWeight[i]=32.066}
  if (atNum[i]==17) {atSym[i]="Cl";atWeight[i]=35.4527}
  if (atNum[i]==18) {atSym[i]="Ar";atWeight[i]=39.948}
  if (atNum[i]==19) {atSym[i]="K";atWeight[i]=39.0983}
  if (atNum[i]==20) {atSym[i]="Ca";atWeight[i]=40.078}
  if (atNum[i]==21) {atSym[i]="Sc";atWeight[i]=44.96}
  if (atNum[i]==22) {atSym[i]="Ti";atWeight[i]=47.867}
  if (atNum[i]==23) {atSym[i]="V";atWeight[i]=50.94}
  if (atNum[i]==24) {atSym[i]="Cr";atWeight[i]=51.9961}
  if (atNum[i]==25) {atSym[i]="Mn";atWeight[i]=54.938}
  if (atNum[i]==26) {atSym[i]="Fe";atWeight[i]=55.845}
  if (atNum[i]==27) {atSym[i]="Co";atWeight[i]=58.933}
  if (atNum[i]==28) {atSym[i]="Ni";atWeight[i]=58.693}
  if (atNum[i]==29) {atSym[i]="Cu";atWeight[i]=63.546}
  if (atNum[i]==30) {atSym[i]="Zn";atWeight[i]=65.38}
```

```
  if (atNum[i]==31) {atSym[i]="Ga";atWeight[i]=69.723}
  if (atNum[i]==32) {atSym[i]="Ge";atWeight[i]=72.64}
  if (atNum[i]==33) {atSym[i]="As";atWeight[i]=74.9216}
  if (atNum[i]==34) {atSym[i]="Se";atWeight[i]=78.96}
  if (atNum[i]==35) {atSym[i]="Br";atWeight[i]=79.904}
  if (atNum[i]==46) {atSym[i]="Pd";atWeight[i]=106.42}
  if (atNum[i]==53) {atSym[i]="I";atWeight[i]=126.90447}
# gets actual weight from freqinHP when possible so a prior calc with readisotopes gets you isotopic substitution
  if ((i<100) && ($9>0)) atWeight[i]=$9
#  if ((i>99) && ($8>0)) atWeight[i]=$8

  if ((diag>1) && (i==1)) print "atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3]" >> "diagnostics"
  if (diag>1) print atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3] >> "diagnostics"
  }

# read in frequencies, scale them, read in Reduced masses, read in force
#constants, replace negative frequencies by 2 wavenumbers
numFreq=3*numAtoms-6
if (geometry=="linear") numFreq=3*numAtoms-5
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempfreqs"
  freq[i]=$0*scaling
  if (freq[i]<0) freq[i]=2
  }
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempredmass"
  redMass[i]=$0
  if (redMass[i]=="") redMass[i]=1.
  }
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempfrc"
  frc[i]=$0
  if (frc[i]=="") frc[i]=0.0001
  if (frc[i]==0) frc[i]=0.0001
  if ((diag>1) && (i==1)) print "freq[i],redMass[i],frc[i]" >> "diagnostics"
  if (diag>1) print freq[i],redMass[i],frc[i] >> "diagnostics"
  }

# read in the modes - note that trajectories always need a freq calc with freq=hpmodes unless classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i+=5) {
    for (j=1;j<=(3*numAtoms);j++) {
      getline < "tempmodes"
      mode[i,$2,$1]=$4; mode[i+1,$2,$1]=$5; mode[i+2,$2,$1]=$6; mode[i+3,$2,$1]=$7; mode[i+4,$2,$1]=$8
      }
    }
  }
if (diag>2) {for (i=1;i<=numFreq;i++) {print mode[i,1,1],mode[i,1,2],mode[i,1,3] >> "modesread"}}

# if doing a cannonball trajectory, read in the vector
if (cannonball>0) {
  for (i=1;i<=numAtoms;i++) {
    getline < "cannontraj"
    cannonArr[i,1]=$1; cannonArr[i,2]=$2; cannonArr[i,3]=$3
    }
  }

# collect a series of random numbers from file temp811, generated from an outside random number generator called by
prodynstarterHP
# read from temp811, starting at a random place
srand(PROCINFO["pid"]); tester=rand()*1000
for (i=1;i<=tester;i++) getline < "temp811"
for (i=1;i<=numFreq;i++) {
  getline < "temp811"; randArr[i]=$1
  getline < "temp811"; randArrB[i]=$1
  getline < "temp811"; randArrC[i]=$1
}
for (i=1;i<=6;i++) {
  getline < "temp811"; randArrR[i]=$1
```

```
}

# for a QM distribution for a harmonic oscillator in its ground state, we want to generate a set of random numbers
#between -1 and 1 weighted such that numbers toward the center are properly more common
i=1
while (i<=numFreq) {
  if ((initialDis==2) || (disMode[i]==2)) {
    getline < "temp811"
    tempNum=2*($1-.5)
    prob=exp(-(tempNum^2))
    getline < "temp811"
    if ($1<prob) {
      randArrD[i]=tempNum
      i++
      }
    }
  if ((initialDis!=2) && (disMode[i]!=2)) i++
  }

# to start without normal modes or frequencies we need to just pick a random direction for the motion of each atom, requiring 3N
random numbers
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
  getline < "temp811"
  if ($1>0.5) randArrE[i,j]=1
  if ($1<.5) randArrE[i,j]=-1
    }
  }

# determine energy in each normal mode
for (i=1;i<=numFreq;i++) {
  zpeJ[i]=0.5*h*c*freq[i]       #units J per molecule
#if classical, treat as modes spaced by classicalSpacing wavenumbers
  if (classical==1) zpeJ[i]=0.5*h*c*classicalSpacing  # the zpe is not used when classical but the spacing is used to calculate the
E in mode
  zpeK[i]=zpeJ[i]*avNum/4184    #units kcal/mol
  if (temp<10) vibN[i]=0        # avoids working with very small temperatures - if the temp is too low, it just acts like 0 K
  if (temp>=10) {
    zpeRat[i]=exp((-2*zpeK[i])/(RgasK*temp))
    if (zpeRat[i]==1) zpeRat[i]=.99999999999
    Q[i]=1/(1-zpeRat[i])
    newRand=randArr[i]
    vibN[i]=0
    tester=1/Q[i]
#     get up to 4000 excitations of low modes
    for (j=1;j<=(4000*zpeRat[i]+2);j++) {
      if (newRand>tester) vibN[i]++
      tester=tester+((zpeRat[i]^j)/Q[i])
      }
    }
  }

# figure out mode energies and maximum classical shift and then actual shift
# also calculated total energy desired for molecule
desiredModeEnK=0
for (i=1;i<=numFreq;i++) {
  modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i]+1) # units here are mDyne Ansgroms for compatability with Gaussian force constants
  if (classical==1) modeEn[i]=(zpeJ[i]*1E18)*2*vibN[i]    #no zpe when classical
  modeEnK[i]=zpeK[i]*(2*vibN[i]+1)
  if (classical==1) modeEnK[i]=zpeK[i]*2*vibN[i]          #no zpe when classical
  desiredModeEnK=desiredModeEnK + modeEnK[i]
# no 1/2 hv for imaginary frequencies
# treating modes with frequencies <10 as translations, ignoring their zero point energies
  if (freq[i]<10) modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i])
  maxShift[i]=(2*modeEn[i]/frc[i])^0.5
# new 2012 initialDis 3 means random phase of normal mode
  if (initialDis==3) shift[i]=maxShift[i]*sin(randArrC[i]*3.141592*2)
  if (initialDis==2) shift[i]=maxShift[i]*randArrD[i]
  if (initialDis==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
  if (initialDis==0) shift[i]=0
# lines below allow for setting of displacement mode for individual modes
```

```
# It used to be necessary to use disMode 10 to turn off displacements for a mode, but hopefully that bug is killed and you can use
disMode 0
  if (disMode[i]==3) shift[i]=maxShift[i]*sin(randArrC[i]*3.141592*2)
  if (disMode[i]==2) shift[i]=maxShift[i]*randArrD[i]
  if (disMode[i]==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
  if (disMode[i]==10) shift[i]=0 #kept for backward compatability
  if (disMode[i]==0) shift[i]=0
# no displacements along imaginary frequencies and very low ones - it is better to treat these
# as translations - employing a shift can give you initial weird geometries
  if (freq[i]<10) shift[i]=0
  if (numimag==1) shift[1]=0
  if (numimag==2) shift[2]=0
  }
for (i=1;i<=numFreq;i++) {
  if ((diag>1) && (i==1)) print "zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i]" >> "diagnostics"
  if (diag>1) print zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i] >> "diagnostics"
  }

# multiply each of the modes by its shift and add them up
# Do not do this if classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        shiftMode[i,j,k]=mode[i,j,k]*shift[i]
        geoArr[j,k]=geoArr[j,k]+shiftMode[i,j,k]
        }
      }
    }
  }

#now start toward velocities
for (i=1;i<=numFreq;i++) {
  kinEn[i]=100000*(modeEn[i]-0.5*frc[i]*shift[i]^2)  # the 100000 converts to g angstrom^2 s^2
  vel[i]=(2*kinEn[i]/(redMass[i]/avNum))^0.5        # in angstrom / s
#use searchdir in progdyn.conf to control the direction for trajectories started from a saddle point
  if (numimag>1) numimag=1  #only the first freq can be sent in the searchdir direction, the rest go in a random direction
  if (i>numimag) {
    if (randArrB[i]<0.5) vel[i]=-vel[i]
    }
  if (i==numimag) {
    if (searchdir=="negative") vel[i]=-vel[i]
    }
  if ((diag>1) && (i==1)) print "vel[i]" >> "diagnostics"
  if (diag>1) print vel[i] >> "diagnostics"
  }

# if controlphase is being used, set the velocity on particular modes as positive or negative as requested
for (i=1;i<=numFreq;i++) {
  if ((controlPhase[i]=="positive") && (vel[i]<0)) vel[i]=-vel[i]
  if ((controlPhase[i]=="negative") && (vel[i]>0)) vel[i]=-vel[i]
  }

# multiply each of the modes by its velocity and add them up
# Do not do this if classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        velMode[i,j,k]=mode[i,j,k]*vel[i]*timestep
        velArr[j,k]=velArr[j,k]+velMode[i,j,k]
        }
      }
    }
  }

# to start without normal modes or frequencies we figure out the energy per atom based on 1/2RT in degree of freedom
if (classical==2) {
# to avoid a bug with a box on, starts without modes should use the input geometry, not the standard
  do {
    getline < "tempinputgeos"
    if (oldline==$0) $0=""
```

```
    oldline=$0
    atom = $1
    geoArr[atom,1]=$4; geoArr[atom,2]=$5; geoArr[atom,3]=$6
    geoArrOrig[atom,1]=$4; geoArrOrig[atom,2]=$5; geoArrOrig[atom,3]=$6
    }
  while (length($0) > 0)
  degFreedomEnK=temp*RgasK
  degFreedomEnJ=degFreedomEnK/(avNum/4184)
  cartEn=degFreedomEnJ*1E18
  kinEnCart=100000*cartEn
#print degFreedomEnK, degFreedomEnJ, cartEn, kinEnCart
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
      velArr[i,j]=randArrE[i,j]*timestep*(2*kinEnCart/(atWeight[i]/avNum))^0.5
      if (DRP==1) velArr[i,j]=0
      }
    }
  }

# calculate the KE in the modes at this point
KEinitmodes=0
for (j=1;j<=numAtoms;j++) {
  KEinitmodes=KEinitmodes + 0.5*atWeight[j]*(velArr[j,1]^2 + velArr[j,2]^2 + velArr[j,3]^2)/((timestep^2)*conver1)
  }

# add molecular rotation if requested
if (rotationmode>0) {
#establish three rotation vectors
  for (j=1;j<=numAtoms;j++) {
    rotateX[j,1]=0
    rotateX[j,2]=-geoArrOrig[j,3]
    rotateX[j,3]=geoArrOrig[j,2]
    rotateY[j,1]=-geoArrOrig[j,3]
    rotateY[j,2]=0
    rotateY[j,3]=geoArrOrig[j,1]
    rotateZ[j,1]=-geoArrOrig[j,2]
    rotateZ[j,2]=geoArrOrig[j,1]
    rotateZ[j,3]=0
    }
#figure out how much energy is in the raw vectors
  eRotX=0;eRotY=0;eRotZ=0
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      eRotX=eRotX + 0.5*atWeight[j]*(rotateX[j,k]^2)/((timestep^2)*conver1)
      eRotY=eRotY + 0.5*atWeight[j]*(rotateY[j,k]^2)/((timestep^2)*conver1)
      eRotZ=eRotZ + 0.5*atWeight[j]*(rotateZ[j,k]^2)/((timestep^2)*conver1)
      }
    }
#  print "rotation energies if raw vector used",eRotX,eRotY,eRotZ
#now deciie how much energy we want in each rotation
  keRx=-0.5*0.001987*temp*log(1-randArrR[1])
  keRy=-0.5*0.001987*temp*log(1-randArrR[2])
  keRz=-0.5*0.001987*temp*log(1-randArrR[3])
  if (eRotX<1) keRx=0;if (eRotY<1) keRy=0;if (eRotZ<1) keRz=0
  rotEdesired=keRx+keRy+keRz
  signX=1;signY=1;signZ=1
  if (randArrR[4]<.5) signX=-1
  if (randArrR[5]<.5) signY=-1
  if (randArrR[6]<.5) signZ=-1

#  print "desired energies",keRx,keRy,keRz,"and random numbers",randArrR[1],randArrR[2],randArrR[3]
#protect against zero rotations
  if (eRotX<1) eRotX=1;if (eRotY<1) eRotY=1;if (eRotZ<1) eRotZ=1
#now scale the rotational vectors
  scaleX=(keRx/eRotX)^.5
  scaleY=(keRy/eRotY)^.5
  scaleZ=(keRz/eRotZ)^.5
#  print "scaling factors" scaleX,scaleY,scaleZ
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      rotateX[j,k]=rotateX[j,k]*scaleX*signX
      rotateY[j,k]=rotateY[j,k]*scaleY*signY
```

```
        rotateZ[j,k]=rotateZ[j,k]*scaleZ*signZ
        }
      }
    for (j=1;j<=numAtoms;j++) {
#     print rotateX[j,1],"   ",rotateX[j,2],"   ",rotateX[j,3]
      }
#   print ""
    for (j=1;j<=numAtoms;j++) {
#     print rotateY[j,1],"   ",rotateY[j,2],"   ",rotateY[j,3]
      }
#   print ""
    for (j=1;j<=numAtoms;j++) {
#     print rotateZ[j,1],"   ",rotateZ[j,2],"   ",rotateZ[j,3]
      }
# now add the rotational vectors  to velArr
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        velArr[j,k]=velArr[j,k]+rotateX[j,k]+rotateY[j,k]+rotateZ[j,k]
        }
      }
    }

# if doing a cannonball, adjust multiplier until extra energy is correct
if (cannonball>0) {
  multiplier=1; tester=0; tolerance=.1
  while (tester==0) {
    KEinittotal=0
    for (j=1;j<=numAtoms;j++) {
      cannonvelArr[j,1]=velArr[j,1]+multiplier*cannonArr[j,1]; cannonvelArr[j,2]=velArr[j,2]+multiplier*cannonArr[j,2];
cannonvelArr[j,3]=velArr[j,3]+multiplier*cannonArr[j,3]
      KEinittotal=KEinittotal + 0.5*atWeight[j]*(cannonvelArr[j,1]^2 + cannonvelArr[j,2]^2 +
cannonvelArr[j,3]^2)/((timestep^2)*conver1)
      }
    if (KEinittotal>(KEinitmodes+cannonball+tolerance)) multiplier=multiplier*0.98901364
    if (KEinittotal<(KEinitmodes+cannonball-tolerance)) multiplier=multiplier*1.01
    if ((KEinittotal<(KEinitmodes+cannonball+tolerance)) && (KEinittotal>(KEinitmodes+cannonball-tolerance))) tester=1
    }
  for (j=1;j<=numAtoms;j++) {
    velArr[j,1]=velArr[j,1]+multiplier*cannonArr[j,1]; velArr[j,2]=velArr[j,2]+multiplier*cannonArr[j,2];
velArr[j,3]=velArr[j,3]+multiplier*cannonArr[j,3]
    }
  }

#output the new geometry.
# ****** this section changed for special experiment for cyclopentadiene.  do not use this for other cases
# atWeight[4]=140.0001
# ****** line below added for special experiment switching mass from 12 to 140, keeping momenta the same
#velArr[4,1]=velArr[4,1]/11.66667; velArr[4,2]=velArr[4,2]/11.66667; velArr[4,3]=velArr[4,3]/11.66667
for (j=1;j<=numAtoms;j++) {
  printf("%2s % .7f % .7f % .7f %9.5f \n",atSym[j],geoArr[j,1],geoArr[j,2],geoArr[j,3],atWeight[j])
  }

#output the velocities and calculate the total kinetic energy overall
KEinittotal=0
for (j=1;j<=numAtoms;j++) {
  KEinittotal=KEinittotal + 0.5*atWeight[j]*(velArr[j,1]^2 + velArr[j,2]^2 + velArr[j,3]^2)/((timestep^2)*conver1)
  printf("% .8f % .8f % .8f \n",velArr[j,1],velArr[j,2],velArr[j,3])
  }

#anything else I add to the file will not affect the trajectories but will keep a record and be good for analysis
for (i=1;i<=numFreq;i++) {
  if (initialDis==0) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i\n", randArr[i], randArrB[i], vibN[i], vel[i], shift[i],
disMode[i])
  if (initialDis==1) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i\n", randArr[i], randArrC[i], vibN[i], vel[i], shift[i],
disMode[i])
  if (initialDis==2) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i\n", randArr[i], randArrD[i], vibN[i], vel[i], shift[i],
disMode[i])
  if (initialDis==3) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i % .6f\n", randArr[i], randArrC[i], vibN[i], vel[i], shift[i],
disMode[i], sin(randArrC[i]*3.141592*2))
  }
print "temp ",temp
print "initialDis",initialDis
```

```
print "classical",classical
print "timestep",timestep
print "numimag",numimag
OFMT = "%.3f"
print "Total mode energy desired=",desiredModeEnK
print "KE initial from modes=",KEinitmodes,"   KE initial total=",KEinittotal,"   Rotational Energy desired=",rotEdesired
if (cannonball>0) print "cannonball",cannonball,"  cannon Energy=",KEinittotal-KEinitmodes
if (boxon>0) print "boxsize",boxsize
if (DRP>0) print "DRP",DRP,"   maxAtomMove",maxAtomMove
if (DRP>0) print maxAtomMove > "maxMove"
}  # End of BEGIN

/Zero-point correction/ {zpeGauss=$3}
/zero-point Energies/ {zpePlusE=$7}
END {
zpeGaussK=zpeGauss*627.509
potentialE=zpePlusE - zpeGauss
OFMT = "%.6f"
print "Gaussian zpe=",zpeGauss,"or",zpeGaussK,"kcal/mol  E + zpe=",zpePlusE,"  potential E=",potentialE
print "" #will use blank line to mark end of geoPlusVel file
}
```

Program prog1stpoint

```
BEGIN {
# aug 2010 changed so that it is more careful in reading in from geoPlusVel
#     removed some default parameters that should always be defined
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# aug 2008 added to atom list so handles H to Cl without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# this program creates the first input file for g09
# the title should be changed as appropriate
# the isomer number comes from a file isomernumber

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
geometry="nonlinear";nonstandard=0
nmrtype=0;nmrevery=9999999

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0
getline < "runpointnumber"
runpointnum = $1

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
```

```
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag==1) print "***************** starting prog1stpoint *****************" >> "diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

getline < "isomernumber"
isomernum = $1
#read in number of atoms, geometry, masses, and velocity from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
# geometry
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  for (j=1;j<=3;j++) {
    geoArr[i,j]=$(1+j)
    }
  }
#velocities not needed for 1st point
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  for (j=1;j<=3;j++) {
    velArr[i,j]=$j
    }
  }

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "# " method " force scf=(tight,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint ",runpointnum
```

```
print "runisomer ", isomernum
print ""
print charge,multiplicity
}

END {
for (i=1;i<=numAtoms;i++) {
   printf("%s %.7f %.7f %.7f",atSym[i],geoArr[i,1],geoArr[i,2],geoArr[i,3])
   if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
   if (i>(highlevel+linkatoms)) printf(" %s","M")
   print ""
   }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
   for (i=1;i<=methodfilelines;i++) {
      getline < "methodfile"
      print $0
      }
   }
if ((nmrtype>0) && ((runpointnum % nmrevery)==0)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod " nmr=giao geom=check"
   if (nmrmethod==method) print "guess=tcheck"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>1) && ((runpointnum % nmrevery)==0)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod2 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>2) && ((runpointnum % nmrevery)==0)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod3 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
}
```

Program prog2ndpoint

```
BEGIN {
#Aug 2010 added etolerance to make it controllable from progdyn.conf, made it so that DRP does not check energy
# aug 2008 added to atom list so handles 1 to 17 without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 9, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# read progdyn.conf for configuration info

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
etolerance=1
geometry="nonlinear";nonstandard=0
NMRtype=none;NMRevery=9999999

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0
getline < "runpointnumber"
runpointnum = $1

blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="DRP") DRP=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="etolerance") etolerance=$2
  if ($1=="reversetraj") reversetraj=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }
```

```
if (diag>=1) print "***************** starting prog2ndpoint *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

#get the isomer number from file
getline < "isomernumber"
isomernum = $1

#get forward or reverse from skipstart if it exists
getline < "skipstart"
trajdirection = $1

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "# " method " force scf=(tight,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
print title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ", isomernum
print ""
print charge,multiplicity

# ok, now we have to figure the second point.  this should be
# x(t) = x + v*t + 1/2*F*t^2/m
# so we need to set up arrays for position, velocity, and force

#read in number of atoms, geometry, masses, and velocity from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
# geometry
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  for (j=1;j<=3;j++) {
    geoArr[i,j]=$(1+j)
    }
  }
#velocities
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  for (j=1;j<=3;j++) {
    velArr[i,j]=$j
    }
  }

#now we go ahead and add the velocities
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
    arr[i,j]=velArr[i,j]+geoArr[i,j]
    if (trajdirection=="reverserestart") arr[i,j]=geoArr[i,j]-velArr[i,j]
    }
  if ((diag>1) && (i==1)) print "geometry after adding velocities" >> "diagnostics"
  if (diag>1) print arr[i,1],arr[i,2],arr[i,3] >> "diagnostics"
  }

#pull out other information useful for testing whether total energy is right or bad
```

```
blankLineTester=10
while (blankLineTester>1) {
  getline < "geoPlusVel"
  if ($4=="desired=") desiredModeEnK=$5
  if ($4=="modes=") {
    KEinitmodes=$5
    KEinittotal=$9
    }
  if ($11=="potential") potentialE=$13
  blankLineTester=length($0)
  }
#get initial geometry into file traj
print numAtoms >> "traj"
print potentialE,title1,title2,title3,title4,"runpoint 1 ","runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  print atSym[i],geoArr[i,1],geoArr[i,2],geoArr[i,3] >> "traj"
  }
#added by Samae on 102910
scfcount=0
} # end of BEGIN

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ {
if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
if (($1=="SCF") && (scfcount==0)) newPotentialE=$5
if ($1=="E2") {
  tempstring=$6
  split(tempstring, arr10, "D")
  newPotentialE=arr10[1]*(10^arr10[2])
  }
newPotentialEK=(newPotentialE-potentialE)*627.509
if ($1=="SCF") {
  if (scfcount==0) {
    pddga=$5
    }
  if (scfcount==1) {
    qm=$5
    }
  if (scfcount==2) {
    pddgb=$5
    pddgc=(pddga-pddgb)
    newPotentialE=(qm+pddgc)
    newPotentialEK=(newPotentialE-potentialE)*627.509
    }
  scfcount++
  }
}

# now we go ahead and translate the forces and add them
(/      1   / || /      2   / || /      3   / || /      4   / || /      5   / || /      6   / || /      7   / || /      8   / || /      9   / || /      10   / || /
11   / || /      12   / || /      13   / || /      14   / || /      15   / || /      16   / || /      17   / || /      18   / || /      19   / || /      20   / || /
21   / || /      22   / || /      23   / || /      24   / || /      25   / || /      26   / || /      27   / || /      28   / || /      29   / || /      30   / || /
31   / || /      32   / || /      33   / || /      34   / || /      35   /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)    #the raw units of the forces are Hartree/Bohr
  }
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
#put out Echeck but only if not a DRP
if (DRP==0) {
  print "trajectory #",isomernum >> "Echeck"
  print "point 1 potential E=",newPotentialEK,"   point 1 kinetic E=",KEinitmodes,"  Total=",newPotentialEK+KEinitmodes >>
"Echeck"
  print "desired total energy=", desiredModeEnK >> "Echeck"
  if ((newPotentialEK+KEinitmodes)>(desiredModeEnK+etolerance)) print "XXXX bad total Energy" >> "Echeck"
  if ((newPotentialEK+KEinitmodes)<(desiredModeEnK-etolerance)) print "XXXX bad total Energy" >> "Echeck"
  }
# turn the forces into motion
```

```
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg to get angstroms
    forceArr[i,j]=0.5*1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
# for simplicity, DRPs will throw away the forces at the second pont.  This means that if we are not at a saddlepoint, point 2 = point 1 but this is a minor waste
    if (DRP==1) forceArr[i,j]=0
    arr[i,j]=arr[i,j]+forceArr[i,j]
# if atoms are fixed, replace calcd new position by original position
    if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4)) arr[i,j]=geoArr[i,j]
    }
  if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
  if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
  printf("%s %.7f %.7f %.7f",atSym[i],arr[i,1],arr[i,2],arr[i,3])
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
if ((nmrtype>0) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod " nmr=giao geom=check"
  if (nmrmethod==method) print "guess=tcheck"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>1) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod2 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>2) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod3 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
```

```
  }
print ""
#get second geometry into file traj
print numAtoms >> "traj"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum,"runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  print atSym[i],arr[i,1],arr[i,2],arr[i,3] >> "traj"
  }
}
```

Program progdynb

```
BEGIN { #this is the main routine for generating new .com files by the Verlet algorithym
# Aug 2010 increased elements handled automatically but only up to bromine!
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# Nov 2008 added ability to handle DRPs
# Aug 2008 added long list of atoms to handle 1-17 without change
# May 2008 added option to put out velocities in vellist - make diag=3
# version Feb 2008 incorporates methodfile, boxon and boxsize
# version Jan 2008 incorporates fixed atoms, oniom, and velocity damping
# version August 2007 incorporates keepevery to decrease size of dyn file
# version Sept 11, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
damping=1;nonstandard=0
nmrtype=0;nmrevery=9999999;nmrcc=0;nmrrand=0;nmrdo=0
thermostat=0;thermostatemult=1.00

#initialization
srand(PROCINFO["pid"])
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
OFS="     "

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="temperature") temp=$2
  if ($1=="thermostat") thermostat=$2
  if ($1=="thermostatmult") thermostatmult=$2
  if (thermostatmult>1) thermostatmult=1/thermostatmult
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="keepevery") keepevery=$2
  if ($1=="fixedatom1") fixedatom1=$2
```

```
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="DRP") DRP=$2
  if ($1=="maxAtomMove") maxAtomMove=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="damping") damping=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="NMRrand") nmrrand=$2
  if ($1=="loadlimit") loadlimit=$2
  if ($1=="NMRcc") nmrcc=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag>=1) print "***************** starting progdynb *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

# get number of atoms and weights from geoPlusVel, and previous geometries from old and older
getline < "geoPlusVel"
numAtoms=$1
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5; atSym[i]=$1
  }

for (at=1;at<=numAtoms;at++) {
  getline < "old"
  oldarr[at,1]=$4; oldarr[at,2]=$5; oldarr[at,3]=$6
  }

for (at=1;at<=numAtoms;at++) {
  getline < "older"
  olderarr[at,1]=$4; olderarr[at,2]=$5; olderarr[at,3]=$6
  }

#for DRPs read in oldAdjForces and maxAtomMove
if (DRP==1) {
  for (at=1;at<=numAtoms;at++) {
    getline < "oldAdjForces"
    oldForce[at,1]=$1; oldForce[at,2]=$2; oldForce[at,3]=$3
    }
  getline < "maxMove"
  if (($1<maxAtomMove) && ($1>0)) maxAtomMove=$1
  if (maxAtomMove<0.000001) maxAtomMove=0.000001
  }

# record atom velocities for IVR analysis.  This is actually the velocity in the previous run, which is the easiest to calculate.
getline < "isomernumber"
isomernum = $1
getline < "runpointnumber"
runpointnum = $1
# routine to control whether NMR calculations are done.
if ((nmrrand==0) && ((runpointnum % nmrevery)==0)) nmrdo=1
if ((nmrrand==1) && (rand()<(1/nmrevery))) nmrdo=1
getline < "uptimelist"
```

```
x=1.0001*substr($10,1,3);if (x<8) x=8
# turn of nmrs if load is too high - this is under control of loadlimit parameter in progdyn.conf and requires proganal to make uptimelist
if ((nmrrand==1) && (x>loadlimit)) nmrdo=0

if (diag==3) print "runpoint ",runpointnum-1,"runisomer ",isomernum >> "vellist"
for (at=1;at<=numAtoms;at++) {
  atomVel=((oldarr[at,1]-olderarr[at,1])^2 + (oldarr[at,2]-olderarr[at,2])^2 +(oldarr[at,3]-olderarr[at,3])^2)^.5
  KEatomstotal=KEatomstotal+0.5*weight[at]*(atomVel^2)/(((timestep^2)*conver1)
  if (diag==3) print atomVel >> "vellist"
  }
apparentTemp=KEatomstotal*2/(3*RgasK*numAtoms)
if (diag==4) print "KEatomstotal",KEatomstotal,"apparent Temperature",apparentTemp >> "vellist"
if (thermostat==1) {
  if (diag<4) print "KEatomstotal",KEatomstotal,"desired temperature",temp,"apparent Temperature",apparentTemp >> "vellist"
  if (apparentTemp>temp) damping=thermostatmult
  if (apparentTemp<temp) damping=1/thermostatmult
  }
}

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ || /ONIOM:/ {
if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
if ($1=="SCF") newPotentialE=$5
if ($2=="extrapolated")  newPotentialE=$5
if ($1=="E2") {
  tempstring=$6
  split(tempstring, arr10, "D")
  newPotentialE=arr10[1]*(10^arr10[2])
  }
}

#must adjust next line for weird atoms
(/    1   / || /    2   / || /    3   / || /    4   / || /    5   / || /    6   / || /    7   / || /    8   / || /    9   / || /    10   / || /
11   / || /    12   / || /    13   / || /    14   / || /    15   / || /    16   / || /    17   / || /    18   / || /    19   / || /    20   / || /
21   / || /    22   / || /    23   / || /    24   / || /    25   / || /    26   / || /    27   / || /    28   / || /    29   / || /    30   / || /
31   / || /    32   / || /    33   / || /    34   / || /    35   /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)   #the raw units of the forces are Hartree/Bohr
  }
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
#############routine for DRPs##############
if (DRP==1) {
  maxForce=0;oscillTest=0
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg to get angstroms
      forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
      oscillTest=oscillTest+forceArr[i,j]*oldForce[i,j]
      if (forceArr[i,j]>maxForce) maxForce=forceArr[i,j]
      if ((0-forceArr[i,j])>maxForce) maxForce=-forceArr[i,j]
      }
    if (i==1) printf("% .8f % .8f % .8f \n",forceArr[1,1],forceArr[1,2],forceArr[1,3])  > "oldAdjForces"
    if (i>1) printf("% .8f % .8f % .8f \n",forceArr[i,1],forceArr[i,2],forceArr[i,3])  >> "oldAdjForces"
    }
  print "oscillTest ",oscillTest >> "oldAdjForces"
  if (oscillTest<0) {
    maxAtomMove = maxAtomMove*0.5
    print maxAtomMove > "maxMove"
    }
  if (oscillTest>0) {
    maxAtomMove = maxAtomMove*1.2
    print maxAtomMove > "maxMove"
    }
  print "maxAtomMove ",maxAtomMove >> "oldAdjForces"
  forceMult=maxAtomMove/maxForce
```

```
   for (i=1;i<=numAtoms;i++) {
     for (j=1;j<=3;j++) {
       newarr[i,j]=oldarr[i,j]+forceMult*forceArr[i,j]
       }
     }
   }
########

#############normal routine for Verlet ##############
if (DRP==0) {
   for (i=1;i<=numAtoms;i++) {
     for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
       forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
       if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
       if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
       newarr[i,j]=oldarr[i,j]+damping*(oldarr[i,j]-olderarr[i,j])+forceArr[i,j]
       if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4)) newarr[i,j]=oldarr[i,j]
#turn around atoms outside the box
       if (boxon==1) {
         if (newarr[i,j]>boxsize) if (oldarr[i,j]>olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-oldarr[i,j])+forceArr[i,j]
         if (newarr[i,j]<-1*boxsize) if (oldarr[i,j]<olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-
oldarr[i,j])+forceArr[i,j]
         }
       }
     }
   }
########

if ((runpointnum % keepevery)==0) system("cat g09.log >> dyn")
print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
   print "# " method " force scf=(tight,nosym) "
   if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
   if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
   print "pop=none "
   if (length(meth3)>2) print meth3
   if (length(meth4)>2) print meth4
   }
if (nonstandard==1) {
   print "# "
   print "nonstd"
   system("cat nonstandard")
   }
print ""
print  title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ",isomernum
if (DRP==1) print "maxForce and forceMult and maxAtomMove",maxForce,forceMult,maxAtomMove
print ""
print charge,multiplicity
print numAtoms >> "traj"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum,"runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
   printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
   printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "traj"
   print "" >> "traj"
   if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
   if (i>(highlevel+linkatoms)) printf(" %s","M")
   print ""
   }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
   for (i=1;i<=methodfilelines;i++) {
     getline < "methodfile"
     print $0
     }
```

```
   }
if ((nmrtype>0) && (nmrdo==1)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod " nmr=giao geom=check"
   if (nmrmethod==method) print "guess=tcheck"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>1) && (nmrdo==1)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod2 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>2) && (nmrdo==1)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod3 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""

if ((nmrcc==1) && (nmrdo==1)) {
   print "CCSD(T) NMR calculation" > "ZMAT"
   for (i=1;i<=numAtoms;i++) {
      printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "ZMAT"
      print "" >> "ZMAT"
      }
   print "" >> "ZMAT"
   print "*ACES2(CALC=CCSD[T],PROP=NMR,BASIS=dzp" >> "ZMAT"
   print "ABCDTYPE=AOBASIS,TREAT_PERT=SEQUENTIAL,CC_PROG=ECC" >> "ZMAT"
   print "COORD=CARTESIAN" >> "ZMAT"
   print "MEM_UNIT=GB,MEMORY=2)" >> "ZMAT"
   print "" >> "ZMAT"
   }
}
```

Program progcfour

The last two lines below would have to be set up for the local environment.

```
#!/bin/bash
origdir=$1
workdir=$2
```

```
cd $origdir
echo "starting cfour calculation"
date
mv x.log tempcfour.log
cd $workdir
rm -f -r tempcfour
mkdir tempcfour
mv CSH* tempcfour
mv GRD tempcfour
mv MOLDEN_NAT tempcfour
mv OPTARC tempcfour
mv AUXMOI tempcfour
mv DERINT tempcfour
mv FILES tempcfour
mv GAMLAM tempcfour
mv IIII tempcfour
mv IIJJ tempcfour
mv IJIJ tempcfour
mv IJKL tempcfour
mv JAINDX tempcfour
mv JMOL.plot tempcfour
mv JOBARC tempcfour
mv MOABCD tempcfour
mv MOINTS tempcfour
mv MOL tempcfour
mv MOLDEN tempcfour
mv MOLECULE.INP tempcfour
mv NEWMOS tempcfour
mv PPPPAA tempcfour
mv PPPHAA tempcfour
mv HHHHAA tempcfour
mv PHPHAA tempcfour
mv PPHHAA tempcfour
mv PHHHAA tempcfour
PATH=/data/d-singleton/cfour/cfour_v1_64bit/bin:$PATH
/data/d-singleton/cfour/cfour_v1_64bit/bin/xcfour > $origdir/x.log
```

Program randgen.c

This is compiled before use to give the service program *randgen*

```
#include <stdio.h>
#include <stdlib.h>

int a,b,c;
double d;

int product(int x, int y);

int main(void)
{
  int count=1;
  srand48(time (0));
  while (count<=100000)
  {
    d = drand48();
    printf ("%.20f\n", d);
    count++;
  }
  return 0;
}
```

Program proganal

```
BEGIN {
firsttitle=1
getline < "isomernumber"
isomer=$1
}
/ alame3/ {
```

```
   if (firsttitle==1) {
      printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
      runpoint=$6
      }
   firsttitle++
   }
/Standard orientation/,/Rotational constants/ {
   if (($1>.5) && ($1<30)) {
      A[$1]=$4;B[$1]=$5;C[$1]=$6
      }
   }
/before annihilation/ {
   printf("%s %.5f ",$1,$6)
   }

END {
   C1N6=Distance(1,6)
   C3C8=Distance(3,8)
   C1C8=Distance(1,8)
   printf("%s %.3f  %s %.3f  %s %.3f ","C1N6",C1N6,"C3C8",C3C8,"C1C8",C1C8)
   if (runpoint>500) {
      print "Too many points.  XXXXN"
#     system("date > nogo")
      }
      if ((C1N6>2.5) && (C3C8<1.8)) {
         getline < "skipstart"
#        if ($1=="reverse") system("date > nogo")
         print "2,3-Rearrangement XXXX23N"
         }
      if ((C1N6>2.5) && (C1C8<1.8)) {
         getline < "skipstart"
#        if ($1=="reverse") system("date > nogo")
         print "1,2-Rearrangement XXXX12N"
         }
      if ((C1N6>3.4) && (C3C8>3.4) && (C1C8>3.4)) {
         getline < "skipstart"
#        if ($1=="reverse") system("date > nogo")
         print "Dissociation XXXXDN"
         }
      if ((C1N6<1.6) && (C3C8>2.8)) {
         getline < "skipstart"
#        if ($1=="reverse") system("date > nogo")
         print "reformed starting material XXXX23N"
         }
   system("date '+%b:%d:%Y %T'")
   system("tail -1 Echeck | grep XXXX")
   }

function Distance(Atom1,Atom2) {
  return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
   value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
   return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
   B1x=A[Atom2]-A[Atom1]
   B1y=B[Atom2]-B[Atom1]
   B1z=C[Atom2]-C[Atom1]
   B2x=A[Atom3]-A[Atom2]
   B2y=B[Atom3]-B[Atom2]
   B2z=C[Atom3]-C[Atom2]
```

```
  B3x=A[Atom4]-A[Atom3]
  B3y=B[Atom4]-B[Atom3]
  B3z=C[Atom4]-C[Atom3]
  modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
  yAx=modB2*(B1x)
  yAy=modB2*(B1y)
  yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
  CP2x=(B2y*B3z)-(B2z*B3y)
  CP2y=(B2z*B3x)-(B2x*B3z)
  CP2z=(B2x*B3y)-(B2y*B3x)
  termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
  CPx=(B1y*B2z)-(B1z*B2y)
  CPy=(B1z*B2x)-(B1x*B2z)
  CPz=(B1x*B2y)-(B1y*B2x)
  termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
 dihed4=(180/3.141592)*atan2(termY,termX)
 return dihed4
}

function killdyn(isomer) {
  system("rm -f dyn")
}
```

progdyn.conf

```
#This is the configuration file for PROGDYN.  This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
#The program has a number of default values but they are unlikely to be what you want.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
#***The keywords are case sensitive.  The following keywords should always be defined:***
#***method, charge, multiplicity, memory, processors, title
#*** method --The following word is copied exactly to the gaussian input file.
method UB3LYP/6-31G*
#To do a nonstandard route, make nonstandard 1.  For normal calcs, use nonstandard 0 or else leave it out.
#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.
nonstandard 0
# NMRoptions As is NMR=1 will add a section for an NMR calc at every NMRevery intervals.  If you want to combine the two
use nonstandard
#NMRtype 1
#NMRmethod B3LYP/cc-pvtz
#NMRevery 4
#geometry linear
rotationmode 1
#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.
method2 unrestricted
charge 0
multiplicity 1
processors 2
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 200mw
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting
#the name after the keyword checkpoint.  This is necessary if you use the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 1
killcheck 1
#checkpoint g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical calculations
diagnostics 0
#*** title -- the title keyword must be followed by exactly four words
title alame3 XC UB3D2PCM 363dis2
```

```
#*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all trajectories start from the same place
# and only the energies and signs of the motion in the modes are randomized
# 1 gives a flat distribution of displacements where all of the possible values are equally likely
# 2 (recommended) gives a QM-like gaussian distribution of displacements, so that displacements in the middle are more likely
that
# those at the end by 1/e
initialdis 2
#*** timestep -- this is the time between points in the trajectory.  Typical values would be 1E-15 or 0.5E-15 or 0.25E-15
timestep 1E-15
#*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 363.15
#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method, and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line.  Here are some examples to uncomment if needed
#method4 IOp(3/76=0572004280)
method3 scrf=(pcm,solvent=acetonitrile)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
#method3 iop(2/9=2000)
method4 iop(3/124=3)
#method5 radii=bondi
#method6
#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files
#such as a gen basis set.  Put after the keyword the number of lines in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0
#*** numimag --This tells the program the number of imaginary frequencies in the starting structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random direction
numimag 1
#*** searchdir -- This keyword says what direction to follow the mode associated with the imaginary frequency.
#The choices are "negative" and "positive".  Positive moves in the direction defined in the gaussian frequency calculation
#for the imaginary frequency, while negative moves in the opposite direction.  The correct choice can be made either
#by a careful inspection of the normal modes and standard orientation geometry, or by trial and error.
searchdir positive
#*** classical --  for quassiclassical dynamics, the default, use 0.  for classical dynamics, use 1
#if there are no normal modes and the velocities are to be generated from scratch, use classical 2
classical 0
#*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0 or comment it
out
#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
#*** cannonball -- The program can "fire" a trajectory from a starting position toward a particular target, such as toward
#a ts.  To use this, make a file cannontraj with numAtom lines and three numbers per line that defines the vector
#for firing the trajectory, relative to the starting geometry's standard orientation.  The number following cannonball sets
#the extra energy being put into the structure in kcal/mol
#cannonball 10
#*** keepevery --This tells the program how often to write the gaussian output file to file dyn, after the first two points.
#Use 1 for most dynamics to start with, but use a higher number to save on disk space or molden loading time.
keepevery 99
#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,
#which must come before the medium level atoms.  Use some high value such as 999 if not using ONIOM
highlevel 999
#*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.
#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms
#fixes one distance and fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0
#fixedatom1 2
#fixedatom2 3
#fixedatom3 19
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle.  Useful for dynamics with solvent molecules.  This is a crude
#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms
boxon 0
```

```
boxsize 7.5
#*** displacements -- This keyword lets you set the initialdis of particular modes by using a series of lines of the format
# displacements NumberOfMode InitialDisForThatMode, as in the example below. You should be able to do as many of these as
you like
# you might consider this for rotations where a straight-line displacement goes wrong at large displacements
# The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as 0 but is maintained for now
because
# a previous version of the program had a bug that made 0 not work.
#displacements 2 0
#displacements 3 0
#*** etolerance --This sets the allowable difference between the desired energy in a trajectory and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in the initial velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems.  For very large and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy in the molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the value.
etolerance 2
#*** controlphase --It is sometimes useful to set the phase of particular modes in the initialization of trajectories.
#The format is controlphase numberOfModeToControl positive or controlphase numberOfModeToControl negative.
#controlphase 2 positive
#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the
velocities
#by the damping factor.  A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values
range
#from 0.95 to 1.05.  The use of damping lets one do simulated annealing - you add energy until the structure is moving enough
#to sample the kinds of possibilities you are interested in, then you take away the energy slowly.
damping 1
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.
reversetraj true


#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword classical
#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size
#update Feb 2008 to include methodfile parameter
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
# update Aug 2010 to include etolerance, damping controlphase and reversetraj
```

Sample Input Files for Gaussrate

The sample input files below are the ones used for B3LYP/6-31G*/D2 calculations for the rearrangement of **2** via the lowest-energy exo s-cis transition structure (as shown in Figure 1 of the main text). In the example shown, the esp.fu71, esp.fu73, and esp.fu75 files are not actually used for the calculation, but these files are shown because they were used in an initial crude calculation to establish the starting geometries. The starting geometries were then taken from the esp.fu61 output file for the crude calculation and put in the poly.fu5 file for the production calculation.

Isotope effect calculations: The calculation shown provides as one of its outputs a poly.fu31 file. To calculate isotope effects, the poly.fu31 file was modified to add the "KIES" command, then the polyrate calculation was reran using the option in poly.fu5

```
*ENERGETICS
        potential  unit31
```

with the various isotopic substitutions denoted in the standard Gaussrate / Polyrate fashion.

poly.fu5

```
*General

  TITLE
23 on parent for isotope effects
 END
```

```
 ATOMS
   1  C
   2  O
   3  C
   4  C
   5  N
   6  C
   7  O
   8  C
   9  C
  10  C
  11  C
  12  H
  13  H
  14  H
  15  H
  16  H
  17  H
  18  H
  19  H
  20  H
  21  H
  22  H
  23  H
  24  H
  25  H
  26  H
 END

 NOSUPERMOL

 WRITEFU31 ON
 INPUNIT AU

*OPTIMIZATION

 OPTMIN  OHOOK
 OPTTS   OHOOK

*SECOND

 HESSCAL HHOOK

*REACT1
 STATUS 2
 SPECIES   NONLINRP
 GEOM
   1        3.85039041    -1.67470171    -4.57817476
   2        5.36839215     0.54831811    -4.64688766
   3        5.56401497     1.68543016    -7.01809061
   4        7.16092270     3.76837714    -6.95650532
   5        7.32483886     5.40477321    -9.21216438
   6        8.93749650     7.64016019    -8.58931252
   7        4.39353621     0.76866367    -8.86481910
   8        8.53638925     3.99721579   -11.36809590
   9        4.72161444     6.35664332   -10.18895270
  10        3.30700582     7.85816685    -8.26222183
  11        1.66673719     6.76860077    -6.68506234
  12        3.89469007    -2.32693299    -2.61710371
  13        1.89571931    -1.28068899    -5.14461587
  14        4.60175798    -3.14970479    -5.82662769
  15        7.70725788     4.67260659    -5.21218459
  16       10.43344040     3.45712315   -10.77083450
  17        7.37922236     2.33136268   -11.72030770
  18        8.60592268     5.22831581   -13.02780280
  19       10.78345730     6.94432980    -7.98763065
  20        9.10894854     8.82557573   -10.27027780
  21        8.03801527     8.68237957    -7.05497100
  22        5.12567058     7.45571597   -11.89227460
  23        3.72646362     4.61848791   -10.66941190
  24        3.68588154     9.87642533    -8.15214797
  25        1.29141107     4.75066204    -6.79925029
```

```
 26        0.65102332      7.84775912     -5.26111852
END

*PROD1
STATUS 2
SPECIES   NONLINRP
GEOM
  1        3.94014407     -1.55165936     -4.34093198
  2        4.74938431      0.95503066     -5.04352795
  3        5.25004493      1.29635872     -7.51457979
  4        5.85836637      4.07752950     -8.03012564
  5        7.49376618      4.29243331    -10.24672930
  6        7.87576351      6.91111027    -11.04206380
  7        5.11334464     -0.37213040     -9.08288042
  8        9.95280078      3.12597138     -9.74575242
  9        2.33235942     10.08890660     -8.84597719
 10        3.28740735      8.17957161     -7.50857040
 11        3.27189395      5.45398801     -8.32779796
 12        3.60729402     -1.47553593     -2.30836939
 13        2.20624768     -2.05047114     -5.35061852
 14        5.41588259     -2.92732315     -4.79177851
 15        6.79039426      4.83580447     -6.31731076
 16       10.95895600      4.05548723     -8.16241540
 17        9.71627353      1.12179007     -9.29693976
 18       11.13171050      3.27808781    -11.44101690
 19        8.70549623      8.09858180     -9.53147264
 20        9.17096946      6.91962367    -12.65809330
 21        6.09145969      7.76705753    -11.62143590
 22        2.33048956     12.01468590     -8.12875707
 23        1.52215376      9.78347471    -10.71353270
 24        4.09883831      8.53875869     -5.64796616
 25        2.63522262      5.26460176    -10.29022150
 26        1.89508964      4.45712645     -7.13414368
END

*START

STATUS 2
SPECIES NONLINTS
GEOM
  1       -1.59273884     -5.45598460      3.45090083
  2       -0.16021435     -3.16988400      3.26261579
  3       -0.00246963     -2.16410217      0.87272281
  4        1.28482578      0.19966195      0.91460003
  5        1.92060183      1.50429079     -1.25566462
  6        3.47959932      3.75117172     -0.72827752
  7       -0.95251551     -3.24966058     -0.97019252
  8        2.88617125      0.06962607     -3.44839837
  9       -1.36155112      3.17567432     -2.83405487
 10       -2.45919904      4.03868695     -0.57547037
 11       -3.36692472      2.32899754      1.14476062
 12       -1.52910733     -5.99272178      5.44324524
 13       -3.55283720     -5.15357987      2.85390866
 14       -0.76596998     -6.94924365      2.27943840
 15        1.80228315      1.03547940      2.70284161
 16        4.81226093     -0.58680698     -3.04784257
 17        1.64577706     -1.53472760     -3.78783287
 18        2.90426784      1.32937425     -5.08605687
 19        5.32073493      3.16917662      0.02746986
 20        3.74207922      4.81122542     -2.47947837
 21        2.49385955      4.92667269      0.65346200
 22       -0.55129957      4.48885484     -4.18946207
 23       -1.95304625      1.35695320     -3.58298087
 24       -2.11903247      5.98314354      0.00946661
 25       -3.87986551      0.43515672      0.55083658
 26       -3.91383792      2.89171194      3.04371007
END

# end of start section

*PATH
```

```
 SCALEMASS  1.00

 RODS ON

 INTMU   3
 SSTEP   0.005
 INH     10

 SRANGE
   SLP   2.61
   SLM  -2.61
 END

 RPM       pagem

 SIGN    REACTANT

 IDIRECT   1

 COORD  CURV3

INTDEF
 11-4 11-3 3-4-11 4-11-10
 2-1 3-2 4-3 5-4 6-5 7-3 8-5 9-5 10-9 11-10 12-1
 13-1 14-1 15-4 16-8 17-8 18-8 19-6 20-6 21-6 22-9
 23-9 24-10 25-11 26-11 3-2-1 4-3-2 5-4-3 6-5-4
 7-3-2 8-5-4 9-5-4 10-9-5 11-10-9 12-1-2 13-1-2
 14-1-2 15-4-3 16-8-5 17-8-5 18-8-5 19-6-5 20-6-5
 21-6-5 22-9-10 23-9-10 24-10-9 25-11-10 26-11-10
 4-3-2-1 5-4-3-2 6-5-4-3 7-3-2-1 8-5-4-3 9-5-4-3
 10-9-5-4 11-10-9-5 12-1-2-3 13-1-2-3 14-1-2-3
 15-4-3-2 16-8-5-4 17-8-5-4 18-8-5-4 19-6-5-4
 20-6-5-4 21-6-5-4 22-9-10-11 23-9-10-11 24-10-9-5
 25-11-10-9 26-11-10-9
END

 FREQSCALE 1.000000

 PRPATH
   COORD 2 4
   INTERVAL 1
   XMOL
 END

#END

*TUNNEL

 QUAD
  NQE   40
  NQTH  40
 END

 SCT

*RATE

  FORWARDK

  SIGMAF        1
  CVT
  PRDELG ON
# PRGIGT ON

  TEMP
    298.15
  END
```

esp.fu70

```
*GRGENERAL

 GRRESTART
 RSTTOL 0.00001

*GRSTART

 CHARGE      0
 MULTIPLICITY  1

*GRREACT1

 CHARGE      0
 MULTIPLICITY  1

*GRPROD1

 CHARGE      0
 MULTIPLICITY  1

*GRCOMMON

 GRENER
     #p B3LYP/6-31G* FCHK NOSYMM UNITS=AU
     scf=tight iop(3/124=3) scrf=(pcm,solvent=n,n-DiMethylFormamide)
     int(grid=ultrafine)
 END

 GRFIRST
     #p B3LYP/6-31G* FORCE FCHK NOSYMM UNITS=AU
     scf=tight iop(3/124=3) scrf=(pcm,solvent=n,n-DiMethylFormamide)
     int(grid=ultrafine)
 END

 GRSEC
     #p B3LYP/6-31G* FREQ=NORAMAN FCHK NOSYMM UNITS=AU
     scf=tight iop(3/124=3) scrf=(pcm,solvent=n,n-DiMethylFormamide)
     int(grid=ultrafine)
 END

 GRLINK0
    %chk=g09.chk
    %nproc=8
    %mem=7gb
 END
```

esp.fu71

```
%nproc=8
%mem=3gb
%chk=g09.chk
#p B3LYP/6-31G* opt=loose fchk NOSYMM
scf=tight int(grid=ultrafine)
scrf=(pcm,solvent=n,n-DiMethylFormamide)
iop(3/124=3)

sm for 23 from opt of ts

0 1
 C,0,2.0375388467,-0.8862139749,-2.4226657382
 O,0,2.840830771,0.2901574472,-2.4590270401
 C,0,2.9443499088,0.8918912279,-3.7138135966
 C,0,3.7893970873,1.9941392954,-3.6812240659
 N,0,3.8761377809,2.8600828001,-4.8748674307
 C,0,4.7295194509,4.0429986429,-4.5452684222
 O,0,2.3249592261,0.406759293,-4.6910602271
 C,0,4.5172626373,2.1152354958,-6.0157372728
 C,0,2.4985707517,3.3637907671,-5.3917615721
 C,0,1.7499921087,4.158362798,-4.3721794846
```

C,0,0.8819993356,3.5817892612,-3.5375826263
H,0,2.0609812186,-1.2313599052,-1.3849116377
H,0,1.0031714503,-0.6777114272,-2.7224134647
H,0,2.4351454424,-1.6667519863,-3.0833185763
H,0,4.0785052086,2.4726369101,-2.7581692899
H,0,5.521138878,1.8294307768,-5.6996801311
H,0,3.9049162892,1.2337039969,-6.2021197346
H,0,4.5540581437,2.7667055673,-6.8940163355
H,0,5.7063598314,3.67478106,-4.226872092
H,0,4.8202479598,4.6702935273,-5.434796919
H,0,4.2535344856,4.5945173864,-3.733329859
H,0,2.7123880505,3.9453949672,-6.293120655
H,0,1.9719596179,2.4439985403,-5.6460096185
H,0,1.9504845071,5.2263791882,-4.3139309066
H,0,0.6833853073,2.513942079,-3.5980082897
H,0,0.3445067045,4.1528552656,-2.7840640136

esp.fu73

%nproc=8
%mem=3gb
%chk=g09.chk
#p B3LYP/6-31G* opt=loose fchk NOSYMM
scf=tight int(grid=ultrafine)
scrf=(pcm,solvent=n,n-DiMethylFormamide)
iop(3/124=3)

23 product

0 1
C,0,2.0850344388,-0.8211027674,-2.2971222658
O,0,2.5132659316,0.5053804567,-2.6689200443
C,0,2.7782041207,0.6860034863,-3.9765443583
C,0,3.100113961,2.1577356774,-4.2493594702
N,0,3.9655302665,2.2714578763,-5.4223356296
C,0,4.1676745503,3.657202043,-5.8432085134
O,0,2.7058654432,-0.1969229265,-4.8064533057
C,0,5.2667953344,1.6541928076,-5.1572300635
C,0,1.2342314461,5.3388194363,-4.6810895166
C,0,1.7396210438,4.328442874,-3.9733643265
C,0,1.7314117053,2.886126149,-4.4068808756
H,0,1.9088977799,-0.7808199834,-1.2215364703
H,0,1.1674959901,-1.0850625948,-2.8314253711
H,0,2.8659616298,-1.549072691,-2.5356999757
H,0,3.5933218785,2.5589975101,-3.3429768749
H,0,5.7992297687,2.1460714141,-4.3193641954
H,0,5.1416305052,0.5936257383,-4.9197286315
H,0,5.890647507,1.7346893566,-6.0543253873
H,0,4.6067501947,4.2855849088,-5.0438380833
H,0,4.8530680213,3.6617071358,-6.6983744651
H,0,3.2234616346,4.1101498203,-6.1497990052
H,0,1.2332419576,6.3578979475,-4.3015529778
H,0,0.8054890768,5.177191837,-5.6693573206
H,0,2.1690118177,4.5185164901,-2.9887749669
H,0,1.3944997525,2.7859072655,-5.4453506671
H,0,1.0028382437,2.3586097323,-3.7752262383

esp.fu75

%nproc=8
%mem=3gb
%chk=g09.chk
#p B3LYP/6-31G* opt=(ts,calcfc,noeigentest) fchk NOSYMM
scrf=(pcm,solvent=n,n-DiMethylFormamide)
int(grid=ultrafine)
iop(3/124=3)

ts for 23 parent

0 1
C,0,1.9736117658,-0.7967995959,-2.3687400088
O,0,2.7316710775,0.4129527354,-2.4683761612
C,0,2.8151459858,0.945189561,-3.7330530571
C,0,3.4963533784,2.1960396602,-3.7108925905
N,0,3.8327915746,2.8864195039,-4.8593471787
C,0,4.6577775155,4.0754176834,-4.5802659421
O,0,2.3124033596,0.3707367886,-4.7082818509
C,0,4.3437489067,2.1272276342,-6.0196919224
C,0,2.0959510367,3.770877575,-5.6945953473
C,0,1.515100776,4.2275641901,-4.4994038813
C,0,1.0347530351,3.3228355195,-3.5890968503
H,0,2.0072841125,-1.0808286802,-1.3144367545
H,0,0.9363723885,-0.6367739069,-2.6846546614
H,0,2.4111190052,-1.5869982518,-2.9886512311
H,0,3.7701800247,2.6383352028,-2.7645959006
H,0,5.3629916871,1.7798582257,-5.8077268786
H,0,3.6873605708,1.2782402373,-6.1993128949
H,0,4.3533252091,2.7938576585,-6.8863034575
H,0,5.6320645427,3.7674391414,-4.1803416558
H,0,4.7966758975,4.6363739415,-5.5069614963
H,0,4.1361464932,4.6974660086,-3.8490808795
H,0,2.5247176932,4.465782776,-6.4118459336
H,0,1.782945297,2.8084518131,-6.0909099038
H,0,1.6951091734,5.256526301,-4.1898685671
H,0,0.7633164601,2.3206581215,-3.9033879127
H,0,0.7453390331,3.6206111562,-2.5842160821

NMR Integration Macro

The listing below shows a sample macro for the output of NMR integrations. The spectra were first carefully phased by hand and the phases were recorded for use in the macro. The integration cut points shown in the macro were in each case used for both the sample and the standard.

Macro “macrokie2”

```
shell('rm /home/singleton/dsingle/dastemp2')
$filename='/nmrdata/singleton/scollins/SEAN-KIE2-STANDARD-ERIK-CUT-OME'
$filenameshort='SEAN-KIE2-STANDARD'
rt($filename)

rp=-21.5
lp=-269.7
$cut[1]=.6
$cut[2]=1.06
$cut[3]=.68
$cut[4]=.44
$cut[5]=.30
$cut[6]=.38
$cut[7]=.57

setlimit('fn',2097152,8,2)
fn=1048576
wft('all')
wc=550
axis='p'

"For this program the argument is the number of spectra to be worked up in the array"
if ($#<1) then $numspec=6 else $numspec=$1 endif
```

```
$multiplier=8

$spectrum=1
repeat
ds($spectrum)

"First, I want to get the full spectrum, set some basics and set the shifts"
$totalwidth=0
$sp=sp $wp=wp
vp=12 f intmod='partial' cz vs=160 th=5 nm

"count lines in case something is going wrong and exit if so"
nll('pos',20):$count
if ($count<5 or $count>15) then
  text
  echo('Problem with wrong number of peaks.')
  return
endif

"----------Setting shifts----------"
"get carbonyl set to 171.6 then find chlororm and set it at 77.00"
getll(1):$ht,$freq
cr=$freq
rl(171.5p)
sp=76.0p wp=4p
repeat
  nll('pos',10):$count
  if ($count<3) then th=th-1 endif
  if ($count>3) then th=th+1 endif
  nll('pos',10):$count
until ($count=3)
getll(2):$ht,$freq
cr=$freq rl(77.00p) f
"----------"

"----------Setting the level----------"
"to turn off this section make the next line false"
if (1<2) then
  f cz intmod='partial'
  z(80p,110p)
  repeat
    integ(79p,111p):$intmid
    echo($intmid)
    if ($intmid>0) then lvl=lvl-1 endif
    integ(69p,111p):$intmid
  until ($intmid<0)
  repeat
    integ(69p,111p):$intmid
    echo($intmid)
    if ($intmid<0) then lvl=lvl+.1 endif
    integ(69p,111p):$intmid
  until ($intmid>0)
  repeat
    integ(69p,111p):$intmid
    echo($intmid)
    if ($intmid>0) then lvl=lvl-.01 endif
```

```
    integ(69p,111p):$intmid
  until ($intmid<0)
  cz
  sp=$sp wp=$wp
endif
"----------------------------------------------------------------"

"-----------------------------Cutting integrations---------------"
"to turn off this section make the next line false, to turn it on make the line true"
if (2>1) then

cz
"1 now focus on carbonyl ono far left and cut it"
sp=170p wp=3p
repeat
  nll('pos',144):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',144):$count
until ($count=1)
$i=1
repeat
  getll($i):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>1)

"2 now focus on second peak from the left"
sp=133p wp=3p
repeat
  nll('pos',20):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',20):$count
until ($count=1)
$i=2
repeat
  getll($i-1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>2)

"Now focus on cutting the third peak, cut them"
sp=114p wp=3p
repeat
  nll('pos',20):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',20):$count
until ($count=1)
$i=3
repeat
```

```
  getll($i-2):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>3)

"now focus on cutting peaks 4"
sp=65p wp=2p
repeat
  nll('pos',50):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',50):$count
until ($count=1)
$i=4
repeat
  getll($i-3):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>4)

"Focus on cutting peaks 5 "
sp=48p wp=3p
repeat
  nll('pos',60):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',60):$count
until ($count=1)
$i=5
repeat
  getll($i-4):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>5)

"Focus on cutting peaks 6 "
sp=39p wp=3p
repeat
  nll('pos',70):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',70):$count
until ($count=1)
$i=6
repeat
  getll($i-5):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
```

```
until ($i>6)

"Focus on cutting peaks 7 "
sp=31p wp=3p
repeat
  nll('pos',20):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',20):$count
until ($count=1)
$i=7
repeat
  getll($i-6):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>7)

endif
"-----------------------------------------------------------------"

sp=$sp wp=$wp

echo('The average line width is ',$totalwidth/5)

"--------------------------Output integrals-------------------------"
"to turn off this section make the next line false, to turn it on make the line true"
if (2>1) then
  intmod='partial'
  f
  nll('pos',20):$count
  printon
  shell('date')
  text(file)
  echo('The average line width is ',$totalwidth/5)
  nli
  setint(5,1000)
  printoff('/home/singleton/dsingle/tempfile')
  shell('cat /home/singleton/dsingle/tempfile >> /home/singleton/dsingle/dastemp2')

endif
"-----------------------------------------------------------------"

$spectrum=$spectrum+1
until ($spectrum>$numspec)

sp=$sp wp=$wp
```

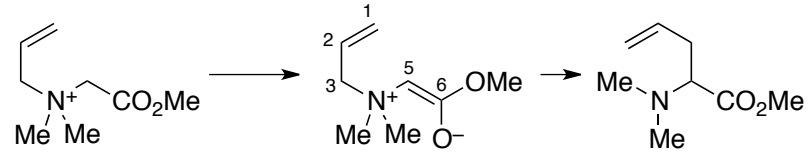
Calculated Structures and Complete Energies

Guide to Structures, Structure Titles and Their Organization

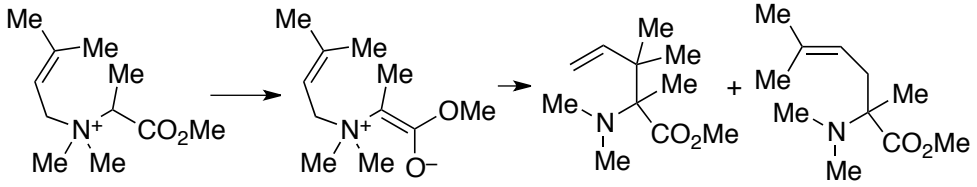
The calculated structures provided are divided into large groups by system, then divided

by method / basis set / solvent model.

The first section below provides structures associated with the rearrangement of **2** (using in all cases the numbering in the main text). Since the purpose of these calculations was to survey the diversity of predicted isotope effects versus transition structure geometry, most combinations of method / basis set / solvent model only involved the calculation of two structures, the lowest-energy starting cation **1** and the lowest-energy transition structure for the [2,3]-sigmatropic rearrangement. Exploratory calculations had identified a lowest-energy conformation for **1** that was the second conformation out of a series that were explored, and this conformation is designated "Conf2" in the structure titles. The complete structure titles for **1** are then labeled as "Cation-" followed by the method, basis set, and solvent model, followed by "Conf2". Exploratory calculations had identified the exo s-cis transition structure for the rearrangement as lowest in energy, and these transition structures are labeled as either "23TS-" or just "TS-" followed by the method, basis set, and solvent model.



1 **2** **3** [2,3]



4 **5** **6** [2,3] **7** [1,2]

The second section below provides structures associated with the rearrangement of **5**. Many of these calculations were explored with the purpose of surveying the diversity of transition structure geometries for the 2,3-rearrangement, and so for many combinations of method / basis set / solvent model only a single structure was calculated, namely the exo s-cis transition structure. Exploratory calculations had indicated that the exo s-cis structure was lowest in energy, out of four possibilities (endo versus exo, s-cis versus s-trans (referring to to the relative orientation of the carbonyl versus the C^5-N bond). In some cases we have provided the alternative possibilities; these are labeled in their title as endo s-trans or endo s-cis or exo s-trans. If a TS is not labeled, it is the exo s-cis. All of titles for 2,3-rearrangement structures start with "TS23". The section also includes transition structures for the simple N-C^3 bond cleavage (with the prenyl fragment oriented in such a way that the 2,3-rearrangement cannot occur). Out of two logical conformations explored for the cleavage, the first was found to be lowest in energy and this is designated in the title as "TSCleavageA". An alternative conformation is labeled "TSCleavageB".

A final section presents structures used in relevant GAUSSRATE / POLYRATE calculations. These are slightly different in structure and energy from their counterparts in other sections, in part because of the use of int(grid=ultrafine) and nosymm options in their calculation, in part because they were often optimized with tight convergence, and in part because the starting materials and / or products were chosen from steepest-descent paths in mass-weighted coordinates. The names in this section are self-explanatory.

We have not included a large number of calculated structures, such as those associated with model systems **A** and **B**, or structures for most higher-energy conformers.

For the purpose of ease in record keeping and data retrieval, the listings here include a file name and complete path for the server on which the calculations are saved.

Structures for the Rearrangement of 2

Cation-B3LYP-D2/6-31+G**/PCM- Conf2

/home/bibaswanbiswas/c8/23parentSM2B3D2PS
parent sm conf 2
B3LYP/6-31+G**
E(RB3LYP) = -519.576987851

Zero-point correction= 0.240438 (Hartree/Particle)
Thermal correction to Energy= 0.253183
Thermal correction to Enthalpy= 0.254128
Thermal correction to Gibbs Free Energy= 0.201260
Sum of electronic and ZPE= -519.336549
Sum of electronic and thermal Energies= -519.323804
Sum of electronic and thermal Enthalpies= -519.322860
Sum of electronic and thermal Free Energies= -519.375728

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.875	46.943	111.270

C,0,2.0118341603,-0.7967810691,-2.241639745
O,0,2.7688990345,0.4347315652,-2.4047463337
C,0,2.7842096205,0.9649270844,-3.623761134
O,0,2.2179839729,0.507229846,-4.5973435544
C,0,3.6294435895,2.2320931766,-3.5835941847
N,0,3.7213850288,2.9921952502,-4.8798104341
C,0,4.4357083946,2.179678611,-5.9306496582
C,0,4.530204375,4.2344162768,-4.6023149496
C,0,2.3411244626,3.4037716527,-5.4314834853
C,0,1.4724256821,4.0714262579,-4.4099085947
C,0,1.1908370164,5.376710319,-4.4452866791
H,0,2.1314987601,-1.064871835,-1.1931442059
H,0,0.9627734765,-0.6145700232,-2.4853120576
H,0,2.423854689,-1.5680492904,-2.8961962755
H,0,4.6482799399,1.9686235028,-3.289840571
H,0,3.2241543707,2.9079267871,-2.8280874685
H,0,3.8509578196,1.2848221256,-6.1326261033
H,0,4.5211255789,2.7957159768,-6.8264746725
H,0,5.4250562258,1.9254852247,-5.5480441456
H,0,5.5041312858,3.9309010763,-4.2174410393
H,0,4.6421611392,4.7778063685,-5.5404062559
H,0,3.9945626682,4.8402084404,-3.8721706699
H,0,2.5626219619,4.0691680792,-6.2680136907
H,0,1.8905905845,2.4830855693,-5.8007027733
H,0,1.0288377989,3.4380463022,-3.6450556813
H,0,1.6085075895,6.0240991344,-5.213362045
H,0,0.5258627739,5.8285215903,-3.7149065922

23TS-B3LYP-D2/6-31+G**/PCM

/home/bibaswanbiswas/c8/23parentTSB3D2PS
parent ts exo s-cis
B3LYP/6-31+G**
E(RB3LYP) = -519.067923267

Zero-point correction= 0.222213 (Hartree/Particle)
Thermal correction to Energy= 0.234910
Thermal correction to Enthalpy= 0.235854
Thermal correction to Gibbs Free Energy= 0.184094
Sum of electronic and ZPE= -518.845711
Sum of electronic and thermal Energies= -518.833013
Sum of electronic and thermal Enthalpies= -518.832069
Sum of electronic and thermal Free Energies= -518.883829

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.408	47.022	108.938

C,0,1.9918091767,-0.809209825,-2.3262079805
O,0,2.725447739,0.419122139,-2.4545316512
C,0,2.8225841576,0.9292027439,-3.7284625127
C,0,3.481175396,2.1933223282,-3.7204134657
N,0,3.8311322247,2.8820187818,-4.864109122
C,0,4.6775828194,4.0572988169,-4.5778370444
O,0,2.354328585,0.3184629103,-4.7021199114
C,0,4.3223591519,2.1288628785,-6.0383123247
C,0,2.0976924831,3.8277104129,-5.7033721897
C,0,1.5097695154,4.2429428785,-4.4957034072
C,0,0.9963178156,3.312392053,-3.627683994
H,0,2.0137716856,-1.0524431442,-1.2624900804
H,0,0.9590383656,-0.6796055152,-2.6658170947
H,0,2.4641252859,-1.6064361108,-2.9089019046
H,0,3.7212115367,2.6526578882,-2.7730789992
H,0,5.3232805008,1.7345376947,-5.8233166193
H,0,3.6372009994,1.3116380315,-6.2519137224
H,0,4.3707213925,2.8165913473,-6.8857002618
H,0,5.6514695998,3.7284567406,-4.195295962
H,0,4.8134577094,4.6279430426,-5.4980852211
H,0,4.1768855947,4.6782371467,-3.8320132122
H,0,2.5606998315,4.5434295872,-6.3763950915
H,0,1.7799387547,2.8867732003,-6.1437161508
H,0,1.6990892512,5.2553373109,-4.1421096933
H,0,0.7332795716,2.3204068951,-3.9798192768
H,0,0.6998848563,3.577810767,-2.6166331063

Cation-B3LYP-D2/6-31+G**/SMD- Conf2

/home/bibaswanbiswas/c8/23parentSM2B3D2PSSMD
parent sm conf 2
B3LYP/6-31+G**
E(RB3LYP) = -519.597337906

Zero-point correction= 0.241141 (Hartree/Particle)
Thermal correction to Energy= 0.253568
Thermal correction to Enthalpy= 0.254512
Thermal correction to Gibbs Free Energy= 0.202903

Sum of electronic and ZPE= -519.356197
Sum of electronic and thermal Energies= -519.343770
Sum of electronic and thermal Enthalpies= -519.342826
Sum of electronic and thermal Free Energies= -519.394435

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.116	46.484	108.621

C,0,1.9652299496,-0.7576776524,-2.2301376274
O,0,2.7191617294,0.4747767898,-2.3948841081
C,0,2.8081880972,0.9569858241,-3.634762971
O,0,2.2983312928,0.4497493669,-4.6157030489
C,0,3.6576127806,2.2177503173,-3.5983559547
N,0,3.7297355644,2.9908131533,-4.8864470241
C,0,4.4474421771,2.2057474241,-5.951866044
C,0,4.5298375254,4.2356031967,-4.6039714402
C,0,2.3457687206,3.391687441,-5.4221243067
C,0,1.4766812339,4.0450285002,-4.3908107459
C,0,1.1749635428,5.3455589845,-4.4282959901
H,0,2.0515002563,-1.0054594181,-1.171937447
H,0,0.9203917538,-0.5909066241,-2.5055106667
H,0,2.3995100144,-1.546029421,-2.8504296121
H,0,4.683192749,1.9452617936,-3.3329201203
H,0,3.2696726655,2.8899373705,-2.8308600722
H,0,3.869962493,1.3120132798,-6.1801973191
H,0,4.5306783026,2.8469743007,-6.8308821646
H,0,5.4357990982,1.9474808987,-5.5679446359
H,0,5.5113016024,3.929059611,-4.2379770436
H,0,4.6202002532,4.7884754083,-5.5399544939
H,0,4.002864993,4.8270577279,-3.8550190432
H,0,2.553891519,4.0644522258,-6.2563156763
H,0,1.8976397655,2.4706158629,-5.7952538462
H,0,1.0616602318,3.4064626139,-3.6128291174
H,0,1.5781291902,5.9943253357,-5.2042088787
H,0,0.509684498,5.7915736888,-3.6927236023

23TS-B3LYP-D2/6-31+G**/SMD

/home/bibaswanbiswas/c8/23parentTSB3D2PSSMD
parent ts exo s-cis
B3LYP/6-31+G**
E(RB3LYP) = -519.072558527

Zero-point correction= 0.222269 (Hartree/Particle)
Thermal correction to Energy= 0.234857
Thermal correction to Enthalpy= 0.235801
Thermal correction to Gibbs Free Energy= 0.184387
Sum of electronic and ZPE= -518.850290
Sum of electronic and thermal Energies= -518.837702
Sum of electronic and thermal Enthalpies= -518.836758
Sum of electronic and thermal Free Energies= -518.888172

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.375	46.897	108.210

C,0,2.0047006433,-0.8044424496,-2.3027812513
O,0,2.7223329922,0.4308067966,-2.4448726789
C,0,2.8250386391,0.9210915309,-3.7257297696
C,0,3.4698023078,2.195292889,-3.7248377997
N,0,3.8248851462,2.8827287127,-4.8658770729
C,0,4.6876410956,4.0461349009,-4.5814234795
O,0,2.3817504562,0.2863329757,-4.6933860752
C,0,4.2996464335,2.1313068673,-6.0464092197
C,0,2.1150828813,3.8617237312,-5.7001923815
C,0,1.5065625233,4.2444559579,-4.4914824762
C,0,0.980783541,3.2908918565,-3.6557957296
H,0,2.0155143257,-1.0288804528,-1.233567435
H,0,0.972228135,-0.6999567944,-2.6542847811
H,0,2.493764266,-1.6105009566,-2.8605698226
H,0,3.6950459969,2.6663354068,-2.7791447584
H,0,5.2868150687,1.702905752,-5.8302246142
H,0,3.5931649333,1.3375478348,-6.2791417453
H,0,4.3764138849,2.8303024677,-6.882679289
H,0,5.6617348028,3.7025672889,-4.2109068464
H,0,4.8213962455,4.6190800748,-5.5009685801
H,0,4.2048760121,4.6703042568,-3.8259319766
H,0,2.596238814,4.5964911963,-6.3398643345
H,0,1.7928345587,2.9419085709,-6.181218657
H,0,1.6976132136,5.2446907347,-4.1041401342
H,0,0.7223176116,2.3072313445,-4.0358289341
H,0,0.666069472,3.5311105068,-2.6427801572

Cation-B3LYP-D2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/23parentSM2B3D2SB
parent sm conf 2
B3LYP/6-31G*
E(RB3LYP) = -519.541373957

Zero-point correction= 0.241730 (Hartree/Particle)
Thermal correction to Energy= 0.254499
Thermal correction to Enthalpy= 0.255443
Thermal correction to Gibbs Free Energy= 0.202324
Sum of electronic and ZPE= -519.299644
Sum of electronic and thermal Energies= -519.286875
Sum of electronic and thermal Enthalpies= -519.285931
Sum of electronic and thermal Free Energies= -519.339050

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.700	46.763	111.799

C,0,2.0243629283,-0.7919080244,-2.2532833654
O,0,2.7865949024,0.4330936219,-2.4083864972
C,0,2.7742877251,0.9772892654,-3.6200782967
O,0,2.1850063012,0.5363730471,-4.5857022996
C,0,3.6207421924,2.2452729313,-3.5782449206
N,0,3.718982322,2.9936657208,-4.8805131823
C,0,4.4358884884,2.1676470057,-5.9167961407
C,0,4.5225235898,4.2396631444,-4.61375006
C,0,2.3385479335,3.3982601218,-5.4408425062
C,0,1.4630752774,4.0570420179,-4.4204755028
C,0,1.2142232602,5.3679051105,-4.4239187567
H,0,2.1579475357,-1.080101455,-1.2111692032
H,0,0.9719319468,-0.6007525211,-2.4773958608
H,0,2.41699461,-1.5573123315,-2.9273357987
H,0,4.638639665,1.9888257822,-3.2746497115
H,0,3.2069849686,2.9282178087,-2.8331775015
H,0,3.8570524605,1.2632673551,-6.0940689131
H,0,4.5109777888,2.7649224879,-6.8268371347

H,0,5.4299225686,1.9305180136,-5.533676887
H,0,5.4903541367,3.9443468,-4.2061510355
H,0,4.6502481141,4.7657823415,-5.5604773496
H,0,3.9721276092,4.8580055828,-3.9044522122
H,0,2.5634055344,4.066681194,-6.274408239
H,0,1.8980254641,2.4744889463,-5.813547338
H,0,0.9947672537,3.4102274423,-3.6818089634
H,0,1.6569712279,6.0269948416,-5.1680718871
H,0,0.5484461949,5.818901749,-3.6931034369

23TS-B3LYP-D2/6-31G*/PCM

/home/bibaswanbiswas/c8/23parentTSB3D2SB
parent ts exo s-cis
B3LYP/6-31G*
E(RB3LYP) = -519.022559562

Zero-point correction= 0.223787 (Hartree/Particle)
Thermal correction to Energy= 0.236342
Thermal correction to Enthalpy= 0.237286
Thermal correction to Gibbs Free Energy= 0.185854
Sum of electronic and ZPE= -518.798772
Sum of electronic and thermal Energies= -518.786218
Sum of electronic and thermal Enthalpies= -518.785274
Sum of electronic and thermal Free Energies= -518.836705

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.307	46.624	108.247

C,0,1.9843757471,-0.8034079907,-2.3643243653
O,0,2.7307391171,0.4134089273,-2.4657521081
C,0,2.8096974076,0.945246613,-3.7311581953
C,0,3.4878519713,2.1975602465,-3.7105020712
N,0,3.8269269367,2.8868606111,-4.8594447179
C,0,4.6584119928,4.071458751,-4.5795224612
O,0,2.3066530007,0.3685880326,-4.704942114
C,0,4.3365020156,2.1240427835,-6.0182498556
C,0,2.1024227713,3.7817537401,-5.6952845874
C,0,1.5169264324,4.2362596519,-4.5009781803
C,0,1.0291738374,3.3279082169,-3.598679955
H,0,2.0220684802,-1.0861628422,-1.309787578
H,0,0.9452793347,-0.653842764,-2.6791114033
H,0,2.4289344341,-1.5900157111,-2.9839381066
H,0,3.7631122529,2.6400654658,-2.7647416184
H,0,5.3544193251,1.7739007678,-5.804666378
H,0,3.6774184051,1.2768582475,-6.1968671913
H,0,4.3490289584,2.7888828793,-6.8861763019
H,0,5.6300244127,3.7579773144,-4.17777547
H,0,4.8017611419,4.6309970071,-5.5063798537
H,0,4.1387078033,4.696721384,-3.8496608805
H,0,2.5380164213,4.4775663103,-6.407621438
H,0,1.7833959454,2.8241047057,-6.0983269923
H,0,1.6995427905,5.2628150226,-4.1851439828
H,0,0.7583996453,2.3280805473,-3.9213617993
H,0,0.7344634195,3.6198330823,-2.5936423947

Cation- B97D3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/23parentSM2B97D3SB
parent sm conf 2
B97D3/6-31G*
E(RB97D3) = -519.191750743

Zero-point correction= 0.236901 (Hartree/Particle)
Thermal correction to Energy= 0.250194
Thermal correction to Enthalpy= 0.251138
Thermal correction to Gibbs Free Energy= 0.195480
Sum of electronic and ZPE= -518.954849
Sum of electronic and thermal Energies= -518.941557
Sum of electronic and thermal Enthalpies= -518.940613
Sum of electronic and thermal Free Energies= -518.996271

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.999	48.119	117.141

C,0,2.0042759519,-0.7911685801,-2.2412586973
O,0,2.7740178964,0.4378099713,-2.3982410602
C,0,2.7776478474,0.9709418054,-3.6257601666
O,0,2.1969883869,0.519494911,-4.5995173743
C,0,3.633958441,2.2378787468,-3.5811881665
N,0,3.7312430636,2.9955367457,-4.8858949575
C,0,4.4478815717,2.1697209954,-5.9320615865
C,0,4.5347943146,4.2478514305,-4.6144459299
C,0,2.3354667853,3.4004931123,-5.441423949
C,0,1.4565518808,4.0521133877,-4.4197235059
C,0,1.1987194767,5.3684893689,-4.4123603823
H,0,2.1290581285,-1.0672984918,-1.1920547565
H,0,0.9513580469,-0.6005242497,-2.4759353852
H,0,2.4049419549,-1.566458843,-2.9033720178
H,0,4.6542875579,1.9739709335,-3.2818270149
H,0,3.2310555842,2.9233363011,-2.8286549375
H,0,3.8771923192,1.2557677551,-6.1005990344
H,0,4.507796255,2.7626858602,-6.8487273253
H,0,5.4512428216,1.9422317603,-5.5610986783
H,0,5.5055058746,3.9558770083,-4.2051888711
H,0,4.6652568706,4.7807589795,-5.5596903036
H,0,3.9842397167,4.8663513133,-3.9018265372
H,0,2.5557241328,4.0695503358,-6.2791618221
H,0,1.8999666847,2.4710823837,-5.8151320446
H,0,0.9752558793,3.3969564072,-3.6909505946
H,0,1.6440167083,6.0445183113,-5.1447170516
H,0,0.5205878483,5.8093503401,-3.6815108497

23TS-B97D3/6-31G*/PCM

/home/bibaswanbiswas/c8/23parentTSB97D3SB
parent ts exo s-cis
B97D3/6-31G*
E(RB97D3) = -518.682459365

Zero-point correction= 0.219801 (Hartree/Particle)
Thermal correction to Energy= 0.232694
Thermal correction to Enthalpy= 0.233638
Thermal correction to Gibbs Free Energy= 0.181304
Sum of electronic and ZPE= -518.462658
Sum of electronic and thermal Energies= -518.449766
Sum of electronic and thermal Enthalpies= -518.448821
Sum of electronic and thermal Free Energies= -518.501156

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 146.018 47.627 110.147

C,0,1.9722204471,-0.8322814371,-2.4121711006
O,0,2.7705079801,0.357220501,-2.4877427541
C,0,2.8539075202,0.9258429356,-3.7589447894
C,0,3.5996165478,2.1303188479,-3.7198191189
N,0,3.8194815775,2.8955481491,-4.8789616287
C,0,4.6408325521,4.0983482248,-4.5813615223
O,0,2.3103217465,0.3842120786,-4.7439941134
C,0,4.3781528455,2.1483239159,-6.0427935664
C,0,2.1687044161,3.6346017954,-5.6164317138
C,0,1.5209910736,4.2356721414,-4.4871209724
C,0,0.9217624491,3.4722984756,-3.531015571
H,0,2.0179892921,-1.1498693168,-1.3642987778
H,0,0.9286933003,-0.6333096339,-2.6972962359
H,0,2.3685221455,-1.6249658855,-3.0626226966
H,0,3.8254037636,2.606513305,-2.7733437701
H,0,5.4083782138,1.8496519685,-5.8088559396
H,0,3.7568915622,1.2665967564,-6.2083882364
H,0,4.3673981207,2.8020214128,-6.9223693936
H,0,5.6251037691,3.7820886839,-4.212113127
H,0,4.7543243993,4.6904572714,-5.4947273812
H,0,4.1292969331,4.6895598214,-3.8155947259
H,0,2.539553277,4.2778096085,-6.4165611057
H,0,1.786204829,2.6691221013,-5.9495841057
H,0,1.6803160319,5.3020213369,-4.3053690641
H,0,0.7182292755,2.416476807,-3.7030422702
H,0,0.5514499315,3.9031811348,-2.5995163189

Cation- N12/6-31+G**/PCM- Conf2

/home/bibaswanbiswas/c8/SM2N12PS
parent sm conf 2
N12/6-31+G**
E(RN12) = -519.407692482

Zero-point correction= 0.239843 (Hartree/Particle)
Thermal correction to Energy= 0.252803
Thermal correction to Enthalpy= 0.253747
Thermal correction to Gibbs Free Energy= 0.200521
Sum of electronic and ZPE= -519.167849
Sum of electronic and thermal Energies= -519.154890
Sum of electronic and thermal Enthalpies= -519.153946
Sum of electronic and thermal Free Energies= -519.207171

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 158.636 47.526 112.022

C,0,2.0714897046,-0.8407639046,-2.278635364
O,0,2.8061443038,0.3809669936,-2.4360077855
C,0,2.7841441775,0.9515683637,-3.6250072628
O,0,2.197845739,0.5217250676,-4.5931266227
C,0,3.6083228695,2.2214214517,-3.5681294851
N,0,3.7084720776,2.9884326525,-4.8476454746
C,0,4.4013331225,2.1769631405,-5.8962885868
C,0,4.5250163173,4.2090616707,-4.5669291908
C,0,2.3370813691,3.4134397705,-5.3862965157
C,0,1.5015609048,4.1598724426,-4.4087141007
C,0,1.1836219568,5.4466550772,-4.5541788526
H,0,2.2858131899,-1.1787829447,-1.2736502
H,0,1.0102003001,-0.6483610188,-2.4000719657
H,0,2.403662779,-1.5701009203,-3.0099766184
H,0,4.6183901086,1.9680291858,-3.258710985
H,0,3.1948740705,2.8808673488,-2.8112371498
H,0,3.8087995797,1.2968792137,-6.1038119037
H,0,4.5006994773,2.7852703672,-6.7869276516
H,0,5.3813899821,1.900894284,-5.525776302
H,0,5.4887801052,3.9049370402,-4.1774055223
H,0,4.6539570844,4.755006705,-5.4932924566
H,0,4.0018602117,4.8228192993,-3.8447370689
H,0,2.5533508306,4.0133724244,-6.2638879686
H,0,1.8569245547,2.490595542,-5.6933491202
H,0,1.0795916867,3.5989804781,-3.5854786464
H,0,1.560506309,6.0374948172,-5.3774838229
H,0,0.5251991879,5.940073452,-3.8555663769

23TS-N12/6-31+G**/PCM

/home/bibaswanbiswas/c8/TSparentN12PS
parent ts exo s-cis
N12/6-31+G**
E(RN12) = -518.906645363

Zero-point correction= 0.222212 (Hartree/Particle)
Thermal correction to Energy= 0.235111
Thermal correction to Enthalpy= 0.236056
Thermal correction to Gibbs Free Energy= 0.183660
Sum of electronic and ZPE= -518.684434
Sum of electronic and thermal Energies= -518.671534
Sum of electronic and thermal Enthalpies= -518.670590
Sum of electronic and thermal Free Energies= -518.722986

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 147.535 47.424 110.277

C,0,2.0564008038,-0.8340301518,-2.3495362104
O,0,2.7287859217,0.4062835961,-2.4739485019
C,0,2.8263414038,0.9218125193,-3.7355218924
C,0,3.4729672503,2.181442418,-3.7220999019
N,0,3.8072613303,2.8830164302,-4.8602357181
C,0,4.677762835,4.026476963,-4.5687300017
O,0,2.3752374237,0.3057777503,-4.7075628004
C,0,4.2881451469,2.1203505386,-6.0194213949
C,0,2.1462231716,3.8139069453,-5.6733577565
C,0,1.5140854742,4.2812450804,-4.5061997931
C,0,0.9207867272,3.4148730948,-3.6379747183
H,0,2.0712070404,-1.0756361934,-1.2925712064
H,0,1.0281920944,-0.7604798853,-2.6973355961
H,0,2.5630659969,-1.6139310063,-2.9142890342
H,0,3.6975392974,2.6442133067,-2.779456683
H,0,5.2852642597,1.7358334363,-5.8092057777
H,0,3.6128424516,1.2960694277,-6.2054322792
H,0,4.3298500079,2.778161461,-6.8810952093
H,0,5.6385700062,3.6730395143,-4.1978580289
H,0,4.827826628,4.6044523189,-5.4731464904
H,0,4.2087779928,4.6498873853,-3.8157224017
H,0,2.5974444757,4.5107521758,-6.3650518242
H,0,1.7951344597,2.8900081198,-6.1098752419
H,0,1.6945670388,5.3017385352,-4.1919454324

H,0,0.6748726773,2.4089171092,-3.9410302632
H,0,0.5751020847,3.7332801107,-2.6654358417

23TS-UN12/6-31+G/PCM**

/home/bibaswanbiswas/c8/TSparentUN12PS
parent ts exo s-cis
UN12/6-31+G**
E(UN12) = -518.906645392

Zero-point correction= 0.222211 (Hartree/Particle)
Thermal correction to Energy= 0.235110
Thermal correction to Enthalpy= 0.236054
Thermal correction to Gibbs Free Energy= 0.183663
Sum of electronic and ZPE= -518.684434
Sum of electronic and thermal Energies= -518.671535
Sum of electronic and thermal Enthalpies= -518.670591
Sum of electronic and thermal Free Energies= -518.722982

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.534	47.424	110.266

C,0,2.0562314234,-0.8341384674,-2.3498227891
O,0,2.7286613326,0.4061597084,-2.4741656537
C,0,2.8263266439,0.9217465195,-3.7356962028
C,0,3.4729797542,2.1813736915,-3.7221539334
N,0,3.8073909481,2.8829435016,-4.8602371409
C,0,4.6775922754,4.0266049027,-4.5686980878
O,0,2.3752718239,0.3058070456,-4.7078170781
C,0,4.288440442,2.1203760863,-6.0194046535
C,0,2.1459508533,3.8135091356,-5.6734184022
C,0,1.5141907307,4.2812295883,-4.5062240298
C,0,0.9210695462,3.4152829918,-3.6374100435
H,0,2.0707044697,-1.0756102683,-1.2928223807
H,0,1.0281333471,-0.7606277306,-2.6979488943
H,0,2.563079461,-1.6141210139,-2.9142986382
H,0,3.6974605392,2.6441013723,-2.7794656866
H,0,5.2856799214,1.7361397345,-5.8092301366
H,0,3.6133543312,1.2959067796,-6.2053758607
H,0,4.3299274535,2.7781636975,-6.8811061874
H,0,5.6383788873,3.6734245838,-4.1975216571
H,0,4.8277681153,4.6044599978,-5.4731742116
H,0,4.2082992147,4.6500536269,-3.8159120456
H,0,2.5969682721,4.5101282547,-6.3654700719
H,0,1.795007477,2.8892884731,-6.1093693893
H,0,1.6946548337,5.3018860171,-4.1924755237
H,0,0.67512946,2.4091485921,-3.9398543473
H,0,0.5756024434,3.7342241793,-2.6649669541

Cation- M06/6-31+G/PCM- Conf2**

/home/bibaswanbiswas/c8/23SMcatUm06pcmdmf
M06/6-31+G**
E(RM06) = -519.181390021

Zero-point correction= 0.239598 (Hartree/Particle)
Thermal correction to Energy= 0.252131
Thermal correction to Enthalpy= 0.253075
Thermal correction to Gibbs Free Energy= 0.201601
Sum of electronic and ZPE= -518.941792
Sum of electronic and thermal Energies= -518.929259
Sum of electronic and thermal Enthalpies= -518.928315
Sum of electronic and thermal Free Energies= -518.979789

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.215	47.047	108.338

C,0,1.8449022255,-0.6202354751,-2.2587965391
O,0,2.653549298,0.5596326055,-2.4164482523
C,0,2.857624907,0.9670456834,-3.6584316879
O,0,2.4207786733,0.4291083116,-4.6513663997
C,0,3.7298770733,2.2021951378,-3.6229354871
N,0,3.7738587923,2.9876199218,-4.8983089406
C,0,4.4871082033,2.2251543877,-5.9774959624
C,0,4.554317142,4.2395541458,-4.6232107253
C,0,1.4967903942,3.9349821651,-4.347557834
C,0,0.3973762362,3.3146767553,-3.9191606785
C,0,2.371657725,3.352501454,-5.4033239894
H,0,1.7950352201,-0.8002957435,-1.1866052159
H,0,0.8466544672,-0.4403973485,-2.6656713981
H,0,2.3095351457,-1.4658326142,-2.7706623205
H,0,4.7567850783,1.9060896296,-3.3796511894
H,0,5.5049191822,2.0197199265,-5.6399798894
H,0,3.9496886874,1.2975544823,-6.1692918168
H,0,4.5101386922,2.8487580723,-6.8731071551
H,0,5.5521526301,3.9593235055,-4.2798093552
H,0,4.6257713577,4.8119159739,-5.5496004358
H,0,4.0510064231,4.826123165,-3.8540617691
H,0,2.5491791786,4.0508354476,-6.2288188021
H,0,1.9436244956,2.4320776298,-5.8065152052
H,0,1.7534193863,4.9189327707,-3.9546863359
H,0,0.1014380287,2.3414406104,-4.31048681
H,0,-0.2530567785,3.7660907643,-3.1754353262
H,0,3.3787311354,2.8610796355,-2.823552479

23TS- UM06/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23TSUm06pcmdmf
experimental system pcm m06 +G**
UM06/6-31+G**
E(UM06) = -518.672218948

Zero-point correction= 0.221418 (Hartree/Particle)
Thermal correction to Energy= 0.234072
Thermal correction to Enthalpy= 0.235017
Thermal correction to Gibbs Free Energy= 0.183563
Sum of electronic and ZPE= -518.450801
Sum of electronic and thermal Energies= -518.438147
Sum of electronic and thermal Enthalpies= -518.437202
Sum of electronic and thermal Free Energies= -518.488656

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.883	47.194	108.292

C,0,1.970228096,-0.746171725,-2.320652426
O,0,2.7138886572,0.4578462826,-2.4575862697
C,0,2.8455666321,0.9308357404,-3.7323189364
C,0,3.4750871328,2.2082126603,-3.7315061733
N,0,3.8255321724,2.8921291851,-4.8748804425

C,0,4.6848178613,4.0477189436,-4.5897630335
O,0,2.422951473,0.289275982,-4.6973658933
C,0,4.3125034756,2.1383997425,-6.0399849742
C,0,2.0899516843,3.8451866391,-5.6893655938
C,0,1.5027604756,4.2015719264,-4.4714539513
C,0,1.0274548926,3.2271183222,-3.6348624496
H,0,1.9503834857,-0.968129213,-1.2527113365
H,0,0.9480044431,-0.6177236985,-2.6934686426
H,0,2.4440512586,-1.5707451583,-2.8626157051
H,0,3.7147174459,2.6699841627,-2.7806019011
H,0,5.3173399979,1.7474151076,-5.8312025334
H,0,3.6363019858,1.3112599221,-6.2516785084
H,0,4.3589887852,2.8154107868,-6.8981176418
H,0,5.6588210654,3.7065763073,-4.2148460994
H,0,4.8306540664,4.6278022282,-5.5045978175
H,0,4.2073777777,4.678309554,-3.8347120819
H,0,2.5283754223,4.5944440246,-6.346482319
H,0,1.7864105014,2.9145992827,-6.1679192638
H,0,1.6720213918,5.2058035996,-4.0797160053
H,0,0.755815771,2.2487220285,-4.0258098728
H,0,0.7342480491,3.4416083664,-2.6098201275

23TS- UM06/6-31+G**/PCM(water)

/home/bibaswanbiswas/c8/Parentcalcs/23TSUm06pcmwater
E(UM06) = -518.672476705

Zero-point correction= 0.221405 (Hartree/Particle)
Thermal correction to Energy= 0.234061
Thermal correction to Enthalpy= 0.235005
Thermal correction to Gibbs Free Energy= 0.183546
Sum of electronic and ZPE= -518.451072
Sum of electronic and thermal Energies= -518.438415
Sum of electronic and thermal Enthalpies= -518.437471
Sum of electronic and thermal Free Energies= -518.488931

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.876	47.199	108.306

C,0,1.9695982163,-0.7456296158,-2.3200625243
O,0,2.7138787945,0.458026488,-2.4576400498
C,0,2.8456119394,0.9308025184,-3.7324546517
C,0,3.4748567005,2.2082544201,-3.7319115827
N,0,3.8260580792,2.8919919096,-4.875004415
C,0,4.6850540651,4.047828855,-4.589717002
O,0,2.4232401792,0.2886829825,-4.6974095327
C,0,4.3129521465,2.1386576628,-6.0403414965
C,0,2.0888615652,3.8458551643,-5.6898126723
C,0,1.5026418738,4.2009711333,-4.4712638065
C,0,1.0280720924,3.2257012984,-3.6349517392
H,0,1.9492396739,-0.9667984534,-1.2519863915
H,0,0.9475357382,-0.6169374533,-2.6932184318
H,0,2.4433635847,-1.5708502445,-2.8610861372
H,0,3.7145771741,2.6699108704,-2.7809550357
H,0,5.3176407955,1.7472479549,-5.8316257564
H,0,3.6365150123,1.3119332834,-6.2527967969
H,0,4.3599499113,2.816046309,-6.8981076807
H,0,5.6592330041,3.706879193,-4.2151066235
H,0,4.8305212448,4.6281405267,-5.5044306738
H,0,4.2075693702,4.6781270889,-3.8344759477
H,0,2.5275237628,4.5954535382,-6.3463272911
H,0,1.7862144645,2.9151140826,-6.1686400452
H,0,1.672315304,5.2048026211,-4.0786978187
H,0,0.7556070662,2.2477520294,-4.0264786104
H,0,0.7356222414,3.4394968371,-2.6095372863

Cation- M052X/6-31+G**/PCM

/home/bibaswanbiswas/c8/Parentcalcs/m052x/m052xsm
sean allyl ester starting material for m05 isotope effects
M052X/6-31+G**
E(RM052X) = -519.458425931

Zero-point correction= 0.244429 (Hartree/Particle)
Thermal correction to Energy= 0.257198
Thermal correction to Enthalpy= 0.258142
Thermal correction to Gibbs Free Energy= 0.205418
Sum of electronic and ZPE= -519.213997
Sum of electronic and thermal Energies= -519.201228
Sum of electronic and thermal Enthalpies= -519.200284
Sum of electronic and thermal Free Energies= -519.253008

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.394	46.517	110.968

C,0,1.8753927368,-0.653356482,-2.262116733
O,0,2.6767889894,0.5449787039,-2.4048214272
C,0,2.8302734595,0.9920222651,-3.6396703478
O,0,2.3491328009,0.4808431155,-4.6262806566
C,0,3.7148547103,2.2236890973,-3.6109402379
N,0,3.7695804993,2.9878272364,-4.8947924428
C,0,4.4782688998,2.2046598567,-5.9610553401
C,0,4.5598708111,4.2352989127,-4.6289714907
C,0,1.499947069,3.9470141828,-4.3501513435
C,0,0.3904728638,3.3291856057,-3.9460576201
C,0,2.3824597572,3.3621705081,-5.4110058485
H,0,1.8880661532,-0.8770341196,-1.2017770858
H,0,0.8643990353,-0.452480746,-2.6082148757
H,0,2.3222353929,-1.458958433,-2.8393002029
H,0,4.7316239643,1.9170587925,-3.3622916506
H,0,5.4904488518,2.0014301033,-5.6199114776
H,0,3.9338930029,1.2829623267,-6.1351936011
H,0,4.5007743534,2.8155189657,-6.8601434295
H,0,5.5430234999,3.9479595132,-4.2642886778
H,0,4.6503681149,4.7843921539,-5.5622165124
H,0,4.0450051088,4.8336595975,-3.8832143747
H,0,2.5659723758,4.0694651792,-6.2202136068
H,0,1.9492889221,2.4527716061,-5.8173098904
H,0,1.7575595144,4.9201196944,-3.9459236071
H,0,0.0994333919,2.3664758427,-4.3527727895
H,0,-0.2611987378,3.7786427279,-3.2077648691
H,0,3.3549274594,2.8893347933,-2.828571861

23TS- M052X/6-31+G**/PCM

/home/bibaswanbiswas/c8/Parentcalcs/m052x/m052xts
sean allyl ester trying to kill m052x
M052X/6-31+G**
E(RM052X) = -518.943406641

Zero-point correction= 0.227481 (Hartree/Particle)
Thermal correction to Energy= 0.239713
Thermal correction to Enthalpy= 0.240657
Thermal correction to Gibbs Free Energy= 0.189859
Sum of electronic and ZPE= -518.715925
Sum of electronic and thermal Energies= -518.703694
Sum of electronic and thermal Enthalpies= -518.702749
Sum of electronic and thermal Free Energies= -518.753548

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.422	45.488	106.914

C,0,2.0214222998,-0.801470997,-2.3436663695
O,0,2.6920040321,0.4592246856,-2.4613388313
C,0,2.7699657924,0.9663735427,-3.7242952189
C,0,3.3442741961,2.2701939876,-3.7241876718
N,0,3.7411570132,2.9195768418,-4.8868343303
C,0,4.6309569671,4.0525916432,-4.5786546222
O,0,2.3202534765,0.3379528755,-4.6871908685
C,0,4.2760879426,2.1201346678,-6.0058787783
C,0,2.1512261715,3.8242141753,-5.6936255173
C,0,1.5332829504,4.2552068717,-4.5079695332
C,0,1.1363014059,3.2610890069,-3.6419244858
H,0,2.0412077778,-1.0429547931,-1.2849102024
H,0,0.9936515017,-0.7206055204,-2.6955861613
H,0,2.5426923356,-1.5662803349,-2.9173733919
H,0,3.6824212148,2.6797841947,-2.7863429004
H,0,5.2570505295,1.7243886643,-5.7348663684
H,0,3.5946863008,1.3061616519,-6.2243960353
H,0,4.371574235,2.7754799723,-6.8710644165
H,0,5.5631239473,3.6804056233,-4.1484891814
H,0,4.8385835963,4.6010428524,-5.4953510396
H,0,4.1321954646,4.7057433756,-3.864886474
H,0,2.593910139,4.5369841137,-6.3821675512
H,0,1.7929387797,2.9053817144,-6.1481182601
H,0,1.7310244274,5.2547601481,-4.1349016844
H,0,0.7878394384,2.3144676581,-4.0377774451
H,0,0.8744220644,3.4776153786,-2.6122436608

Cation M062X/6-31+G**/PCM Conf1

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM1m062x SSpcm
try at new ts's with small basis
m062X/6-31+G**
E(RM062X) = -519.293599561

Zero-point correction= 0.242639 (Hartree/Particle)
Thermal correction to Energy= 0.255413
Thermal correction to Enthalpy= 0.256357
Thermal correction to Gibbs Free Energy= 0.203557
Sum of electronic and ZPE= -519.050961
Sum of electronic and thermal Energies= -519.038186
Sum of electronic and thermal Enthalpies= -519.037242
Sum of electronic and thermal Free Energies= -519.090042

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.274	46.678	111.128

C,0,1.849223013,-0.6188169651,-2.2621308349
O,0,2.6606202547,0.5626727661,-2.4077677231
C,0,2.8234429286,1.0062399898,-3.6431787688
O,0,2.3379450616,0.5038532678,-4.6307662106
C,0,3.728264934,2.2252443523,-3.6144898326
N,0,3.7798387297,2.9935116574,-4.8997112637
C,0,4.4832181769,2.2061944663,-5.9685684755
C,0,4.5685749377,4.2446351055,-4.6367230942
C,0,1.497676587,3.9134462822,-4.3335105962
C,0,0.4007832547,3.2710286601,-3.9320590757
C,0,2.3855731262,3.3664405391,-5.4092690223
H,0,1.8434744057,-0.8343517523,-1.1970046035
H,0,0.8402812973,-0.4164012566,-2.6237104802
H,0,2.2917964463,-1.4420646717,-2.8240002122
H,0,4.745515658,1.9040693351,-3.3753778555
H,0,5.5018987492,2.0079858558,-5.6358763057
H,0,3.9401671153,1.2783279732,-6.1324475844
H,0,4.495741449,2.810415033,-6.8754548565
H,0,5.551809646,3.9627077119,-4.2606424563
H,0,4.666990662,4.7897545742,-5.5743289395
H,0,4.0459267708,4.8505843838,-3.8983638166
H,0,2.5623699749,4.0959254757,-6.2038299793
H,0,1.963114415,2.4603281426,-5.8410394482
H,0,1.7473061035,4.8825532228,-3.9069911153
H,0,0.1178975948,2.3101716648,-4.3563570069
H,0,-0.252243492,3.6958757141,-3.1770532778
H,0,3.3856552185,2.8953194721,-2.8243191645

Cation- M062X/6-31+G**/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM2M062 XSS
parent sm
M062X/6-31+G**
E(RM062X) = -519.292775633

Zero-point correction= 0.243092 (Hartree/Particle)
Thermal correction to Energy= 0.255685
Thermal correction to Enthalpy= 0.256630
Thermal correction to Gibbs Free Energy= 0.204183
Sum of electronic and ZPE= -519.049683
Sum of electronic and thermal Energies= -519.037090
Sum of electronic and thermal Enthalpies= -519.036146
Sum of electronic and thermal Free Energies= -519.088593

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.445	46.378	110.383

C,0,1.9991012581,-0.7446404209,-2.259699165
O,0,2.7746449214,0.4608314914,-2.4080355116
C,0,2.7764752357,1.0065000642,-3.6126826673
O,0,2.1822035176,0.5747384982,-4.5733649137
C,0,3.6397917839,2.2561533747,-3.584392107
N,0,3.7300377836,2.9918314704,-4.8856522347
C,0,4.439955203,2.1636346937,-5.9178217952
C,0,4.5370394966,4.232044221,-4.6275557578
C,0,2.3611652444,3.395750662,-5.4427532979
C,0,1.462128603,4.0088496952,-4.4135005246
C,0,1.1851919223,5.3118105524,-4.3865830858
H,0,2.1220664504,-1.0398098054,-1.2211170058

H,0,0.9524227288,-0.5370376996,-2.4844292693
H,0,2.3829650687,-1.513323233,-2.9311899834
H,0,4.6539311343,1.9758130129,-3.2894278981
H,0,3.2478346394,2.9416301204,-2.829403239
H,0,3.8702886525,1.2534151264,-6.0908343918
H,0,4.5045099774,2.75058318,-6.8338843052
H,0,5.4393070758,1.9341326502,-5.5481511672
H,0,5.5039437003,3.9387332156,-4.2200863163
H,0,4.669180799,4.7562160329,-5.5732038185
H,0,3.9979384042,4.8593576785,-3.9186506606
H,0,2.579477771,4.0993142796,-6.2488226153
H,0,1.9273193218,2.4880766755,-5.8604652531
H,0,0.9839517466,3.3369971895,-3.7033204504
H,0,1.6276870289,6.0008534451,-5.1021136848
H,0,0.498472531,5.724861829,-3.6551818808

TS M062X/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23iparentTSm062xpcmSS
try at new ts's with small basis
m062X/6-31+G**
E(RM062X) = -518.778953134

Zero-point correction= 0.225580 (Hartree/Particle)
Thermal correction to Energy= 0.237903
Thermal correction to Enthalpy= 0.238847
Thermal correction to Gibbs Free Energy= 0.187871
Sum of electronic and ZPE= -518.553373
Sum of electronic and thermal Energies= -518.541050
Sum of electronic and thermal Enthalpies= -518.540106
Sum of electronic and thermal Free Energies= -518.591082

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.286	45.846	107.287

C,0,2.0079655936,-0.7935153283,-2.3536069007
O,0,2.6975626855,0.4497499733,-2.4681593401
C,0,2.7778222507,0.9662920821,-3.7264353507
C,0,3.3727023027,2.2636023109,-3.7181223987
N,0,3.7608795511,2.9160434216,-4.8795746054
C,0,4.635873307,4.0629593683,-4.5812225016
O,0,2.3169154317,0.3566302452,-4.6938582812
C,0,4.2912041559,2.1186818033,-6.0026370172
C,0,2.1363527999,3.8099041901,-5.6957164935
C,0,1.5289269331,4.2407474105,-4.5064796523
C,0,1.126822727,3.2624229175,-3.6269326029
H,0,2.0431572378,-1.0544553011,-1.2969439024
H,0,0.9707950185,-0.6914397995,-2.6824126833
H,0,2.4992479247,-1.5659040525,-2.9495537368
H,0,3.7050144967,2.6764631329,-2.7768767993
H,0,5.2776284891,1.7243438741,-5.7381170746
H,0,3.610329159,1.2997941286,-6.2185802697
H,0,4.380961365,2.7729776131,-6.8722610405
H,0,5.580107906,3.708171632,-4.1558620402
H,0,4.8297675761,4.6153519924,-5.501526219
H,0,4.1319340065,4.7128595861,-3.8637747667
H,0,2.5720906557,4.5224305677,-6.3927925744
H,0,1.7923420512,2.877502255,-6.140222008
H,0,1.7149338327,5.2506948297,-4.1477159113
H,0,0.7912029524,2.301032558,-4.0057355428
H,0,0.8617135905,3.494119589,-2.5989202865

Cation- SOGGA11/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMSOGGA11gasSB
parent sm conf 2
SOGGA11/6-31G*
E(RSOGGA11) = -519.439679577

C,0,1.9798202338,-0.7762095285,-2.2151157052
O,0,2.7012436396,0.4541253901,-2.4094230064
C,0,2.8049988195,0.9064345208,-3.6526952863
O,0,2.3280223489,0.4111642095,-4.6483309619
C,0,3.6741118238,2.1728556777,-3.6024352308
N,0,3.741949616,2.9881076067,-4.8738456249
C,0,4.4274303364,2.216056744,-5.972857282
C,0,4.5616349058,4.2144008088,-4.5739155584
C,0,2.3385523732,3.424649043,-5.3860290314
C,0,1.4815267505,4.1171740421,-4.3803295744
C,0,1.1285978751,5.4017673622,-4.4730298394
H,0,1.9783252877,-0.9482402721,-1.1375477318
H,0,0.9566560721,-0.6839083377,-2.5916467598
H,0,2.4831241533,-1.598479862,-2.733242176
H,0,4.7008419712,1.8877787259,-3.3542242628
H,0,3.3160655034,2.8286588484,-2.8090057388
H,0,3.846796158,1.3225896996,-6.1922948711
H,0,4.4927388035,2.8575083045,-6.8530397177
H,0,5.431270583,1.9489071086,-5.6367165869
H,0,5.537320105,3.9050603396,-4.1952521109
H,0,4.6876263947,4.7815176563,-5.4974539013
H,0,4.0394286412,4.8210611381,-3.8347454116
H,0,2.5488466981,4.0692033288,-6.2411470881
H,0,1.8747456118,2.5024995474,-5.7372046811
H,0,1.0606175198,3.5040745793,-3.5857543603
H,0,1.4890386175,6.047239101,-5.2722683568
H,0,0.437701157,5.8513222178,-3.7627721441

Zero-point correction= 0.238319 (Hartree/Particle)
Thermal correction to Energy= 0.251473
Thermal correction to Enthalpy= 0.252417
Thermal correction to Gibbs Free Energy= 0.198953
Sum of electronic and ZPE= -519.201361
Sum of electronic and thermal Energies= -519.188207
Sum of electronic and thermal Enthalpies= -519.187262
Sum of electronic and thermal Free Energies= -519.240726

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	157.802	48.044	112.524

TS- SOGGA11/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSSOGGA11gasSB
parent ts exo s-cis
SOGGA11/6-31G*
E(RSOGGA11) = -518.995048971

Zero-point correction= 0.221969 (Hartree/Particle)

Thermal correction to Energy= 0.234854
Thermal correction to Enthalpy= 0.235798
Thermal correction to Gibbs Free Energy= 0.183306
Sum of electronic and ZPE= -518.773080
Sum of electronic and thermal Energies= -518.760195
Sum of electronic and thermal Enthalpies= -518.759251
Sum of electronic and thermal Free Energies= -518.811743

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.373	47.269	110.480

C,0,2.0668125601,-0.8699958378,-2.3949887683
O,0,2.8055590313,0.3290931946,-2.4907774755
C,0,2.8735089101,0.8662156656,-3.7581064081
C,0,3.5767088903,2.1038383569,-3.7234236662
N,0,3.8033493162,2.8751101419,-4.8620823723
C,0,4.6479561761,4.0475495586,-4.5570456062
O,0,2.3647409063,0.3044500071,-4.7315973275
C,0,4.3357863934,2.1398937755,-6.0360403834
C,0,2.1899713945,3.6792621873,-5.6084659827
C,0,1.5161777438,4.3001082119,-4.5110203628
C,0,0.8224150887,3.5946490011,-3.5861107169
H,0,2.0854127953,-1.1589960154,-1.3396295487
H,0,1.0273973765,-0.7348254806,-2.7220826024
H,0,2.5043873474,-1.6709008558,-3.0045546317
H,0,3.7723845074,2.5764315677,-2.7745382116
H,0,5.3565996967,1.8135453254,-5.815298802
H,0,3.7015356856,1.2731450533,-6.2079763226
H,0,4.3364364197,2.7999139331,-6.9063937099
H,0,5.6271890004,3.7081298844,-4.2057370523
H,0,4.7661422239,4.6547759786,-5.4561324921
H,0,4.1643840525,4.6379703543,-3.7788518199
H,0,2.5792527864,4.3181698051,-6.3983353189
H,0,1.7814100718,2.7378480939,-5.9632579432
H,0,1.694026347,5.361589017,-4.338810724
H,0,0.6013579429,2.5414882109,-3.7259886299
H,0,0.4133513358,4.0690018654,-2.6967931205

Cation- M11/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMM11gasSB
parent sm conf 2
M11/6-31G*
E(RM11) = -519.142571310

Zero-point correction= 0.241770 (Hartree/Particle)
Thermal correction to Energy= 0.254466
Thermal correction to Enthalpy= 0.255410
Thermal correction to Gibbs Free Energy= 0.202889
Sum of electronic and ZPE= -518.900801
Sum of electronic and thermal Energies= -518.888106
Sum of electronic and thermal Enthalpies= -518.887161
Sum of electronic and thermal Free Energies= -518.939682

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.680	46.631	110.538

C,0,1.9777653427,-0.724564256,-2.2697283594
O,0,2.7644748543,0.4849157165,-2.4058020397
C,0,2.7800558254,1.0284344229,-3.605373081
O,0,2.197323612,0.6111407864,-4.5793859447
C,0,3.6508301703,2.2821720087,-3.5753892338
N,0,3.7392644197,2.9936208194,-4.8916761776
C,0,4.4491430357,2.1453357192,-5.9059859817
C,0,4.5291515871,4.2471006541,-4.6630192358
C,0,2.3607710458,3.3775792004,-5.4519117832
C,0,1.4575323012,3.9676195651,-4.4086456984
C,0,1.2091478735,5.272964765,-4.3272031703
H,0,2.0783060943,-1.021131132,-1.2236455195
H,0,0.9333567333,-0.5116267349,-2.523845206
H,0,2.3739510009,-1.4945506306,-2.941054651
H,0,4.6692052301,2.0075247347,-3.2685419395
H,0,3.2485765464,2.9820484049,-2.8314000884
H,0,3.8873447831,1.2167699119,-6.0414061679
H,0,4.4939226244,2.7045790366,-6.8477003666
H,0,5.4647629868,1.9408712053,-5.5463292408
H,0,5.4964933939,3.985257209,-4.2186481311
H,0,4.6853506927,4.742387762,-5.6282338547
H,0,3.9621839132,4.9001229133,-3.9898238223
H,0,2.5703126184,4.0955819709,-6.2558762662
H,0,1.9396877488,2.4610612708,-5.8759580559
H,0,0.9457579364,3.2665942988,-3.7431522247
H,0,1.6702062376,5.9896337601,-5.0128104685
H,0,0.5141533917,5.6758746174,-3.5897762916

TS- M11/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSM11gasSB
parent ts exo s-cis
M11/6-31G*
E(RM11) = -518.681738827

Zero-point correction= 0.225643 (Hartree/Particle)
Thermal correction to Energy= 0.237656
Thermal correction to Enthalpy= 0.238600
Thermal correction to Gibbs Free Energy= 0.188571
Sum of electronic and ZPE= -518.456096
Sum of electronic and thermal Energies= -518.444083
Sum of electronic and thermal Enthalpies= -518.443139
Sum of electronic and thermal Free Energies= -518.493167

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.131	45.275	105.293

C,0,1.9891134653,-0.8093901821,-2.4488932146
O,0,2.7070229288,0.4200475128,-2.4866945061
C,0,2.765405726,0.9995430201,-3.7156832699
C,0,3.3875988892,2.2833395402,-3.6771745216
N,0,3.7481725741,2.921696739,-4.864553138
C,0,4.5868813635,4.0965560758,-4.5906438888
O,0,2.2461124317,0.4672150204,-4.6972788123
C,0,4.311828711,2.1035493414,-5.9559156176
C,0,2.1518926684,3.6950105842,-5.6691014682
C,0,1.5487853978,4.2469954885,-4.5225144534
C,0,1.1950642762,3.3349593906,-3.5594354206
H,0,2.0138825675,-1.1425089673,-1.4060518138
H,0,0.9523946859,-0.6648980083,-2.781793654
H,0,2.4611112764,-1.5551415419,-3.1022938667
H,0,3.8010437438,2.6572188581,-2.7468082112

H,0,5.3318486052,1.7874184157,-5.6924014585
H,0,3.6723294771,1.2300130511,-6.1046590573
H,0,4.3407826217,2.7152588416,-6.8685939124
H,0,5.5400617114,3.7785560409,-4.1429106453
H,0,4.7777456351,4.6354044452,-5.5273922923
H,0,4.0502124445,4.7488890899,-3.891114336
H,0,2.5444667778,4.340470511,-6.4621241519
H,0,1.7790684728,2.7240293595,-6.0137324483
H,0,1.7225607029,5.2942802939,-4.2640794072
H,0,0.8393544739,2.3490592398,-3.8625225706
H,0,0.9495123722,3.6398888401,-2.5396738631

Cation- SOGGA11X/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMSOGGA11XgasSB
parent sm conf 2
SOGGA11X/6-31G*
E(RSOGGA11X) = -519.282912340

Zero-point correction= 0.246556 (Hartree/Particle)
Thermal correction to Energy= 0.259214
Thermal correction to Enthalpy= 0.260159
Thermal correction to Gibbs Free Energy= 0.207596
Sum of electronic and ZPE= -519.036356
Sum of electronic and thermal Energies= -519.023698
Sum of electronic and thermal Enthalpies= -519.022754
Sum of electronic and thermal Free Energies= -519.075316

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.660	46.153	110.628

C,0,2.0346290851,-0.8052187547,-2.2744266965
O,0,2.7798372036,0.4271214551,-2.4180481469
C,0,2.783383088,0.9695801425,-3.6180540196
O,0,2.2211340968,0.5441651978,-4.598339211
C,0,3.6267510831,2.2415403963,-3.5671917205
N,0,3.7201950627,2.9909512364,-4.8641618568
C,0,4.4145260975,2.161008048,-5.9049953949
C,0,4.5351958172,4.2223575564,-4.6089408928
C,0,2.3413290031,3.4024544034,-5.4074555797
C,0,1.4761337744,4.0946492165,-4.4000964787
C,0,1.192153366,5.3967875287,-4.4575718715
H,0,2.1563386387,-1.0862445989,-1.2309185839
H,0,0.985214809,-0.6313809143,-2.5149498917
H,0,2.4496266477,-1.565370226,-2.937246478
H,0,4.6434020769,1.9816957645,-3.2589329609
H,0,3.2155630252,2.9167622552,-2.8132524146
H,0,3.8334823429,1.2575235556,-6.0793081771
H,0,4.4870539979,2.749960652,-6.8204886154
H,0,5.4156608138,1.9143374003,-5.5462133974
H,0,5.5049290463,3.9302699871,-4.2027160911
H,0,4.6753517609,4.7487851157,-5.5542433955
H,0,4.0033993626,4.8607273357,-3.9031335815
H,0,2.5564218572,4.0512096541,-6.2603115065
H,0,1.8810957098,2.479219093,-5.760363031
H,0,0.9990250355,3.472014199,-3.645143831
H,0,1.6078749826,6.0455647463,-5.2256769479
H,0,0.509324215,5.8568475542,-3.7501422279

TS- SOGGA11X/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSSOGGA11XgasSB
parent ts exo s-cis
SOGGA11X/6-31G*
E(RSOGGA11X) = -518.818183233

Zero-point correction= 0.229415 (Hartree/Particle)
Thermal correction to Energy= 0.241663
Thermal correction to Enthalpy= 0.242607
Thermal correction to Gibbs Free Energy= 0.191836
Sum of electronic and ZPE= -518.588768
Sum of electronic and thermal Energies= -518.576520
Sum of electronic and thermal Enthalpies= -518.575576
Sum of electronic and thermal Free Energies= -518.626347

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.646	45.392	106.857

C,0,2.0337956752,-0.8187408272,-2.3949807224
O,0,2.7180805973,0.4236866169,-2.4739637608
C,0,2.773443403,0.9659157892,-3.7215106847
C,0,3.4063919793,2.2454924329,-3.6981029262
N,0,3.7645657372,2.9103700611,-4.8651545267
C,0,4.6379809469,4.0537689972,-4.5789114214
O,0,2.2807844988,0.3956795036,-4.69325368
C,0,4.2907408998,2.1019757374,-5.9793170045
C,0,2.1477188206,3.7859572252,-5.686533522
C,0,1.5265065228,4.2673873471,-4.5177777758
C,0,1.076673442,3.3466883371,-3.6097101842
H,0,2.0716764058,-1.1070857628,-1.3432247689
H,0,0.9950507205,-0.7198215734,-2.7225121952
H,0,2.5220269049,-1.5773289759,-3.0129346484
H,0,3.7415074933,2.6610344708,-2.7596500419
H,0,5.2991249677,1.7477658166,-5.7356020282
H,0,3.6299508578,1.2523574658,-6.1390331721
H,0,4.3310371666,2.7278634638,-6.8757105221
H,0,5.582805209,3.707154576,-4.1444599574
H,0,4.8388529528,4.5991286422,-5.5039700156
H,0,4.1337230432,4.7147805558,-3.8708055681
H,0,2.5638686248,4.4797492496,-6.4155815945
H,0,1.790135353,2.8466999687,-6.1026417233
H,0,1.6984491657,5.297389436,-4.2085335832
H,0,0.7771653502,2.3568544215,-3.9368977865
H,0,0.7821972621,3.6327380251,-2.6032661855

Cation- M11L/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMM11LgasSB
parent sm conf 2
M11L/6-31G*
E(RM11L) = -519.255175775

Zero-point correction= 0.235966 (Hartree/Particle)
Thermal correction to Energy= 0.249184
Thermal correction to Enthalpy= 0.250128
Thermal correction to Gibbs Free Energy= 0.195337
Sum of electronic and ZPE= -519.019210
Sum of electronic and thermal Energies= -519.005991
Sum of electronic and thermal Enthalpies= -519.005047

Sum of electronic and thermal Free Energies= -519.059839

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.366	47.624	115.319

C,0,2.0249147956,-0.7192511392,-2.300208613
O,0,2.7830186235,0.4827623455,-2.4221330613
C,0,2.7835477207,1.007634739,-3.6116546375
O,0,2.2161253562,0.5894905091,-4.5754859232
C,0,3.633177064,2.2599182229,-3.5752519294
N,0,3.7207070389,2.979459038,-4.867257703
C,0,4.4075019531,2.1567610104,-5.8852386471
C,0,4.5172082092,4.1998834618,-4.6280670379
C,0,2.3595395452,3.3816085125,-5.409560424
C,0,1.4822239535,4.0181077826,-4.3996037916
C,0,1.2051102439,5.315454341,-4.3986103643
H,0,2.149706884,-1.0318233023,-1.2590035086
H,0,0.9676862451,-0.5224064929,-2.5265731952
H,0,2.4139315682,-1.4821342216,-2.9884588403
H,0,4.6592027506,2.0032521956,-3.2630047457
H,0,3.2370436649,2.958675112,-2.820321011
H,0,3.8348381228,1.2382766831,-6.0603969479
H,0,4.4735419438,2.7384503028,-6.8150093297
H,0,5.4211089847,1.9193348446,-5.5325203503
H,0,5.4949821761,3.920236815,-4.2117441472
H,0,4.6621624918,4.724563835,-5.5825479297
H,0,3.9810527841,4.8510339901,-3.9237934385
H,0,2.5817914243,4.0686418923,-6.2439053264
H,0,1.9157819206,2.4613828366,-5.8176175697
H,0,0.9770031942,3.3536359843,-3.6853427584
H,0,1.6444746864,6.0014659965,-5.1339984131
H,0,0.5016486542,5.7529027051,-3.6850133562

TS- M11L/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSM11LgasSB
parent ts exo s-cis
M11L/6-31G*
E(RM11L) = -518.813902185

Zero-point correction= 0.219337 (Hartree/Particle)
Thermal correction to Energy= 0.232165
Thermal correction to Enthalpy= 0.233109
Thermal correction to Gibbs Free Energy= 0.181072
Sum of electronic and ZPE= -518.594565
Sum of electronic and thermal Energies= -518.581737
Sum of electronic and thermal Enthalpies= -518.580793
Sum of electronic and thermal Free Energies= -518.632830

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.686	47.472	109.521

C,0,2.0005719324,-0.7485365973,-2.4426445577
O,0,2.742958879,0.4319150475,-2.4901268005
C,0,2.8420877931,0.9494421424,-3.7263555714
C,0,3.5623865725,2.1730797313,-3.6975902581
N,0,3.8367406597,2.8657306597,-4.8363407126
C,0,4.6381675029,4.0372883549,-4.5802791724
O,0,2.349549803,0.4014241047,-4.6902734874
C,0,4.3260254718,2.1167975711,-5.9766336208
C,0,2.1139310834,3.7163874351,-5.6644085453
C,0,1.5289998968,4.2110635575,-4.492862903
C,0,1.0094709782,3.3697748706,-3.5658674332
H,0,2.0094864201,-1.0665215251,-1.3909913357
H,0,0.961693272,-0.5878204298,-2.7783806163
H,0,2.4439086491,-1.533643631,-3.0775203529
H,0,3.7560864057,2.6690506336,-2.7483698432
H,0,5.3564892449,1.7668468572,-5.7809278421
H,0,3.6737773083,1.2537186896,-6.1533665782
H,0,4.3272495644,2.7761072388,-6.8591994662
H,0,5.632658852,3.7493229201,-4.1921300074
H,0,4.7626493405,4.6129316609,-5.5094675658
H,0,4.1302671163,4.6651300519,-3.8323630904
H,0,2.4955567164,4.4040818315,-6.4302352538
H,0,1.7758408228,2.7414356712,-6.0383592099
H,0,1.698354791,5.264529982,-4.2255532245
H,0,0.7545099446,2.3389365408,-3.8330279672
H,0,0.6848349794,3.718987631,-2.5807645839

Cation- MN12L/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMMN12LgasSB
parent sm conf 2
MN12L/6-31G*
E(RMN12L) = -518.878893022

Zero-point correction= 0.243781 (Hartree/Particle)
Thermal correction to Energy= 0.256324
Thermal correction to Enthalpy= 0.257269
Thermal correction to Gibbs Free Energy= 0.205211
Sum of electronic and ZPE= -518.635112
Sum of electronic and thermal Energies= -518.622569
Sum of electronic and thermal Enthalpies= -518.621624
Sum of electronic and thermal Free Energies= -518.673682

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.846	46.202	109.565

C,0,1.982134696,-0.6898426066,-2.2606374093
O,0,2.7814197438,0.4950011646,-2.4133649704
C,0,2.7647421192,1.0483673982,-3.6011724494
O,0,2.1457677112,0.6593302107,-4.5600651829
C,0,3.6466517985,2.2822574125,-3.5814425652
N,0,3.7410069395,2.9866473258,-4.8983366183
C,0,4.450049639,2.1414510338,-5.906332346
C,0,4.5349044362,4.2302470095,-4.6641876294
C,0,2.3708407484,3.3916277727,-5.4734184211
C,0,1.4488009829,3.9285191179,-4.4317097179
C,0,1.1950508761,5.2283637095,-4.2949113784
H,0,2.1124466052,-0.9940357112,-1.2236706304
H,0,0.9353355799,-0.4602190776,-2.4750099681
H,0,2.3356979391,-1.4645650755,-2.9455666334
H,0,4.6644488956,2.009725848,-3.2756374682
H,0,3.2618861105,2.9964354257,-2.8426727816
H,0,3.8919387791,1.2146987444,-6.050977395
H,0,4.4992227879,2.7007813353,-6.8451846103
H,0,5.4627214551,1.9358506377,-5.5463732593
H,0,5.4897009942,3.9648963616,-4.2009996046

H,0,4.7131680133,4.7186255415,-5.6262298907
H,0,3.9636290097,4.8915369341,-4.0051979295
H,0,2.6056230976,4.1445481356,-6.2362826087
H,0,1.9691149074,2.4962628402,-5.9542118535
H,0,0.930323994,3.1936420422,-3.8122501762
H,0,1.6660377387,5.9748886034,-4.936758713
H,0,0.4863664016,5.6022758659,-3.5597207896

TS- MN12L/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSMN12LgasSB
parent ts exo s-cis
MN12L/6-31G*
E(RMN12L) = -518.430596673

Zero-point correction= 0.225642 (Hartree/Particle)
Thermal correction to Energy= 0.238139
Thermal correction to Enthalpy= 0.239083
Thermal correction to Gibbs Free Energy= 0.187929
Sum of electronic and ZPE= -518.204955
Sum of electronic and thermal Energies= -518.192458
Sum of electronic and thermal Enthalpies= -518.191514
Sum of electronic and thermal Free Energies= -518.242668

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.434	46.378	107.663

C,0,1.9478226148,-0.7680069572,-2.4484615478
O,0,2.7271891489,0.407736052,-2.4937929803
C,0,2.8308958241,0.9656074106,-3.7228223348
C,0,3.569497527,2.1782221256,-3.6837587388
N,0,3.8579146469,2.869804375,-4.8375990226
C,0,4.6241725409,4.0819853814,-4.5822755942
O,0,2.3019736506,0.4555964719,-4.7071366689
C,0,4.3643466891,2.1245989844,-5.9917725842
C,0,2.078862244,3.6752397134,-5.6749358345
C,0,1.5331491583,4.2027144903,-4.4981659585
C,0,1.0627783473,3.3637568485,-3.5299113797
H,0,1.9563689,-1.0925457019,-1.4058044224
H,0,0.9196199243,-0.5744343671,-2.7769294217
H,0,2.3699774433,-1.54722473,-3.0933971624
H,0,3.8265330922,2.6396618578,-2.7378888254
H,0,5.3998473641,1.8048350325,-5.8036405319
H,0,3.7319322879,1.2521431756,-6.1627031884
H,0,4.3414215554,2.7843177103,-6.8674562051
H,0,5.621556246,3.8322755214,-4.1905390956
H,0,4.7284219047,4.6501346646,-5.5123900345
H,0,4.0870533912,4.6869934679,-3.8436719635
H,0,2.4710371565,4.3216841523,-6.460995412
H,0,1.7839012825,2.6706754247,-5.982544383
H,0,1.6949138813,5.2582295,-4.2675626212
H,0,0.8060203073,2.3352026433,-3.7761457009
H,0,0.7770468718,3.7182577527,-2.5417383875

Cation- N12/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMN12gasSB
parent sm conf 2
N12/6-31G*
E(RN12) = -519.298176840

Zero-point correction= 0.241070 (Hartree/Particle)
Thermal correction to Energy= 0.253204
Thermal correction to Enthalpy= 0.254148
Thermal correction to Gibbs Free Energy= 0.202914
Sum of electronic and ZPE= -519.057107
Sum of electronic and thermal Energies= -519.044973
Sum of electronic and thermal Enthalpies= -519.044028
Sum of electronic and thermal Free Energies= -519.095263

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.888	45.268	107.831

C,0,2.059856015,-0.8262562526,-2.2923624338
O,0,2.7934728317,0.4010963822,-2.4373966514
C,0,2.7878456781,0.9628714489,-3.6246860965
O,0,2.2228646096,0.5465605028,-4.6079118481
C,0,3.6166863846,2.237734902,-3.5589343712
N,0,3.7163160055,2.9898559463,-4.8493959032
C,0,4.4008880016,2.1611747867,-5.8894396309
C,0,4.5267611147,4.2166820338,-4.5940611027
C,0,2.3312228264,3.4022100176,-5.3849391727
C,0,1.4932104758,4.1321874268,-4.3989768129
C,0,1.2010091727,5.4283504441,-4.5048925767
H,0,2.2277134011,-1.1415052139,-1.2706231515
H,0,1.0046247544,-0.6462022764,-2.4748394882
H,0,2.4334735551,-1.5645816117,-2.9952394849
H,0,4.6276816917,1.9936291123,-3.2406005433
H,0,3.1941282197,2.90769644,-2.8149807181
H,0,3.8122473911,1.2693091357,-6.0619881038
H,0,4.4776977498,2.7488796157,-6.7979912786
H,0,5.3936180237,1.9050989379,-5.5324763091
H,0,5.4880065936,3.9287702755,-4.1810274254
H,0,4.6721701779,4.7370413664,-5.5349528914
H,0,3.9894591887,4.853587062,-3.900257469
H,0,2.5439041612,4.0106944055,-6.2597477656
H,0,1.8678519889,2.4701198896,-5.6929422745
H,0,1.0380318972,3.5457460782,-3.610771825
H,0,1.5936270266,6.0433267043,-5.3041579261
H,0,0.5346630633,5.9132404402,-3.8067297458

TS- N12/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSN12gasSB
parent ts exo s-cis
N12/6-31G*
E(RN12) = -518.850311079

Zero-point correction= 0.223991 (Hartree/Particle)
Thermal correction to Energy= 0.236726
Thermal correction to Enthalpy= 0.237670
Thermal correction to Gibbs Free Energy= 0.185716
Sum of electronic and ZPE= -518.626320
Sum of electronic and thermal Energies= -518.613585
Sum of electronic and thermal Enthalpies= -518.612641
Sum of electronic and thermal Free Energies= -518.664596

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 148.548 46.890 109.348

C,0,2.0432916881,-0.8451035306,-2.4454135796
O,0,2.7402871057,0.3787150029,-2.4998686936
C,0,2.8189259179,0.9465613132,-3.7346546297
C,0,3.5146914936,2.1789017487,-3.693552363
N,0,3.7927970122,2.8903745549,-4.8492593075
C,0,4.62799759,4.0589385695,-4.5724749815
O,0,2.3120175886,0.4102621972,-4.7207350884
C,0,4.314306732,2.110305683,-5.9810457707
C,0,2.1651498674,3.6863875275,-5.6392528991
C,0,1.5341870422,4.2777095948,-4.5207485308
C,0,0.9708551756,3.4985970545,-3.5631162237
H,0,2.0634967121,-1.1539618195,-1.4044854617
H,0,1.0132621228,-0.7328769916,-2.7819753982
H,0,2.5210454435,-1.600325607,-3.0687922825
H,0,3.771408036,2.6328425939,-2.7551804899
H,0,5.3295602305,1.784347169,-5.7575373483
H,0,3.6718846435,1.2484563379,-6.1196997601
H,0,4.31719364,2.7346765504,-6.8711639953
H,0,5.5866011554,3.7393237887,-4.1652822987
H,0,4.7862602532,4.617719147,-5.4900439568
H,0,4.1180661133,4.6877361163,-3.8490770482
H,0,2.5524482335,4.3176097252,-6.4294464613
H,0,1.7909162015,2.7267941379,-5.9699187188
H,0,1.691256693,5.3327431922,-4.3289346834
H,0,0.7405085037,2.4629882055,-3.758415575
H,0,0.6258388048,3.9077387386,-2.6239644539

Cation- N12SX/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMN12SXgasSB
parent sm conf 2
N12SX/6-31G*
E(RN12SX) = -519.152815042

Zero-point correction= 0.245562 (Hartree/Particle)
Thermal correction to Energy= 0.258294
Thermal correction to Enthalpy= 0.259239
Thermal correction to Gibbs Free Energy= 0.206509
Sum of electronic and ZPE= -518.907253
Sum of electronic and thermal Energies= -518.894521
Sum of electronic and thermal Enthalpies= -518.893576
Sum of electronic and thermal Free Energies= -518.946306

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.082	46.416	110.978

C,0,2.0425604974,-0.8052785082,-2.2769344952
O,0,2.7756716394,0.4215287286,-2.4312262312
C,0,2.7867889466,0.9686901233,-3.6252396823
O,0,2.2304965601,0.5422448947,-4.607373687
C,0,3.6227705187,2.2370744476,-3.570254777
N,0,3.7177972538,2.9897075073,-4.8600894305
C,0,4.40835375,2.1665991074,-5.9020847652
C,0,4.5279014626,4.2180131072,-4.6020443805
C,0,2.3393573086,3.4011882712,-5.3973045127
C,0,1.4872588232,4.1049764716,-4.3983032405
C,0,1.2002367547,5.4022303214,-4.4710387085
H,0,2.1613041348,-1.0846822231,-1.2370119741
H,0,0.9956035607,-0.6422729071,-2.5182322305
H,0,2.4560408762,-1.56638468,-2.9331678538
H,0,4.6346304492,1.981224154,-3.2594474605
H,0,3.2103243184,2.9061452076,-2.8182950918
H,0,3.8291485205,1.2680233026,-6.0788892505
H,0,4.4807012595,2.7553160812,-6.812034935
H,0,5.4052762064,1.9173118696,-5.5478944
H,0,5.4931443033,3.9297025897,-4.1950692804
H,0,4.6695446023,4.7446828933,-5.5415127561
H,0,3.9949234873,4.8527932209,-3.9010584775
H,0,2.5499158722,4.0347556145,-6.2563532469
H,0,1.8763257664,2.4785210209,-5.7346305655
H,0,1.0227834093,3.4963083365,-3.6309479259
H,0,1.6033546366,6.0387448183,-5.2494766343
H,0,0.5268170816,5.8701542291,-3.7664070069

TS- N12SX/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSN12SXgasSB
parent ts exo s-cis
N12SX/6-31G*
E(RN12SX) = -518.693748885

Zero-point correction= 0.228453 (Hartree/Particle)
Thermal correction to Energy= 0.240818
Thermal correction to Enthalpy= 0.241762
Thermal correction to Gibbs Free Energy= 0.190717
Sum of electronic and ZPE= -518.465296
Sum of electronic and thermal Energies= -518.452931
Sum of electronic and thermal Enthalpies= -518.451987
Sum of electronic and thermal Free Energies= -518.503031

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.116	45.706	107.433

C,0,2.0342013524,-0.8156767844,-2.4030759169
O,0,2.7174901676,0.4176494315,-2.485695148
C,0,2.7817290626,0.9673869813,-3.7258277046
C,0,3.4226632692,2.2342488281,-3.700232991
N,0,3.7703428624,2.9063045649,-4.8614357202
C,0,4.6304689721,4.0549899545,-4.5788061692
O,0,2.2883260217,0.4036060082,-4.7006734088
C,0,4.2890531059,2.106025795,-5.9791414569
C,0,2.1602709532,3.7657018984,-5.6731762803
C,0,1.5370316123,4.2622972939,-4.5153440952
C,0,1.0648295368,3.3666961502,-3.6029522552
H,0,2.0652786412,-1.107598369,-1.3566637341
H,0,1.0003554722,-0.717535903,-2.7335169848
H,0,2.5167739039,-1.5749786129,-3.0179075582
H,0,3.7426376356,2.6542111971,-2.7638257399
H,0,5.2981613676,1.7622881424,-5.7462260915
H,0,3.6363158683,1.2531190473,-6.1262210249
H,0,4.3136991406,2.7250100126,-6.8746084716
H,0,5.575247152,3.7174136863,-4.1497263248
H,0,4.8234486717,4.6015270832,-5.4988817438
H,0,4.1249279567,4.7072851555,-3.8711735794
H,0,2.5733712232,4.4466529114,-6.4087858767
H,0,1.8004055985,2.8270610359,-6.0760828292
H,0,1.7015125101,5.2943907972,-4.2258204037

H,0,0.7835659699,2.369855645,-3.9092442086
H,0,0.7621459725,3.6695290497,-2.6089942825

Cation- MN12SX/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMMN12SXgasSB
parent sm conf 2
MN12SX/6-31G*
E(RMN12SX) = -518.982546949

Zero-point correction= 0.243079 (Hartree/Particle)
Thermal correction to Energy= 0.255846
Thermal correction to Enthalpy= 0.256790
Thermal correction to Gibbs Free Energy= 0.203916
Sum of electronic and ZPE= -518.739468
Sum of electronic and thermal Energies= -518.726701
Sum of electronic and thermal Enthalpies= -518.725757
Sum of electronic and thermal Free Energies= -518.778631

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.546	46.628	111.283

C,0,1.9988732249,-0.7305065565,-2.2600201146
O,0,2.771498644,0.4737052925,-2.4119993288
C,0,2.7743736917,1.0122810745,-3.6105058473
O,0,2.1878656314,0.5981585411,-4.5802953329
C,0,3.6413666086,2.2626871745,-3.5803765591
N,0,3.7338020949,2.9878940953,-4.8871157883
C,0,4.4374836103,2.1533149433,-5.9117573479
C,0,4.5363126396,4.2261305113,-4.6414857312
C,0,2.3612299291,3.3956450148,-5.4452497141
C,0,1.45926989,3.9938279471,-4.4156552435
C,0,1.1904278466,5.2962012901,-4.357553421
H,0,2.1174369565,-1.0189807117,-1.2140955523
H,0,0.9481160247,-0.5306084736,-2.4958878629
H,0,2.386498369,-1.5071144994,-2.9279663095
H,0,4.6603147109,1.9903056714,-3.2735589017
H,0,3.2471302011,2.9588065948,-2.8283981335
H,0,3.8689299849,1.2349743651,-6.080024512
H,0,4.5018640198,2.7317417363,-6.8395905556
H,0,5.4464278925,1.9253735656,-5.5506472645
H,0,5.5036257273,3.9479854786,-4.2094599377
H,0,4.6930088576,4.7390711657,-5.5961678777
H,0,3.9858710098,4.8757423611,-3.9526735908
H,0,2.5860999065,4.1100562309,-6.2481154371
H,0,1.9302749552,2.4879381432,-5.880609699
H,0,0.9532915171,3.2990237591,-3.740045468
H,0,1.6412281477,6.0104645992,-5.0507844263
H,0,0.4864099079,5.7031986853,-3.6322830433

TS- MN12SX/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSMN12SXgasSB
parent ts exo s-cis
MN12SX/6-31G*
E(RMN12SX) = -518.531483626

Zero-point correction= 0.225892 (Hartree/Particle)
Thermal correction to Energy= 0.238352
Thermal correction to Enthalpy= 0.239297
Thermal correction to Gibbs Free Energy= 0.188205
Sum of electronic and ZPE= -518.305591
Sum of electronic and thermal Energies= -518.293131
Sum of electronic and thermal Enthalpies= -518.292187
Sum of electronic and thermal Free Energies= -518.343279

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.568	46.295	107.532

C,0,1.9726834518,-0.7773424101,-2.4245075482
O,0,2.7166557363,0.4221360397,-2.4852083679
C,0,2.8093143302,0.9686307902,-3.7246066717
C,0,3.5056606665,2.2085097573,-3.6936803286
N,0,3.820737446,2.8879819157,-4.8521859064
C,0,4.6306943811,4.0742789889,-4.5860776173
O,0,2.2979154396,0.4295420185,-4.7038338531
C,0,4.3396305043,2.1187458941,-5.9895327473
C,0,2.1058275696,3.7170551612,-5.6771827594
C,0,1.5309037527,4.215593553,-4.4984708419
C,0,1.0751224359,3.338370215,-3.5576454418
H,0,1.9901522475,-1.0878662433,-1.3750583839
H,0,0.9368718247,-0.620709321,-2.7544939029
H,0,2.4199570187,-1.5553362332,-3.0568979214
H,0,3.7937572798,2.6504730858,-2.7473018634
H,0,5.3662885708,1.7856359095,-5.7749942323
H,0,3.6983760993,1.2516593305,-6.1626710079
H,0,4.3466822454,2.7660106268,-6.8757018649
H,0,5.6116490023,3.7843764261,-4.179632822
H,0,4.7733810988,4.6380483254,-5.5149941964
H,0,4.1095964325,4.7038062628,-3.8554842692
H,0,2.4984841628,4.3917525279,-6.4410687205
H,0,1.7812845848,2.7379872308,-6.0374213772
H,0,1.6952030325,5.2624052181,-4.2297838042
H,0,0.7945877496,2.3245715378,-3.8401564277
H,0,0.7928369367,3.6611443929,-2.5554471221

Cation- APFD/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMAPFDgasSB
parent sm conf 2
APFD/6-31G*
E(RAPFD) = -519.013400141

Zero-point correction= 0.242905 (Hartree/Particle)
Thermal correction to Energy= 0.255680
Thermal correction to Enthalpy= 0.256624
Thermal correction to Gibbs Free Energy= 0.203691
Sum of electronic and ZPE= -518.770496
Sum of electronic and thermal Energies= -518.757720
Sum of electronic and thermal Enthalpies= -518.756776
Sum of electronic and thermal Free Energies= -518.809709

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.442	46.721	111.407

C,0,2.0028096039,-0.7579125726,-2.2619185322
O,0,2.7603587791,0.4632020043,-2.4162455456

C,0,2.7814091688,0.9845453544,-3.6278764353
O,0,2.2243469114,0.5511981515,-4.6111524054
C,0,3.6394540636,2.2468650025,-3.5829164071
N,0,3.7310386336,2.9917105354,-4.8811400198
C,0,4.4338062747,2.166178101,-5.9144079196
C,0,4.5255772785,4.2326999792,-4.6263395243
C,0,2.3478707997,3.3889209554,-5.4252883833
C,0,1.46762644,4.0318123241,-4.4039247237
C,0,1.209095971,5.3404113688,-4.3911779487
H,0,2.1094193454,-1.0273131388,-1.2133331446
H,0,0.9563104665,-0.5799938579,-2.5165562483
H,0,2.4146420213,-1.5338731464,-2.9098979408
H,0,4.6563985044,1.9808971814,-3.2798347384
H,0,3.2379070529,2.9309169026,-2.8310324275
H,0,3.8745514656,1.2448743635,-6.0672911412
H,0,4.4801146622,2.7402879783,-6.8410143846
H,0,5.4448562406,1.9509435322,-5.5636323562
H,0,5.4880401968,3.9595136035,-4.1908958582
H,0,4.6835576703,4.7469831526,-5.5754653531
H,0,3.9659466567,4.8742082667,-3.9447142233
H,0,2.5573080645,4.063118037,-6.2599547591
H,0,1.9100098486,2.4657368777,-5.806549687
H,0,0.9733685399,3.3714318976,-3.6924462413
H,0,1.6499418317,6.0223583055,-5.1162701516
H,0,0.5232655079,5.7775968403,-3.6710465001

TS- APFD/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSAPFDgasSB
parent ts exo s-cis
APFD/6-31G*
E(RAPFD) = -518.557977027

Zero-point correction= 0.225785 (Hartree/Particle)
Thermal correction to Energy= 0.238257
Thermal correction to Enthalpy= 0.239201
Thermal correction to Gibbs Free Energy= 0.187940
Sum of electronic and ZPE= -518.332192
Sum of electronic and thermal Energies= -518.319720
Sum of electronic and thermal Enthalpies= -518.318776
Sum of electronic and thermal Free Energies= -518.370037

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.508	46.168	107.888

C,0,1.9937289045,-0.8020044167,-2.4291077463
O,0,2.730001606,0.4091235159,-2.490541345
C,0,2.8010410311,0.9681860397,-3.7338620599
C,0,3.483428446,2.2139905361,-3.6963200822
N,0,3.7891938175,2.902452745,-4.8615945172
C,0,4.6247519225,4.0741334529,-4.5835182219
O,0,2.2850676704,0.4367967457,-4.7201842394
C,0,4.3277308793,2.1152582729,-5.9832572318
C,0,2.1416049357,3.707520644,-5.6634083882
C,0,1.5287765357,4.2402313405,-4.5076307153
C,0,1.0672342554,3.3741322208,-3.5600127737
H,0,2.0288149283,-1.1166398442,-1.3845637083
H,0,0.955214864,-0.6528735846,-2.7427419856
H,0,2.4383568592,-1.5700981119,-3.0699169686
H,0,3.7882668961,2.6478031367,-2.7557179326
H,0,5.349508428,1.7972716314,-5.7481842925
H,0,3.6918729659,1.2437924058,-6.1299061051
H,0,4.332997185,2.7387005427,-6.8818152713
H,0,5.5849078712,3.7560638818,-4.1620234374
H,0,4.7942747803,4.629331006,-5.5086115034
H,0,4.1041126913,4.7127929495,-3.8671037246
H,0,2.5281912802,4.3716465983,-6.4355923111
H,0,1.784992369,2.7452624533,-6.0255997171
H,0,1.6851457731,5.2897273208,-4.2580546778
H,0,0.8039093523,2.3559138448,-3.825891861
H,0,0.7711277521,3.7089456728,-2.5688791825

Cation- B3LYPGD2/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMB3LYPGD2
gasSB
parent sm conf 2
B3LYP/6-31G*
E(RB3LYP) = -519.469063285

Zero-point correction= 0.241552 (Hartree/Particle)
Thermal correction to Energy= 0.254302
Thermal correction to Enthalpy= 0.255247
Thermal correction to Gibbs Free Energy= 0.202380
Sum of electronic and ZPE= -519.227512
Sum of electronic and thermal Energies= -519.214761
Sum of electronic and thermal Enthalpies= -519.213817
Sum of electronic and thermal Free Energies= -519.266683

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.577	46.829	111.267

C,0,2.0120125523,-0.795658184,-2.2551387652
O,0,2.7660835457,0.4423961786,-2.4085147979
C,0,2.7805059796,0.9723774595,-3.6214478802
O,0,2.2223442461,0.5353866401,-4.6051757308
C,0,3.629536459,2.2451117016,-3.5723325053
N,0,3.7243172827,2.9931565026,-4.8781997381
C,0,4.4355366868,2.164726503,-5.9176363181
C,0,4.5253941253,4.2413702177,-4.6212595586
C,0,2.3334138209,3.3949467721,-5.4314836681
C,0,1.4667659089,4.0598441364,-4.4082461922
C,0,1.2145591692,5.3707201481,-4.4161492273
H,0,2.1250810206,-1.065377556,-1.2058834009
H,0,0.9645973227,-0.6186678448,-2.5111421068
H,0,2.4321578927,-1.5614798409,-2.9115863339
H,0,4.6490988739,1.9911570342,-3.2683822414
H,0,3.2137381728,2.9291006616,-2.8288961489
H,0,3.857168671,1.2584547265,-6.0903821455
H,0,4.5055751575,2.7606471781,-6.8299442196
H,0,5.4349374075,1.929918175,-5.5436037466
H,0,5.493663564,3.9555702056,-4.2048265746
H,0,4.6614570664,4.7590423601,-5.5728805917
H,0,3.9702137735,4.8702982072,-3.9238561587
H,0,2.5529339766,4.0596256108,-6.2710861051
H,0,1.8926135173,2.4667009538,-5.7944006229
H,0,0.9922163053,3.4134335677,-3.67258706
H,0,1.6487203239,6.0300416977,-5.1660294403
H,0,0.5443891776,5.8244747876,-3.6912517215

TS- B3LYPGD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSB3LYPGD2gasSB
parent ts exo s-cis
B3LYP/6-31G*
E(RB3LYP) = -519.013995617

Zero-point correction= 0.224309 (Hartree/Particle)
Thermal correction to Energy= 0.236757
Thermal correction to Enthalpy= 0.237702
Thermal correction to Gibbs Free Energy= 0.186590
Sum of electronic and ZPE= -518.789686
Sum of electronic and thermal Energies= -518.777238
Sum of electronic and thermal Enthalpies= -518.776294
Sum of electronic and thermal Free Energies= -518.827405

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.568	46.386	107.573

C,0,1.968310092,-0.8109111111,-2.425166266
O,0,2.7409934651,0.3892709681,-2.4832019702
C,0,2.8217528981,0.9561725669,-3.7296063155
C,0,3.5403315374,2.1853934614,-3.6909183361
N,0,3.8288211149,2.8880237222,-4.8514167211
C,0,4.6343896871,4.0901946489,-4.5844726125
O,0,2.2885725718,0.4354416434,-4.7162031972
C,0,4.3587890581,2.1225294781,-6.0013669114
C,0,2.1130234799,3.6881080094,-5.6684033134
C,0,1.5220204607,4.2300425766,-4.5057667756
C,0,1.0303953882,3.3928050458,-3.5460792146
H,0,2.003336823,-1.1333925891,-1.3814175982
H,0,0.9324967276,-0.62724625,-2.7337884803
H,0,2.3905506298,-1.5820013809,-3.0793384586
H,0,3.8159147133,2.6312645644,-2.7472902076
H,0,5.386304037,1.8049971112,-5.7826725392
H,0,3.7203565928,1.2544957804,-6.1592115806
H,0,4.3485855006,2.7730448915,-6.8816467222
H,0,5.6141279136,3.8009410622,-4.1831313794
H,0,4.7621929051,4.6485066667,-5.5154417384
H,0,4.1021008337,4.7067489124,-3.8559080086
H,0,2.5101548702,4.3413679984,-6.4426476188
H,0,1.7801858552,2.7076315302,-5.9994403179
H,0,1.685951876,5.2820702843,-4.2734467772
H,0,0.785190152,2.3649409519,-3.789143672
H,0,0.729404817,3.7570204567,-2.5669132673

Cation- PBEPBEGD2/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMPBEPBEGD2gasSB
parent sm conf 2
PBEPBE/6-31G*
E(RPBE-PBE) = -518.800218864

Zero-point correction= 0.234765 (Hartree/Particle)
Thermal correction to Energy= 0.247834
Thermal correction to Enthalpy= 0.248779
Thermal correction to Gibbs Free Energy= 0.195258
Sum of electronic and ZPE= -518.565454
Sum of electronic and thermal Energies= -518.552384
Sum of electronic and thermal Enthalpies= -518.551440
Sum of electronic and thermal Free Energies= -518.604961

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	155.518	48.181	112.644

C,0,2.0073738919,-0.8046730628,-2.2613028956
O,0,2.760987967,0.4412790062,-2.3952965637
C,0,2.7887544964,0.9634314176,-3.6231387302
O,0,2.2423855586,0.5098664036,-4.6190996397
C,0,3.6362625114,2.242466652,-3.5675058886
N,0,3.7281321409,2.9931885727,-4.8759949344
C,0,4.4352785081,2.164416207,-5.9202870541
C,0,4.5250466868,4.2462520182,-4.6215634262
C,0,2.3260454423,3.3893468236,-5.4191979557
C,0,1.4721297477,4.0717876803,-4.3961061523
C,0,1.2152475222,5.3908575164,-4.4247729182
H,0,2.1063945331,-1.080900631,-1.2041060605
H,0,0.9549209018,-0.6315676601,-2.5341776958
H,0,2.4423173702,-1.5723970436,-2.9196748633
H,0,4.6656079508,1.9926397206,-3.26087614
H,0,3.2164827748,2.9331956172,-2.8188017728
H,0,3.8548310831,1.2471351737,-6.0837600916
H,0,4.4940248537,2.7606814853,-6.8429197645
H,0,5.4472221215,1.9344615092,-5.5532036288
H,0,5.5011353136,3.9645895391,-4.1991311107
H,0,4.6625823626,4.7658066472,-5.5815290999
H,0,3.9613420345,4.8813424071,-3.9226862016
H,0,2.5380807458,4.0439614349,-6.2801806175
H,0,1.8809954398,2.4442358209,-5.7633404146
H,0,0.9980268613,3.4343365801,-3.6393963604
H,0,1.6421081092,6.0423486239,-5.1973602959
H,0,0.5453150705,5.8592295404,-3.6969127237

TS- PBEPBEGD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSPBEPBEGD2gasSB
parent ts exo s-cis
PBEPBE/6-31G*
E(RPBE-PBE) = -518.358258699

Zero-point correction= 0.218331 (Hartree/Particle)
Thermal correction to Energy= 0.231054
Thermal correction to Enthalpy= 0.231999
Thermal correction to Gibbs Free Energy= 0.180342
Sum of electronic and ZPE= -518.139928
Sum of electronic and thermal Energies= -518.127204
Sum of electronic and thermal Enthalpies= -518.126260
Sum of electronic and thermal Free Energies= -518.177917

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.989	47.587	108.720

C,0,1.9656135653,-0.8300421215,-2.4518385062
O,0,2.756856815,0.3653123498,-2.4809800332
C,0,2.8360280592,0.9470999469,-3.7344072178
C,0,3.5770563543,2.165946513,-3.6878333077
N,0,3.8168888188,2.895107686,-4.8577710727

C,0,4.6184309905,4.1062358742,-4.5873970733
O,0,2.2869551665,0.4365712247,-4.7316916538
C,0,4.3665863547,2.1276279199,-6.0047584715
C,0,2.1537260072,3.629318623,-5.6359764469
C,0,1.5312642697,4.240530165,-4.5069493337
C,0,1.0076880224,3.455190891,-3.5158379578
H,0,2.0042902035,-1.1826261622,-1.4096642636
H,0,0.9212835331,-0.625981061,-2.7501079854
H,0,2.3734337437,-1.5959894161,-3.1350878524
H,0,3.8253921343,2.6379323855,-2.7393873936
H,0,5.4056158139,1.8319217615,-5.776052695
H,0,3.7360803042,1.2385372945,-6.1452211687
H,0,4.341753624,2.7703378219,-6.9006025241
H,0,5.6050555879,3.8150254095,-4.1851691282
H,0,4.7414729868,4.6725299896,-5.5237474026
H,0,4.0768622306,4.7180702229,-3.8493651884
H,0,2.527728158,4.254253635,-6.457186469
H,0,1.788933156,2.6375721298,-5.9312837613
H,0,1.6809875476,5.3145667151,-4.3333786612
H,0,0.7933816884,2.399265173,-3.7027561778
H,0,0.6748888647,3.8731460291,-2.5595882538

Cation- BLYPGD2/6-31G*/Gas-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMBLYPGD2gasSB
parent sm conf 2
BLYP/6-31G*
E(RB-LYP) = -519.246526000

Zero-point correction= 0.233764 (Hartree/Particle)
Thermal correction to Energy= 0.246919
Thermal correction to Enthalpy= 0.247863
Thermal correction to Gibbs Free Energy= 0.194107
Sum of electronic and ZPE= -519.012762
Sum of electronic and thermal Energies= -518.999607
Sum of electronic and thermal Enthalpies= -518.998663
Sum of electronic and thermal Free Energies= -519.052419

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	154.944	48.505	113.139

C,0,2.0020733179,-0.8342278411,-2.2399661743
O,0,2.7642518002,0.4241074837,-2.3873351283
C,0,2.781192391,0.9542301473,-3.6191664494
O,0,2.2239891854,0.5077753807,-4.6154117603
C,0,3.6358800055,2.2398941888,-3.5612457205
N,0,3.732166468,2.9973940987,-4.8812135516
C,0,4.4484508407,2.1613744333,-5.9334759605
C,0,4.537689949,4.2604126701,-4.6222111149
C,0,2.3163266975,3.4029166335,-5.4383755511
C,0,1.4556417791,4.0799053239,-4.4081271361
C,0,1.2066295076,5.4023766198,-4.4223047193
H,0,2.1143523456,-1.1025611498,-1.1824998333
H,0,0.9492277009,-0.6551338239,-2.5046211844
H,0,2.4332152568,-1.5999431009,-2.9020503237
H,0,4.6644399409,1.9906714225,-3.2576124556
H,0,3.2130919865,2.9318050572,-2.8184836948
H,0,3.8632287764,1.2498763243,-6.1007111865
H,0,4.5133311527,2.7642593631,-6.8502929563
H,0,5.4551494398,1.9282302242,-5.5565099571
H,0,5.5111223927,3.9721984874,-4.2004062992
H,0,4.6730100294,4.777219739,-5.5827925081
H,0,3.9720352653,4.8905240419,-3.9228314938
H,0,2.5412099687,4.064046856,-6.2887897274
H,0,1.8789735008,2.4600941747,-5.7897161882
H,0,0.9836167839,3.4347541866,-3.65905253
H,0,1.6399543994,6.0583356536,-5.1861555425
H,0,0.5387811178,5.8667814051,-3.6909638532

TS- BLYPGD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSBLYPGD2gasSB
parent ts exo s-cis
BLYP/6-31G*
E(RB-LYP) = -518.802483883

Zero-point correction= 0.217751 (Hartree/Particle)
Thermal correction to Energy= 0.230467
Thermal correction to Enthalpy= 0.231411
Thermal correction to Gibbs Free Energy= 0.179669
Sum of electronic and ZPE= -518.584733
Sum of electronic and thermal Energies= -518.572017
Sum of electronic and thermal Enthalpies= -518.571073
Sum of electronic and thermal Free Energies= -518.622815

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.620	47.562	108.901

C,0,1.9526796919,-0.8589732551,-2.4611378494
O,0,2.7669889982,0.334230627,-2.4850139691
C,0,2.8530930814,0.9381958996,-3.7433024552
C,0,3.6487427001,2.1160139839,-3.6947519963
N,0,3.8050882369,2.9012980677,-4.8753423121
C,0,4.6114762734,4.1273889928,-4.5899498741
O,0,2.2663247113,0.4555567391,-4.742185424
C,0,4.393806834,2.1486312149,-6.0394217975
C,0,2.2047178956,3.5436870819,-5.5775384101
C,0,1.5330923785,4.2399043554,-4.4960265774
C,0,0.9444332011,3.5377702343,-3.4885042566
H,0,1.9931115995,-1.2185237057,-1.4211803794
H,0,0.9103510171,-0.6374822461,-2.7529523497
H,0,2.3477279189,-1.6245128677,-3.1521774969
H,0,3.876080684,2.6051140883,-2.7514354819
H,0,5.4294441001,1.8715464375,-5.7856775497
H,0,3.7778300748,1.2538154634,-6.1920859799
H,0,4.3721686366,2.8028856662,-6.9266314472
H,0,5.6038255981,3.8233865008,-4.2189984477
H,0,4.7060737671,4.7140695379,-5.5162516485
H,0,4.0806993149,4.7100247171,-3.8233231656
H,0,2.5389764639,4.1358999744,-6.4389646446
H,0,1.7976695041,2.5599865041,-5.8368379737
H,0,1.6608799668,5.3260134762,-4.4101658887
H,0,0.7916861932,2.4601469888,-3.5787179168
H,0,0.5472851585,4.0313865234,-2.5954647077

Cation- BP86GD2/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMBP86GD2gasSB
parent sm conf 2
BP86/6-31G*
E(RB-P86) = -519.455853943

Zero-point correction= 0.233913 (Hartree/Particle)
Thermal correction to Energy= 0.246996
Thermal correction to Enthalpy= 0.247940
Thermal correction to Gibbs Free Energy= 0.194389
Sum of electronic and ZPE= -519.221941
Sum of electronic and thermal Energies= -519.208858
Sum of electronic and thermal Enthalpies= -519.207914
Sum of electronic and thermal Free Energies= -519.261465

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	154.992	48.284	112.707

C,0,2.0052877382,-0.8108729891,-2.2580323634
O,0,2.759767265,0.4408860792,-2.3929050776
C,0,2.7870508145,0.9632755588,-3.6224776026
O,0,2.2410504503,0.5086667685,-4.6196073905
C,0,3.6342563584,2.2454910787,-3.5658547032
N,0,3.7268865988,2.9940615434,-4.8784479222
C,0,4.4387653046,2.1630784333,-5.9218692857
C,0,4.5221022187,4.2518850204,-4.6248239011
C,0,2.3221599071,3.3877557774,-5.4256407806
C,0,1.4692484632,4.0687145083,-4.3975007103
C,0,1.2239396362,5.3912811836,-4.4183606513
H,0,2.1027522685,-1.0828806386,-1.1985684166
H,0,0.9532480359,-0.6376842882,-2.5361737032
H,0,2.4464032973,-1.5776627219,-2.9149821863
H,0,4.6648125326,1.9984366321,-3.2583338232
H,0,3.2095894448,2.9388175666,-2.8211149649
H,0,3.8565446359,1.2458606874,-6.0852377038
H,0,4.4991934272,2.7614895771,-6.8442786698
H,0,5.4499369284,1.9343185557,-5.5487895232
H,0,5.4987608129,3.9706382273,-4.2006819172
H,0,4.6576204356,4.7687387546,-5.5876769622
H,0,3.9531200682,4.8851282919,-3.9269586044
H,0,2.5363376489,4.0449890449,-6.2852561675
H,0,1.8803409234,2.4404389789,-5.7695884901
H,0,0.9941116707,3.4284894593,-3.6429946664
H,0,1.6567739433,6.0416417252,-5.1899138871
H,0,0.5589711713,5.862335185,-3.6862529259

TS- BP86GD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSBP86GD2gasSB
parent ts exo s-cis
BP86/6-31G*
E(RB-P86) = -519.013386628

Zero-point correction= 0.217497 (Hartree/Particle)
Thermal correction to Energy= 0.230215
Thermal correction to Enthalpy= 0.231159
Thermal correction to Gibbs Free Energy= 0.179558
Sum of electronic and ZPE= -518.795890
Sum of electronic and thermal Energies= -518.783172
Sum of electronic and thermal Enthalpies= -518.782227
Sum of electronic and thermal Free Energies= -518.833828

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.462	47.673	108.604

C,0,1.954864405,-0.8317341601,-2.4541109656
O,0,2.7560388656,0.3622973541,-2.4800428328
C,0,2.8361995055,0.9493221631,-3.733461069
C,0,3.5858886904,2.1640218513,-3.684856936
N,0,3.8220446112,2.8943605146,-4.8569996344
C,0,4.6159785945,4.1137786549,-4.5886062755
O,0,2.2810020811,0.4455846899,-4.7327653771
C,0,4.3744023315,2.1291577173,-6.0076786406
C,0,2.1471019453,3.6201415957,-5.6375820664
C,0,1.5314486002,4.2375369696,-4.5067923282
C,0,1.0162178615,3.4529020367,-3.5085854761
H,0,1.9879759055,-1.1836728205,-1.4102936503
H,0,0.9129098183,-0.6191119,-2.7581897804
H,0,2.3630354803,-1.5993519578,-3.1370440852
H,0,3.8331343691,2.6378719693,-2.7362335949
H,0,5.4152995229,1.8353494488,-5.7789597345
H,0,3.7432009572,1.239673389,-6.1495128046
H,0,4.3462714373,2.7772049202,-6.9011338441
H,0,5.6057324949,3.8298158077,-4.185325984
H,0,4.7327720414,4.6779830602,-5.5283808731
H,0,4.0664783731,4.7218600583,-3.8515440292
H,0,2.5222725864,4.2394970331,-6.4635662267
H,0,1.7880696945,2.62175879,-5.9202078688
H,0,1.6825421245,5.3130679744,-4.3382709419
H,0,0.8037976263,2.395676698,-3.6941304596
H,0,0.6895740767,3.8724691426,-2.5497645207

Cation- B3LYPGD3/6-31G*/Gas-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMB3LYPGD3gasSB
parent sm conf 2
B3LYP/6-31G*
E(RB3LYP) = -519.456328353

Zero-point correction= 0.242189 (Hartree/Particle)
Thermal correction to Energy= 0.254978
Thermal correction to Enthalpy= 0.255922
Thermal correction to Gibbs Free Energy= 0.202923
Sum of electronic and ZPE= -519.214139
Sum of electronic and thermal Energies= -519.201351
Sum of electronic and thermal Enthalpies= -519.200406
Sum of electronic and thermal Free Energies= -519.253405

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.001	46.841	111.545

C,0,1.9956002557,-0.7824858409,-2.2507694813
O,0,2.7598802421,0.4486715626,-2.4066987088
C,0,2.7817240827,0.9776737163,-3.6203144884
O,0,2.2214690534,0.544739125,-4.6045627973
C,0,3.6432231698,2.2417888666,-3.5739962916

N,0,3.7372452635,2.9951502333,-4.8814621022
C,0,4.4441603345,2.1617566452,-5.926162202
C,0,4.5434551802,4.2447796764,-4.6247560875
C,0,2.338923547,3.4007123817,-5.432556237
C,0,1.4583823837,4.0489398175,-4.4097933162
C,0,1.1872997804,5.3564216695,-4.4012529242
H,0,2.1049787198,-1.0504588944,-1.2017931393
H,0,0.9495800028,-0.6011593733,-2.5054016295
H,0,2.4078989974,-1.5561582893,-2.9013784132
H,0,4.6589579508,1.971783428,-3.2727231864
H,0,3.2429703496,2.9225050407,-2.820188564
H,0,3.8770490418,1.2472235017,-6.0868884859
H,0,4.4996849036,2.7429269655,-6.847805854
H,0,5.4510190909,1.9357862858,-5.569932307
H,0,5.5087737232,3.9652311322,-4.1997367269
H,0,4.6928574366,4.7625824035,-5.5732653534
H,0,3.9924012616,4.8836300754,-3.9344944919
H,0,2.553412571,4.0712662369,-6.2679473906
H,0,1.9011007292,2.4768813679,-5.8083005325
H,0,0.97746107,3.388602294,-3.6906326486
H,0,1.6176005796,6.0394991754,-5.1309260036
H,0,0.5019222788,5.7890287966,-3.678583637

TS- B3LYPGD3/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSB3LYPGD3gasSB
parent ts exo s-cis
B3LYP/6-31G*
E(RB3LYP) = -519.003002963

Zero-point correction= 0.225100 (Hartree/Particle)
Thermal correction to Energy= 0.237522
Thermal correction to Enthalpy= 0.238467
Thermal correction to Gibbs Free Energy= 0.187365
Sum of electronic and ZPE= -518.777903
Sum of electronic and thermal Energies= -518.765481
Sum of electronic and thermal Enthalpies= -518.764536
Sum of electronic and thermal Free Energies= -518.815638

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.048	46.265	107.553

C,0,1.9734601032,-0.8146708279,-2.4318504227
O,0,2.7518366146,0.3812562479,-2.4883390538
C,0,2.831870372,0.9560898236,-3.7329369335
C,0,3.5638621201,2.1749037102,-3.6937655888
N,0,3.8310529442,2.8920096087,-4.8560740662
C,0,4.6478431771,4.0905662383,-4.5851561224
O,0,2.2889094235,0.4429682352,-4.7194483523
C,0,4.3641262834,2.1210010882,-6.0061707231
C,0,2.1249105065,3.6734867924,-5.6516724745
C,0,1.5095573482,4.2278136493,-4.5003028837
C,0,0.9875756196,3.4165243124,-3.5391365312
H,0,2.0128128183,-1.143150745,-1.3911547655
H,0,0.9358558153,-0.6282449772,-2.7298464793
H,0,2.384812211,-1.5876275607,-3.0893459372
H,0,3.8300305003,2.6239106454,-2.7494434989
H,0,5.390090831,1.8049233491,-5.7856222582
H,0,3.7313871849,1.2494479964,-6.160368252
H,0,4.3562369613,2.7586856615,-6.8945024997
H,0,5.6268730086,3.7942155431,-4.1910989585
H,0,4.7790107593,4.6580355829,-5.5088136798
H,0,4.1300700709,4.7093064578,-3.8497928252
H,0,2.498500898,4.3293171702,-6.4354381846
H,0,1.7821262759,2.6988845269,-5.9877493937
H,0,1.6589366001,5.2861622412,-4.2872404671
H,0,0.7621216305,2.3775069698,-3.7505356307
H,0,0.6603839221,3.8041392606,-2.578234017

Cation- M06GD3/6-31G*/Gas-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMM06GD3gasSB
parent sm conf 2
M06/6-31G*
E(RM06) = -519.081480703

Zero-point correction= 0.240007 (Hartree/Particle)
Thermal correction to Energy= 0.252846
Thermal correction to Enthalpy= 0.253791
Thermal correction to Gibbs Free Energy= 0.200825
Sum of electronic and ZPE= -518.841474
Sum of electronic and thermal Energies= -518.828634
Sum of electronic and thermal Enthalpies= -518.827690
Sum of electronic and thermal Free Energies= -518.880656

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.664	47.167	111.477

C,0,2.0361820788,-0.7854522717,-2.2739412444
O,0,2.7905348192,0.4361442766,-2.4180171651
C,0,2.7780446864,0.9867111562,-3.6146648135
O,0,2.1984037178,0.5718387102,-4.5894133394
C,0,3.6217079359,2.2490073561,-3.5651365728
N,0,3.7182918776,2.9902114165,-4.8654198967
C,0,4.4192373124,2.1553270728,-5.8960687886
C,0,4.5274208366,4.2245459595,-4.615896273
C,0,2.3377224084,3.3999996821,-5.4222829188
C,0,1.4642520902,4.062588633,-4.4163432285
C,0,1.2078786099,5.3691732607,-4.4343866417
H,0,2.1976130711,-1.1071662424,-1.2457631988
H,0,0.9768723782,-0.589709812,-2.4607985926
H,0,2.4031355831,-1.534067122,-2.9811217369
H,0,4.642172494,1.9934343743,-3.2529064013
H,0,3.2135548253,2.9327789175,-2.8115602317
H,0,3.8473258059,1.2395170878,-6.0583847773
H,0,4.4809476475,2.7341835861,-6.8220555557
H,0,5.4268197798,1.9261598029,-5.5355826205
H,0,5.4979660687,3.937873894,-4.2003427193
H,0,4.6714186361,4.7458881703,-5.5667218411
H,0,3.990094186,4.8690695574,-3.9148913293
H,0,2.5662825374,4.0658510402,-6.263623776
H,0,1.8936610379,2.4759486127,-5.8020997163
H,0,0.9652704916,3.4169644511,-3.6909719958
H,0,1.6542685677,6.0320656687,-5.1770404467
H,0,0.5219525162,5.8284307611,-3.7268871786

TS- M06GD3/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSM06GD3gas
SB
parent ts exo s-cis
M06/6-31G*
E(RM06) = -518.628058088

Zero-point correction= 0.223114 (Hartree/Particle)
Thermal correction to Energy= 0.235669
Thermal correction to Enthalpy= 0.236613
Thermal correction to Gibbs Free Energy= 0.185271
Sum of electronic and ZPE= -518.404944
Sum of electronic and thermal Energies= -518.392389
Sum of electronic and thermal Enthalpies= -518.391445
Sum of electronic and thermal Free Energies= -518.442787

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.884	46.719	108.058

C,0,1.9680973176,-0.7562911585,-2.3940205037
O,0,2.7174962985,0.4404042769,-2.4762215963
C,0,2.8276949231,0.9549171915,-3.7333229112
C,0,3.491852852,2.2148792881,-3.7043735915
N,0,3.8114920455,2.9000953347,-4.8625959103
C,0,4.6526040606,4.0661389357,-4.592111598
O,0,2.3549411054,0.3797123017,-4.7099201997
C,0,4.3246075128,2.1221826146,-6.0002601979
C,0,2.1181759487,3.7600939161,-5.6714219251
C,0,1.5170923377,4.2087357998,-4.48608746
C,0,1.0619163276,3.290028212,-3.5856106593
H,0,1.991236352,-1.0564327926,-1.3431640282
H,0,0.9308747905,-0.5966953514,-2.7160643061
H,0,2.4016642004,-1.54402016,-3.0212089057
H,0,3.7717356038,2.6590411094,-2.7561032367
H,0,5.3503454323,1.7899970192,-5.7865451435
H,0,3.6801840268,1.2546613037,-6.1530596878
H,0,4.3242754684,2.7604446472,-6.8920388968
H,0,5.6255226306,3.7444140858,-4.1941271785
H,0,4.8043664949,4.6322867595,-5.5174291899
H,0,4.153743541,4.7038530817,-3.8547466618
H,0,2.5143593772,4.4673687305,-6.4021855995
H,0,1.7905604582,2.8044361963,-6.0831934044
H,0,1.6721895444,5.2433596187,-4.1712872794
H,0,0.7942020592,2.2866721368,-3.9105967131
H,0,0.7630232911,3.5671779026,-2.5763432155

Cation- PBE1PBEGD3/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMPBE1PBEG
D3gasSB
parent sm conf 2
PBE1PBE/6-31G*
E(RPBE1PBE) = -518.839019773

Zero-point correction= 0.243689 (Hartree/Particle)
Thermal correction to Energy= 0.256408
Thermal correction to Enthalpy= 0.257352
Thermal correction to Gibbs Free Energy= 0.204571
Sum of electronic and ZPE= -518.595331
Sum of electronic and thermal Energies= -518.582612
Sum of electronic and thermal Enthalpies= -518.581668
Sum of electronic and thermal Free Energies= -518.634449

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.898	46.506	111.087

C,0,2.0062944289,-0.7613827417,-2.2724209515
O,0,2.7591869686,0.4618729034,-2.4155711566
C,0,2.7894438218,0.9831321489,-3.6245625071
O,0,2.2424930871,0.5427192163,-4.6082294921
C,0,3.639323947,2.2456140433,-3.5784938179
N,0,3.7285628498,2.9901989474,-4.8751266103
C,0,4.4281817148,2.1649959744,-5.9112409728
C,0,4.5261403328,4.2298446911,-4.6228436781
C,0,2.3453531284,3.3869470817,-5.4142035333
C,0,1.4770421226,4.047370064,-4.3961801678
C,0,1.2030521139,5.3518984096,-4.4102217876
H,0,2.1026128875,-1.0344641632,-1.2235956957
H,0,0.9617243152,-0.5873344071,-2.5376504706
H,0,2.4274868238,-1.5337859324,-2.9187264294
H,0,4.6564794727,1.9808615047,-3.2742411179
H,0,3.2359980144,2.9252831224,-2.8235117834
H,0,3.8612164404,1.2495819795,-6.073614578
H,0,4.4839168003,2.7457682949,-6.8335528545
H,0,5.4361064794,1.9379015315,-5.5578487474
H,0,5.4942067892,3.9532130586,-4.2012690505
H,0,4.6725535,4.7496844659,-5.5712179065
H,0,3.9770369578,4.869109256,-3.9301324301
H,0,2.5501700892,4.0496537771,-6.2594259541
H,0,1.8984949692,2.4610450907,-5.7790840972
H,0,0.9979120617,3.4009069078,-3.6624820982
H,0,1.625837531,6.0213338342,-5.1570135927
H,0,0.5222043521,5.795348941,-3.6898615192

TS- PBE1PBEGD3/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSPBE1PBEGD
3gasSB
parent ts exo s-cis
PBE1PBE/6-31G*
E(RPBE1PBE) = -518.383597958

Zero-point correction= 0.226786 (Hartree/Particle)
Thermal correction to Energy= 0.239069
Thermal correction to Enthalpy= 0.240013
Thermal correction to Gibbs Free Energy= 0.189232
Sum of electronic and ZPE= -518.156812
Sum of electronic and thermal Energies= -518.144529
Sum of electronic and thermal Enthalpies= -518.143585
Sum of electronic and thermal Free Energies= -518.194366

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.018	45.789	106.878

C,0,2.0081444154,-0.8045555354,-2.4259872825
O,0,2.727654208,0.4153097902,-2.4851389159
C,0,2.7932890595,0.9704163051,-3.7270980651
C,0,3.4554100645,2.2280760581,-3.6947838153
N,0,3.7778938964,2.9067230744,-4.8612469822

C,0,4.6223056692,4.0712702873,-4.5841781788
O,0,2.2851027154,0.4226301634,-4.7063027994
C,0,4.3118423029,2.1093994506,-5.9768979334
C,0,2.1517551861,3.7245304755,-5.667366125
C,0,1.535305838,4.245536357,-4.5110590487
C,0,1.07490222,3.3666502165,-3.5745718316
H,0,2.0423354662,-1.1184127022,-1.3810333419
H,0,0.9693848366,-0.669632798,-2.7450846799
H,0,2.4657054038,-1.5668427202,-3.0645679535
H,0,3.7700038529,2.6561115044,-2.7546999488
H,0,5.3285150475,1.7780906158,-5.73713261
H,0,3.6653930813,1.2453380117,-6.1248994223
H,0,4.3298034978,2.7305614862,-6.8772786454
H,0,5.5793983516,3.7465819703,-4.1601064015
H,0,4.798489322,4.6232762054,-5.5103099162
H,0,4.1069812561,4.7166421555,-3.8694800175
H,0,2.5464346704,4.3950792987,-6.4297017377
H,0,1.7905774886,2.7688022718,-6.0427776918
H,0,1.7002368577,5.2888513992,-4.2444950745
H,0,0.7951948481,2.3575399549,-3.8590370028
H,0,0.7821944444,3.6894877038,-2.5788045783

Cation1- wB97XD/6-31G*/PCM-Conf1

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM1wB97XDSB
parent sm
wb97xd/6-31G*
E(RwB97XD) = -519.349039668

Zero-point correction= 0.245416 (Hartree/Particle)
Thermal correction to Energy= 0.257894
Thermal correction to Enthalpy= 0.258839
Thermal correction to Gibbs Free Energy= 0.206853
Sum of electronic and ZPE= -519.103624
Sum of electronic and thermal Energies= -519.091145
Sum of electronic and thermal Enthalpies= -519.090201
Sum of electronic and thermal Free Energies= -519.142186

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.831	46.030	109.412

C,0,1.9237085968,-0.7009911841,-2.2712416557
O,0,2.7085673332,0.4952306192,-2.4214923847
C,0,2.8061396053,0.9783279222,-3.6474467082
O,0,2.2917186597,0.495846093,-4.6309260638
C,0,3.6754462451,2.2254345317,-3.6033039181
N,0,3.7611743803,2.990802584,-4.8890243394
C,0,4.4754660646,2.1901266305,-5.9391171667
C,0,4.5565129968,4.2335136101,-4.6159653947
C,0,1.4906611062,4.0036861638,-4.4010772706
C,0,0.4054360219,3.387745163,-3.9368372433
C,0,2.380633248,3.3745411543,-5.4282565373
H,0,1.9827105981,-0.9531009281,-1.2149635608
H,0,0.8907043472,-0.5058868744,-2.5638679446
H,0,2.3401216038,-1.5020365205,-2.8837677637
H,0,4.6904796475,1.9394457793,-3.3181237434
H,0,5.4817143637,1.9674646524,-5.5843323304
H,0,3.919734502,1.2725777742,-6.1177851052
H,0,4.5251112857,2.7897304618,-6.8476511901
H,0,5.5391889023,3.9460949835,-4.2428930723
H,0,4.6594435649,4.7891968827,-5.5473289851
H,0,4.0399267517,4.8382874085,-3.8722122518
H,0,2.5802307889,4.0527080015,-6.2611005226
H,0,1.9425648701,2.4563234284,-5.8148981458
H,0,1.7305965328,5.0112693463,-4.0709339623
H,0,0.133577658,2.3872005751,-4.2645197922
H,0,-0.2532874758,3.8690135637,-3.2211862953
H,0,3.2845808013,2.893099178,-2.8347186519

Cation3/wb97xd /6-31G */PCM-Conf3

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM3wB97XDSB
parent sm
wb97xd/6-31G*
E(RwB97XD) = -519.347492531

Zero-point correction= 0.245361 (Hartree/Particle)
Thermal correction to Energy= 0.257882
Thermal correction to Enthalpy= 0.258826
Thermal correction to Gibbs Free Energy= 0.206739
Sum of electronic and ZPE= -519.102132
Sum of electronic and thermal Energies= -519.089611
Sum of electronic and thermal Enthalpies= -519.088667
Sum of electronic and thermal Free Energies= -519.140753

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.823	46.032	109.625

C,0,1.840545096,-0.6285851552,-2.211902471
O,0,2.7078788401,0.4998145189,-2.4221271907
C,0,2.7821632562,0.9583173153,-3.6596763483
O,0,2.1787776926,0.5110340675,-4.6075668602
C,0,3.7670113997,2.1201761753,-3.674215779
N,0,3.8631137516,2.8680628286,-4.9682628563
C,0,4.4033853687,1.9888745483,-6.0573175161
C,0,2.5220292297,3.4091745521,-5.3724515476
C,0,4.7958656997,4.0667583194,-4.7680706143
C,0,6.1618983327,3.7121023219,-4.265276736
C,0,7.2366810194,3.7155484761,-5.0504435815
H,0,1.9210055669,-0.8570634331,-1.1516621644
H,0,0.8147790508,-0.3636387181,-2.4729061316
H,0,2.1731689801,-1.4741613791,-2.8159011911
H,0,4.7569711118,1.7258106805,-3.4360291158
H,0,3.4884980755,2.8304871614,-2.8929872687
H,0,3.7163150059,1.1590003225,-6.2021855108
H,0,4.4816256,2.5833740767,-6.9674254881
H,0,5.3882044118,1.630558635,-5.7611271974
H,0,2.1237605189,4.003141198,-4.549609873
H,0,2.6573444111,4.0361035134,-6.2532646092
H,0,1.8604395578,2.5769621726,-5.5987274538
H,0,4.84929848,4.5555977974,-5.7423275854
H,0,4.2768913893,4.7308381598,-4.0727492777
H,0,6.2638844803,3.5009066149,-3.203885888
H,0,7.1712724523,3.947067107,-6.1108016402
H,0,8.222796221,3.4944441231,-4.6546011039

Cation4wb97xd /6-31G */PCM-Conf4

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM4wB97XDSB
parent sm
wb97xd/6-31G*
E(RwB97XD) = -519.344298249

Zero-point correction= 0.244933 (Hartree/Particle)
Thermal correction to Energy= 0.257625
Thermal correction to Enthalpy= 0.258569
Thermal correction to Gibbs Free Energy= 0.205721
Sum of electronic and ZPE= -519.099365
Sum of electronic and thermal Energies= -519.086674
Sum of electronic and thermal Enthalpies= -519.085729
Sum of electronic and thermal Free Energies= -519.138577

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.662	46.229	111.228

C,0,1.7464201509,-0.8957098538,-2.4876160473
O,0,2.4918759703,0.3340159924,-2.4033943576
C,0,2.7556024597,0.9391587238,-3.5520406776
O,0,2.4093437436,0.5497820682,-4.6396957985
C,0,3.5140627841,2.2560900964,-3.4348913183
N,0,4.2431245201,2.5833843818,-2.162261507
C,0,3.2892665687,2.8529279121,-1.0362258881
C,0,5.1819698861,1.476200684,-1.7808853949
C,0,5.0960457714,3.8337310888,-2.4104450655
C,0,4.324819643,5.0197927501,-2.9018941523
C,0,4.055138571,6.0667325495,-2.125439149
H,0,1.6491917334,-1.2400621535,-1.4608630092
H,0,0.7670148169,-0.70466481,-2.9278538095
H,0,2.2952390408,-1.6199643007,-3.0907278798
H,0,2.7911886859,3.054851687,-3.6153856472
H,0,4.2422838102,2.2705445775,-4.2472879659
H,0,2.6989643096,1.9587507894,-0.8561951498
H,0,3.8723661006,3.1089091584,-0.1519830152
H,0,2.6477470035,3.6880525426,-1.3136514177
H,0,5.8191325627,1.2480260689,-2.6355037804
H,0,5.7886680635,1.8163116549,-0.9423086483
H,0,4.6017969719,0.6028112071,-1.4941030653
H,0,5.5806765364,4.0460626011,-1.4556872039
H,0,5.8600476406,3.5300204934,-3.1299925742
H,0,4.0312969207,5.0275443871,-3.9485544901
H,0,4.3581500591,6.0977193385,-1.0815514889
H,0,3.5295196754,6.933579365,-2.5128564986

CationB971/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2B971SB
parent sm
b971/6-31G*
E(RB971) = -519.341196575

Zero-point correction= 0.241515 (Hartree/Particle)
Thermal correction to Energy= 0.254421
Thermal correction to Enthalpy= 0.255365
Thermal correction to Gibbs Free Energy= 0.202002
Sum of electronic and ZPE= -519.099682
Sum of electronic and thermal Energies= -519.086775
Sum of electronic and thermal Enthalpies= -519.085831
Sum of electronic and thermal Free Energies= -519.139195

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.652	47.113	112.313

C,0,2.0481997595,-0.8355963614,-2.263900018
O,0,2.7941523524,0.3964101093,-2.4107127832
C,0,2.7795414196,0.9488040728,-3.6188778442
O,0,2.1972678847,0.5085253903,-4.589467928
C,0,3.6206381908,2.2271585476,-3.566717081
N,0,3.7151889278,2.9931654679,-4.8634080951
C,0,4.4192398404,2.1704702681,-5.9165444907
C,0,4.5350860199,4.2306443813,-4.5898832342
C,0,2.3289463272,3.4097902687,-5.4097076538
C,0,1.4700905054,4.1280598209,-4.4079619933
C,0,1.1914761198,5.4339900459,-4.4942711652
H,0,2.1794611951,-1.1247473466,-1.2212529619
H,0,0.9927908593,-0.6614395289,-2.489554239
H,0,2.4537946567,-1.5987344422,-2.933438732
H,0,4.639980205,1.9673565834,-3.2641197353
H,0,3.2095599299,2.89811029,-2.8068888959
H,0,3.8358897258,1.2692818522,-6.1022374931
H,0,4.496524302,2.7722056957,-6.8244701981
H,0,5.4163623942,1.9185666315,-5.548453884
H,0,5.505786144,3.9265564412,-4.1930140109
H,0,4.6656293114,4.770646325,-5.5297645055
H,0,4.0038313797,4.8532405099,-3.8682424628
H,0,2.5453373661,4.0410192992,-6.2757834232
H,0,1.8621936736,2.4808824008,-5.7438456452
H,0,1.0115397452,3.5266982693,-3.6230343663
H,0,1.6077059459,6.0605762007,-5.2821896778
H,0,0.5228178187,5.9156768076,-3.7845804825

TS B971/6-31G */PCM-

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSB971SB
23 parent ts
b971/6-31G*
E(RB971) = -518.822074086

Zero-point correction= 0.223785 (Hartree/Particle)
Thermal correction to Energy= 0.236477
Thermal correction to Enthalpy= 0.237422
Thermal correction to Gibbs Free Energy= 0.185598
Sum of electronic and ZPE= -518.598289
Sum of electronic and thermal Energies= -518.585597
Sum of electronic and thermal Enthalpies= -518.584653
Sum of electronic and thermal Free Energies= -518.636476

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.392	46.819	109.072

C,0,2.0308067342,-0.8195092802,-2.3373156405
O,0,2.7284035646,0.4215035118,-2.4541475247
C,0,2.799840733,0.9354309965,-3.7274355177
C,0,3.4429724765,2.2124303111,-3.7167152171

N,0,3.8000538586,2.8999576265,-4.8688369853
C,0,4.6828773078,4.0494947273,-4.5756156907
O,0,2.3256662866,0.3239756617,-4.6942404749
C,0,4.3015366393,2.1137359438,-6.0205865095
C,0,2.1327231281,3.8383212769,-5.6954797921
C,0,1.5032504573,4.2629573876,-4.5048138132
C,0,0.9908575714,3.3301394466,-3.6385841234
H,0,2.0723122913,-1.0823338952,-1.2772190766
H,0,0.9866177272,-0.7200756311,-2.6567756556
H,0,2.5092531967,-1.6027745859,-2.9363681829
H,0,3.719205138,2.6568519319,-2.7700237615
H,0,5.3098341742,1.7402343265,-5.7982344932
H,0,3.6273370924,1.2758595831,-6.1949825672
H,0,4.338622474,2.7651675025,-6.8990463535
H,0,5.6395459299,3.6930711414,-4.1722593737
H,0,4.8590721652,4.6125430353,-5.495757275
H,0,4.194245945,4.6952561816,-3.8410121573
H,0,2.5684712754,4.5640026709,-6.3809988723
H,0,1.7945428688,2.9118706983,-6.1568439202
H,0,1.6738657159,5.2825170552,-4.1553390285
H,0,0.7202699855,2.3375660041,-3.9891603157
H,0,0.6620692628,3.5992673715,-2.6362476778

CationB972/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2B972SB
parent sm
b972/6-31G*
E(RB972) = -519.313755427

Zero-point correction= 0.243801 (Hartree/Particle)
Thermal correction to Energy= 0.256659
Thermal correction to Enthalpy= 0.257603
Thermal correction to Gibbs Free Energy= 0.204252
Sum of electronic and ZPE= -519.069955
Sum of electronic and thermal Energies= -519.057096
Sum of electronic and thermal Enthalpies= -519.056152
Sum of electronic and thermal Free Energies= -519.109504

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.056	46.762	112.288

C,0,2.0651958293,-0.8361186311,-2.2650402841
O,0,2.8024293002,0.3922849441,-2.4217434659
C,0,2.7767927358,0.9448394976,-3.6248086606
O,0,2.1899072107,0.50653375,-4.5878753458
C,0,3.6108389211,2.2178141732,-3.5737523304
N,0,3.7077103294,2.98987629,-4.8574913237
C,0,4.4081341543,2.1791104727,-5.9107523228
C,0,4.5271215855,4.216016881,-4.5746124078
C,0,2.3330446636,3.4140049375,-5.3998284107
C,0,1.4822507299,4.1445661142,-4.4114501747
C,0,1.1942486208,5.4419218368,-4.5209559793
H,0,2.2073158606,-1.1219111174,-1.226773732
H,0,1.0102560133,-0.6674601081,-2.4779241348
H,0,2.4645891172,-1.5981833357,-2.9332007961
H,0,4.626051375,1.9582338515,-3.2713952915
H,0,3.2033140535,2.8808593529,-2.8107843238
H,0,3.8225329675,1.2884792832,-6.1157288398
H,0,4.4992579616,2.7885839799,-6.8074603624
H,0,5.3966907745,1.9121309289,-5.5417994633
H,0,5.4967262782,3.9091743647,-4.1881652411
H,0,4.6535394981,4.7667927934,-5.5041378218
H,0,4.004659975,4.8299621815,-3.8452443399
H,0,2.551138876,4.0329658936,-6.2694790626
H,0,1.8568233778,2.4921001316,-5.7278745064
H,0,1.0305563358,3.5591049836,-3.6156550997
H,0,1.6013654551,6.0559564584,-5.3185418951
H,0,0.5265400001,5.9296780919,-3.8198473842

TS B972/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSB972SB
23 parent ts
b972/6-31G*
E(RB972) = -518.792886842

Zero-point correction= 0.226030 (Hartree/Particle)
Thermal correction to Energy= 0.238612
Thermal correction to Enthalpy= 0.239556
Thermal correction to Gibbs Free Energy= 0.187975
Sum of electronic and ZPE= -518.566857
Sum of electronic and thermal Energies= -518.554275
Sum of electronic and thermal Enthalpies= -518.553331
Sum of electronic and thermal Free Energies= -518.604911

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.731	46.437	108.561

C,0,2.0531245275,-0.8163374453,-2.330327741
O,0,2.7280617697,0.4286151403,-2.4587459408
C,0,2.8009378682,0.9303098773,-3.7322155494
C,0,3.432212062,2.2066113043,-3.7261546257
N,0,3.7921655312,2.8952948378,-4.8691799346
C,0,4.6815195245,4.0286144516,-4.5699852242
O,0,2.342107168,0.3057175689,-4.6921930626
C,0,4.2870482675,2.1164629314,-6.0185931503
C,0,2.1410185584,3.8514128437,-5.6906697105
C,0,1.5076205674,4.2697029086,-4.5059099668
C,0,0.9730450606,3.343150142,-3.656188388
H,0,2.0941448915,-1.0656872963,-1.2707341928
H,0,1.0118013143,-0.7393701695,-2.6520958049
H,0,2.5445462201,-1.5974960701,-2.914472787
H,0,3.6952374132,2.6544132652,-2.7812614041
H,0,5.283710975,1.7251013202,-5.7937493325
H,0,3.6062207582,1.2927661779,-6.2085779045
H,0,4.3424560936,2.7717094029,-6.8882504403
H,0,5.6333328521,3.662024604,-4.1748120798
H,0,4.860528935,4.5981195718,-5.4809465174
H,0,4.2055898094,4.6707589586,-3.8299724669
H,0,2.582435606,4.5789085749,-6.3649509579
H,0,1.7958648061,2.938115423,-6.1641078362
H,0,1.6819478687,5.2823755292,-4.1492412784
H,0,0.7008379894,2.3565360356,-4.0113952767
H,0,0.6367375625,3.6096311116,-2.6593084264

Cation B97D/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2B97DSB
parent sm
b97d/6-31G*
E(RB97D) = -519.163158799

Zero-point correction= 0.236252 (Hartree/Particle)
Thermal correction to Energy= 0.249247
Thermal correction to Enthalpy= 0.250192
Thermal correction to Gibbs Free Energy= 0.196526
Sum of electronic and ZPE= -518.926907
Sum of electronic and thermal Energies= -518.913911
Sum of electronic and thermal Enthalpies= -518.912967
Sum of electronic and thermal Free Energies= -518.966633

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.405	47.862	112.949

C,0,2.0226896537,-0.8189659294,-2.232896756
O,0,2.7826617643,0.4187469055,-2.3989550608
C,0,2.7720819106,0.9522320877,-3.6271450243
O,0,2.1890576655,0.4982150426,-4.5986125614
C,0,3.6212722947,2.2298140395,-3.5791068391
N,0,3.7213592309,2.9946477193,-4.8827559862
C,0,4.4420133063,2.1747989724,-5.9334515999
C,0,4.5298426899,4.2448405865,-4.602845122
C,0,2.3277114638,3.4090732118,-5.4432601055
C,0,1.4565817842,4.0809353604,-4.4230819506
C,0,1.2092247484,5.4002012961,-4.4380052937
H,0,2.1558105488,-1.0899046477,-1.1811933283
H,0,0.9657883604,-0.6357788962,-2.4660425637
H,0,2.4285731734,-1.5923332608,-2.8978371229
H,0,4.6452406709,1.9744700848,-3.2788447944
H,0,3.2064907621,2.9137349004,-2.8288807629
H,0,3.8572327409,1.2717922886,-6.1242758062
H,0,4.5214435438,2.7878332387,-6.8379771462
H,0,5.4373935544,1.9291513874,-5.5464613698
H,0,5.5033606803,3.9417602959,-4.2024751081
H,0,4.6515726807,4.7831342334,-5.548624205
H,0,3.9791040324,4.8551473933,-3.8800635634
H,0,2.5593576474,4.0713299593,-6.2859277931
H,0,1.8833156635,2.4785600435,-5.809008981
H,0,0.9845327131,3.4393645034,-3.6751012195
H,0,1.6545753767,6.0547436297,-5.1917924847
H,0,0.5407433385,5.8597735539,-3.7077004514

TS B97D/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSB97DSB
23 parent ts
b97d/6-31G*
E(RB97D) = -518.652802726

Zero-point correction= 0.218558 (Hartree/Particle)
Thermal correction to Energy= 0.231416
Thermal correction to Enthalpy= 0.232361
Thermal correction to Gibbs Free Energy= 0.180264
Sum of electronic and ZPE= -518.434244
Sum of electronic and thermal Energies= -518.421386
Sum of electronic and thermal Enthalpies= -518.420442
Sum of electronic and thermal Free Energies= -518.472538

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.216	47.762	109.645

C,0,1.9690473826,-0.8287584544,-2.3837629976
O,0,2.7700282427,0.3621798328,-2.4771141184
C,0,2.8427714347,0.9213842748,-3.7510720594
C,0,3.5882247362,2.1351933919,-3.7165196333
N,0,3.8407480504,2.8841964158,-4.868240979
C,0,4.6528136075,4.0933533276,-4.5759207522
O,0,2.2959764435,0.3796533377,-4.7320560102
C,0,4.3832840242,2.1489071815,-6.045268765
C,0,2.1288423127,3.6796445196,-5.6524473203
C,0,1.5071890389,4.2387651013,-4.4983175173
C,0,0.9347301001,3.4321316129,-3.5525354591
H,0,2.0227493005,-1.1361059781,-1.3313458945
H,0,0.9235478976,-0.6271257605,-2.6673315466
H,0,2.3629046443,-1.6257172402,-3.0339025933
H,0,3.8247909967,2.6018700784,-2.7659589481
H,0,5.4150044652,1.8343634315,-5.8240914932
H,0,3.7496024572,1.2776657011,-6.2296968745
H,0,4.3726223535,2.8253692852,-6.9102192762
H,0,5.6438689499,3.787872144,-4.2065239384
H,0,4.7563040224,4.6809743403,-5.4959781601
H,0,4.1319293395,4.6838080944,-3.8123080672
H,0,2.535669056,4.3351580849,-6.4256242567
H,0,1.7778046422,2.7042808362,-5.9953600201
H,0,1.6752533863,5.2971613267,-4.2757942572
H,0,0.7213379065,2.385807867,-3.7722870295
H,0,0.5872092086,3.8254282475,-2.5943620324

Cation B97D/6-31+G/PCM-Conf2**

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2B97DSS
parent sm
b97d/6-31+G**
E(RB97D) = -519.197401760

Zero-point correction= 0.235116 (Hartree/Particle)
Thermal correction to Energy= 0.248095
Thermal correction to Enthalpy= 0.249039
Thermal correction to Gibbs Free Energy= 0.195683
Sum of electronic and ZPE= -518.962286
Sum of electronic and thermal Energies= -518.949307
Sum of electronic and thermal Enthalpies= -518.948363
Sum of electronic and thermal Free Energies= -519.001719

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	155.682	48.081	112.297

C,0,2.0076945986,-0.8205454672,-2.2221865418
O,0,2.7631441439,0.4233686939,-2.3949424763
C,0,2.783621811,0.9417091154,-3.6306834428
O,0,2.2265966381,0.4701339888,-4.6107363015
C,0,3.6310018547,2.2184754652,-3.5843181267

N,0,3.7240257258,2.9934231153,-4.882986676
C,0,4.4427615318,2.1856943121,-5.9466955699
C,0,4.5357217272,4.2416542284,-4.5943732799
C,0,2.3299434327,3.4120657582,-5.4351124407
C,0,1.464615024,4.0905381425,-4.4129789521
C,0,1.1899969665,5.4052543755,-4.4531124932
H,0,2.1254840453,-1.0725320551,-1.1648997746
H,0,0.9549042758,-0.6459406165,-2.475382476
H,0,2.4324918594,-1.5989785131,-2.8675511314
H,0,4.6556332917,1.9568151871,-3.2937244941
H,0,3.2242567244,2.8955334491,-2.8246377382
H,0,3.8541772047,1.2903237882,-6.1572571239
H,0,4.5290565971,2.8141485694,-6.8388227549
H,0,5.4345265528,1.927183715,-5.5614518551
H,0,5.5146443074,3.9333237428,-4.2142054728
H,0,4.6425926308,4.7947810802,-5.5322009395
H,0,3.9972970971,4.8401770492,-3.8540614191
H,0,2.5569863657,4.0719490193,-6.2801838822
H,0,1.8774091882,2.4842155469,-5.7975553936
H,0,1.013018573,3.4600782485,-3.6440277413
H,0,1.6145465724,6.0502612092,-5.2258405304
H,0,0.5228832597,5.8642068517,-3.7223939721

TS B97D/6-31+G **/ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSB97DSS
23 parent ts
B97D/6-31+G**
E(RB97D) = -518.696707820

Zero-point correction= 0.217204 (Hartree/Particle)
Thermal correction to Energy= 0.230198
Thermal correction to Enthalpy= 0.231142
Thermal correction to Gibbs Free Energy= 0.178710
Sum of electronic and ZPE= -518.479504
Sum of electronic and thermal Energies= -518.466510
Sum of electronic and thermal Enthalpies= -518.465566
Sum of electronic and thermal Free Energies= -518.517998

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.451	48.161	110.354

C,0,1.9798755105,-0.8480299921,-2.35685013
O,0,2.7658999532,0.3578682374,-2.4711999942
C,0,2.8462504077,0.9061500604,-3.7507819627
C,0,3.5697244056,2.1337729604,-3.7226019974
N,0,3.8383117896,2.879903219,-4.8716463925
C,0,4.6651344623,4.0800776964,-4.5718596487
O,0,2.3213629263,0.3410369967,-4.7334779575
C,0,4.3703824437,2.1500430419,-6.0583060956
C,0,2.1250593563,3.714513854,-5.6625936116
C,0,1.5060686538,4.2578476635,-4.4991536592
C,0,0.9131954857,3.4425081801,-3.57045451
H,0,2.0241358657,-1.1229759336,-1.2965016293
H,0,0.9383953333,-0.665272175,-2.6607616149
H,0,2.4012420778,-1.6520345996,-2.978021079
H,0,3.7935497375,2.6032119331,-2.7707251108
H,0,5.3886830018,1.8003932583,-5.8317502087
H,0,3.7162309963,1.3023643115,-6.2737332094
H,0,4.3913717634,2.8449538743,-6.9066748274
H,0,5.655924055,3.7600682536,-4.2167482385
H,0,4.7661611509,4.6761892301,-5.485414992
H,0,4.1603958243,4.6682563752,-3.7970021005
H,0,2.5577078387,4.3797965994,-6.4114458584
H,0,1.7662626709,2.7514175528,-6.0294709111
H,0,1.686045065,5.3085000717,-4.2548405882
H,0,0.6971081559,2.4000120283,-3.8036829553
H,0,0.5697750689,3.8268883022,-2.6083407169

Cation B98/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2B98SB
parent sm
b98/6-31G*
E(RB98) = -519.297732939

Zero-point correction= 0.241750 (Hartree/Particle)
Thermal correction to Energy= 0.254650
Thermal correction to Enthalpy= 0.255594
Thermal correction to Gibbs Free Energy= 0.202269
Sum of electronic and ZPE= -519.055983
Sum of electronic and thermal Energies= -519.043083
Sum of electronic and thermal Enthalpies= -519.042139
Sum of electronic and thermal Free Energies= -519.095464

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.795	47.061	112.232

C,0,2.0511520949,-0.8384620976,-2.2639335555
O,0,2.7947074989,0.3932776758,-2.4135007396
C,0,2.7792421129,0.9470487766,-3.6192617027
O,0,2.1969559895,0.508328807,-4.5889027448
C,0,3.6197415104,2.2253425322,-3.5664110666
N,0,3.7142066001,2.9929613558,-4.8618557916
C,0,4.4175943779,2.1712294835,-5.9161811474
C,0,4.535297041,4.2292661254,-4.5870102661
C,0,2.3284795708,3.4112466434,-5.4079750519
C,0,1.4709015842,4.1336859804,-4.4083463941
C,0,1.1903226772,5.4377896238,-4.5007330085
H,0,2.1846069419,-1.126600535,-1.2218540184
H,0,0.9955821013,-0.6658870919,-2.487329396
H,0,2.45616358,-1.6014509366,-2.9330890547
H,0,4.6384732172,1.9650009772,-3.2643334111
H,0,3.2092023223,2.8944690506,-2.8056072501
H,0,3.8335953909,1.2716131273,-6.1039749549
H,0,4.4964499314,2.7740422465,-6.8225688936
H,0,5.4136707454,1.9171059896,-5.548424771
H,0,5.5060037646,3.9241537246,-4.1924949591
H,0,4.664779615,4.7711044532,-5.5253173525
H,0,4.0062716472,4.8505911853,-3.8635780573
H,0,2.545216563,4.0393657688,-6.2754247168
H,0,1.8598974626,2.4830581522,-5.7395153558
H,0,1.0140965468,3.5361470811,-3.6203318549
H,0,1.6043484755,6.0612908047,-5.291476956
H,0,0.5220726368,5.9215990963,-3.7928905292

TS B98/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSB98SB
23 parent ts
b98/6-31G*
E(RB98) = -518.778127035

Zero-point correction= 0.224009 (Hartree/Particle)
Thermal correction to Energy= 0.236695
Thermal correction to Enthalpy= 0.237640
Thermal correction to Gibbs Free Energy= 0.185806
Sum of electronic and ZPE= -518.554118
Sum of electronic and thermal Energies= -518.541432
Sum of electronic and thermal Enthalpies= -518.540488
Sum of electronic and thermal Free Energies= -518.592321

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.529	46.748	109.093

C,0,2.0351915029,-0.8199621689,-2.3344432231
O,0,2.7266413509,0.422673644,-2.4552158271
C,0,2.7996908645,0.9343133892,-3.7276172516
C,0,3.439543792,2.2120700238,-3.7180254457
N,0,3.7988004862,2.8993535806,-4.868964433
C,0,4.6858576417,4.0450461523,-4.5744597175
O,0,2.3300928962,0.3195786426,-4.693045269
C,0,4.2975507558,2.1130335139,-6.021546311
C,0,2.1341690469,3.845453199,-5.6946417408
C,0,1.5026782756,4.2656020793,-4.5042407364
C,0,0.98585198,3.3312692607,-3.6439036039
H,0,2.0744628231,-1.0776374792,-1.2735342148
H,0,0.9920362705,-0.7271847763,-2.6572815925
H,0,2.5191146524,-1.6035597215,-2.9276462143
H,0,3.7141424658,2.6565390461,-2.7715624032
H,0,5.303558683,1.7347527723,-5.7993564134
H,0,3.6206238852,1.2785709134,-6.1977229862
H,0,4.3382781019,2.7652465147,-6.8985571399
H,0,5.6412126181,3.6846784938,-4.1728513251
H,0,4.8634408437,4.609089247,-5.4930489118
H,0,4.2010139373,4.6910731773,-3.8384797952
H,0,2.5720488361,4.5735066329,-6.3753021154
H,0,1.795294042,2.9229135515,-6.1616488199
H,0,1.6732859554,5.2831316116,-4.1505973805
H,0,0.7152845933,2.3406726597,-3.9981556954
H,0,0.6543876994,3.5972370402,-2.6421914327

Cation B98/6-31+G* */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2B98SS
parent sm
b98/6-31+G**
E(RB98) = -519.330102315

Zero-point correction= 0.240167 (Hartree/Particle)
Thermal correction to Energy= 0.253178
Thermal correction to Enthalpy= 0.254123
Thermal correction to Gibbs Free Energy= 0.200411
Sum of electronic and ZPE= -519.089935
Sum of electronic and thermal Energies= -519.076924
Sum of electronic and thermal Enthalpies= -519.075980
Sum of electronic and thermal Free Energies= -519.129691

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.872	47.378	113.045

C,0,2.0450435856,-0.8438261167,-2.2514978415
O,0,2.7855741189,0.3919503897,-2.4110161534
C,0,2.7835625983,0.9389173373,-3.6208642759
O,0,2.2115251152,0.4911307794,-4.5942157179
C,0,3.6232682861,2.2160897102,-3.5711435091
N,0,3.7155216955,2.9917328526,-4.8624738276
C,0,4.4176219765,2.1784979748,-5.9261902622
C,0,4.5421548553,4.2240415271,-4.5779200664
C,0,2.333075693,3.4200709572,-5.4060969951
C,0,1.4772143564,4.1450643922,-4.4058711479
C,0,1.1705343792,5.4433163892,-4.5162274646
H,0,2.1757358284,-1.1187418556,-1.2062100138
H,0,0.9906208736,-0.6757183276,-2.4805952297
H,0,2.4582110355,-1.6106674694,-2.9101233536
H,0,4.6420289956,1.9505571625,-3.2748146264
H,0,3.2181326288,2.879766778,-2.8034282973
H,0,3.8262463555,1.288974103,-6.1357246497
H,0,4.510857665,2.7956918579,-6.8206633625
H,0,5.407189435,1.9067507003,-5.5555549644
H,0,5.5179661186,3.9117792167,-4.2041403895
H,0,4.65717726,4.7816508914,-5.5078953601
H,0,4.0265379934,4.8334094645,-3.8358609827
H,0,2.5519310566,4.0496877214,-6.2715173033
H,0,1.8557547401,2.4981103667,-5.7421620211
H,0,1.038016093,3.5557079056,-3.6022222747
H,0,1.5668265811,6.0606458036,-5.3201575804
H,0,0.5007026797,5.9227274882,-3.8077353292

TS B98/6-31+G **/ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSB98SS
23 parent ts
b98/6-31+G**
E(RB98) = -518.819267263

Zero-point correction= 0.222269 (Hartree/Particle)
Thermal correction to Energy= 0.235138
Thermal correction to Enthalpy= 0.236082
Thermal correction to Gibbs Free Energy= 0.183823
Sum of electronic and ZPE= -518.596999
Sum of electronic and thermal Energies= -518.584129
Sum of electronic and thermal Enthalpies= -518.583185
Sum of electronic and thermal Free Energies= -518.635444

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.551	47.257	109.988

C,0,2.0412593518,-0.8267692261,-2.3008137363
O,0,2.7190278056,0.4260191141,-2.4465444468
C,0,2.8149821644,0.9158214068,-3.7260214799
C,0,3.4390770886,2.2031873612,-3.7276469734
N,0,3.8088367451,2.8904031776,-4.871452986

C,0,4.7039598834,4.0301849209,-4.5710538603
O,0,2.3823501301,0.2702665079,-4.6915996997
C,0,4.2899686952,2.118488755,-6.0416133272
C,0,2.121164167,3.8847659106,-5.7040955003
C,0,1.4958322248,4.2725832317,-4.500377354
C,0,0.9507901039,3.327221729,-3.6660957999
H,0,2.0625881891,-1.0475448506,-1.2322592323
H,0,1.0054493406,-0.7548936703,-2.6478627509
H,0,2.552942135,-1.6181270278,-2.8573736186
H,0,3.6774918205,2.6629131817,-2.7786773971
H,0,5.2797821021,1.6995524141,-5.8213458399
H,0,3.5912812062,1.3119609791,-6.2546053745
H,0,4.3627897419,2.7946387344,-6.8968185888
H,0,5.6641030908,3.6602639015,-4.1909250764
H,0,4.8698339524,4.6082159939,-5.4820486516
H,0,4.2355700886,4.666575482,-3.8173392102
H,0,2.5811594768,4.6272986847,-6.352209248
H,0,1.7879226145,2.9742864537,-6.1964816921
H,0,1.67564128,5.2774920731,-4.1179039433
H,0,0.6787563818,2.3445318943,-4.0402643938
H,0,0.62169422,3.5781238673,-2.660609818

Cation wB97/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2wB97SB
parent sm
wb97/6-31G*
E(RwB97) = -519.414979918

Zero-point correction= 0.245716 (Hartree/Particle)
Thermal correction to Energy= 0.258387
Thermal correction to Enthalpy= 0.259332
Thermal correction to Gibbs Free Energy= 0.206296
Sum of electronic and ZPE= -519.169264
Sum of electronic and thermal Energies= -519.156592
Sum of electronic and thermal Enthalpies= -519.155648
Sum of electronic and thermal Free Energies= -519.208684

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.141	46.124	111.624

C,0,2.027264072,-0.7818090359,-2.2746428635
O,0,2.7964059745,0.4324154631,-2.411527894
C,0,2.7752324748,0.989122438,-3.6139720138
O,0,2.1743214336,0.5576888068,-4.5747646762
C,0,3.6246608842,2.253090682,-3.5759765845
N,0,3.7193050049,2.9940831032,-4.8741495637
C,0,4.4283885243,2.1628687254,-5.9015625403
C,0,4.5257106615,4.2319491902,-4.6175014917
C,0,2.3524997067,3.3934596299,-5.4274080012
C,0,1.4687606399,4.0560766068,-4.4103891753
C,0,1.2017410043,5.3606069905,-4.4307777236
H,0,2.1773223714,-1.1038478471,-1.2440361874
H,0,0.9711804255,-0.5746521922,-2.4672529062
H,0,2.3948508867,-1.5358232078,-2.9756398828
H,0,4.6414302752,1.9859732941,-3.2700271664
H,0,3.2183340121,2.9335539517,-2.8210307355
H,0,3.8567645921,1.2493654465,-6.0687323533
H,0,4.4967454112,2.7431522473,-6.8249303675
H,0,5.4299928937,1.9309849451,-5.5308797365
H,0,5.4936951962,3.942262444,-4.2021057288
H,0,4.6666096827,4.7554447871,-5.5659103248
H,0,3.9834264232,4.8672011451,-3.9138096345
H,0,2.5651588927,4.0640194603,-6.2659872998
H,0,1.901550771,2.4735988762,-5.805539994
H,0,0.9935100093,3.4125129641,-3.6685078846
H,0,1.6389455281,6.023289565,-5.1782074461
H,0,0.5252242481,5.8107295207,-3.7070528244

TS WB97/6-31G */ PCM-TS

home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentT
SwB97SB
23 parent ts
wb97/6-31G*
E(RwB97) = -518.876911794

Zero-point correction= 0.229013 (Hartree/Particle)
Thermal correction to Energy= 0.240985
Thermal correction to Enthalpy= 0.241929
Thermal correction to Gibbs Free Energy= 0.191754
Sum of electronic and ZPE= -518.647899
Sum of electronic and thermal Energies= -518.635927
Sum of electronic and thermal Enthalpies= -518.634983
Sum of electronic and thermal Free Energies= -518.685157

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.220	44.788	105.601

C,0,2.0647973152,-0.8397152466,-2.3884806782
O,0,2.7186324101,0.4262440472,-2.4845413274
C,0,2.7190795111,0.9818967749,-3.7294304435
C,0,3.2515619291,2.3130375028,-3.7040519631
N,0,3.6830072335,2.9465244389,-4.8925948633
C,0,4.5854705612,4.0675706801,-4.572208716
O,0,2.2148794265,0.3970282587,-4.6908063013
C,0,4.2696863181,2.1047983286,-5.9551671426
C,0,2.1813682645,3.7812811284,-5.6941129518
C,0,1.5324294751,4.2953791521,-4.5512289291
C,0,1.2028388577,3.3214392224,-3.6270402817
H,0,2.1473311126,-1.1377865395,-1.3405912436
H,0,1.010449279,-0.7595860105,-2.6747960464
H,0,2.5515527928,-1.5818681297,-3.0301898615
H,0,3.7121043067,2.6571118689,-2.7841855214
H,0,5.2528503125,1.7363985693,-5.6389766098
H,0,3.6040434238,1.2648956983,-6.1534248608
H,0,4.3835485864,2.7163079062,-6.8570555472
H,0,5.4955621267,3.6877227101,-4.0932747124
H,0,4.8467692955,4.59643196,-5.4940217149
H,0,4.0703735543,4.7515208202,-3.8915045191
H,0,2.61885162,4.4537817486,-6.4361190914
H,0,1.787498261,2.8552326542,-6.1218154965
H,0,1.7594197233,5.3097126477,-4.2201704534
H,0,0.7866147028,2.3760155581,-3.9748880605
H,0,0.9635336004,3.5760852505,-2.5933626629

Cation wB97XD/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2wB97XDSB
parent sm
wb97xd/6-31G*
E(RwB97XD) = -519.348291809

Zero-point correction= 0.244927 (Hartree/Particle)
Thermal correction to Energy= 0.257599
Thermal correction to Enthalpy= 0.258543
Thermal correction to Gibbs Free Energy= 0.205559
Sum of electronic and ZPE= -519.103365
Sum of electronic and thermal Energies= -519.090693
Sum of electronic and thermal Enthalpies= -519.089749
Sum of electronic and thermal Free Energies= -519.142733

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.646	46.168	111.515

C,0,2.0403547456,-0.7867962794,-2.2668301088
O,0,2.8041856281,0.4228924401,-2.4216470239
C,0,2.7693074886,0.9853819402,-3.6166718377
O,0,2.1607071269,0.5610826954,-4.5723325102
C,0,3.6131878276,2.2505046315,-3.5772362448
N,0,3.7156704256,2.9935485937,-4.8748035216
C,0,4.4291701538,2.1629293654,-5.901018312
C,0,4.5218658988,4.2309520664,-4.6100797711
C,0,2.3483565629,3.3971941767,-5.436540455
C,0,1.4619365898,4.0613303066,-4.4292966264
C,0,1.2123560028,5.3685965162,-4.4345820445
H,0,2.2309259681,-1.1191490322,-1.2489713514
H,0,0.9795417257,-0.5760891329,-2.4114406418
H,0,2.3744398038,-1.5350992163,-2.9869045452
H,0,4.6264220906,1.9891580328,-3.264507918
H,0,3.2014749402,2.9297894177,-2.8280326271
H,0,3.8556868633,1.2556848434,-6.0776825928
H,0,4.5088583147,2.7453729103,-6.8187167879
H,0,5.4233012587,1.9234806082,-5.5236323095
H,0,5.486786437,3.9412875014,-4.1949099981
H,0,4.6638423405,4.758609696,-5.5526315392
H,0,3.9796012575,4.8610688732,-3.9062359041
H,0,2.5686731507,4.0593743359,-6.2755872844
H,0,1.8999900098,2.4784012293,-5.8112517626
H,0,0.972038497,3.4166768656,-3.7030601209
H,0,1.665440842,6.0358740006,-5.1638445589
H,0,0.5349100498,5.8152606142,-3.7138746023

WB97XD/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSwB97XDSB
glycine allyl TSfreq
wb97xd/6-31G*
E(RwB97XD) = -518.818252298

Zero-point correction= 0.227675 (Hartree/Particle)
Thermal correction to Energy= 0.239819
Thermal correction to Enthalpy= 0.240763
Thermal correction to Gibbs Free Energy= 0.190399
Sum of electronic and ZPE= -518.590577
Sum of electronic and thermal Energies= -518.578434
Sum of electronic and thermal Enthalpies= -518.577489
Sum of electronic and thermal Free Energies= -518.627854

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.488	45.456	106.000

C,0,2.0142989125,-0.7958060399,-2.3641659798
O,0,2.711634185,0.4381595342,-2.4762017862
C,0,2.7803116218,0.959587034,-3.7337312741
C,0,3.3875172225,2.2489364786,-3.7178403505
N,0,3.7729411004,2.9115393467,-4.8740432652
C,0,4.6409939234,4.0601898382,-4.575828495
O,0,2.3081801512,0.3582182663,-4.7002946578
C,0,4.3000605232,2.1166898535,-5.9964975015
C,0,2.1295999673,3.8068074742,-5.6969127528
C,0,1.5230595358,4.2431118646,-4.5111421398
C,0,1.1031006121,3.2894966388,-3.6195930458
H,0,2.0513860109,-1.062555839,-1.3076170661
H,0,0.9739551785,-0.692250158,-2.6857291704
H,0,2.492675602,-1.5758891964,-2.9627531652
H,0,3.7234357748,2.6577855144,-2.7763202792
H,0,5.3007313618,1.7451422969,-5.7509659543
H,0,3.6317415666,1.2793626874,-6.182060697
H,0,4.3569695255,2.7561916477,-6.8803461497
H,0,5.5844255383,3.7148927115,-4.1401452366
H,0,4.8414391448,4.6101033469,-5.4966970748
H,0,4.1303378232,4.7155151035,-3.8680122479
H,0,2.5504230853,4.5199078396,-6.4023156174
H,0,1.7907978273,2.8716356812,-6.1371650561
H,0,1.7098087575,5.2584419727,-4.1662084386
H,0,0.7734548698,2.3178212197,-3.9726473748
H,0,0.8309741785,3.5444258826,-2.5988052232

Cation wB97XD/6-31+G **/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2wB97XDSS
parent sm
wb97xd/6-31+G**
E(RwB97XD) = -519.379062031

Zero-point correction= 0.243470 (Hartree/Particle)
Thermal correction to Energy= 0.256170
Thermal correction to Enthalpy= 0.257114
Thermal correction to Gibbs Free Energy= 0.204264
Sum of electronic and ZPE= -519.135592
Sum of electronic and thermal Energies= -519.122892
Sum of electronic and thermal Enthalpies= -519.121948
Sum of electronic and thermal Free Energies= -519.174798

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.749	46.433	111.233

C,0,2.0281293843,-0.7863721771,-2.2529988938
O,0,2.7911535574,0.4252327463,-2.4182452221
C,0,2.7763381389,0.9754952203,-3.6199554132
O,0,2.1828585502,0.5377711058,-4.5808939298
C,0,3.6201820071,2.2391083105,-3.5841410717

N,0,3.7180947506,2.9918551932,-4.8765676076
C,0,4.4323251679,2.1745110928,-5.9143231153
C,0,4.5263986848,4.2269549039,-4.6010660011
C,0,2.3515453701,3.4013178072,-5.4331993999
C,0,1.4676958764,4.0666127736,-4.4238230381
C,0,1.1950947567,5.3702017465,-4.4467400474
H,0,2.2165466026,-1.1064420806,-1.2314422709
H,0,0.9682709699,-0.5766560723,-2.402303379
H,0,2.3672635707,-1.5404796027,-2.9637932876
H,0,4.6339982417,1.9720538635,-3.2787829492
H,0,3.2153167712,2.9129388176,-2.826834865
H,0,3.8559316063,1.2746304928,-6.1146684597
H,0,4.5216477063,2.7741388699,-6.8193230684
H,0,5.4219499736,1.9218569666,-5.5354585774
H,0,5.4959733915,3.9313947338,-4.2028025327
H,0,4.6561110091,4.7689842514,-5.5363793634
H,0,3.9937200527,4.845914149,-3.8810852519
H,0,2.5711564849,4.0658025836,-6.270384143
H,0,1.897328593,2.4863513842,-5.8106609812
H,0,0.9946790378,3.4282521689,-3.6811087802
H,0,1.6314233022,6.0318371689,-5.1906864237
H,0,0.5178984421,5.8140515823,-3.7246549271

TS WB97XD/6-31+G **/ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSwB97SDSS
23 parent ts
wB97xD/6-31+G**
E(RwB97XD) = -518.856711302

Zero-point correction= 0.225781 (Hartree/Particle)
Thermal correction to Energy= 0.238136
Thermal correction to Enthalpy= 0.239081
Thermal correction to Gibbs Free Energy= 0.188120
Sum of electronic and ZPE= -518.630930
Sum of electronic and thermal Energies= -518.618575
Sum of electronic and thermal Enthalpies= -518.617631
Sum of electronic and thermal Free Energies= -518.668591

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.433	46.011	107.256

C,0,2.0089085743,-0.79561239,-2.3373730977
O,0,2.7030905924,0.4428211763,-2.4699512709
C,0,2.7909823498,0.9483538925,-3.7322269943
C,0,3.3905335106,2.2426879308,-3.7267149683
N,0,3.786101013,2.9042598198,-4.875669322
C,0,4.6585188323,4.0497433533,-4.5740132981
O,0,2.3466248635,0.3238485041,-4.7004090288
C,0,4.2969821442,2.121217749,-6.0139776092
C,0,2.1132098054,3.8395638969,-5.7066715256
C,0,1.5202629807,4.242477767,-4.5045649932
C,0,1.0848920454,3.273465002,-3.6332181558
H,0,2.0335749313,-1.0341410229,-1.2747892065
H,0,0.9738367892,-0.7005702923,-2.6751366819
H,0,2.5026534426,-1.5844726251,-2.9098300666
H,0,3.6970687527,2.6640778616,-2.7806398626
H,0,5.2868601032,1.7194244731,-5.7733139154
H,0,3.6127157737,1.3042747566,-6.2275258246
H,0,4.3741703217,2.7800141987,-6.880930494
H,0,5.6069886747,3.6997272901,-4.1537250652
H,0,4.8483165322,4.6092953984,-5.49042632
H,0,4.1591718596,4.6991293697,-3.8534976175
H,0,2.5482474309,4.5684301561,-6.3855334972
H,0,1.7838566139,2.9110256268,-6.1662266421
H,0,1.7129216978,5.2474028363,-4.1342723954
H,0,0.755154883,2.3092335149,-4.0058430288
H,0,0.8186094818,3.5117827559,-2.6075591183

Cation wB97X/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2wB97XSB
parent sm
wb97x/6-31G*
E(RwB97X) = -519.373462601

Zero-point correction= 0.245540 (Hartree/Particle)
Thermal correction to Energy= 0.258240
Thermal correction to Enthalpy= 0.259184
Thermal correction to Gibbs Free Energy= 0.206043
Sum of electronic and ZPE= -519.127923
Sum of electronic and thermal Energies= -519.115223
Sum of electronic and thermal Enthalpies= -519.114279
Sum of electronic and thermal Free Energies= -519.167419

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.048	46.151	111.843

C,0,2.0413972326,-0.7945103089,-2.2775796753
O,0,2.8020144345,0.4208797263,-2.4172706499
C,0,2.7761660057,0.9815270416,-3.614571658
O,0,2.1769739038,0.552019516,-4.574329743
C,0,3.6182736522,2.2475186299,-3.5728766926
N,0,3.7144545745,2.9929216119,-4.8678585174
C,0,4.4210593006,2.1642960158,-5.8984892658
C,0,4.5238187865,4.2272672345,-4.6071549332
C,0,2.3472540979,3.3965141857,-5.4199362321
C,0,1.4713200604,4.0779762002,-4.4129364175
C,0,1.203923097,5.38033531,-4.4554815415
H,0,2.2053140473,-1.1214697123,-1.252777242
H,0,0.9837375199,-0.5915271182,-2.454580335
H,0,2.4014523875,-1.542590624,-2.9857592697
H,0,4.6334276738,1.9847267625,-3.2649196212
H,0,3.2090567725,2.9234592662,-2.8183888557
H,0,3.8456045969,1.2573201771,-6.0737022728
H,0,4.49681842,2.7489877275,-6.815984253
H,0,5.4180191156,1.9234187849,-5.5271396299
H,0,5.4905919915,3.9347069384,-4.1963822454
H,0,4.6635044494,4.7544272304,-5.5513226068
H,0,3.9864728796,4.8597352956,-3.9005456411
H,0,2.5613815783,4.0516793529,-6.2672877692
H,0,1.8906290982,2.476035727,-5.7833593078
H,0,0.9988026818,3.4500703046,-3.6591273084
H,0,1.6368531031,6.0299901442,-5.2137302412
H,0,0.5307105387,5.8416025803,-3.7388310749

TS wB97x/6-31G*/PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSwB97xSB
23 parent ts
wb97x/6-31G*
E(RwB97X) = -518.839136984

Zero-point correction= 0.228505 (Hartree/Particle)
Thermal correction to Energy= 0.240607
Thermal correction to Enthalpy= 0.241551
Thermal correction to Gibbs Free Energy= 0.191103
Sum of electronic and ZPE= -518.610632
Sum of electronic and thermal Energies= -518.598530
Sum of electronic and thermal Enthalpies= -518.597586
Sum of electronic and thermal Free Energies= -518.648034

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.983	45.169	106.176

C,0,2.0392631875,-0.8147728155,-2.3740740216
O,0,2.7144533461,0.4348897983,-2.4773640026
C,0,2.7513968478,0.9720060946,-3.7287903311
C,0,3.3243847463,2.2800981033,-3.7113197289
N,0,3.7337319621,2.9258125976,-4.880010738
C,0,4.618078319,4.0605140935,-4.5744437174
O,0,2.2637115654,0.3781464254,-4.6914495461
C,0,4.2843844744,2.1094603426,-5.9762166106
C,0,2.1490882964,3.8028944059,-5.6980254947
C,0,1.5275046017,4.2661713676,-4.5289151535
C,0,1.1500940974,3.2999020693,-3.6264192833
H,0,2.0963729801,-1.0974964744,-1.322176329
H,0,0.9932959499,-0.7231490757,-2.6806787815
H,0,2.5232578692,-1.5752239923,-2.9930657919
H,0,3.7181632452,2.6583834982,-2.7774695608
H,0,5.2794771442,1.7414009855,-5.7035561869
H,0,3.6190845848,1.2693981822,-6.1636509746
H,0,4.3622408252,2.7345221309,-6.8699971139
H,0,5.5452505542,3.7007133586,-4.1158090469
H,0,4.8496793674,4.5976663473,-5.4967396119
H,0,4.1055613447,4.7321866191,-3.8824942155
H,0,2.5780584198,4.5002916109,-6.4167462351
H,0,1.790477557,2.8708425981,-6.1336018654
H,0,1.7227000427,5.2821888878,-4.1884173813
H,0,0.786274875,2.3398846711,-3.9823261485
H,0,0.8882677964,3.5507291699,-2.6002821289

Cation wb97x /6-31+G **/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SM2wB97XSS
parent sm
wb97x/6-31+G**
E(RwB97X) = -519.406513476

Zero-point correction= 0.243947 (Hartree/Particle)
Thermal correction to Energy= 0.256704
Thermal correction to Enthalpy= 0.257648
Thermal correction to Gibbs Free Energy= 0.204398
Sum of electronic and ZPE= -519.162567
Sum of electronic and thermal Energies= -519.149810
Sum of electronic and thermal Enthalpies= -519.148866
Sum of electronic and thermal Free Energies= -519.202115

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.084	46.401	112.073

C,0,2.0303271615,-0.7932456544,-2.2629029431
O,0,2.7893332396,0.4251491313,-2.4138539885
C,0,2.7816572643,0.9749763353,-3.6170420288
O,0,2.1950482311,0.5332519975,-4.5811868043
C,0,3.6238052887,2.2392881506,-3.5801392237
N,0,3.7171545757,2.9919536905,-4.8712450891
C,0,4.4230255746,2.1726391328,-5.9113250661
C,0,4.5310881444,4.222634355,-4.6010517598
C,0,2.3519503028,3.4036573302,-5.4202875875
C,0,1.4746805726,4.0798359626,-4.4102047577
C,0,1.185798628,5.3785662808,-4.460111764
H,0,2.1835252702,-1.1002987149,-1.230827623
H,0,0.9749544257,-0.5948170487,-2.4560338649
H,0,2.404558453,-1.5503499006,-2.953452863
H,0,4.6393168139,1.9710108415,-3.2780176696
H,0,3.2205933576,2.9111404097,-2.8189980807
H,0,3.8425749403,1.2731078259,-6.1066320635
H,0,4.5091534611,2.7717945099,-6.8181094975
H,0,5.4154091576,1.9181966107,-5.5379464739
H,0,5.5023350703,3.9226097615,-4.2076437806
H,0,4.6587613632,4.7636971997,-5.5384097078
H,0,4.00505958,4.8451724036,-3.8778689603
H,0,2.5676805663,4.0656560813,-6.2619343097
H,0,1.8907047584,2.48896155,-5.7932298057
H,0,1.0147139581,3.45305484,-3.6475083413
H,0,1.605963871,6.0281593719,-5.2253358687
H,0,0.50985797,5.8315155463,-3.7410230775

TSwB97x/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSwB97xSS
23 parent ts
wB97x/6-31+G**
E(RwB97X) = -518.879949446

Zero-point correction= 0.226475 (Hartree/Particle)
Thermal correction to Energy= 0.238794
Thermal correction to Enthalpy= 0.239739
Thermal correction to Gibbs Free Energy= 0.188772
Sum of electronic and ZPE= -518.653474
Sum of electronic and thermal Energies= -518.641155
Sum of electronic and thermal Enthalpies= -518.640211
Sum of electronic and thermal Free Energies= -518.691177

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.846	45.759	107.268

C,0,2.0338231588,-0.8112522384,-2.336653686
O,0,2.6986914702,0.4465865879,-2.4654764794
C,0,2.7658618417,0.9578768879,-3.7267977614
C,0,3.332566666,2.2692221281,-3.7245613077
N,0,3.7502469375,2.9171437834,-4.8826541058

C,0,4.6445145277,4.0438653786,-4.5728059848
O,0,2.3169383227,0.3299635249,-4.6905110387
C,0,4.2765332039,2.1145908315,-6.0008245891
C,0,2.1351735115,3.8504537227,-5.7070808756
C,0,1.5243566719,4.264458023,-4.5164337051
C,0,1.1193381183,3.2756201549,-3.6485257206
H,0,2.0759285181,-1.0587119333,-1.2761012556
H,0,0.9934889097,-0.7357899076,-2.6638915506
H,0,2.5409691455,-1.5810284365,-2.9236091994
H,0,3.68332659,2.6691091754,-2.7825396153
H,0,5.2579420891,1.705619026,-5.7366158451
H,0,3.5884975991,1.3014008166,-6.2208209118
H,0,4.3788804114,2.7640485798,-6.8736853878
H,0,5.5774036564,3.6743581887,-4.1336008491
H,0,4.8645931267,4.5931894915,-5.4900127378
H,0,4.1482762831,4.7095585574,-3.8637992785
H,0,2.5806142571,4.5743109908,-6.3874681113
H,0,1.7869338484,2.9317944044,-6.1765853767
H,0,1.7215515622,5.2667558882,-4.1386112225
H,0,0.7649511152,2.3243689241,-4.0363089111
H,0,0.852852458,3.4999484501,-2.618064493

Cation LC-B97D /6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
SMLCB97DSB
parent sm
LC-B97D/6-31G*
E(RB97D) = -518.216650707

Zero-point correction= 0.246785 (Hartree/Particle)
Thermal correction to Energy= 0.258980
Thermal correction to Enthalpy= 0.259924
Thermal correction to Gibbs Free Energy= 0.208322
Sum of electronic and ZPE= -517.969866
Sum of electronic and thermal Energies= -517.957670
Sum of electronic and thermal Enthalpies= -517.956726
Sum of electronic and thermal Free Energies= -518.008329

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.513	45.152	108.607

C,0,1.989353905,-0.6828483473,-2.262528349
O,0,2.7986906503,0.4989901678,-2.4193588055
C,0,2.7496440793,1.0716964133,-3.6018873459
O,0,2.0944100652,0.6792326828,-4.5350597143
C,0,3.6240122751,2.3056134941,-3.5913970923
N,0,3.727002951,3.0014406935,-4.9088994951
C,0,4.4585373694,2.1455042585,-5.8906045163
C,0,4.5100354273,4.2537876781,-4.6763147198
C,0,2.3712543039,3.3773940958,-5.5060133651
C,0,1.432512444,3.8966873563,-4.4655360898
C,0,1.2544763563,5.1898574512,-4.2600055694
H,0,2.1483337983,-1.0140221655,-1.2370355169
H,0,0.9405093128,-0.4312208595,-2.439813655
H,0,2.3127403792,-1.4425635146,-2.9787280122
H,0,4.6366518324,2.0328079359,-3.283583681
H,0,3.2218815991,3.0134588224,-2.8624670364
H,0,3.902178674,1.2158475755,-6.0127811366
H,0,4.5108389442,2.6911211376,-6.8353126117
H,0,5.4615690488,1.958152212,-5.5007689291
H,0,5.4609673234,3.9858121876,-4.2108134917
H,0,4.6777906636,4.7312808185,-5.6435248562
H,0,3.9250346931,4.904850131,-4.0234814896
H,0,2.594761528,4.1318030612,-6.2648406009
H,0,1.9856088945,2.4759782427,-5.977601708
H,0,0.9036311499,3.1509024453,-3.8743743508
H,0,1.7855263223,5.9281617676,-4.8600468803
H,0,0.5710780094,5.5575922583,-3.4995439812

TS LC-B97D/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parent
TSLCB97DSB
23 parent ts
LC-B97D/6-31G*
E(RB97D) = -517.680577010

Zero-point correction= 0.229305 (Hartree/Particle)
Thermal correction to Energy= 0.241036
Thermal correction to Enthalpy= 0.241980
Thermal correction to Gibbs Free Energy= 0.192564
Sum of electronic and ZPE= -517.451272
Sum of electronic and thermal Energies= -517.439541
Sum of electronic and thermal Enthalpies= -517.438597
Sum of electronic and thermal Free Energies= -517.488013

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.252	44.463	104.005

C,0,1.8665656953,-0.7084827635,-2.4386998118
O,0,2.7072902216,0.4380079121,-2.5108465806
C,0,2.8305665286,0.981802071,-3.7444684079
C,0,3.4680533718,2.2485069801,-3.7029343693
N,0,3.8173604732,2.9064894862,-4.867086469
C,0,4.5801502552,4.1242225241,-4.601073593
O,0,2.3289673586,0.4403776491,-4.72662376
C,0,4.3831357478,2.1523017176,-5.9906338484
C,0,2.0640614183,3.6501951248,-5.6729481568
C,0,1.5315939855,4.1365281349,-4.4863810902
C,0,1.2503823742,3.2089393585,-3.5146804522
H,0,1.852616292,-1.0084835273,-1.389196827
H,0,0.8548262135,-0.4608072811,-2.7797978123
H,0,2.2581655607,-1.5169304356,-3.0638956091
H,0,3.8577381941,2.6213448109,-2.7657876336
H,0,5.4227679257,1.8803089802,-5.7668983737
H,0,3.7830916724,1.2594428242,-6.1561559108
H,0,4.3548983786,2.7962751437,-6.8761667047
H,0,5.5579600816,3.8656544844,-4.1749070445
H,0,4.7135253983,4.6709601629,-5.5391002976
H,0,4.0165369452,4.7403206388,-3.8945069468
H,0,2.4484842482,4.3164887052,-6.4432050277
H,0,1.7812815192,2.6502386321,-6.0002687691
H,0,1.7270445248,5.1708646613,-4.2064555611
H,0,0.8767705219,2.2298102864,-3.7999240743
H,0,1.0804190939,3.503084719,-2.4813968683

Cation- B3LYP /6-31+G/PCM-Conf2**

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM2B3LYPSS
parent sm
B3LYP/6-31+G**
E(RB3LYP) = -519.536967748

Zero-point correction= 0.240197 (Hartree/Particle)
Thermal correction to Energy= 0.253276
Thermal correction to Enthalpy= 0.254221
Thermal correction to Gibbs Free Energy= 0.199879
Sum of electronic and ZPE= -519.296770
Sum of electronic and thermal Energies= -519.283691
Sum of electronic and thermal Enthalpies= -519.282747
Sum of electronic and thermal Free Energies= -519.337089

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.933	47.446	114.371

C,0,2.0567111022,-0.8679876245,-2.2528599574
O,0,2.796051203,0.3733597139,-2.4118368817
C,0,2.7866344848,0.9295161946,-3.6201584389
O,0,2.2101830471,0.4845457872,-4.5935833724
C,0,3.6191443785,2.2068828839,-3.5671505481
N,0,3.7107970344,2.9914219293,-4.8544286647
C,0,4.4103552921,2.1838482363,-5.9250945069
C,0,4.5409646282,4.2207797237,-4.5643798171
C,0,2.3262510403,3.4247968442,-5.3935402348
C,0,1.4863126127,4.1776356596,-4.4056544417
C,0,1.1679050496,5.4671008014,-4.554365488
H,0,2.1935558471,-1.1452895965,-1.2100951562
H,0,1.0021855652,-0.7004035175,-2.4761365337
H,0,2.4682535926,-1.6301854027,-2.9159062534
H,0,4.6375253279,1.9449305258,-3.2716426849
H,0,3.2132958016,2.8646222135,-2.7970340897
H,0,3.8146491992,1.3023683994,-6.1476028198
H,0,4.5123832558,2.8093184031,-6.811184128
H,0,5.3951058772,1.9001245027,-5.5543718602
H,0,5.5183560127,3.9047600312,-4.201976995
H,0,4.6488202376,4.7870184544,-5.4884684017
H,0,4.0330690572,4.8230334041,-3.8135731996
H,0,2.5436130135,4.0329539254,-6.2726125778
H,0,1.839026617,2.5017043708,-5.7069289851
H,0,1.065428755,3.6148788878,-3.5752533719
H,0,1.5457673256,6.0597966939,-5.3838872164
H,0,0.5066866416,5.9657865549,-3.8525963752

TS- B3LYP/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23parentTSB3LYPSS
23 parent ts
B3LYP/6-31+G**
E(RB3LYP) = -519.030461902

Zero-point correction= 0.222429 (Hartree/Particle)
Thermal correction to Energy= 0.235288
Thermal correction to Enthalpy= 0.236233
Thermal correction to Gibbs Free Energy= 0.183971
Sum of electronic and ZPE= -518.808033
Sum of electronic and thermal Energies= -518.795173
Sum of electronic and thermal Enthalpies= -518.794229
Sum of electronic and thermal Free Energies= -518.846491

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.646	47.282	109.994

C,0,2.0464163806,-0.8404928319,-2.3029579915
O,0,2.7308080223,0.4128404119,-2.4453893647
C,0,2.8273741842,0.9117607462,-3.7266111398
C,0,3.4654026925,2.1860789655,-3.7255076312
N,0,3.8208471062,2.8832849213,-4.8665259223
C,0,4.7132744981,4.0259671603,-4.5688935975
O,0,2.385320975,0.2721326076,-4.6948047545
C,0,4.2960271129,2.1187232574,-6.0443986626
C,0,2.1168394678,3.8755825629,-5.6983323958
C,0,1.4889082395,4.2807756554,-4.5022817705
C,0,0.9065949286,3.3672315433,-3.6656474406
H,0,2.0705016078,-1.0656095875,-1.2364122536
H,0,1.0109504262,-0.7627408857,-2.6459924636
H,0,2.5524331476,-1.6306357383,-2.864208327
H,0,3.6923551141,2.6497326321,-2.7772679816
H,0,5.2871383863,1.7019403186,-5.831547437
H,0,3.5995235294,1.3120250644,-6.2565750038
H,0,4.3628180595,2.7974072509,-6.8962440417
H,0,5.6789058711,3.6583667551,-4.2041153657
H,0,4.8653966213,4.6111560314,-5.4760087306
H,0,4.2529195316,4.6535375176,-3.8050270754
H,0,2.5806312337,4.6083004309,-6.3521704184
H,0,1.7818858019,2.9624588415,-6.1804654629
H,0,1.6691797097,5.2912043751,-4.1376569459
H,0,0.6507166766,2.372773325,-4.0152556285
H,0,0.5610846756,3.643659669,-2.673742193

TS- UB3LYP/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/tsUB3BBPCM
sean allyl ester checking ts for u instability
UB3LYP/6-31+G**
E(UB3LYP) = -519.030461924

Zero-point correction= 0.222428 (Hartree/Particle)
Thermal correction to Energy= 0.235288
Thermal correction to Enthalpy= 0.236232
Thermal correction to Gibbs Free Energy= 0.183970
Sum of electronic and ZPE= -518.808034
Sum of electronic and thermal Energies= -518.795174
Sum of electronic and thermal Enthalpies= -518.794230
Sum of electronic and thermal Free Energies= -518.846492

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.646	47.283	109.995

C,0,2.047329036,-0.8406727389,-2.3028548348
O,0,2.7309139453,0.4131264398,-2.4450550182
C,0,2.8281345915,0.9117958482,-3.7263243397
C,0,3.4652710447,2.1865658354,-3.7250375863
N,0,3.8208861261,2.8837848455,-4.8659889232
C,0,4.7121228876,4.0273148946,-4.5680549793
O,0,2.387296342,0.2716067618,-4.6947099101

C,0,4.2975640363,2.1193084221,-6.0433107027
C,0,2.1166392585,3.8743420473,-5.6992785075
C,0,1.4875970393,4.2797034653,-4.5038563906
C,0,0.9052483996,3.3662262677,-3.667178332
H,0,2.0707028621,-1.0654902546,-1.2362301607
H,0,1.0120884651,-0.7637757561,-2.6467620919
H,0,2.5543888488,-1.6305924017,-2.8634787924
H,0,3.6910951999,2.6506593498,-2.7767433707
H,0,5.2888856181,1.7034435374,-5.8296467996
H,0,3.6019095276,1.3119464055,-6.2557469716
H,0,4.3643700568,2.7978070455,-6.8953023339
H,0,5.6778752369,3.6606342205,-4.2026724884
H,0,4.8642304205,4.6124870415,-5.4751830084
H,0,4.2507787726,4.6546005885,-3.8045531044
H,0,2.5802828342,4.6070790157,-6.3531957333
H,0,1.7826712835,2.9607167835,-6.1811562034
H,0,1.6668758242,5.2904577714,-4.1396453837
H,0,0.6502713104,2.371407809,-4.0163929492
H,0,0.5588250323,3.6429777555,-2.6756810841

Cation- M06/6-31+G**/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM2M06SS
parent sm
M06/6-31+G**
E(RM06) = -519.180677407

Zero-point correction= 0.239200 (Hartree/Particle)
Thermal correction to Energy= 0.251979
Thermal correction to Enthalpy= 0.252923
Thermal correction to Gibbs Free Energy= 0.200158
Sum of electronic and ZPE= -518.941477
Sum of electronic and thermal Energies= -518.928698
Sum of electronic and thermal Enthalpies= -518.927754
Sum of electronic and thermal Free Energies= -518.980519

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.119	47.201	111.054

C,0,2.0548077151,-0.8069902191,-2.2666049013
O,0,2.8042002784,0.4132329487,-2.4169704966
C,0,2.7767769764,0.9741099188,-3.6145031516
O,0,2.1789685075,0.5448848039,-4.5756764332
C,0,3.6117059705,2.234379581,-3.5719550411
N,0,3.7059292067,2.9892979165,-4.8615985659
C,0,4.4132653722,2.1714935893,-5.9030286037
C,0,4.5220684648,4.2184481893,-4.5911351054
C,0,2.3363538577,3.4068587399,-5.4182216501
C,0,1.4685027424,4.0941182983,-4.4220648267
C,0,1.2035284449,5.3984864012,-4.4817630139
H,0,2.2212763118,-1.1280261754,-1.2401402504
H,0,0.9941604072,-0.6152356987,-2.4434531556
H,0,2.4205114662,-1.5582436038,-2.9699646958
H,0,4.6313822239,1.9732069988,-3.2679626584
H,0,3.2109844681,2.9064684808,-2.8059489456
H,0,3.8331762872,1.270505657,-6.1036627102
H,0,4.5018498274,2.7754423874,-6.8082184424
H,0,5.4062535888,1.9163463418,-5.5270639405
H,0,5.4974961666,3.9149976588,-4.2064444092
H,0,4.6421597563,4.7641830166,-5.5287204052
H,0,4.0035202716,4.8397068741,-3.8590811267
H,0,2.5659587835,4.0587900065,-6.2673954754
H,0,1.8777191292,2.4867097177,-5.7875349027
H,0,0.9930654158,3.4773129776,-3.6584156872
H,0,1.6432417987,6.0330394061,-5.2506616709
H,0,0.530168561,5.8737937869,-3.7741327345

TS-M06/6-31+G**/PCM

/home/bibaswanbiswas/c8/Parentcalcs/23parentTSM06SS
23 parent ts
M06/6-31+G**
E(RM06) = -518.672218980

Zero-point correction= 0.221419 (Hartree/Particle)
Thermal correction to Energy= 0.234073
Thermal correction to Enthalpy= 0.235017
Thermal correction to Gibbs Free Energy= 0.183564
Sum of electronic and ZPE= -518.450800
Sum of electronic and thermal Energies= -518.438146
Sum of electronic and thermal Enthalpies= -518.437202
Sum of electronic and thermal Free Energies= -518.488655

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.883	47.194	108.293

C,0,1.9671225433,-0.7456365185,-2.3212418089
O,0,2.7121118167,0.4575732541,-2.4580435898
C,0,2.8440248132,0.9307112903,-3.732700632
C,0,3.4751729877,2.2072828396,-3.7317548961
N,0,3.8260521409,2.8911200613,-4.8750453534
C,0,4.6869114038,4.0455297489,-4.5899015879
O,0,2.4203389841,0.2898949598,-4.6977734322
C,0,4.3115944948,2.1371405277,-6.0405883066
C,0,2.0913624163,3.8466371973,-5.6885836532
C,0,1.5051064714,4.2034505334,-4.47035176
C,0,1.0287798396,3.2294026594,-3.6338746784
H,0,1.9471634658,-0.9677734744,-1.2533398869
H,0,0.9449958083,-0.6159793616,-2.6939085579
H,0,2.4399600841,-1.5706304821,-2.8634277195
H,0,3.7157110883,2.6684792338,-2.7808011922
H,0,5.3160508015,1.7448935292,-5.832348679
H,0,3.6342971012,1.3108832667,-6.2522231421
H,0,4.3585222749,2.814341629,-6.8985471319
H,0,5.660634486,3.7030408787,-4.2154868607
H,0,4.8331125829,4.6257257532,-5.5046068256
H,0,4.2105695377,4.6764772218,-3.83445581
H,0,2.5305003811,4.5955002016,-6.34566916
H,0,1.7864595411,2.9165570342,-6.1672448899
H,0,1.6757988694,5.2073624813,-4.0784145853
H,0,0.755718025,2.2514859249,-4.0250261538
H,0,0.7361820408,3.44399061,-2.6086797064

Cation/ APFD/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2APFDPCMSB
parent sm conf 2

APFD/6-31G*
E(RAPFD) = -519.085647732

Zero-point correction= 0.242905 (Hartree/Particle)

Zero-point correction= 0.242996 (Hartree/Particle)
Thermal correction to Energy= 0.255824
Thermal correction to Enthalpy= 0.256768
Thermal correction to Gibbs Free Energy= 0.203415
Sum of electronic and zero-point Energies= -518.842652
Sum of electronic and thermal Energies= -518.829824
Sum of electronic and thermal Enthalpies= -518.828880
Sum of electronic and thermal Free Energies= -518.882233

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.532	46.701	112.290

C,0,2.0183189617,-0.7563565164,-2.2586730326
O,0,2.783518533,0.4524034038,-2.4162229495
C,0,2.7726308215,0.990634896,-3.6254178874
O,0,2.1802290993,0.5560312753,-4.5893280946
C,0,3.6274444359,2.248747365,-3.5886001182
N,0,3.724240861,2.9927182072,-4.8841586239
C,0,4.4336071642,2.1683038338,-5.9128069429
C,0,4.5221686616,4.2309961967,-4.6201075918
C,0,2.3519752871,3.3926952127,-5.4379188305
C,0,1.4611410001,4.0278132734,-4.4203097719
C,0,1.2125089887,5.3376025827,-4.3961435796
H,0,2.148582737,-1.0447555898,-1.2176588233
H,0,0.9664810655,-0.5634547827,-2.4784109112
H,0,2.4015097069,-1.5307037398,-2.9260566854
H,0,4.642483961,1.9820335843,-3.2834641281
H,0,3.2264065853,2.9326792008,-2.8367244642
H,0,3.8735290519,1.2491854106,-6.0709807328
H,0,4.4876566496,2.7439202271,-6.8371083068
H,0,5.4386792253,1.9496631447,-5.5509136004
H,0,5.4847540738,3.9470314827,-4.1949516377
H,0,4.6709763197,4.7542775452,-5.564401883
H,0,3.9690042536,4.8623971795,-3.925276023
H,0,2.5680434967,4.0716730628,-6.265397622
H,0,1.9161958184,2.4742042832,-5.8307330849
H,0,0.9671782519,3.3652974542,-3.7112520088
H,0,1.6693150965,6.0208992862,-5.1090504213
H,0,0.5304518925,5.7713805207,-3.6702552443

TS/ APFD /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSAPFDPCMSB
parent ts exo s-cis
APFD/6-31G*
E(RAPFD) = -518.566897926

Zero-point correction= 0.225645 (Hartree/Particle)
Thermal correction to Energy= 0.237974
Thermal correction to Enthalpy= 0.238919
Thermal correction to Gibbs Free Energy= 0.188069
Sum of electronic and ZPE= -518.341253
Sum of electronic and thermal Energies= -518.328924
Sum of electronic and thermal Enthalpies= -518.327979
Sum of electronic and thermal Free Energies= -518.378829

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	149.331	46.128	107.023

C,0,1.9999359942,-0.7903283736,-2.3782242315
O,0,2.724075863,0.4282193717,-2.4803738468
C,0,2.7932427007,0.9588664256,-3.7396778803
C,0,3.4471177992,2.2200405452,-3.7171421347
N,0,3.7906714559,2.902620653,-4.8711210136
C,0,4.6445197283,4.0610883551,-4.5793847854
O,0,2.2970650728,0.3821402607,-4.7136473317
C,0,4.3177508345,2.121031544,-6.001274973
C,0,2.1296616196,3.7761281229,-5.6826316634
C,0,1.5216866715,4.2387279153,-4.5008074724
C,0,1.0648429184,3.3165133145,-3.5990562224
H,0,2.0420203736,-1.0731350642,-1.3253564313
H,0,0.957625708,-0.6606409401,-2.6871834842
H,0,2.4517285474,-1.5749545574,-2.9932142948
H,0,3.7491126643,2.6509222832,-2.7736548576
H,0,5.3328072622,1.7806811562,-5.769042725
H,0,3.6691185765,1.2642236736,-6.1693754564
H,0,4.3401269643,2.7583378302,-6.8883837478
H,0,5.598417391,3.7249494313,-4.1587574329
H,0,4.8254445606,4.618514077,-5.4998888252
H,0,4.1336678089,4.7045138586,-3.86065706
H,0,2.5457282208,4.4748511898,-6.4058321653
H,0,1.7885709799,2.8312582183,-6.1005542062
H,0,1.6947151192,5.2671323759,-4.1841812319
H,0,0.7803345964,2.3212922128,-3.9259764806
H,0,0.7742645687,3.5944671207,-2.5886400456

Cation-B3LYPGD2/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2B3LYPPCMSB GD2
parent sm conf 2
B3LYP/6-31G*
E(RB3LYP) = -519.541373957

Zero-point correction= 0.241730 (Hartree/Particle)
Thermal correction to Energy= 0.254499
Thermal correction to Enthalpy= 0.255443
Thermal correction to Gibbs Free Energy= 0.202324
Sum of electronic and zero-point Energies= -519.299644
Sum of electronic and thermal Energies= -519.286875
Sum of electronic and thermal Enthalpies= -519.285931
Sum of electronic and thermal Free Energies= -519.339050

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	159.700	46.763	111.799

C,0,2.0243628679,-0.7919076275,-2.2532830939
O,0,2.7865950862,0.433093851,-2.4083865448
C,0,2.7742874194,0.9772896663,-3.6200782559
O,0,2.1850053133,0.5363738108,-4.5857019749
C,0,3.6207420756,2.2452731397,-3.5782450973
N,0,3.7189823465,2.9936657389,-4.8805134428
C,0,4.4358886691,2.1676469014,-5.9167961454
C,0,4.5225235979,4.2396631405,-4.6137503115
C,0,2.3385480653,3.3982602508,-5.4408430236
C,0,1.4630749419,4.0570411579,-4.4204759789
C,0,1.2142234089,5.3679042803,-4.4239178528
H,0,2.1579478252,-1.0801010673,-1.2111689693
H,0,0.9719318482,-0.6007518815,-2.4773951853
H,0,2.4169941438,-1.5573120149,-2.9273356856
H,0,4.6386395063,1.9888258649,-3.2746498205
H,0,3.206984996,2.9282181215,-2.8331777256
H,0,3.8570528482,1.2632670978,-6.0940687402
H,0,4.510977935,2.764922138,-6.826837298
H,0,5.4299227803,1.9305181398,-5.5336768218
H,0,5.4903540485,3.9443468648,-4.2061509834
H,0,4.6502483999,4.765782228,-5.5604776327
H,0,3.9721274981,4.8580057597,-3.9044527152
H,0,2.5634059103,4.0666819261,-6.2744082265
H,0,1.8980259783,2.4744892804,-5.8135487545
H,0,0.99476643,3.4102260052,-3.6818103797
H,0,1.6569719606,6.0269948334,-5.1680700052
H,0,0.5484460989,5.8189003941,-3.6931023349

TS/ B3LYPGD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSB3LYPPCMSBGD2
parent ts exo s-cis
B3LYP/6-31G*
E(RB3LYP) = -519.022559409

Zero-point correction= 0.223789 (Hartree/Particle)
Thermal correction to Energy= 0.236342
Thermal correction to Enthalpy= 0.237287
Thermal correction to Gibbs Free Energy= 0.185860
Sum of electronic and ZPE= -518.798770
Sum of electronic and thermal Energies= -518.786217
Sum of electronic and thermal Enthalpies= -518.785273
Sum of electronic and thermal Free Energies= -518.836700

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.307	46.622	108.237

C,0,1.9841384717,-0.8034473331,-2.3646308064
O,0,2.7305885842,0.4133293752,-2.4658945835
C,0,2.8094879254,0.9454087977,-3.7311980735
C,0,3.4880055004,2.197521651,-3.7104448392
N,0,3.8269326628,2.8868539471,-4.8594396022
C,0,4.6582953075,4.0715292515,-4.5795028541
O,0,2.3061396933,0.3691158586,-4.705045214
C,0,4.336690105,2.1240451039,-6.0181670759
C,0,2.1022583012,3.781443345,-5.6952081653
C,0,1.5171272083,4.2363656361,-4.5009133427
C,0,1.0294298577,3.3281291338,-3.5984179891
H,0,2.0219181727,-1.0864147652,-1.310154135
H,0,0.9450218547,-0.6537457208,-2.6792861075
H,0,2.4285853592,-1.5899645775,-2.9844391755
H,0,3.7639138356,2.6396956,-2.7647136647
H,0,5.3549129896,1.7746496052,-5.8048097841
H,0,3.6780988972,1.2763819795,-6.1963593004
H,0,4.3485243365,2.788623082,-6.8863113399
H,0,5.6298919205,3.758149816,-4.1776342263
H,0,4.8017149926,4.6310221409,-5.5063804205
H,0,4.1384763177,4.696803853,-3.8497345584
H,0,2.5377515118,4.4768759158,-6.4079743698
H,0,1.7830612279,2.8236241043,-6.0977192485
H,0,1.7001065178,5.2629118754,-4.1852737898
H,0,0.7581176035,2.3284396361,-3.9210927846
H,0,0.7350648453,3.6201136888,-2.5932945491

Cation/ PBEGD2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2PBEPCMSBGD2
parent sm conf 2
PBEPBE/6-31G*
E(RPBE-PBE) = -518.871680499
Zero-point correction= 0.234868 (Hartree/Particle)
Thermal correction to Energy= 0.247970
Thermal correction to Enthalpy= 0.248915
Thermal correction to Gibbs Free Energy= 0.195083
Sum of electronic and zero-point Energies= -518.636813
Sum of electronic and thermal Energies= -518.623710
Sum of electronic and thermal Enthalpies= -518.622766
Sum of electronic and thermal Free Energies= -518.676598

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	155.604	48.161	113.299

C,0,2.0157960413,-0.8005460685,-2.259521803
O,0,2.7753264908,0.434631849,-2.3930369619
C,0,2.7876740065,0.9638435832,-3.6232436459
O,0,2.222020114,0.4992189312,-4.6047580961
C,0,3.630211618,2.2393272993,-3.5740167089
N,0,3.7218534521,2.993383041,-4.8777132949
C,0,4.4351039459,2.1714566594,-5.9220547593
C,0,4.5192011544,4.2450448066,-4.6121206001
C,0,2.3280139852,3.3889722174,-5.4245152391
C,0,1.4696399951,4.071823844,-4.4044688026
C,0,1.2173594287,5.3910903066,-4.4363321089
H,0,2.1231660248,-1.0878851992,-1.2059393391
H,0,0.9604244096,-0.6184223603,-2.5155440767
H,0,2.4350771446,-1.5703324189,-2.9259240829
H,0,4.6590413274,1.9876644927,-3.2707131399
H,0,3.2137805644,2.926878081,-2.8211485489
H,0,3.8553733265,1.2562010875,-6.0939930484

H,0,4.4984008316,2.773090478,-6.8399194091
H,0,5.4419370056,1.9390959301,-5.5462570314
H,0,5.496613589,3.9537527109,-4.2024603633
H,0,4.6450457925,4.7765712267,-5.5657200612
H,0,3.9619987634,4.866264485,-3.8972117085
H,0,2.5420656573,4.0418079645,-6.2845928805
H,0,1.8814734555,2.4461685702,-5.7709866017
H,0,1.0050790963,3.4389682206,-3.6386228657
H,0,1.6516186757,6.0368741308,-5.2088701392
H,0,0.5557361033,5.8623741312,-3.7026376832

TS/ PBEGD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSPBEPCMSBGD2
parent ts exo s-cis
PBEPBE/6-31G*
E(RPBE-PBE) = -518.366686658

Zero-point correction= 0.217743 (Hartree/Particle)
Thermal correction to Energy= 0.230580
Thermal correction to Enthalpy= 0.231524
Thermal correction to Gibbs Free Energy= 0.179576
Sum of electronic and ZPE= -518.148943
Sum of electronic and thermal Energies= -518.136107
Sum of electronic and thermal Enthalpies= -518.135163
Sum of electronic and thermal Free Energies= -518.187111

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	144.691	47.902	109.334

Charge = 0 Multiplicity = 1
Redundant internal coordinates found in file.
C,0,1.9839941672,-0.8238953816,-2.3879762833
O,0,2.7462379833,0.3909225266,-2.4619780914
C,0,2.8138799616,0.9415034663,-3.7339240465
C,0,3.512256651,2.186830635,-3.7029674964
N,0,3.8217363723,2.8933790112,-4.8604243743
C,0,4.6485280814,4.086594473,-4.580972098
O,0,2.2895198387,0.3793309889,-4.7176634904
C,0,4.3444002213,2.1253717268,-6.0155616537
C,0,2.1290251253,3.7348790411,-5.6796562045
C,0,1.5228969361,4.248239435,-4.5060652547
C,0,1.0093374492,3.3800916472,-3.5722620424
H,0,2.0312180916,-1.1383415507,-1.334552077
H,0,0.9343110498,-0.6555191317,-2.6883834426
H,0,2.4129977755,-1.6053567766,-3.0396206638
H,0,3.7778943679,2.6441416502,-2.7515215968
H,0,5.3774909427,1.7995882649,-5.7988545657
H,0,3.694596986,1.2546422646,-6.1730464772
H,0,4.3362173385,2.7806279924,-6.9009857084
H,0,5.6283446134,3.7745595685,-4.1777785109
H,0,4.7878866182,4.6514458441,-5.5147817265
H,0,4.1208244515,4.7112693644,-3.8440656529
H,0,2.5517500004,4.4083759268,-6.43401332
H,0,1.7872167351,2.760957932,-6.0499889163
H,0,1.6988089994,5.2975108385,-4.2346079485
H,0,0.7581669772,2.3531434205,-3.8539257808
H,0,0.6947162655,3.7171678227,-2.5784625765

Cation/ BLYPGD2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2BLYPPCMSBGD2
parent sm conf 2
BLYP/6-31G*
E(RB-LYP) = -519.318058822
Zero-point correction= 0.233919 (Hartree/Particle)
Thermal correction to Energy= 0.247103
Thermal correction to Enthalpy= 0.248047
Thermal correction to Gibbs Free Energy= 0.193936
Sum of electronic and zero-point Energies= -519.084140
Sum of electronic and thermal Energies= -519.070956
Sum of electronic and thermal Enthalpies= -519.070011
Sum of electronic and thermal Free Energies= -519.124123

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.060	48.455	113.887

C,0,2.0041728129,-0.8228240244,-2.2375598515
O,0,2.7734811555,0.4229584498,-2.384605604
C,0,2.7817368085,0.9561892662,-3.6206278081
O,0,2.2091801894,0.4958601335,-4.6033807637
C,0,3.6338781119,2.2364996479,-3.5697890405
N,0,3.7286346218,2.9976305148,-4.884480686
C,0,4.449995304,2.1687442835,-5.9376990194
C,0,4.5348108986,4.2593863449,-4.6143772208
C,0,2.3214234254,3.4022957897,-5.4428439441
C,0,1.4551135414,4.0745368314,-4.4130876063
C,0,1.2034998329,5.3957209692,-4.4281312122
H,0,2.1201118612,-1.1002658804,-1.1826406054
H,0,0.9495980107,-0.6349433884,-2.4898350781
H,0,2.4210012842,-1.5930936639,-2.903881832
H,0,4.6617394072,1.9826980773,-3.2714756431
H,0,3.217062738,2.925539828,-2.821724227
H,0,3.8674833378,1.2570710113,-6.109101532
H,0,4.5137861055,2.7749741947,-6.851305808
H,0,5.4536038395,1.9370730388,-5.5554789269
H,0,5.5091528003,3.9615408786,-4.2047158583
H,0,4.6592040139,4.7875739605,-5.5687708317
H,0,3.9748740318,4.8759525996,-3.8998753832
H,0,2.5459508845,4.0650933113,-6.290209379
H,0,1.8832056282,2.4625837774,-5.7998416262
H,0,0.9957832088,3.4307209426,-3.6556577273
H,0,1.6384876266,6.049803116,-5.1917726866
H,0,0.5420605193,5.8579979901,-3.6894530992

TS/ BLYPGD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSBLYPPCMSBGD2
parent ts exo s-cis
BLYP/6-31G*
E(RB-LYP) = -518.811650515

Zero-point correction= 0.216786 (Hartree/Particle)
Thermal correction to Energy= 0.229707

Thermal correction to Enthalpy= 0.230651
Thermal correction to Gibbs Free Energy= 0.178524
Sum of electronic and ZPE= -518.594865
Sum of electronic and thermal Energies= -518.581944
Sum of electronic and thermal Enthalpies= -518.580999
Sum of electronic and thermal Free Energies= -518.633126

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.143	48.136	109.711

C,0,1.9450451684,-0.830533539,-2.3951735216
O,0,2.7697226486,0.3574345904,-2.4680368836
C,0,2.8434892981,0.9344973867,-3.7423573283
C,0,3.6039148659,2.1415029095,-3.7040441176
N,0,3.8557261059,2.8869726922,-4.8635268064
C,0,4.6582032905,4.1119035536,-4.5823143321
O,0,2.2779407524,0.4101393278,-4.7310462835
C,0,4.3946112479,2.1436322123,-6.0455983809
C,0,2.1186771046,3.6650252288,-5.6545507253
C,0,1.5045188163,4.2291469374,-4.4966712143
C,0,0.9477473192,3.4214647168,-3.5371045034
H,0,1.9997791953,-1.1612335012,-1.3471694754
H,0,0.8997680792,-0.6052622985,-2.6718462477
H,0,2.324243255,-1.6192484136,-3.0680275947
H,0,3.85450302,2.6048007489,-2.7529712644
H,0,5.4354475643,1.8424688055,-5.8349196462
H,0,3.7643413756,1.2624096925,-6.2107489736
H,0,4.3634858091,2.8143074222,-6.9179121175
H,0,5.6532857225,3.8210011305,-4.2037005386
H,0,4.7590680101,4.6890046122,-5.5124521018
H,0,4.1245661842,4.7068148015,-3.8270799235
H,0,2.5231184535,4.3140257226,-6.4372001446
H,0,1.7831924062,2.6753770674,-5.9786739852
H,0,1.6663827717,5.2928985009,-4.2832253784
H,0,0.7394087313,2.3708296823,-3.7513726391
H,0,0.6040668045,3.8180810102,-2.5763158721

Cation/ BP86GD2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2BP86PCMSBGD2
parent sm conf 2
BP86/6-31G*
E(RB-P86) = -519.527335985
Zero-point correction= 0.234056 (Hartree/Particle)
Thermal correction to Energy= 0.247167
Thermal correction to Enthalpy= 0.248111
Thermal correction to Gibbs Free Energy= 0.194269
Sum of electronic and zero-point Energies= -519.293280
Sum of electronic and thermal Energies= -519.280169
Sum of electronic and thermal Enthalpies= -519.279225
Sum of electronic and thermal Free Energies= -519.333067

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	155.099	48.247	113.319

C,0,2.0129905536,-0.806028919,-2.2561888253
O,0,2.7719166871,0.4355540545,-2.3902539509
C,0,2.7869913935,0.9630266253,-3.6230404905
O,0,2.2251143039,0.495005513,-4.6066354132
C,0,3.6283368292,2.242270385,-3.57255966
N,0,3.7202529208,2.9942640214,-4.8801700265
C,0,4.4386938758,2.170663897,-5.9237452049
C,0,4.5151158136,4.2512866147,-4.6155888788
C,0,2.3235901342,3.3861862608,-5.4308281665
C,0,1.4664325839,4.0684916027,-4.4060942262
C,0,1.228062736,5.3916569398,-4.4293259876
H,0,2.1194820968,-1.0897703338,-1.2004945906
H,0,0.957584927,-0.6247156969,-2.5167140087
H,0,2.4385992842,-1.5743627328,-2.9218522211
H,0,4.6584255489,1.993723304,-3.2683764725
H,0,3.2066185688,2.9319763466,-2.823487024
H,0,3.8577635518,1.2550263589,-6.0951921259
H,0,4.502871181,2.7744993353,-6.8413115718
H,0,5.4448379724,1.9402449393,-5.5420096337
H,0,5.4940690489,3.960945586,-4.20618961
H,0,4.6365627206,4.7811093272,-5.5718257214
H,0,3.9532081674,4.8695144853,-3.9002772688
H,0,2.5394161728,4.0405015702,-6.29045421
H,0,1.8806807854,2.4405551591,-5.7760013263
H,0,0.9996498195,3.4333242234,-3.6427493112
H,0,1.669481779,6.0363327894,-5.2000458559
H,0,0.5722825436,5.8660363434,-3.6909112178

TS/ BP86GD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSBP86PCMSBGD2
parent ts exo s-cis
BP86/6-31G*
E(RB-P86) = -519.021844990

Zero-point correction= 0.216846 (Hartree/Particle)
Thermal correction to Energy= 0.229709
Thermal correction to Enthalpy= 0.230654
Thermal correction to Gibbs Free Energy= 0.178653
Sum of electronic and ZPE= -518.804999
Sum of electronic and thermal Energies= -518.792136
Sum of electronic and thermal Enthalpies= -518.791191
Sum of electronic and thermal Free Energies= -518.843192

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.145	48.034	109.444

C,0,1.9754168932,-0.8287999233,-2.3896795892
O,0,2.7444856205,0.3872940752,-2.460900231
C,0,2.812249073,0.9426429397,-3.7330465669
C,0,3.5156023018,2.1868405879,-3.6994277285
N,0,3.8275202427,2.8914014679,-4.8583465692
C,0,4.6459095506,4.0935191662,-4.5810051569
O,0,2.2840747728,0.3857386765,-4.719454277
C,0,4.3524016962,2.1248609761,-6.0164767917
C,0,2.1171535783,3.7308245898,-5.6860392088

C,0,1.5235395408,4.2488648424,-4.5080504564
C,0,1.0206275209,3.380247323,-3.5655340074
H,0,2.0201405897,-1.1435684968,-1.3351005414
H,0,0.926868126,-0.65404666,-2.6937525229
H,0,2.4055172225,-1.6098942261,-3.0428029366
H,0,3.7819111106,2.6440711292,-2.7473285633
H,0,5.3872700556,1.8001740933,-5.7998035648
H,0,3.7015084627,1.2540448151,-6.1753800253
H,0,4.3416928937,2.7850458204,-6.8996566006
H,0,5.6285179205,3.7898993472,-4.1745265781
H,0,4.7804133195,4.6554155539,-5.5186165897
H,0,4.1086768849,4.7154353583,-3.8468823187
H,0,2.5430688353,4.3982962648,-6.4448719029
H,0,1.7828603409,2.7482993869,-6.0425752275
H,0,1.7039321495,5.2992945108,-4.2406721573
H,0,0.7659427832,2.3532684604,-3.8464828173
H,0,0.716952515,3.7182909213,-2.5676270706

Cation/ B3LYPGD3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2B3LYPPCMSBGD3
parent sm conf 2
B3LYP/6-31G*
E(RB3LYP) = -519.528552243
Zero-point correction= 0.242322 (Hartree/Particle)
Thermal correction to Energy= 0.255129
Thermal correction to Enthalpy= 0.256073
Thermal correction to Gibbs Free Energy= 0.202846
Sum of electronic and zero-point Energies= -519.286230
Sum of electronic and thermal Energies= -519.273424
Sum of electronic and thermal Enthalpies= -519.272479
Sum of electronic and thermal Free Energies= -519.325707

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.096	46.797	112.026

C,0,2.0071022247,-0.776382545,-2.2475641334
O,0,2.7802617735,0.4411707824,-2.4058465496
C,0,2.7742781201,0.9846673246,-3.6182711913
O,0,2.1806066683,0.5486663872,-4.5834078193
C,0,3.6346685899,2.2432126723,-3.580670352
N,0,3.7327104093,2.9960608849,-4.8850859586
C,0,4.4452722385,2.1643409319,-5.9261205285
C,0,4.542001335,4.2433046725,-4.6189665001
C,0,2.3449951647,3.4041037702,-5.4437368399
C,0,1.4528567462,4.0418596774,-4.4235802743
C,0,1.1866528596,5.3495416847,-4.4041314277
H,0,2.1371008719,-1.0628610283,-1.2056387024
H,0,0.9562389812,-0.5801931479,-2.4700287023
H,0,2.3912060882,-1.5498577025,-2.9157644363
H,0,4.6483949695,1.9699710437,-3.2792859015
H,0,3.2375178935,2.9240817428,-2.8258318497
H,0,3.8797028422,1.249798288,-6.088345609
H,0,4.5027212983,2.7452367188,-6.8467608867
H,0,5.4482776864,1.939233658,-5.5624424167
H,0,5.5056327465,3.9536496221,-4.200082511
H,0,4.6862994476,4.7680091573,-5.563066279
H,0,3.9946986569,4.8734377724,-3.9190156756
H,0,2.5639035617,4.0811513476,-6.271052845
H,0,1.9093421741,2.4852578897,-5.8322729478
H,0,0.9740357179,3.3778611461,-3.7070491127
H,0,1.6294457915,6.0358152895,-5.1222779496
H,0,0.5031071424,5.7761799596,-3.6760256004

TS/ B3LYPGD3 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSB3LYPPCMSBGD3
parent ts exo s-cis
B3LYP/6-31G*
E(RB3LYP) = -519.011856695

Zero-point correction= 0.224523 (Hartree/Particle)
Thermal correction to Energy= 0.237051
Thermal correction to Enthalpy= 0.237995
Thermal correction to Gibbs Free Energy= 0.186593
Sum of electronic and ZPE= -518.787334
Sum of electronic and thermal Energies= -518.774806
Sum of electronic and thermal Enthalpies= -518.773862
Sum of electronic and thermal Free Energies= -518.825264

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	148.752	46.541	108.185

C,0,1.9866846467,-0.8015225046,-2.3669378769
O,0,2.7412570102,0.4094627254,-2.4690339087
C,0,2.8184042089,0.9479447164,-3.733921268
C,0,3.5093184178,2.1909031702,-3.7129085486
N,0,3.8327248315,2.8918089264,-4.8632179052
C,0,4.6762030536,4.0716894223,-4.5806906754
O,0,2.3063549903,0.3764456728,-4.7071852919
C,0,4.340996961,2.1233313228,-6.0232718209
C,0,2.1097103892,3.7729455719,-5.6829787854
C,0,1.5023653673,4.2286754139,-4.4950232621
C,0,0.9896523656,3.3364742385,-3.5949018789
H,0,2.0283818312,-1.0883825688,-1.3146522924
H,0,0.9459704744,-0.6473413973,-2.6713209823
H,0,2.4186206923,-1.592630499,-2.9883025513
H,0,3.7795834301,2.6337124602,-2.7663263314
H,0,5.3567282935,1.7706865553,-5.8101993241
H,0,3.6843765219,1.2750298114,-6.1994126786
H,0,4.3564293874,2.7771783264,-6.8980707305
H,0,5.6466770861,3.751462259,-4.1848400888
H,0,4.8244975744,4.6381499319,-5.5011846436
H,0,4.1708338851,4.701099242,-3.8461222957
H,0,2.5241815033,4.4775310782,-6.3990899215
H,0,1.7860123278,2.8225622243,-6.0974880062
H,0,1.669824969,5.2605525083,-4.187904618
H,0,0.7359750628,2.3262885636,-3.8971618144
H,0,0.6724887185,3.6434038287,-2.6018924991

Cation/ M06GD3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2M06PCMSBGD3
parent sm conf 2
M06/6-31G*
E(RM06) = -519.153693058
Zero-point correction= 0.240263 (Hartree/Particle)
Thermal correction to Energy= 0.253066
Thermal correction to Enthalpy= 0.254010
Thermal correction to Gibbs Free Energy= 0.200939
Sum of electronic and zero-point Energies= -518.913430
Sum of electronic and thermal Energies= -518.900627
Sum of electronic and thermal Enthalpies= -518.899683
Sum of electronic and thermal Free Energies= -518.952754

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	158.801	47.046	111.697

C,0,2.0455191788,-0.7824688665,-2.2736836244
O,0,2.8073855096,0.42681895,-2.4187059667
C,0,2.7747204393,0.9886404351,-3.6148319811
O,0,2.168559344,0.5672155385,-4.5724415938
C,0,3.6171754479,2.2453239062,-3.5718128528
N,0,3.7127282613,2.9906642058,-4.8665914065
C,0,4.4189825183,2.1622443883,-5.8980702741
C,0,4.5230869859,4.2240403233,-4.6070984084
C,0,2.3402975794,3.400326728,-5.4256402855
C,0,1.4626331018,4.0632222767,-4.4227185167
C,0,1.2074696891,5.36933152,-4.4458473339
H,0,2.2094918964,-1.1120002763,-1.2481534726
H,0,0.9855772451,-0.5784108837,-2.4489664623
H,0,2.3994048548,-1.5360000816,-2.9826074863
H,0,4.6371898701,1.9849602238,-3.2653138959
H,0,3.21611523,2.9257730238,-2.8120154249
H,0,3.8479374067,1.2478689885,-6.0671930803
H,0,4.4846065527,2.7465184995,-6.8194146989
H,0,5.4220543397,1.9306463218,-5.5303997
H,0,5.4939969952,3.9288503504,-4.2016562129
H,0,4.6567777862,4.7541615228,-5.5532691794
H,0,3.9905912044,4.8567794985,-3.8931543976
H,0,2.569063657,4.0649322424,-6.2662148639
H,0,1.8950465333,2.4783911678,-5.8077106484
H,0,0.9758274121,3.4224964663,-3.6852909445
H,0,1.6576477382,6.0259985625,-5.1910343292
H,0,0.5291452224,5.8309929679,-3.7324859592

TS/ M06GD3 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSM06PCMSBGD3
parent ts exo s-cis
M06/6-31G*
E(RM06) = -518.636532007
Zero-point correction= 0.222776 (Hartree/Particle)
Thermal correction to Energy= 0.235400
Thermal correction to Enthalpy= 0.236344
Thermal correction to Gibbs Free Energy= 0.184630
Sum of electronic and ZPE= -518.413756
Sum of electronic and thermal Energies= -518.401132
Sum of electronic and thermal Enthalpies= -518.400188
Sum of electronic and thermal Free Energies= -518.451902

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	147.716	46.776	108.841

C,0,1.9687402095,-0.735901955,-2.3381080529
O,0,2.714598796,0.4622698015,-2.4611407738
C,0,2.8329816531,0.9417399961,-3.7348623201
C,0,3.4646191692,2.2169739513,-3.7266952061
N,0,3.8125749001,2.900102372,-4.8747522137
C,0,4.6731788603,4.0531098462,-4.5916999336
O,0,2.3915643397,0.3141327407,-4.6971365788
C,0,4.3085005006,2.1326811389,-6.0257958101
C,0,2.1128160148,3.8288892221,-5.6801159045
C,0,1.5094433467,4.1984372726,-4.4735282658
C,0,1.0581723224,3.2211798605,-3.6295642329
H,0,1.9791593152,-0.993009333,-1.2762334932
H,0,0.9341564602,-0.5933982801,-2.6754117842
H,0,2.4152043352,-1.5492123669,-2.9217322006
H,0,3.7328953931,2.6672546987,-2.7774234389
H,0,5.3247568828,1.7694451398,-5.8184397591
H,0,3.6449777128,1.2859662781,-6.2034643039
H,0,4.3294912044,2.7896224806,-6.9022218347
H,0,5.6417745378,3.7117941402,-4.2011399737
H,0,4.8310802808,4.6247860416,-5.5114934659
H,0,4.1865982861,4.6916022487,-3.8474214218
H,0,2.5364684089,4.5746832519,-6.3533675377
H,0,1.7994976012,2.8993972573,-6.1576335792
H,0,1.6727258168,5.207986358,-4.0899348123
H,0,0.7822745821,2.2425844388,-4.0191668983
H,0,0.7560030703,3.4343443996,-2.6055562038

Cation/ PBE0GD3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2PBE0PCMSBGD3
parent sm conf 2
PBE1PBE/6-31G*
E(RPBE1PBE) = -518.911312025
Zero-point correction= 0.243794 (Hartree/Particle)
Thermal correction to Energy= 0.256526
Thermal correction to Enthalpy= 0.257470
Thermal correction to Gibbs Free Energy= 0.204542
Sum of electronic and zero-point Energies= -518.667518
Sum of electronic and thermal Energies= -518.654786
Sum of electronic and thermal Enthalpies= -518.653842
Sum of electronic and thermal Free Energies= -518.706770

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.973	46.479	111.396

C,0,2.0149126296,-0.7571899549,-2.2693600272
O,0,2.7748845503,0.4544501958,-2.4141465477
C,0,2.7851715512,0.9853049554,-3.6241313143
O,0,2.2127928843,0.537146961,-4.5917018791
C,0,3.6329359825,2.2431200121,-3.5851480135
N,0,3.723870322,2.9906532391,-4.8772207773
C,0,4.4289794016,2.1708848288,-5.9129734682
C,0,4.5232590544,4.2281786666,-4.6138584148
C,0,2.3494474189,3.3892224325,-5.4213729963
C,0,1.4740771538,4.04545354,-4.4059825894
C,0,1.2013316902,5.3496665706,-4.4203695351
H,0,2.1274446644,-1.0450305099,-1.2259206501
H,0,0.9659317829,-0.5709054368,-2.5083407315
H,0,2.4136620937,-1.5301240991,-2.9294026408
H,0,4.6490407198,1.975107461,-3.2835754566
H,0,3.2340155873,2.9207670669,-2.8265381284
H,0,3.8621814612,1.2575101128,-6.082375925
H,0,4.4892912386,2.756151265,-6.8312101203
H,0,5.4320759099,1.940923676,-5.551514414
H,0,5.492259521,3.9413269242,-4.2044739181
H,0,4.65872052,4.7594030474,-5.556175536
H,0,3.9805983573,4.854550903,-3.9057952823
H,0,2.5578615842,4.0543372328,-6.2622183824
H,0,1.9028656939,2.4668609995,-5.7936039045
H,0,1.0046842248,3.4008056386,-3.6650371633
H,0,1.6307845071,6.0159734013,-5.1653251848
H,0,0.5259514949,5.7927688702,-3.694549999

TS/ PBE0GD3 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSPBE0PCMSBGD3
parent ts exo s-cis
PBE1PBE/6-31G*
E(RPBE1PBE) = -518.392479456

Zero-point correction= 0.226405 (Hartree/Particle)
Thermal correction to Energy= 0.238737
Thermal correction to Enthalpy= 0.239681
Thermal correction to Gibbs Free Energy= 0.188764
Sum of electronic and ZPE= -518.166074
Sum of electronic and thermal Energies= -518.153743
Sum of electronic and thermal Enthalpies= -518.152798
Sum of electronic and thermal Free Energies= -518.203716

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	149.810	45.920	107.164

C,0,2.0145562325,-0.7913118165,-2.3718084097
O,0,2.7201242151,0.4366837062,-2.4733323536
C,0,2.7859948012,0.9602679804,-3.7320044668
C,0,3.4143454864,2.2353887925,-3.7168002437
N,0,3.7767889675,2.9076773035,-4.8716482687
C,0,4.6412266428,4.0569340951,-4.5794916535
O,0,2.3019165306,0.3648549915,-4.6981191734
C,0,4.2965082005,2.1170355324,-5.9972030348
C,0,2.145150778,3.7958460254,-5.6853552582
C,0,1.5291806279,4.2427954714,-4.5044461232
C,0,1.0782328154,3.3030529032,-3.616947438
H,0,2.0523749073,-1.069998597,-1.3175457629
H,0,0.9731137467,-0.6785222755,-2.6899556748
H,0,2.4828549078,-1.5707792471,-2.9807683046
H,0,3.725397308,2.6615117889,-2.7739769182
H,0,5.3046103198,1.7582984097,-5.7612081474
H,0,3.6343503049,1.2708923894,-6.1695072577
H,0,4.3347640207,2.7540485966,-6.8843872894
H,0,5.5904103039,3.712579564,-4.1541860229
H,0,4.8317781845,4.6104475493,-5.5008131647
H,0,4.1355137299,4.7082263123,-3.8637194482
H,0,2.5703765824,4.5032628788,-6.3946348841
H,0,1.798939724,2.8610411401,-6.1220599752
H,0,1.7099087689,5.2625772103,-4.1669415955
H,0,0.7760514863,2.319991988,-3.9653567153
H,0,0.7897844072,3.5646583073,-2.6018224152

Cation/ B3LYP /6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2B3LYPPSPCMSB
parent sm conf 2
B3LYP/6-31G*
E(RB3LYP) = -519.501174619

Zero-point correction= 0.241778 (Hartree/Particle)
Thermal correction to Energy= 0.254736
Thermal correction to Enthalpy= 0.255680
Thermal correction to Gibbs Free Energy= 0.202048
Sum of electronic and ZPE= -519.259397
Sum of electronic and thermal Energies= -519.246439
Sum of electronic and thermal Enthalpies= -519.245495
Sum of electronic and thermal Free Energies= -519.299126

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	159.849	47.134	112.878

C,0,2.057310332,-0.8525210663,-2.2644215254
O,0,2.8004239017,0.3836051209,-2.4133833706
C,0,2.7811731767,0.9430577525,-3.618858864
O,0,2.196147222,0.5059513815,-4.5887552883
C,0,3.6175854908,2.2194814405,-3.5641303376
N,0,3.7125583763,2.9930236554,-4.8571188975
C,0,4.4128834307,2.1733844154,-5.9158875469
C,0,4.5368527192,4.227047812,-4.5795129339
C,0,2.3249993452,3.4161127604,-5.3999901168
C,0,1.4775098647,4.1532393317,-4.4079726935
C,0,1.1854150316,5.4507017515,-4.523475005
H,0,2.1946047229,-1.1423502822,-1.2244671487
H,0,1.0021190179,-0.6807220039,-2.4841088156
H,0,2.461033324,-1.6120347478,-2.9362773631
H,0,4.6352669684,1.9608902164,-3.2626365805
H,0,3.2078664526,2.8848422748,-2.8020791317
H,0,3.8269071757,1.2778770232,-6.1076533313
H,0,4.4940904395,2.7791455699,-6.8183711727
H,0,5.4068489108,1.9140964916,-5.5500692251
H,0,5.5063919083,3.9194221315,-4.1880586108

H,0,4.6657064237,4.7713277048,-5.514880347
H,0,4.0113098307,4.8465578523,-3.8544571307
H,0,2.5412489232,4.0317356399,-6.2744482588
H,0,1.8510950239,2.4882231086,-5.7190619141
H,0,1.0351231637,3.5703576534,-3.6027360935
H,0,1.5847069846,6.0610956377,-5.3302437229
H,0,0.5218538388,5.9437693743,-3.8192675742

TS/ B3LYP/6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSB3LYPPSPCMS
B
parent ts exo s-cis
B3LYP/6-31G*
E(RB3LYP) = -518.984732518

Zero-point correction= 0.224070 (Hartree/Particle)
Thermal correction to Energy= 0.236778
Thermal correction to Enthalpy= 0.237722
Thermal correction to Gibbs Free Energy= 0.185859
Sum of electronic and ZPE= -518.760663
Sum of electronic and thermal Energies= -518.747955
Sum of electronic and thermal Enthalpies= -518.747011
Sum of electronic and thermal Free Energies= -518.798874

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 148.580 46.847 109.155
C,0,2.036326266,-0.8273470306,-2.3371917288
O,0,2.7383275449,0.4126488013,-2.4535910539
C,0,2.8112976155,0.9339679026,-3.7268721839
C,0,3.4742243681,2.1939486613,-3.7153756902
N,0,3.8161979518,2.8917848668,-4.8627768863
C,0,4.6993609501,4.0414038579,-4.5735449359
O,0,2.3271350897,0.3295760773,-4.693978429
C,0,4.3050334079,2.1132864994,-6.02497574
C,0,2.1287052447,3.8367035771,-5.6875491085
C,0,1.4944377057,4.2670291683,-4.5032165916
C,0,0.9404699723,3.3611140797,-3.6436048471
H,0,2.0819040609,-1.0938451002,-1.2798134553
H,0,0.9924168064,-0.724546189,-2.6505133129
H,0,2.5080435058,-1.6094425911,-2.9400318655
H,0,3.7370555229,2.6429043213,-2.769327603
H,0,5.3129187747,1.7369086231,-5.8141777511
H,0,3.6299157112,1.2787320813,-6.1978464715
H,0,4.3362921509,2.7678431748,-6.8986918264
H,0,5.6612609436,3.6853948294,-4.1873131794
H,0,4.8615948605,4.6115290266,-5.4893981531
H,0,4.2220427584,4.6794049961,-3.8279856004
H,0,2.5661072001,4.5590549983,-6.3718244395
H,0,1.7924817197,2.9113322098,-6.1460772055
H,0,1.6589167755,5.2901196078,-4.1661107056
H,0,0.6938230932,2.3582881637,-3.9754079135
H,0,0.5879639995,3.6496663871,-2.6568433221

Cation/M11/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2M11
parent sm conf 2
M11/6-31G*
E(RM11) = -519.215307678

Zero-point correction= 0.241865 (Hartree/Particle)
Thermal correction to Energy= 0.254549
Thermal correction to Enthalpy= 0.255493
Thermal correction to Gibbs Free Energy= 0.202879
Sum of electronic and ZPE= -518.973442
Sum of electronic and thermal Energies= -518.960759
Sum of electronic and thermal Enthalpies= -518.959814
Sum of electronic and thermal Free Energies= -519.012428

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 159.732 46.564 110.735
C,0,2.013806569,-0.7434856016,-2.2705517241
O,0,2.7993331706,0.4596143627,-2.4088108433
C,0,2.7645167358,1.032736886,-3.5991101612
O,0,2.1346744659,0.6217342909,-4.548558019
C,0,3.6261132855,2.2867533376,-3.5757093088
N,0,3.7248902429,2.994888796,-4.8903262262
C,0,4.4412938844,2.1437312634,-5.8964992964
C,0,4.5228935216,4.2430065377,-4.651455869
C,0,2.3597294168,3.3845848485,-5.4649368007
C,0,1.4471026475,3.9820840322,-4.4333738678
C,0,1.2233994629,5.2913174387,-4.3491196041
H,0,2.1525431586,-1.0683316058,-1.237246996
H,0,0.9605051198,-0.5203671706,-2.4742769724
H,0,2.3777177804,-1.5017713835,-2.972910936
H,0,4.6419490586,2.0166956705,-3.2605357112
H,0,3.2172728579,2.9872328449,-2.8360616535
H,0,3.8754340011,1.2192683976,-6.0383814519
H,0,4.499446002,2.7033408263,-6.8362188558
H,0,5.4485944109,1.9323823316,-5.5215326827
H,0,5.4890086446,3.9657715371,-4.2168489018
H,0,4.6725463785,4.7476631077,-5.6115371164
H,0,3.9646820028,4.8880366093,-3.9648344073
H,0,2.5800950538,4.0987240646,-6.2678561992
H,0,1.9385594964,2.4708745975,-5.8929686747
H,0,0.9258220151,3.2891474507,-3.7673407634
H,0,1.7123163756,5.9983318894,-5.0246124749
H,0,0.5347862408,5.7033526405,-3.6107074824

TS M11 /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentRM11
parent ts exo s-cis
M11/6-31G*
E(RM11) = -518.690990016

Zero-point correction= 0.225201 (Hartree/Particle)
Thermal correction to Energy= 0.237309
Thermal correction to Enthalpy= 0.238253
Thermal correction to Gibbs Free Energy= 0.187899
Sum of electronic and ZPE= -518.465789
Sum of electronic and thermal Energies= -518.453681
Sum of electronic and thermal Enthalpies= -518.452737
Sum of electronic and thermal Free Energies= -518.503091

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 148.914 45.420 105.979

C,0,1.9990917477,-0.8112708507,-2.4148524687

O,0,2.7001513553,0.4302106947,-2.4859167187
C,0,2.7495685992,0.993033897,-3.7243880246
C,0,3.3430589892,2.2914997784,-3.6957182915
N,0,3.7370903755,2.925646042,-4.8752369696
C,0,4.5914363378,4.0892728446,-4.5839555614
O,0,2.2389276698,0.4314893392,-4.6965288329
C,0,4.304068565,2.110158674,-5.9670670415
C,0,2.1506683135,3.7345696062,-5.6833049862
C,0,1.5461271804,4.2530791161,-4.5250848203
C,0,1.2116856179,3.304505757,-3.5820433471
H,0,2.0324822657,-1.119247934,-1.365125744
H,0,0.9581539807,-0.6883524325,-2.7420112782
H,0,2.4821726422,-1.5668193404,-3.0480770708
H,0,3.7613038927,2.65800439,-2.7636197539
H,0,5.3143666309,1.7742682083,-5.6932017149
H,0,3.655136416,1.249791411,-6.1426587714
H,0,4.3590426437,2.7334071112,-6.8693983809
H,0,5.5369242546,3.7537462161,-4.1344128266
H,0,4.7948015714,4.6315184871,-5.5151569955
H,0,4.0611508985,4.7441266682,-3.8823751498
H,0,2.5620728306,4.3967247893,-6.4517186358
H,0,1.7830493066,2.7732873481,-6.0603788629
H,0,1.743098458,5.2857706078,-4.2278544805
H,0,0.8218071774,2.3397580505,-3.9132593075
H,0,0.9768162801,3.5792825208,-2.5506939644

Cation/M11L/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2M11L
parent sm conf 2
M11L/6-31G*
E(RM11L) = -519.327287478
Zero-point correction= 0.236445 (Hartree/Particle)
Thermal correction to Energy= 0.249534
Thermal correction to Enthalpy= 0.250478
Thermal correction to Gibbs Free Energy= 0.196184
Sum of electronic and ZPE= -519.090842
Sum of electronic and thermal Energies= -519.077754
Sum of electronic and thermal Enthalpies= -519.076809
Sum of electronic and thermal Free Energies= -519.131103

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.585	47.456	114.271

C,0,2.0340726827,-0.7141607078,-2.2956807733
O,0,2.7975032983,0.4751438145,-2.4216748932
C,0,2.7789965695,1.0081121502,-3.613020059
O,0,2.1871339235,0.5800854356,-4.5592651837
C,0,3.6262127796,2.2555072033,-3.5833596618
N,0,3.7158436265,2.979869074,-4.8698050726
C,0,4.4092253537,2.1645056277,-5.8883078243
C,0,4.5124352099,4.1991356037,-4.6181554417
C,0,2.363157209,3.3829515876,-5.4171054596
C,0,1.4793288015,4.0166038477,-4.4101481697
C,0,1.2056823388,5.3141635285,-4.4100191268
H,0,2.1714024365,-1.0385321175,-1.2592295894
H,0,0.9735114883,-0.5084838496,-2.4988183743
H,0,2.4027966811,-1.4801262934,-2.9922017889
H,0,4.6504699593,1.9938725382,-3.2736468666
H,0,3.2342121104,2.9502944273,-2.8234833588
H,0,3.8348356963,1.2502436169,-6.0751540558
H,0,4.4834926659,2.7536043489,-6.8117514936
H,0,5.416091875,1.9194670255,-5.5256989758
H,0,5.4897379563,3.9118707302,-4.2093409584
H,0,4.6490877471,4.733725536,-5.5669352691
H,0,3.978894462,4.8381307623,-3.9022942272
H,0,2.5875306608,4.0710919679,-6.2481830219
H,0,1.920389963,2.4656868419,-5.8310136926
H,0,0.9848582509,3.3561711575,-3.6851868708
H,0,1.6520761694,5.996229451,-5.1439171394
H,0,0.510052084,5.7521546916,-3.688925652

TS/ M11L /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentM11L
parent ts exo s-cis
M11L/6-31G*
E(RM11L) = -518.821863825

Zero-point correction= 0.219343 (Hartree/Particle)
Thermal correction to Energy= 0.232208
Thermal correction to Enthalpy= 0.233152
Thermal correction to Gibbs Free Energy= 0.180989
Sum of electronic and ZPE= -518.602521
Sum of electronic and thermal Energies= -518.589656
Sum of electronic and thermal Enthalpies= -518.588712
Sum of electronic and thermal Free Energies= -518.640875

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.713	47.624	109.786

C,0,2.0095406451,-0.72564397,-2.3735716423
O,0,2.731754584,0.4662964057,-2.4699275684
C,0,2.8367125147,0.9396694693,-3.727091124
C,0,3.5210538354,2.1825241292,-3.7206445947
N,0,3.8350356761,2.8686153217,-4.8491774867
C,0,4.6679071403,4.0188828505,-4.5812113521
O,0,2.37709327,0.33050037,-4.6735954095
C,0,4.2982578508,2.1249668546,-6.0027468325
C,0,2.116740734,3.8101927789,-5.6776950658
C,0,1.5206337475,4.2028141153,-4.4784315519
C,0,0.9955289859,3.282645183,-3.62800938
H,0,2.0163858236,-0.9981143903,-1.3097786909
H,0,0.9691545833,-0.5968832365,-2.7177991351
H,0,2.4719401923,-1.5316791614,-2.9668747524
H,0,3.7171352259,2.6753565977,-2.7697082489
H,0,5.3166917913,1.7377680333,-5.8161416154
H,0,3.6215786873,1.2865124428,-6.1999039035
H,0,4.3233798739,2.8003556143,-6.8711198931
H,0,5.6547037726,3.6999271946,-4.1995566528
H,0,4.8067942001,4.5980744093,-5.5049976716
H,0,4.1803589147,4.654721741,-3.8272146509
H,0,2.5369292548,4.5499492148,-6.3692604597
H,0,1.7933034264,2.8679295877,-6.1387058921
H,0,1.6995887121,5.2250808643,-4.1139468787
H,0,0.7343641301,2.2812458317,-3.9880619001
H,0,0.6616864279,3.5457527485,-2.6188676466

Cation/MN12L/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2MN12L

parent sm conf 2
MN12L/6-31G*
E(RMN12L) = -518.951419795

Zero-point correction= 0.243871 (Hartree/Particle)
Thermal correction to Energy= 0.256423
Thermal correction to Enthalpy= 0.257367
Thermal correction to Gibbs Free Energy= 0.205228
Sum of electronic and ZPE= -518.707549
Sum of electronic and thermal Energies= -518.694997
Sum of electronic and thermal Enthalpies= -518.694053
Sum of electronic and thermal Free Energies= -518.746192

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.908	46.170	109.736

C,0,2.0169828434,-0.7049087757,-2.2646252304
O,0,2.8214020853,0.4688281021,-2.421525019
C,0,2.7473463566,1.0593237716,-3.5941676346
O,0,2.0742201311,0.6835027372,-4.5237617892
C,0,3.6215110641,2.292299404,-3.5805403752
N,0,3.7304764188,2.9893785149,-4.8974695711
C,0,4.4439388277,2.1340062105,-5.8924629489
C,0,4.5354299227,4.226101261,-4.6561476084
C,0,2.375961661,3.4023031116,-5.4890249093
C,0,1.4405066955,3.9377820435,-4.4578548506
C,0,1.1979407051,5.23852889,-4.3143488262
H,0,2.2028163389,-1.0523615892,-1.2497499573
H,0,0.9619720487,-0.4545475411,-2.4031232884
H,0,2.315630011,-1.461045135,-2.9952848126
H,0,4.6348888965,2.023795922,-3.2613690998
H,0,3.2274952561,3.0085075336,-2.848846377
H,0,3.8792340087,1.2114559982,-6.0344115308
H,0,4.5054567972,2.6860273103,-6.8337363302
H,0,5.4484894764,1.9222221105,-5.5175272614
H,0,5.4863332028,3.9455736066,-4.1967145379
H,0,4.7129607197,4.7183498625,-5.6149824195
H,0,3.9712686967,4.8848383834,-3.9899332592
H,0,2.621360098,4.1562353184,-6.2457295124
H,0,1.9767818243,2.5120784534,-5.9800775181
H,0,0.9201506744,3.2043932581,-3.8386948965
H,0,1.6868017534,5.9832118681,-4.9439749433
H,0,0.4916754857,5.6114373694,-3.5762384927

TS MN12L /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentMN12L
parent ts exo s-cis
MN12L/6-31G*
E(RMN12L) = -518.439201710

Zero-point correction= 0.224956 (Hartree/Particle)
Thermal correction to Energy= 0.237571
Thermal correction to Enthalpy= 0.238515
Thermal correction to Gibbs Free Energy= 0.187105
Sum of electronic and ZPE= -518.214246
Sum of electronic and thermal Energies= -518.201631
Sum of electronic and thermal Enthalpies= -518.200687
Sum of electronic and thermal Free Energies= -518.252097

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.078	46.711	108.202

C,0,1.9325265401,-0.7508724864,-2.4177255391
O,0,2.7170502308,0.4228731216,-2.4924549408
C,0,2.8277003282,0.9613161688,-3.7321307835
C,0,3.5506798141,2.1827082858,-3.6992814757
N,0,3.8753187468,2.8671519167,-4.8406527571
C,0,4.6383874729,4.0820319173,-4.5779163876
O,0,2.3142950986,0.4212165155,-4.7118213978
C,0,4.3704887247,2.1363986189,-6.0074113063
C,0,2.0513133216,3.7074753426,-5.694436471
C,0,1.5301949616,4.1859552394,-4.4927277437
C,0,1.0772902443,3.3116195317,-3.5408447492
H,0,1.9336110014,-1.046796882,-1.3671227755
H,0,0.9059275494,-0.561921754,-2.7528625601
H,0,2.357600805,-1.5512155504,-3.0338360351
H,0,3.8113550426,2.634157997,-2.749150699
H,0,5.4026389585,1.8015658996,-5.8283307079
H,0,3.7303831307,1.2747687489,-6.198188285
H,0,4.3565031475,2.8115284725,-6.8700028638
H,0,5.6393024901,3.8330449033,-4.1965601213
H,0,4.7343930399,4.6573539976,-5.5034037427
H,0,4.1058646098,4.6799040948,-3.8309618009
H,0,2.4541346334,4.3739779979,-6.4564170948
H,0,1.7835271296,2.7014370055,-6.022651614
H,0,1.705070261,5.2299114483,-4.2228516363
H,0,0.7947015077,2.297662185,-3.8189691612
H,0,0.8139952099,3.6342082642,-2.5353273505

Cation/MN12SX/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2MN12SX
parent sm conf 2
MN12SX/6-31G*
E(RMN12SX) = -519.055212320

Zero-point correction= 0.243315 (Hartree/Particle)
Thermal correction to Energy= 0.256065
Thermal correction to Enthalpy= 0.257009
Thermal correction to Gibbs Free Energy= 0.203999
Sum of electronic and ZPE= -518.811897
Sum of electronic and thermal Energies= -518.799148
Sum of electronic and thermal Enthalpies= -518.798203
Sum of electronic and thermal Free Energies= -518.851213

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.683	46.526	111.568

C,0,2.0281694498,-0.7407991288,-2.2597276378
O,0,2.8045796994,0.4532522075,-2.4152862507
C,0,2.7613065696,1.0185275437,-3.6058803058
O,0,2.1298370753,0.6081280331,-4.55095102
C,0,3.6201832717,2.2684272683,-3.582887212
N,0,3.7223891657,2.9896468148,-4.8883232399
C,0,4.4333645787,2.1518370637,-5.9040637475
C,0,4.5304091009,4.2239768983,-4.6334600956
C,0,2.3627073007,3.4013170035,-5.4604974291
C,0,1.4487959128,3.9987531627,-4.4400784115

C,0,1.2034057908,5.3045625773,-4.3689791727
H,0,2.1781859981,-1.0535024724,-1.2247177199
H,0,0.9708519164,-0.5281763601,-2.4511840208
H,0,2.3831491218,-1.5113184309,-2.9526235966
H,0,4.6364182629,1.9997729765,-3.2674002712
H,0,3.21887838,2.9648759309,-2.8351381606
H,0,3.8613161089,1.2371373718,-6.0759034449
H,0,4.5092105174,2.7284893397,-6.8311637816
H,0,5.4344609597,1.9181770637,-5.5285291764
H,0,5.4960734437,3.9340197119,-4.2083652411
H,0,4.6815417218,4.7444494503,-5.5836470014
H,0,3.9858448762,4.8655335844,-3.9338950254
H,0,2.5962554744,4.1161178581,-6.2590217599
H,0,1.9342173749,2.4973665256,-5.9040192549
H,0,0.9324569263,3.3065492853,-3.7702438898
H,0,1.6815144361,6.0164458883,-5.0452024419
H,0,0.5035085656,5.7137508328,-3.6411336914

TS MN12SX /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentMN12SX
parent ts exo s-cis
MN12SX/6-31G*
E(RMN12SX) = -518.540322510

Zero-point correction= 0.225346 (Hartree/Particle)
Thermal correction to Energy= 0.237939
Thermal correction to Enthalpy= 0.238883
Thermal correction to Gibbs Free Energy= 0.187252
Sum of electronic and ZPE= -518.314977
Sum of electronic and thermal Energies= -518.302383
Sum of electronic and thermal Enthalpies= -518.301439
Sum of electronic and thermal Free Energies= -518.353071

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.309	46.521	108.668

C,0,1.9797597537,-0.7607466632,-2.3636653209
O,0,2.7068764343,0.4484683514,-2.4699473142
C,0,2.8065465414,0.9550897391,-3.729179851
C,0,3.4687007415,2.2132052718,-3.7179805179
N,0,3.8202691512,2.8885693683,-4.8642165818
C,0,4.6537565714,4.058653194,-4.5825581064
O,0,2.3273241175,0.3579310035,-4.6941428454
C,0,4.3195655022,2.1282363583,-6.0151205034
C,0,2.1035482905,3.7958027652,-5.6914997539
C,0,1.5254505726,4.2113985371,-4.4877797194
C,0,1.0700142336,3.2691759675,-3.6060422852
H,0,1.991149565,-1.026584899,-1.3023718482
H,0,0.9439217018,-0.6331807508,-2.7050365473
H,0,2.4464725746,-1.5599257412,-2.9537869379
H,0,3.7452542253,2.6579355953,-2.7687815146
H,0,5.33263677,1.7543215702,-5.8043811019
H,0,3.6526987193,1.2885348183,-6.2172830897
H,0,4.3559352452,2.7958185214,-6.8840505323
H,0,5.6271434187,3.7448778595,-4.1772982293
H,0,4.8103455344,4.6261897868,-5.5060135854
H,0,4.1444481376,4.6933123873,-3.8484839849
H,0,2.5261139463,4.5121895872,-6.3979942571
H,0,1.7917921472,2.8409199235,-6.1205722109
H,0,1.7025671126,5.2330418057,-4.1414345896
H,0,0.7751561533,2.2817328888,-3.9603882233
H,0,0.7868068391,3.5224937541,-2.5840305481

Cation/N12/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2N12
parent sm conf 2
N12/6-31G*
E(RN12) = -519.370120061

Zero-point correction= 0.241625 (Hartree/Particle)
Thermal correction to Energy= 0.254409
Thermal correction to Enthalpy= 0.255353
Thermal correction to Gibbs Free Energy= 0.202643
Sum of electronic and ZPE= -519.128495
Sum of electronic and thermal Energies= -519.115711
Sum of electronic and thermal Enthalpies= -519.114767
Sum of electronic and thermal Free Energies= -519.167477

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.644	47.072	110.937

C,0,2.0693624114,-0.826735041,-2.2909997007
O,0,2.8064644555,0.3910494327,-2.4372418608
C,0,2.7836144465,0.960275659,-3.6254962199
O,0,2.1978976052,0.5330626786,-4.5935661753
C,0,3.6091030077,2.2311816792,-3.5647845136
N,0,3.7095908004,2.9896712112,-4.8486298422
C,0,4.4036552881,2.1707538984,-5.8886983733
C,0,4.5183011185,4.2158805194,-4.5792579416
C,0,2.3327333353,3.4001914924,-5.3873340375
C,0,1.4956115765,4.1405063755,-4.4074346088
C,0,1.2032425912,5.4344107797,-4.5308925466
H,0,2.2818971901,-1.1759089232,-1.2885874733
H,0,1.0075835416,-0.6317159765,-2.4115605567
H,0,2.3966527867,-1.5518029303,-3.0299190452
H,0,4.6194798172,1.9829015174,-3.2508074657
H,0,3.1905285347,2.8963751551,-2.8148614811
H,0,3.8185085826,1.2799104661,-6.07308101
H,0,4.4863479581,2.7656242327,-6.7910388045
H,0,5.3912550714,1.9137069111,-5.5219890913
H,0,5.477772567,3.9206029587,-4.1703597297
H,0,4.6594028669,4.7458490933,-5.5142578778
H,0,3.9812286754,4.8404324406,-3.8754474012
H,0,2.543492918,3.9998697861,-6.2670982487
H,0,1.8642342176,2.4688445687,-5.6882927384
H,0,1.0578805687,3.568139052,-3.5998993158
H,0,1.5964210801,6.0348103394,-5.340336609
H,0,0.5467689872,5.9294306236,-3.8304503317

TS N12 /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentN12
parent ts exo s-cis
N12/6-31G*
E(RN12) = -518.859025806

Zero-point correction= 0.223923 (Hartree/Particle)

Thermal correction to Energy= 0.236612
Thermal correction to Enthalpy= 0.237556
Thermal correction to Gibbs Free Energy= 0.185827
Sum of electronic and ZPE= -518.635102
Sum of electronic and thermal Energies= -518.622414
Sum of electronic and thermal Enthalpies= -518.621469
Sum of electronic and thermal Free Energies= -518.673198

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.476	46.954	108.873

C,0,2.0490754923,-0.8202855069,-2.378918837
O,0,2.7342699992,0.4095184195,-2.4793800431
C,0,2.8104394534,0.9437152042,-3.7336248204
C,0,3.4795834048,2.1904879947,-3.7123869101
N,0,3.8016935943,2.8913013774,-4.8569241793
C,0,4.6655550566,4.0398059666,-4.5734471815
O,0,2.3226615837,0.3586069398,-4.7040651241
C,0,4.2938783878,2.1146141628,-6.0014822734
C,0,2.1588480051,3.781536903,-5.6633740417
C,0,1.5197493012,4.2672374683,-4.5069511675
C,0,0.9517219228,3.4040540935,-3.6220041577
H,0,2.0892314482,-1.1014986488,-1.331178372
H,0,1.0109620185,-0.7256565957,-2.6954215837
H,0,2.5240920646,-1.5896732011,-2.9863934128
H,0,3.7382992329,2.6408111724,-2.7723104552
H,0,5.3027675852,1.7603653875,-5.7918744266
H,0,3.6329878472,1.2707460757,-6.1541514988
H,0,4.309376853,2.7517521444,-6.8809088502
H,0,5.6211398458,3.6954426987,-4.1799050337
H,0,4.8283095699,4.6019937125,-5.4868517795
H,0,4.1795941225,4.6747575992,-3.8396880426
H,0,2.5868118889,4.4702649037,-6.3792910895
H,0,1.8070636777,2.8485678231,-6.0816725312
H,0,1.6868628046,5.2968150047,-4.2134599841
H,0,0.7112737352,2.3933106164,-3.9149505409
H,0,0.5980051046,3.7288692844,-2.6534236632

Cation/N12SX/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2N12SX
parent sm conf 2
N12SX/6-31G*
E(RN12SX) = -519.225340548

Zero-point correction= 0.245635 (Hartree/Particle)
Thermal correction to Energy= 0.258387
Thermal correction to Enthalpy= 0.259331
Thermal correction to Gibbs Free Energy= 0.206316
Sum of electronic and ZPE= -518.979705
Sum of electronic and thermal Energies= -518.966954
Sum of electronic and thermal Enthalpies= -518.966009
Sum of electronic and thermal Free Energies= -519.019024

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.140	46.381	111.579

C,0,2.0562441811,-0.8101113042,-2.2769408091
O,0,2.7892076254,0.4100953084,-2.4307669779
C,0,2.7834968007,0.9646651572,-3.6261628454
O,0,2.2078879347,0.5260615174,-4.5938503898
C,0,3.6142948463,2.2305015704,-3.5757234577
N,0,3.7094841649,2.9895402465,-4.8589049351
C,0,4.4058618069,2.1749494645,-5.9027436964
C,0,4.5209116361,4.2155375503,-4.5876463182
C,0,2.3387959085,3.4022207212,-5.3976529024
C,0,1.4895077728,4.1181758801,-4.4041243941
C,0,1.2028196126,5.4136776323,-4.4965873271
H,0,2.1849475624,-1.0999904892,-1.2408793037
H,0,1.0058667076,-0.6433998364,-2.5008893963
H,0,2.4581086681,-1.570997414,-2.94087206
H,0,4.6258538726,1.9720088542,-3.2691879871
H,0,3.2056171774,2.8946548067,-2.8178895742
H,0,3.8261683233,1.2797743606,-6.0906431187
H,0,4.4852150663,2.7716251764,-6.8059493879
H,0,5.3971145439,1.9205396477,-5.5400448482
H,0,5.4859042158,3.9174630823,-4.1903475916
H,0,4.6541407465,4.7535363129,-5.5206192089
H,0,3.9923636656,4.8369506672,-3.8728015368
H,0,2.5487228074,4.0267691632,-6.2618736083
H,0,1.8697947514,2.4807636325,-5.7283328605
H,0,1.043921468,3.5247739116,-3.6145140687
H,0,1.6054222514,6.0339116227,-5.2877631358
H,0,0.5413578819,5.8936207574,-3.7886112604

TS N12SX /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentN12SX
parent ts exo s-cis
N12SX/6-31G*
E(RN12SX) = -518.702689131

Zero-point correction= 0.227999 (Hartree/Particle)
Thermal correction to Energy= 0.240447
Thermal correction to Enthalpy= 0.241391
Thermal correction to Gibbs Free Energy= 0.190073
Sum of electronic and ZPE= -518.474690
Sum of electronic and thermal Energies= -518.462242
Sum of electronic and thermal Enthalpies= -518.461298
Sum of electronic and thermal Free Energies= -518.512616

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.883	45.859	108.009

C,0,2.0354877349,-0.8004177525,-2.3548270511
O,0,2.7090309373,0.4379353926,-2.476326576
C,0,2.7766300822,0.9589915667,-3.7313466413
C,0,3.3870970636,2.2406442464,-3.7214866376
N,0,3.770800411,2.9073320703,-4.8712943284
C,0,4.6468972515,4.0436032668,-4.5746232581
O,0,2.3058012098,0.3522465495,-4.6945766119
C,0,4.2782297406,2.1150453827,-5.998356289
C,0,2.1527298599,3.8258004201,-5.6885034773
C,0,1.5307091608,4.2554871924,-4.5093572803
C,0,1.0720582713,3.3055370504,-3.6391989501
H,0,2.0766919133,-1.0647083282,-1.301945607
H,0,0.9970190545,-0.7179210948,-2.674383178
H,0,2.5208450307,-1.5733210211,-2.9496218665
H,0,3.7012800612,2.6600013709,-2.7822775499
H,0,5.2778618294,1.7440439005,-5.7669845835
H,0,3.6102091454,1.2802865896,-6.171239081

H,0,4.3252605947,2.7500242149,-6.8803206207
H,0,5.5855776519,3.6897707663,-4.1462369962
H,0,4.8503021892,4.5925707967,-5.4899705923
H,0,4.149785493,4.699156285,-3.8644626444
H,0,2.5908945663,4.5382148577,-6.3768752926
H,0,1.8106312451,2.9041123066,-6.1428261101
H,0,1.7078224175,5.265878805,-4.1577425788
H,0,0.7699903031,2.3329034338,-4.000834061
H,0,0.7746107819,3.5542427317,-2.6284221365

Cation/ SOGGA11/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2SOGGA11
parent sm conf 2
SOGGA11/6-31G*
E(RSOGGA11) = -519.511656104

Zero-point correction= 0.238437 (Hartree/Particle)
Thermal correction to Energy= 0.251627
Thermal correction to Enthalpy= 0.252571
Thermal correction to Gibbs Free Energy= 0.198804
Sum of electronic and ZPE= -519.273219
Sum of electronic and thermal Energies= -519.260029
Sum of electronic and thermal Enthalpies= -519.259085
Sum of electronic and thermal Free Energies= -519.312852

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	157.898	48.019	113.162

C,0,1.9820036548,-0.7625748243,-2.2069933209
O,0,2.6997561064,0.4624778074,-2.4017430785
C,0,2.8065637154,0.905543301,-3.653163056
O,0,2.3274245157,0.3840177386,-4.6358261264
C,0,3.6674515272,2.1700688296,-3.6121448478
N,0,3.7362689209,2.9869346089,-4.8796345008
C,0,4.4296816875,2.2235036397,-5.9788337023
C,0,4.5567612281,4.2113811565,-4.5697834717
C,0,2.342227481,3.425410937,-5.3960855501
C,0,1.476682946,4.1080205336,-4.3896226502
C,0,1.1320607194,5.3949704568,-4.4691662196
H,0,1.9792150731,-0.9360317997,-1.1295661817
H,0,0.9568555966,-0.6734240805,-2.5795750521
H,0,2.4839072826,-1.5879926048,-2.7217461326
H,0,4.6936309659,1.8852929563,-3.3644480054
H,0,3.311547633,2.8237849162,-2.8167502212
H,0,3.8495256684,1.3345307002,-6.2120558916
H,0,4.5023931214,2.8735534331,-6.8509317524
H,0,5.4279317738,1.951831097,-5.6330730594
H,0,5.5341961279,3.8936586196,-4.2063556919
H,0,4.669271638,4.7892487369,-5.4870333996
H,0,4.0415138055,4.8035006432,-3.8154887125
H,0,2.5559069586,4.0758663944,-6.2446323738
H,0,1.8773626679,2.5091794745,-5.7591571107
H,0,1.0565554752,3.4898110527,-3.5991799926
H,0,1.5077732133,6.045356907,-5.2565309771
H,0,0.4445624962,5.8393973688,-3.7528019215

TS SOGGA11 /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentRSOGGA11
parent ts exo s-cis
SOGGA11/6-31G*
E(RSOGGA11) = -519.003299829

Zero-point correction= 0.221265 (Hartree/Particle)
Thermal correction to Energy= 0.234291
Thermal correction to Enthalpy= 0.235235
Thermal correction to Gibbs Free Energy= 0.182513
Sum of electronic and ZPE= -518.782035
Sum of electronic and thermal Energies= -518.769009
Sum of electronic and thermal Enthalpies= -518.768065
Sum of electronic and thermal Free Energies= -518.820786

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.020	47.582	110.962

C,0,2.0564797802,-0.8334529944,-2.32627083
O,0,2.7798781402,0.3718212073,-2.4720904918
C,0,2.8464312617,0.8687242218,-3.7596730876
C,0,3.5079333273,2.1301560287,-3.7458859324
N,0,3.8106087223,2.8758132106,-4.8738969335
C,0,4.6734602068,4.0320772245,-4.5564802909
O,0,2.3662910416,0.2513817392,-4.7157485035
C,0,4.3217330871,2.1466528706,-6.0553619746
C,0,2.1641414241,3.7846330871,-5.6572731194
C,0,1.5092894797,4.281797856,-4.5023037846
C,0,0.8617998268,3.4627421462,-3.6298899216
H,0,2.0818860756,-1.0816607265,-1.2609291967
H,0,1.0134859762,-0.723010491,-2.6509419358
H,0,2.5039766371,-1.6529530331,-2.9024837616
H,0,3.7272461067,2.5898336618,-2.7954762567
H,0,5.336361283,1.7919793432,-5.845972402
H,0,3.6715317448,1.299571084,-6.2539206387
H,0,4.3410592722,2.8240478598,-6.9106085252
H,0,5.6437616676,3.6767147101,-4.1948353037
H,0,4.8149408403,4.6345792767,-5.4544068259
H,0,4.1936405708,4.6348907035,-3.7856811625
H,0,2.6019405668,4.4815175471,-6.3671436283
H,0,1.7874668747,2.866108758,-6.0968123791
H,0,1.6982949106,5.3148221019,-4.2117654923
H,0,0.6137750433,2.4398303315,-3.8917277591
H,0,0.4868401325,3.8288432755,-2.6764598624

Cation/ SOGGA11X /6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2SOGGA11X
parent sm conf 2
SOGGA11X/6-31G*
E(RSOGGA11X) = -519.355548556

Zero-point correction= 0.246551 (Hartree/Particle)
Thermal correction to Energy= 0.259250
Thermal correction to Enthalpy= 0.260194
Thermal correction to Gibbs Free Energy= 0.207270
Sum of electronic and ZPE= -519.108998
Sum of electronic and thermal Energies= -519.096299
Sum of electronic and thermal Enthalpies= -519.095355
Sum of electronic and thermal Free Energies= -519.148278

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 162.682 46.145 111.387
C,0,2.0445472635,-0.8050728211,-2.2729718075
O,0,2.7943086836,0.4170624491,-2.418203596
C,0,2.7801603675,0.9681703745,-3.6191716474
O,0,2.1951968675,0.5325976289,-4.5838313072
C,0,3.6209361403,2.236052061,-3.5738105675
N,0,3.7143797523,2.9911294324,-4.8645330794
C,0,4.4144901202,2.1694072974,-5.9070359922
C,0,4.5304587942,4.2206370186,-4.5965052789
C,0,2.3431000174,3.4035840898,-5.4099054623
C,0,1.4766734171,4.1005745696,-4.4061185134
C,0,1.1912214898,5.4012364499,-4.476681724
H,0,2.1787095322,-1.0982353716,-1.2340845878
H,0,0.9915819716,-0.6229906338,-2.4917567908
H,0,2.4416943276,-1.5665317015,-2.9454387939
H,0,4.6369742361,1.9718831901,-3.2705668252
H,0,3.2145459495,2.9071689653,-2.8141568103
H,0,3.8332861621,1.2688173632,-6.091518739
H,0,4.4926701606,2.7654193963,-6.8164920727
H,0,5.4102421807,1.9181929814,-5.540310264
H,0,5.4994826802,3.9191214035,-4.1987937577
H,0,4.6628401223,4.7574411625,-5.5357420861
H,0,4.0021646628,4.846188684,-3.8779831236
H,0,2.5580830294,4.0484445339,-6.2641102073
H,0,1.8798757388,2.4820020401,-5.7616746725
H,0,1.0167590748,3.4877322577,-3.6331617476
H,0,1.606991312,6.039209732,-5.2531605665
H,0,0.5176579456,5.8680754468,-3.7646029797

TS SOGGA11X /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentRSOGGA11X
parent ts exo s-cis
SOGGA11X/6-31G*
E(RSOGGA11X) = -518.827279415

Zero-point correction= 0.228862 (Hartree/Particle)
Thermal correction to Energy= 0.241196
Thermal correction to Enthalpy= 0.242141
Thermal correction to Gibbs Free Energy= 0.191092
Sum of electronic and ZPE= -518.598417
Sum of electronic and thermal Energies= -518.586083
Sum of electronic and thermal Enthalpies= -518.585139
Sum of electronic and thermal Free Energies= -518.636188

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.353	45.547	107.442

C,0,2.0392457432,-0.8076916123,-2.3491661653
O,0,2.7124331903,0.4409415815,-2.4664164491
C,0,2.7679561999,0.9573465487,-3.7272756887
C,0,3.3682397852,2.2521112242,-3.7190483075
N,0,3.760402671,2.9129515553,-4.8760681687
C,0,4.6508850053,4.042684253,-4.57361537
O,0,2.2959892859,0.3462591075,-4.6877666119
C,0,4.2782730798,2.110791222,-5.9978119679
C,0,2.1435972704,3.8414664962,-5.6996449459
C,0,1.5210129559,4.2647360704,-4.5141626895
C,0,1.085143923,3.2943627455,-3.6447188412
H,0,2.0837639747,-1.0668626306,-1.2906734721
H,0,0.997172443,-0.7261969259,-2.6701062895
H,0,2.533846945,-1.5798093337,-2.9443437534
H,0,3.7004796442,2.6657470546,-2.7781122655
H,0,5.2725229504,1.7221408992,-5.7498473071
H,0,3.597851255,1.2844575228,-6.1887392907
H,0,4.3500081925,2.7531372709,-6.8790720819
H,0,5.5885101513,3.6780969951,-4.1394626632
H,0,4.8630696591,4.59170167,-5.4928960097
H,0,4.1547510374,4.7058230514,-3.8622160849
H,0,2.5836476199,4.5615178555,-6.3865471614
H,0,1.7997449393,2.9189713456,-6.162500555
H,0,1.7071996006,5.2735070392,-4.1486469551
H,0,0.7638379763,2.3283292147,-4.0211907286
H,0,0.7946685018,3.5309407794,-2.623990176

Structures for Reactions of 5

TSCleavageA/ UB3LYP-D2/6-31G*/PCM

/home/bibaswanbiswas/c11/cleavageAB3D2SB
trimethyl pure cleavage conf A
UB3LYP/6-31G*
E(UB3LYP) = -636.975962660

Zero-point correction= 0.306380 (Hartree/Particle)
Thermal correction to Energy= 0.323922
Thermal correction to Enthalpy= 0.324867
Thermal correction to Gibbs Free Energy= 0.261199
Sum of electronic and zero-point Energies= -636.669583
Sum of electronic and thermal Energies= -636.652040
Sum of electronic and thermal Enthalpies= -636.651096
Sum of electronic and thermal Free Energies= -636.714763

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	203.264	63.657	133.999

C	0.96186	0.05852	-1.11585
C	2.23451	-0.54129	-1.02972
C	3.39921	0.03075	-0.56925
C	3.51838	1.46587	-0.13722
C	4.67058	-0.76706	-0.49488
N	-0.15945	-0.24764	0.82847
C	0.79745	0.38775	1.74175
C	-1.41773	0.34013	0.71215
C	-1.64495	1.68974	1.34161
C	-2.33513	-0.2014	-0.24274
C	-0.07123	-1.71616	0.94601
H	4.52065	-1.80463	-0.81505
H	5.45483	-0.31884	-1.1254
H	5.07099	-0.77378	0.53108
H	4.27061	1.98828	-0.74808
H	2.57645	2.01639	-0.2078
H	3.87	1.52592	0.90379
H	2.29362	-1.59289	-1.3139

H	0.83883	1.12812	-0.98334
H	0.14725	-0.46113	-1.60582
H	0.84583	1.46082	1.55765
H	0.50921	0.20546	2.78626
H	1.78074	-0.04876	1.55089
H	0.96555	-2.00953	0.76267
H	-0.36575	-2.01269	1.9625
H	-0.72796	-2.17443	0.21135
H	-2.69582	1.96685	1.25076
H	-1.37769	1.69542	2.40647
H	-1.04977	2.48384	0.85964
O	-2.14357	-1.15262	-1.02073
O	-3.54574	0.4606	-0.24836
C	-4.49635	-0.02563	-1.19845
H	-5.37992	0.60622	-1.08043
H	-4.10769	0.05236	-2.22009
H	-4.75037	-1.07316	-1.00045

TSCleavageB/ UB3LYP-D2/6-31G*/ PCM

/home/bibaswanbiswas/c11/cleavageBB3D2SB
trimethyl pure cleavage conf B
UB3LYP/6-31G*
E(UB3LYP) = -636.976342409

Zero-point correction= 0.306776 (Hartree/Particle)
Thermal correction to Energy= 0.324136
Thermal correction to Enthalpy= 0.325081
Thermal correction to Gibbs Free Energy= 0.262236
Sum of electronic and ZPE= -636.669566
Sum of electronic and thermal Energies= -636.652206
Sum of electronic and thermal Enthalpies= -636.651262
Sum of electronic and thermal Free Energies= -636.714106

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.399	63.496	132.268

C,0,0.872752882,-0.1728587055,-0.9621135773
C,0,2.2132613596,-0.6034704406,-0.8936508531
C,0,3.2954914666,0.1615617617,-0.5204870944
C,0,3.1953871901,1.6169224157,-0.1541050529
C,0,4.6764237146,-0.4274655639,-0.4692327916
N,0,-0.1531187028,-0.3376171624,1.0517264683
C,0,0.885524265,0.1799987806,1.9611467536
C,0,-1.3653416886,0.3462921175,0.9509834669
C,0,-2.6200090805,-0.4478824324,0.6960161764
C,0,-1.3278519825,1.7618122989,0.7632261062
C,0,-0.219054196,-1.8020164959,1.1583648557
H,0,4.6811108953,-1.4859345184,-0.7541818128
H,0,5.3606376409,0.1155024686,-1.1404861591
H,0,5.1049325726,-0.3359392166,0.5412906538
H,0,3.6811499388,2.242565822,-0.9198575582
H,0,2.1640375766,1.9574621605,-0.0276407449
H,0,3.73631287,1.8058485073,0.7851569425
H,0,2.408888652,-1.6535462354,-1.1155033037
H,0,0.6203996585,0.8789900306,-0.9188992882
H,0,0.1233612353,-0.8350748306,-1.3824390426
H,0,0.9098348206,1.2641029922,1.9048136664
H,0,0.6564907127,-0.1491278083,2.9843484124
H,0,1.8491039273,-0.2310980077,1.6505648484
H,0,0.7969758786,-2.1907191648,1.0586038325
H,0,-0.6299364426,-2.0957134823,2.1341728129
H,0,-0.8388507763,-2.2155876131,0.3625780878
H,0,-3.4852284107,0.2157789245,0.7116017041
H,0,-2.6045627682,-0.9494849493,-0.2865844199
H,0,-2.77456105,-1.2309943697,1.4497252153
O,0,-0.3189578801,2.4851691844,0.6599410403
O,0,-2.5866848245,2.3233117166,0.6923076181
C,0,-2.6078423368,3.7349978289,0.4713573216
H,0,-3.6642704646,4.0123238703,0.4405246306
H,0,-2.099059324,4.2685511301,1.2821139524
H,0,-2.1203973287,3.9926879865,-0.4758198676

TSCleavageA/ UM062X/6-31G*/PCM

/home/bibaswanbiswas/c11/cleavageAM062XSB
trimethyl pure cleavage conf A
UM062X/6-31G*
E(UM062X) = -636.614382233

Zero-point correction= 0.309673 (Hartree/Particle)
Thermal correction to Energy= 0.327207
Thermal correction to Enthalpy= 0.328151
Thermal correction to Gibbs Free Energy= 0.264503
Sum of electronic and ZPE= -636.304709
Sum of electronic and thermal Energies= -636.287176
Sum of electronic and thermal Enthalpies= -636.286232
Sum of electronic and thermal Free Energies= -636.349879

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	205.325	63.518	133.958

C,0,0.9507872778,0.0350160376,-1.0699864052
C,0,2.2372713318,-0.5447608178,-1.0078149658
C,0,3.4000723239,0.0450081421,-0.582448903
C,0,3.5086078426,1.4828491599,-0.1645613874
C,0,4.6818456566,-0.7338274147,-0.52575822
N,0,-0.1685744879,-0.269482346,0.8491206837
C,0,0.779346658,0.3503788638,1.7754044303
C,0,-1.4074764822,0.3353680996,0.7191925326
C,0,-1.6282153773,1.6928077109,1.3232652317
C,0,-2.330644737,-0.2052535351,-0.2311742876
C,0,-0.1008117135,-1.7349295241,0.9557577721
H,0,4.5414088782,-1.7720212755,-0.8380848072
H,0,5.446608044,-0.2802793067,-1.1701948155
H,0,5.0965980532,-0.7327920482,0.4911366314
H,0,4.279598364,1.9936766555,-0.7557221038
H,0,2.5745419416,2.0370668036,-0.2754084118
H,0,3.8233752955,1.5568680822,0.8850243676
H,0,2.3036375106,-1.5960675264,-1.2909369962
H,0,0.8117828012,1.105886779,-0.9581578047
H,0,0.1470194547,-0.4951675505,-1.5681000675
H,0,0.8474902442,1.4224059852,1.5934978576
H,0,0.4729811992,0.1734187572,2.813902463
H,0,1.7595686441,-0.1007057278,1.6058757236
H,0,0.9355164429,-2.0400976309,0.7966459891
H,0,-0.4200171826,-2.0348470125,1.9613111677
H,0,-0.7442313522,-2.1853350074,0.2064760298
H,0,-2.6756260941,1.9701961694,1.2175392037
H,0,-1.3771277378,1.715911625,2.3891736314
H,0,-1.0299588159,2.4753892174,0.8327171179

O,0,-2.1522139399,-1.1649994016,-0.9894014664
O,0,-3.5177248817,0.4747470681,-0.256209482
C,0,-4.4603748888,-0.000966734,-1.2063715106
H,0,-5.3284286121,0.6519498703,-1.1171153938
H,0,-4.0543865503,0.0486079254,-2.2198565687
H,0,-4.7448141106,-1.034635093,-0.9932512357

TS23/ N12/6-31G*/ exo s-cis /PCM(DMF)

/home/bibaswanbiswas/c11/obscure/me3TSN12normal
trimethyl ts exo s-cis
N12/6-31G*
E(RN12) = -636.780168187

Zero-point correction= 0.308671 (Hartree/Particle)
Thermal correction to Energy= 0.325512
Thermal correction to Enthalpy= 0.326456
Thermal correction to Gibbs Free Energy= 0.265870
Sum of electronic and ZPE= -636.471498
Sum of electronic and thermal Energies= -636.454656
Sum of electronic and thermal Enthalpies= -636.453712
Sum of electronic and thermal Free Energies= -636.514298

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	204.262	62.915	127.514

C,0,-0.1715715268,0.7048441087,0.52463348
C,0,0.3956347491,0.4590627633,1.7919959173
C,0,1.7360901208,0.4423714881,2.0614517443
C,0,2.7769006932,0.4468338518,0.9906072038
C,0,2.2259502437,0.3323638344,3.4679095638
N,0,-0.4345184883,2.7541455998,0.4109040105
C,0,-1.866494884,2.8470203983,0.7195816899
C,0,0.384799222,3.4776027871,1.2841602816
C,0,-0.1478383238,3.8051260704,2.6428463348
C,0,1.7392138823,3.7227458393,0.9563546077
C,0,-0.2414480376,2.9799460698,-1.0296467312
H,0,1.4149352407,0.3554253238,4.1927057986
H,0,2.7911192029,-0.5920334297,3.6158440676
H,0,2.9173654446,1.1445741005,3.7045900093
H,0,2.5064872338,-0.213981913,0.166205217
H,0,2.9009695793,1.4471133222,0.5580837988
H,0,3.740562466,0.1222096793,1.3792003032
H,0,-0.2838329321,0.3860838374,2.6339930877
H,0,0.4608833068,0.6202726746,-0.3474395771
H,0,-1.203078142,0.4302262819,0.3558564852
H,0,-2.0703474087,2.4681402897,1.7134149672
H,0,-2.1965267738,3.8832110624,0.6514936257
H,0,-2.4170592711,2.2541617298,-0.0028086891
H,0,-0.815309818,2.2390344361,-1.5780903365
H,0,-0.6016078057,3.9767579663,-1.2859210178
H,0,0.8127462336,2.9045403882,-1.2557974073
H,0,0.6346474704,4.2771392801,3.224664212
H,0,-1.0007413287,4.4879329754,2.6243133688
H,0,-0.468879854,2.913856106,3.1892526878
O,0,2.377506623,3.3526885492,-0.0439797526
O,0,2.3777371766,4.4888818402,1.9042693502
C,0,3.7194135881,4.8127539821,1.6246494253
H,0,4.0439719445,5.4631584531,2.4318383175
H,0,4.3528579387,3.9266841697,1.5946605451
H,0,3.8158612348,5.3322670838,0.6717774105

TSCleavageA/ UM06/6-31G*/PCM

/home/bibaswanbiswas/c11/cleavageAM06SB
trimethyl pure cleavage conf A
UM06/6-31G*
E(UM06) = -636.475361474

Zero-point correction= 0.305133 (Hartree/Particle)
Thermal correction to Energy= 0.322776
Thermal correction to Enthalpy= 0.323720
Thermal correction to Gibbs Free Energy= 0.259429
Sum of electronic and ZPE= -636.170229
Sum of electronic and thermal Energies= -636.152585
Sum of electronic and thermal Enthalpies= -636.151641
Sum of electronic and thermal Free Energies= -636.215932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	202.545	64.024	135.312

C,0,0.9542306862,0.0057639336,-1.0119187567
C,0,2.24991062,-0.5521893838,-0.9587657612
C,0,3.4143391943,0.0691959403,-0.588011801
C,0,3.5196206388,1.5193088512,-0.2441285314
C,0,4.7006349861,-0.6876519124,-0.5297595624
N,0,-0.1680881961,-0.2984112868,0.8474078459
C,0,0.7582583438,0.2847245778,1.8139019715
C,0,-1.4127142358,0.324818327,0.7217473897
C,0,-1.6043156566,1.6846435698,1.3143904115
C,0,-2.326531863,-0.1960708768,-0.2428130057
C,0,-0.1469649522,-1.7636127417,0.9630595076
H,0,4.5747297917,-1.743610966,-0.7967426981
H,0,5.45139678,-0.2498371442,-1.2064663584
H,0,5.1422426107,-0.640521849,0.4784295576
H,0,4.2887187345,2.0061931665,-0.8632268107
H,0,2.5833812274,2.0720088469,-0.3760087642
H,0,3.8437528158,1.6515787335,0.800265847
H,0,2.3264121228,-1.6156101964,-1.2065932235
H,0,0.8083222247,1.0826874072,-0.9225212361
H,0,0.1597005882,-0.5265768672,-1.5307055912
H,0,0.8417677235,1.3641770575,1.6689998824
H,0,0.4231490225,0.0823902582,2.8424318002
H,0,1.7445683201,-0.1680724317,1.6635773181
H,0,0.8818046581,-2.1133481363,0.8251595295
H,0,-0.496086824,-2.0520801198,1.9654744365
H,0,-0.7946622288,-2.1971891793,0.2022061601
H,0,-2.634176194,2.0109755206,1.1553536478
H,0,-1.4111906251,1.7111061375,2.3964554578
H,0,-0.9512192012,2.4494540731,0.8571963065
O,0,-2.1502692076,-1.1454088397,-1.0153814736
O,0,-3.5149625173,0.4878859035,-0.2601251289
C,0,-4.4579344396,0.0277272255,-1.2099813934
H,0,-5.3302782647,0.6785531581,-1.1104547509
H,0,-4.0625064515,0.0905759203,-2.230935972
H,0,-4.7476092315,-1.012191677,-1.0160302503

TS23/ UM062X/6-31G*/ endo s-cis /PCM

/home/bibaswanbiswas/c11/allme3NCM062XSB
endo s-cis isomer of trimethylalanine system

um062X/6-31G*
E(UM062X) = -636.627660384

Zero-point correction= 0.311847 (Hartree/Particle)
Thermal correction to Energy= 0.328356
Thermal correction to Enthalpy= 0.329300
Thermal correction to Gibbs Free Energy= 0.269695
Sum of electronic and ZPE= -636.315814
Sum of electronic and thermal Energies= -636.299305
Sum of electronic and thermal Enthalpies= -636.298361
Sum of electronic and thermal Free Energies= -636.357965

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.046	62.322	125.449

C,0,-0.1804468171,0.4762427891,0.2513172089
C,0,0.0990370625,0.1782666755,1.5850693798
C,0,1.3390772718,0.3893285586,2.1528033852
C,0,1.501886509,0.3106574506,3.6459649546
C,0,0.8669272977,2.9180892638,1.3790320534
C,0,2.2252721579,3.3728523419,0.9169020567
C,0,2.6300593947,0.2975170779,1.3884084469
N,0,-0.0832557506,2.5796879381,0.4199190688
C,0,0.2341333775,2.9758628389,-0.9612075318
C,0,0.4968056772,3.0155573952,2.7644622146
O,0,1.5308611425,3.4877948811,3.5368280676
C,0,1.2227782525,3.6426642416,4.9148259471
C,0,-1.5052520339,2.8668294854,0.7023011221
O,0,-0.5803597538,2.7468082195,3.298964544
H,0,0.5520682817,0.4889300261,4.1579692105
H,0,1.8849990478,-0.6743203774,3.946338628
H,0,2.2273000721,1.0564665427,3.9921900791
H,0,3.3544030512,1.0376665688,1.7446332732
H,0,3.07987674,-0.6910173437,1.5571550963
H,0,2.5116803712,0.4278035166,0.310797452
H,0,-0.7470266118,0.0887281193,2.2650807637
H,0,0.5996965009,0.4279387452,-0.5033866773
H,0,-1.188841474,0.3451760265,-0.1328484942
H,0,-1.8265639984,2.3174464595,1.5798620599
H,0,-1.636658058,3.9403364949,0.8778912431
H,0,-2.0868073896,2.5673921752,-0.1709398117
H,0,-0.4973600247,2.5141216083,-1.6259318657
H,0,0.1831840817,4.0656783949,-1.0680439821
H,0,1.2265886281,2.6309378731,-1.2447061105
H,0,2.1851771522,4.336185587,0.390446258
H,0,2.8822905893,3.4911054292,1.7764945105
H,0,2.7043442685,2.657654973,0.2393177076
H,0,2.136843684,4.0080183151,5.3836228552
H,0,0.4143453607,4.3650919276,5.0560919618
H,0,0.9256649393,2.6914347808,5.3631239248

TS23/ UM06/6-31G*/ endo s-trans /PCM

/home/bibaswanbiswas/c11/allme3NTM06SB
endo s-trans isomer of trimethylalanine system
um06/6-31G*
E(UM06) = -636.483393128

Zero-point correction= 0.308783 (Hartree/Particle)
Thermal correction to Energy= 0.324717
Thermal correction to Enthalpy= 0.325661
Thermal correction to Gibbs Free Energy= 0.268103
Sum of electronic and ZPE= -636.174611
Sum of electronic and thermal Energies= -636.158676
Sum of electronic and thermal Enthalpies= -636.157732
Sum of electronic and thermal Free Energies= -636.215290

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.763	62.069	121.142

C,0,-0.0473749285,0.4816483307,0.0764154437
C,0,0.1192851936,0.085816142,1.4065039041
C,0,1.2920684298,0.1838640465,2.1158664475
C,0,2.6490573679,0.2605484762,1.4991386548
C,0,1.3066643629,0.0277928524,3.5985877754
N,0,-0.1333667834,2.6043766603,0.3704621091
C,0,-1.5776854671,2.7684042343,0.6152726887
C,0,0.7787260635,2.9893720367,1.3536863828
C,0,0.5439873816,2.9863597736,2.7666292153
O,0,1.3915707633,3.3008818531,3.611307226
C,0,2.1510157495,3.3982863344,0.9167004882
C,0,0.1745950013,3.0784508521,-0.9869558254
O,0,-0.718792924,2.6510637042,3.1803619756
C,0,-0.9694409404,2.82330213,4.5629967697
H,0,0.3198420176,-0.2300468464,4.0024817747
H,0,2.0266520812,-0.7413409146,3.9175805472
H,0,1.6320717551,0.9763869404,4.0635657645
H,0,3.2447781445,1.0648318605,1.9572770211
H,0,3.197549849,-0.6748285654,1.6937988526
H,0,2.6393460971,0.4174672556,0.415427533
H,0,-0.7902513682,-0.0879550123,1.9885501357
H,0,0.8072386322,0.5345146281,-0.5978277407
H,0,-1.0057472905,0.3285137455,-0.4190512666
H,0,-1.9025882839,2.1331340773,1.4354739147
H,0,-1.7982542369,3.8160870962,0.8616273066
H,0,-2.1131588162,2.4910404663,-0.2976016384
H,0,-0.5029723563,2.5868737462,-1.6912948764
H,0,0.0334417746,4.1672627712,-1.0525376762
H,0,1.2001082291,2.8329887768,-1.2676650508
H,0,2.1548529548,4.3241484627,0.3211205706
H,0,2.7584946091,3.5752848259,1.8074562216
H,0,2.665458134,2.6324253361,0.3144106194
H,0,-2.0164738276,2.5473411979,4.7150066531
H,0,-0.3272019684,2.1832416425,5.1784128639
H,0,-0.8145234003,3.8652320828,4.8688902152

TSCleavageA/ UM06/6-31+G**/ PCM

/home/bibaswanbiswas/c11/cleavageAM06PS
trimethyl pure cleavage conf A
UM06/6-31+G**
E(UM06) = -636.521859139

Zero-point correction= 0.303596 (Hartree/Particle)
Thermal correction to Energy= 0.320985
Thermal correction to Enthalpy= 0.321929
Thermal correction to Gibbs Free Energy= 0.258927
Sum of electronic and ZPE= -636.218263
Sum of electronic and thermal Energies= -636.200874
Sum of electronic and thermal Enthalpies= -636.199930

Sum of electronic and thermal Free Energies= -636.262932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	201.421	64.267	132.600

C,0,0.9923676419,0.0280016999,-1.0227931804
C,0,2.2841265363,-0.5389304493,-0.9591626444
C,0,3.4473439242,0.0799201121,-0.5744867839
C,0,3.5479906647,1.5272665269,-0.2199926923
C,0,4.7326148457,-0.6777528454,-0.5099830016
N,0,-0.1774651443,-0.3058482098,0.8226917602
C,0,0.729735531,0.256321184,1.8239399222
C,0,-1.4151821326,0.3282231636,0.686921027
C,0,-1.5709053579,1.7132273029,1.2329965439
C,0,-2.3606925641,-0.2072754344,-0.2381748119
C,0,-0.1545108663,-1.7741046139,0.9203638649
H,0,4.6063353819,-1.7324469936,-0.7757401282
H,0,5.4833337068,-0.2393781672,-1.1838394175
H,0,5.1668859818,-0.6262943671,0.4995669905
H,0,4.3128633982,2.0179362779,-0.8384919917
H,0,2.6104340248,2.0768138713,-0.3439244844
H,0,3.8768764432,1.6481667757,0.8228225822
H,0,2.3599680536,-1.5993855266,-1.2149888686
H,0,0.8508806323,1.1021873755,-0.9154106182
H,0,0.2055261957,-0.4955017763,-1.5587518535
H,0,0.8457464095,1.3330087177,1.6944017084
H,0,0.3520922401,0.0523435673,2.8361643997
H,0,1.7088307994,-0.2177717248,1.70885191
H,0,0.8812708342,-2.1131318015,0.8255925579
H,0,-0.5432908671,-2.0742167555,1.9038674517
H,0,-0.7637064528,-2.2117493341,0.1318929315
H,0,-2.5828847141,2.0725256015,1.0443934937
H,0,-1.3952963937,1.7697686117,2.3152006224
H,0,-0.8808247267,2.4318737179,0.7591059524
O,0,-2.2182511089,-1.1826852124,-0.9901923876
O,0,-3.5428067701,0.4901778625,-0.2452409183
C,0,-4.5336397268,0.0109941136,-1.1416875489
H,0,-5.3956569516,0.6684377851,-1.0154100199
H,0,-4.1853121001,0.050922041,-2.1791166868
H,0,-4.8173663679,-1.0202580961,-0.9058996804

TS23/ UM062X/6-31G*/ endo s-trans / Gas

/home/bibaswanbiswas/c11/allme3NTM062XSB
endo s-trans isomer of trimethylalanine system
um062X/6-31G*
E(UM062X) = -636.617219503

Zero-point correction= 0.313451 (Hartree/Particle)
Thermal correction to Energy= 0.329430
Thermal correction to Enthalpy= 0.330374
Thermal correction to Gibbs Free Energy= 0.272567
Sum of electronic and ZPE= -636.303769
Sum of electronic and thermal Energies= -636.287789
Sum of electronic and thermal Enthalpies= -636.286845
Sum of electronic and thermal Free Energies= -636.344652

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.720	61.600	121.665

C,0,0.0062835006,0.5084784462,0.0103230279
C,0,0.1140253217,0.0868351913,1.3415343534
C,0,1.2403593838,0.2611286523,2.1104218977
C,0,2.6390346254,0.3361341275,1.5701283842
C,0,1.1735761233,0.0986157702,3.600060813
N,0,-0.1230321983,2.5630800213,0.3600411144
C,0,-1.5629934645,2.674950966,0.6669682797
C,0,0.8051226048,2.9302629844,1.3270302519
C,0,0.5847591858,2.9580801219,2.7494984401
O,0,1.4325619367,3.3058893285,3.5670955932
C,0,2.1640369528,3.3822079737,0.8729387045
C,0,0.1325968174,3.101610945,-0.9852842331
O,0,-0.6617727269,2.5862773068,3.1869659773
C,0,-0.8775499708,2.783057501,4.5772472715
H,0,0.1458770578,-0.0435695536,3.9457264222
H,0,1.7782826936,-0.7562888994,3.9301848669
H,0,1.5869115753,0.9940072475,4.087449942
H,0,3.1943769844,1.1535736877,2.0447171423
H,0,3.1700370795,-0.5941474022,1.8137807119
H,0,2.6843001547,0.4678159684,0.4874494467
H,0,-0.8129455637,-0.1318263641,1.8707921428
H,0,0.8959712767,0.589488948,-0.6090806018
H,0,-0.9104084543,0.3141999396,-0.5421394373
H,0,-1.8267976405,1.9906761757,1.4656731667
H,0,-1.7981117092,3.6981201047,0.9768443965
H,0,-2.1178127748,2.4235355366,-0.2389490833
H,0,-0.5536548988,2.6214965498,-1.6851630393
H,0,-0.0311784943,4.1858445028,-0.997840684
H,0,1.1535573492,2.8884100248,-1.2949417734
H,0,2.1338711916,4.3332109223,0.3245290486
H,0,2.7812680609,3.5319695894,1.7581418749
H,0,2.6678474035,2.6508506228,0.2266171261
H,0,-1.912363262,2.4889336747,4.7585254598
H,0,-0.2001187634,2.1692570042,5.1748081529
H,0,-0.7269453581,3.8306033839,4.8499798431

TS23/ UM062X/6-31G*/ exo s-trans / PCM

/home/bibaswanbiswas/c11/allme3XTM062XSB
exo s-trans isomer of trimethylalanine system
um062X/6-31G*
E(UM062X) = -636.624650896

Zero-point correction= 0.313316 (Hartree/Particle)
Thermal correction to Energy= 0.329255
Thermal correction to Enthalpy= 0.330200
Thermal correction to Gibbs Free Energy= 0.272424
Sum of electronic and ZPE= -636.311335
Sum of electronic and thermal Energies= -636.295396
Sum of electronic and thermal Enthalpies= -636.294451
Sum of electronic and thermal Free Energies= -636.352227

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.611	61.497	121.600

C,0,-0.275612224,0.7099609689,0.214439431
C,0,0.302817612,0.3601804197,1.44552669
C,0,1.5831002556,0.7226815506,1.7867793782
C,0,2.039390644,0.6992475665,3.2153831741

C,0,2.7041362241,0.8943190753,0.7985286108
N,0,-0.4554111078,2.7460830653,0.4949062461
C,0,-0.2765610898,3.2428718281,-0.8865855921
C,0,-1.8860902857,2.8434829438,0.8551345218
C,0,0.4101048297,3.1667852146,1.5117771601
C,0,1.7458098793,3.6462625811,1.3364796638
O,0,2.1977892277,3.7305886165,0.0473890131
C,0,3.5083518879,4.2583348358,-0.102864373
C,0,-0.1094918889,3.176561683,2.9241078576
O,0,2.496783868,3.9821903707,2.2595481848
H,0,1.2192590409,0.4890392179,3.9074605744
H,0,2.8314295778,-0.0451663056,3.3708237141
H,0,2.4676198657,1.6815971832,3.4620634695
H,0,3.3849438311,1.6852557962,1.1320661847
H,0,3.2891304548,-0.0348798036,0.7603389377
H,0,2.3728044231,1.1338982889,-0.2128177209
H,0,-0.3747260839,0.0907114277,2.2558061041
H,0,0.3467971058,0.7921652527,-0.6718716312
H,0,-1.3055470483,0.4280049291,0.0102956942
H,0,-2.0900850775,2.2556944515,1.7481537836
H,0,-2.1602960558,3.8893718174,1.0286287099
H,0,-2.4790070735,2.4460123738,0.0314345249
H,0,-1.0539942144,2.7887131185,-1.5029499498
H,0,-0.378379038,4.3324232001,-0.9081982907
H,0,0.6989337046,2.9644920792,-1.267471074
H,0,0.7225854268,3.3990292018,3.5912094811
H,0,-0.8857947854,3.9352293966,3.0905355504
H,0,-0.5322718131,2.209618167,3.2230737749
H,0,3.696598895,4.2815676563,-1.1763868304
H,0,3.5725256594,5.2665509791,0.3134781245
H,0,4.2502963729,3.6268538522,0.3923629027

TS23/ UM06/6-31G*/ endo s-cis / PCM

/home/bibaswanbiswas/c11/allme3NCM06SB
endo s-cis isomer of trimethylalanine system
um06/6-31G*
E(UM06) = -636.484358520

Zero-point correction= 0.308491 (Hartree/Particle)
Thermal correction to Energy= 0.324683
Thermal correction to Enthalpy= 0.325627
Thermal correction to Gibbs Free Energy= 0.266985
Sum of electronic and ZPE= -636.175868
Sum of electronic and thermal Energies= -636.159676
Sum of electronic and thermal Enthalpies= -636.158731
Sum of electronic and thermal Free Energies= -636.217373

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.742	62.327	123.422

C,0,-0.1640312234,0.4768482549,0.2603814875
C,0,0.1168982902,0.1722108962,1.5929735355
C,0,1.3560176428,0.2805656923,2.1780481914
C,0,1.5091665717,0.1794089891,3.6599848824
C,0,0.8301649431,3.0253543136,1.3714146958
C,0,2.1994238511,3.4153376121,0.905450222
C,0,2.6456359895,0.2570223272,1.4260975358
N,0,-0.1059411095,2.6375254061,0.4141239939
C,0,0.2124050958,2.9918005678,-0.9731719603
C,0,0.4820757194,3.0587014667,2.7618464358
O,0,1.5471662377,3.4639639549,3.5398119842
C,0,1.248779168,3.6536829011,4.910103271
C,0,-1.5292751903,2.9232173952,0.6666644151
O,0,-0.5972866622,2.8119131377,3.3049379152
H,0,0.5416353373,0.1663220752,4.1752461211
H,0,2.0702253356,-0.7246472321,3.9456110708
H,0,2.0864349612,1.0375773346,4.0395850812
H,0,3.3347483591,1.0327578,1.7922964267
H,0,3.1548594384,-0.7060716664,1.5927982735
H,0,2.5331548463,0.386765047,0.3441484291
H,0,-0.7368025128,0.0778479822,2.2688555559
H,0,0.6173428433,0.4402973545,-0.4981258888
H,0,-1.1751339975,0.3492410881,-0.1241651374
H,0,-1.830690437,2.5021406513,1.622863524
H,0,-1.6834741412,4.012422651,0.6913168342
H,0,-2.1194444883,2.4957945392,-0.1497811959
H,0,-0.5190615185,2.5115568484,-1.6303366634
H,0,0.1591286353,4.0814715912,-1.1153842532
H,0,1.2077330096,2.6420088745,-1.2542033983
H,0,2.1931738294,4.3229072788,0.2815280957
H,0,2.8401087078,3.6144449003,1.7660898308
H,0,2.6969066203,2.6312725823,0.3133193206
H,0,2.1793643197,3.9869347408,5.377367213
H,0,0.4724532937,4.4165143907,5.0471132342
H,0,0.9088672344,2.7258232534,5.3859399211

TS23/ UM062X/6-31G* exo s-cis /PCM

/home/bibaswanbiswas/c11/allme3XCM062XSB
exo s-cis isomer of trimethylalanine system
um062X/6-31G*
E(UM062X) = -636.626820538

Zero-point correction= 0.312284 (Hartree/Particle)
Thermal correction to Energy= 0.328784
Thermal correction to Enthalpy= 0.329728
Thermal correction to Gibbs Free Energy= 0.270034
Sum of electronic and ZPE= -636.314537
Sum of electronic and thermal Energies= -636.298037
Sum of electronic and thermal Enthalpies= -636.297092
Sum of electronic and thermal Free Energies= -636.356787

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.315	62.172	125.637

C,0,-0.3466438234,0.6263672319,0.4011987831
C,0,0.2702460329,0.394603681,1.6402136746
C,0,1.5764714181,0.7446195511,1.8883971097
C,0,2.6484855275,0.7597666592,0.8335574088
C,0,2.0967111922,0.8147969383,3.2959669683
N,0,-0.4004384262,2.6956318046,0.4310453921
C,0,-1.8205305623,2.932519804,0.757353468
C,0,0.5021107905,3.1753715635,1.3852994592
C,0,-0.0002425345,3.3515668546,2.793179493
C,0,1.8211162245,3.5890057559,1.0246668788
C,0,-0.1721735806,3.0097838421,-0.9944354387
H,0,1.2957364499,0.7151464293,4.0339770856
H,0,2.8431028965,0.0310869014,3.4824966848

H,0,2.5976175707,1.7795545082,3.4509488406
H,0,3.4010917285,1.5249200373,1.0484571028
H,0,3.1631760803,-0.2109478373,0.8362464023
H,0,2.2724959255,0.9491608913,-0.1727887886
H,0,-0.3802137062,0.2401476698,2.5009713014
H,0,0.2353261695,0.5701974352,-0.5138001395
H,0,-1.3981953612,0.3805248085,0.2756900061
H,0,-2.0735222199,2.476725442,1.7129318998
H,0,-2.0226282476,4.0085432088,0.7955759257
H,0,-2.4338188381,2.4773176396,-0.0208092274
H,0,-0.9345692559,2.4864245001,-1.5743221669
H,0,-0.2633468355,4.0891044929,-1.1554690388
H,0,0.818988065,2.6892787249,-1.2939819264
H,0,0.8371094009,3.5571004234,3.4574990002
H,0,-0.7171142838,4.1781071243,2.8915632536
H,0,-0.4977650305,2.4469220837,3.1625247708
O,0,2.3609636267,3.6017277435,-0.084649857
O,0,2.5409298619,4.0136149048,2.1194678
C,0,3.8451264017,4.4933811604,1.8278860078
H,0,4.2607015706,4.820009209,2.7813506215
H,0,4.4725977609,3.7085763928,1.3970066349
H,0,3.8074970116,5.3325034202,1.1283586092

TSCleavageA/ UB3LYP-D2/6-31+G/ PCM**

/home/bibaswanbiswas/c11/cleavageAB3D2PS
trimethyl pure cleavage conf A
UB3LYP/6-31+G**

E(UB3LYP) = -637.029163479

Zero-point correction= 0.304002 (Hartree/Particle)
Thermal correction to Energy= 0.321694
Thermal correction to Enthalpy= 0.322638
Thermal correction to Gibbs Free Energy= 0.258567
Sum of electronic and zero-point Energies= -636.725161
Sum of electronic and thermal Energies= -636.707469
Sum of electronic and thermal Enthalpies= -636.706525
Sum of electronic and thermal Free Energies= -636.770597

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	201.866	64.199	134.851

C	0.97015	0.07593	-1.12899
C	2.24082	-0.53003	-1.04338
C	3.40525	0.03581	-0.56898
C	3.52406	1.46586	-0.12123
C	4.67356	-0.76628	-0.4895
N	-0.16151	-0.25434	0.82581
C	0.79556	0.3839	1.73999
C	-1.41902	0.33448	0.70547
C	-1.63442	1.69629	1.31545
C	-2.34672	-0.2143	-0.23368
C	-0.06274	-1.72343	0.9424
H	4.5257	-1.79751	-0.82755
H	5.46516	-0.30722	-1.10094
H	5.0563	-0.78766	0.54222
H	4.29355	1.98445	-0.7117
H	2.58907	2.02398	-0.20755
H	3.85417	1.51145	0.92684
H	2.29874	-1.57818	-1.33803
H	0.84653	1.14172	-0.97254
H	0.15672	-0.43863	-1.62628
H	0.84639	1.4558	1.5562
H	0.50464	0.20094	2.78315
H	1.7781	-0.05398	1.55278
H	0.97771	-2.00747	0.76881
H	-0.36075	-2.01955	1.95765
H	-0.70753	-2.19402	0.20561
H	-2.68153	1.98349	1.22234
H	-1.36519	1.71417	2.37841
H	-1.03109	2.47261	0.81732
O	-2.16378	-1.18047	-1.00165
O	-3.55487	0.45576	-0.24677
C	-4.52503	-0.02849	-1.18495
H	-5.39529	0.61969	-1.06445
H	-4.14259	0.03449	-2.20908
H	-4.79272	-1.06787	-0.96771

TS23/ UM06/6-31G*/ exo s-cis /PCM

/home/bibaswanbiswas/c11/allme3XCM06SB
exo s-cis isomer of trimethylalanine system
um06/6-31G*
E(UM06) = -636.484224568

Zero-point correction= 0.308363 (Hartree/Particle)
Thermal correction to Energy= 0.324628
Thermal correction to Enthalpy= 0.325572
Thermal correction to Gibbs Free Energy= 0.266850
Sum of electronic and ZPE= -636.175862
Sum of electronic and thermal Energies= -636.159596
Sum of electronic and thermal Enthalpies= -636.158652
Sum of electronic and thermal Free Energies= -636.217374

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	203.707	62.325	123.591

C,0,-0.3596457928,0.6022817651,0.5648361268
C,0,0.3659359376,0.4437868886,1.7559747168
C,0,1.7114489264,0.6772257898,1.8788822937
C,0,2.6652157752,0.6553570904,0.7321288603
C,0,2.3420387391,0.8152271056,3.2257442818
N,0,-0.4379026409,2.7088519458,0.4250820902
C,0,-1.873862657,2.9425072091,0.6510900934
C,0,0.4058302294,3.3031054826,1.3710007595
C,0,-0.1418906199,3.4661531525,2.7560375792
C,0,1.7485777001,3.658925252,1.0639045029
C,0,-0.1425070394,2.9030545049,-1.0049715224
H,0,1.6044670618,0.7563169586,4.0355911855
H,0,3.1116230317,0.0469206332,3.3980160653
H,0,2.8509945775,1.7903852223,3.3021917217
H,0,3.4439473075,-0.1005419152,0.9170983671
H,0,2.1845485674,0.418824218,-0.224407518
H,0,3.1769712132,1.6208513524,0.5995135561

H,0,-0.2119148787,0.3713830822,2.681936853
H,0,0.1364292158,0.4748242114,-0.3965758553
H,0,-1.4237627425,0.368832496,0.5547096443
H,0,-2.178911237,2.5798942817,1.6344185509
H,0,-2.1001930739,4.0152248468,0.5691106878
H,0,-2.4407441295,2.3968739929,-0.1089438713
H,0,-0.8637136661,2.3171758577,-1.5838230708
H,0,-0.2437161373,3.9660073837,-1.264961829
H,0,0.8740836123,2.5844294803,-1.2257433711
H,0,0.6576519869,3.7474978296,3.4435048025
H,0,-0.9259748958,4.2368697818,2.8262334456
H,0,-0.5835949805,2.5307228666,3.1347059426
O,0,2.356286745,3.5912578344,-0.0113876941
O,0,2.4102155184,4.1551450306,2.171099764
C,0,3.7562223264,4.5260294056,1.948521487
H,0,4.1060248817,4.9696816008,2.8848148825
H,0,4.3796762012,3.6560283543,1.7027213343
H,0,3.8465439371,5.2560500083,1.1355191369

TS23/ B3LYP-D2/6-31G*/exo-cis/ PCM

/home/bibaswanbiswas/c11/exocistsB3D2SB
2,3-rearrangement looking at effect of B3D3
freq=hpmodes
E(RB3LYP) = -636.982869586

Zero-point correction= 0.308691 (Hartree/Particle)
Thermal correction to Energy= 0.325316
Thermal correction to Enthalpy= 0.326260
Thermal correction to Gibbs Free Energy= 0.266139
Sum of electronic and ZPE= -636.674178
Sum of electronic and thermal Energies= -636.657554
Sum of electronic and thermal Enthalpies= -636.656610
Sum of electronic and thermal Free Energies= -636.716730

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	204.139	62.583	126.535

C,0,-0.0899092224,0.6691163789,0.2394521644
C,0,0.3590730144,0.4114130625,1.5502554545
C,0,1.624665994,0.6901420473,2.0019436078
C,0,2.8445240202,0.7554358233,1.1267465305
C,0,1.910499675,0.7605568769,3.4753937631
N,0,-0.4517482639,2.732391293,0.4098857455
C,0,-1.8530156894,2.706364318,0.8805075589
C,0,0.4566105365,3.3153454917,1.3096259337
C,0,0.0095396691,3.5351444895,2.7349079741
C,0,1.7952203232,3.5684918424,0.8962645745
C,0,-0.4270707426,3.1606213827,-1.0095753923
H,0,1.0074471304,0.6126458524,4.0780098366
H,0,2.6625663928,0.0152357574,3.7761597363
H,0,2.3308785859,1.7489803633,3.7134285245
H,0,3.3839949715,-0.2030418609,1.1871015002
H,0,2.6190559919,0.9697064277,0.0813175516
H,0,3.5290613952,1.5331551567,1.4846398624
H,0,-0.408542523,0.2360416655,2.3048740986
H,0,0.6278477838,0.7592669375,-0.5694608412
H,0,-1.0865913183,0.3574853721,-0.0601771234
H,0,-1.9214927372,2.163945885,1.8230883763
H,0,-2.2245652777,3.7292628295,1.0127159468
H,0,-2.456619418,2.1942752554,0.1288092697
H,0,-1.0471180414,2.4653880551,-1.5822174276
H,0,-0.843357424,4.1736229216,-1.086812538
H,0,0.5991929631,3.1500737307,-1.3636446224
H,0,0.8325102737,3.9545978839,3.3128123529
H,0,-0.8394296059,4.2306149053,2.8057279345
H,0,-0.2971260965,2.6019025981,3.2273159173
O,0,2.3058263343,3.402040553,-0.2260917421
O,0,2.5844883925,4.0614875421,1.928132907
C,0,3.9123417646,4.4244593276,1.5488406292
H,0,4.3889006972,4.7903893016,2.461923405
H,0,4.4636805187,3.5640387447,1.1550342072
H,0,3.9050589327,5.2125627888,0.7866383236

TS23/ MPW1KSCF/6-31G*/ endo s-cis /PCM

/home/bibaswanbiswas/c11/me3alaMPW1KSBSCF
endo s-cis isomer of trimethylalanine system
mpwpw91/6-31G(d)
E(RmPW+HF-PW91) = -636.737347303

Zero-point correction= 0.318063 (Hartree/Particle)
Thermal correction to Energy= 0.334605
Thermal correction to Enthalpy= 0.335550
Thermal correction to Gibbs Free Energy= 0.275616
Sum of electronic and ZPE= -636.419284
Sum of electronic and thermal Energies= -636.402742
Sum of electronic and thermal Enthalpies= -636.401798
Sum of electronic and thermal Free Energies= -636.461731

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	209.968	61.469	126.140

C,0,-0.3918180362,0.5312768287,0.5587274461
C,0,0.3240129352,0.4098914181,1.741119056
C,0,1.6605225566,0.70673373,1.8595892442
C,0,2.6175916743,0.6257694082,0.716396911
C,0,2.2873978926,0.8344045786,3.2098651689
N,0,-0.3998350809,2.7085603546,0.4365447837
C,0,-1.8169528023,2.9753055147,0.6678112371
C,0,0.4652676434,3.2051298295,1.3912452905
C,0,-0.0820873914,3.4020099503,2.7697475262
C,0,1.7840417176,3.637065299,1.080460137
C,0,-0.0908025586,2.8932076477,-0.9788742079
H,0,1.5420931563,0.8626693665,4.0018093174
H,0,2.9676302883,0.0020721445,3.4084032435
H,0,2.8808820068,1.7482354957,3.2703009891
H,0,3.4379030338,-0.0451559626,0.9806684563
H,0,2.153621918,0.2411990591,-0.1883962623
H,0,3.0564238835,1.5936469623,0.4683531066
H,0,-0.2467089189,0.330787715,2.6588221749
H,0,0.1018302067,0.4418457238,-0.3969880947
H,0,-1.4502244613,0.3145982527,0.5489385497
H,0,-2.1258909375,2.6200676547,1.6419473762
H,0,-2.0210002974,4.0446642646,0.5924831337
H,0,-2.3952358567,2.4527977756,-0.0869317252
H,0,-0.817651764,2.331566789,-1.5575441421
H,0,-0.160685113,3.9481280096,-1.2458466485
H,0,0.908331,2.5493786231,-1.1944965682
H,0,0.7255573266,3.5985471133,3.4631456058

H,0,-0.7825063187,4.2391713446,2.8320605537
H,0,-0.6103184727,2.5159611375,3.1220945802
O,0,2.3775041006,3.6047378861,0.0042484053
O,0,2.4218108232,4.1504261968,2.1689979699
C,0,3.7197984431,4.6445459097,1.9320212413
H,0,4.0667083919,5.0307842628,2.8846085406
H,0,4.3895855129,3.8604712772,1.5887265985
H,0,3.7096024985,5.4426594394,1.1935150053

TS23/BH AND HLYP/6-31G*/exo s-cis/PCM

/home/bibaswanbiswas/c11/obscure/exocistsBHHSB
2,3-rearrangement looking at effect of B3D3
freq=hpmodes
E(RBHandHLYP) = -636.513957631

Zero-point correction= 0.319942 (Hartree/Particle)
Thermal correction to Energy= 0.336476
Thermal correction to Enthalpy= 0.337420
Thermal correction to Gibbs Free Energy= 0.277422
Sum of electronic and ZPE= -636.194016
Sum of electronic and thermal Energies= -636.177482
Sum of electronic and thermal Enthalpies= -636.176538
Sum of electronic and thermal Free Energies= -636.236536

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	211.142	61.221	126.277

C,0,-0.3945931961,0.5040270207,0.5884458678
C,0,0.3351528964,0.4093571411,1.7647453402
C,0,1.6776786577,0.6729249805,1.8724547449
C,0,2.6279170362,0.5841433442,0.7202607674
C,0,2.3158047967,0.8120150875,3.2199003822
N,0,-0.4112232938,2.7336840072,0.4275431243
C,0,-1.8368020631,2.9957460238,0.644257516
C,0,0.4480986764,3.2483450773,1.3807286118
C,0,-0.1066406837,3.4599614236,2.7593281706
C,0,1.7785134029,3.6464180921,1.0780114478
C,0,-0.0938299443,2.8907516796,-0.9951783788
H,0,1.5778822807,0.8380254522,4.0162333855
H,0,3.003726788,-0.0119589753,3.4163656488
H,0,2.9003933996,1.7301833618,3.2706952208
H,0,3.4481169466,-0.0856092678,0.9797760504
H,0,2.156627088,0.1991473582,-0.178091241
H,0,3.0633726159,1.5501920138,0.4692503024
H,0,-0.2278338863,0.3546377465,2.685887265
H,0,0.0827978574,0.4057502242,-0.3705888215
H,0,-1.4524286018,0.3002109422,0.5986711937
H,0,-2.1497578363,2.6610661315,1.6214008043
H,0,-2.0478345264,4.0599883271,0.5444142898
H,0,-2.4042061852,2.4539278593,-0.1014644364
H,0,-0.8237252481,2.3285290179,-1.5647466815
H,0,-0.1516368386,3.9398670355,-1.2801461313
H,0,0.8985920112,2.5326758885,-1.2025744014
H,0,0.6940111199,3.670788832,3.452684485
H,0,-0.8117140105,4.2916026682,2.8068379086
H,0,-0.6320291176,2.5781832129,3.1201778966
O,0,2.3779930529,3.591919021,0.0053915707
O,0,2.42522664,4.1568597387,2.1667275107
C,0,3.7330343164,4.6400594305,1.9371097906
H,0,4.0747392878,5.0269119443,2.8892474763
H,0,4.3965610705,3.8496171868,1.6034473815
H,0,3.7344144909,5.4332119724,1.1963699379

TS23/B3LYP-D2/6-31+G/exo s-cis/PCM**

/home/bibaswanbiswas/c11/exocistsB3D2PS
2,3-rearrangement looking at effect of B3D3
freq=hpmodes
E(RB3LYP) = -637.035481289

Zero-point correction= 0.306093 (Hartree/Particle)
Thermal correction to Energy= 0.322938
Thermal correction to Enthalpy= 0.323882
Thermal correction to Gibbs Free Energy= 0.263479
Sum of electronic and ZPE= -636.729389
Sum of electronic and thermal Energies= -636.712544
Sum of electronic and thermal Enthalpies= -636.711600
Sum of electronic and thermal Free Energies= -636.772002

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	202.646	63.272	127.127

C,0,-0.067782467,0.6438793263,0.2095712575
C,0,0.3607156802,0.3948797499,1.5261344387
C,0,1.6207229041,0.6800744877,2.0019746911
C,0,2.8532063375,0.7488466238,1.1465469998
C,0,1.8782815566,0.7401670166,3.4809303081
N,0,-0.4532708928,2.7467387769,0.4128672849
C,0,-1.8487853768,2.6990181637,0.8995131042
C,0,0.4659511905,3.30526068,1.313505178
C,0,0.0283054351,3.5251015987,2.7427609974
C,0,1.798052359,3.5782948913,0.8891187955
C,0,-0.4469689442,3.186547402,-1.0032407993
H,0,0.965260334,0.5799693419,4.0633952497
H,0,2.6282603138,-0.0049995508,3.7841448227
H,0,2.2884137843,1.7266127169,3.7405967762
H,0,3.4033615291,-0.200235193,1.2381791437
H,0,2.6402657909,0.9321249762,0.0928474325
H,0,3.5225174312,1.541967314,1.497648823
H,0,-0.4167776062,0.2121544717,2.2680452211
H,0,0.6581086506,0.7707460351,-0.5862243929
H,0,-1.0659856935,0.3515189018,-0.1010319792
H,0,-1.9048570209,2.1399130947,1.8324095544
H,0,-2.2285875157,3.7156229649,1.0544006847
H,0,-2.4561437939,2.1954349386,0.1461942027
H,0,-1.0863698925,2.5046137654,-1.5691952974
H,0,-0.8520651959,4.2050639322,-1.0656413497
H,0,0.568795632,3.1653624442,-1.3850844513
H,0,0.8636203461,3.9078706009,3.3269533986
H,0,-0.7955458042,4.2482499881,2.8178886531
H,0,-0.3092629157,2.5973980732,3.2213999619
O,0,2.3013056409,3.4001017271,-0.2387834934
O,0,2.587598835,4.1003964747,1.9042618591
C,0,3.9232738132,4.4570465597,1.5291671998
H,0,4.3940824808,4.8250129141,2.4432633387
H,0,4.4699072838,3.5905708599,1.1442890431
H,0,3.9187947908,5.2418349316,0.7647673426

TS23/UM06/6-31G*/exo-trans/PCM

/home/bibaswanbiswas/c11/allme3XTM06SB
exo s-trans isomer of trimethylalanine system
um06/6-31G*
E(UM06) = -636.480877828

Zero-point correction= 0.308387 (Hartree/Particle)
Thermal correction to Energy= 0.324463
Thermal correction to Enthalpy= 0.325407
Thermal correction to Gibbs Free Energy= 0.267388
Sum of electronic and ZPE= -636.172491
Sum of electronic and thermal Energies= -636.156415
Sum of electronic and thermal Enthalpies= -636.155471
Sum of electronic and thermal Free Energies= -636.213490

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.604	62.335	122.112

C,0,0.049256444,0.8198435278,-0.0649637651
C,0,0.412715011,0.3869881749,1.2078889044
C,0,1.6156071485,0.6653828277,1.8196186631
C,0,1.7673415624,0.525457904,3.2978734618
C,0,2.9047042721,0.8774781447,1.0987802175
N,0,-0.4828817527,2.8664567848,0.5277530097
C,0,-0.5632079996,3.5601510922,-0.7676991
C,0,-1.8469035128,2.6308329414,1.0117491153
C,0,0.4148144088,3.300393913,1.5059570329
C,0,1.7703415099,3.6593460662,1.2304863105
O,0,2.1576827322,3.5183459465,-0.0787147957
C,0,3.4595201599,3.9844717934,-0.3872399571
C,0,-0.0296722588,3.4067206794,2.9341106131
O,0,2.5856845603,4.0593970093,2.0676495623
H,0,0.817395605,0.3075719489,3.8014233535
H,0,2.4873290313,-0.2656608746,3.5606160548
H,0,2.172677807,1.4619484279,3.7151214695
H,0,3.4407374243,1.7474363632,1.5088955504
H,0,3.5564333776,0.0042353434,1.2645971574
H,0,2.7905177278,1.0138330986,0.01932425
H,0,-0.3956607277,0.0323706735,1.8561710228
H,0,0.8034262383,1.1599352203,-0.774109683
H,0,-0.9060233261,0.5264053149,-0.4980760413
H,0,-1.8464230078,1.9281538239,1.8482038109
H,0,-2.3134743456,3.5737103199,1.3315004311
H,0,-2.4410525323,2.2068494167,0.1969963304
H,0,-1.1555940702,2.9447921862,-1.4544659531
H,0,-1.0646644432,4.5306927805,-0.6354406863
H,0,0.428656556,3.7154606323,-1.1823187872
H,0,0.8076479774,3.7931588803,3.5208902611
H,0,-0.8749715114,4.0986322591,3.069624372
H,0,-0.3285194967,2.4468803643,3.3825940638
H,0,3.5755537122,3.8585804929,-1.4668729828
H,0,3.5760169926,5.0418078738,-0.1224748526
H,0,4.2329297262,3.4076716486,0.133137586

TSCleavageA/UM062X/6-31+G**/PCM

/home/bibaswanbiswas/c11/cleavageAM062XPS
trimethyl pure cleavage conf A
UM062X/6-31+G**
E(UM062X) = -636.657086476

Zero-point correction= 0.307011 (Hartree/Particle)
Thermal correction to Energy= 0.324770
Thermal correction to Enthalpy= 0.325714
Thermal correction to Gibbs Free Energy= 0.260977
Sum of electronic and ZPE= -636.350075
Sum of electronic and thermal Energies= -636.332316
Sum of electronic and thermal Enthalpies= -636.331372
Sum of electronic and thermal Free Energies= -636.396109

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.796	64.043	136.250

C,0,0.9553871407,0.0689996306,-1.0727349545
C,0,2.2372577473,-0.5260308032,-1.0216998846
C,0,3.4055144541,0.0462303844,-0.5822540643
C,0,3.5255356054,1.4743935779,-0.1354349497
C,0,4.680368427,-0.7449695972,-0.5371336616
N,0,-0.1696421495,-0.2682691109,0.8479627406
C,0,0.7710958592,0.3547099394,1.7823746669
C,0,-1.4100220561,0.333004453,0.7122904676
C,0,-1.6220331827,1.7051102716,1.288579426
C,0,-2.3413561651,-0.2206046386,-0.2217171913
C,0,-0.0869258022,-1.7344823517,0.951629873
H,0,4.5315338329,-1.7754676656,-0.8687116222
H,0,5.4487081155,-0.2840780463,-1.1710704882
H,0,5.0897442951,-0.763971888,0.4812711394
H,0,4.3046567352,1.9863649319,-0.7138371237
H,0,2.5984150868,2.0403468539,-0.2390406641
H,0,3.8372531277,1.5216072973,0.9163628406
H,0,2.2944955413,-1.5716767215,-1.326286438
H,0,0.8253083783,1.1371093582,-0.9290647205
H,0,0.1481241753,-0.445011923,-1.5825839198
H,0,0.8373890196,1.4269833304,1.6059927269
H,0,0.4576601057,0.1711540714,2.8175746427
H,0,1.753497885,-0.0928680326,1.6187258458
H,0,0.9574682058,-2.0244642834,0.8213833187
H,0,-0.4275289074,-2.03879509,1.9490130828
H,0,-0.7020560658,-2.1970309813,0.1866198681
H,0,-2.6656842223,1.9905244221,1.1726334862
H,0,-1.3744788508,1.7477116988,2.3539069001
H,0,-1.0137946473,2.4680757583,0.7804463934
O,0,-2.1689841428,-1.1972231614,-0.9652771375
O,0,-3.5270598947,0.4631247539,-0.2575475515
C,0,-4.4848927476,-0.0197071962,-1.1934632127
H,0,-5.3440931836,0.6441981211,-1.1051399094
H,0,-4.0861842686,0.0123650608,-2.2102485469
H,0,-4.7772464512,-1.0459774238,-0.9580353784

Polyrate structures for rearrangement of 5: B3LYP-D2/6-31+G**/PCM

23 Starting Material

pb3lypd2/geom/sm/ g091.log
sm for 23 from opt of ts
B3LYP/6-31+G**
E(RB3LYP) = -637.056800173
Zero-point correction= 0.309833 (Hartree/Particle)
Thermal correction to Energy= 0.326548

Thermal correction to Enthalpy= 0.327492
Thermal correction to Gibbs Free Energy= 0.266676
Sum of electronic and zero-point Energies= -636.746968
Sum of electronic and thermal Energies= -636.730252
Sum of electronic and thermal Enthalpies= -636.729308
Sum of electronic and thermal Free Energies= -636.790124

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.912	62.890	127.999

C,0,1.4846763454,0.9475808171,-1.3323944738
C,0,1.0457625478,2.0602645145,-0.4362992417
C,0,-0.2247591393,2.4277829553,-0.1911145892
C,0,-1.4472766018,1.7870875597,-0.7923237938
C,0,-0.5201024856,3.5460217453,0.7761402919
N,0,1.7647051994,-0.367360139,-0.5598126214
C,0,2.848375725,-0.1025848522,0.445098352
C,0,0.5235136685,-0.9018982347,0.1044084261
C,0,0.3683447106,-0.656214674,1.5825758622
C,0,-0.5191519974,-1.2615102035,-0.7406196032
C,0,2.3394193708,-1.3613127071,-1.5407037273
H,0,0.3941822551,3.9790982931,1.1949080609
H,0,-1.096894036,4.3402983594,0.2831778995
H,0,-1.142238737,3.1720078837,1.6015184845
H,0,-2.1274267716,2.563885481,-1.1664475318
H,0,-1.2222015308,1.0868409173,-1.5974443973
H,0,-1.9888294007,1.2319358135,-0.0143804201
H,0,1.8389051845,2.6043487301,0.0731422918
H,0,0.737963203,0.667662139,-2.0733689619
H,0,2.4244942817,1.1968764731,-1.8353505011
H,0,2.5083843399,0.6365641997,1.1659558884
H,0,3.0877279077,-1.0393238184,0.9480190634
H,0,3.7180255391,0.2734945894,-0.0963296101
H,0,3.2386745346,-0.9270640938,-1.9848747274
H,0,2.5822976972,-2.2667808203,-0.9835708845
H,0,1.5817069385,-1.5635650896,-2.2936442408
H,0,-0.5853680967,-1.0817825015,1.8986633081
H,0,1.1510071235,-1.1257220057,2.1939972652
H,0,0.351282542,0.4157013795,1.83900044
O,0,-0.5435163311,-1.2804192408,-2.0051325647
O,0,-1.6798845343,-1.6404121468,-0.0485799211
C,0,-2.8105480152,-1.9478775344,-0.8648925241
H,0,-3.6138192188,-2.2031725664,-0.1687135202
H,0,-3.1047606153,-1.0861055233,-1.4747640023
H,0,-2.6084466028,-2.7963906992,-1.5283197762

23 Product

pb3lypd2/geom/p/g091.log
B3LYP/6-31+G**
E(RB3LYP) = -637.085989816

Zero-point correction= 0.309693 (Hartree/Particle)
Thermal correction to Energy= 0.326159
Thermal correction to Enthalpy= 0.327103
Thermal correction to Gibbs Free Energy= 0.267762
Sum of electronic and zero-point Energies= -636.776297
Sum of electronic and thermal Energies= -636.759831
Sum of electronic and thermal Enthalpies= -636.758886
Sum of electronic and thermal Free Energies= -636.818228

C,0,1.9035878192,2.2318895432,-1.3352584808
C,0,1.2449339646,2.0374675082,-0.1893731577
C,0,-0.1731308191,1.5229975942,-0.0275924204
C,0,-0.8041345181,1.0067820133,-1.3405003258
C,0,-1.0092886502,2.7730391766,0.3679617463
N,0,1.0430854135,-0.4450273805,1.0425955787
C,0,1.2085964292,-1.4004733754,2.1471599109
C,0,-0.1689028241,0.4017785246,1.1288270414
C,0,-0.1838756322,1.079341469,2.5219794608
C,0,-1.4648630119,-0.4420071879,1.0044078342
C,0,1.3340234945,-1.0991575591,-0.2401649416
H,0,-0.5496730281,3.3326721591,1.1874429526
H,0,-1.059504702,3.4344167836,-0.5031926586
H,0,-2.0253837588,2.4911677198,0.6562919954
H,0,-0.6991226504,1.7701273814,-2.1175341427
H,0,-0.3682649598,0.0780097981,-1.7083132666
H,0,-1.8767882093,0.8442244457,-1.1904020908
H,0,1.7212408331,2.3243970359,0.7461683297
H,0,1.4814279079,1.9565120224,-2.298283643
H,0,2.9000549061,2.6660246969,-1.3381228467
H,0,1.3255586724,-0.8849565082,3.1025913062
H,0,0.374613001,-2.1171077192,2.2276797579
H,0,2.1277643003,-1.9676155356,1.9722208929
H,0,1.4969522051,-0.3556131354,-1.0183328243
H,0,2.2721820469,-1.6525584936,-0.1262808043
H,0,0.5521124808,-1.8031337877,-0.55902938
H,0,-1.0200389923,1.7696126979,2.6084969712
H,0,-0.2944550608,0.3414320301,3.318813033
H,0,0.7556429266,1.6192404475,2.6712512993
O,0,-1.5183570476,-1.6074534412,0.6525010617
O,0,-2.5658689681,0.2622691655,1.3321484324
C,0,-3.8315611563,-0.4246968558,1.2009819499
H,0,-4.5873925296,0.3038284828,1.4944659991
H,0,-3.9783041027,-0.7426072462,0.1650046021
H,0,-3.8543787796,-1.2968224698,1.8596808277

23 Transition State

pb3lypd2/geom/ts/ g091.log
alanine prenyl TSfreq
B3LYP/6-31+G**
E(RB3LYP) = -637.038443161

Zero-point correction= 0.306141 (Hartree/Particle)
Thermal correction to Energy= 0.322963
Thermal correction to Enthalpy= 0.323907
Thermal correction to Gibbs Free Energy= 0.263544
Sum of electronic and zero-point Energies= -636.732302

Sum of electronic and thermal Energies= -636.715480
Sum of electronic and thermal Enthalpies= -636.714536
Sum of electronic and thermal Free Energies= -636.774900

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	202.662	63.207	127.046

C,0,-0.0711494365,0.6534223104,0.2120586619
C,0,0.3595368194,0.4000549812,1.5285831057
C,0,1.6196556726,0.6842974269,2.0019265126
C,0,2.8513470929,0.7559656259,1.1455036
C,0,1.8789860945,0.7506965606,3.4799959512
N,0,-0.4528476097,2.7418043194,0.411096931
C,0,-1.8488283417,2.6996356121,0.898461198
C,0,0.4660189769,3.3047588665,1.3114069961
C,0,0.0298750619,3.5121485453,2.7430267345
C,0,1.7974245305,3.5774569654,0.8876441811
C,0,-0.4459486683,3.1811858806,-1.0055674053
H,0,0.9679817991,0.5867040981,4.0647677797
H,0,2.6351962351,0.0127604754,3.7851837328
H,0,2.2815861882,1.7419948628,3.7328745375
H,0,3.4068761238,-0.1894547678,1.2417036216
H,0,2.6367034935,0.9336315729,0.0913102846
H,0,3.5153034605,1.5551989341,1.4930524807
H,0,-0.4173153709,0.220517796,2.2718030331
H,0,0.6544450008,0.7732114235,-0.5855002641
H,0,-1.0689614779,0.3582940612,-0.0978809993
H,0,-1.9074218015,2.1344438237,1.827570635
H,0,-2.2213214054,3.7176260342,1.0605961552
H,0,-2.4597832037,2.2049092123,0.1422905692
H,0,-1.0920806912,2.5039135035,-1.5694695513
H,0,-0.842286767,4.2030342238,-1.0673997637
H,0,0.5691744301,3.1512301523,-1.3886168593
H,0,0.8664122524,3.8868531585,3.3308078059
H,0,-0.7931185344,4.235474489,2.8265066651
H,0,-0.3084542661,2.5788808935,3.2101309294
O,0,2.3011075583,3.4036560171,-0.2409739939
O,0,2.5882896464,4.093225861,1.9055303063
C,0,3.9241808282,4.4500013951,1.5321242688
H,0,4.3941583104,4.8161548947,2.4474763248
H,0,4.4709082461,3.5837085426,1.1469095366
H,0,3.9207487529,5.2357632482,0.7686402981

Polyrate structures for rearrangement of 5: M06/6-31+G**/PCM

23 Starting Material

pm06only23/geom/sm/alanineprenyl23smm06631plusgstarstarpcm
sm for 23 from opt of ts
M06/6-31+G**
E(RM06) = -636.554189139

Zero-point correction= 0.308245 (Hartree/Particle)
Thermal correction to Energy= 0.325010
Thermal correction to Enthalpy= 0.325954
Thermal correction to Gibbs Free Energy= 0.265694
Sum of electronic and ZPE= -636.245944
Sum of electronic and thermal Energies= -636.229179
Sum of electronic and thermal Enthalpies= -636.228235
Sum of electronic and thermal Free Energies= -636.288495

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	203.947	63.374	126.827

C,0,1.4534289807,0.9419096635,-1.3197179856
C,0,1.0429666568,2.0639055153,-0.4355663187
C,0,-0.2139456443,2.4742702393,-0.1964388234
C,0,-1.4513208212,1.8650120562,-0.776306911
C,0,-0.4714327515,3.6091480972,0.7461992758
N,0,1.7462703963,-0.3634412715,-0.5535198845
C,0,2.8220278385,-0.0966405521,0.4438821289
C,0,0.5188693013,-0.9233259722,0.1118183056
C,0,0.3563125672,-0.7247349551,1.5871005339
C,0,-0.5187699018,-1.2813682105,-0.7417175141
C,0,2.3256104103,-1.344456203,-1.5308997444
H,0,0.4537136084,4.0338988143,1.1486946586
H,0,-1.0382898198,4.4096782028,0.2524705456
H,0,-1.0897042019,3.2670403193,1.5884915059
H,0,-2.0864022917,2.6452636719,-1.2166530956
H,0,-1.2597800256,1.0969303211,-1.5308070177
H,0,-2.0423738811,1.3996613499,0.0267970918
H,0,1.8516713926,2.6061735746,0.0590452313
H,0,0.6917750011,0.6616666854,-2.0511855552
H,0,2.3817300291,1.183639628,-1.8532728959
H,0,2.4747494583,0.6078786615,1.198222343
H,0,3.1039328485,-1.0390257674,0.9176801029
H,0,3.6808932695,0.3240207582,-0.0855386197
H,0,3.2300727709,-0.9150334106,-1.9722389898
H,0,2.5668454725,-2.2568152203,-0.9817605049
H,0,1.5767444291,-1.5507479018,-2.2941858192
H,0,-0.5806765725,-1.2014784962,1.8837913364
H,0,1.1455580777,-1.1843051632,2.198308938
H,0,0.2823437136,0.3341748265,1.8939375228
O,0,-0.5432664496,-1.2730445263,-1.9963889037
O,0,-1.6602459666,-1.6943857044,-0.0606645297
C,0,-2.7713506708,-2.0204347761,-0.8724749572
H,0,-3.5696646089,-2.3159231682,-0.1872098435
H,0,-3.103044588,-1.1610666861,-1.4683854083
H,0,-2.551023027,-2.8500894,-1.5539821986

23 Product

pm06only23/geom/p/alanineprenyl23pdtm06631plusgstarstarpcm
23 product
M06/6-31+G**
E(RM06) = -636.584166461

Zero-point correction= 0.307900 (Hartree/Particle)
Thermal correction to Energy= 0.324587
Thermal correction to Enthalpy= 0.325531
Thermal correction to Gibbs Free Energy= 0.265848
Sum of electronic and ZPE= -636.276266
Sum of electronic and thermal Energies= -636.259580

Sum of electronic and thermal Enthalpies= -636.258636
Sum of electronic and thermal Free Energies= -636.318318

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.681	63.899	125.613

C,0,1.8862740754,2.233417533,-1.347090206
C,0,1.239496733,2.0216864595,-0.2013407867
C,0,-0.1752422235,1.5180726303,-0.0263320537
C,0,-0.8096444633,1.0094071305,-1.3284553596
C,0,-0.989157259,2.7699326929,0.3665041454
N,0,1.0225774361,-0.4470130149,1.0442833738
C,0,1.189209052,-1.3819110438,2.1507891388
C,0,-0.1778062177,0.4070728857,1.1235674078
C,0,-0.1936549231,1.0675006112,2.5111294614
C,0,-1.4657851323,-0.4268687777,0.9836030017
C,0,1.3426992311,-1.1125875348,-0.2137721759
H,0,-0.5218688213,3.338339189,1.1773740068
H,0,-1.0376659883,3.4321589383,-0.5059784108
H,0,-2.0136228342,2.5163142552,0.6597576825
H,0,-0.7254395543,1.7753601375,-2.1076133005
H,0,-0.3718238286,0.0860194701,-1.7151199169
H,0,-1.8833748254,0.833350682,-1.1837852118
H,0,1.7323674079,2.3046620836,0.7316672157
H,0,1.4644744005,1.9739319549,-2.3169419538
H,0,2.8819174047,2.6703880176,-1.353372385
H,0,1.3028365264,-0.8664189959,3.1078819676
H,0,0.364545842,-2.1121740459,2.2393117812
H,0,2.1119257615,-1.947571877,1.9865532802
H,0,1.4458939425,-0.3941291613,-1.0279365781
H,0,2.3226436269,-1.5899133764,-0.0985119383
H,0,0.6165433993,-1.8888381853,-0.5028333398
H,0,-1.0046860678,1.7882943259,2.6042357405
H,0,-0.3451750113,0.328325238,3.3024610337
H,0,0.7602013159,1.5739355443,2.6965222477
O,0,-1.5269976856,-1.5609389981,0.556555661
O,0,-2.5546052985,0.2471588766,1.3829486337
C,0,-3.8077407687,-0.4235081904,1.2096490386
H,0,-4.5685842756,0.2659907175,1.5743010901
H,0,-3.9738432954,-0.6485912284,0.1514796817
H,0,-3.8284006812,-1.3528549433,1.7847980271

23 Transition State

pm06only23/geom/ts/alanineprenyl23tsm06631plusgstarstarpcm
alanine prenyl TSfreq
M06/6-31+G**
E(RM06) = -636.529717334

Zero-point correction= 0.303801 (Hartree/Particle)
Thermal correction to Energy= 0.321062
Thermal correction to Enthalpy= 0.322006
Thermal correction to Gibbs Free Energy= 0.260154
Sum of electronic and ZPE= -636.225916
Sum of electronic and thermal Energies= -636.208655
Sum of electronic and thermal Enthalpies= -636.207711
Sum of electronic and thermal Free Energies= -636.269563

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	201.469	64.166	130.179

C,0,-0.0967635102,0.5733433215,0.2479843634
C,0,0.3560741693,0.3734367964,1.552212669
C,0,1.6271619764,0.6628581776,1.9994840886
C,0,2.8288262866,0.7116961137,1.1151795494
C,0,1.9270550387,0.6812857028,3.4625831317
N,0,-0.4441797728,2.7513925886,0.4228822161
C,0,-1.8419709342,2.7486209027,0.8708871376
C,0,0.4693372423,3.2872262733,1.3313657656
C,0,0.0209606377,3.5563301171,2.7383390102
C,0,1.8005761836,3.583661651,0.9113156818
C,0,-0.3944807243,3.1583022193,-0.9915825953
H,0,1.0311544896,0.533191449,4.0750442098
H,0,2.6585994743,-0.0975743827,3.725229657
H,0,2.3853506673,1.6399315175,3.7480793153
H,0,3.3279352015,-0.2694525631,1.129354306
H,0,2.6062761683,0.9712741117,0.0773851763
H,0,3.5606938321,1.4401167785,1.4879420422
H,0,-0.4038469289,0.1883770631,2.3166906055
H,0,0.6047845178,0.6883705706,-0.575644125
H,0,-1.1089370139,0.2898303092,-0.0321680433
H,0,-1.9545243519,2.208974511,1.8124759563
H,0,-2.2082687216,3.7770990726,0.9966249432
H,0,-2.4515393668,2.2516809902,0.112761705
H,0,-1.0605137778,2.5033309633,-1.5612484484
H,0,-0.7442843618,4.1966070351,-1.087685474
H,0,0.6210010449,3.081536116,-1.3713252802
H,0,0.8727329636,3.8653947133,3.3446203297
H,0,-0.7315811049,4.3566243771,2.7989253741
H,0,-0.4149853967,2.6728773322,3.2234977508
O,0,2.3167817448,3.3878343672,-0.1978729349
O,0,2.5514315935,4.1610793458,1.9105448389
C,0,3.8667734619,4.5487486919,1.5459657395
H,0,4.3127473105,4.9779752546,2.4452605227
H,0,4.4628339179,3.6928666325,1.2115310368
H,0,3.8531870433,5.2983128795,0.7469337784

Polyrate structures for rearrangement of 5: M062X/6-31+G**/PCM

23 Starting Material

pm0623/geom/sm/alanineprenyl23smm062x631plusgstarstarpcm
sm for 23 from opt of ts
m062x/6-31+G**
E(RM062X) = -636.700911132

Zero-point correction= 0.313391 (Hartree/Particle)
Thermal correction to Energy= 0.330063
Thermal correction to Enthalpy= 0.331007
Thermal correction to Gibbs Free Energy= 0.270419
Sum of electronic and ZPE= -636.387521
Sum of electronic and thermal Energies= -636.370848
Sum of electronic and thermal Enthalpies= -636.369904
Sum of electronic and thermal Free Energies= -636.430493

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 207.118 62.441 127.519

C,0,1.4584992874,0.9297615226,-1.3432165067
C,0,1.0565837422,2.0684336546,-0.4593737405
C,0,-0.2006833018,2.4436681586,-0.1781096807
C,0,-1.4420819195,1.7723778809,-0.6991304425
C,0,-0.4606140274,3.5974123671,0.7537525743
N,0,1.7456763513,-0.3581883775,-0.5615850793
C,0,2.8104173671,-0.0777779167,0.4482418744
C,0,0.5098562453,-0.8944585761,0.0979998108
C,0,0.3309932941,-0.674052431,1.5734403763
C,0,-0.5166636392,-1.2675725626,-0.7544943714
C,0,2.3290134829,-1.358499082,-1.5195196147
H,0,0.465734649,4.0379121925,1.1290432174
H,0,-1.0423258903,4.3764701589,0.2485994891
H,0,-1.05889224,3.2600459748,1.6086057497
H,0,-2.1592860365,2.5272476796,-1.039546008
H,0,-1.2506476944,1.0695481985,-1.5112778009
H,0,-1.9220006793,1.2134763837,0.1149978673
H,0,1.8694781028,2.6385361226,-0.0121441787
H,0,0.6893363935,0.6495311282,-2.062511619
H,0,2.3819118076,1.1672090256,-1.8805315995
H,0,2.4481151869,0.6399242145,1.1796216073
H,0,3.0771292083,-1.0127806729,0.9397548074
H,0,3.6745062349,0.3300155122,-0.0777700457
H,0,3.2435035681,-0.9412134019,-1.9452830155
H,0,2.5495210854,-2.2636595293,-0.9549430465
H,0,1.5915565207,-1.5611459456,-2.2909462229
H,0,-0.6123692625,-1.1372943806,1.8620974181
H,0,1.1124157809,-1.1302896037,2.1920603868
H,0,0.2681146803,0.3899070152,1.8514308385
O,0,-0.5284621147,-1.2802995016,-2.0139974213
O,0,-1.6690787466,-1.662932635,-0.0831250787
C,0,-2.7770591758,-1.978308216,-0.9105307161
H,0,-3.5864536047,-2.2488762365,-0.2314314983
H,0,-3.0756258373,-1.1184316956,-1.5175387227
H,0,-2.5558938186,-2.8177414253,-1.5751156078

23 Product

pm0623/geom/p/alanineprenyl23pdtm062x631plusgstarstarpcm
23 product
m062x/6-31+G**
E(RM062X) = -636.730284009

Zero-point correction= 0.312703 (Hartree/Particle)
Thermal correction to Energy= 0.329204
Thermal correction to Enthalpy= 0.330148
Thermal correction to Gibbs Free Energy= 0.270955
Sum of electronic and ZPE= -636.417581
Sum of electronic and thermal Energies= -636.401080
Sum of electronic and thermal Enthalpies= -636.400136
Sum of electronic and thermal Free Energies= -636.459329

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 206.579 63.125 124.582

C,0,1.8793957426,2.2109073683,-1.3632725251
C,0,1.2451660138,2.0222859089,-0.2062587707
C,0,-0.1744416023,1.5244843344,-0.0155512312
C,0,-0.8269192102,1.016692385,-1.3148692872
C,0,-0.9845996273,2.778273967,0.3975885675
N,0,1.0422827026,-0.4332982717,1.0452480794
C,0,1.2096509049,-1.3679896982,2.1589564865
C,0,-0.1649232701,0.4074503646,1.1295332952
C,0,-0.2006912837,1.0613740392,2.526045063
C,0,-1.4511831555,-0.4358696637,0.9905341751
C,0,1.3247677124,-1.1060415274,-0.22386756
H,0,-0.5060081909,3.3291135707,1.2107887532
H,0,-1.0376789884,3.4465142795,-0.4667274507
H,0,-2.0026947556,2.5165932654,0.6969343434
H,0,-0.7463436921,1.7812493413,-2.0922933883
H,0,-0.396203816,0.0917677027,-1.6997435977
H,0,-1.8960564339,0.8474701341,-1.1486240492
H,0,1.7491435251,2.3073767014,0.7171671248
H,0,1.4400258188,1.940773313,-2.3196845153
H,0,2.8782501987,2.6352129972,-1.3854293495
H,0,1.3701527903,-0.839687671,3.0994517959
H,0,0.3613871926,-2.0603480238,2.2785398863
H,0,2.1045088847,-1.9643582683,1.9694115174
H,0,1.4502330652,-0.3801190381,-1.0243689899
H,0,2.2818199442,-1.6234537665,-0.1158226054
H,0,0.5634077608,-1.8433188691,-0.5110449097
H,0,-1.0355957598,1.7522783099,2.6122551162
H,0,-0.3269872533,0.3113380823,3.3083863368
H,0,0.7356488589,1.5967428753,2.707843191
O,0,-1.5003102381,-1.5937072146,0.6347436242
O,0,-2.5514756569,0.2609564815,1.3095006626
C,0,-3.799267196,-0.4277868202,1.1538012298
H,0,-4.5672497288,0.2860987939,1.4431433981
H,0,-3.9312980654,-0.7343494467,0.1140591804
H,0,-3.8274261908,-1.3066259359,1.7999164029

23 Transition State

pm0623/geom/ts/alanineprenyl23tsm062x631plusgstarstarpcm
alanine prenyl TSfreq
M062x/6-31+G**
E(RM062X) = -636.669052060

Zero-point correction= 0.310285 (Hartree/Particle)
Thermal correction to Energy= 0.326670
Thermal correction to Enthalpy= 0.327615
Thermal correction to Gibbs Free Energy= 0.268567
Sum of electronic and ZPE= -636.358767
Sum of electronic and thermal Energies= -636.342382
Sum of electronic and thermal Enthalpies= -636.341437
Sum of electronic and thermal Free Energies= -636.400486

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 204.989 62.372 124.277

C,0,-0.3044454378,0.5661859359,0.4335824281
C,0,0.3117070217,0.3894461711,1.6811629742
C,0,1.6116351182,0.7763004301,1.9270903852
C,0,2.6882809513,0.7876243167,0.8773580043
C,0,2.1219511777,0.88649285,3.3355380128

N,0,-0.4136766219,2.6604975751,0.4198765702
C,0,-1.8382639263,2.8704440583,0.7486704839
C,0,0.483607709,3.167439842,1.3637646054
C,0,-0.0201257197,3.3687612474,2.7689201608
C,0,1.7928178691,3.6047609818,0.9919245768
C,0,-0.1984724756,2.9417328411,-1.0150623904
H,0,1.3182693163,0.7939336764,4.0707859205
H,0,2.8742268936,0.1135814489,3.5406858696
H,0,2.6139308949,1.8581500383,3.4736228624
H,0,3.2063150443,-0.1807690251,0.8923677239
H,0,2.3173662872,0.9661143392,-0.132715371
H,0,3.4366635888,1.5570140534,1.092420703
H,0,-0.3383874594,0.2416296319,2.5431596604
H,0,0.284263686,0.5217756267,-0.4772626086
H,0,-1.3510310405,0.2994486557,0.3122485987
H,0,-2.0781915856,2.4285025666,1.7135667978
H,0,-2.0653298007,3.9421695306,0.7667169675
H,0,-2.4431591263,2.3861194528,-0.0174365824
H,0,-0.9642323262,2.4016190967,-1.5739695932
H,0,-0.2958943917,4.0163700031,-1.2025530266
H,0,0.7893390956,2.6169755359,-1.3213775655
H,0,0.8137351208,3.5971432272,3.4292943686
H,0,-0.7434299329,4.1911643969,2.8439915005
H,0,-0.5095631473,2.4681437101,3.1557873576
O,0,2.3227106271,3.6146093617,-0.1261554295
O,0,2.5127410336,4.056301066,2.0730766297
C,0,3.8183986158,4.5409621723,1.7817306646
H,0,4.2347043411,4.8569636685,2.737757578
H,0,4.4418154424,3.7579465512,1.3429413878
H,0,3.7761221576,5.3876059654,1.0920637746

Polyrate structures for C-N Bond Cleavage in 5: B3LYP-D2/6-31+G**/PCM

Cleavage A Starting Material

SM_Ylide_Cleavage/ Ab3lyp_d2ps1.log
SM Alanine ammonium dimethyl allyl ylide
b3lyp/6-31+g**
E(RB3LYP) = -637.054742510

Zero-point correction= 0.309431 (Hartree/Particle)
Thermal correction to Energy= 0.326397
Thermal correction to Enthalpy= 0.327341
Thermal correction to Gibbs Free Energy= 0.265483
Sum of electronic and zero-point Energies= -636.745311
Sum of electronic and thermal Energies= -636.728346
Sum of electronic and thermal Enthalpies= -636.727402
Sum of electronic and thermal Free Energies= -636.789260

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.817	63.124	130.191

C,0,0.7503973531,-0.4733121616,-0.4453787405
C,0,2.1318469562,-0.9407591219,-0.1076912437
C,0,3.2843811244,-0.3267548752,-0.4343809345
C,0,3.3869605786,0.9760597734,-1.1839345861
C,0,4.6118493423,-0.9218399061,-0.0390324679
N,0,0.0289885937,0.2999389941,0.6884557427
C,0,0.8427313192,1.5122023897,1.0400427685
C,0,-1.3485546938,0.6997944273,0.2258757009
C,0,-1.4587041714,2.0570952452,-0.42231885
C,0,-2.2441240671,-0.3423021669,-0.0224220165
C,0,-0.0186275443,-0.5458867826,1.9365493365
H,0,4.4897314779,-1.8564353559,0.5176654141
H,0,5.2238662363,-1.1175752372,-0.9300014816
H,0,5.1767807272,-0.2120644294,0.580989555
H,0,4.0601319639,0.8621225465,-2.0433324321
H,0,2.4274498431,1.353308131,-1.542855851
H,0,3.8323755734,1.7416059292,-0.5335266446
H,0,2.1928729832,-1.8740784843,0.4486334364
H,0,0.727487572,0.2128494372,-1.2926828738
H,0,0.0876363181,-1.3160741382,-0.6439470937
H,0,0.9855371016,2.1257406023,0.1537546884
H,0,0.3039837063,2.0696661419,1.8063375204
H,0,1.8078670429,1.1722492022,1.4132542874
H,0,1.0060903669,-0.772818508,2.236506999
H,0,-0.5254678037,0.0410978972,2.7034178655
H,0,-0.580168279,-1.4483441119,1.710778516
H,0,-2.4762527901,2.1763230571,-0.7973497801
H,0,-1.260284765,2.8928045247,0.2615719055
H,0,-0.7798321168,2.1813406291,-1.2856733467
O,0,-2.1048649723,-1.5763066919,0.2035860696
O,0,-3.4501707154,0.0993812151,-0.5849043899
C,0,-4.4462004625,-0.9064304642,-0.782703749
H,0,-5.2995770478,-0.3890847375,-1.2285664463
H,0,-4.0912230294,-1.6936385886,-1.4569572451
H,0,-4.7431457215,-1.3654113819,0.1675223673

Cleavage A Product

SM_Ylide_Cleavage_pdt/apps1.log

ub3lyp/6-31+g**
E(UB3LYP) = -637.032309571

Zero-point correction= 0.301659 (Hartree/Particle)
Thermal correction to Energy= 0.321232
Thermal correction to Enthalpy= 0.322176
Thermal correction to Gibbs Free Energy= 0.252304
Sum of electronic and zero-point Energies= -636.730651
Sum of electronic and thermal Energies= -636.711078
Sum of electronic and thermal Enthalpies= -636.710134
Sum of electronic and thermal Free Energies= -636.780005

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	201.576	67.836	147.057

C,0,0.7965536274,-0.7737096786,-0.802977391
C,0,2.0434101084,-1.0562752399,-0.2615785688
C,0,3.1976082271,-0.2737627921,-0.3309081377
C,0,3.2729331374,1.0329037146,-1.0680156413
C,0,4.4683278927,-0.7179542809,0.3353311074
N,0,-0.4207760186,0.7914280154,1.2544073424
C,0,0.6580310046,1.7728420202,1.2187088049
C,0,-1.6482771225,1.0889422373,0.7162269222
C,0,-1.8699969368,2.4767230654,0.1719137122
C,0,-2.615084735,0.0436312436,0.5005838827
C,0,-0.2200397985,-0.2103746453,2.3027370345
H,0,4.3445161276,-1.6761794076,0.8516328892
H,0,5.2821916673,-0.8211234411,-0.3992008855
H,0,4.809662916,0.0304010576,1.0672392749
H,0,4.0257365133,0.9774652389,-1.8688798304
H,0,2.3206086958,1.3289024728,-1.5144508764
H,0,3.5986597001,1.836968739,-0.3917028103
H,0,2.1333390298,-1.9831608276,0.3070104216
H,0,0.6056612879,0.1349348243,-1.3644790018
H,0,-0.0499380464,-1.426551871,-0.6214584821
H,0,0.6408932279,2.3387215352,0.2876833801
H,0,0.5898492674,2.4687706536,2.0687845438
H,0,1.6063243444,1.2315180637,1.2766466805
H,0,0.7400249098,-0.706782682,2.1304380783
H,0,-0.190071301,0.2924980481,3.2817482205
H,0,-1.0182983448,-0.9467430196,2.2835468625
H,0,-2.9306965642,2.6478056125,-0.0102566374
H,0,-1.3385507689,2.6300097002,-0.7799611363
H,0,-1.5055909784,3.2359697315,0.8730135476
O,0,-2.4548765837,-1.175998272,0.6855465918
O,0,-3.8144806891,0.5261821937,0.0251739017
C,0,-4.8187040762,-0.4627595298,-0.2456161426
H,0,-5.681133431,0.0928664635,-0.6181711674
H,0,-4.4678220629,-1.1745273007,-0.9998943894
H,0,-5.0811212269,-1.008311643,0.6666068997

Cleavage ATransition State

SM_Ylide_Cleavage_ts/atspcmps1.log
alanine prenyl TSfreq
UB3LYP/6-31+G**
E(UB3LYP) = -637.029145424
Zero-point correction= 0.303912 (Hartree/Particle)
Thermal correction to Energy= 0.321624
Thermal correction to Enthalpy= 0.322568
Thermal correction to Gibbs Free Energy= 0.258533
Sum of electronic and zero-point Energies= -636.725234
Sum of electronic and thermal Energies= -636.707522
Sum of electronic and thermal Enthalpies= -636.706577
Sum of electronic and thermal Free Energies= -636.770613

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	201.822	64.244	134.774

C,0,0.9631906469,-0.7669448014,-0.8301175942
C,0,2.243089843,-1.1128395882,-0.3491918605
C,0,3.4020765477,-0.3735932901,-0.4560786194
C,0,3.5015020738,0.9318626831,-1.1944511423
C,0,4.6830665281,-0.8565337892,0.1637080209
N,0,-0.1508335904,0.4264048875,0.7650837899
C,0,0.8080438653,1.5285070138,0.922844939
C,0,-1.4124135741,0.7452089037,0.2655972281
C,0,-1.6305689415,2.1241554927,-0.3035465377
C,0,-2.3438251887,-0.3128805367,0.0272595597
C,0,-0.0430085067,-0.4987963153,1.9114805342
H,0,4.549337182,-1.8097406188,0.6862137326
H,0,5.4639190595,-0.9828673987,-0.6014989015
H,0,5.0718717042,-0.1164680781,0.879621364 8
H,0,4.2621143666,0.8619440883,-1.9858173573
H,0,2.5584725297,1.2424185431,-1.6497018098
H,0,3.8331599799,1.7306112494,-0.5151297568
H,0,2.314667627,-2.0442872225,0.2129776622
H,0,0.8253395768,0.0768056326,-1.4969838853
H,0,0.1536061511,-1.4853071054,-0.7835246323
H,0,0.8557887955,2.1292190022,0.0161137047
H,0,0.521324172,2.1628136157,1.7723212687
H,0,1.7908248497,1.0910781753,1.1097977814
H,0,0.997344259,-0.823324952,1.9878626433
H,0,-0.3297637908,0.0363721654,2.8272530757
H,0,-0.692106823,-1.3554963091,1.7543393197
H,0,-2.6798889474,2.255489729,-0.5667979158
H,0,-1.3538990658,2.9085339786,0.4112029623
H,0,-1.0353173897,2.2946948606,-1.2154832061
O,0,-2.1619422922,-1.53483807,0.2019814739
O,0,-3.5549635499,0.1395339302,-0.4600445046
C,0,-4.5299138318,-0.8735163511,-0.7414405814
H,0,-5.4025551639,-0.3397744088,-1.1230392463
H,0,-4.1555887607,-1.5770768803,-1.4924123422
H,0,-4.7903783413,-1.4269022354,0.1668838327

Polyrate structures for C-N Bond Cleavage in 5: M06/6-31+G**/PCM

Cleavage A Starting Material

SM_Ylide_Cleavage/alanineprenylcleavageAsmm06631plusgstarstarpcm
SM Alanine ammonium dimethyl allyl ylide
m06/6-31+g**
E(RM06) = -636.552177221

Zero-point correction= 0.307731 (Hartree/Particle)
Thermal correction to Energy= 0.324900
Thermal correction to Enthalpy= 0.325844
Thermal correction to Gibbs Free Energy= 0.263370
Sum of electronic and ZPE= -636.244446
Sum of electronic and thermal Energies= -636.227278
Sum of electronic and thermal Enthalpies= -636.226334
Sum of electronic and thermal Free Energies= -636.288808

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	203.878	63.675	131.488

C,0,0.7641437801,-0.4285014282,-0.3859347284

C,0,2.1398391687,-0.8830888352,-0.0470216589
C,0,3.2921094585,-0.3282488124,-0.4621019477
C,0,3.402935776,0.8999492819,-1.3109025326
C,0,4.6090237697,-0.9277538359,-0.0763220584
N,0,0.0170227086,0.3155082372,0.7368587957
C,0,0.7983279105,1.5223538666,1.1335556993
C,0,-1.3533878461,0.7138264852,0.254724314
C,0,-1.4762296033,2.0694122866,-0.3723805035
C,0,-2.2244366078,-0.3390777407,-0.0318141852
C,0,-0.0602232182,-0.5460312771,1.9622279655
H,0,4.4919126528,-1.8027004,0.5706453704
H,0,5.1730926289,-1.229140955,-0.9691793213
H,0,5.2308361026,-0.1884744886,0.4465664096
H,0,4.0497122667,0.7063313039,-2.1762457859
H,0,2.446333838,1.2781598103,-1.6814720258
H,0,3.8845777952,1.705760805,-0.7393462909
H,0,2.2073771778,-1.7836821583,0.566739743
H,0,0.7407044887,0.2618194447,-1.2345278378
H,0,0.1099647161,-1.2767052668,-0.6107284765
H,0,0.9469567734,2.175847612,0.2737866807
H,0,0.2436070312,2.0511024018,1.9116668746
H,0,1.7675626672,1.1981042481,1.5169475917
H,0,0.9528961633,-0.756670065,2.31362182
H,0,-0.6139506554,0.0133745945,2.7193277954
H,0,-0.5929739276,-1.46149572,1.7096674214
H,0,-2.4924711253,2.1686851143,-0.7594124829
H,0,-1.3185846778,2.9078602176,0.3197281901
H,0,-0.7991735268,2.2314391798,-1.2318008532
O,0,-2.0693419516,-1.5651988174,0.1698724665
O,0,-3.4164334533,0.0936424632,-0.6010234716
C,0,-4.380686283,-0.9126869227,-0.8462576843
H,0,-5.2378440717,-0.4053471738,-1.2954342269
H,0,-4.0057158656,-1.6765265651,-1.5368300311
H,0,-4.6957160606,-1.4073838903,0.0800809651

Cleavage A Product

SM_Ylide_Cleavage_pdt/alanineprenylcleavageApdtm06631plusgstarstarpcm
Pdt Alanine ammonium dimethyl allyl ylide
um06/6-31+g**
E(UM06) = -636.530381159
Zero-point correction= 0.300024 (Hartree/Particle)
Thermal correction to Energy= 0.320057
Thermal correction to Enthalpy= 0.321002
Thermal correction to Gibbs Free Energy= 0.248323
Sum of electronic and zero-point Energies= -636.230357
Sum of electronic and thermal Energies= -636.210324
Sum of electronic and thermal Enthalpies= -636.209379
Sum of electronic and thermal Free Energies= -636.282058

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.839	68.482	152.965

C	0.788524	-0.745480	-0.756150
C	2.061067	-1.027741	-0.293953
C	3.220938	-0.274400	-0.477519
C	3.260697	1.002263	-1.249789
C	4.520815	-0.716409	0.108370
N	-0.541974	0.880252	1.552228
C	0.598875	1.773010	1.514043
C	-1.662397	1.120586	0.804809
C	-1.808527	2.454129	0.146953
C	-2.589271	0.054839	0.543054
C	-0.450537	-0.133977	2.587437
H	4.424260	-1.647140	0.677644
H	5.277540	-0.871881	-0.675725
H	4.935304	0.052917	0.777692
H	4.012925	0.949022	-2.050284
H	2.301775	1.266106	-1.705532
H	3.565151	1.837621	-0.600697
H	2.177774	-1.941478	0.296263
H	0.566841	0.141446	-1.348632
H	-0.049132	-1.397265	-0.520387
H	0.665479	2.293628	0.556831
H	0.559573	2.515942	2.325595
H	1.513865	1.178831	1.633819
H	0.200106	-0.961819	2.271682
H	-0.017900	0.323471	3.487132
H	-1.432875	-0.536876	2.826393
H	-2.843246	2.615646	-0.158192
H	-1.187072	2.543777	-0.758142
H	-1.518009	3.267539	0.822033
O	-2.455259	-1.135945	0.845844
O	-3.702852	0.487903	-0.123075
C	-4.656144	-0.516411	-0.441686
H	-5.462678	-0.007872	-0.972162
H	-4.217089	-1.288009	-1.082612
H	-5.047672	-0.990955	0.464146

Cleavage A Transition State

SM_Ylide_Cleavage_ts/alanineprenylcleavageAtsm06631plusgstarstarpcm
alanine prenyl TSfreq
UM06/6-31+G**
E(UM06) = -636.521890517

Zero-point correction= 0.302763 (Hartree/Particle)
Thermal correction to Energy= 0.320520
Thermal correction to Enthalpy= 0.321464
Thermal correction to Gibbs Free Energy= 0.257307
Sum of electronic and ZPE= -636.219128
Sum of electronic and thermal Energies= -636.201371
Sum of electronic and thermal Enthalpies= -636.200426
Sum of electronic and thermal Free Energies= -636.264583

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	201.129	64.591	135.030

C,0,0.9741155078,-0.7469290698,-0.7177303483
C,0,2.2791967219,-1.0719821452,-0.2881627843
C,0,3.4267470259,-0.3456381407,-0.4895988684
C,0,3.4897464075,0.9178207493,-1.2836977437
C,0,4.7315548061,-0.8040648496,0.0740545055
N,0,-0.1601997931,0.3838372892,0.8048811019
C,0,0.7653604066,1.4890784249,1.0539571805

C,0,-1.4033411981,0.7279340447,0.2669416445
C,0,-1.5606560918,2.0786263997,-0.3593437142
C,0,-2.3530675192,-0.30896855,0.0256183634
C,0,-0.1267441106,-0.5435159444,1.9465420205
H,0,4.6310555966,-1.7263818215,0.655488188
H,0,5.466401604,-0.9784266506,-0.7256588603
H,0,5.1704411795,-0.0325589567,0.7240424625
H,0,4.2396520305,0.8299078873,-2.0826168561
H,0,2.5371287101,1.1961673451,-1.7433307199
H,0,3.8170868421,1.7556380703,-0.6501633722
H,0,2.3813130279,-1.9870170523,0.3016289396
H,0,0.8061886283,0.0614898526,-1.4276494708
H,0,0.1949577306,-1.5034626792,-0.6800478352
H,0,0.8714974869,2.1219856016,0.1718719193
H,0,0.4135937831,2.0984373106,1.8987530488
H,0,1.7452760435,1.070004167,1.3020379074
H,0,0.9091060579,-0.8540524775,2.1125633239
H,0,-0.4952970059,-0.0231538456,2.8419929801
H,0,-0.7479976215,-1.4127627629,1.7410343499
H,0,-2.5848670957,2.2048775709,-0.7114616087
H,0,-1.3456999928,2.8992733582,0.3371041829
H,0,-0.9007118779,2.2188685139,-1.2325997998
O,0,-2.2149093042,-1.5251625123,0.2234967309
O,0,-3.5326386272,0.1674687039,-0.4899637305
C,0,-4.523876527,-0.8109727057,-0.7637677308
H,0,-5.3771540481,-0.2674208928,-1.1734007666
H,0,-4.1670558613,-1.5457735419,-1.4932789167
H,0,-4.8244309226,-1.3387046904,0.1477472769

Polyrate structures for C-N Bond Cleavage in 5: M062X/6-31+G**/PCM

Cleavage A Starting Material

SM_Ylide_Cleavage/alanineprenylcleavageAsmm062x631plusgstarstarpcm
SM Alanine ammonium dimethyl allyl ylide
m062x/6-31+g**
E(RM062X) = -636.698102848

Zero-point correction= 0.313086 (Hartree/Particle)
Thermal correction to Energy= 0.330026
Thermal correction to Enthalpy= 0.330970
Thermal correction to Gibbs Free Energy= 0.269062
Sum of electronic and ZPE= -636.385017
Sum of electronic and thermal Energies= -636.368077
Sum of electronic and thermal Enthalpies= -636.367132
Sum of electronic and thermal Free Energies= -636.429041

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	207.095	62.664	130.297

C,0,0.747521742,-0.4348997736,-0.4459999366
C,0,2.1199326319,-0.9234106488,-0.0966483499
C,0,3.2828206896,-0.3435762732,-0.4342826248
C,0,3.4163136471,0.94722555,-1.196758635
C,0,4.5944713013,-0.967449975,-0.0380639789
N,0,0.0299085751,0.3214789156,0.6782479157
C,0,0.8220653817,1.5364845074,1.0391098485
C,0,-1.3435003748,0.7119328852,0.2167639684
C,0,-1.4983005814,2.0767387566,-0.3950363102
C,0,-2.2229131309,-0.3369760684,-0.031796017
C,0,-0.0179574247,-0.5259582848,1.9174031375
H,0,4.4517330212,-1.8817954013,0.5416487751
H,0,5.1876569301,-1.2050992022,-0.928106092
H,0,5.1854025074,-0.262532433,0.5577313788
H,0,4.1112238766,0.8175383517,-2.0329587824
H,0,2.473267283,1.3262502146,-1.5919621845
H,0,3.8457686123,1.7176840449,-0.5448947182
H,0,2.161943132,-1.8576512481,0.4609885768
H,0,0.744437131,0.2548607312,-1.2916569835
H,0,0.0814803908,-1.2701038839,-0.6683566284
H,0,0.9447621429,2.1717750266,0.1644593621
H,0,0.2846452423,2.0734104665,1.8205153879
H,0,1.796992087,1.2133349181,1.4015924091
H,0,1.0034117477,-0.7049287849,2.2549961671
H,0,-0.5750447091,0.032887484,2.6687743025
H,0,-0.5281746495,-1.4547620406,1.6813486299
H,0,-2.5244690605,2.1648113033,-0.7507335082
H,0,-1.3261760684,2.9029704653,0.3037878579
H,0,-0.8442289952,2.2463914107,-1.2663325571
O,0,-2.0630867092,-1.5647256606,0.1830790882
O,0,-3.4283461653,0.0843015225,-0.5807295713
C,0,-4.3992360489,-0.931796737,-0.777148801
H,0,-5.2637169063,-0.4336675156,-1.2172750323
H,0,-4.0339266195,-1.7080365932,-1.4544166211
H,0,-4.6849106292,-1.3982400301,0.1699935271

Cleavage A Product

SM_Ylide_Cleavage_pdt/alanineprenylcleavageApdtm062x631plusgstarstarpcm
Pdt Alanine ammonium dimethyl allyl ylide
um062x/6-31+g**
E(UM062X) = -636.665411694
Zero-point correction= 0.304695 (Hartree/Particle)
Thermal correction to Energy= 0.324605
Thermal correction to Enthalpy= 0.325549
Thermal correction to Gibbs Free Energy= 0.253918
Sum of electronic and zero-point Energies= -636.360717
Sum of electronic and thermal Energies= -636.340807
Sum of electronic and thermal Enthalpies= -636.339863
Sum of electronic and thermal Free Energies= -636.411493

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.692	67.834	150.759
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.384626
C	1.107222	0.000000	2.232264
C	0.934996	0.016486	3.721017
C	2.523045	-0.015710	1.741828
N	0.112607	3.070949	-0.553587
C	-1.065275	3.425594	0.224545
C	1.353934	3.088724	0.204125
C	0.095620	2.788570	-1.885595

C	-1.115142	2.345301	-2.513740
O	-0.981794	2.208761	-3.869932
C	-2.141799	1.744720	-4.552442
C	1.389919	2.837266	-2.646576
O	-2.188741	2.081594	-1.956820
H	-0.118778	0.020803	4.010027
H	1.415856	-0.856815	4.181092
H	1.416698	0.900487	4.159786
H	3.049108	-0.902243	2.118576
H	2.601417	-0.012800	0.653619
H	3.070192	0.856177	2.124207
H	-0.974415	0.015563	1.874278
H	0.915284	-0.006662	-0.582869
H	-0.931819	0.046698	-0.551570
H	2.118310	2.485686	-0.284416
H	1.726456	4.112909	0.333497
H	1.161670	2.656567	1.191344
H	-1.453438	2.554104	0.764676
H	-0.771503	4.190256	0.949950
H	-1.845893	3.818688	-0.421314
H	1.190855	2.939197	-3.711964
H	1.984064	1.923800	-2.507899
H	2.002139	3.683773	-2.323401
H	-1.861570	1.682637	-5.603045
H	-2.442180	0.761169	-4.183426
H	-2.972998	2.442409	-4.424861

Cleavage A Transition State

SM_Ylide_Cleavage_ts/alanineprenylcleavageAtsm062x63
1plusgstarstarpcm
alanine prenyl TSfreq
UM062X/6-31+G**
E(UM062X) = -636.657111959

Zero-point correction= 0.307282 (Hartree/Particle)
Thermal correction to Energy= 0.324985
Thermal correction to Enthalpy= 0.325929
Thermal correction to Gibbs Free Energy= 0.261888
Sum of electronic and ZPE= -636.349830
Sum of electronic and thermal Energies= -636.332127
Sum of electronic and thermal Enthalpies= -636.331183
Sum of electronic and thermal Free Energies= -636.395224

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.931	64.003	134.785

C,0,0.9543247591,-0.725193676,-0.7985209082
C,0,2.2417647169,-1.0959935489,-0.345422005
C,0,3.405594593,-0.3775053144,-0.4666751392
C,0,3.5094320564,0.9350483123,-1.1875999658
C,0,4.6907614796,-0.8870857039,0.1179598918
N,0,-0.1580602163,0.433757153,0.7803333779
C,0,0.7804298115,1.5437451598,0.9652002873
C,0,-1.4034079941,0.7470558766,0.2618557626
C,0,-1.6188507022,2.1060497398,-0.3436082712
C,0,-2.3396172335,-0.3111101802,0.0367348371
C,0,-0.0625103828,-0.4985533267,1.9156894381
H,0,4.5534793543,-1.8390584129,0.6363257775
H,0,5.4476686979,-1.0242498686,-0.6649883528
H,0,5.1086786567,-0.1623884899,0.8287261739
H,0,4.2765045956,0.8779543127,-1.969760586
H,0,2.573224774,1.2479178361,-1.652230176
H,0,3.8278799665,1.7270720369,-0.4972140885
H,0,2.307866518,-2.0389565474,0.1981835458
H,0,0.8170632552,0.1167352926,-1.4696175614
H,0,0.1482507234,-1.4499394599,-0.7706636672
H,0,0.8451911036,2.1499311653,0.0632705044
H,0,0.4654438008,2.1714446755,1.8079100266
H,0,1.7638049719,1.1207344214,1.1792225879
H,0,0.9842624246,-0.7857430061,2.0307788319
H,0,-0.4012825715,0.0139703227,2.8243638774
H,0,-0.6724498222,-1.3761306693,1.7305719638
H,0,-2.6625258642,2.2142122198,-0.6313224424
H,0,-1.3731998442,2.9126211085,0.3542611557
H,0,-1.0105183232,2.25878654,-1.2472643383
O,0,-2.1667846388,-1.5223143436,0.2343204054
O,0,-3.5325876597,0.1348383669,-0.4661820275
C,0,-4.5016805297,-0.8739251451,-0.7306816716
H,0,-5.3687302715,-0.351349328,-1.1325365018
H,0,-4.1245289247,-1.5947165153,-1.4600216768
H,0,-4.7731192805,-1.4031950036,0.1858839344

Polyrate structures for rearrangement of 2: M06/6-31+G**/PCM(DMF)

23 Starting Material

/g/home/biswas85/parentdmfm06/sm/g09.log
sm for 23 from opt of ts
M06/6-31+G**
E(RM06) = -518.694746359

Zero-point correction= 0.223875 (Hartree/Particle)
Thermal correction to Energy= 0.236917
Thermal correction to Enthalpy= 0.237861
Thermal correction to Gibbs Free Energy= 0.184158
Sum of electronic and ZPE= -518.470871
Sum of electronic and thermal Energies= -518.457829
Sum of electronic and thermal Enthalpies= -518.456885
Sum of electronic and thermal Free Energies= -518.510589

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.668	47.606	113.029

C,0,1.1333071034,-0.1218041045,2.2064736122
C,0,0.0000933671,0.0326690312,1.5220872205
C,0,-0.047768062,-0.0071633904,0.0354155882
N,0,-0.131398525,1.3843791958,-0.6153483973
C,0,1.0395596613,2.2399093241,-0.3350302844
C,0,2.3088823221,1.7771417278,-0.6612243047
O,0,3.2972129854,2.610343799,-0.164251276
C,0,4.628824054,2.248251984,-0.484027493
C,0,-1.3491782563,2.08477429,-0.1201183413
C,0,-0.2967356606,1.171366675,-2.090028071
O,0,2.6238708087,0.7659426221,-1.3222093789
H,0,0.8595729485,-0.4516936169,-0.3840109545
H,0,-0.9233939406,-0.5621344851,-0.3228546894
H,0,-0.9412142358,0.1729148895,2.0547282923
H,0,1.1511140466,-0.1082158632,3.2932473258

H,0,2.08387299,-0.274037335,1.6953626709
H,0,-1.2453061905,2.2752581971,0.9495823324
H,0,-2.224802973,1.4584105434,-0.309859651
H,0,-1.436868616,3.0343601354,-0.6523079255
H,0,-1.1789549197,0.5493744809,-2.2689146993
H,0,-0.4165303885,2.150844872,-2.556360578
H,0,0.6051424569,0.6844316774,-2.4629264389
H,0,4.8903416346,1.2661848778,-0.0731431755
H,0,5.2666192138,3.0118431856,-0.0333408849
H,0,4.7938065027,2.2276111707,-1.5673607619
H,0,0.8771776727,2.9881461163,0.4300172631

23 Product

/g/home/biswas85/parentdmfm06/p/g09.log
23 product
M06/6-31+G**
E(RM06) = -518.742159479

Zero-point correction= 0.223726 (Hartree/Particle)
Thermal correction to Energy= 0.236854
Thermal correction to Enthalpy= 0.237798
Thermal correction to Gibbs Free Energy= 0.184675
Sum of electronic and ZPE= -518.518434
Sum of electronic and thermal Energies= -518.505305
Sum of electronic and thermal Enthalpies= -518.504361
Sum of electronic and thermal Free Energies= -518.557485

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.628	47.081	111.808

C,0,0.248569026,0.1136980282,1.9585947295
C,0,0.5810526322,0.5139119792,0.5516588156
C,0,1.4829518537,-0.1172518565,-0.2011163179
N,0,-0.3509756572,2.094078552,3.3886020017
C,0,-0.916195782,2.8743330853,2.3009523105
C,0,0.6685419158,1.1187845757,3.0588438653
C,0,2.0285207211,1.6953505816,2.6839142054
O,0,2.2438670974,2.8169540825,2.2745605061
C,0,0.0017425704,2.9199325248,4.5294745891
O,0,2.9835199911,0.7685342633,2.8363855663
C,0,4.2950980678,1.1320048808,2.3921779129
H,0,2.031522176,-0.980237549,0.1776748281
H,0,1.7031314895,0.2007895908,-1.2172548827
H,0,0.0630272084,1.3794490129,0.1341369413
H,0,-0.8311290668,-0.0524686401,2.0776067804
H,0,0.7451077383,-0.8406958306,2.1717226977
H,0,0.3679930227,2.2869759032,5.34679906
H,0,-0.8904302817,3.4479418329,4.8860854284
H,0,0.7753996489,3.6750730397,4.3027152484
H,0,-1.7282384913,3.4898721524,2.7047200069
H,0,-0.1894061859,3.5442503473,1.8109286735
H,0,-1.3588969668,2.2186549574,1.5441576919
H,0,4.2774158229,1.3708354706,1.3243197181
H,0,4.9257013509,0.2625659108,2.5754419505
H,0,4.665355605,1.994536644,2.9526588523
H,0,0.8359234937,0.5278064607,3.9721138207

23 Transition State

/g/home/biswas85/parentdmfm06/ts/g09.log
glycine allyl TSfreq
M06/6-31+G**
E(RM06) = -518.672174429

Zero-point correction= 0.220896 (Hartree/Particle)
Thermal correction to Energy= 0.233692
Thermal correction to Enthalpy= 0.234636
Thermal correction to Gibbs Free Energy= 0.182582
Sum of electronic and ZPE= -518.451279
Sum of electronic and thermal Energies= -518.438483
Sum of electronic and thermal Enthalpies= -518.437539
Sum of electronic and thermal Free Energies= -518.489593

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.644	47.372	109.557

C,0,1.1208611714,-0.0012050587,2.1125085329
C,0,-0.1136273499,-0.2699158874,1.583957285
C,0,-0.3554501247,-0.0432927865,0.2254035237
N,0,-0.2145010566,2.0936215391,0.285248748
C,0,0.7811094194,2.4599781681,1.1635019884
C,0,2.1687937195,2.4265017896,0.8465109637
O,0,2.9104516828,2.9412969162,1.8715621034
C,0,4.3210402146,2.8385615063,1.7252096105
C,0,-1.5492321603,2.4601461294,0.7736762782
C,0,-0.0607426848,2.4096405313,-1.1429723496
O,0,2.7071323417,1.9863243866,-0.1723725164
H,0,0.4778537571,-0.0945258587,-0.4744652149
H,0,-1.3442334769,-0.1937334883,-0.2048344085
H,0,-0.9648707932,-0.3941218825,2.2551627538
H,0,1.2950406927,0.0104094622,3.1859679052
H,0,2.001846206,0.0291700209,1.4746665458
H,0,-1.6902623575,2.0613683712,1.782007574
H,0,-2.3089365272,2.0395412735,0.109954053
H,0,-1.6520779981,3.5531027327,0.7990406872
H,0,-0.8402921118,1.8839539589,-1.7024796709
H,0,-0.1727722291,3.4917198855,-1.2934349281
H,0,0.9239864679,2.0932252987,-1.4854614339
H,0,4.6303283239,1.7909198975,1.6392737064
H,0,4.7501679912,3.2779259748,2.6268805815
H,0,4.6701219697,3.3848655609,0.8431640978
H,0,0.4788829119,2.8076695588,2.1446875837

Polyrate structures for rearrangement of 2: M062X/6-31+G**/PCM(DMF)

23 Starting Material

/g/home/biswas85/parentdmfm062x/sm/g09.log
sm for 23 from opt of ts
M062X/6-31+G**
E(RM062X) = -518.806416442

Zero-point correction= 0.227816 (Hartree/Particle)
Thermal correction to Energy= 0.240698
Thermal correction to Enthalpy= 0.241642
Thermal correction to Gibbs Free Energy= 0.188327
Sum of electronic and ZPE= -518.578601

Sum of electronic and thermal Energies= -518.565718
Sum of electronic and thermal Enthalpies= -518.564774
Sum of electronic and thermal Free Energies= -518.618090

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.040	46.846	112.212

C,0,1.1269700984,-0.0927661204,2.1998380003
C,0,-0.0129008803,0.0125338672,1.5175752732
C,0,-0.0474883799,-0.0139001263,0.0217496431
N,0,-0.130397807,1.3815076267,-0.6083299145
C,0,1.0402761819,2.2251171138,-0.3064318215
C,0,2.3061181091,1.7665970479,-0.6273198589
O,0,3.3019343985,2.6117448535,-0.1653461172
C,0,4.6299404757,2.2359724569,-0.5004037323
C,0,-1.3514869522,2.0757612902,-0.1048728894
C,0,-0.2819664972,1.1879828851,-2.0893205159
O,0,2.6202448181,0.7321195871,-1.2614781342
H,0,0.865124861,-0.4474256871,-0.3888032588
H,0,-0.9175385479,-0.5654183413,-0.345174927
H,0,-0.9598725925,0.1034004429,2.04542985
H,0,1.1427029289,-0.0861498449,3.2852017015
H,0,2.0793006265,-0.1905753062,1.6828505618
H,0,-1.2443265185,2.2440897797,0.9659222639
H,0,-2.2223069758,1.451383924,-0.3082977721
H,0,-1.4356258969,3.0309022681,-0.6227101229
H,0,-1.1599319664,0.5679842643,-2.2807280317
H,0,-0.398897612,2.1720384785,-2.5405527157
H,0,0.6238601914,0.7067678981,-2.45347295
H,0,4.8865725466,1.2615621939,-0.0761469306
H,0,5.2729916426,3.0053859662,-0.0726067502
H,0,4.7705520983,2.1963548627,-1.5840976165
H,0,0.8633976499,3.0361386192,0.3811237656

23 Product

/g/home/biswas85/parentdmfm062x/p/g09.log
23 product
M062X/6-31+G**
E(RM062X) = -518.851309696

Zero-point correction= 0.227403 (Hartree/Particle)
Thermal correction to Energy= 0.240398
Thermal correction to Enthalpy= 0.241342
Thermal correction to Gibbs Free Energy= 0.188355
Sum of electronic and ZPE= -518.623907
Sum of electronic and thermal Energies= -518.610912
Sum of electronic and thermal Enthalpies= -518.609967
Sum of electronic and thermal Free Energies= -518.662954

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.852	46.437	111.520

C,0,0.2296425962,0.1020687292,1.9668478427
C,0,0.5907750045,0.5243331986,0.565772539
C,0,1.5554705386,-0.0573767365,-0.1486883418
N,0,-0.3749900539,2.0828218482,3.4010598736
C,0,-0.8988159124,2.8625203808,2.285368259
C,0,0.6445902369,1.1004877434,3.0830345889
C,0,2.0107571184,1.6785164431,2.7104668553
O,0,2.2324637013,2.8175059376,2.3599329444
C,0,-0.0063993852,2.9257444314,4.5318839158
O,0,2.9572061051,0.735249234,2.7865595158
C,0,4.2628239655,1.1153961192,2.3335295749
H,0,2.1299130182,-0.8896672003,0.2528152446
H,0,1.7986930697,0.2782469706,-1.15204944
H,0,0.0470001625,1.3605850866,0.1298552668
H,0,-0.8501343369,-0.0556355602,2.0658316226
H,0,0.7230128483,-0.8510680536,2.1756191971
H,0,0.3357397267,2.2963081181,5.3590029712
H,0,-0.8882415714,3.4786140709,4.8673817744
H,0,0.786853976,3.6499042275,4.2911055698
H,0,-1.6780779637,3.5257379674,2.6704993707
H,0,-0.1361815918,3.4756046751,1.7835547196
H,0,-1.3684646599,2.202609606,1.5522652973
H,0,4.2183854803,1.4120907916,1.2834182847
H,0,4.8865462295,0.2326996962,2.4556848845
H,0,4.6455458043,1.9422884459,2.9340047246
H,0,0.8050548933,0.5100938292,3.9931179445

23 Transition State

/g/home/biswas85/parentdmfm062x/ts/g09.log
glycine allyl TSfreq
M062X/6-31+G**
E(RM062X) = -518.778941294

Zero-point correction= 0.225591 (Hartree/Particle)
Thermal correction to Energy= 0.237921
Thermal correction to Enthalpy= 0.238865
Thermal correction to Gibbs Free Energy= 0.187954
Sum of electronic and ZPE= -518.553350
Sum of electronic and thermal Energies= -518.541021
Sum of electronic and thermal Enthalpies= -518.540076
Sum of electronic and thermal Free Energies= -518.590988

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.297	45.928	107.152

C,0,1.0484463717,0.0846688271,2.1132030365
C,0,-0.1614101495,-0.2705747472,1.5631550875
C,0,-0.3432959294,0.0074895744,0.1999510948
N,0,-0.2054615318,2.0278568246,0.2999088228
C,0,0.7865572134,2.3597890321,1.2112700485
C,0,2.1728387466,2.3656063811,0.8720067357
O,0,2.9221821971,2.9288160568,1.8606939005
C,0,4.3350319755,2.8658711801,1.6763663018
C,0,-1.5377715433,2.4131060033,0.7965743704
C,0,-0.0334413512,2.4102371604,-1.1151786067
O,0,2.703664216,1.8865099367,-0.1322570412
H,0,0.5204906799,-0.0616541795,-0.4589825337
H,0,-1.3062367022,-0.1505056361,-0.2805148502
H,0,-1.0325621222,-0.3953812359,2.202425432
H,0,1.1947828465,0.1228165415,3.1892115398
H,0,1.9486300614,0.0549147309,1.5059560129
H,0,-1.6870080919,1.9720379731,1.7833393342
H,0,-2.2992672025,2.0402242754,0.1106424521
H,0,-1.6057018553,3.5032650623,0.8678237248
H,0,-0.8167434569,1.920250442,-1.6971625777

H,0,-0.1287442173,3.4961346546,-1.215509852
H,0,0.9454032707,2.0895274085,-1.4610260274
H,0,4.669196238,1.8280426814,1.6060366101
H,0,4.7687044122,3.3417313268,2.5544406899
H,0,4.6326640346,3.4009332869,0.7719360636
H,0,0.4796698898,2.8014344387,2.1480542311

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