SUPPORTING INFORMATION

Controlling Selectivity by Controlling the Path of Trajectories

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Experimental Procedures

Syntheses of Ylide Precursors

1a: To a mixture of 12.95 g (60 mmol) of 4-nitrobenzyl bromide and 50 mL of dichloromethane (dried over 4 Å molecular sieves) under N_2 at 25 °C was added 7.02 g (60 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 12 h. During the stirring solid precipitated out from the solution. The liquid phase was decanted off. The solid was then washed two 10-mL portions of dichloromethane to afford 15.92 g (79%) of **1a**. ^{1}H NMR ($CDCl_3$): δ 3.60 (s, 6 H), 3.83 (s, 3H), 5.13 (s, 2 H), 5.61 (s, 2 H), 8.00 (d, J=8.6 Hz, 2 H), 8.34 (d, J=8.6 Hz, 2 H). ^{13}C NMR (d_6-DMSO): δ 50.5, 53.0, 60.6, 65.8, 123.9, 134.6, 134.7, 148.7, 165.2. The nonintegrated peaks in the ^{1}H NMR spectrum shown below are $CHCl_3$ (7.26) and water (1.61). HRMS (+ESI) m/z calculated for $C_{12}H_{17}N_2O_4^+$: 253.1188; found: 253.1187.

1b: To a mixture of 2.05 g (10 mmol) of 4-chlorobenzyl bromide and 10 mL of diethyl ether (dried over sodium followed by distillation) under N_2 at 25 °C was added 1.20 g (10.2 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 12 h. During the stirring solid precipitated out from the solution. The volatiles were then removed on a rotatory evaporator. The solid was then washed with two 20-mL portions of diethyl ether. The residual solvent was then removed on a rotatory evaporator to afford 2.21 g (69%) of **1b**. ^{1}H NMR ($CDCl_3$): δ 3.49 (s, 6 H), 3.73 (s, 3H), 5.09 (s, 2 H), 5.32 (s, 2 H), 7.40 (d, J=8.4 Hz, 2 H), 7.61 (d, J=8.4 Hz, 2 H). ^{13}C NMR ($CDCl_3$): δ 49.6, 52.8, 60.5, 66.6, 125.6, 129.2, 134.5, 137.0, 165.3. HRMS (+ESI) m/z calculated for $C_{12}H_{17}ClNO_2^+$: 242.0948; found: 242.0956

1c: To a mixture of 2.38 g (9.95 mmol) of 4-(trifuoromethyl)benzyl bromide and 5 mL of dicholoromethane under N_2 at 25 °C was added 1.19 g (10.15 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 12 h. During the stirring solid precipitated out from the solution. The volatiles were then removed on a rotatory evaporator. The solid was then washed with two 10-mL portions of dichloromethane. The residual solvent was then removed on a rotatory evaporator to afford 3.1 g (87%) of **1c**. ^{1}H NMR ($CDCl_3$): δ 3.57 (s, 6 H), 3.78 (s, 3H), 5.13 (s, 2 H), 5.52 (s, 2 H), 7.73 (d, J=8.1 Hz, 2 H), 7.87 (d, J=8.1 Hz, 2 H). ^{13}C NMR ($CDCl_3$): δ 42.7, 44.6, 52.9, 59.3, 115.6 (q, $J_{C\text{-}F}$=276.2 Hz), 117.9 (q, $J_{C\text{-}F}$=3.6 Hz), 112.9, 124.4 (q, $J_{C\text{-}F}$=33.4 Hz), 125.6, 157.0. The nonintegrated peaks in the ^{1}H NMR spectrum shown below are $CHCl_3$ (7.26) and water (1.70). The identity of impurity was confirmed by ^{1}H NMR analysis in d_6-DMSO where the impurities have the chemical shifts, δ 3.33 (water). HRMS (+ESI) m/z calculated for $C_{13}H_{17}F_3NO_2^+$: 276.1211; found: 276.1226

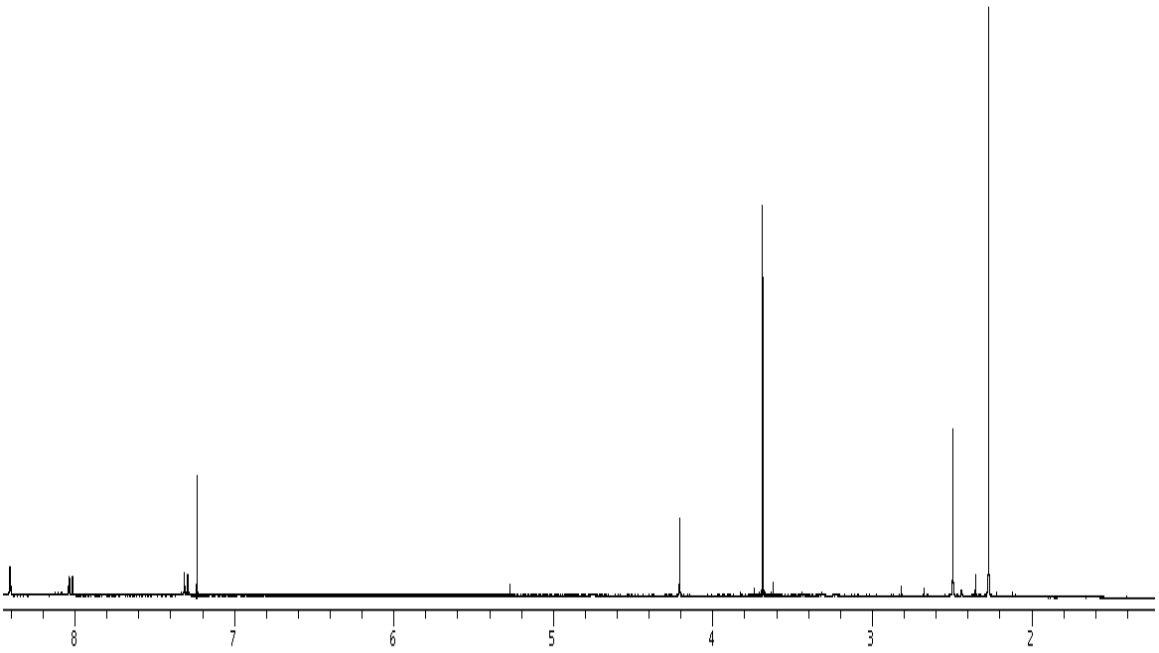
1d: To a mixture of 8.55 g (50 mmol) of benzyl bromide in 25 mL of diethyl ether (dried over sodium followed by distilled under nitrogen) under N_2 at 25 °C was added 5.90 g (50.36 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 24 h. During the stirring solid precipitated out from the solution. The solid was then washed two 10-mL portions of diethyl ether to afford 12.20 g (85%) of **1d**. ^{1}H NMR ($CDCl_3$): δ 3.53 (s, 6 H), 3.74 (s, 3H), 5.07 (s, 2 H), 5.30 (s, 2 H), 7.45 (m, 3 H), 7.63 (m, 2 H). ^{13}C NMR ($CDCl_3$): 49.3, 52.6, 59.9, 67.0, 126.4, 128.7, 130.4, 132.7, 164.8. The nonintegrated peak in the ^{1}H NMR spectrum shown below is $CHCl_3$ (7.26). HRMS (+ESI) m/z calculated for $C_{12}H_{18}NO_2^+$: 208.1332; found: 208.1340

1e: To a mixture of 1.96 g (10.00 mmol) of 4-(bromomethyl)benzonitrile and 5 mL of dicholoromethane under N_2 at 25 °C was added 1.19 g (10.15 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 12 h. During the stirring solid precipitated out from the solution. The volatiles were then removed on a rotatory evaporator. The solid was washed with two 10-mL portions of dichloromethane. The residual solvent was then removed on a rotatory evaporator to afford 2.60 g (83%) **1e**. ^{1}H NMR ($CDCl_3$): δ 3.56 (s, 6 H), 3.80 (s, 3H), 5.09 (s, 2 H), 5.53 (s, 2 H), 7.78 (d, J=7.9 Hz, 2 H), 7.90 (d, J=7.9 Hz, 2 H). ^{13}C NMR (d_4-Methanol): δ 52.1, 53.8, 62.2 (broad due to transesterification by d_4-Methanol), 68.6, 115.9, 118.9, 133.3, 134.2, 135.2, 166.4. The nonintegrated peaks in the ^{1}H NMR spectrum shown below are $CHCl_3$ (7.26), dichloromethane (5.29) and water (1.67). The identities of impurities were confirmed by ^{1}H NMR analysis in d_6-DMSO where the impurities have the chemical shifts, δ 3.30 (water), 5.75 (dichloromethane). HRMS (+ESI) m/z calculated for $C_{13}H_{17}N_2O_2^+$: 233.1290; found: 233.1302.

Procedures for Isolated Yields Maximizing the [2,3]-Product 5.

5a: To a mixture of 1.00 g (3.0 mmol) of **1a**, 5 mL of anhydrous carbon tetrachloride and 10 mL of dichloromethane at 25 °C was added 900 mg (5.91 mmol) of DBU. The mixture was stirred for 1 h at 25 °C. Then 100 mL of diethyl ether was added to the reaction mixture and shaken. After that the ether layer was washed with 25 mL of water and by three 25-mL portions of brine, then dried over K_2CO_3. The volatiles were removed on a rotatory evaporator to afford a mixture of **4a** and **5a** in the ratio 3:97. The residue was chromatographed on silica gel using 25% ethyl acetate in hexanes as eluent to afford 686 mg (91%) of pure **5a**: ^{1}H NMR ($CDCl_3$): δ 2.30 (s, 6 H), 2.52 (s, 3H), 3.72 (s, 3 H), 4.24 (s, 1 H), 7.33 (d, J=9.9 Hz, 1 H), 8.05 (dd, J=9.9 Hz, J=2.64 Hz, 1 H), 8.43 (d, J=2.64 Hz, 1H). ^{13}C NMR ($CDCl_3$): 19.4, 42.6, 51.7, 69.6, 122.3, 123.0, 131.2, 136.9, 144.8, 146.4, and 170.8. (+ESI) m/z calculated for $C_{12}H_{17}N_2O_4^+$: 253.1188 found: 253.1195.

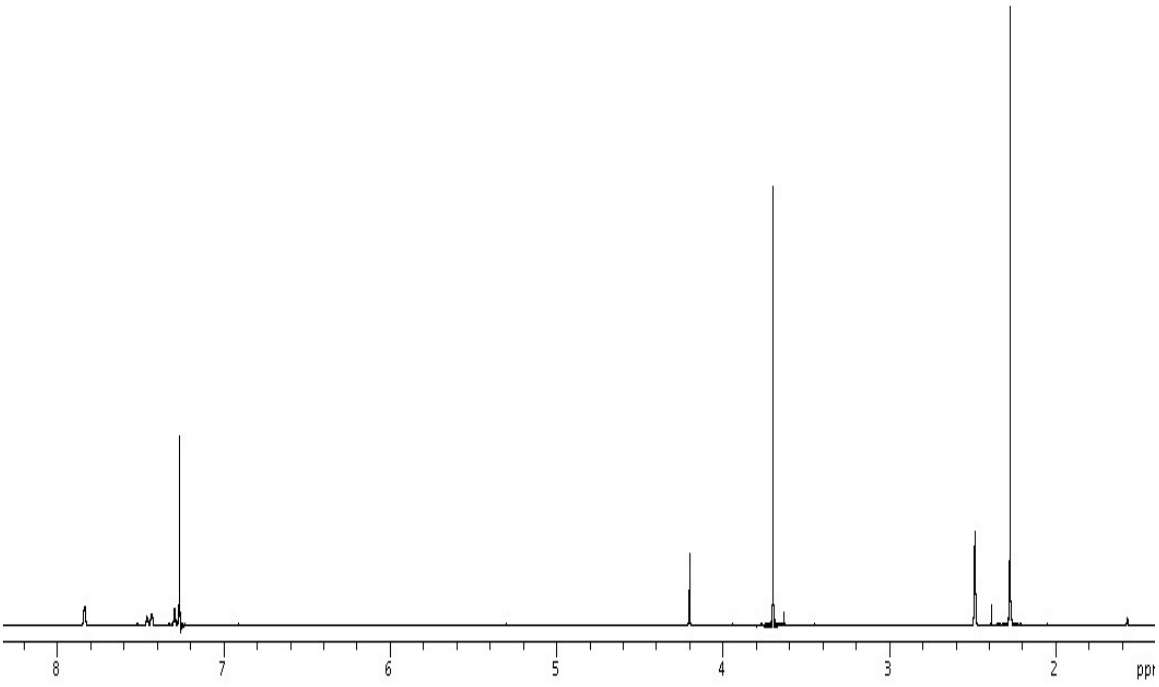
The NMR spectra of purified **5a** are presented in a later section. The ^{1}H NMR spectrum below is of the crude material before any purification. This is shown to illustrate the cleanliness of the reaction.



5b: To a mixture of 963 mg (2.98 mmol) of **1b** and 15 mL of dichloromethane at 25 °C was added 3.00 g (19.7 mmol) of DBU. The mixture was sonicated for 1 h at 43 °C. During the sonication the solid in the reaction mixture dissolved. After that the reaction mixture was stirred at 25 °C for 1 h. The volatiles were removed on a rotatory evaporator and the residue was directly chromatographed on silica gel using 20% ethyl acetate in hexanes as eluent to afford 551 mg (76%) of pure **5b**: ^{1}H NMR ($CDCl_3$): δ 2.20 (s, 6 H), 2.32 (s, 3H), 3.62 (s, 3 H), 4.06 (s, 1 H), 7.02 (d, J=8.1 Hz, 1 H), 7.09 (dd, J=8.1 Hz, J=2.3 Hz, 1 H), 7.50 (d, J=2.3 Hz, 1H). ^{13}C NMR ($CDCl_3$): 19.1, 43.1, 51.9, 70.2, 127.9, 128.1, 131.7, 132.1, 135.4, 136.8 and 171.6. m/z (+ESI) calculated for $C_{12}H_{17}ClNO_2^+$: 242.0948 found: 242.0945.

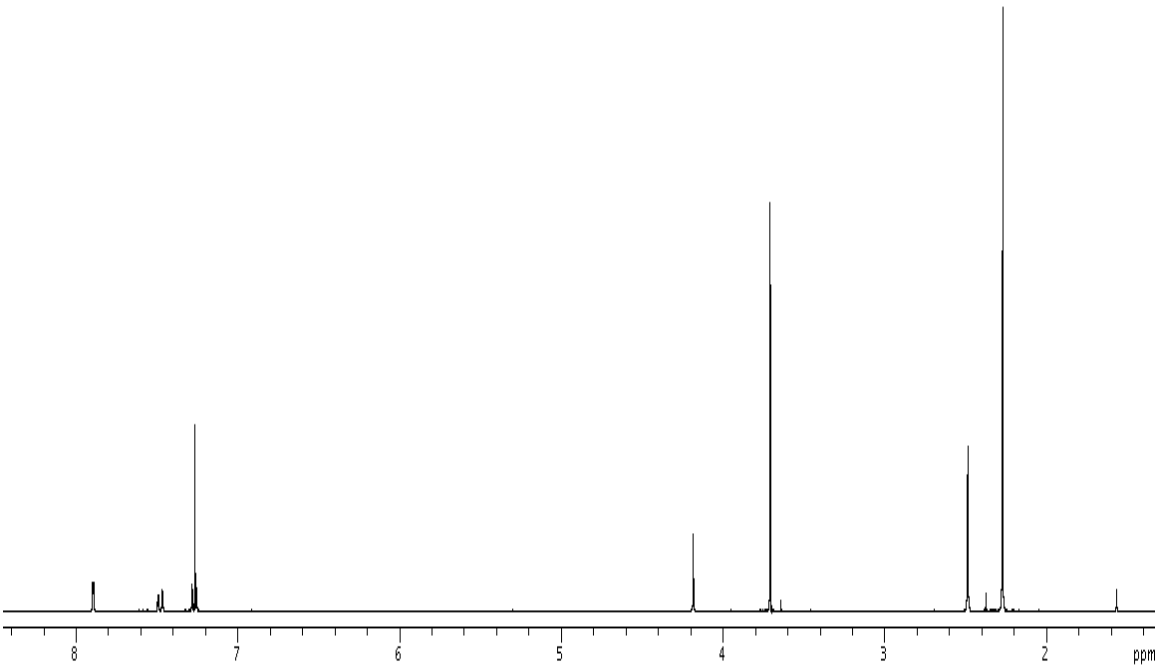
5c: To a mixture of 1.10 g (3.09 mmol) of **1c** and 10 mL of dichloromethane at 25 °C was added 3.00 g (19.7 mmol) of DBU. The mixture was sonicated until all solid dissolved and then stirred at 25 °C for 1 h. The mixture was then partitioned between 150 mL of diethyl ether and 25 mL of water. The organic layer was rinsed with four 25-mL portions of brine, then dried over K_2CO_3. The volatiles were removed on a rotatory evaporator to afford 790 mg of a mixture of **4c** and **5c** in the ratio 2:98. The residue was chromatographed on silica gel using 25% ethyl acetate in hexanes as eluent to afford 734 mg (86%) of pure **5c**: ^{1}H NMR ($CDCl_3$): δ 2.27 (s, 6 H), 2.48 (s, 3H), 3.70 (s, 3 H), 4.20 (s, 1 H), 7.28 (d, J=7.9 Hz, 1 H), 7.44 (dd, J=7.9 Hz, J=1.5 Hz, 1 H), 7.83 (d, J=1.5 Hz, 1H). ^{13}C NMR ($CDCl_3$): 19.9, 43.4, 52.2, 70.4, 124.1 (J_{C-F}=278.0 Hz), 124.8 (J_{C-F}=3.8 Hz), 125.3 (J_{C-F}=3.8 Hz), 129.0 (J_{C-F}=33.0 Hz), 131.1, 136.1, 141.3 and 171.8. m/z (+ESI) calculated for $C_{13}H_{17}F_3NO_2^+$: 276.1211 found: 276.1199.

The NMR spectra of purified **5c** are presented in a later section. The ^{1}H NMR spectrum below is of the crude material before any purification. This is shown to illustrate the cleanliness of the reaction.



5e: To a mixture of 928 g (2.96 mmol) of **1b** and 8 mL of dichloromethane at 25 °C was added 4.00 g (26.27 mmol) of DBU. The mixture was sonicated until all solid dissolved and then stirred at 25 °C for 1 h. The mixture was then partitioned between 150 mL of diethyl ether and 25 mL of water. The organic layer was rinsed with four 25-mL portions of brine, then dried over K_2CO_3. The volatiles were removed on a rotatory evaporator to afford 678 mg of a mixture of **4e** and **5e** in the ratio 2:98. The residue was chromatographed on silica gel using 25% ethyl acetate in hexanes as eluent to afford 617 mg (90%) of **5e**: ^{1}H NMR ($CDCl_3$): δ 2.27 (s, 6 H), 2.48 (s, 3H), 3.70 (s, 3 H), 4.18 (s, 1 H), 7.26 (d, J=8.0 Hz, 1 H), 7.47 (dd, J=8.0 Hz, J=1.8 Hz, 1 H), 7.89 (d, J=1.8 Hz, 1H). ^{13}C NMR ($CDCl_3$): 20.1, 43.2, 52.2, 70.1, 110.5, 118.9, 131.4, 131.5, 132.3, 136.9, 143.0 and 171.4. m/z (+ESI) calculated for $C_{13}H_{17}N_2O_2^+$: 233.1290 found: 233.1285

The NMR spectra of purified **5e** are presented in a later section. The ^{1}H NMR spectrum below is of the crude material before any purification. This is shown to illustrate the cleanliness of the reaction.



Procedures for Isolated Yields Maximizing the [1,2]-Product 4.

4a: To a mixture of 665 mg (1.99 mmol) of **1a** and 2 mL of DMSO was added 200 mg (2.0 mmol) of 40% KH in paraffin oil (washed with hexanes) at room temperature. The reaction mixture was stirred for 15 min at room temperature. The mixture was then partitioned between 50 mL of diethyl ether and 25 mL water. The organic layer was dried over anhydrous potassium carbonate. The volatiles were removed on a rotatory evaporator, and the residue was flash chromatographed on silica gel using 50% ethyl acetate in hexanes as eluent to afford 351 mg (70%) of pure **4a**: ^{1}H NMR ($CDCl_3$): δ 2.37 (s, 6H), 3.01 (dd, J=12.5 Hz, J=6.5 Hz, 1 H), 3.13 (dd, J=12.5 Hz, J=8.2 Hz, 1 H), 3.44 (dd, J=6.5 Hz, J=8.2 Hz, 1 H), 3.64 (s, 3 H), 7.36 (d, J=9.1 Hz, 2 H), 8.15 (d, J=9.1 Hz, 2 H). ^{13}C NMR ($CDCl_3$): 35.3, 41.7, 51.3, 68.7, 123.6, 130.0, 146.3, 146.7 and 171.2. m/z (+ESI) calculated for $C_{12}H_{17}N_2O_4^+$: 253.1188 found: 253.1189.

4b: To a mixture of 970 mg (3.0 mmol) of **1b** and 5 mL of dichloromethane was added 300 mg (3.0 mmol) of 40% KH in paraffin oil (washed with hexanes) at 25 °C. The reaction mixture was sonicated for 2 h at 25 °C. The mixture was partitioned between 25 mL of dichloromethane and 25 mL water. The organic layer was dried (K_2CO_3) and the volatiles were removed on a rotatory evaporator to afford 610 mg of crude **4b**. The crude mixture was chromatographed on silica gel using 25% ethyl acetate in hexanes as eluent to afford 507 mg (70%) of pure **4b**: ^{1}H NMR ($CDCl_3$): δ 2.38 (s, 6H), 2.90 (dd, J=13.3 Hz, J=5.9 Hz, 1 H), 3.01 (dd, J=13.3 Hz, J=9.4 Hz, 1 H), 3.39 (dd, J=5.9 Hz, J=9.4 Hz, 1 H), 3.61 (s, 3 H), 7.12 (d, J=8.4 Hz, 2 H), 7.23 (d, J=8.4 Hz, 2 H). ^{13}C NMR ($CDCl_3$): 35.0, 41.8, 51.2, 69.3, 128.5, 130.4, 132.3, 136.5 and 171.5. m/z (+ESI) calculated for $C_{12}H_{17}ClNO_2^+$: 242.0948 found: 242.0956.

4c: To a mixture of 710 mg (2.0 mmol) of **1c** and 2 mL of dichloromethane was added 300 mg (3.0 mmol) of 40% KH in paraffin oil (washed with hexanes) at 25 °C. The reaction mixture was sonicated for 2 h at 43 °C. The mixture was partitioned between 25 mL of dichloromethane and 25 mL water. The organic layer was dried (K_2CO_3) and the volatiles were

removed on a rotatory evaporator to afford 388 mg of crude mixture of **4c** and **5c**. The ratio of **4c** to **5c** was found to be 92:8 by ^{1}H-NMR analysis. The crude mixture was flash chromatographed on silica gel using 25% ethyl acetate in hexanes as eluent to afford 308 mg (56%) of pure **4c**: ^{1}H NMR ($CDCl_3$): δ 2.39 (s, 6H), 2.97 (dd, J=14.0 Hz, J=6.0 Hz, 1 H), 3.10 (dd, J=14.0 Hz, J=9.0 Hz, 1 H), 3.44 (dd, J=6.0 Hz, J=9.0 Hz, 1 H), 3.63 (s, 3 H), 7.31 (d, J=8.0 Hz, 2 H), 7.53 (d, J=8.0 Hz, 2 H). ^{13}C NMR ($CDCl_3$): 35.3, 41.6, 52.0, 68.9, 124.2 (J_{C-F}=272.3 Hz), 125.2 (J_{C-F}=3.9 Hz), 128.7 (J_{C-F}=32.5 Hz), 129.4, 142.5 and 171.4. m/z (+ESI) calculated for $C_{13}H_{17}F_3NO_2^+$: 276.1211 found: 276.1201.

4d: To a mixture of 580 mg (2.01 mmol) of **1d** and 5 mL of dichloromethane was added 240 mg (2.4 mmol) of 40% KH in paraffin oil (washed with hexanes) at room temperature. The reaction mixture was sonicated for 2 h at 25 °C, then the unreacted KH was quenched by slow addition of water at 0 °C. The mixture was partitioned between 50 mL of dichloromethane and 25 mL of water. The dichloromethane layer was washed with 25-mL portions of brine and dried over anhydrous potassium carbonate. The volatiles were removed on a rotatory evaporator to afford 390 mg of crude **4d**. The crude mixture was flash chromatographed on silica gel using 50% ethyl acetate in hexanes as eluent to afford 270 mg (65%) of pure **4d**: ^{1}H NMR ($CDCl_3$): δ 2.39 (s, 6H), 2.94 (dd, J=13.8 Hz, J=5.9 Hz, 1 H), 3.05 (dd, J=13.8 Hz, J=9.0 Hz, 1 H), 3.43 (dd, J=5.9 Hz, J=9.0 Hz, 1 H), 3.59 (s, 3 H), 7.19 (m, 3 H), 7.27 (m, 2H) ^{13}C NMR ($CDCl_3$): 35.8, 41.9, 51.0, 69.6, 126.4, 128.4, 129.1, 138.2 and 171.9. m/z (+ESI) calculated for $C_{12}H_{18}NO_2^+$: 208.1338 found: 208.1332.

4e: To a mixture 625 mg (2.00 mmol) of **1e** and 2 mL of dichloromethane was added 200 mg (2.00 mmol) of KH in paraffin oil (hexanes washed). The mixture was sonicated for 3 h at room temperature, then added to 50 mL of dichloromethane. The organic layer was washed with two 25-mL portions of water and dried with anhydrous potassium carbonate. The volatiles were removed on a rotatory evaporator to afford 375 mg of a crude mixture of **4e** and **5e**. The ratio of **4e** to **5e** was determined to be 95:5 by ^{1}H NMR analysis. The crude product was flash chromatographed on silica gel using 50% ethyl acetate in hexanes as eluent to afford 265 mg (57%) of **4e**: ^{1}H NMR ($CDCl_3$): δ 2.37 (s, 6H), 2.97 (dd, J=13.5 Hz, J=6.6 Hz, 1 H), 3.09 (dd, J=13.5 Hz, J=8.9 Hz, 1 H), 3.42 (dd, J=6.6 Hz, J=8.9 Hz, 1 H), 3.64 (s, 3 H), 7.31 (d, J=8.3 Hz, 2 H), 7.57 (d, J=8.3 Hz, 2 H). ^{13}C NMR ($CDCl_3$): 35.6, 41.7, 51.2, 68.7, 110.4, 118.9, 129.9, 132.1, 144.1 and 171.3. m/z (+ESI) calculated for $C_{13}H_{17}N_2O_2^+$: 233.1290 found: 233.1279.

Product Distribution, Rate Observations, and Control Experiments

The [2,3] / [1,2] product distributions were generally determined in small-scale exploratory reactions. Example procedure: To a mixture of 1 mL of dichloromethane and 167 mg (0.50 mmol) of **1a** was added 75 mg (0.49 mmol) of DBU was added at 25 °C. The reaction was stirred for 1 h, then partitioned between 5 mL of ether and 5 mL of water. The ether layer was then washed with two 5-mL portions of water and dried with anhydrous potassium carbonate. Then volatiles were removed on a rotatory evaporator. The relative ratio of **4a** and **5a** was found to be 6:94 by comparing the relative integration of the $-OCH_3$ groups of **4a** [$-OCH_3$, 3.64 (s, 3 H)] and **5a** [$-OCH_3$, 3.72 (s, 3 H)] in the ^{1}H-NMR.

The product ratios did not change with time. In a control experiment to test the limits of this statement, a 1:2 mixture of **4d** and **5d** was heated at 85 °C for 20 h in acetonitrile in presence of DBU. The proportion of **4d** to **5d** was unaltered based on ^{1}H-NMR analysis.

Due to the rapidity of many of the reactions, no detailed kinetics experiments were undertaken. However, qualitative observations are consistent with a strong role of hydrogen

bonding in increasing the barrier for reaction of the ylide.

Reactions using alkoxide or hydride bases were complete when first checked. In an attempt to observe the rate of one of these reactions, a solution of 332 mg (1.00 mmol) of **1a** and 21 mg (0.15 mmol) of 1,4-dimethoxybenzene (internal standard) was prepared at 25 °C in 2 mL of d_6-DMSO. The mixture was made homogenous by sonication, and the ratio of **1a** to 1,4-dimethoxybenzene was found to be 50:7 by comparing the relative integration of aromatic protons of **1a** [8.34 (d, J=8.6 Hz, 2 H)] and 1,4-dimethoxybenzene [6.85 (s, 4 H)] in ^{1}H-NMR. To this mixture was added 2 mL of a 0.5 M solution of potassium methoxide in d_6-DMSO, and the ^{1}H NMR was taken immediately (≈1 min). No peak associated with **1a** could be detected. The conversion of **1a** to **4a** was determined by integrating aromatic peaks of **4a** and 1,4-dimethoxybenzene. The conversion of **1a** to **4a** was found to be 66%.

In contrast to reactions of naked ylides, reactions in methanol were very slow. In an exploratory reaction, a solution of 835 mg (2.51 mmol) of **1a** and 28 mg (0.20 mmol) of 1,4-dimethoxybenzene was prepared in 3 mL of methanol, and the mixture was made homogenous by sonication. Then 300 mg (5.55 mmol) of sodium methoxide was added to the mixture and was it was stirred for 14 h at 25 °C. A 1-mL aliquot of the reaction mixture was quenched with 5 mL of water and the organics were extracted in 5 mL of ether. The ether layer was dried over anhydrous potassium carbonate and the volatiles were removed on a rotatory evaporator. ^{1}H-NMR analysis was done on the residue. The conversion of **1a** to **4a** and **5a** was determined by integrating $-OCH_3$ peaks of **4a**, **5a** and 1,4-dimethoxybenzene. The conversion of **1a** to **4a** and **5a** was found to be 21% and the ratio of **4a** to **5a** was found to be 1:3.

From these observations, the reaction in methanol was at least three orders of magnitude slower than the reaction in DMSO.

The reactions mediated by DBU in non-polar solvents are not homogeneous, but they are certainly much faster than the reactions in methanol. The reaction of **5a** is complete in high yield with a reaction time of 1 h.

Effects of Varying the Amount of Base and of Ultraviolet Irradiation

Substoichiometric DBU in Dichloromethane. To a mixture of 171 mg (0.51 mmol) of **1a** and 1 mL of dichloromethane at 25 °C was added 37 mg (0.24 mmol) of DBU. The mixture was stirred for 15 min and was analyzed directly by ^{1}H-NMR. The ratio of **4a** to **5a** was found to be 6:94 by ^{1}H-NMR analysis.

Excess DBU in Dichloromethane. To a mixture of 159 mg (1.04 mmol) of DBU and 4 mL of dichloromethane at 25 °C was added 151 mg (0.45 mmol) of **1a**. The mixture was stirred for 15 minutes and was analyzed directly by ^{1}H-NMR. The ratio of **4a** to **5a** was found to be 9:91 by ^{1}H-NMR analysis.

It is uncertain whether the small product ratio difference between the two reactions above is a real effect, but it should be noted that the direction of the change is opposite that expected for DBU catalysis of rearomatization.

Excess DBU in DMSO. To a mixture of 2 mL of DMSO and 211 mg (1.39 mmol) of DBU was added 162 mg (0.49 mmol) of **1a** at 25 °C. The mixture was stirred for 5 min, and then partitioned between 5 mL of ether and 5 mL of water. The ether layer was then washed with two 5-mL portions of water and dried with anhydrous potassium carbonate. Then volatiles were removed on a rotatory evaporator. The relative ratio of **4a** and **5a** was found to be 66:34 by ^{1}H-NMR analysis of the residue.

In a duplicate reaction (with excess DBU) the product ratio was determined directly from the reaction mixture. The ratio of **4a** to **5a** was found to be 62:38 by ^{1}H-NMR analysis.

Substoichiometric DBU in DMSO. During the measurement of intramolecular kinetic isotope effect below the reaction was carried out using 36 mol % of DBU versus **1a** in DMSO. The ratio of **4a** to **5a** was found to be 67:33.

Excess NaOMe in DMSO. To a mixture of 1 mL of DMSO and 59 mg (1.09 mmol) of NaOMe was added 148 mg (0.44 mmol) of **1a** at 25 °C. The reaction mixture was stirred for 5 min, and then partitioned between 5 mL of ether and 5 mL of water. The ether layer was then washed with two 5-mL portions of water and dried with anhydrous potassium carbonate. Then volatiles were removed on a rotatory evaporator. ^{1}H-NMR analysis on the residue showed exclusive formation of **4a**.

Excess NaOMe in MeOH. For a procedure using 2.2 equiv of NaOMe, see above. The ratio of **4a** to **5a** was found to be 25:75.

Stoichiometric NaOMe in MeOH. To a mixture of 162 (0.49 mmol) mg of **1a** and 2 mL of methanol was added 0.35 mL (0.56 mmol) of a 1.6 M sodium methoxide solution in methanol. The reaction mixture was stirred for 1 h, and then partitioned between 5 mL of dichloromethane and 5 mL of water. The ether layer was then washed with two 5-mL portions of water and dried with anhydrous potassium carbonate. Then volatiles were removed on a rotatory evaporator. The ratio of **4a** to **5a** was found to be 25:75 by ^{1}H-NMR analysis.

Excess DBU in Dichloromethane with UV-Irradiation. To a mixture of 136 mg (0.89 mmol) of DBU and 1 mL of dichloromethane at 25 °C was added 168 mg (0.50 mmol) of **1a**. The mixture was stirred and irradiated with a UV-light (λ_{max}=350 nm) through the sidewall of a borosilicate flask using a Rayonet photochemical reactor for 15 min. The reaction mixture was directly analyzed and the ratio of **4a** to **5a** was found to be 5:95 by ^{1}H-NMR analysis .

Substoichiometric DBU in Dichloromethane with UV-Irradiation. To a mixture of 175 mg (0.53 mmol) of **1a** and 1 mL of dichloromethane at 25 °C was added 65 mg (0.43 mmol) of DBU. The mixture was stirred and irradiated with a UV-light (λ_{max}=350 nm) through the sidewall of a borosilicate flask using Rayonet photochemical reactor for 15 min. The reaction mixture was analyzed and the ratio of **4a** to **5a** was found to be 6:94 by ^{1}H-NMR analysis.

Crossover Experiment and Related Procedures

Benzyl bromide-d_7 was synthesized from toluene-d_8 and NBS (N-bromosuccinimide) following a method previously reported. (Meddour, A.; Courtieu, J. *Tetrahedron: Asymmetry* **2000**, *11*, 3635-3644.)

1d-D$_{13}$: To a mixture of 920 mg (10.5 mmol) of bis(methyl-d_3)amine hydrogen chloride, 2 mL of water, and 600 mg (15 mmol) of ground sodium hydroxide at 0 °C was added a solution of 850 mg (4.77 mmol) of benzyl bromide-d_7 in 5 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 288 mg (41%) of crude *N*,*N*-bis(methyl-d_3) benzyl-d_7-amine, which was used in the next step without further purification.

To a mixture of 288 mg (1.94 mmol) of *N*,*N*-bis(methyl-d_3) benzyl-d_7-amine and 5 mL ether (dried over sodium followed by distilled under nitrogen), 425 mg (2.78 mmol) of methyl bromoacetate was added at 25 °C. The mixture was stirred for 24 h. During stirring solid

precipitated out. The solid was then was with three 10-mL portions of ether. The residual ether was removed on a rotatory evaporator to afford 360 mg (61%) of 1d-d_{13}. The identity of the species was confirmed by comparing its ^{1}H-NMR with the non-deuterated sample. ^{1}H NMR ($CDCl_3$): 3.78 (s, 3H), 5.07 (s, 2 H).

Crossover Experiment: To a mixture of 306 mg (1.06 mmol) of **1d**, 350 mg (1.16 mmol) of **1d-D_{13}**, and 4 mL of acetonitrile under N_2 at 80 °C was added 3.66 g (24.04 mmol) of DBU. The stirring of the reaction mixture continued for additional 1 h at 80 °C. After cooling to 25 °C the reaction mixture was partitioned between 50 mL of ether and 25 mL of water. The ether layer was washed with five 25-mL portions of water and dried (anhydrous potassium carbonate), and the volatiles were removed on a rotary evaporator to afford 252 mg of mixture of **4d** and **5d**. The ratio of **4d** to **5d** was found to be 3:1 by ^{1}H-NMR analysis. The residue was flash chromatographed on silica gel using 50% ethyl acetate in hexanes as eluent, and the separated components **4d** and **5d** were characterized by ^{1}H-NMR and ESI-MS. In each case the extent of crossover was based on the sum of the peak intensities at M=214 and M=215 to sum of intensities at M=208, M=214, M=215 and M=221 peaks. The extent of crossover in **4d** and **5d** was found to be 13.66% and 1.07% (averaging two measurements) respectively.

Table 1. Raw crossover results and calculated percentage crossover.

	Peak Intensites				Extent of
Sample	208	214	215	221	Crossover
5d	2849.652	47.7946	23.3482	2238.821	1.38
5d, second sample	2747.702	23.7895	10.00	1646.544	0.76
4d	1462.328	429.0259	229.319	2699.853	13.66

The reaction of a mixture of **1d** and **1d-D_{13}** was also used to look for an H/D isotope effect on the product ratio. A crude product mixture from a reaction of **1d** / **1d-D_{13}** was analyzed by ^{1}H NMR. For the [1,2] product **4d**, the relative integrations of the methyl ester, the methine proton, and the methylene group were 288.27, 106.84, and 140.77, respectively. From these numbers, the deuteration in **4d** was either 27% based on the methyl ester or 34% based on the methine, averaging to 30.5%. For the [2,3] product **5d**, the relative integrations of the methyl ester, the aromatic methyl group and the NMe_2 were 100, 71.68, and 141.51, respectively. From these numbers, the deuteration in **5d** was 28% based on the aromatic methyl and 29% based on the NMe_2. The deuteration of **4d** versus **5d** was judged to be equivalent within the limits of the experiment.

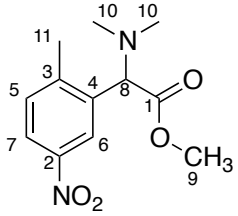
Intramolecular KIE Determination

Sample 1. To a mixture of 10.00 g (30.1 mmol) of **1a** and 60 mL of DMSO (dried over 4 Å molecular sieves) under N_2 at 25 °C was added 1.63 g (10.7 mmol) of DBU. The reaction was stirred for 3 h, then partitioned between 50 mL of ether and 25 mL of water. The ether layer was washed with three 25-mL portions of water, dried (K_2CO_3), and the volatiles were removed on a rotatory evaporator to afford 1.89 g (25%) of mixture of **4a** and **5a**. The ratio of the [2,3] product **5a** and the [1,2] product **4a** was determined to be approximately 4:9 by ^{1}H-NMR analysis. The isomers were separated by column chromatography on silica gel using 30% ethyl acetate in hexanes as eluent to afford 470 mg (6.1%) of **5a**.

Sample 2. In a procedure closely analogous to that for Sample 1, 13.13 g (39.43mmol) of **1a**, 70 mL of DMSO and 2.00 g (13.17 mmol) of DBU were employed and the isolated amount of **5a** was 510 mg.

NMR Measurements. All NMR samples consisted of approximately 400 mg of **5a** 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 and calibrated $\pi/2$ pulses. For Sample 1, 37 s delays and an 8 s acquisition time was employed to collect 512820 points. For Sample 2, 41.1 s delays and an 5 s acquisition time was employed to collect 320512 points. Six spectra were recorded for each sample. The integrations were obtained numerically by 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.

Peak Assignments. The ^{13}C NMR signals for **5a** were assigned as shown below based on DEPT-135 and HMBC spectrum. The numbers refer to the order of the peaks from high field to low field in the spectrum.



NMR Results and Calculation of KIEs. For the integrations of the peaks for carbon 4 versus carbon 5, the integration of carbon 5 was set to 1000 and the integration of carbon 4 was recorded. The raw results are shown in the first section of the tables below.

A complication in the raw results for carbon 4 versus carbon 5 is that carbon 5 is subject to two ^{13}C-^{13}C couplings leading to satellites not included in the integration range, while carbon 4 is subject to three such couplings. As a result, the integration of carbon 4 is diminished by the natural abundance of ^{13}C at the additional. To allow for this, the integrations at carbon 4 were adjusted by the 0.0107(8) natural abundance of ^{13}C. The second section of the first table below shows the adjusted results.

The isotope effects were then calculated as 1000 divided by the integration, the results were averaged, and 95% confidence ranges were calculated in a standard way. (See: http://www.iupac.org/publications/analytical_compendium/Cha02sec3.pdf.)

Table of Results for Carbon 4, Setting Carbon 5 at 1000, and KIEs

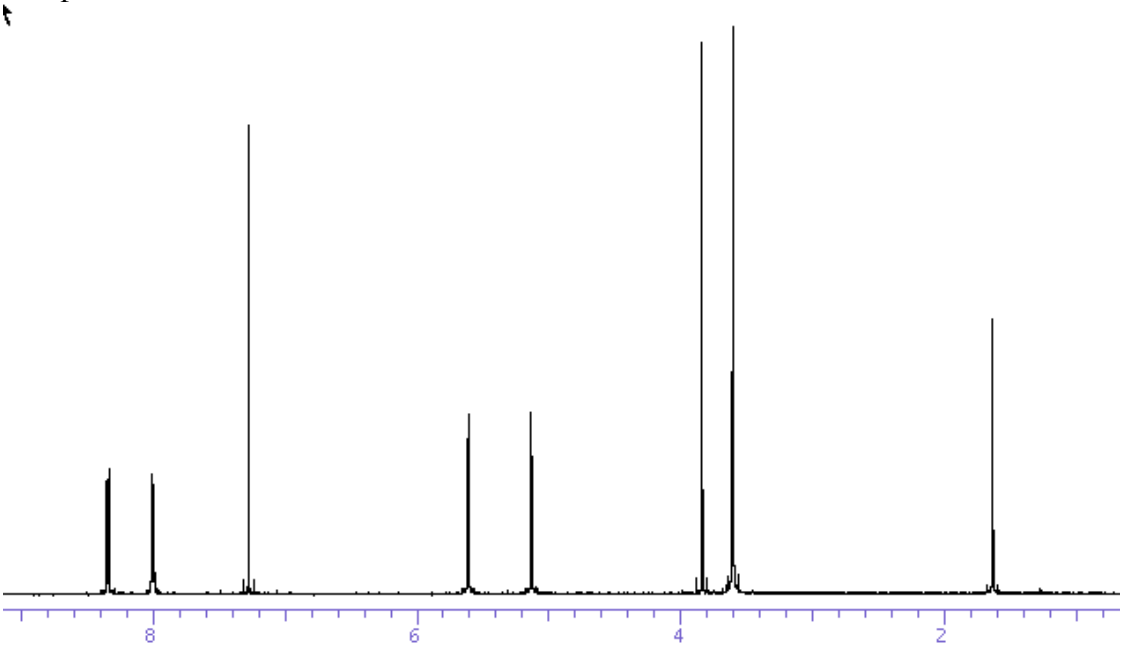
Raw Integrations		Adjusted for Satellites	
Sample 1	Sample 2	Sample 1	Sample 2
984.836	985.207	995.49	995.86
984.214	983.773	994.86	994.41
986.437	981.441	997.11	992.06
988.788	986.867	999.48	997.54
983.769	983.564	994.41	994.20
983.66	978.353	994.30	988.93
		Average	
		995.94	993.83
		standard deviation	
		2.0	3.0
		95% confidence	
		2.1	3.2

KIE	
Sample 1	Sample 2
1.004	1.006
Uncertainty	
0.002	0.003

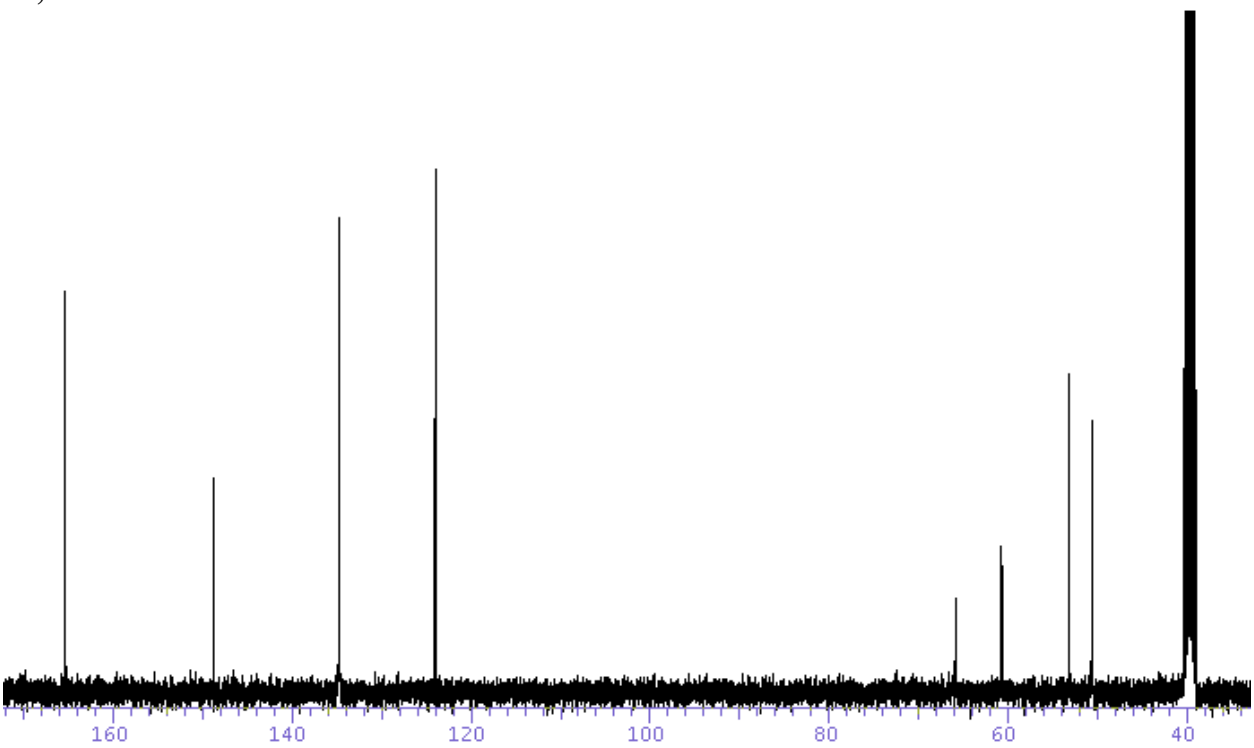
NMR Spectra of New Compounds

1a, ^{1}H NMR

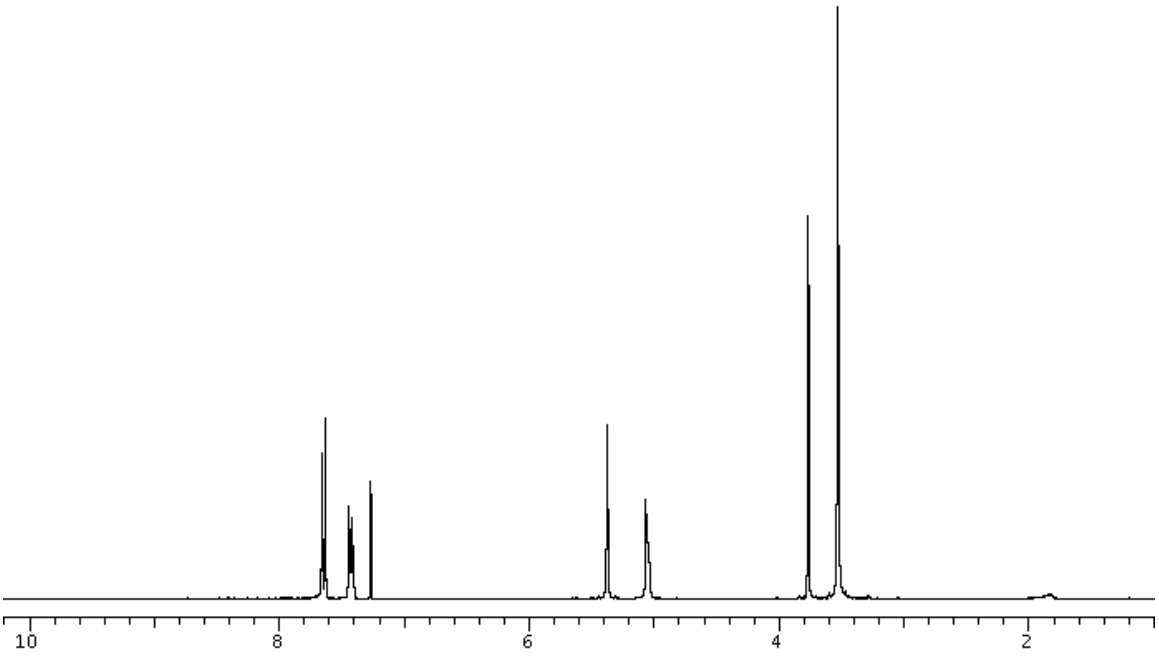
The peak at δ 1.8 is water.



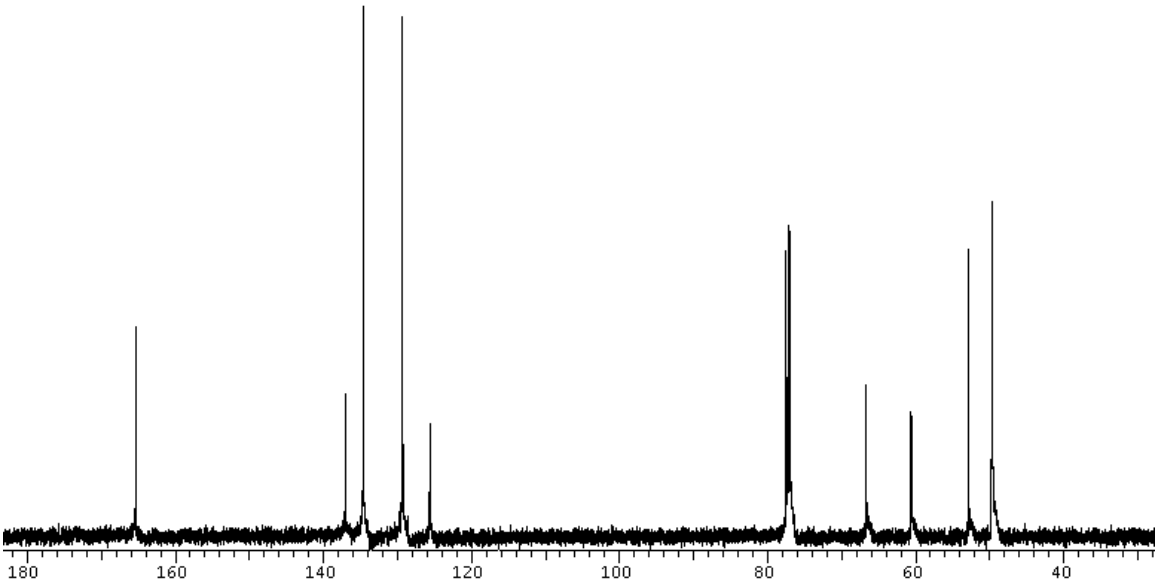
1a, ^{13}C NMR



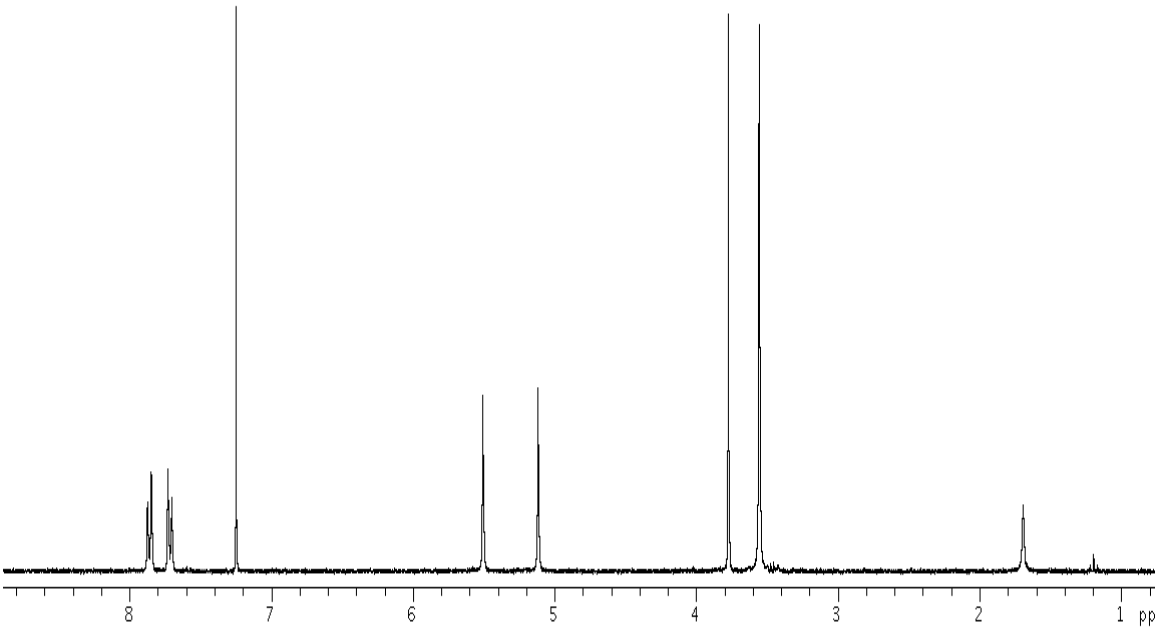
1b, ^{1}H NMR



1b, ^{13}C NMR



1c, ^{1}H NMR



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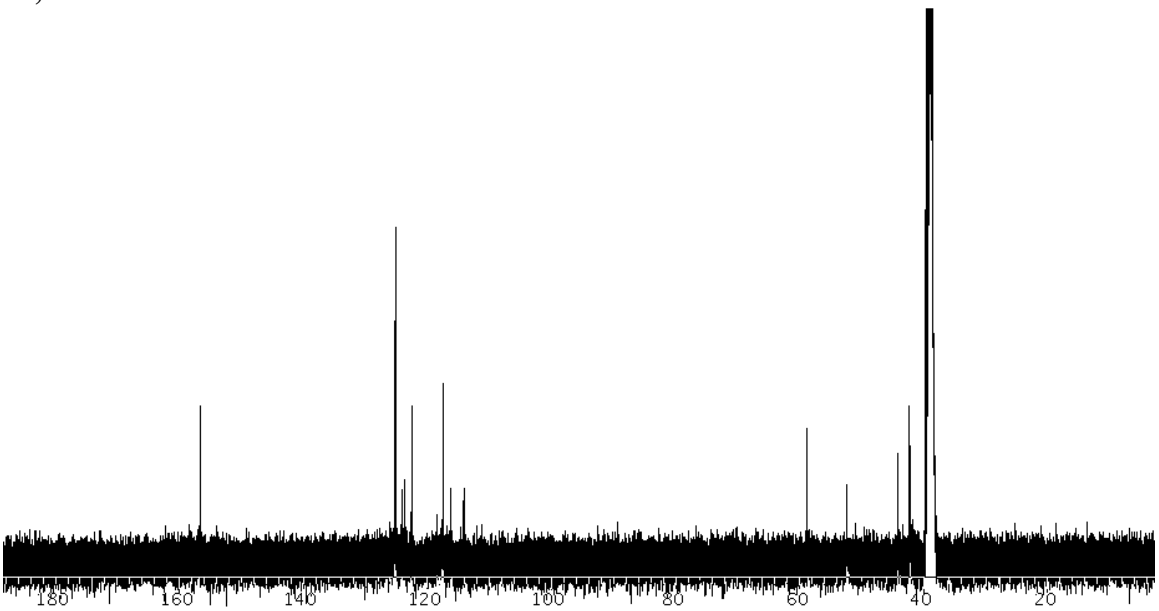

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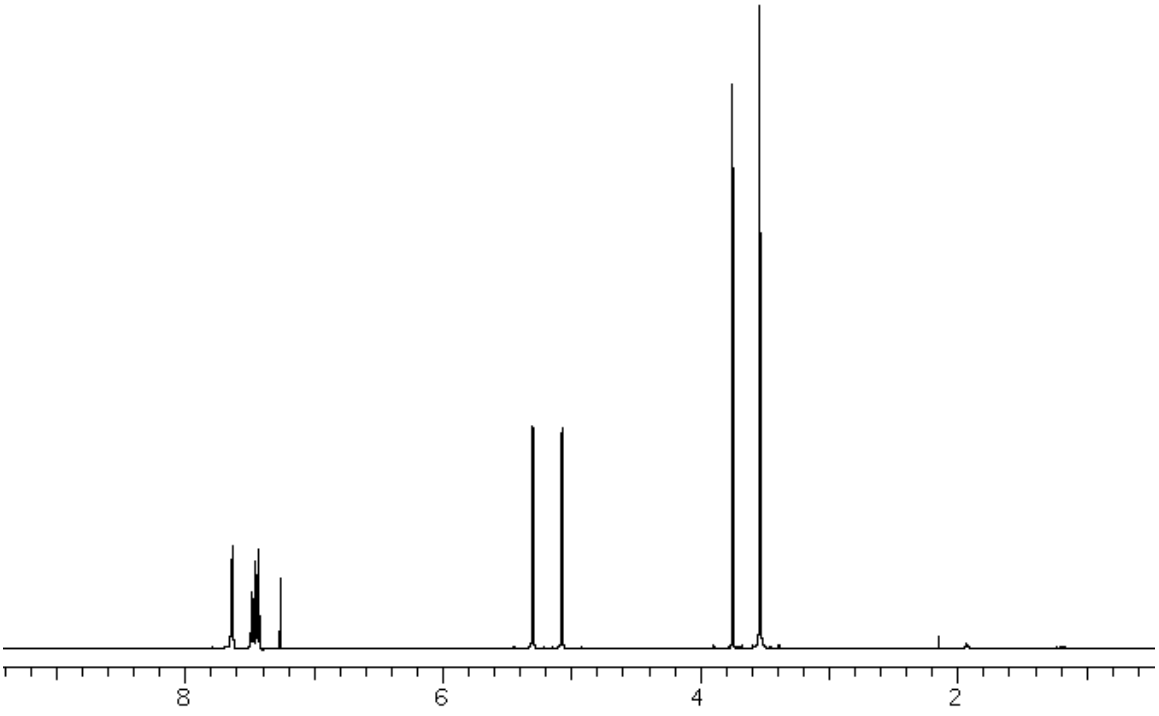

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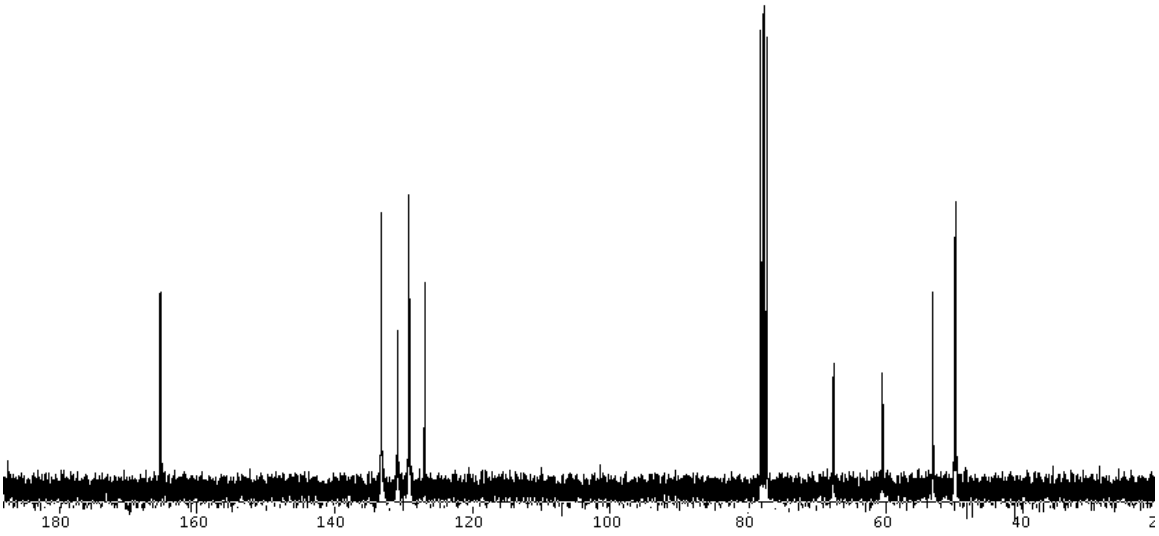

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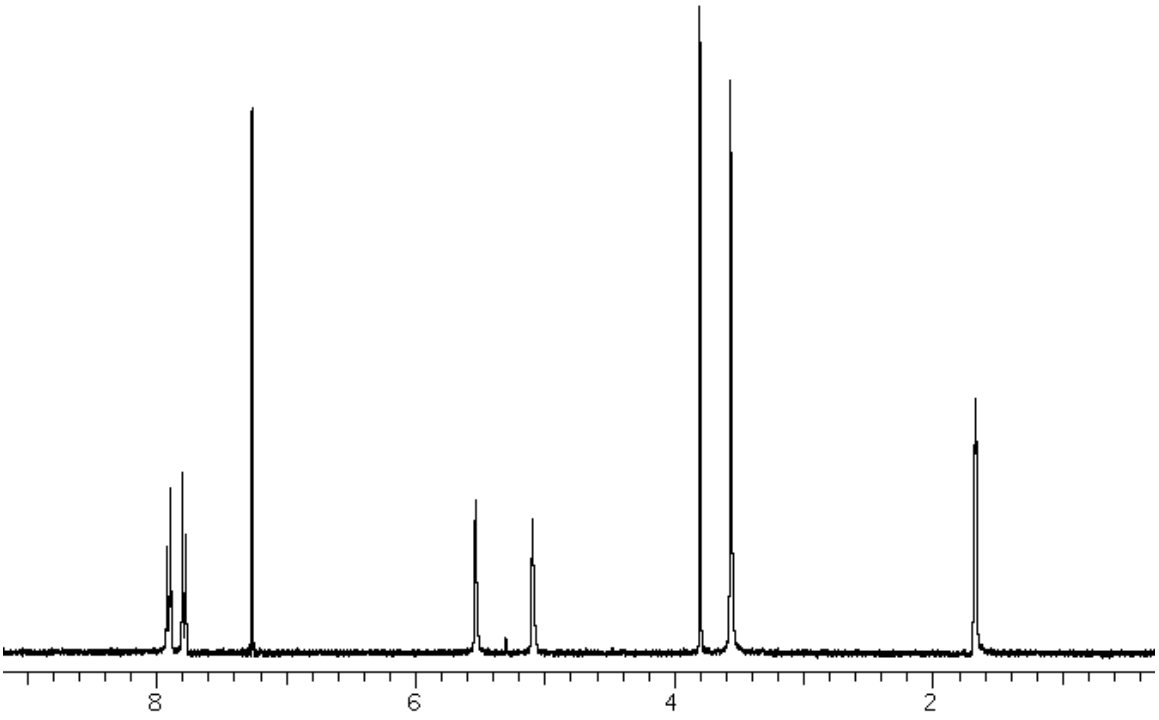

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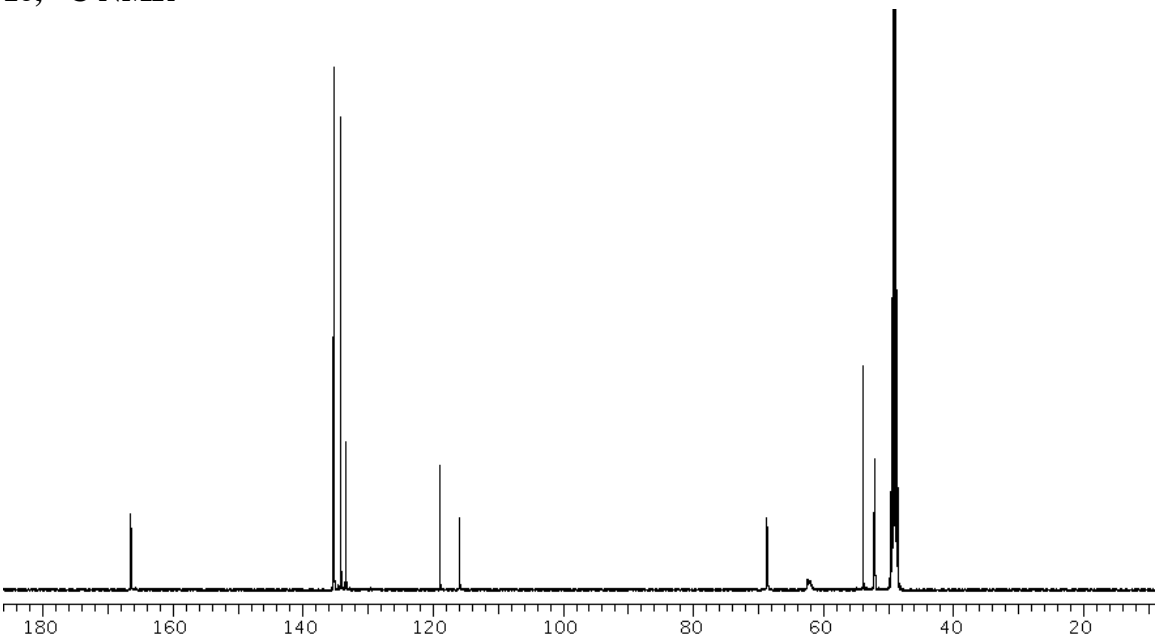
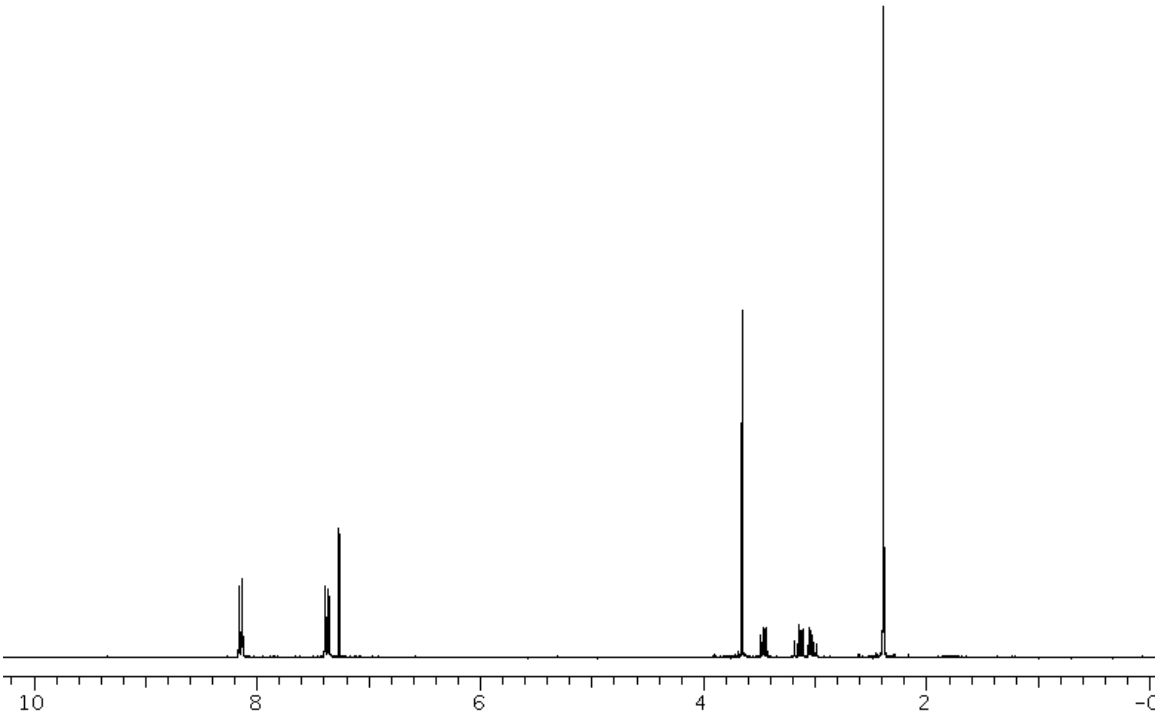
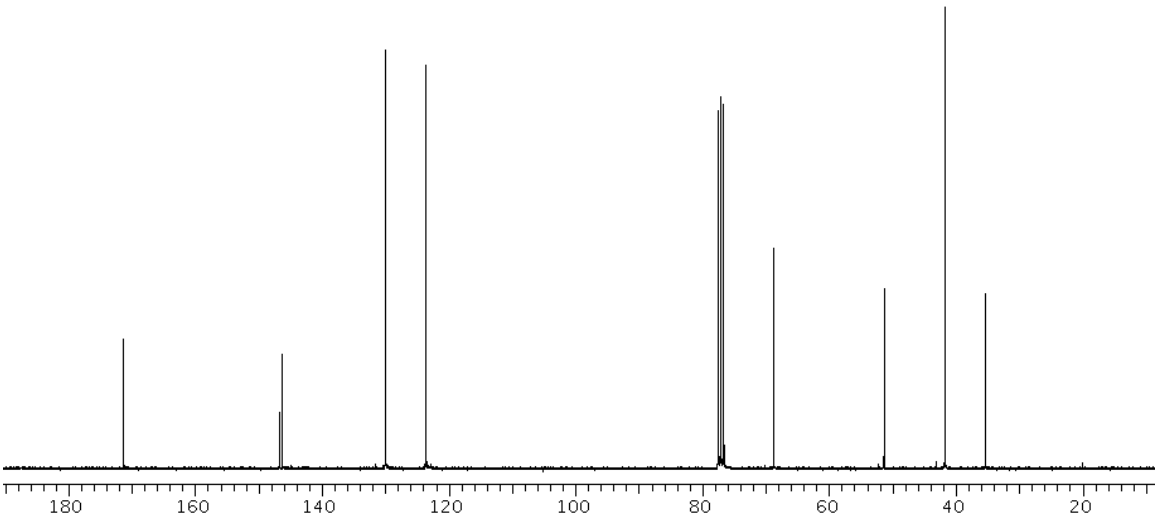


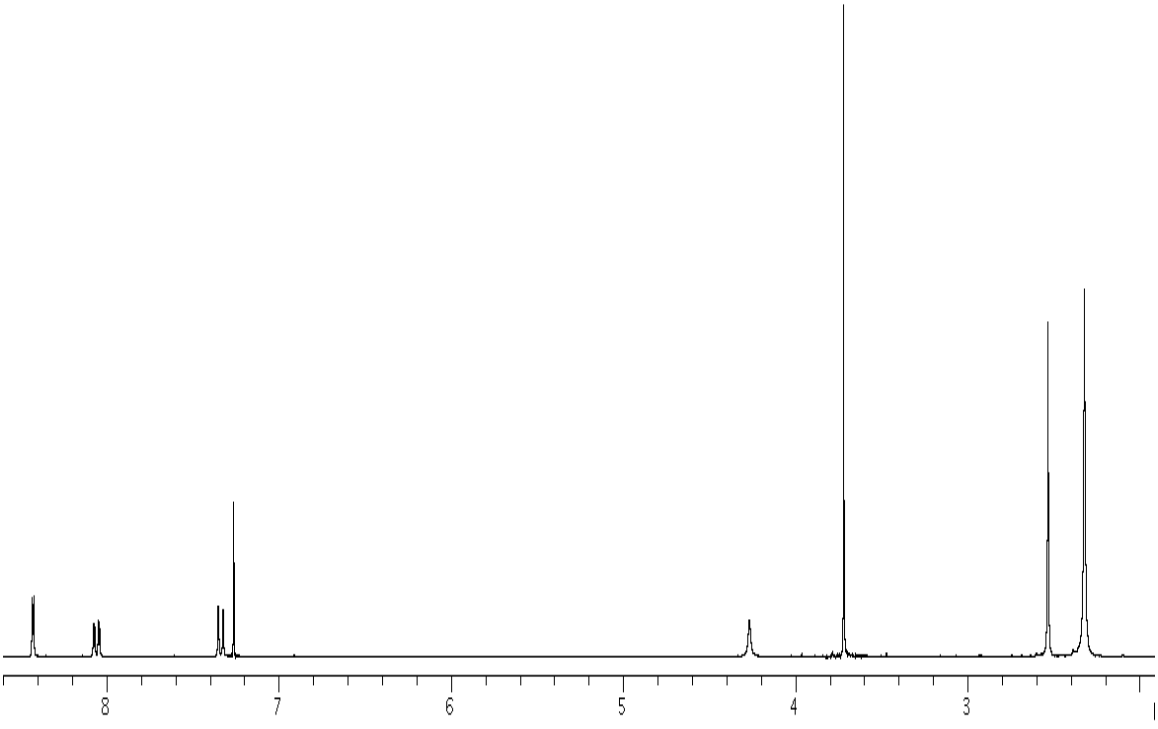
4a, ^{1}H NMR



4a, ^{13}C NMR



5a, ^{1}H NMR



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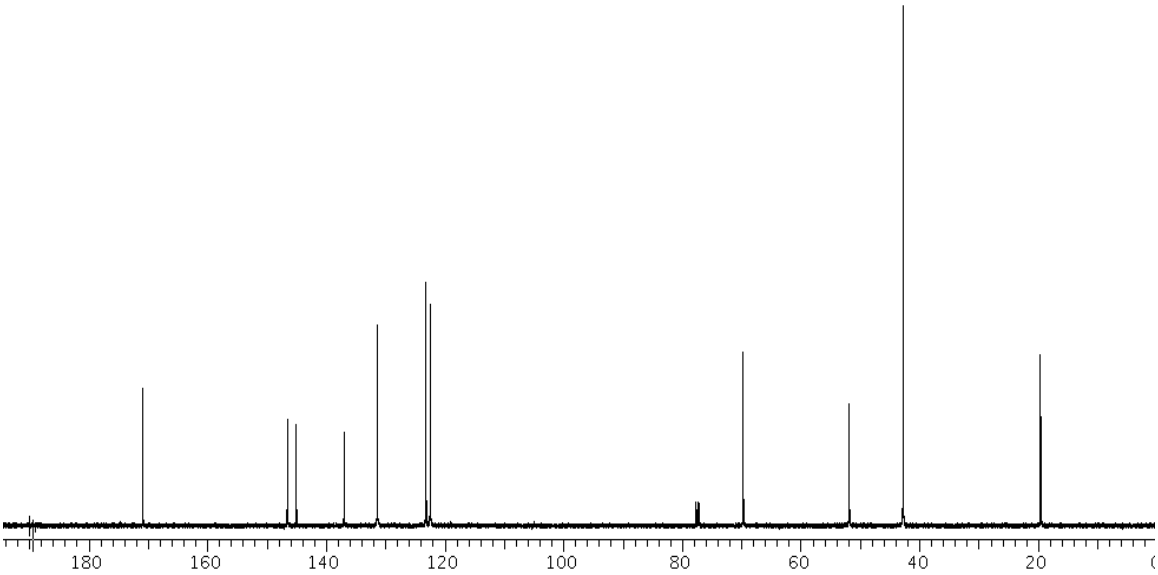
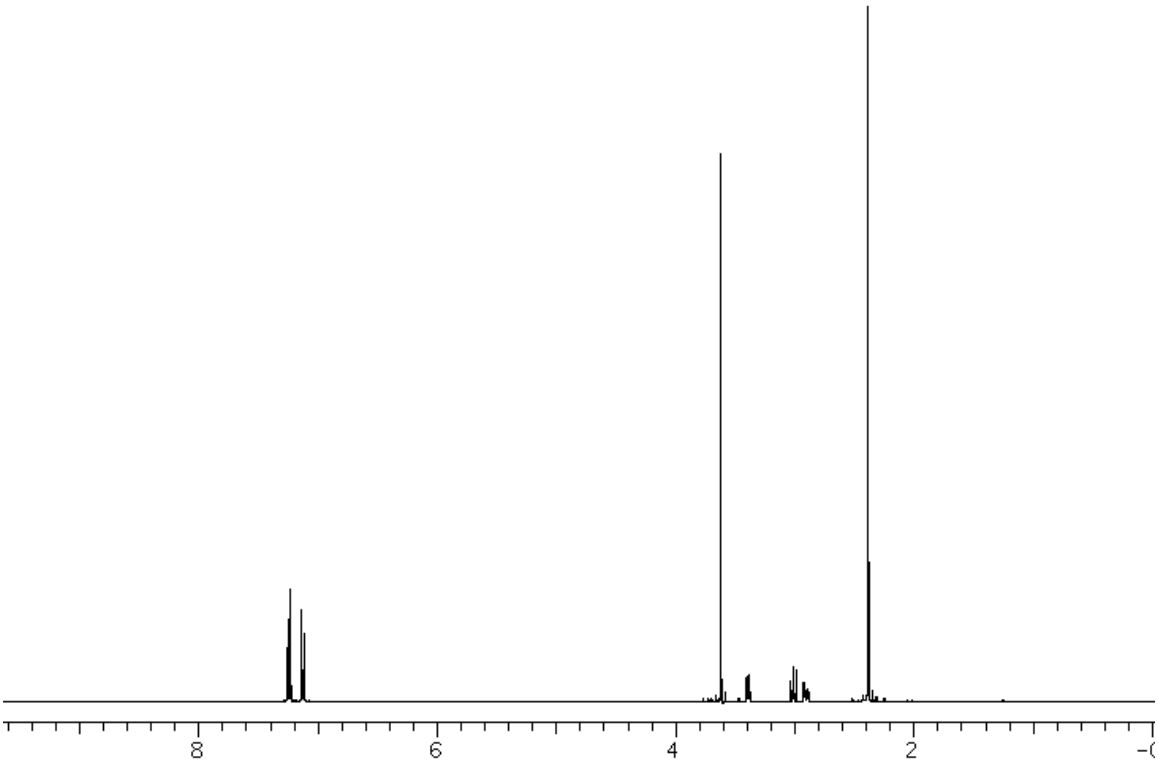


4b, ^{1}H NMR



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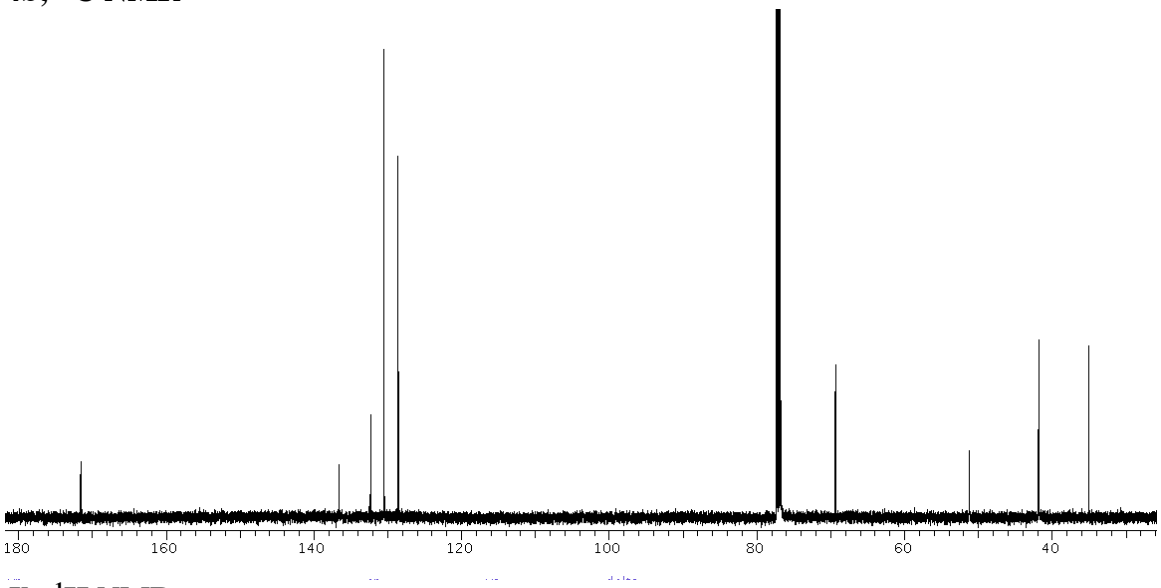

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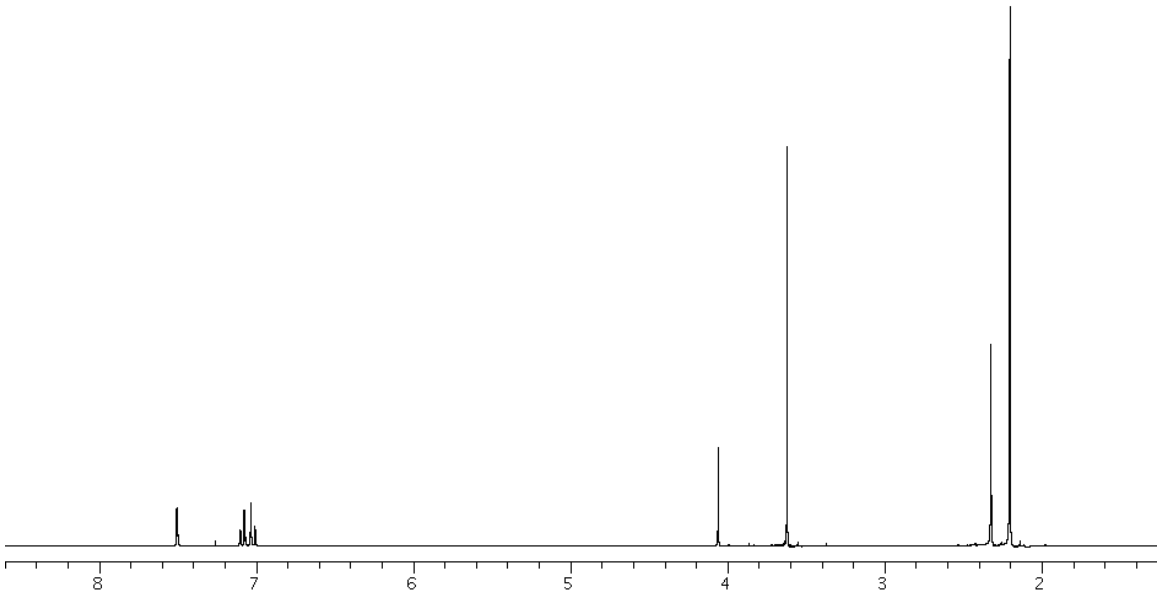

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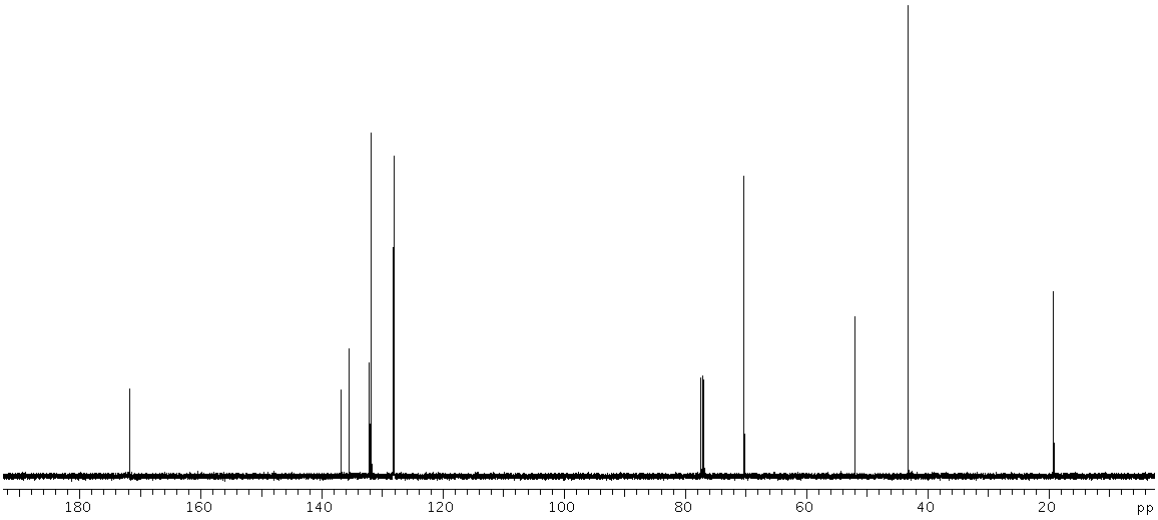

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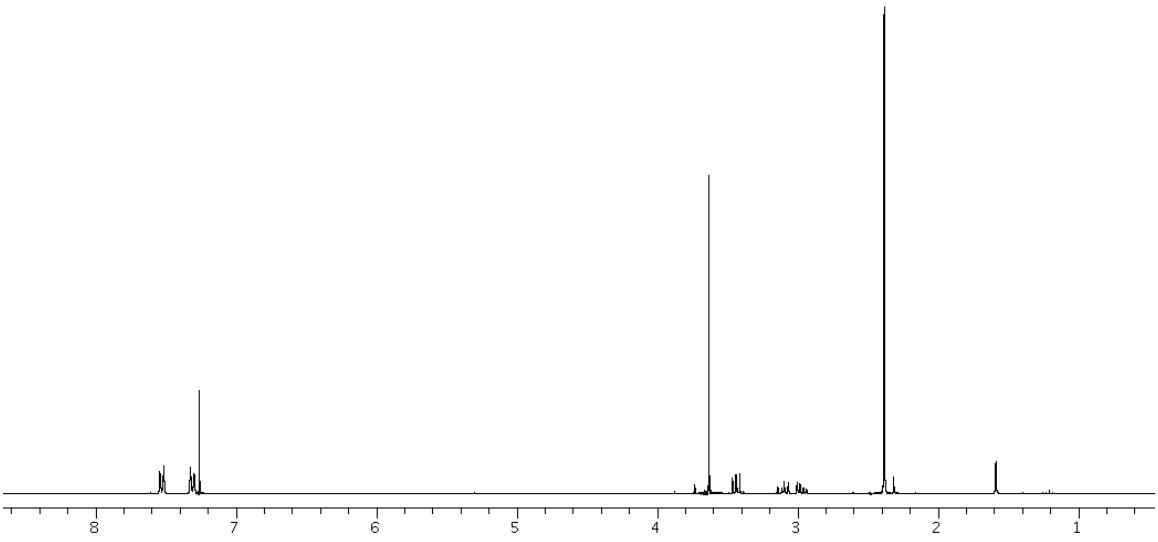

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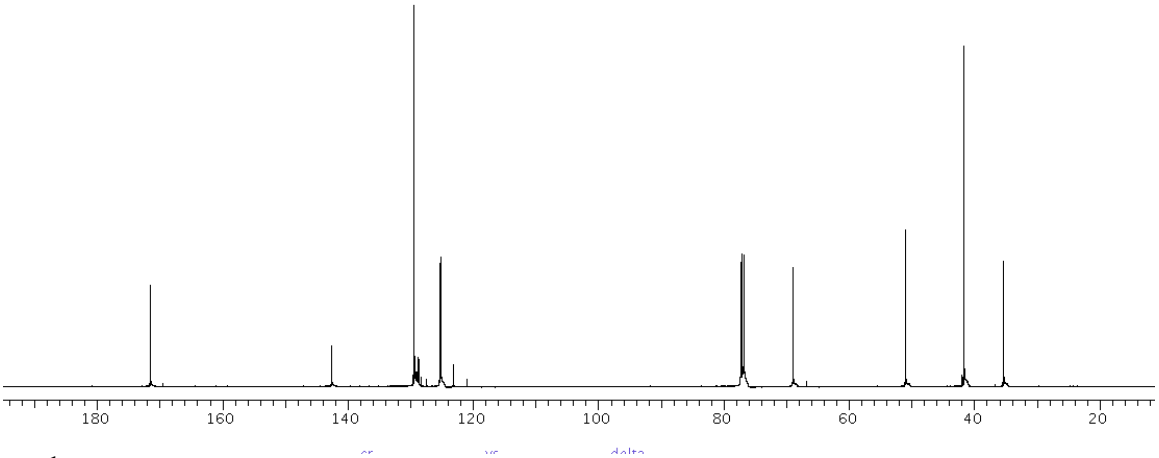

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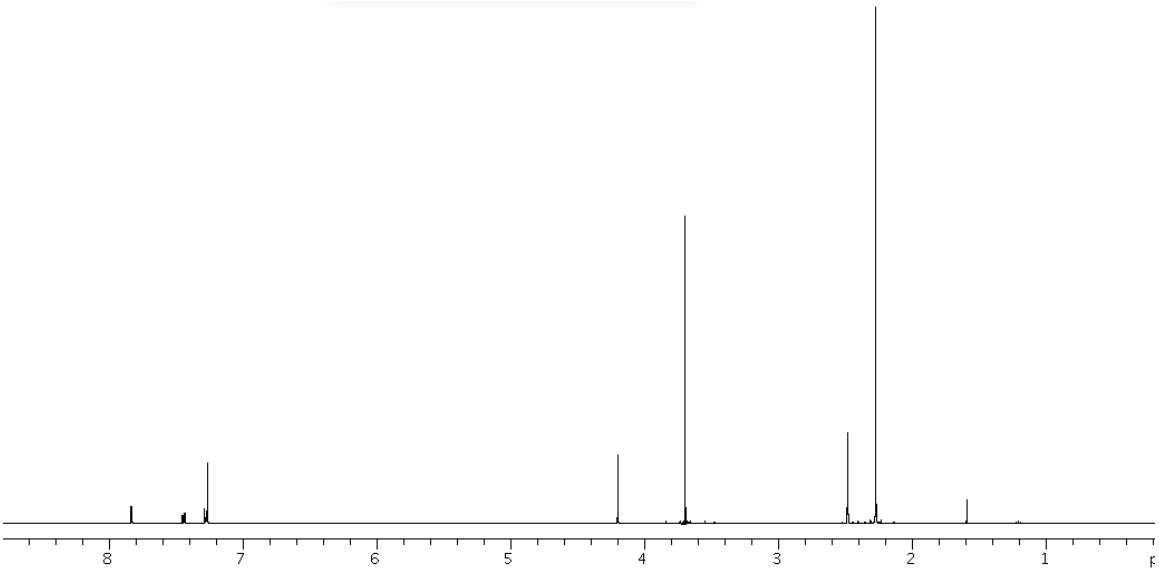

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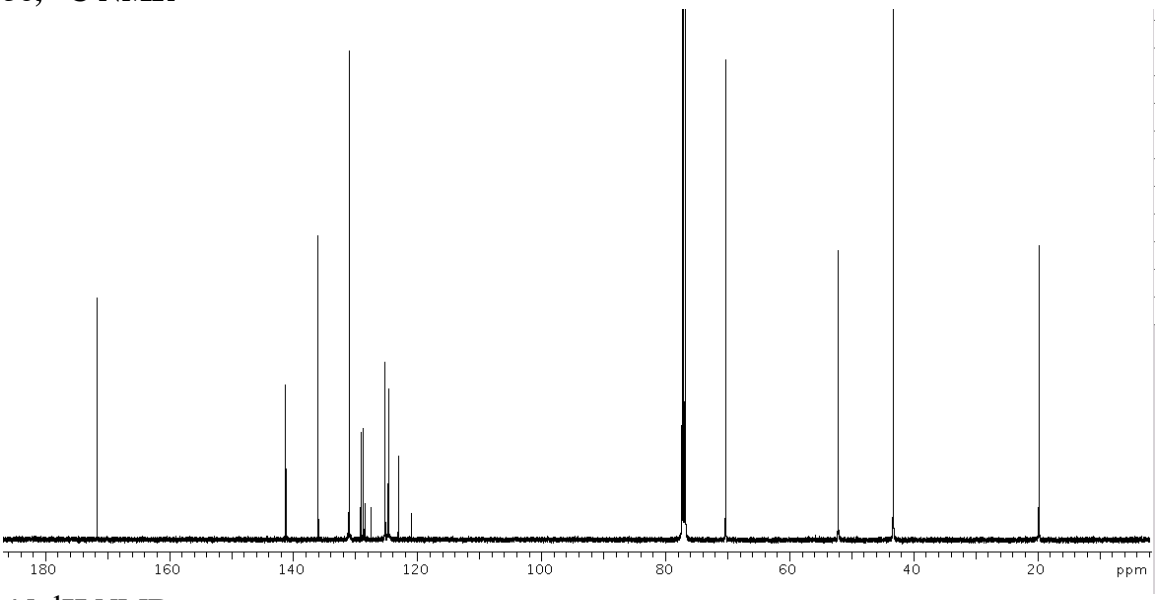

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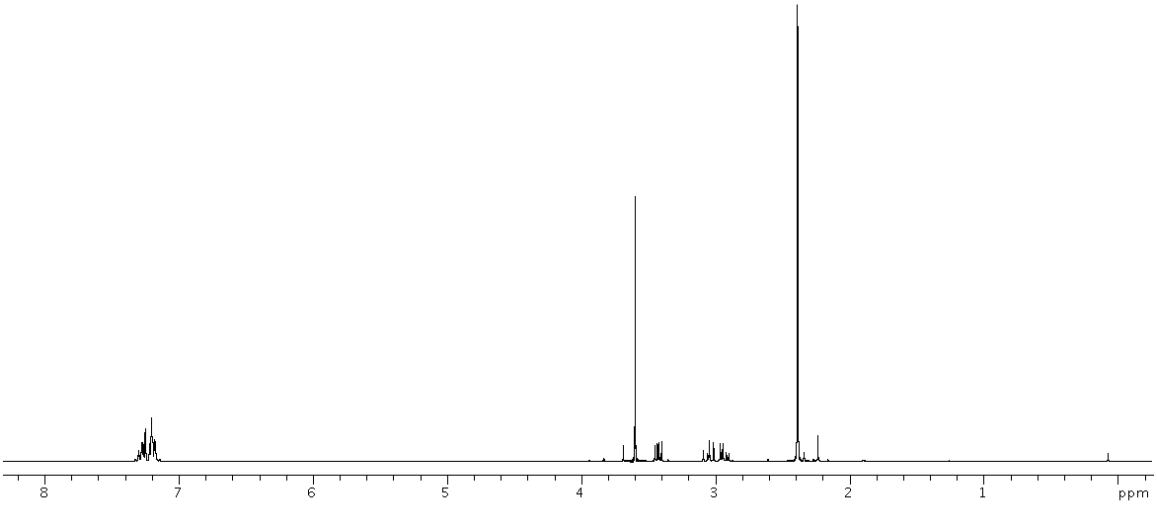

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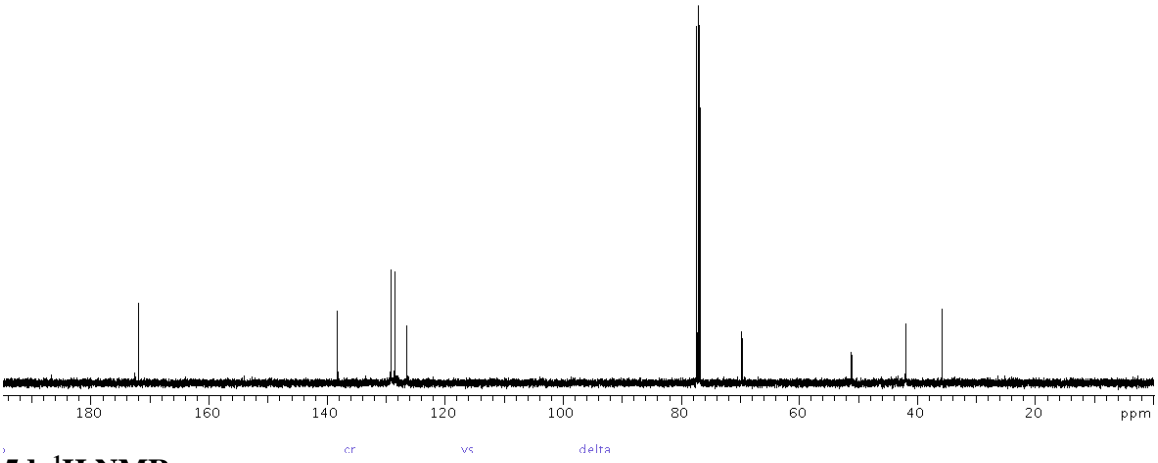

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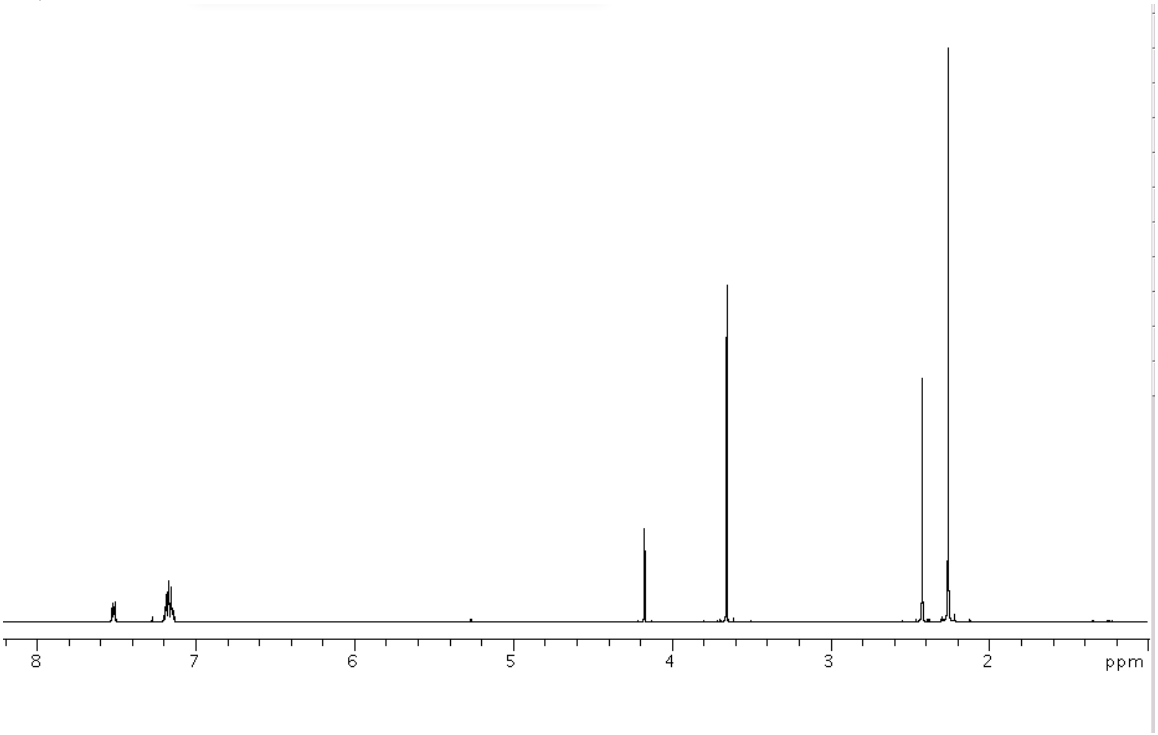

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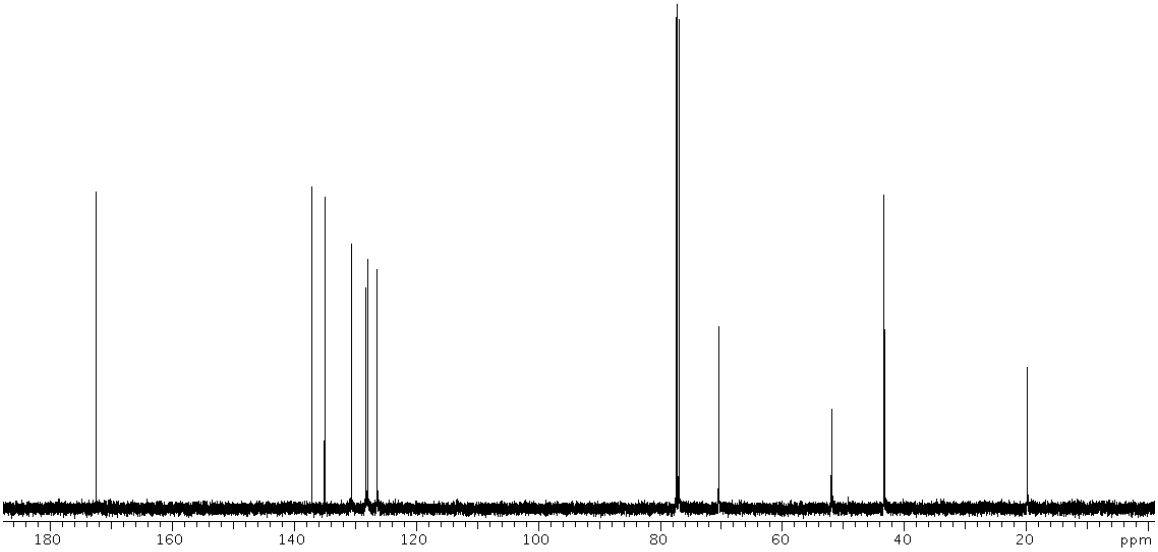

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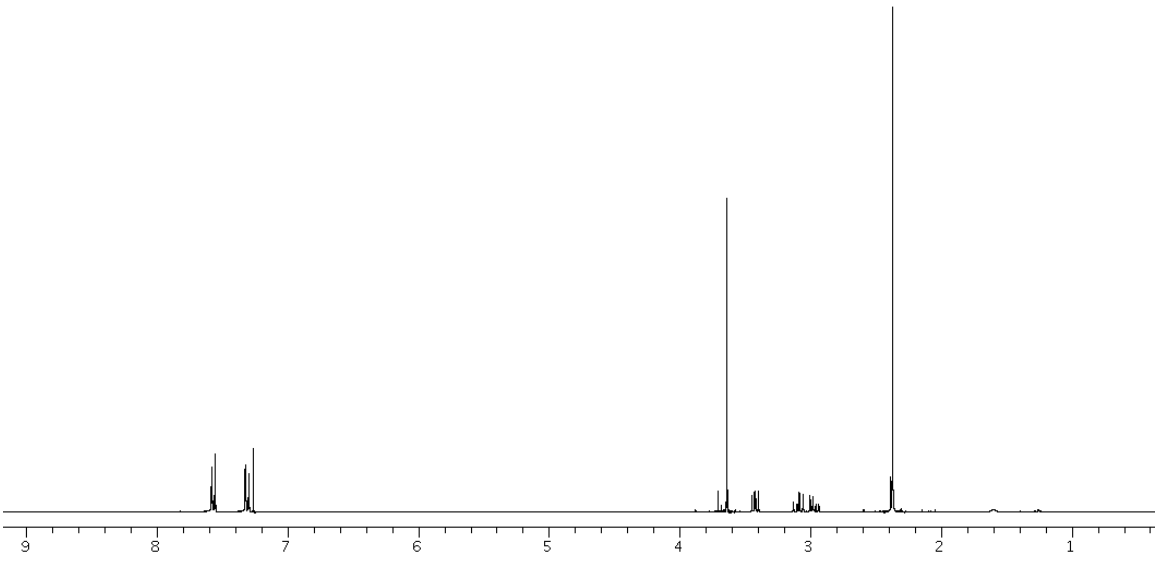

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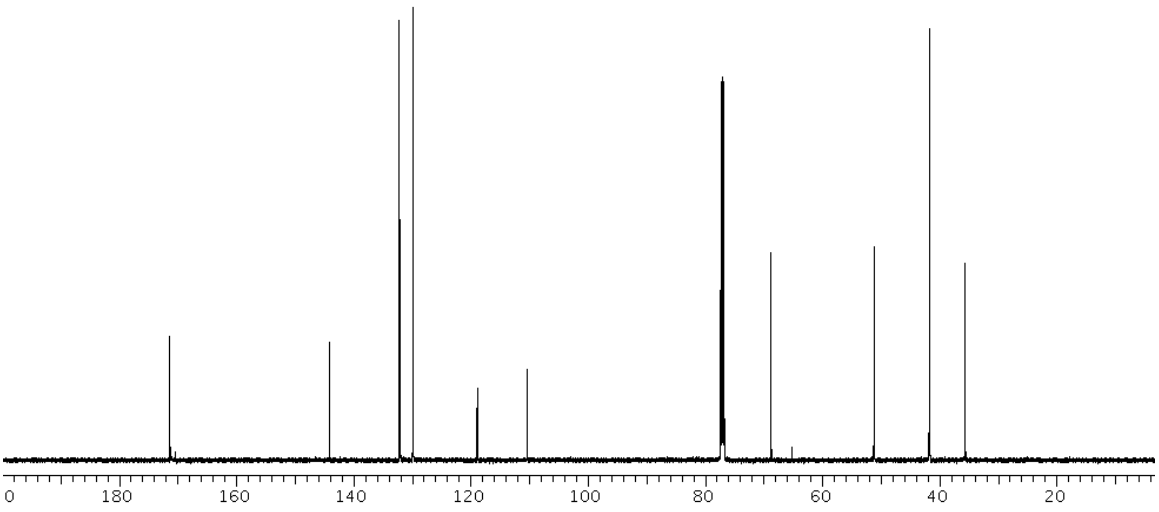
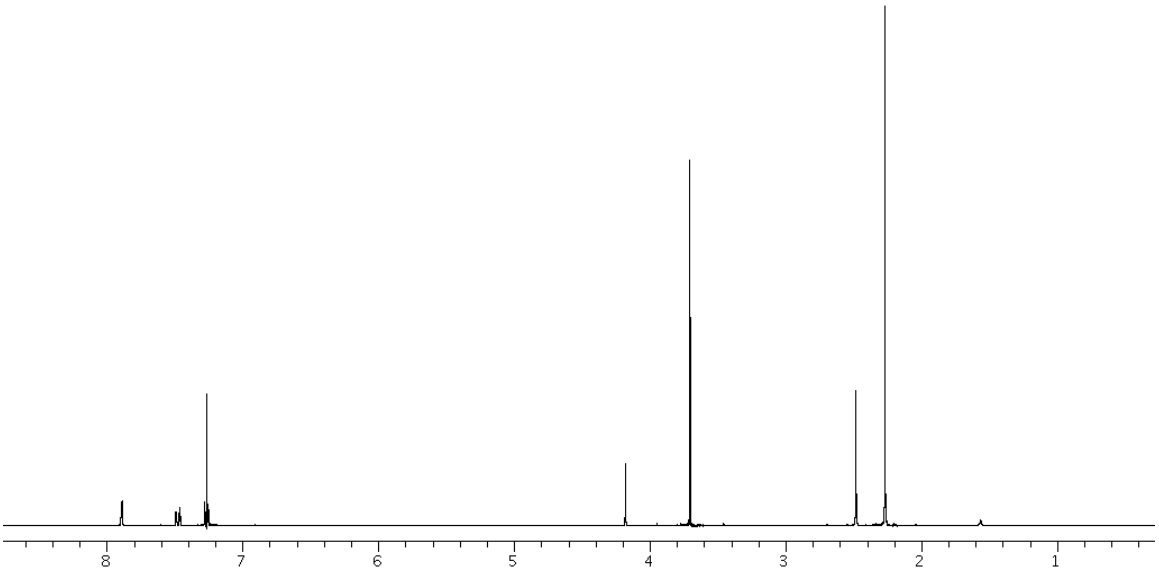


5e, ^{1}H NMR



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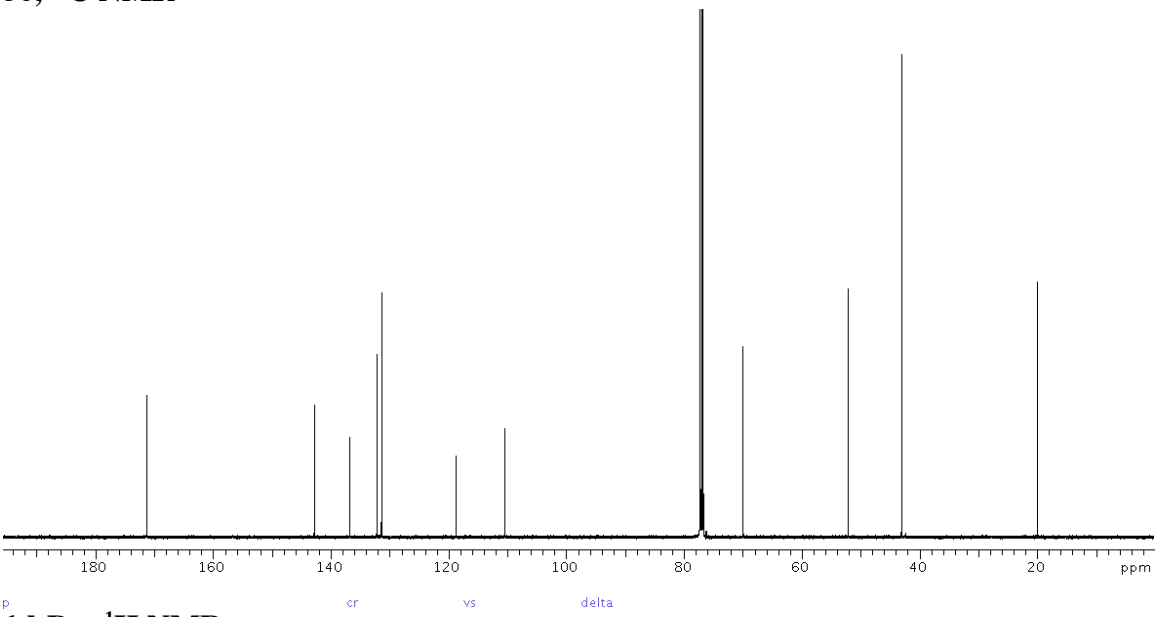
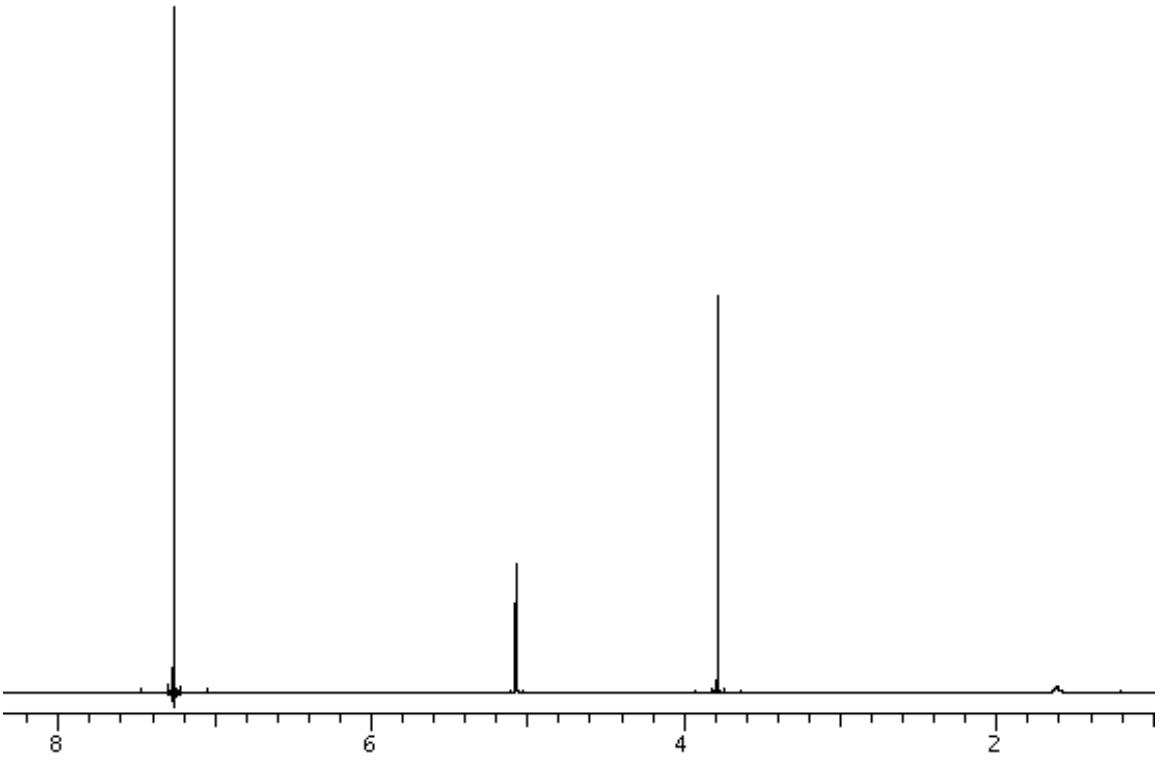


1d-D_{13}, ^{1}H NMR



Computational Procedures and Supporting Computational Results

General

Calculations of structures, energies, and frequencies employed default procedures in Gaussian09[1,2,3] unless otherwise noted. Complete structures and energetics are provided in sections 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.[4]

KIE Prediction

For the prediction of the intramolecular isotope effect based on **6**‡----H-DBU^{+}, conventional TST isotope effects for each competing isotopomer were calculated by the method of Bigeleisen and Mayer[5] using the program QUIVER,[6] modified for easier use with Gaussian 09 and compilation on modern compilers. The conventional TST isotope effects were then corrected by a one-dimensional infinite-parabola tunneling correction.[7] The modified QUIVER program, macros that aid in running the program, and a spreadsheet that carries out the isotope effect calculations is available on request, and we have supplied this material to over 20 groups. A single scaling factor of 0.9614 in all cases. The choice of scaling factor has a negligible effect on the predicted isotope effect, within roundoff error in the current case.

Initialization of Trajectories and Additional Details on Trajectories

The trajectories in DMSO, CH_2Cl_2, and CCl_4 were quasiclassical, i. e. including zero-point energy plus a Boltzmann distribution of quantized vibrational energies for each mode. These trajectories were initated from the area of **6**‡ or **6**‡----H-DBU^{+}. The desired energy in each of the normal modes of **6**‡ or **6**‡----H-DBU^{+} 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.[8]) The mode corresponding to the transition vector was treated classically. A sample PROGDYN parameter file (progdyn.conf) is given in a later section.

The trajectories were initiated from the area of **6**‡ or **6**‡----H-DBU^{+} and integrated both forward and backward in time to obtain complete trajectories connecting the starting **2a** to either **3a** or dissociation. A significant proportion of the trajectories were not productive. With **6**‡ in

CH_2Cl_2, 23% of the trajectories connected dissociation with dissociation. With **6**‡ in DMSO, 6% of the trajectories connected dissociation with dissociation. With **6**‡----H-DBU$^+$ in CCl_4, 10% of the trajectories connected **3a** with **3a**. 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 more serious complication occurred with the **6**‡----H-DBU$^+$ trajectories in that 22% passed from starting material into the area of **7----8** and remained there for the trajectory time limit of 500 fs. Continuing quasiclassical trajectories longer than this time was judged unphysical due to the rise in unphysical redistribution of energy out of the initially quantized normal modes. We cannot know the long-term disposition of such trajectories but even if they all dissociated, it would not significantly affect the discussion in the main text.

For trajectories in a sphere of 101 methanol molecules, the distances *a* and *b* in **6**‡ were constrained to 2.26 Å and 2.64 Å by a harmonic potential (with k = 474 kcal/mol/Å^2), and the centroid of **6**‡ was contrained by a weak harmonic potential (with k = 0.119 kcal/mol/Å^2) to the middle of the sphere. The sphere was maintained with a density of 0.79 by a harmonic restoring potential (with k = 11.86 kcal/mol/Å^2) on atoms outside of 11.9 Å from the center of the sphere. That is, a force is applied to atoms that are outside of 11.9 Å from the center of the sphere, along a vector toward the center of the sphere. The magnitude of the force was set to (distance to center -11.9 Å) x 11.86 kcal/mol/Å^2. These parameters are set with the "sphereon 1", "spheresize 11.9", and "sphereforce 0.01" keywords in PROGDYN. A later section gives the complete PROGDYN parameter file (prodyn.conf) for these trajectories.

A series of six trajectories in 101 methanol molecules were started in PM3 calculations giving each of the atoms a Boltzmann-random motion for 1000 K. These six trajectories were then equilibrated for 5 ps at 1000 K, then they were slowly cooled to 298.15 K using the thermostat facility in PROGDYN with thermostatmult set at 0.999 (removing 0.1% of the energy per fs), and equilibration at 298 K was continued for 5 ps. The method for force calculation was then switched to ONIOM using M06-2X/6-31G* for all of the atoms of **6**‡ and using PM3 for the methanol molecules, and the trajectories were continued for 5 ps.

The six trajectories were then continued and at 250 fs intervals the helper program *prodynsam* (listed in a later section) was used to create a *geoPlusVel* file for use in PROGDYN. The *progdynsam* program leads to trajectories with all atoms moving at their current velocity. Each resulting unconstrained velocity was integrated forward and backward in time.

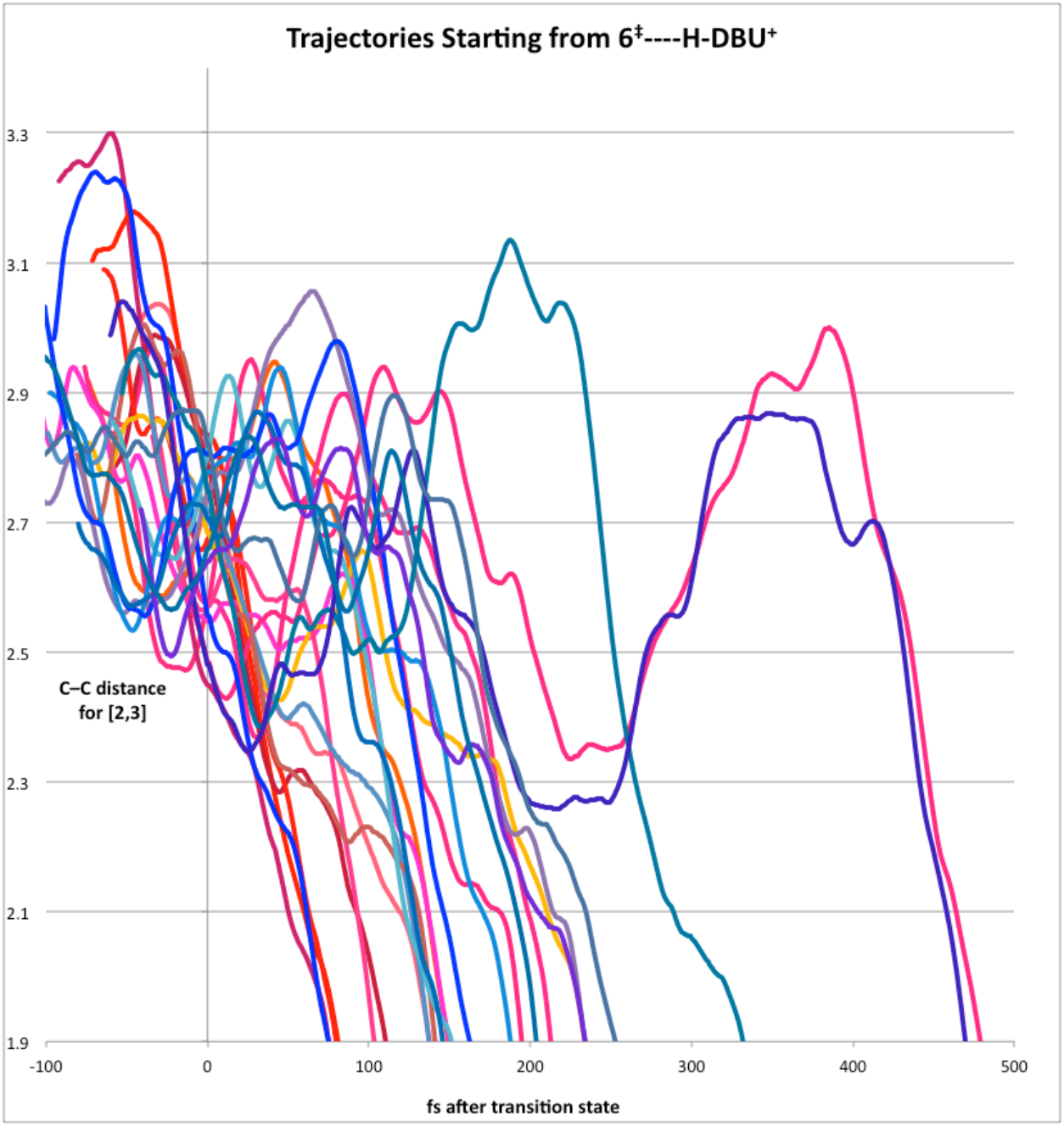
A large proportion of the trajectories in methanol, 65%, were recrossing trajectories. This is normal for trajectories started in solvent since setting limited dimensions (here just *a* and *b*) is not sufficient to consistently place the initial trajectory point at the transition state. The recrossing trajectories are of no particular significance and were ignored.

Plots of Trajectories

Starting from 6‡----H-DBU$^+$

The graph below shows plots of the C–C distance *b* in the main text associated with formation of the [2,3] intial product **3a** versus time. The 0 point on the horizontal axis nominally represents the transition state **6**‡ and in practice is the initialization point for the trajectories. The

point is derived from **6**‡ by displacements along the normal modes as described in a previous section. The plot only shows through the 500 fs time limit; as discussed above 22% of trajectories extended beyone this time limit. As discussed in the main text, most of the trajectories forming **3a** do so quickly, with a mediate time of 160 fs. The graph shows how these trajectories tend to pass directly to **3a** with a consistent closure of the C-C distance as the reaction coordinate progresses.



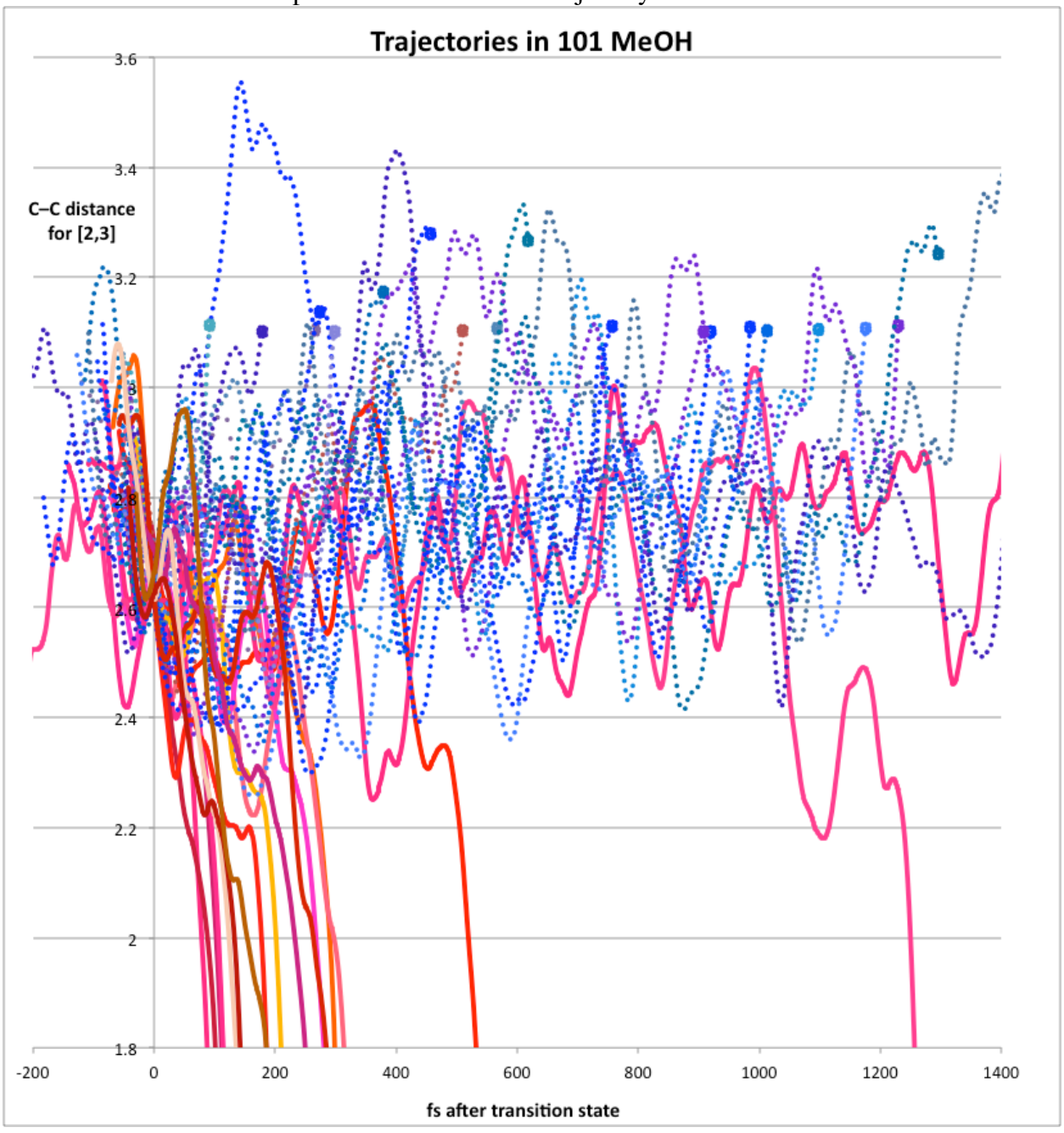
In Methanol

The graph below shows plots of the C–C distance *b* in the main text associated with formation of the [2,3] intial product **3a** versus time. The 0 point on the horizontal axis nominally

represents the transition state **6**‡ and in practice represents the geometry at which the constraints were removed to intiate integrations forward and backward in time. The plot only shows through 1400 fs past the transition transition state; trajectories that took longer than this were cut off. As discussed in the main text, most of the trajectories forming **3a** do so quickly, with a mediate time of 210 fs and with 80% finishing within 300 fs. However, dissociative trajectories are slow, taking a median time of 560 fs.

KEY:

dotted lines	dissociative trajectories
solid lines	[2,3] trajectories leading to **3a**
	end point for a dissociative trajectory



Programs for Calculations and NMR Integrations

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. This pathway for initialization is important here because it is used when the program progdynsam, described later, is used to generate the geoPlusVel file.
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 sometimes 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.

The following helper programs were used for the current study.
progdynsam – an awk program that generates a geoPlusVel file based on input from a *traj* file. Typically, the traj file is a trajectory performed with constraints, and the new geoPlusVel will be started without constraints. *progdynsam* must be modified for the desired temperature, and it takes as input the variable pt to decide which points in the traj file are used to define the geoPlusVel. For previously constrained atoms, *progdynsam* gives the atoms a Boltzmann-random velocity and direction of motion appropriate for the desired temperature. The program is invoked with awk –v pt=## –f progdynsam traj where ## is the trajectory point used to start a new geoPlusVel, and traj is the output file from above containing the list of trajectory points.
progtrajlength – an awk program used to analyze the output data in *dynfollowfile*. It is involked with awk –f progtrajlength dynfollowfile where dynfollowfile is a list of one or more of the dynfollowfile output files described above.

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
#version Aug 2011 runpointnumber starts better, restart better if died during first few points, awk bug fix
#version Aug 2012 freqinHP reads with only 3 freqs, goingwell and other temp files moved to $scratchdir
#version Aug 2013 adds ability to automatically run a CFOUR program if the file ZMAT exists
#
#version Nov 2013 adds ability to bypass generation of geoPlusVel using the signal file bypassproggen
#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, set the scratch, program, and other directores, remove errant control files
#    start outermost loop L1L1L1L1L1L1L1L1
#    start loop 2 L2L2L2L2L2L2L2L2
# B. branch on whether there is a file named "skipstart"
#    if there is, skip B1, B2, B3 entirely
#    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
#  B1. generates geoPlusVel, isomernumber, runpointnumber=1, then makes g09.com for point 1
```

```
#  B2. checks for success of B1 or exits, then sets geoRecord then runs g09.com.  Checks for its success or exits.
#  B3. runpointnumber=2, kills run if XXXX in dynfollowfile due to bad energy probably, makes g09.com for point 2, runs it
#      checks for its success or exits
#      runpointnumber=3, uses progdynb to make g09.com for point 3
#      sets skipstart=forward
#  B4. Only runs if skipstart=ireverserestart, performs reverserestart, ends with runpointnumber=3
#      sets skipstart=reverse
# C. loop over propagation steps
#
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAA
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAA
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAA
#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=/software/lms/g09_D01
. $g09root/g09/bsd/g09.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
proggramdir=~/binall500
freqfile=~/binall500/freqinHP
echo
echo ORIGDIR at the beginning of run:
echo $origdir
ls $origdir
echo
echo SCRATCHDIR at the beginning of run:
echo $scratchdir
ls $scratchdir
echo
echo PROGGRAMDIR at the beginning of run::
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
#L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1
L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1
while (true)
do
# As long as there is a file "goingwell" the program will not exit entirely by itself
rm -f $scratchdir/goingwell
#L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2
L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2
while (true)
do
```

```
#  BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
  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
```

```
#  B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3 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
        if (test -f bypassproggen) then
          cat bypassproggen > runpointnumber
          echo 3 > bypassproggen
        fi
        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
#
B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4
B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4
# 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
        if (test -f bypassproggen) then
          cat bypassproggen > runpointnumber
        fi
        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___

#  CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC  propagation loop
  while (true)
  do
    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
      #increment runpointnumber
      cp runpointnumber $scratchdir/temp533
```

```
      awk 'BEGIN {getline;i=$1+1;print i}' $scratchdir/temp533 > runpointnumber
      rm $scratchdir/temp533
      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 {
# 2014 - avoids bug with a box on, so that starts without modes use input geometry, not standard orientation
# aug 2013 summary of changes
#includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, handling of linear molecules using geometry linear, fixed but with atoms over 99 but
#bug varies with version of Gaussian, randomization based on PROCINFO (solved many problems), added initialDiss 3 for
random
#phase of normal modes
# 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 {
# 2014 added ONIOMcharge, more reliable convergence commands
# 2013 added multiple NMR calculations, molecular rotations
# 2012 added NMR calculations
# 2011 added linkatoms in ONIOM
# 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
oniomcharge=0; oniommult=0

#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=="oniomchargemult") {
    oniomcharge=$2
    oniommult=$3
    }
  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=(xqc,maxconven=55,fulllinear,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 ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult
}

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 {
# 2014 added ONIOMcharge, more reliable convergence commands
# aug 2013 includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, checks more kinds of energies at point 2
#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
oniomcharge=0; oniommult=0

#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=="oniomchargemult") {
    oniomcharge=$2
    oniommult=$3
    }
  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=(xqc,maxconven=55,fulllinear,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 ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult

# 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
# May 2015 added ability to force solvent into a sphere
# Feb 2015 added zeroatom ability to make solute centered in solvent
# Jan 2015 added applyforce to apply forces on motion of atoms and allow PMF calculations
# Dec 2014 added oniom charge specifications
# 2013 added multiple NMR calculations, molecular rotations, thermostat commands
# 2012 added NMR calculations
# 2011 added linkatoms in ONIOM
# 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
oniomcharge=0; oniommult=0
applyforce=0; applyforceB=0; applyforceC=0; zeroatomon=0
sphereon=0; spheresize=999; sphereforceK=0.01

#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; pi=3.14159265359
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=="oniomchargemult") {
  oniomcharge=$2
  oniommult=$3
  }
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=="sphereon") sphereon=$2
if ($1=="spheresize") spheresize=$2
if ($1=="sphereforce") sphereforceK=$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=="applyforce") {
  applyforce=$2; apforce=$3; apforceX0=$4; apforce2=$5; apforce3=$6
  }
if ($1=="applyforceB") {
  applyforceB=$2; apforceB=$3; apforceX0B=$4; apforce2B=$5; apforce3B=$6
  }
if ($1=="applyforceC") {
  applyforceC=$2; apforceC=$3; apforceX0C=$4; apforce2C=$5; apforce3C=$6
  }
if ($1=="afatoms") {
  for (i=1;i<8;i++) {
    if ($(i+1)>0) afatom[i]=$(i+1)
    }
  }
```

```
  if ($1=="afatomsB") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) afatomB[i]=$(i+1)
      }
    }
  if ($1=="afatomsC") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) afatomC[i]=$(i+1)
      }
    }
  if ($1=="zeroatom") {
    zeroatomon=1
    zeroatom=$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
  }
blankLineTester=10
while (blankLineTester>1) {
  getline < "geoPlusVel"
  if ($11=="potential") potentialE=$13
  blankLineTester=length($0)
  }

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
  KEold=KEold+0.5*weight[at]*(atomVel^2)/((timestep^2)*conver1)
  if (diag==3) print atomVel >> "vellist"
  }
}

#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])
  }
newPotEK=(newPotentialE-potentialE)*627.509
}

#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 to apply a force to bring atoms within a sphere - note that if atoms are too far outside of a sphere then the force on them
will be very large
#unless sphereforce is turned down
if (sphereon==1) {
  sphereforcetotal=0; totalweight=0
  for (i=1;i<=numAtoms;i++) {
    distToOrig=((oldarr[i,1]^2+oldarr[i,2]^2+oldarr[i,3]^2)^.5)
    if (distToOrig>spheresize) {
#originally tried a harmonic restortation to the sphere but this is too big for atoms far outside the sphere
      sphereforce=sphereforceK*(distToOrig-spheresize)
      if (sphereforce>0.01) sphereforce=0.01
```

```
        sphereforcetotal=sphereforcetotal+sphereforce
# tried a constant force outside of sphere but am worried about what this means since the potential is discontinuous and steps are
discrete
#        sphereforce=sphereforceK

unitX=sphereforce*oldarr[i,1]/distToOrig;unitY=sphereforce*oldarr[i,2]/distToOrig;unitZ=sphereforce*oldarr[i,3]/distToOrig
        forceArr[i,1]=forceArr[i,1]-unitX;forceArr[i,2]=forceArr[i,2]-unitY;forceArr[i,3]=forceArr[i,3]-unitZ
        }
# calculate the density at 0.9*spheresize
      if (distToOrig<0.9*spheresize) {
        totalweight=totalweight+weight[i]
        }
      }
   density=(totalweight/avNum)/((4/3)*pi*(0.9*spheresize*1E-8)^3)
   }
# routine to apply forces between atoms, used for umbrella sampling
# the next few lines are a kludge to apply the force to one of a series of atoms, whichever is closest to afatom[1]
for (i=3;i<8;i++) {
   if (afatom[i]>0) {
      if(Distance(afatom[1],afatom[i])<Distance(afatom[1],afatom[2])) afatom[2]=afatom[i]
      }
   if (afatomB[i]>0) {
      if(Distance(afatomB[1],afatomB[i])<Distance(afatomB[1],afatomB[2])) afatomB[2]=afatomB[i]
      }
   if (afatomC[i]>0) {
      if(Distance(afatomC[1],afatomC[i])<Distance(afatomC[1],afatomC[2])) afatomC[2]=afatomC[i]
      }
   }
# applyforce 1 puts a linear constant force.
# applyforce 2 puts on a harmonic restoring force to apforceX0
if (applyforce>0) {
   delX=oldarr[afatom[1],1]-oldarr[afatom[2],1];delY=oldarr[afatom[1],2]-oldarr[afatom[2],2];delZ=oldarr[afatom[1],3]-
oldarr[afatom[2],3];
   distatoms=(delX^2+delY^2+delZ^2)^.5
   if (applyforce==2) apforce=apforce*(distatoms-apforceX0)
   if (applyforce==3) apforce=apforce*(distatoms-apforceX0) + apforce2*(distatoms-apforceX0)^2
   if (applyforce==4) apforce=apforce*(distatoms-apforceX0) + apforce2*(distatoms-apforceX0)^2 + apforce3*(distatoms-
apforceX0)^3
   unitX=apforce*delX/distatoms;unitY=apforce*delY/distatoms;;unitZ=apforce*delZ/distatoms;
   forceArr[afatom[1],1]=forceArr[afatom[1],1]-unitX;forceArr[afatom[1],2]=forceArr[afatom[1],2]-
unitY;forceArr[afatom[1],3]=forceArr[afatom[1],3]-unitZ

forceArr[afatom[2],1]=forceArr[afatom[2],1]+unitX;forceArr[afatom[2],2]=forceArr[afatom[2],2]+unitY;forceArr[afatom[2],3]=
forceArr[afatom[2],3]+unitZ
   }
if (applyforceB>0) {
   delX=oldarr[afatomB[1],1]-oldarr[afatomB[2],1];delY=oldarr[afatomB[1],2]-oldarr[afatomB[2],2];delZ=oldarr[afatomB[1],3]-
oldarr[afatomB[2],3];
   distatoms=(delX^2+delY^2+delZ^2)^.5
   if (applyforceB==2) apforceB=apforceB*(distatoms-apforceX0B)
   if (applyforceB==3) apforceB=apforceB*(distatoms-apforceX0B) + apforce2B*(distatoms-apforceX0B)^2
   if (applyforceB==4) apforceB=apforceB*(distatoms-apforceX0B) + apforce2B*(distatoms-apforceX0B)^2 +
apforce3B*(distatoms-apforceX0B)^3
   unitX=apforceB*delX/distatoms;unitY=apforceB*delY/distatoms;;unitZ=apforceB*delZ/distatoms;
   forceArr[afatomB[1],1]=forceArr[afatomB[1],1]-unitX;forceArr[afatomB[1],2]=forceArr[afatomB[1],2]-
unitY;forceArr[afatomB[1],3]=forceArr[afatomB[1],3]-unitZ

forceArr[afatomB[2],1]=forceArr[afatomB[2],1]+unitX;forceArr[afatomB[2],2]=forceArr[afatomB[2],2]+unitY;forceArr[afatom
B[2],3]=forceArr[afatomB[2],3]+unitZ
   }
if (applyforceC>0) {
   delX=oldarr[afatomC[1],1]-oldarr[afatomC[2],1];delY=oldarr[afatomC[1],2]-oldarr[afatomC[2],2];delZ=oldarr[afatomC[1],3]-
```

```
oldarr[afatomC[2],3];
  distatoms=(delX^2+delY^2+delZ^2)^.5
  if (applyforceC==2) apforceC=apforceC*(distatoms-apforceX0C)
  if (applyforceC==3) apforceC=apforceC*(distatoms-apforceX0C) + apforce2C*(distatoms-apforceX0C)^2
  if (applyforceC==4) apforceC=apforceC*(distatoms-apforceX0C) + apforce2C*(distatoms-apforceX0C)^2 +
apforce3C*(distatoms-apforceX0C)^3
  unitX=apforceC*delX/distatoms;unitY=apforceC*delY/distatoms;;unitZ=apforceC*delZ/distatoms;
  forceArr[afatomC[1],1]=forceArr[afatomC[1],1]-unitX;forceArr[afatomC[1],2]=forceArr[afatomC[1],2]-
unitY;forceArr[afatomC[1],3]=forceArr[afatomC[1],3]-unitZ

forceArr[afatomC[2],1]=forceArr[afatomC[2],1]+unitX;forceArr[afatomC[2],2]=forceArr[afatomC[2],2]+unitY;forceArr[afatom
C[2],3]=forceArr[afatomC[2],3]+unitZ
  }
#routine to slowly move an atom toward the origin as set by a harmonic potential
if (zeroatomon==1) {
  multiple=0.99996
  oldarr[zeroatom,1]=multiple*oldarr[zeroatom,1]
  oldarr[zeroatom,2]=multiple*oldarr[zeroatom,2]
  oldarr[zeroatom,3]=multiple*oldarr[zeroatom,3]
  }
#print out some things to vellist and do thermostat
apparentTemp=KEold*2/(3*RgasK*numAtoms)
# the damping in the thermostat is based on temperature based on old geo vs older geo
if (thermostat==1) {
  if (diag<4) print "KEold",KEold,"desired temperature",temp,"apparent Temperature",apparentTemp >> "vellist"
  if (apparentTemp>temp) damping=thermostatmult
  if (apparentTemp<temp) damping=1/thermostatmult
  }

#############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]
        }
      }
    }
  for (at=1;at<=numAtoms;at++) {
    atomVel=((oldarr[at,1]-newarr[at,1])^2 + (oldarr[at,2]-newarr[at,2])^2 +(oldarr[at,3]-newarr[at,3])^2)^.5
    KEnew=KEnew+0.5*weight[at]*(atomVel^2)/((timestep^2)*conver1)
    }
    KEave=0.5*KEold+0.5*KEnew
    Etotal=newPotEK+KEave
#still basing apparent Temperature on velocities from old vs older, even though the KE now represents an average of old and new
    if (diag==4) print runpointnum,"KEave",KEave,"apparent
Temperature",apparentTemp,"newPotEK",newPotEK,"Etotal",Etotal,"TotalSphereForce",sphereforcetotal,"density in
0.9r",density >> "vellist"
  }
########

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 "#p " method " force scf=(xqc,maxconven=55,fulllinear,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 ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult
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"
  }
}

function Distance(Atom1,Atom2) {
 return sqrt((oldarr[Atom1,1]-oldarr[Atom2,1])^2+(oldarr[Atom1,2]-oldarr[Atom2,2])^2+(oldarr[Atom1,3]-oldarr[Atom2,3])^2)
}
```

Program progcfour

This module calls an outside calculation with CFOUR but was not used for the current paper. 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
}
/ NO2BnDBUfull/ {
  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<99)) {
    A[$1]=$4;B[$1]=$5;C[$1]=$6
    }
  }
#/before annihilation/ {
#   printf("%s %.5f ",$1,$6)
#   }

END {
  CN=Distance(7,8)
  CC23=Distance(1,9)
  CC12=Distance(7,9)
  printf("%s %.3f  %s %.3f  %s %.3f ","CN",CN,"CC23",CC23,"CC12",CC12)
  if (runpoint>500) {
    print "Too many points.  XXXXN"
    }
  if ((CN>2.5) && (CC23<1.9)) {
    print "2,3-Rearrangement XXXX23N"
    }
  if ((CN>2.5) && (CC12<1.9)) {
    print "1,2-Rearrangement XXXX12N"
    }
  if ((CN>3.2) && (CC12>3.2) && (CC23>3.2)) {
    print "Dissociation XXXXDN"
    }
```

```
  if ((CN<1.8) && (CC23>2.6)) {
    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 M062X/6-31+G**
#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 NMRtype=1 will add a section for an NMR calc at every NMRevery intervals.  If you want to combine the
two use nonstandard
#NMRtype 1
#NMRmethod2 B97D/6-31G*
#NMRmethod LC-wPBE/6-31G*
#NMRmethod3 B3LYP/cc-pvtz
#NMRevery 4
#NMRrand 1
#NMRcc 1
#loadlimit 10.0
#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 restricted
charge 1
multiplicity 1
#oniomchargemult 1 1
processors 5
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 10gb
#*** 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 NO2BnDBUfull TS 2XPS 298dis2
#*** 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 298.15
#*** thermostat 1 puts in a damping factor so as to bring the classical temperature toward the desired temperature.
#*** use a thermostatmult between 0.95 and 1, typically 0.995, so the damping happens slowly - otherwise there will be
#*** overadjustment in response to random variation
```

```
#*** the thermostat is not exact.  The second traj point ignores this, so it only applies to later points handled by progdynb.
thermostat 0
#thermostatmult 0.999
#*** 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
#method3 IOp(3/76=0572004280)
method3 scrf=(pcm,solvent=ccl4)
#method3 scrf=(pcm,Solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method4 iop(2/9=2000)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmso,read)
#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 99999
#*** 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 60
#*** 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 16
#fixedatom2 1
#fixedatom3 4
#fixedatom4 20
#applyforce 1 lets one push atoms together or appart - a positive force pushes them together
#format is applyforce 1 firstatom secondatom force    - with the units on force the same as in the Gaussian output file
```

```
#applyforce 2 or 3 or 4 applys a polynomical force centered at dist0.  2 is just harmonic, 3 is second order, 4 is third order
#format is applyforce 4 firstatom secondatom forcecoefficient dist0 forcecoefficient2 forcecoefficient3
#applyforce 2 0.2 1.6
#afatoms 2 4
#applyforceB 4 0.1 2.8 0.0 0.05
#afatomsB 1 3
#*** 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 1
#boxsize 10.2
#*** 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
#displacements 4 0
#displacements 5 0
#displacements 6 0
#displacements 7 0
#displacements 8 0
#displacements 9 0
#displacements 10 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 1
#*** 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 1.000
#at a damping of .9995, the energy is cut in half in 693 points
#*** 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
```

progdyn.conf for equilibrating trajectories in methanol

```
#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 ONIOM(M062X/6-31G*:PM3)
#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 NMRtype=1 will add a section for an NMR calc at every NMRevery intervals.  If you want to combine the
two use nonstandard
#NMRtype 1
#NMRmethod2 B97D/6-31G*
#NMRmethod LC-wPBE/6-31G*
#NMRmethod3 B3LYP/cc-pvtz
#NMRevery 4
#NMRrand 1
#NMRcc 1
#loadlimit 10.0
#geometry linear
rotationmode 0
#*** 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 restricted
charge 0
multiplicity 1
#oniomchargemult 1 1
processors 6
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 13gb
#*** 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 4
#*** title -- the title keyword must be followed by exactly four words
title 23arom ONIOM sphere 101MeOH
#*** 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 0
#*** 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 298.15
#*** thermostat 1 puts in a damping factor so as to bring the classical temperature toward the desired temperature.
#*** use a thermostatmult between 0.95 and 1, typically 0.995, so the damping happens slowly - otherwise there will be
#*** overadjustment in response to random variation
#*** the thermostat is not exact.  The second traj point ignores this, so it only applies to later points handled by progdynb.
thermostat 1
```

```
thermostatmult 0.999
#*** 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
#method3 IOp(3/76=0572004280)
#method3 scrf=(pcm,solvent=ethanol)
#method3 scrf=(pcm,Solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method4 iop(2/9=2000)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmso,read)
#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 0
#*** 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 2
#*** 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 99999
#*** 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 40
#*** 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 16
#fixedatom2 1
#fixedatom3 4
#fixedatom4 20
#applyforce 1 lets one push atoms together or appart - a positive force pushes them together
#format is applyforce 1 firstatom secondatom force    - with the units on force the same as in the Gaussian output file
#applyforce 2 or 3 or 4 applys a polynomical force centered at dist0.  2 is just harmonic, 3 is second order, 4 is third order
#format is applyforce 4 firstatom secondatom forcecoefficient dist0 forcecoefficient2 forcecoefficient3
```

```
applyforce 2 0.4 2.26
afatoms 7 8
applyforceB 2 0.4 2.64
afatomsB 1 9
applyforceC 2 0.2 1.85
afatomsC 15 35
#zeroatom pushes the numbered atom toward the origin with a small harmonic potential  - good with boxon when you want to keep the reaction in the center
zeroatom 6
#*** 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 1
#boxsize 10.2
#*** sphereon and spheresize and sphereforce - uses a force to push atoms within a sphere.  notice that if the atom is far outside of
#the sphere then the force is large unless sphereforce is set small
sphereon 1
spheresize 11.9
sphereforce .01
#*** 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
#displacements 4 0
#displacements 5 0
#displacements 6 0
#displacements 7 0
#displacements 8 0
#displacements 9 0
#displacements 10 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 9999999
#*** 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 1.000
#at a damping of .9995, the energy is cut in half in 693 points
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.
reversetraj false
```

progdynsam

```
BEGIN {
```

```
temp=298.15
if (pt<1) startpoint=6363
if (pt>1) startpoint=pt
line=0
printon=0
pointline=0
secondpoint=0
}

{
line++
if (line==1) numAtoms=$1
pointline++
if (printon==1) {
  if ($1=="H") atWeight[pointline]=1.00783
  if ($1=="C") atWeight[pointline]=12.0000
  if ($1=="B") atWeight[pointline]=10.81
  if ($1=="O") atWeight[pointline]=15.99940
  if ($1=="F") atWeight[pointline]=18.9984
  if ($1=="P") atWeight[pointline]=30.9738
  if ($1=="S") atWeight[pointline]=31.972
  if ($1=="N") atWeight[pointline]=14.0030740
  if ($1=="Al") atWeight[pointline]=26.981
  if ($1=="Cl") atWeight[pointline]=35.4527
  if (($1=="C") || ($1=="H") || ($1=="O") || ($1=="P") || ($1=="N") || ($1=="Cl")  || ($1=="B") || ($1=="F") || ($1=="S") ||
($1=="Al")) {
    Arr0[pointline,0]=$1
    Arr0[pointline,1]=$2
    Arr0[pointline,2]=$3
    Arr0[pointline,3]=$4
    Arr1[pointline,0]=$1
    Arr1[pointline,1]=$2
    Arr1[pointline,2]=$3
    Arr1[pointline,3]=$4
    }
  }
if (secondpoint==1) {
  if (($1=="C") || ($1=="H") || ($1=="O") || ($1=="P") || ($1=="N") || ($1=="Cl")  || ($1=="B") || ($1=="F") || ($1=="S") ||
($1=="Al")) {
    Arr1[pointline,1]=$2-Arr1[pointline,1]
    Arr1[pointline,2]=$3-Arr1[pointline,2]
    Arr1[pointline,3]=$4-Arr1[pointline,3]
    }
  }
if ($8=="runisomer") {
  pointline=0
  }
if ($7==startpoint) {
  pointline=0
  printon=1
  }
if ($7==startpoint+1) {
  secondpoint=1
  pointline=0
  printon=0
  }
if ($7==startpoint+2) {
  secondpoint=0
  printon=0
  }

}
```

```
END {
print numAtoms
for (i=1;i<=numAtoms;i++) {
  print Arr0[i,0],Arr0[i,1],Arr0[i,2],Arr0[i,3],atWeight[i]
  }
conver1=4.184E26
srand()
timestep=1E-15
for (i=1;i<=100;i++) {
  newRand=rand()
  newRand2=rand()
  randArr[i]=newRand
  sign[i]=1
  if (newRand2<0.5) sign[i]=-1
}
for (i=1;i<=numAtoms;i++) {
  if ((Arr1[i,1]==0) && (Arr1[i,2]==0) && (Arr1[i,3]==0)) {
    for (j=1;j<=3;j++) {
      KE=-0.001987*temp*log(1-randArr[3*i+j])
      Vel=sign[3*i+j]*timestep*(2*KE*conver1/atWeight[i])^0.5
      Arr1[i,j]=Vel
      }
    }
  print Arr1[i,1],Arr1[i,2],Arr1[i,3]
  }
printf("%s %i %i %s ","generated from points",startpoint,startpoint+1,"in a trajectory, so no modes to print out")
system("pwd")
print "Total mode energy desired=",0
for (i=1;i<=700;i++) {
  velsq= Arr1[i,1]^2+Arr1[i,2]^2+Arr1[i,3]^2
  KE=1E30*0.5*atWeight[i]*velsq/conver1
  KE=2.388E3*0.5*atWeight[i]*velsq
  #print i,KE
  }
print ""
}
```

NMR Integration Macro

The listing below shows the macro used to calculate and output the NMR integrations for Sample 1. 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 used for both samples, so the only differences from sample to sample were the phases and baseline lvl.

Macro “bintra5das”

```
plotter='LaserJet_1318_PSR'
shell('rm /home/singleton/dsingle/vnmrsys/maclib/tempbintra5')
$filename='/nmrdata/singleton/biswas/ammonium_sigmatropic_shift/2014/08_14/sampl1.fid'
rt($filename)

lvl=0.05
rp=-38
lp=-42
$cut[1]=10.
$cut[2]=10.
$cut[3]=10.
$cut[4]=12.15
```

```
$cut[5]=13.75
$cut[6]=10
$cut[7]=10
$cut[8]=10
$cut[9]=10.
$cut[10]=10
$cut[11]=10

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=1

$spectrum=1
repeat
ds($spectrum)
echo('new spectrum')

"spectrum-specific phases"
if (1>2) then
  if ($spectrum=1) then rp=-60.40 endif
  if ($spectrum=2) then rp=-60.40 endif
  if ($spectrum=3) then rp=-60.40 endif
  if ($spectrum=3) then  rp=-60.40 endif
  if ($spectrum=4) then rp=-60.40 endif
  if ($spectrum=4) then lvl=0.05 endif
  if ($spectrum=5) then rp=-60.40 endif
  if ($spectrum=6) then rp=-60.40 endif
endif

"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):$count
echo('here1')
if ($count<5 or $count>25) then
  text
  echo('Problem with wrong number of peaks.')
  return
endif

"----------Setting shifts----------"
"get carbonyl set to 170p then find chlororm and set it at 77.00"
getll(1):$ht,$freq
cr=$freq
rl(170.6p)
"sp=75.0p wp=4p"
"repeat"
```

```
"   nll('pos',1):$count"
"   if ($count<3) then th=th-1 endif"
"   if ($count>3) then th=th+1 endif"
"   nll('pos',1):$count"
"until ($count=3)"
"getll(2):$ht,$freq"
"cr=$freq rl(77.00p) f"
"-----------------------------------------------------------------"

"----------------------------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=167p wp=6p
repeat
  nll('pos',4):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',4):$count
until ($count=1)
$i=1
  getll(1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"2 now focus on second peak from the left"
sp=145p wp=6p
repeat
  nll('pos',40):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',40):$count
until ($count=1)
$i=2
  getll(1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"Now focus on cutting the third peak, cut them"
sp=143p wp=2p
repeat
  nll('pos',16):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',16):$count
until ($count=1)
$i=3
  getll(1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
```

```
"peak 4"
sp=134p wp=4p
repeat
  nll('pos',1):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',1):$count
until ($count=1)
$i=4
  getll(1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"peak 5"
sp=128p wp=6p
repeat
  nll('pos',10):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',10):$count
until ($count=1)
$i=5
  getll(1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"peak 6 and 7"
sp=120p wp=6p
repeat
  nll('pos',1):$count
  if ($count<2) then th=th-1 endif
  if ($count>2) then th=th+1 endif
  nll('pos',1):$count
until ($count=2)
$i=6
  getll(1):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
$i=7
  getll(2):$ht,$freq
  dres($freq):$lw
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"peak 8"
sp=66p wp=6p
repeat
  nll('pos',10):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',10):$count
until ($count=1)
$i=8
```

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

"peak 9"
sp=48p wp=6p
repeat
   nll('pos',10):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',10):$count
until ($count=1)
$i=9
   getll(1):$ht,$freq
   dres($freq):$lw
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"peak 10"
sp=40p wp=6p
repeat
   nll('pos',10):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',10):$count
until ($count=1)
$i=10
   getll(1):$ht,$freq
   dres($freq):$lw
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

"peak 11"
sp=16p wp=6p
repeat
   nll('pos',10):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',10):$count
until ($count=1)
$i=11
   getll(1):$ht,$freq
   dres($freq):$lw
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)

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

echo('The average line width is ',$totalwidth/6)

"-------------------------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/6)
  nli
  setint(5,1000)
  printoff('/home/singleton/dsingle/vnmrsys/maclib/temp')
  shell('cat /home/singleton/dsingle/vnmrsys/maclib/temp >> /home/singleton/dsingle/vnmrsys/maclib/tempbintra5')

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

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

sp=$sp wp=$wp
sp=130.6p wp=1.1p intmod='full'
is=10000000
vs=1600

" peaks 170.6 146.3 144.9 136.7 131.1 122.9 122.2 69.5 51.6 42.5 19.3 "
```

Calculated Structures and Complete Energies

Guide to Structures, Structure Titles and Their Organization

The sections below are divided into "naked" structures, meaning structures lacking hydrogen bonding to extra molecules, structures including one explicit methanol molecule, structures coordinated to H-DBU$^+$, and ancilliary structures (**7** and **8**) in the main text. Aside from the structures from the main text (**2a**, **6**‡, **3a**, and **7**----**8**), the listings include alternative conformers to the transition structure **6**‡, including structures labeled as "Dissociation" in which the carboxylate group is turned away from the aromatic so that there is no [2,3] character. These structures, obtained in unrestricted calculations, are much higher in energy.

It should be noted that all of the relevant structures for **6**‡ and **7----8** are RHF→UHF stable. To gauge how close the diradical surface is to the close-shell species for **7---8**, single-point triplet energies for these structures were calculated. In each case the triplet energy was 18-23 kcal/mol higher than than the closed-shell singlet.

The listings also include potential energy saddle points connecting **7**----**8** to **3a**. It should be noted that for the naked systems, these saddle points are never traversed (because the trajectories rapidly dissociate) and for the hydrogen bonded systems these saddle points are either bypassed or overcome on the time scale of a few hundred femtoseconds, and it is not clear that a "real" transition state, that is a free-energy saddle point, lies in this area.

For the structures coordinated to H-DBU$^+$, an ultrafine grid was used in their calculation. Other calculations were completed with a default grid.

Tabulated Energies

Table S1 CCl4

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Naked 2a	-876.599491	0.0
Naked 6‡	-876.57945	12.6
Naked 3a	-876.601647	-1.4
Naked (7+8)	-876.524389	47.1
Naked TS opposite Side	-876.580048	12.2

Table S2 CCl4

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Ylide (2a) ----H-DBU+	-1338.744157	0.00
TS (6‡) ----H-DBU+	-1338.719182	15.7
Product (3a) ----H-DBU$^+$	-1338.728922	9.6
Complex 7----8----H-DBU$^+$	-1338.721597	14.2
TS to 23 ----H-DBU$^+$	-1338.720754	14.7
[Nitro(benzyl anion){8}----H-DBU+]+8	-1338.701726	26.6

Table S3 CH2Cl2

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Naked 2a	-876.611618	0.0
Naked 6‡	-876.587984	14.8
Naked 3a	-876.607164	2.8
Naked 7----8	-876.594019	11.0
naked TS to 23	-876.590963	13.0
Naked (7+8)	-876.581694	18.8
TS opposite Side in Naked TS Dissociation	-876.587433	15.2
(Unrestricted)	-876.581951	18.6

Table S4 CH2Cl2

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Ylide (2a) ----H-DBU+	-1338.76871	0.0
TS (6‡) ----H-DBU+	-1338.741031	17.4
Product (3a) ----H-DBU$^+$	-1338.752531	10.2
Complex 7----8----H-DBU$^+$	-1338.74414	15.4
TS to 23 ----H-DBU$^+$	-1338.740963	17.4
[Nitro(benzyl anion){8}----H-	-1338.744926	14.9

DBU+]+8

Table S5 DMSO

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Naked 2a	-876.615691	0.0
Naked 6‡	-876.591202	15.4
Naked 3a	-876.609281	4.0
Naked 7----8	-876.599273	10.3
naked TS to 23	-876.593838	13.7
Naked (7+8)	-876.597716	11.3
TS opposite Side in Naked TS Dissociation (Unrestricted)	-876.589964 -876.584549	16.1 19.5

Table S6 DMSO

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Ylide (2a) ----H-DBU+	-1338.776739	0.0
TS (6‡) ----H-DBU+	-1338.748282	17.9
Product (3a) ----H-DBU$^+$	-1338.763677	8.2
Complex 7----8----H-DBU$^+$	-1338.753377	14.7
TS to 23 ----H-DBU$^+$	-1338.748331	17.8
[Nitro(benzyl anion){8}----H-DBU+]+8	-1338.757906	11.8

Table S7 MeOH

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Ylide (2a) ----H–OMe	-992.257985	0.0
TS (6‡) ----H–OMe	-992.232032	16.3
23 product (3a) ----H–OMe	-992.243503	9.1
Complex 7----8----H–OMe	-992.236661	13.4
TS Dissociation ----H–OMe in methanol (Unrestricted)	-992.226363	19.8

Table S8 gas phase

Structure	Free Energy (Hartrees)	Relative Free Energy (kcal/mol)
Naked 2a	-876.589514	0.0
Naked 6‡	-876.571372	11.4

Naked 3a	-876.596674	-4.5
Naked TS opposite Side	-876.572277	10.8

Naked Structures for 2a, 3a, 6‡, and 7---8

Naked ylide (2a) gas phase

/home/biswas/23arom_Doc_first_download/nitro/gas/ylidegas
starting material opt
M062X/6-31+g**
E(RM062X) = -876.822077832

Zero-point correction= 0.279027 (Hartree/Particle)
Thermal correction to Energy= 0.296502
Thermal correction to Enthalpy= 0.297447
Thermal correction to Gibbs Free Energy= 0.232564
Sum of electronic and ZPE= -876.543051
Sum of electronic and thermal Energies= -876.525575
Sum of electronic and thermal Enthalpies= -876.524631
Sum of electronic and thermal Free Energies= -876.589514

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	186.058	65.462	136.557

C,0,1.3360110737,0.989313973,-1.6886866553
C,0,-0.0374463389,1.0706849906,-1.8778068783
C,0,-0.7955216046,1.7203841525,-0.9130217267
C,0,-0.2389953651,2.304471517,0.2162484912
C,0,1.1359933504,2.2096446493,0.3884462054
C,0,1.9255670442,1.5338071871,-0.544712111
C,0,3.3994434243,1.3741183069,-0.3171455536
N,0,3.769019993,0.0769807991,0.4133376016
C,0,3.3108843131,-1.1385198582,-0.2836173018
C,0,1.985911255,-1.5720254675,-0.1735210156
O,0,1.7347324111,-2.6157776199,-1.0352250974
C,0,0.4286372469,-3.1640683154,-0.9384120424
C,0,3.2786841206,0.1398876126,1.8310660811
C,0,5.2601402112,0.0330265107,0.4620836957
O,0,1.0841324751,-1.1480685827,0.5671232646
N,0,-2.2554232875,1.8102865675,-1.1048453585
O,0,-2.7254797608,1.298362783,-2.1048094008
O,0,-2.9008276575,2.3936189282,-0.2521681652
H,0,1.9507809285,0.4686181657,-2.4159895254
H,0,-0.5230330192,0.6391765116,-2.7445800815
H,0,-0.8755842363,2.8101757777,0.9316659027
H,0,1.5958750108,2.6547549661,1.2669554188
H,0,3.9311036626,1.318225055,-1.2697252814
H,0,3.800007501,2.2061218182,0.2728061329
H,0,2.1909937819,0.1395472581,1.8230177609
H,0,3.6958362224,1.0354219256,2.3000370883
H,0,3.6300043602,-0.7632744829,2.3299579321
H,0,5.6338599991,0.9346757899,0.9523786649
H,0,5.5497296497,-0.8609454983,1.0124940166
H,0,5.6406340395,-0.0254685339,-0.5584142461
H,0,3.9804904996,-1.4929737167,-1.0514766936
H,0,0.2390542654,-3.5548676389,0.0649958102
H,0,-0.3321739521,-2.4118190598,-1.1654319839
H,0,0.3928963829,-3.9715654713,-1.6704269485

Naked TS (6‡) gas phase

/home/biswas/23arom_Doc_first_download/nitro/gas/TSgas
nitrobenzyl rearr uncoordinated
M062X/6-31+G**
E(RM062X) = -876.803832315

Zero-point correction= 0.276485 (Hartree/Particle)
Thermal correction to Energy= 0.293541
Thermal correction to Enthalpy= 0.294485
Thermal correction to Gibbs Free Energy= 0.232460
Sum of electronic and ZPE= -876.527347
Sum of electronic and thermal Energies= -876.510291
Sum of electronic and thermal Enthalpies= -876.509347
Sum of electronic and thermal Free Energies= -876.571372

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.200	65.277	130.543

C,0,-1.143800153,-0.4634423163,1.9392033137
C,0,-1.0747743209,-0.8265684376,3.2848667926
C,0,0.1495048805,-0.7674406641,3.9233403906
C,0,1.3099318888,-0.2812462134,3.2947469101
C,0,1.2340358898,0.0867828491,1.9755193294
C,0,0.0105583952,-0.0113031844,1.2490129764
C,0,-0.0271634072,0.0756577304,-0.1536526051
N,0,-0.0666427136,-2.0713476757,-0.5028555179
C,0,-0.8812848052,-2.6918172932,0.3843501102
C,0,-0.4588498025,-3.283756502,1.636135472
O,0,-1.5288243721,-3.8353038977,2.2597961847
C,0,-1.2588097907,-4.4083697704,3.5403570424
C,0,1.382492908,-2.3342950562,-0.4368455415
C,0,-0.5723534652,-2.0494324189,-1.8833379237
O,0,0.6644027687,-3.3214631856,2.1135581277
N,0,0.2387623449,-1.2080277424,5.3143770997
O,0,-0.7515069442,-1.7224523459,5.8163299758
O,0,1.2985721398,-1.0477567267,5.896505481
H,0,-2.1058352667,-0.4529465236,1.4376191663
H,0,-1.9473355644,-1.1800204479,3.8222706794
H,0,2.2349700706,-0.228835522,3.855486445
H,0,2.121224161,0.4493740615,1.4627453381
H,0,-0.9843708555,0.2207549475,-0.6466122188
H,0,0.8463433602,0.4308814461,-0.6957502943
H,0,1.7615889948,-2.0476108252,0.5421611051
H,0,1.8637899897,-1.7572384297,-1.2273008613
H,0,1.5621053644,-3.4041195853,-0.5828600478
H,0,-0.0134634464,-1.3087494293,-2.4571376356
H,0,-0.4532675676,-3.0408974318,-2.3329848463
H,0,-1.6290794783,-1.7794724738,-1.8750117198
H,0,-1.9319750329,-2.7442959153,0.1319322702
H,0,-0.4494230662,-5.1378988694,3.471175424

H,0,-0.984886652,-3.6307589224,4.2589463723
H,0,-2.1863474519,-4.8905972284,3.845501205

Naked 23 product (3a) gas phase

/home/biswas/23arom_Doc_first_download/nitro/gas/23prodgas
product opt
M062X/6-31+g**
E(RM062X) = -876.826228771

Zero-point correction= 0.277801 (Hartree/Particle)
Thermal correction to Energy= 0.295736
Thermal correction to Enthalpy= 0.296680
Thermal correction to Gibbs Free Energy= 0.229555
Sum of electronic and ZPE= -876.548427
Sum of electronic and thermal Energies= -876.530493
Sum of electronic and thermal Enthalpies= -876.529549
Sum of electronic and thermal Free Energies= -876.596674

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.577	66.030	141.277

C,0,-2.5259293736,-0.7383769176,-1.1275944783
C,0,-1.2981699009,-0.6716189373,-1.9924444593
C,0,-0.1491938134,-1.2107220282,-1.5696492761
C,0,-0.0114542059,-1.9786309885,-0.3381532354
C,0,-1.1194020253,-2.2585196306,0.3679822086
C,0,-2.4486315765,-1.8242185676,-0.072374435
C,0,-3.5613278899,-2.3822009478,0.4270120617
N,0,-3.966077525,0.781588961,0.2781253353
C,0,-2.7871561634,0.7138063638,-0.5691854871
C,0,-1.4951532219,1.2659316049,0.0379489759
O,0,-0.9769214358,2.2351155734,-0.7331201581
C,0,0.3095752554,2.7163750737,-0.3281786783
C,0,-3.7544508004,0.6481519038,1.7188892756
C,0,-4.7813831439,1.9568412738,-0.0025886011
O,0,-0.9683660325,0.867617882,1.0483402676
N,0,1.0573353732,-1.027584265,-2.4017446327
O,0,0.9584115823,-0.3833785012,-3.4314420686
O,0,2.090852593,-1.5291227013,-1.9948986193
H,0,-3.402866931,-0.9280382509,-1.7554353978
H,0,-1.3226662282,-0.1085093936,-2.920367559
H,0,0.9722413169,-2.3182728026,-0.0423682536
H,0,-1.0560062321,-2.8611210919,1.2697941754
H,0,-4.5451121555,-2.0876333752,0.075064798
H,0,-3.5064330199,-3.1301017198,1.2132134178
H,0,-3.0622634926,-0.1621782209,1.9363019977
H,0,-4.7192337853,0.4289134022,2.1863659918
H,0,-3.3487513536,1.5702152245,2.1675106327
H,0,-5.7039798711,1.892883182,0.5808298329
H,0,-4.2754362147,2.9024882045,0.2611911995
H,0,-5.0509385379,1.9863842443,-1.0616558752
H,0,-2.984038038,1.3238030554,-1.4557051519
H,0,0.260853689,3.1257434446,0.6823850296
H,0,1.0345874707,1.8987511654,-0.3510575782
H,0,0.575431688,3.4864027806,-1.0493612551

Naked TSopposite Side Gas phase

This is an alternative conformation of **6**‡ that is lower in energy in the gas phase but is higher in energy in PCM calculations.
home/biswas/nitrodoc2/gas/TSoppSideGas
TS conf C with ester on other side of ring
M062X/6-31+g**
E(RM062X) = -876.802541278

Zero-point correction= 0.276089 (Hartree/Particle)
Thermal correction to Energy= 0.293653
Thermal correction to Enthalpy= 0.294597
Thermal correction to Gibbs Free Energy= 0.230265
Sum of electronic and ZPE= -876.526452
Sum of electronic and thermal Energies= -876.508889
Sum of electronic and thermal Enthalpies= -876.507945
Sum of electronic and thermal Free Energies= -876.572277

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.270	65.608	135.398

C,0,-1.025879193,-0.3489184122,2.2200699083
C,0,-0.45509286,-0.7360955172,3.4058063412
C,0,0.9422626988,-0.9274509357,3.4594491227
C,0,1.7509985392,-0.742022864,2.3570661506
C,0,1.1610478217,-0.3896783005,1.1375586382
C,0,-0.2375747877,-0.1382146114,1.0430418573
C,0,-0.8102846869,0.0335756863,-0.2158030535
N,0,-0.4755919241,-2.2013982634,-0.7227967126
C,0,0.6331169198,-2.6186665553,-0.0837065997
C,0,1.9773209518,-2.4991317499,-0.6216402935
O,0,2.8551867573,-3.1428020132,0.1756474509
C,0,4.226682861,-3.0090819328,-0.1949673455
C,0,-0.5116253872,-2.083471813,-2.1898023508
C,0,-1.7272185725,-2.7093856969,-0.1526015743
O,0,2.3212346309,-1.8904374468,-1.6234769107
N,0,1.5491596386,-1.3315034567,4.7241723982
O,0,0.8060294575,-1.5143127769,5.6771560478
O,0,2.7623507841,-1.4688476237,4.7625661312
H,0,-2.0983849378,-0.177669508,2.1683285906
H,0,-1.0436770284,-0.8880034341,4.3024622146
H,0,2.8206748079,-0.893862202,2.4452715233
H,0,1.7940770016,-0.1562481902,0.2866609476
H,0,-1.8818443319,0.1836866555,-0.3192275361
H,0,-0.1889742255,0.3403935873,-1.0513891146
H,0,0.3783939414,-1.5698120329,-2.5412473057
H,0,-1.4097135897,-1.5269818669,-2.4604607405
H,0,-0.5510291242,-3.0878369957,-2.628450781
H,0,-2.5668019392,-2.1850971594,-0.6091805524
H,0,-1.8121038168,-3.7851993786,-0.345370344
H,0,-1.7281224179,-2.5278237596,0.9247027929
H,0,0.5114173044,-3.1022055547,0.8768387437
H,0,4.3949347506,-3.4139834179,-1.1952381095
H,0,4.5233670694,-1.9570506393,-0.1832580034
H,0,4.7866898866,-3.5728398203,0.549023469

Naked ylide (2a) in DMSO

/home/biswas/23arom_Doc_first_download/nitro /ylideDMSO
starting material opt
M062X/6-31+g**

E(RM062X) = -876.847914470

Zero-point correction= 0.278826 (Hartree/Particle)
Thermal correction to Energy= 0.296349
Thermal correction to Enthalpy= 0.297293
Thermal correction to Gibbs Free Energy= 0.232224
Sum of electronic and ZPE= -876.569088
Sum of electronic and thermal Energies= -876.551566
Sum of electronic and thermal Enthalpies= -876.550621
Sum of electronic and thermal Free Energies= -876.615691

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.962	65.549	136.950

C,0,1.2859487011,0.9744121364,-1.6656100078
C,0,-0.0830885107,1.1074910783,-1.8593925548
C,0,-0.8142129554,1.8095000792,-0.9075301536
C,0,-0.2330692915,2.3929257646,0.2116934095
C,0,1.138193274,2.2467256602,0.3861072488
C,0,1.9006462674,1.52234133,-0.5349698653
C,0,3.3793634271,1.3520826156,-0.3294832095
N,0,3.7503381137,0.0728465287,0.4216609354
C,0,3.297775214,-1.1463254076,-0.272465123
C,0,2.0047035419,-1.6401500188,-0.1510160105
O,0,1.7909017753,-2.6749786747,-1.0527709816
C,0,0.5252321556,-3.3132874125,-0.9663586062
C,0,3.2613449727,0.1531394135,1.8376668879
C,0,5.2481592858,0.0373171539,0.47299419
O,0,1.0838149163,-1.3089869649,0.6233320391
N,0,-2.263434901,1.9559007976,-1.102307831
O,0,-2.7625831913,1.4552225599,-2.0969806888
O,0,-2.8964305714,2.5705699183,-0.2591300616
H,0,1.8815446629,0.4329093813,-2.3932949388
H,0,-0.5774814871,0.6831353793,-2.7245680988
H,0,-0.8390972033,2.9456608647,0.9186108743
H,0,1.6154420748,2.7011796129,1.2495103896
H,0,3.8927003223,1.2785788325,-1.2901929442
H,0,3.7958516485,2.189881445,0.2368641159
H,0,2.175906459,0.1758568772,1.8366556475
H,0,3.6888120169,1.0471113528,2.295299261
H,0,3.6063341428,-0.7442821471,2.3505856032
H,0,5.6104220832,0.944715027,0.9576838181
H,0,5.5428554511,-0.8467193469,1.0360186625
H,0,5.6302440831,-0.0244102234,-0.5457930356
H,0,3.9421967837,-1.4427091327,-1.086421574
H,0,0.372418723,-3.7634120442,0.0185594869
H,0,-0.2890588059,-2.6101761303,-1.1628623276
H,0,0.5332448212,-4.0921353059,-1.7294965569

Naked TS (6‡) in DMSO

/home/biswas/23arom_Doc_first_download/nitro /TSDMSO
nitrobenzyl rearr uncoordinated
M062X/6-31+G**
E(RM062X) = -876.822188916

Zero-point correction= 0.275744 (Hartree/Particle)
Thermal correction to Energy= 0.292996
Thermal correction to Enthalpy= 0.293940
Thermal correction to Gibbs Free Energy= 0.230987
Sum of electronic and ZPE= -876.546445
Sum of electronic and thermal Energies= -876.529193
Sum of electronic and thermal Enthalpies= -876.528249
Sum of electronic and thermal Free Energies= -876.591202

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.858	65.435	132.496

C,0,-1.1446920281,-0.4743877968,1.9506932627
C,0,-1.0669459527,-0.8317301028,3.2936216701
C,0,0.1613729531,-0.7550184922,3.9339612955
C,0,1.3158109735,-0.2555718135,3.2959518933
C,0,1.2322908798,0.1025322156,1.9754229956
C,0,0.005447858,-0.0136305776,1.2517395854
C,0,-0.0408920026,0.0731490471,-0.1466603684
N,0,-0.0570965567,-2.0844879588,-0.5015495685
C,0,-0.8687436511,-2.7082386916,0.3787230589
C,0,-0.4597236178,-3.3014825932,1.6303726521
O,0,-1.5372840408,-3.8587039423,2.2426278594
C,0,-1.2914822549,-4.4216500491,3.5315290957
C,0,1.3966464883,-2.3269694645,-0.4410703306
C,0,-0.5680943679,-2.0419422116,-1.8860007027
O,0,0.6589742621,-3.3517134361,2.1276430278
N,0,0.2563952247,-1.1867169849,5.3121089079
O,0,-0.7375219369,-1.6691663246,5.8481223471
O,0,1.3319286124,-1.0651475918,5.8893426721
H,0,-2.1070457897,-0.4839253494,1.4498398325
H,0,-1.9380581471,-1.1905581177,3.8299812964
H,0,2.2453641949,-0.1818064656,3.846733498
H,0,2.1137939454,0.4714398143,1.4581975801
H,0,-1.0014555605,0.1913849121,-0.638456079
H,0,0.8309518931,0.4149728842,-0.6985614232
H,0,1.7765246591,-2.0370274181,0.5361299959
H,0,1.8680206171,-1.7399076588,-1.2283415641
H,0,1.5868453225,-3.3923089388,-0.6014102491
H,0,-0.0154814537,-1.2882723888,-2.4462817599
H,0,-0.432417146,-3.02516867,-2.3458033118
H,0,-1.6272610285,-1.7860073128,-1.8701610364
H,0,-1.9191647675,-2.754310428,0.1234345541
H,0,-0.5253734412,-5.197633208,3.4749074723
H,0,-0.9729763916,-3.6449371446,4.2333113561
H,0,-2.2403687488,-4.8490717415,3.8514884849

Naked 7----8 complex in DMSO

/home/biswas/nitrodoc2/ComplexDMSO
opt of complex found in ch2cl2
M062X/6-31+g**
E(RM062X) = -876.827787533
(Potential energy of triplet for this geometry: -876.790872551)

Zero-point correction= 0.274989 (Hartree/Particle)
Thermal correction to Energy= 0.293606
Thermal correction to Enthalpy= 0.294551
Thermal correction to Gibbs Free Energy= 0.228515
Sum of electronic and ZPE= -876.552798
Sum of electronic and thermal Energies= -876.534181
Sum of electronic and thermal Enthalpies= -876.533237
Sum of electronic and thermal Free Energies= -876.599273

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.241	68.558	138.984

C,0,-1.0673763244,1.3601157034,-0.38254811
C,0,-1.0184638047,0.9135196075,0.9149278833
C,0,0.2041245541,0.9144223502,1.6201757279
C,0,1.3869138658,1.419701797,0.9963916051
C,0,1.3396942507,1.893240979,-0.2757213683
C,0,0.1055684561,1.9053194246,-1.0522254894
C,0,0.0618682025,2.333786583,-2.3438754673
N,0,0.0087956121,-0.6394178907,-2.7354192648
C,0,-0.7799914948,-1.0123241947,-1.7824189974
C,0,-0.3273004619,-1.597265822,-0.4854622823
O,0,-1.3886654635,-2.0929710513,0.1441202994
C,0,-1.1424354106,-2.6775041608,1.4343164357
C,0,1.4771250062,-0.6631000457,-2.6380347594
C,0,-0.5519752278,-0.3452154985,-4.0648593039
O,0,0.8128608155,-1.6556750445,-0.0851776198
N,0,0.2584885191,0.4326516537,2.9245507847
O,0,-0.7792161456,-0.008730161,3.4655603266
O,0,1.3444688081,0.4393687223,3.5393593337
H,0,-2.0227596498,1.4002438613,-0.9001188683
H,0,-1.9110938146,0.5369136151,1.4032245745
H,0,2.3141994497,1.4150859909,1.5574957532
H,0,2.2403731799,2.2862281467,-0.7405924212
H,0,-0.8730625001,2.3480736967,-2.8964291562
H,0,0.9497208446,2.7144109134,-2.8403293834
H,0,1.7879989445,-0.1572246606,-1.7237868559
H,0,1.8737831838,-0.1537768835,-3.5134289227
H,0,1.8180919879,-1.700316598,-2.6159066511
H,0,-0.0465844278,0.5249531127,-4.4774867101
H,0,-0.3792934776,-1.2163465619,-4.7027010638
H,0,-1.619666584,-0.1521195062,-3.9756109407
H,0,-1.8480932185,-1.0147726959,-1.9723683609
H,0,-0.347020108,-3.4203533606,1.3619112207
H,0,-0.8713880337,-1.8929183465,2.1462176088
H,0,-2.0815565331,-3.1440376753,1.7225754434

Naked TS to 23 in DMSO

This is a saddle point for conversion of **7----8** to **3a**.
/home/biswas/nitrodoc2/2ndTSto23DMSO
search for 23 ts
M062X/6-31+g**
E(RM062X) = -876.824744558

Zero-point correction= 0.275948 (Hartree/Particle)
Thermal correction to Energy= 0.293576
Thermal correction to Enthalpy= 0.294520
Thermal correction to Gibbs Free Energy= 0.230907
Sum of electronic and ZPE= -876.548797
Sum of electronic and thermal Energies= -876.531169
Sum of electronic and thermal Enthalpies= -876.530225
Sum of electronic and thermal Free Energies= -876.593838

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.221	65.813	133.885

C,0,-0.9386520521,1.3385219903,-0.4955076247
C,0,-1.0330450005,1.0656841288,0.8948852944
C,0,0.0905969743,1.1405538392,1.6788485078
C,0,1.3477551943,1.6132025195,1.1603567721
C,0,1.4193027385,2.028250011,-0.1264054634
C,0,0.2597718967,2.0078906528,-1.009722931
C,0,0.3152172713,2.4597649831,-2.2859929945
N,0,-0.0474906174,-0.3555557877,-2.5845569508
C,0,-0.7653863497,-0.5366975171,-1.4668315658
C,0,-0.247945953,-1.3450209784,-0.3228287816
O,0,-1.2769912594,-1.821940445,0.3851473895
C,0,-0.9351085506,-2.5352752262,1.5825015199
C,0,1.3981673671,-0.5475311835,-2.6420261011
C,0,-0.7464929141,-0.2148779576,-3.8586841407
O,0,0.9125921736,-1.5364348353,-0.0328250237
N,0,0.0029860588,0.7752486987,3.0642349522
O,0,-1.0590209789,0.33299138,3.5047642102
O,0,1.0035451626,0.9108637933,3.7673829781
H,0,-1.8717112834,1.5483408875,-1.0116940448
H,0,-1.971406475,0.734798189,1.326296522
H,0,2.210246445,1.6422720551,1.8144275505
H,0,2.353340442,2.4231041926,-0.5174688592
H,0,-0.567894456,2.4676385492,-2.917263228
H,0,1.234099963,2.8659728849,-2.6986060724
H,0,1.871018274,-0.0972928757,-1.7684697603
H,0,1.76625513,-0.0631978025,-3.5467823657
H,0,1.6491602701,-1.6137961829,-2.6685751424
H,0,-0.2090044275,0.4923098377,-4.4920223067
H,0,-0.8076218792,-1.1831313384,-4.3695784407
H,0,-1.7552994645,0.1627213303,-3.685362241
H,0,-1.833187596,-0.6482223215,-1.6190934365
H,0,-0.3210096425,-3.403722395,1.3399526421
H,0,-0.3958414439,-1.8776705747,2.2675364693
H,0,-1.8829530175,-2.8420905019,2.0188126671

Naked 23 product (3a) in DMSO

/home/biswas/23arom_Doc_first_download/nitro
/23prodDMSO
product opt
M062X/6-31+g**
E(RM062X) = -876.838907733

Zero-point correction= 0.277130 (Hartree/Particle)
Thermal correction to Energy= 0.295138
Thermal correction to Enthalpy= 0.296082
Thermal correction to Gibbs Free Energy= 0.229627
Sum of electronic and ZPE= -876.561778
Sum of electronic and thermal Energies= -876.543770
Sum of electronic and thermal Enthalpies= -876.542826
Sum of electronic and thermal Free Energies= -876.609281

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.202	66.274	139.866

C,0,-2.5245823453,-0.7507528728,-1.1284144146
C,0,-1.2907652382,-0.6915546765,-1.9834009638
C,0,-0.1467285612,-1.2339373623,-1.5467870447
C,0,-0.0226213594,-1.9961976502,-0.3092331174
C,0,-1.140123343,-2.2751797169,0.3837709844
C,0,-2.4627887421,-1.844503935,-0.0811403388
C,0,-3.579717139,-2.422967329,0.3850593245
N,0,-3.9533619613,0.7844019924,0.279434717
C,0,-2.7819751701,0.7063677438,-0.577465664
C,0,-1.4923581342,1.2833371072,0.0129309834
O,0,-1.002797977,2.260860148,-0.7593205378
C,0,0.2612018972,2.806018299,-0.3536180162

C,0,-3.7352498236,0.6143910458,1.7158918339
C,0,-4.7309393657,1.9967760355,0.0346416861
O,0,-0.9483853375,0.90094101,1.0246647856
N,0,1.0593385062,-1.073103412,-2.3732050716
O,0,0.9899396261,-0.4086628981,-3.3950626862
O,0,2.0820190917,-1.6158164529,-1.9850219126
H,0,-3.3940231734,-0.9300398331,-1.7685910202
H,0,-1.3169214548,-0.1391185928,-2.9173051294
H,0,0.9546251046,-2.3392976804,0.0037035262
H,0,-1.0883258931,-2.8796641837,1.2852620909
H,0,-4.5580931381,-2.1444245042,0.0056838583
H,0,-3.5340053184,-3.1755033155,1.1674966875
H,0,-3.0696379318,-0.2239968543,1.9105568594
H,0,-4.702200095,0.4163730927,2.1876394597
H,0,-3.300522104,1.5155291711,2.1788740422
H,0,-5.6508893205,1.9488326739,0.6232934417
H,0,-4.1889902053,2.9140365774,0.322828133
H,0,-5.0019256551,2.0646966002,-1.0216761191
H,0,-2.9932277513,1.3021221168,-1.4694010068
H,0,0.1825253432,3.2366966672,0.6457299421
H,0,1.0206411568,2.0207665645,-0.3575992037
H,0,0.4988118123,3.5733594242,-1.0865901091

Naked TS opposite Side in DMSO

This is an alternative conformation of **6**‡ that is lower in energy in the gas phase but is higher in energy in PCM calculations.
/home/biswas/nitrodoc2/TSoppSideDMSO
TS conf C with ester on other side of ring
M062X/6-31+G**
E(RM062X) = -876.819621831

Zero-point correction= 0.275564 (Hartree/Particle)
Thermal correction to Energy= 0.293123
Thermal correction to Enthalpy= 0.294067
Thermal correction to Gibbs Free Energy= 0.229658
Sum of electronic and ZPE= -876.544058
Sum of electronic and thermal Energies= -876.526499
Sum of electronic and thermal Enthalpies= -876.525555
Sum of electronic and thermal Free Energies= -876.589964

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.937	65.714	135.561

C,0,-1.0136593441,-0.3816732059,2.2184979923
C,0,-0.4430278228,-0.7452990855,3.412587033
C,0,0.9586105671,-0.8982960711,3.4819309629
C,0,1.7733033766,-0.6951961095,2.3769684126
C,0,1.1862962779,-0.351953102,1.162064179
C,0,-0.2198709636,-0.1551598122,1.049363989
C,0,-0.7871385578,-0.0103840874,-0.2183426316
N,0,-0.4847722853,-2.2038234556,-0.734600133
C,0,0.6169575523,-2.6685564324,-0.1238686195
C,0,1.9640938083,-2.5201735312,-0.6366389895
O,0,2.8363328866,-3.1904490354,0.1461663554
C,0,4.2178516471,-3.0252934656,-0.1815541544
C,0,-0.5357053309,-2.0519692951,-2.2025483197
C,0,-1.7464134116,-2.7117491714,-0.1700125135
O,0,2.3226222491,-1.8774401756,-1.6164208391
N,0,1.5610903675,-1.2792477077,4.7376490667
O,0,0.8274230361,-1.4647817965,5.7047126
O,0,2.7812148493,-1.4054211351,4.7946068215
H,0,-2.090889377,-0.2545481777,2.1537673712
H,0,-1.0446120701,-0.9117876142,4.2976693513
H,0,2.8467024078,-0.8180756394,2.4641313667
H,0,1.8197212945,-0.1324389729,0.3079983338
H,0,-1.860305625,0.1146497754,-0.3315114577
H,0,-0.1641966828,0.3102385061,-1.0476479209
H,0,0.3526601835,-1.5360262157,-2.5521358237
H,0,-1.4323046843,-1.4854865713,-2.4518918997
H,0,-0.5894933793,-3.0491161802,-2.6519990965
H,0,-2.5789137467,-2.1584619155,-0.6014990415
H,0,-1.8434254191,-3.7758001992,-0.406952495
H,0,-1.7339242621,-2.5741987601,0.9128309447
H,0,0.4905597247,-3.1545328564,0.8349566502
H,0,4.4180546779,-3.3839899122,-1.1930667151
H,0,4.5011676084,-1.9726272786,-0.1057923485
H,0,4.765017448,-3.6193093129,0.5477865687

Naked TS Dissociation in DMSO (Unrestricted)

This is an alternative conformation of **6**‡ with the ylide twisted away from the aromatic ring, making this a purely dissociative transition state. It is 4.2 kcal/mol less stable than **6**‡. Its S**2 value is 0.05.
Nitro TS
um062x/6-31+G**
E(UM062X) = -876.810702539

Zero-point correction= 0.274327 (Hartree/Particle)
Thermal correction to Energy= 0.292384
Thermal correction to Enthalpy= 0.293328
Thermal correction to Gibbs Free Energy= 0.226154
Sum of electronic and ZPE= -876.536376
Sum of electronic and thermal Energies= -876.518319
Sum of electronic and thermal Enthalpies= -876.517374
Sum of electronic and thermal Free Energies= -876.584549

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.474	66.276	141.380

C,0,1.2330509266,-0.1749723466,3.4311705136
C,0,1.2184713465,-0.2537516217,2.0554773986
C,0,-0.0075137204,-0.3244877491,1.3309931981
C,0,-1.2223866682,-0.3076816426,2.0777449677
C,0,-1.2163048649,-0.2268202635,3.4526095518
C,0,0.013709632,-0.1636300853,4.1238535084
C,0,-0.0197249766,-0.4598558244,-0.0727901548
N,0,0.023940476,-0.076010643,5.5597941268
O,0,1.1074159314,-0.0253517023,6.1389705974
O,0,-1.0516007055,-0.054954937,6.1555773516
N,0,0.0298392726,-2.6366299684,-0.7023123609
C,0,-0.0694574144,-2.6317739904,-2.0561623463
C,0,-1.2893098557,-2.3392413171,-2.7563707418
O,0,-1.1021059827,-2.4146828978,-4.0967078564
C,0,-2.246326426,-2.1161405188,-4.8976838738
C,0,1.3421239022,-3.0336083449,-0.176081985
O,0,-2.3759481521,-2.037356214,-2.2661181217
H,0,0.8972098012,-0.315524881,-0.6343752101

H,0,-0.956071739,-0.3696104453,-0.6144466264
H,0,-2.1676040967,-0.3556306037,1.5448683918
H,0,-2.1394085891,-0.2080822246,4.0190301645
H,0,2.1641989171,-0.1172996275,3.9816345706
H,0,2.1560543684,-0.2552057795,1.5069757856
H,0,0.8549784009,-2.6560280292,-2.6186439837
H,0,-1.9148551282,-2.2092305717,-5.930179308
H,0,-3.0521534811,-2.8241996945,-4.6919097274
H,0,-2.5977305786,-1.1009223632,-4.7010169313
C,0,-1.0770343615,-3.1487005761,0.1212066417
H,0,-0.8646497577,-2.9103476199,1.1638215009
H,0,-2.0127329186,-2.6930267687,-0.1902570617
H,0,-1.1298942863,-4.2362241165,-0.0022156392
H,0,1.4096905379,-2.7293863318,0.8695199683
H,0,1.4509243031,-4.1208233924,-0.2473686214
H,0,2.1287438875,-2.5451749077,-0.7517296878

Naked ylide (2a) in CH2Cl2

/home/biswas/23arom_Doc_first_download/nitro
/ylideCH2Cl2
nitrobenzyl sm naked in CH2Cl2
M062X/6-31+G**
E(RM062X) = -876.843676287

Zero-point correction= 0.278849 (Hartree/Particle)
Thermal correction to Energy= 0.296385
Thermal correction to Enthalpy= 0.297329
Thermal correction to Gibbs Free Energy= 0.232058
Sum of electronic and ZPE= -876.564827
Sum of electronic and thermal Energies= -876.547291
Sum of electronic and thermal Enthalpies= -876.546347
Sum of electronic and thermal Free Energies= -876.611618

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.985	65.535	137.374

C,0,1.2881510841,0.961092326,-1.6629636969
C,0,-0.0816517006,1.0881752036,-1.855141261
C,0,-0.8139868475,1.7924292511,-0.9063759464
C,0,-0.2339505713,2.3819506692,0.2097929246
C,0,1.1377985386,2.2408524375,0.383404583
C,0,1.9020157917,1.5160449034,-0.5354975661
C,0,3.3809675493,1.3504369368,-0.3286900215
N,0,3.756323768,0.0723583989,0.4229557916
C,0,3.3069356506,-1.149116252,-0.2691631806
C,0,2.0085426127,-1.6338422096,-0.1503722734
O,0,1.7882211339,-2.6671877624,-1.0496271437
C,0,0.508088379,-3.2773177731,-0.9737775075
C,0,3.2660030106,0.1526233393,1.8387107356
C,0,5.253112619,0.0403639006,0.4744350756
O,0,1.0911903037,-1.2908267094,0.6204377423
N,0,-2.2644266628,1.9345695037,-1.1011630344
O,0,-2.7612626396,1.429501252,-2.0943258172
O,0,-2.8970315221,2.5513759978,-0.2597154049
H,0,1.8842714374,0.415350009,-2.3870884389
H,0,-0.5768252257,0.656938615,-2.7164627936
H,0,-0.8424661024,2.9338546948,0.9151927174
H,0,1.6144770879,2.6984738256,1.2455772977
H,0,3.8953035068,1.2776096564,-1.2890543754
H,0,3.7941324999,2.1907205101,0.237186804
H,0,2.1802341306,0.1699210987,1.8359018534
H,0,3.6903015463,1.0488522776,2.2957694416
H,0,3.6128801377,-0.7438285115,2.3519670874
H,0,5.6143082844,0.9487428108,0.958583164
H,0,5.5496604983,-0.8432996495,1.0371105614
H,0,5.6355193968,-0.0217121477,-0.5443867148
H,0,3.9544599283,-1.4505746042,-1.0786121733
H,0,0.3366902886,-3.7212083903,0.0106635899
H,0,-0.2874176402,-2.5545746178,-1.1763028196
H,0,0.5053677279,-4.0568179905,-1.7363712003

Naked TS (6‡) in CH2Cl2

/home/biswas/23arom_Doc_first_download/nitro /TSCH2Cl2
nitrobenzyl rearr naked in CH2Cl2
M062X/6-31+G**
E(RM062X) = -876.819242748

Zero-point correction= 0.275904 (Hartree/Particle)
Thermal correction to Energy= 0.293122
Thermal correction to Enthalpy= 0.294066
Thermal correction to Gibbs Free Energy= 0.231259
Sum of electronic and ZPE= -876.543339
Sum of electronic and thermal Energies= -876.526121
Sum of electronic and thermal Enthalpies= -876.525176
Sum of electronic and thermal Free Energies= -876.587984

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.937	65.400	132.189

C,0,-1.1436487214,-0.4711533411,1.94423616
C,0,-1.0738558406,-0.8287863785,3.2884202627
C,0,0.1512234276,-0.7579477399,3.9332204109
C,0,1.3111599149,-0.2666094162,3.3003579073
C,0,1.2351328891,0.093171108,1.9797500833
C,0,0.0109072748,-0.0141935514,1.2511945798
C,0,-0.0294401999,0.0758550407,-0.1476507953
N,0,-0.060374956,-0.2827490262,-0.5034152353
C,0,-0.8699103946,-2.7030400944,0.3820244538
C,0,-0.4535899259,-3.2976153025,1.631701343
O,0,-1.527394737,-3.8544506638,2.249853872
C,0,-1.2715306248,-4.4196438239,3.5362059747
C,0,1.3922331783,-2.3323380577,-0.4491203559
C,0,-0.5777939657,-2.0406442662,-1.8843347236
O,0,0.6677109608,-3.3460132938,2.12073562
N,0,0.2379622216,-1.1868603003,5.3155926041
O,0,-0.7585665871,-1.6718720871,5.8425506644
O,0,1.3077585767,-1.0573081803,5.8989095042
H,0,-2.1043593329,-0.4735170959,1.4400370555
H,0,-1.9487490157,-1.182829656,3.8217239575
H,0,2.2384766424,-0.2007941836,3.855825906
H,0,2.121143049,0.4571434766,1.4666591925
H,0,-0.987132624,0.203751071,-0.642722516
H,0,0.8462407412,0.4159873414,-0.6947490935
H,0,1.7776125841,-2.0418523224,0.5258133383
H,0,1.8624793895,-1.7497076795,-1.2406202433
H,0,1.5775924599,-3.3991488365,-0.6059548651
H,0,-0.0248634585,-1.290252884,-2.4490892367
H,0,-0.4504450632,-3.0250735941,-2.344336604
H,0,-1.6357593042,-1.7791726272,-1.8637742461
H,0,-1.9214171943,-2.7492545971,0.1315071106

H,0,-0.4968567288,-5.1865251978,3.4737710176
H,0,-0.9586150988,-3.6425866227,4.2398758091
H,0,-2.215040537,-4.8579812177,3.8573890877

Naked 7----8 complex in CH2Cl2

/home/biswas/nitrodoc2/ComplexCH2Cl2
opt from irc of naked ts
M062X/6-31+g**
E(RM062X) = -876.823041194
(Potential energy of triplet for this geometry: -876.786699998)

Zero-point correction= 0.275255 (Hartree/Particle)
Thermal correction to Energy= 0.293764
Thermal correction to Enthalpy= 0.294708
Thermal correction to Gibbs Free Energy= 0.229022
Sum of electronic and ZPE= -876.547786
Sum of electronic and thermal Energies= -876.529278
Sum of electronic and thermal Enthalpies= -876.528333
Sum of electronic and thermal Free Energies= -876.594019

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.339	68.361	138.247

C,0,-1.0561277768,1.3204499618,-0.4006752001
C,0,-1.0126565594,0.8957221863,0.9130416528
C,0,0.1996126806,0.9134257834,1.613959774
C,0,1.3833979562,1.4220033422,1.00062945
C,0,1.3399130509,1.8848747555,-0.2765714045
C,0,0.112308424,1.8796005986,-1.0582590184
C,0,0.0766697464,2.2855037238,-2.3599800552
N,0,0.0091110977,-0.5845410334,-2.7234545033
C,0,-0.7783147883,-0.9580285229,-1.7565760076
C,0,-0.3261702308,-1.5778584618,-0.4833387694
O,0,-1.3905663751,-2.0804408865,0.1453392061
C,0,-1.1389678819,-2.6868631981,1.4232356941
C,0,1.4742788914,-0.6371780995,-2.6371146948
C,0,-0.560996452,-0.3387944164,-4.0561807789
O,0,0.8138560559,-1.6578755615,-0.0825931913
N,0,0.2497265541,0.4414742513,2.9403934582
O,0,-0.7818478305,-0.0131673882,3.4640229993
O,0,1.3243165722,0.4832801989,3.5560534587
H,0,-2.0141369526,1.3748408174,-0.9112589403
H,0,-1.9053644643,0.5213761343,1.4028409039
H,0,2.3053950666,1.429007279,1.5699973974
H,0,2.2390692247,2.2856427368,-0.7375482766
H,0,-0.8567622104,2.300134215,-2.9147089026
H,0,0.9639046882,2.6725020339,-2.8525289169
H,0,1.8016790018,-0.1698819295,-1.7081309784
H,0,1.8762979972,-0.1036221675,-3.4960514543
H,0,1.8023341249,-1.6798389171,-2.6516565787
H,0,-0.0299788899,0.4867648614,-4.5253990404
H,0,-0.444129987,-1.2472196206,-4.6550622833
H,0,-1.6176603471,-0.0919711563,-3.9610550579
H,0,-1.845334015,-0.9719207868,-1.9491354113
H,0,-0.3483984092,-3.4332866528,1.3349777297
H,0,-0.8572627491,-1.9181544496,2.1476920597
H,0,-2.0790622132,-3.1519936309,1.7114206801

Naked TS to 23 in CH2Cl2

This is a saddle point for conversion of **7----8** to **3a**.
/home/biswas/nitrodoc2/2ndTSto23CH2Cl2
search for 23 ts
M062X/6-31+g**
E(RM062X) = -876.821928722

Zero-point correction= 0.276018 (Hartree/Particle)
Thermal correction to Energy= 0.293646
Thermal correction to Enthalpy= 0.294590
Thermal correction to Gibbs Free Energy= 0.230965
Sum of electronic and ZPE= -876.545911
Sum of electronic and thermal Energies= -876.528283
Sum of electronic and thermal Enthalpies= -876.527339
Sum of electronic and thermal Free Energies= -876.590963

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.266	65.824	133.910

C,0,-0.9514065678,1.3559360144,-0.4780313893
C,0,-1.0305662218,1.0700167279,0.9072610436
C,0,0.1024852805,1.1393733012,1.6799033605
C,0,1.3518601365,1.6132054199,1.1499499189
C,0,1.410769483,2.0304374149,-0.1374918094
C,0,0.2436465151,2.0106163589,-1.0092396281
C,0,0.2902215365,2.4483145566,-2.2925103732
N,0,-0.0393808924,-0.3557420001,-2.5842808407
C,0,-0.7669346048,-0.5565708358,-1.4804171913
C,0,-0.2565268387,-1.3485968258,-0.3251426963
O,0,-1.2907248282,-1.8241206878,0.3774687616
C,0,-0.9547264466,-2.5289980534,1.5816441239
C,0,1.4082080587,-0.5428982949,-2.6267551007
C,0,-0.7255556616,-0.209737723,-3.8651046542
O,0,0.902294618,-1.5340745434,-0.0256159002
N,0,0.0306645281,0.7648422631,3.0648672939
O,0,-1.026097897,0.3162269939,3.5108633888
O,0,1.0373102561,0.8996501937,3.7577651337
H,0,-1.8877325438,1.5491648306,-0.9944234758
H,0,-1.9637859288,0.7366792196,1.3478355103
H,0,2.2209290679,1.6397064272,1.79541731
H,0,2.3413728534,2.4248609659,-0.5370640456
H,0,-0.60017588,2.4590866811,-2.9135440218
H,0,1.2057826718,2.8500668497,-2.7165795028
H,0,1.8686576848,-0.0941781686,-1.7459160658
H,0,1.7837618915,-0.0554584898,-3.526548829
H,0,1.6613290822,-1.6084764091,-2.6516029504
H,0,-0.1782416801,0.495463233,-4.4917241294
H,0,-0.7870728053,-1.1775281604,-4.3768649447
H,0,-1.7336914841,0.1732528993,-3.6999037825
H,0,-1.8351808279,-0.6541354985,-1.6372025983
H,0,-0.3309280327,-3.3932528203,1.3486738359
H,0,-0.4280863802,-1.8641652715,2.2692306396
H,0,-1.9044861419,-2.8412945685,2.0099336089

Naked 23 product (3a) in CH2Cl2

/home/biswas/23arom_Doc_first_download/nitro
/23prodCH2Cl2
nitrobenzyl 23 prod naked ch2cl2
M062X/6-31+G**
E(RM062X) = -876.836977053

Zero-point correction= 0.277224 (Hartree/Particle)
Thermal correction to Energy= 0.295207
Thermal correction to Enthalpy= 0.296151
Thermal correction to Gibbs Free Energy= 0.229813
Sum of electronic and ZPE= -876.559753
Sum of electronic and thermal Energies= -876.541770
Sum of electronic and thermal Enthalpies= -876.540826
Sum of electronic and thermal Free Energies= -876.607164

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.245	66.248	139.620

C,0,-2.5240529052,-0.7491667046,-1.1311203822
C,0,-1.2906682179,-0.6852348481,-1.9867324325
C,0,-0.1450819637,-1.2250480517,-1.5516705252
C,0,-0.0182976961,-1.9885107547,-0.3153230767
C,0,-1.1344295976,-2.271365934,0.3779544206
C,0,-2.4586970484,-1.8440199525,-0.0851901085
C,0,-3.5741795742,-2.4239780273,0.3823616944
N,0,-3.9567187291,0.7797712779,0.2788212716
C,0,-2.784018175,0.705817833,-0.5765615839
C,0,-1.4951370277,1.2805696472,0.0175597954
O,0,-1.0037382949,2.2602745681,-0.7520445408
C,0,0.2620486694,2.7989573111,-0.3444274108
C,0,-3.7398623784,0.6071262204,1.7152405946
C,0,-4.7363083125,1.990703007,0.0360166299
O,0,-0.953143809,0.8945587601,1.028204472
N,0,1.0613868759,-1.0576807436,-2.3779251681
O,0,0.9876259115,-0.3931042212,-3.3990746821
O,0,2.0858737072,-1.5950734965,-1.9884962529
H,0,-3.3941019373,-0.9301335684,-1.7701659213
H,0,-1.3168771691,-0.1299559425,-2.9190015215
H,0,0.9605771441,-2.327794876,-0.0033929222
H,0,-1.080173008,-2.8753602887,1.2795818018
H,0,-4.5536019678,-2.1447869337,0.0061760956
H,0,-3.5263386073,-3.1774416173,1.1637628008
H,0,-3.0702257081,-0.2281046783,1.909052334
H,0,-4.7067040715,0.4033794243,2.1848496779
H,0,-3.309337612,1.5088064738,2.1810804299
H,0,-5.6571249853,1.9394084696,0.6230802714
H,0,-4.1968877982,2.9087386064,0.3269983568
H,0,-5.0064303484,2.0609399891,-1.0204467468
H,0,-2.9943028084,1.3045384898,-1.4669426003
H,0,0.1863429529,3.2229171084,0.6580352715
H,0,1.0190301553,2.0112712116,-0.3533803394
H,0,0.5014983349,3.569766241,-1.0732487034

Naked TS opposite Side in CH2Cl2

This is an alternative conformation of **6**‡ that is lower in energy in the gas phase but is higher in energy in PCM calculations.
/home/biswas/nitrodoc2/TSoppSideCH2Cl2
TS conf C with ester on other side of ring
M062X/6-31+G**
E(RM062X) = -876.817025877

Zero-point correction= 0.275623 (Hartree/Particle)
Thermal correction to Energy= 0.293208
Thermal correction to Enthalpy= 0.294152
Thermal correction to Gibbs Free Energy= 0.229592
Sum of electronic and ZPE= -876.541403
Sum of electronic and thermal Energies= -876.523818
Sum of electronic and thermal Enthalpies= -876.522874
Sum of electronic and thermal Free Energies= -876.587433

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.991	65.715	135.877

C,0,-1.0155663567,-0.3779455383,2.2196799087
C,0,-0.4424569864,-0.7453980933,3.4113220158
C,0,0.9587782877,-0.9028075851,3.4759037994
C,0,1.7704007104,-0.700664704,2.3700654544
C,0,1.1805762781,-0.3554978336,1.1558716514
C,0,-0.2249546002,-0.1518377572,1.0481196038
C,0,-0.7951073597,-0.0019884634,-0.2171070636
N,0,-0.4838035919,-2.2038890022,-0.733481139
C,0,0.6183577419,-2.6602182443,-0.1170831549
C,0,1.9660929131,-2.517335961,-0.632551492
O,0,2.8370368661,-3.1837247607,0.1544015361
C,0,4.2181233684,-3.024799185,-0.1768157703
C,0,-0.5304590724,-2.0551048513,-2.2011291291
C,0,-1.7445715651,-2.7122058016,-0.1699663858
O,0,2.3238980439,-1.8814253026,-1.6161877527
N,0,1.5645384622,-1.2878594462,4.7316661722
O,0,0.8313038643,-1.4757816758,5.6974522737
O,0,2.7838033772,-1.4135893556,4.7839679098
H,0,-2.0923978841,-0.2448206237,2.1591302952
H,0,-1.0405284025,-0.9104711478,4.2990690769
H,0,2.8435160927,-0.8273196987,2.4552179315
H,0,1.8120375433,-0.1332368483,0.3010491697
H,0,-1.8684680818,0.1248872013,-0.3273396003
H,0,-0.1739468712,0.3176373606,-1.0480728874
H,0,0.3574359013,-1.5368916686,-2.5488841757
H,0,-1.4281827809,-1.4917877404,-2.4542641366
H,0,-0.5788193676,-3.052755604,-2.650660574
H,0,-2.5774768462,-2.1615311055,-0.6045447772
H,0,-1.8405357586,-3.7775602626,-0.4027501792
H,0,-1.7345655655,-2.5705854654,0.9125235338
H,0,0.4920720325,-3.1439871244,0.8428447525
H,0,4.415609229,-3.3916526318,-1.1859785388
H,0,4.5045100367,-1.9722289532,-0.1111151181
H,0,4.7647773421,-3.6140001265,0.5568517901

Naked TS Dissociation in CH2Cl2 (Unrestricted)

This is an alternative conformation of **6**‡ with the ylide twisted away from the aromatic ring, making this a purely dissociative transition state. It is 3.8 kcal/mol less stable than **6**‡. Its S**2 value is 0.05.
/home/bibaswanbiswas/medusa/bibaswanbiswas/Nitro/TSdiss/m062x.log
Alanine ammonium dimethyl allyl cation
um062x/6-31+G**
E(UM062X) = -876.808142563

Zero-point correction= 0.274426 (Hartree/Particle)
Thermal correction to Energy= 0.292493
Thermal correction to Enthalpy= 0.293437
Thermal correction to Gibbs Free Energy= 0.226192
Sum of electronic and ZPE= -876.533717

Sum of electronic and thermal Energies= -876.515650
Sum of electronic and thermal Enthalpies= -876.514705
Sum of electronic and thermal Free Energies= -876.581951

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.542	66.250	141.530

C,0,1.2250556894,-0.1728020112,3.4337722668
C,0,1.2161144508,-0.2508903822,2.0573264948
C,0,-0.0060214903,-0.3238053142,1.3280135862
C,0,-1.223423487,-0.3086596127,2.0693889423
C,0,-1.2230460239,-0.2287316814,3.4449577236
C,0,0.0035061529,-0.1647253767,4.1203217951
C,0,-0.0126571841,-0.4603749048,-0.0767083891
N,0,0.0077872737,-0.0796059995,5.5600114803
O,0,1.0888879718,-0.0299283209,6.1407430746
O,0,-1.0701384283,-0.0607567201,6.1483391801
N,0,0.0409127936,-2.6394832959,-0.7057410064
C,0,-0.0643127093,-2.6388960879,-2.060048383
C,0,-1.2868074045,-2.3364348902,-2.751715214
O,0,-1.1126521198,-2.4191493355,-4.0934645935
C,0,-2.2615996226,-2.1095759683,-4.8828044972
C,0,1.3547301151,-3.0337148565,-0.183732665
O,0,-2.3646109634,-2.0205627675,-2.2522814276
H,0,0.9064487574,-0.315225198,-0.6346798168
H,0,-0.9465957025,-0.3716812571,-0.6226926219
H,0,-2.1662350732,-0.3572115637,1.5322352603
H,0,-2.1478320175,-0.2111315542,4.0087389125
H,0,2.1531364608,-0.1128112,3.9892183835
H,0,2.1559684494,-0.2487664286,1.5125538147
H,0,0.8568368886,-2.6699741904,-2.6275485028
H,0,-1.9441178583,-2.2165440352,-5.9184417341
H,0,-3.0762715593,-2.8023313456,-4.6605033259
H,0,-2.5950047154,-1.0874440287,-4.6900689012
C,0,-1.0618383911,-3.1533503055,0.1217626225
H,0,-0.85005554,-2.9084611672,1.1631128306
H,0,-2.0002148155,-2.7042266578,-0.1916311878
H,0,-1.1093595931,-4.2418084078,0.0035144728
H,0,1.4260905515,-2.726732927,0.8609985695
H,0,1.4660888168,-4.1210813021,-0.2526830998
H,0,2.1387683275,-2.5454889053,-0.763386044

Naked ylide (2a) in CCl4

/home/biswas/23arom_Doc_first_download/nitro /ylideCCl4
starting material opt
M062X/6-31+g**
E(RM062X) = -876.832689103

Zero-point correction= 0.279212 (Hartree/Particle)
Thermal correction to Energy= 0.296597
Thermal correction to Enthalpy= 0.297541
Thermal correction to Gibbs Free Energy= 0.233198
Sum of electronic and ZPE= -876.553477
Sum of electronic and thermal Energies= -876.536092
Sum of electronic and thermal Enthalpies= -876.535148
Sum of electronic and thermal Free Energies= -876.599491

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	186.117	65.379	135.421

C,0,1.333071328,0.9944409438,-1.6933704503
C,0,-0.0399237456,1.0810956939,-1.8829944514
C,0,-0.7960711447,1.7280532844,-0.9138054635
C,0,-0.2371239834,2.3055467926,0.2183116086
C,0,1.1376713187,2.2056819308,0.3898500396
C,0,1.9249133892,1.5313921234,-0.5466478368
C,0,3.3999818668,1.3711841378,-0.3226454474
N,0,3.7657639431,0.0801715013,0.4165833096
C,0,3.3000021402,-1.1362037597,-0.2741850839
C,0,1.9814250474,-1.5770404529,-0.1633078075
O,0,1.7408346934,-2.6301096292,-1.0260015467
C,0,0.4379091997,-3.1881348771,-0.9408425299
C,0,3.279613879,0.1543435867,1.8348086554
C,0,5.2593995232,0.0317675218,0.4615676585
O,0,1.0686937965,-1.1660615176,0.5749374931
N,0,-2.2533199858,1.8224700822,-1.1040888231
O,0,-2.7296002774,1.3216311035,-2.1081497669
O,0,-2.9020047835,2.3985560252,-0.2474469179
H,0,1.9462140506,0.4815391959,-2.4273440699
H,0,-0.5231572491,0.656334829,-2.7542922241
H,0,-0.8683126922,2.8112278485,0.9383683206
H,0,1.5988685031,2.6473177244,1.2689559144
H,0,3.9287669507,1.3097792013,-1.2761859426
H,0,3.8035232698,2.2049962548,0.2613494021
H,0,2.1927347292,0.159267272,1.8316521096
H,0,3.6979748802,1.052909217,2.2948839979
H,0,3.6328998886,-0.742966845,2.3422506289
H,0,5.6344641714,0.9348411259,0.9465521645
H,0,5.5490616329,-0.8582625853,1.0179994694
H,0,5.6369634101,-0.0318216284,-0.5593885662
H,0,3.966814889,-1.4899776854,-1.0449691251
H,0,0.242760181,-3.5864549001,0.0586187294
H,0,-0.3271625973,-2.4419504719,-1.1728587542
H,0,0.4122877772,-3.9936320434,-1.6755666942

Naked TS (6‡) in CCl4

/home/biswas/23arom_Doc_first_download/nitro /TSCCl4
nitrobenzyl rearr uncoordinated
M062X/6-31+G**
E(RM062X) = -876.811451502

Zero-point correction= 0.276247 (Hartree/Particle)
Thermal correction to Energy= 0.293368
Thermal correction to Enthalpy= 0.294313
Thermal correction to Gibbs Free Energy= 0.232002
Sum of electronic and ZPE= -876.535205
Sum of electronic and thermal Energies= -876.518083
Sum of electronic and thermal Enthalpies= -876.517139
Sum of electronic and thermal Free Energies= -876.579450

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.092	65.340	131.144

C,0,-1.1430517881,-0.4668148038,1.9374277871
C,0,-1.0786106817,-0.8272362186,3.2829143065
C,0,0.1440278005,-0.7651808759,3.9280696393
C,0,1.3077400998,-0.2810108758,3.3002077349
C,0,1.23642753,0.0842770074,1.9805499246

C,0,0.0140584206,-0.0129757538,1.2494823084
C,0,-0.0216809228,0.0801925838,-0.150576809
N,0,-0.0648101113,-2.0785426035,-0.5046037934
C,0,-0.8748862499,-2.6948463535,0.3855773681
C,0,-0.4514220876,-3.2897356884,1.634821516
O,0,-1.5213054192,-3.844197061,2.2588315743
C,0,-1.2538154727,-4.4120192521,3.5422906932
C,0,1.3857906867,-2.3364767295,-0.449213546
C,0,-0.5817643609,-2.0438360525,-1.8830255441
O,0,0.672296046,-3.3330331005,2.1136913772
N,0,0.226306408,-1.1972326112,5.3163774491
O,0,-0.7697700147,-1.6945067857,5.8281709178
O,0,1.2888503537,-1.0518164736,5.9028556017
H,0,-2.1034377777,-0.4584956922,1.4325828199
H,0,-1.9551140643,-1.1779328468,3.8157060453
H,0,2.2329022199,-0.2263070799,3.860404789
H,0,2.1257612806,0.4450122782,1.4705938659
H,0,-0.977541456,0.2191335553,-0.6469171893
H,0,0.8553204854,0.4255757473,-0.6927937289
H,0,1.7717488121,-2.0464487996,0.525860762
H,0,1.8592440995,-1.758686341,-1.2430849908
H,0,1.5671855419,-3.4052369854,-0.599175215
H,0,-0.0260041962,-1.2992736666,-2.4537768454
H,0,-0.4633120073,-3.0315642777,-2.3396493005
H,0,-1.6383560364,-1.7750687482,-1.864418614
H,0,-1.9267559647,-2.7439776262,0.1374007566
H,0,-0.4576061964,-5.1560119445,3.4753714419
H,0,-0.9633193432,-3.6327475019,4.2526845609
H,0,-2.1868066334,-4.8769924222,3.856950337

Naked 23 product (3a) in CCl4

product opt
M062X/6-31+g**
E(RM062X) = -876.831663411

Zero-point correction= 0.277544 (Hartree/Particle)
Thermal correction to Energy= 0.295494
Thermal correction to Enthalpy= 0.296438
Thermal correction to Gibbs Free Energy= 0.230016
Sum of electronic and ZPE= -876.554119
Sum of electronic and thermal Energies= -876.536170
Sum of electronic and thermal Enthalpies= -876.535225
Sum of electronic and thermal Free Energies= -876.601647

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.425	66.135	139.796

C,0,2.0904726969,0.7114963341,1.8050627649
C,0,0.7637029357,0.9821794286,2.1136226727
C,0,-0.1119848977,-0.0913292732,2.2373249918
C,0,0.2922776277,-1.4148233839,2.1137551607
C,0,1.6204939894,-1.6621326655,1.7905808809
C,0,2.514780046,-0.6052587655,1.5983627323
C,0,3.9225356918,-0.890001399,1.1595124544
N,0,4.0964608776,-0.8469341375,-0.3598795314
C,0,3.8501500895,0.4942273576,-0.9172087987
C,0,2.605153803,0.9692346052,-1.267224223
O,0,2.6959985051,2.2451495978,-1.793943255
C,0,1.4851954998,2.9787550233,-1.8316248166
C,0,3.2574609961,-1.9050114299,-1.0134607352
C,0,5.5328735757,-1.1884352498,-0.6263581948
O,0,1.4723892259,0.4218829775,-1.1801066501
N,0,-1.5352637567,0.1809789998,2.4767749076
O,0,-1.8916488204,1.3460059365,2.5605559009
O,0,-2.299067114,-0.7692522613,2.5474547744
H,0,2.7943260784,1.5289204782,1.6877675068
H,0,0.408084082,1.9973095684,2.2443729852
H,0,-0.4166516115,-2.2212109046,2.2566213513
H,0,1.9570464065,-2.6882511897,1.6760672264
H,0,4.6148388459,-0.1413611124,1.5480638121
H,0,4.2401069545,-1.8836999227,1.4881406158
H,0,2.2087553878,-1.6574389258,-0.8757389634
H,0,3.508029666,-2.8690288216,-0.5671354777
H,0,3.499556863,-1.8993540715,-2.0757223307
H,0,5.7420935633,-2.1800688994,-0.2250025921
H,0,5.6885096259,-1.1654123275,-1.7036402213
H,0,6.1625680007,-0.4431606055,-0.1409800356
H,0,4.7291282362,1.1150966714,-0.9840117649
H,0,0.7384974002,2.4878666958,-2.4638460262
H,0,1.0823040245,3.1123941083,-0.8197299004
H,0,1.733905252,3.9532626119,-2.2510291793
H,0,-0.2103825227,0.9832109917,-0.8876204985
N,0,-1.2119402314,1.1144545446,-0.669598314
C,0,-1.9543832776,0.0218740518,-0.5840458154
N,0,-3.2383539498,0.0687211858,-0.2600220276
C,0,-4.0459517158,-1.1545762664,-0.1165611967
C,0,-3.9257592241,1.351257923,-0.036641914
C,0,-1.7416261147,2.4616380491,-0.461778095
C,0,-1.3023786575,-1.2928792982,-0.9077269149
C,0,-1.877189805,-1.9202744472,-2.1935120495
H,0,-1.4393305954,-1.978248962,-0.0628578367
H,0,-0.2310584042,-1.1068118146,-1.0120178161
H,0,-4.9518550968,1.2340636842,-0.3914599834
H,0,-3.9497236804,1.549427604,1.0409480897
H,0,-1.5709673668,2.7630470831,0.5777452545
H,0,-1.1965736146,3.1431717377,-1.1158257011
C,0,-3.2253249905,2.4669294825,-0.7934705395
H,0,-3.6663456654,3.4272749561,-0.5212485053
H,0,-3.360922153,2.3217606557,-1.8701067717
C,0,-4.3468171953,-1.8344552346,-1.4527452421
H,0,-3.5395724956,-1.837601393,0.5731138864
H,0,-4.9689532239,-0.8422345239,0.3738519379
H,0,-5.2197754859,-2.4796871018,-1.3118122919
H,0,-4.6310074529,-1.066728715,-2.1835767815
C,0,-3.1874488353,-2.6809832594,-1.9809468648
H,0,-2.0056545494,-1.1373614941,-2.9510485108
H,0,-1.1273122022,-2.6136743772,-2.5846494985
H,0,-3.485149733,-3.1450770158,-2.9264873422
H,0,-3.0034175078,-3.5010620937,-1.2738186991

Naked 23 product (3a) in CCl4

/home/biswas/nitrodoc2/23prodCCl4UF
attempt to find complex in CCl4
M062X/6-31+G**
E(RM062X) = -876.833106859

Zero-point correction= 0.277499 (Hartree/Particle)
Thermal correction to Energy= 0.295488
Thermal correction to Enthalpy= 0.296432
Thermal correction to Gibbs Free Energy= 0.230434

Sum of electronic and ZPE= -876.555607
Sum of electronic and thermal Energies= -876.537619
Sum of electronic and thermal Enthalpies= -876.536675
Sum of electronic and thermal Free Energies= -876.602672

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.421	66.190	138.903
C,0,-0.5682738234,1.2397703648,-0.674680729			
C,0,-1.0984497442,1.2953010925,0.7304550889			
C,0,-0.2967808005,1.5729004281,1.7630071916			
C,0,1.1235052901,1.8711686032,1.6365855102			
C,0,1.6501079922,1.9554766358,0.4047411881			
C,0,0.841881366,1.7992066663,-0.8090494441			
C,0,1.3189203425,2.2036827827,-1.9961772153			
N,0,-0.4946270069,-0.3093977296,-2.6581848064			
C,0,-0.797921248,-0.1992145231,-1.2314676289			
C,0,-0.0764134039,-1.2720601614,-0.4213357631			
O,0,-0.6229349867,-2.4757923406,-0.6454151329			
C,0,0.037138395,-3.5804674737,-0.0131801929			
C,0,0.8165957721,-0.8714838237,-2.9752726034			
C,0,-1.5392260671,-0.9911508924,-3.4144356361			
O,0,0.888956045,-1.0962585935,0.2827677179			
N,0,-0.8809129934,1.5827551054,3.1158973627			
O,0,-2.0649984204,1.3174654584,3.244473978			
O,0,-0.1362536074,1.8584096334,4.0415970131			
H,0,-1.2315106471,1.8487129589,-1.3014962457			
H,0,-2.1476560567,1.0757007402,0.9039180187			
H,0,1.7100340262,2.0221313594,2.5328912702			
H,0,2.7023368983,2.194287672,0.2773733164			
H,0,0.7150883022,2.1435316615,-2.8962943481			
H,0,2.3312192208,2.5878555091,-2.0851199546			
H,0,1.5885741668,-0.4097560951,-2.3593147508			
H,0,1.0441149776,-0.6621834286,-4.0242531445			
H,0,0.8488318397,-1.9655365804,-2.8281211173			
H,0,-1.3055877928,-0.9191652988,-4.4802397377			
H,0,-1.6275942142,-2.0570720602,-3.1477179813			
H,0,-2.5019872749,-0.5022780356,-3.2442850352			
H,0,-1.8690969308,-0.3972994922,-1.1081395867			
H,0,1.0692051996,-3.6496474464,-0.3629459441			
H,0,0.0297175322,-3.4512039957,1.0703488597			
H,0,-0.5278693476,-4.4644227,-0.3006045175			

Naked TS opposite Side in CCl4

This is an alternative conformation of **6**‡ that is lower in energy in the CCl_4 but is higher in energy in more polar solvent calculations.
home/biswas/nitrodoc2/TSoppSideCCl4
TS conf C with ester on other side of ring
M062X/6-31+G**
E(RM062X) = -876.809847516

Zero-point correction= 0.275808 (Hartree/Particle)
Thermal correction to Energy= 0.293411
Thermal correction to Enthalpy= 0.294355
Thermal correction to Gibbs Free Energy= 0.229799
Sum of electronic and ZPE= -876.534040
Sum of electronic and thermal Energies= -876.516437
Sum of electronic and thermal Enthalpies= -876.515493
Sum of electronic and thermal Free Energies= -876.580048

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.118	65.706	135.868
C,0,-1.0199099629,-0.3645769627,2.2207047585			
C,0,-0.4444297474,-0.7430601457,3.4073326913			
C,0,0.95519232,-0.9167621967,3.4625860571			
C,0,1.7621124584,-0.7209124403,2.3564650942			
C,0,1.16879653,-0.3709985198,1.14173788			
C,0,-0.2339430946,-0.1439121328,1.0442798475			
C,0,-0.808844741,0.0198023741,-0.2153912982			
N,0,-0.4808466899,-2.2046658735,-0.7295608787			
C,0,0.6236143364,-2.6388199697,-0.0996755594			
C,0,1.9712139301,-2.510005204,-0.6249924261			
O,0,2.8424199668,-3.1638698213,0.1710293925			
C,0,4.2207455996,-3.0165002251,-0.1728120099			
C,0,-0.5198227293,-2.0678562521,-2.1965729241			
C,0,-1.7381149877,-2.7115906913,-0.1643432751			
O,0,2.3241044005,-1.8913324807,-1.6191870612			
N,0,1.5652006579,-1.3130053972,4.720580505			
O,0,0.8296964027,-1.5020343384,5.6813154722			
O,0,2.7816668031,-1.4426270028,4.7631344546			
H,0,-2.0948924914,-0.2120668087,2.1680858185			
H,0,-1.0354227176,-0.9022805087,4.3009706773			
H,0,2.8338960112,-0.8597118665,2.4397472327			
H,0,1.7984874481,-0.1420906886,0.2872598352			
H,0,-1.8819110893,0.1561820286,-0.319130294			
H,0,-0.1901040296,0.3334634978,-1.0503171164			
H,0,0.3682345989,-1.548619886,-2.5434500134			
H,0,-1.4187603675,-1.5096410803,-2.4586956064			
H,0,-0.5598206793,-3.0678064405,-2.6435220831			
H,0,-2.5731553219,-2.1722971242,-0.6103695487			
H,0,-1.8301436728,-3.7820884837,-0.3779888761			
H,0,-1.7342380908,-2.5508350823,0.9159038412			
H,0,0.4988869899,-3.119469417,0.8619957551			
H,0,4.4094916625,-3.4031846038,-1.1763671413			
H,0,4.5112824166,-1.9635668323,-0.133487252			
H,0,4.7703448801,-3.5916374241,0.5699390514			

Structures for 2a, 3a, 6‡, and 7---8 coordinated to one explicit methanol molecule

Each of the following structures used a PCM model for methanol solvent.

Ylide (2a) ----H–OMe in methanol

/home/biswas/23arom_Doc_first_download/nitro/
ylidemethanolmethanol
sm with methanol in methanol
M062X/6-31+g**
E(RM062X) = -992.542177910

Zero-point correction= 0.334262 (Hartree/Particle)
Thermal correction to Energy= 0.355519
Thermal correction to Enthalpy= 0.356463
Thermal correction to Gibbs Free Energy= 0.284193
Sum of electronic and ZPE= -992.207916
Sum of electronic and thermal Energies= -992.186659
Sum of electronic and thermal Enthalpies= -992.185714

Sum of electronic and thermal Free Energies= -992.257985

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	223.092	78.138	152.105

C,0,-0.5625667821,-0.9495584099,-1.4483692644
C,0,0.8075629778,-1.144809548,-1.5653912553
C,0,1.4650403298,-1.8014639707,-0.5327570834
C,0,0.808341696,-2.3003391889,0.584240079
C,0,-0.5622076217,-2.0915462928,0.6837264758
C,0,-1.2463959735,-1.3848517649,-0.308702019
C,0,-2.702723802,-1.0614678155,-0.147977478
N,0,-2.9388989516,0.2887813386,0.5391053137
C,0,-2.2957601225,1.4101591722,-0.1677200668
C,0,-0.9582613855,1.7270341363,-0.0158225432
O,0,-0.574265382,2.7197975227,-0.8976498666
C,0,0.7775644983,3.1468743416,-0.800761599
C,0,-2.5309458718,0.2062945887,1.9811057572
C,0,-4.4192616902,0.5229772493,0.5092832975
O,0,-0.1111212471,1.2617547622,0.7883000443
N,0,2.9220702353,-1.9598572163,-0.617733899
O,0,3.4882550658,-1.5396092487,-1.6130870755
O,0,3.4952574455,-2.5096024409,0.3081603147
H,0,-1.1007347377,-0.4290353569,-2.2338992537
H,0,1.3606557845,-0.7858656727,-2.424397584
H,0,1.3613026733,-2.8189223209,1.3572884683
H,0,-1.096430287,-2.4644076246,1.5527757643
H,0,-3.1913716428,-0.9768688082,-1.120319655
H,0,-3.2179542208,-1.8181149834,0.4504829725
H,0,-1.4593439294,0.0379355226,2.0344056484
H,0,-3.0959819936,-0.6011362672,2.4500061993
H,0,-2.7731618368,1.1637887937,2.4416341383
H,0,-4.9203732053,-0.313943033,0.9967071404
H,0,-4.6228446554,1.4546304212,1.0348073134
H,0,-4.7392206946,0.6008642501,-0.5296248092
H,0,-2.8876442813,1.8248537198,-0.9689665924
H,0,1.0102635434,3.5025575412,0.2071503754
H,0,1.4694626886,2.3386767764,-1.0608490572
H,0,0.8823670431,3.9633879612,-1.5153780359
H,0,1.5837410722,0.8040085741,0.640878787
O,0,2.5365582531,0.5740203536,0.688263856
C,0,3.2327529386,1.6604346253,1.2663621528
H,0,4.2346765221,1.3149897092,1.5334162982
H,0,3.334310412,2.5008018155,0.5664229468
H,0,2.7377806356,2.023885788,2.1756123943

23 product (3a) ----H–OMe in methanol

/home/biswas/23arom_Doc_first_download/nitro
/23prodmethanolmethanol
prod with methanol in methanol
M062X/6-31+g**
E(RM062X) = -992.522054803

Zero-point correction= 0.330957 (Hartree/Particle)
Thermal correction to Energy= 0.353434
Thermal correction to Enthalpy= 0.354378
Thermal correction to Gibbs Free Energy= 0.278552
Sum of electronic and ZPE= -992.191098
Sum of electronic and thermal Energies= -992.168621
Sum of electronic and thermal Enthalpies= -992.167676
Sum of electronic and thermal Free Energies= -992.243503

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	221.783	80.285	159.589

C,0,-1.2373235079,-0.676373006,-1.1472178386
C,0,0.242437821,-0.672900904,-1.4140606086
C,0,1.0725120355,-1.1598472804,-0.4812795489
C,0,0.6356766981,-1.8176302223,0.7443389339
C,0,-0.6713557671,-2.0935275618,0.8904298453
C,0,-1.6276605956,-1.7724362602,-0.1772452338
C,0,-2.7674927596,-2.4622644111,-0.3162497872
N,0,-2.8621805329,0.9972240672,0.0817992572
C,0,-1.6628640003,0.8115969407,-0.6939817157
C,0,-0.4764880163,1.5257227386,-0.0522959591
O,0,0.1614513017,2.2671959783,-0.9579505413
C,0,1.3892637243,2.8825053333,-0.5406315942
C,0,-2.9626735098,0.4637457081,1.4389506204
C,0,-4.1014673782,0.8770657922,-0.6679984074
O,0,-0.1145051554,1.4326091523,1.1036785858
N,0,2.5167295569,-1.0664363597,-0.712829487
O,0,2.9337044813,-0.1789403771,-1.4437994436
O,0,3.2304622884,-1.889820169,-0.1662187533
H,0,-1.7750028167,-0.8423936949,-2.0851983291
H,0,0.6327979965,-0.1976014452,-2.3083546635
H,0,1.3798364592,-2.069120729,1.4887356738
H,0,-1.0309909897,-2.6230051409,1.7685739013
H,0,-3.4417823065,-2.2871248173,-1.1494498401
H,0,-3.0523079378,-3.2206809797,0.4079806006
H,0,-1.9701850384,0.2984321224,1.857874561
H,0,-3.5215777443,-0.4794235427,1.4740734008
H,0,-3.4826826655,1.1944112476,2.0695236933
H,0,-4.3858566381,-0.16590431,-0.8756139772
H,0,-4.9091016317,1.3357426249,-0.0887374941
H,0,-4.0168560463,1.4124089336,-1.6179588595
H,0,-1.8234733233,1.3393331936,-1.6376203775
H,0,1.2454436904,3.4243390663,0.3952501568
H,0,2.1541530532,2.1102116974,-0.4248150875
H,0,1.6650980019,3.5626124409,-1.3431518853
H,0,1.7201446383,0.9505351113,1.5961976463
O,0,2.4680304895,0.3483353907,1.7298067373
C,0,3.7010062574,1.0365050711,1.5951351893
H,0,4.4746534734,0.4069806754,2.0391824464
H,0,3.9562774864,1.2018323519,0.5398529411
H,0,3.6910418075,1.9997710736,2.1166532415

TS (6‡) ----H–OMe in methanol

/home/biswas/23arom_Doc_first_download/nitro
/methanolTSmethanol
Nitro 23 ts methanol with methanol
m062x/6-31+G**
E(RM062X) = -992.512419036

Zero-point correction= 0.329966 (Hartree/Particle)
Thermal correction to Energy= 0.351501
Thermal correction to Enthalpy= 0.352445
Thermal correction to Gibbs Free Energy= 0.280388
Sum of electronic and ZPE= -992.182453
Sum of electronic and thermal Energies= -992.160918
Sum of electronic and thermal Enthalpies= -992.159974
Sum of electronic and thermal Free Energies= -992.232032

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	220.570	79.180	151.658

C,0,-1.0270270097,-0.6009155444,1.9877116723
C,0,-0.7276569228,-0.9970468529,3.2910310383
C,0,0.5555884667,-0.8019398873,3.7757644495
C,0,1.5626996952,-0.1711401977,3.0087570912
C,0,1.2703009143,0.2193356167,1.7313012273
C,0,-0.0384121095,0.0284703461,1.168034039
C,0,-0.2971991736,0.2491600132,-0.1779089484
N,0,-0.2138538296,-2.0603467202,-0.6515323196
C,0,-0.8507172119,-2.7006994618,0.3323111901
C,0,-0.2274192354,-3.3181793316,1.4870331456
O,0,-1.1579834081,-3.9469387383,2.2309134706
C,0,-0.6933333001,-4.535022733,3.4492745538
C,0,1.2473013954,-2.1503777447,-0.7906793793
C,0,-0.9316562953,-1.9613704001,-1.9335272121
O,0,0.9631012984,-3.3212226068,1.7851068414
N,0,0.8563744068,-1.1947986977,5.1323824731
O,0,0.1020339174,-1.9875419115,5.6938268216
O,0,1.842506524,-0.7134816882,5.6760095797
H,0,-2.0529059296,-0.6564942941,1.6388593513
H,0,-1.4828397615,-1.4502884962,3.9241466389
H,0,2.5471155415,-0.0301197389,3.4383766782
H,0,2.0357744546,0.6889706363,1.1193493457
H,0,-1.3196203206,0.2486339399,-0.5413541163
H,0,0.4580009993,0.6908357151,-0.8222772348
H,0,1.7263068181,-1.8326980232,0.1334125674
H,0,1.5439155951,-1.5050225209,-1.616107715
H,0,1.5274014867,-3.1868203813,-1.0045033103
H,0,-0.507093891,-1.1439067783,-2.514832725
H,0,-0.8219213536,-2.9037860896,-2.4796331727
H,0,-1.9869377863,-1.767241323,-1.7432813334
H,0,-1.9231329316,-2.8126186916,0.2349912341
H,0,0.1106076334,-5.247358207,3.2481331422
H,0,-0.3437496933,-3.7571046292,4.136115934
H,0,-1.5540253665,-5.047982349,3.8740830333
H,0,1.952429872,-3.3516514018,3.3460370465
O,0,2.5842774064,-3.2258338017,4.074212837
C,0,2.4409326589,-4.2597441916,5.0306169723
H,0,3.2562046733,-4.1551781689,5.7499937598
H,0,1.4904581322,-4.1797594209,5.5740827817
H,0,2.5096836403,-5.2545182439,4.5732135513

Complex 7----8----H–OMe in methanol

/home/biswas/nitrodoc2/methanolComplexmethanol
complex from methanol ts in methanol
M062X/6-31+G**
E(RM062X) = -992.514172176
(Potential energy of triplet for this geometry: -992.480655949)

Zero-point correction= 0.329272 (Hartree/Particle)
Thermal correction to Energy= 0.352189
Thermal correction to Enthalpy= 0.353133
Thermal correction to Gibbs Free Energy= 0.277511
Sum of electronic and ZPE= -992.184900
Sum of electronic and thermal Energies= -992.161983
Sum of electronic and thermal Enthalpies= -992.161039
Sum of electronic and thermal Free Energies= -992.236661

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	221.002	82.189	159.161

C,0,-1.0877996009,-0.6269942451,1.8801640377
C,0,-0.8175719564,-1.0757719196,3.1545851964
C,0,0.4743824962,-0.9388365401,3.6902314319
C,0,1.5032242457,-0.29494607,2.9372168366
C,0,1.238337478,0.1744114064,1.6898633725
C,0,-0.0807511697,0.0551762814,1.0829332948
C,0,-0.3389766122,0.4838332442,-0.1846902233
N,0,-0.1953803557,-2.3814646157,-0.6849529068
C,0,-0.8356835003,-2.8503685228,0.3415666532
C,0,-0.1918096042,-3.4297844271,1.5471404057
O,0,-1.1136186188,-4.0400249648,2.283252733
C,0,-0.656356918,-4.6294673764,3.510959788
C,0,1.2710193771,-2.3034492384,-0.7661181122
C,0,-0.9290452808,-2.1275484112,-1.9356714384
O,0,0.9949489553,-3.3966799856,1.807146343
N,0,0.7397563248,-1.3849924959,4.9932690782
O,0,-0.1340610994,-2.026767351,5.6106022023
O,0,1.839418828,-1.1364023282,5.5120090012
H,0,-2.1073597714,-0.6669003658,1.5054757415
H,0,-1.5938329272,-1.5423433662,3.7520068519
H,0,2.489431396,-0.1971184415,3.3760204413
H,0,2.0216709033,0.6659662525,1.1187443274
H,0,-1.3358466911,0.4044512933,-0.6080068513
H,0,0.4287220236,0.9665156139,-0.7822914584
H,0,1.6619750814,-1.8107690882,0.124100962
H,0,1.5211026861,-1.735241536,-1.659400469
H,0,1.6820522335,-3.3137021,-0.8324102749
H,0,-0.5417491896,-1.2215509913,-2.3966079998
H,0,-0.7712709477,-2.9815065176,-2.6005824505
H,0,-1.9899559529,-2.0129794377,-1.7196209211
H,0,-1.9141145864,-2.9428004853,0.2728590866
H,0,0.1706816284,-5.3137043364,3.3108207972
H,0,-0.3500976261,-3.8415048864,4.2069300698
H,0,-1.5118455117,-5.1712426356,3.9075056478
H,0,2.2092214933,-3.7058594225,3.2433886221
O,0,2.9711577232,-3.839901347,3.827158562
C,0,2.5355662616,-4.3825754015,5.0631178252
H,0,3.4033152317,-4.4207039014,5.725013948
H,0,1.7691788309,-3.7581738689,5.5368609342
H,0,2.1481297224,-5.4026744708,4.9447959142

TS----H–OMe in methanol, Alternative Conformation 2

methanolTSmethanolconf2
ts with methanol in methanol conf 2
M062X/6-31+g**
E(RM062X) = -992.499049003

Zero-point correction= 0.328794 (Hartree/Particle)
Thermal correction to Energy= 0.350915
Thermal correction to Enthalpy= 0.351859
Thermal correction to Gibbs Free Energy= 0.277865
Sum of electronic and ZPE= -992.170255
Sum of electronic and thermal Energies= -992.148134
Sum of electronic and thermal Enthalpies= -992.147190
Sum of electronic and thermal Free Energies= -992.221184

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 220.203 80.207 155.734

C,0,-1.0252922727,-0.6819014469,1.8317635226
C,0,-0.6661436886,-1.0567756773,3.1215818219
C,0,0.6038397539,-0.7562053362,3.6020877046
C,0,1.5213188513,0.0152977075,2.825470629
C,0,1.154782292,0.4511415668,1.5919848617
C,0,-0.1523420199,0.1540063305,1.0267262329
C,0,-0.5082958019,0.5616799598,-0.2252450317
N,0,-0.0201205354,-2.2112878534,-0.7683546464
C,0,-0.4933830718,-2.7480374659,0.3311801075
C,0,0.3330843082,-3.2021390964,1.4675976566
O,0,-0.2659101228,-3.9302460743,2.4195217117
C,0,-1.6586547734,-4.2594125147,2.3899925183
C,0,1.3954082008,-1.8807301971,-0.9765940947
C,0,-0.8971354314,-2.1961434259,-1.9581531849
O,0,1.526813432,-2.9919312677,1.5909535407
N,0,0.9590324224,-1.1421267235,4.9270848009
O,0,0.1623442779,-1.8068225926,5.5964633012
O,0,2.051122605,-0.7817508541,5.3743439888
H,0,-2.0515874362,-0.8250158931,1.5038541126
H,0,-1.3544038517,-1.6048974583,3.7560721772
H,0,2.4961105702,0.2470469215,3.2375647758
H,0,1.8407724264,1.0557505458,1.0045700787
H,0,-1.5071009632,0.3760985341,-0.6063402203
H,0,0.1647689153,1.1543711293,-0.8372174687
H,0,1.7967881916,-1.3886289042,-0.0929171244
H,0,1.4581528838,-1.2207459027,-1.8390461153
H,0,1.9580237793,-2.8006684726,-1.1633229327
H,0,-1.540486881,-1.3182052151,-1.9531043703
H,0,-0.2664289835,-2.1798643718,-2.8454329327
H,0,-1.5042419556,-3.1016389299,-1.9684842068
H,0,-1.5361783026,-3.0379431042,0.296946237
H,0,-2.272270673,-3.3546678889,2.3716016828
H,0,-1.8877206557,-4.8999417742,1.5356877467
H,0,-1.8417148717,-4.8030746449,3.3147947306
H,0,1.9437840801,-3.6580816922,3.3844190108
O,0,2.2969039558,-3.9619419107,4.2363373345
C,0,1.3374479019,-4.7886804312,4.8733421991
H,0,1.7746130183,-5.1204057555,5.8180802344
H,0,0.4136766178,-4.2396736641,5.0873835057
H,0,1.0975158084,-5.6727081555,4.2697741046

TS----H–OMe in methanol, Alternative Conformation 3

methanolTSmethanolconf3
ts with methanol in methanol conf 3
M062X/6-31+g**
E(RM062X) = -992.506854672

Zero-point correction= 0.330031 (Hartree/Particle)
Thermal correction to Energy= 0.351793
Thermal correction to Enthalpy= 0.352737
Thermal correction to Gibbs Free Energy= 0.278352
Sum of electronic and ZPE= -992.176824
Sum of electronic and thermal Energies= -992.155062
Sum of electronic and thermal Enthalpies= -992.154117
Sum of electronic and thermal Free Energies= -992.228502

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 220.753 78.936 156.556

C,0,-1.0569552064,-1.0891021224,2.1446503026
C,0,-0.5193226929,-1.4473019794,3.3772486787
C,0,0.6961663404,-0.8990410377,3.7664694987
C,0,1.3815672918,0.0494901763,2.9739000557
C,0,0.8468151039,0.4071476991,1.7656004897
C,0,-0.3883452559,-0.1521919012,1.2993805846
C,0,-0.8266355408,0.0274788492,-0.0101018717
N,0,-0.0789173246,-2.0444012491,-0.6761729922
C,0,-0.4138569638,-2.9556412922,0.247232522
C,0,0.3777755584,-3.5176922393,1.3255828107
O,0,1.5683093688,-2.9575776035,1.5623471871
C,0,2.3389449464,-3.5311680065,2.6257538125
C,0,1.3268753145,-1.6713030653,-0.9059136589
C,0,-0.8761402388,-2.0896435779,-1.9181399737
O,0,-0.0438603111,-4.473785773,1.9777982189
N,0,1.2796578147,-1.3071037158,5.0209771874
O,0,0.6936128153,-2.1467925334,5.7012926503
O,0,2.3539261044,-0.8146774956,5.3549396679
H,0,-2.0393823769,-1.4545905886,1.8649642476
H,0,-1.0217332116,-2.1600830416,4.0219889619
H,0,2.315917982,0.4680719824,3.3271757477
H,0,1.3624180735,1.1289129733,1.137922241
H,0,-1.8353346873,-0.2638432468,-0.2845956408
H,0,-0.3170618385,0.7229714887,-0.6714241883
H,0,1.7629417588,-1.2831774697,0.0116609202
H,0,1.3474514719,-0.9106278454,-1.6847179022
H,0,1.8850175495,-2.5549998794,-1.2302953346
H,0,-0.7699737292,-1.1409782637,-2.4421399064
H,0,-0.5090179694,-2.9075265277,-2.5456987924
H,0,-1.9235089821,-2.2580913534,-1.6697813333
H,0,-1.4019014168,-3.3899700753,0.1599338528
H,0,1.7404323849,-3.6042142072,3.537906382
H,0,2.6927870951,-4.5248678666,2.3411793019
H,0,3.1794684578,-2.8546190648,2.7728012194
H,0,0.5529218842,-5.68886096,3.2540267742
O,0,0.6560851557,-6.1689539254,4.0921412993
C,0,-0.1716230342,-5.5129081149,5.0388313056
H,0,-0.0201175532,-5.9989085644,6.0051316488
H,0,0.0875494014,-4.4510846017,5.1385309818
H,0,-1.2327285399,-5.59258098,4.7714650437

TS----H–OMe in methanol, Alternative Conformation 4

methanolTSmethanolconf4
ts with methanol in methanol conf 4
M062X/6-31+g**
E(RM062X) = -992.506557461

Zero-point correction= 0.329476 (Hartree/Particle)
Thermal correction to Energy= 0.351593
Thermal correction to Enthalpy= 0.352537
Thermal correction to Gibbs Free Energy= 0.276642
Sum of electronic and ZPE= -992.177081
Sum of electronic and thermal Energies= -992.154965

Sum of electronic and thermal Enthalpies= -992.154021
Sum of electronic and thermal Free Energies= -992.229915

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	220.628	79.304	159.734

C,0,-1.7344684391,-1.131160047,1.4270181404
C,0,-1.6733339501,-1.4703891233,2.7766119027
C,0,-0.6254450668,-0.9825536301,3.5431562077
C,0,0.3641379155,-0.1333310784,2.9975908327
C,0,0.27899267,0.2274296526,1.6774753791
C,0,-0.7891126893,-0.2372270929,0.8415522976
C,0,-0.7870172398,-0.0601787173,-0.5378447544
N,0,0.0863366596,-2.2083426496,-0.8560120304
C,0,-0.2935316664,-2.9851232913,0.1653975242
C,0,-1.5262233537,-3.744735658,0.2231111656
O,0,-1.5338806718,-4.5432125095,1.302839132
C,0,-2.7375223686,-5.2806194206,1.5362808121
C,0,1.5035539488,-1.8124041383,-0.8282492238
C,0,-0.4437218777,-2.4065274665,-2.2179356899
O,0,-2.4654873618,-3.6930672916,-0.5692182906
N,0,-0.5405078895,-1.3547715979,4.9345847683
O,0,-1.4022901055,-2.0936844723,5.4034149711
O,0,0.3951032783,-0.9177669357,5.5996030931
H,0,-2.5834077007,-1.4572712845,0.8334926464
H,0,-2.41716076,-2.1190488354,3.2256033989
H,0,1.1686375422,0.22389758,3.6287406813
H,0,1.0269606272,0.8906718961,1.2512320642
H,0,-1.6727575274,-0.3084428867,-1.1138315564
H,0,-0.0478229812,0.5770942777,-1.0143033595
H,0,1.7438374863,-1.4159035622,0.1603816016
H,0,1.6747271297,-1.0470613923,-1.5833064347
H,0,2.127368204,-2.6872819382,-1.0368290789
H,0,-0.1434620239,-1.5517024597,-2.8224193951
H,0,-0.0126023075,-3.3242646441,-2.6325375317
H,0,-1.5254088332,-2.4900118148,-2.1876294888
H,0,0.3794902934,-3.0661535284,1.0097602332
H,0,-3.5710565728,-4.5973546258,1.7191490988
H,0,-2.9667737173,-5.9197407841,0.6811252214
H,0,-2.5440262758,-5.8828903495,2.4212778369
H,0,-4.3267017725,-3.9702129011,-0.5226156748
O,0,-5.2670261473,-3.7935327039,-0.3580049937
C,0,-5.3414206873,-2.5456868633,0.3073174929
H,0,-6.3963349473,-2.3216657695,0.4778017845
H,0,-4.8339129728,-2.5716184982,1.2818173351
H,0,-4.9050398478,-1.7376884444,-0.2935091191

TS----H–OMe in methanol, Alternative Conformation 5

methanolTSmethanolconf5
ts with methanol in methanol conf 5
M062X/6-31+g**
E(RM062X) = -992.500385982

Zero-point correction= 0.329551 (Hartree/Particle)
Thermal correction to Energy= 0.351645
Thermal correction to Enthalpy= 0.352589
Thermal correction to Gibbs Free Energy= 0.277315
Sum of electronic and ZPE= -992.170835
Sum of electronic and thermal Energies= -992.148741
Sum of electronic and thermal Enthalpies= -992.147797
Sum of electronic and thermal Free Energies= -992.223071

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	220.660	79.494	158.426

C,0,-1.6539277412,-1.0401298788,1.3101481681
C,0,-1.6799238784,-1.548327927,2.6068196533
C,0,-0.6271368631,-1.2691891724,3.4676372218
C,0,0.4550483171,-0.4411338702,3.0687712486
C,0,0.4585756171,0.0977653164,1.8131782055
C,0,-0.6102306432,-0.1525330261,0.8762486665
C,0,-0.5455301366,0.2488306845,-0.439507503
N,0,0.189513365,-2.1383976183,-0.9437372601
C,0,-0.3605873607,-2.8765890182,0.0109502579
C,0,-1.67848503,-3.5088247273,-0.0847158651
O,0,-2.0175541038,-4.3996896367,0.8585448731
C,0,-1.0805314283,-4.8703052469,1.8363533738
C,0,1.6205223871,-1.8456041374,-0.7812556895
C,0,-0.2855201892,-2.111472458,-2.3370690808
O,0,-2.505905669,-3.26367337,-0.9552066431
N,0,-0.6240974399,-1.8475630301,4.7784050413
O,0,-1.5139337037,-2.6446267741,5.0792626134
O,0,0.2749111608,-1.5335127852,5.5582349624
H,0,-2.5133947433,-1.1893397384,0.662671588
H,0,-2.5013194692,-2.1720329585,2.9439749999
H,0,1.2610955102,-0.2481457272,3.7663085935
H,0,1.2773790031,0.7429015935,1.5061332546
H,0,-1.3935302359,0.1056939061,-1.1013116884
H,0,0.2756527167,0.8623156993,-0.7983755216
H,0,1.8180312427,-1.578331305,0.258834426
H,0,1.8897669322,-1.0139271428,-1.4294192994
H,0,2.2032645722,-2.732044877,-1.0523583994
H,0,0.1908647638,-1.2671666543,-2.8325242271
H,0,0.0117546501,-3.0441802124,-2.8285803368
H,0,-1.3647231119,-2.009969297,-2.3667357078
H,0,0.2546666442,-3.059132263,0.8821661192
H,0,-0.1864035829,-5.2707438951,1.353729599
H,0,-0.8184910966,-4.0743358596,2.5386152296
H,0,-1.5984554236,-5.6648937244,2.3690595851
H,0,-4.2583589358,-3.8646998831,-0.5498568991
O,0,-5.1336868365,-3.9204630148,-0.1309682857
C,0,-5.0916348062,-3.0867668969,1.0133224616
H,0,-6.0541980855,-3.1688481774,1.5221961953
H,0,-4.3015280406,-3.4005003666,1.7071645715
H,0,-4.9319143273,-2.0344395296,0.744589498

TS Dissociation ----H–OMe in methanol (Unrestricted)

This is an alternative conformation of **6**‡ with the ylide twisted away from the aromatic ring, making this a purely dissociative transition state. It is 3.6 kcal/mol less stable than **6**‡. Its S**2 value is 0.06.
/general/home/bibaswanbiswas/diss_Nitromeohm062xpsmeoh/m062x.log
#p um062x/6-31+G** opt=(modredun,loose) guess=(mix,always) scf SCRF=(S
um062x/6-31+G**

E(UM062X) = -992.496998581

Zero-point correction= 0.327968 (Hartree/Particle)
Thermal correction to Energy= 0.350775
Thermal correction to Enthalpy= 0.351719
Thermal correction to Gibbs Free Energy= 0.270636
Sum of electronic and ZPE= -992.169031
Sum of electronic and thermal Energies= -992.146224
Sum of electronic and thermal Enthalpies= -992.145279
Sum of electronic and thermal Free Energies= -992.226363

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	220.115	79.971	170.654

C,0,0.9451551585,-0.1985799666,3.3799712054
C,0,1.0982130545,-0.3318251825,2.0161823182
C,0,-0.0239574068,-0.2913382628,1.1394897415
C,0,-1.313492495,-0.1008542073,1.7155875916
C,0,-1.4745739017,0.0363330485,3.0772341371
C,0,-0.3425108163,-0.0176008579,3.9020054592
C,0,0.1276587702,-0.4872695274,-0.2499806292
N,0,-0.5076390101,0.1243401447,5.3276091078
O,0,0.4899240337,0.0689331597,6.0422546435
O,0,-1.6398961528,0.294615125,5.77248203
N,0,-0.0039109264,-2.7028398458,-0.7810893834
C,0,0.0405466109,-2.7560727687,-2.1385238019
C,0,-1.0460959948,-2.3461825843,-2.9719511726
O,0,-0.7610281623,-2.5189746692,-4.2808439122
C,0,-1.7784051363,-2.1179528614,-5.2004497901
C,0,1.1931558858,-3.2106329883,-0.0996487288
O,0,-2.1223827749,-1.8679814251,-2.5940081937
H,0,1.1190152805,-0.4800408607,-0.6903369932
H,0,-0.7160607694,-0.3236625551,-0.9126439876
H,0,-2.1810712444,-0.0601248099,1.0630507157
H,0,-2.4533653364,0.1859889914,3.5164631844
H,0,1.7978910766,-0.2277153379,4.0473016988
H,0,2.0913660768,-0.4645258838,1.5967468455
H,0,1.0041356869,-2.9376083056,-2.5967197235
H,0,-1.3733783934,-2.3139888487,-6.1910796509
H,0,-2.6888605759,-2.7015110997,-5.042932764
H,0,-2.0000133371,-1.0537589677,-5.0878081253
C,0,-1.2410617009,-3.0487563623,-0.0631014938
H,0,-1.1102380003,-2.7875443315,0.9874546071
H,0,-2.0829775228,-2.5071761537,-0.4857948138
H,0,-1.4070549403,-4.1280065299,-0.1535749362
H,0,1.185458084,-2.8612355286,0.9340116098
H,0,1.187077171,-4.3057008991,-0.1131890008
H,0,2.085168537,-2.8395407945,-0.6048474473
H,0,-3.7560389381,-1.3868021734,-3.2879240238
O,0,-4.7032892042,-1.1867668965,-3.3773640278
C,0,-5.3056064294,-1.4812060096,-2.1288802969
H,0,-6.3677962887,-1.2402562328,-2.2066547761
H,0,-5.2066730542,-2.543021955,-1.8714364177
H,0,-4.8708169136,-0.8827067859,-1.3186738049

Structure 7

Iminium cation 7 in DMSO

/home/biswas/nitrodoc2/dissociation/iminiumcationdmso
iminiumcation 2
opt
E(RM062X) = -401.407650215

Zero-point correction= 0.155829 (Hartree/Particle)
Thermal correction to Energy= 0.165186
Thermal correction to Enthalpy= 0.166130
Thermal correction to Gibbs Free Energy= 0.121338
Sum of electronic and ZPE= -401.251821
Sum of electronic and thermal Energies= -401.242464
Sum of electronic and thermal Enthalpies= -401.241520
Sum of electronic and thermal Free Energies= -401.286312

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	103.656	32.128	94.272

C,0,0.2594667472,-0.8642259691,-0.0761691142
N,0,1.3714668978,-0.4484920643,-0.5430453871
C,0,-0.7393430789,0.0220907082,0.629183293
C,0,1.8462033313,0.9503302216,-0.5075238478
C,0,2.3157960445,-1.3938603446,-1.1647159493
H,0,3.2750801037,-1.2812827674,-0.6577427223
H,0,1.942277774,-2.4095576181,-1.0623045401
H,0,2.4188825326,-1.1213499355,-2.2156892778
H,0,2.4945506435,1.0885073725,-1.3703255635
H,0,1.0070901117,1.6373162832,-0.5322705388
H,0,2.4164932509,1.0852300754,0.4133843267
O,0,-0.4687551888,1.0741208256,1.1521150445
O,0,-1.9166363564,-0.5670873971,0.6031895748
C,0,-2.9887588619,0.1392448465,1.2624791128
H,0,-3.8644414337,-0.491610982,1.1408725259
H,0,-2.7399156472,0.2699851515,2.3161176944
H,0,-3.1329886987,1.1088140175,0.784855209
H,0,0.0166814584,-1.9188459541,-0.1724098505

Iminium cation 7 in CCl4

/home/biswas/nitrodoc2/dissociation/iminiumcationccl4
iminiumcation 2
opt
E(RM062X) = -401.370802531

Zero-point correction= 0.155961 (Hartree/Particle)
Thermal correction to Energy= 0.165346
Thermal correction to Enthalpy= 0.166290
Thermal correction to Gibbs Free Energy= 0.121279
Sum of electronic and ZPE= -401.214842
Sum of electronic and thermal Energies= -401.205456
Sum of electronic and thermal Enthalpies= -401.204512
Sum of electronic and thermal Free Energies= -401.249524

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	103.756	32.075	94.735

C,0,0.0380211826,-0.7713170932,-0.0080786558
N,0,1.2972149243,-0.8898859,-0.188987218
C,0,-0.7191322969,0.5332926213,0.162459293
C,0,2.2779076449,0.2117547686,-0.2701089124
C,0,1.899770454,-2.2287028668,-0.3397696466
H,0,2.6395246372,-2.3536059944,0.4522144524
H,0,1.1310456342,-2.9950149792,-0.2713758722

H,0,2.3945388544,-2.265247222,-1.3113373318
H,0,3.0128966599,0.0435009808,0.5190668976
H,0,2.7678312112,0.1319753163,-1.2421862684
H,0,1.7894500848,1.1716481182,-0.1539427853
O,0,-0.2371304009,1.6356738367,0.1506543826
O,0,-1.9893721494,0.2270828556,0.3236909847
C,0,-2.8915919268,1.3429357347,0.5049532182
H,0,-3.875178201,0.8971520896,0.6193418369
H,0,-2.6021208526,1.8997438489,1.396848936
H,0,-2.8481121967,1.9883522659,-0.3730296394
H,0,-0.5599398728,-1.6784193109,0.0295863586

Iminium cation 7 in MeOH

/home/biswas/nitrodoc2/dissociation/iminiumcationmeoh
iminiumcation 2
opt
E(RM062X) = -401.406822324

Zero-point correction= 0.155826 (Hartree/Particle)
Thermal correction to Energy= 0.165183
Thermal correction to Enthalpy= 0.166127
Thermal correction to Gibbs Free Energy= 0.121347
Sum of electronic and ZPE= -401.250997
Sum of electronic and thermal Energies= -401.241639
Sum of electronic and thermal Enthalpies= -401.240695
Sum of electronic and thermal Free Energies= -401.285476

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	103.654	32.131	94.249

C,0,0.258484417,-0.8632358482,-0.0779872036
N,0,1.3713272143,-0.4481798973,-0.5436256283
C,0,-0.7405098076,0.023497558,0.6269156138
C,0,1.8474839131,0.9502080149,-0.5069605704
C,0,2.3157252351,-1.3940429039,-1.1646244108
H,0,3.2746831606,-1.282163047,-0.6568181362
H,0,1.9416704066,-2.4096333069,-1.0628820609
H,0,2.4200297372,-1.1212840699,-2.2154535103
H,0,2.4985580865,1.0875309308,-1.3678663495
H,0,1.0092857008,1.6382318876,-0.533773156
H,0,2.4153528865,1.0846298203,0.4155420473
O,0,-0.470194947,1.0767239382,1.1473516429
O,0,-1.9168912892,-0.5674966059,0.6039109204
C,0,-2.9890565028,0.138282628,1.2640245652
H,0,-3.8638827261,-0.4943267641,1.145346868
H,0,-2.7382197471,0.2715493904,2.316877948
H,0,-3.1357889283,1.1067510838,0.7849339719
H,0,0.0150928205,-1.9177163392,-0.1749125618

Iminium cation 7 in CH2Cl2

/home/biswas/nitrodoc2/dissociation/iminiumcationdcm
iminiumcation 2
opt
E(RM062X) = -401.399119500

Zero-point correction= 0.155835 (Hartree/Particle)
Thermal correction to Energy= 0.165290
Thermal correction to Enthalpy= 0.166234
Thermal correction to Gibbs Free Energy= 0.120751
Sum of electronic and ZPE= -401.243285
Sum of electronic and thermal Energies= -401.233829
Sum of electronic and thermal Enthalpies= -401.232885
Sum of electronic and thermal Free Energies= -401.278369

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	103.721	32.109	95.729

C,0,0.0401811705,-0.7704033983,-0.0083719777
N,0,1.2983489345,-0.8883665408,-0.1890756608
C,0,-0.7173144237,0.5316053836,0.16205292
C,0,2.2787536885,0.2109368338,-0.2702439035
C,0,1.8981643791,-2.2277589749,-0.3394960088
H,0,2.636575561,-2.3522838083,0.4532690104
H,0,1.1266656825,-2.9904122852,-0.2705694406
H,0,2.3915049778,-2.2638538297,-1.3113731501
H,0,3.012782434,0.0421186285,0.5190810806
H,0,2.767744523,0.1306117871,-1.2422383999
H,0,1.7904308156,1.17021191,-0.1541272575
O,0,-0.2437135262,1.6391952463,0.1516281924
O,0,-1.9888813178,0.2259982747,0.3235839123
C,0,-2.8885213343,1.3403679085,0.5044273951
H,0,-3.8731234077,0.8967481559,0.6191370989
H,0,-2.6002798955,1.8973042907,1.3966352684
H,0,-2.8464168955,1.9858667208,-0.3735559227
H,0,-0.5572779754,-1.6769672327,0.0292368736

Structure 8

Nitro benzyl anion (8) in CCl4

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionnakedm
062xpsccl4
Free Nirto tol
opt
E(RM062X) = -475.359060455

Zero-point correction= 0.117683 (Hartree/Particle)
Thermal correction to Energy= 0.125846
Thermal correction to Enthalpy= 0.126790
Thermal correction to Gibbs Free Energy= 0.084196
Sum of electronic and ZPE= -475.241377
Sum of electronic and thermal Energies= -475.233214
Sum of electronic and thermal Enthalpies= -475.232270
Sum of electronic and thermal Free Energies= -475.274865

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	78.970	31.291	89.648

C,0,-1.0823456257,0.1186084415,0.0001717436
C,0,0.2779762602,0.1211651333,0.0006240035
C,0,1.0065784083,1.3482935171,0.0001129373
C,0,0.2781078462,2.5754992399,-0.0009265144
C,0,-1.0822142137,2.5782008099,-0.001380947
C,0,-1.8679043822,1.3484469279,-0.0008156002
H,0,-1.6197197122,-0.8268915226,0.0005514342
H,0,0.836229678,-0.8085497566,0.0013577397
H,0,0.8364598223,3.5051550895,-0.0013667283
H,0,-1.6194867176,3.5237582132,-0.0021941487
C,0,-3.2314331462,1.3485192737,-0.0011808098
N,0,2.3837443736,1.3482200465,0.0006583863

O,0,3.0093948163,0.2585115557,0.0014989246
O,0,3.0095116241,2.4378614882,0.0001195598
H,0,-3.7932563275,2.27746058,-0.0019108095
H,0,-3.7933557039,0.4196379628,-0.0007381712

Nitro benzyl anion (8) in methanol

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionnakedm062xpsmeoh
Free Nirto tol
opt
E(RM062X) = -475.394890879

Zero-point correction= 0.117673 (Hartree/Particle)
Thermal correction to Energy= 0.125809
Thermal correction to Enthalpy= 0.126753
Thermal correction to Gibbs Free Energy= 0.084329
Sum of electronic and ZPE= -475.277218
Sum of electronic and thermal Energies= -475.269082
Sum of electronic and thermal Enthalpies= -475.268138
Sum of electronic and thermal Free Energies= -475.310562

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	78.946	31.286	89.289
C,0,-1.0810614305,0.1131300717,0.0002037093			
C,0,0.2756523966,0.1144454316,0.0006659039			
C,0,1.0077951322,1.3482938441,0.0001510919			
C,0,0.27578531,2.582219251,-0.0008935365			
C,0,-1.0809295773,2.5836798547,-0.0013563169			
C,0,-1.8637719641,1.3484480946,-0.0008137833			
H,0,-1.6207024632,-0.8305939992,0.0005857707			
H,0,0.8315756892,-0.816241714,0.0014142851			
H,0,0.831806403,3.5128481343,-0.0013205205			
H,0,-1.6204670353,3.5274629558,-0.0021649025			
C,0,-3.2228766042,1.3485181245,-0.0012261937			
N,0,2.3682556765,1.3482206803,0.0006577597			
O,0,3.0079427854,0.2542854413,0.0014257388			
O,0,3.0080609873,2.4420867303,0.0000459651			
H,0,-3.784341201,2.2777122448,-0.0019836567			
H,0,-3.7844371046,0.4193818543,-0.0008103144			

Nitro benzyl anion (8) in DMSO

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionnakedm062xpsdmso
Free Nirto tol
opt
E(RM062X) = -475.395770955

Zero-point correction= 0.117684 (Hartree/Particle)
Thermal correction to Energy= 0.125813
Thermal correction to Enthalpy= 0.126757
Thermal correction to Gibbs Free Energy= 0.084367
Sum of electronic and ZPE= -475.278087
Sum of electronic and thermal Energies= -475.269958
Sum of electronic and thermal Enthalpies= -475.269014
Sum of electronic and thermal Free Energies= -475.311404

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	78.949	31.281	89.217
C,0,-1.0810261512,0.112943562,0.000206071			
C,0,0.2755699785,0.1142042448,0.0006683625			
C,0,1.0078363037,1.3482938493,0.000152663			
C,0,0.2757029441,2.5824604431,-0.0008913052			
C,0,-1.0808942782,2.5838663828,-0.0013542804			
C,0,-1.8636352155,1.3484481333,-0.0008134673			
H,0,-1.6207617043,-0.8307122382,0.000589419			
H,0,0.8314594555,-0.8164877598,0.0014183811			
H,0,0.8316902042,3.5130942033,-0.0013167353			
H,0,-1.6205261977,3.5275812675,-0.0021616686			
C,0,-3.2225949058,1.3485180891,-0.0012290501			
N,0,2.3677378575,1.3482207004,0.0006554637			
O,0,3.0078992244,0.2540880026,0.001420142			
O,0,3.0080174389,2.4422841593,0.0000406871			
H,0,-3.7840460788,2.2777210153,-0.0019884735			
H,0,-3.7841418753,0.4193729452,-0.0008152089			

Nitro benzyl anion (8) in CH2Cl2

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionnakedm062xpsdcm
Free Nirto tol
opt
E(RM062X) = -475.387412984

Zero-point correction= 0.117612 (Hartree/Particle)
Thermal correction to Energy= 0.125793
Thermal correction to Enthalpy= 0.126737
Thermal correction to Gibbs Free Energy= 0.084088
Sum of electronic and ZPE= -475.269801
Sum of electronic and thermal Energies= -475.261620
Sum of electronic and thermal Enthalpies= -475.260676
Sum of electronic and thermal Free Energies= -475.303325

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	78.936	31.315	89.762
C,0,-1.0813566015,0.1146078122,0.0001847132			
C,0,0.2762944296,0.1163168431,0.0006453925			
C,0,1.0074811459,1.348293765,0.0001375925			
C,0,0.2764269639,2.5803477404,-0.0009116174			
C,0,-1.0812248775,2.5822019311,-0.0013727582			
C,0,-1.8648564071,1.3484477784,-0.0008162939			
H,0,-1.6202871074,-0.8296375348,0.0005581311			
H,0,0.8325500805,-0.8142896077,0.0013819595			
H,0,0.8327805806,3.5108957671,-0.0013498344			
H,0,-1.6200522892,3.52650588,-0.0021898674			
C,0,-3.2251162285,1.3485184276,-0.001202673			
N,0,2.3723593433,1.3482205335,0.0006739702			
O,0,3.0083147246,0.2557066745,0.0014703425			
O,0,3.0084326218,2.4406657105,0.0000868136			
H,0,-3.7866812827,2.2776438848,-0.001944111			
H,0,-3.7867780962,0.4194513944,-0.0007707597			

Structures for 2a, 3a, 6‡, and 7---8 coordinated to H-DBU+

The listing here only includes the lowest-energy conformations, referred to in file titles as "confB".

Ylide (2a) ----H-DBU+ in CH2Cl2

/home/biswas/23arom_Doc_first_download/nitro
/ylideDBUfullconfbCH2Cl2UF
nitrobenzyl SM with DBU actual conf B
M062X/6-31+G**
E(RM062X) = -1339.25509991

Zero-point correction= 0.544269 (Hartree/Particle)
Thermal correction to Energy= 0.572456
Thermal correction to Enthalpy= 0.573400
Thermal correction to Gibbs Free Energy= 0.486390
Sum of electronic and ZPE= -1338.710831
Sum of electronic and thermal Energies= -1338.682644
Sum of electronic and thermal Enthalpies= -1338.681700
Sum of electronic and thermal Free Energies= -1338.768710

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	359.221	109.905	183.127

C,0,2.0904726969,0.7114963341,1.8050627649
C,0,0.7637029357,0.9821794286,2.1136226727
C,0,-0.1119848977,-0.0913292732,2.2373249918
C,0,0.2922776277,-1.4148233839,2.1137551607
C,0,1.6204939894,-1.6621326655,1.7905808809
C,0,2.514780046,-0.6052587655,1.5983627323
C,0,3.9225356918,-0.890001399,1.1595124544
N,0,4.0964608776,-0.8469341375,-0.3598795314
C,0,3.8501500895,0.4942273576,-0.9172087987
C,0,2.605153803,0.9692346052,-1.267224223
O,0,2.6959985051,2.2451495978,-1.793943255
C,0,1.4851954998,2.9787550233,-1.8316248166
C,0,3.2574609961,-1.9050114299,-1.0134607352
C,0,5.5328735757,-1.1884352498,-0.6263581948
O,0,1.4723892259,0.4218829775,-1.1801066501
N,0,-1.5352637567,0.1809789998,2.4767749076
O,0,-1.8916488204,1.3460059365,2.5605559009
O,0,-2.299067114,-0.7692522613,2.5474547744
H,0,2.7943260784,1.5289204782,1.6877675068
H,0,0.408084082,1.9973095684,2.2443729852
H,0,-0.4166516115,-2.2212109046,2.2566213513
H,0,1.9570464065,-2.6882511897,1.6760672264
H,0,4.6148388459,-0.1413611124,1.5480638121
H,0,4.2401069545,-1.8836999227,1.4881406158
H,0,2.2087553878,-1.6574389258,-0.8757389634
H,0,3.508029666,-2.8690288216,-0.5671354777
H,0,3.499556863,-1.8993540715,-2.0757223307
H,0,5.7420935633,-2.1800688994,-0.2250025921
H,0,5.6885096259,-1.1654123275,-1.7036402213
H,0,6.1625680007,-0.4431606055,-0.1409800356
H,0,4.7291282362,1.1150966714,-0.9840117649
H,0,0.7384974002,2.4878666958,-2.4638460262
H,0,1.0823040245,3.1123941083,-0.8197299004
H,0,1.733905252,3.9532626119,-2.2510291793
H,0,-0.2103825227,0.9832109917,-0.8876204985
N,0,-1.2119402314,1.1144545446,-0.669598314
C,0,-1.9543832776,0.0218740518,-0.5840458154
N,0,-3.2383539498,0.0687211858,-0.2600220276
C,0,-4.0459517158,-1.1545762664,-0.1165611967
C,0,-3.9257592241,1.351257923,-0.036641914
C,0,-1.7416261147,2.4616380491,-0.461778095
C,0,-1.3023786575,-1.2928792982,-0.9077269149
C,0,-1.877189805,-1.9202744472,-2.1935120495
H,0,-1.4393305954,-1.978248962,-0.0628578367
H,0,-0.2310584042,-1.1068118146,-1.0120178161
H,0,-4.9518550968,1.2340636842,-0.3914599834
H,0,-3.9497236804,1.549427604,1.0409480897
H,0,-1.5709673668,2.7630470831,0.5777452545
H,0,-1.1965736146,3.1431717377,-1.1158257011
C,0,-3.2253249905,2.4669294825,-0.7934705395
H,0,-3.6663456654,3.4272749561,-0.5212485053
H,0,-3.360922153,2.3217606557,-1.8701067717
C,0,-4.3468171953,-1.8344552346,-1.4527452421
H,0,-3.5395724956,-1.837601393,0.5731138864
H,0,-4.9689532239,-0.8422345239,0.3738519379
H,0,-5.2197754859,-2.4796871018,-1.3118122919
H,0,-4.6310074529,-1.066728715,-2.1835767815
C,0,-3.1874488353,-2.6809832594,-1.9809468648
H,0,-2.0056545494,-1.1373614941,-2.9510485108
H,0,-1.1273122022,-2.6136743772,-2.5846494985
H,0,-3.485149733,-3.1450770158,-2.9264873422
H,0,-3.0034175078,-3.5010620937,-1.2738186991

TS (6‡) ----H-DBU+ in CH2Cl2

/home/biswas/23arom_Doc_first_download/nitro
/DBUfullTSPSCH2Cl2confbUF
DBUfullTSPSCH2Cl2confb UF
M062X/6-31+G**
E(RM062X) = -1339.22522116

Zero-point correction= 0.541380 (Hartree/Particle)
Thermal correction to Energy= 0.569550
Thermal correction to Enthalpy= 0.570494
Thermal correction to Gibbs Free Energy= 0.484190
Sum of electronic and ZPE= -1338.683841
Sum of electronic and thermal Energies= -1338.655671
Sum of electronic and thermal Enthalpies= -1338.654727
Sum of electronic and thermal Free Energies= -1338.741031

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.398	110.175	181.642

C,0,-2.2289072618,-0.6646682262,-1.6590058612
C,0,-0.9246562359,-0.4683527978,-2.104357662
C,0,0.1109928682,-1.1281951078,-1.4574688011
C,0,-0.1213376286,-2.0507713067,-0.4126079457
C,0,-1.4034158777,-2.2423236226,0.0253214867
C,0,-2.5073356762,-1.5501122306,-0.5741443635
C,0,-3.7775102302,-1.5534851444,-0.0033894257
N,0,-3.5153252017,0.5255191778,0.9282608327
C,0,-2.9204462701,1.3302190486,0.0348400681
C,0,-1.5086758446,1.6267158883,-0.0319834206
O,0,-1.2637932667,2.5034174377,-1.0252131042
C,0,0.1065532168,2.8378942233,-1.2473215492
C,0,-2.7967259499,0.096676568,2.1393679921
C,0,-4.9502655447,0.7804144899,1.1556544369

O,0,-0.6113268077,1.1960040893,0.6921884726
N,0,1.4676917111,-0.8865330441,-1.8839968741
O,0,1.6727235535,-0.0204512552,-2.7321256421
O,0,2.3740806384,-1.5341432418,-1.3653726034
H,0,-3.0503833634,-0.2136157742,-2.2052791567
H,0,-0.7102571544,0.1999433136,-2.9307602408
H,0,0.7153215772,-2.5868537967,0.0194638729
H,0,-1.6010463095,-2.9379649415,0.8365058205
H,0,-4.6249852037,-1.183457227,-0.5710889228
H,0,-3.9971475595,-2.1980781182,0.8433990865
H,0,-1.8930991531,-0.4414981784,1.8583653634
H,0,-3.4614681491,-0.550508668,2.7097712065
H,0,-2.5254166209,0.9759645121,2.7312450428
H,0,-5.4012884298,-0.1019123323,1.6076486994
H,0,-5.0573153729,1.63943485,1.8249108098
H,0,-5.434403555,0.9947859119,0.2033792921
H,0,-3.5605632242,1.8234768141,-0.6848950402
H,0,0.549444585,3.2573835729,-0.340387611
H,0,0.6674812136,1.9542664833,-1.5729949884
H,0,0.102796839,3.582714279,-2.040362957
H,0,1.2590941906,1.0621554711,0.7106921833
N,0,2.2123471419,0.6933921449,0.7007247143
C,0,2.4488620847,-0.3678421861,1.4583480093
N,0,3.6238850496,-0.9737655987,1.4590488719
C,0,3.8803187159,-2.1655103466,2.2854473283
C,0,4.7409949722,-0.4625594717,0.6474414569
C,0,3.2247417324,1.3346793744,-0.1404986715
C,0,1.3601196822,-0.818494503,2.3920601176
C,0,1.7421953429,-0.5717565604,3.8659045997
H,0,1.1533721149,-1.882404839,2.2359610236
H,0,0.4536987669,-0.2708671257,2.1278264294
H,0,5.6625343998,-0.6867599674,1.1882030371
H,0,4.7524672622,-0.9999235084,-0.3068068813
H,0,3.146426873,0.959882785,-1.1662953663
H,0,3.0214662447,2.4073872418,-0.1454918668
C,0,4.5978644727,1.0361565455,0.4376925474
H,0,5.3745427061,1.386167377,-0.244332329
H,0,4.721671051,1.5547332802,1.393975548
C,0,3.9867471422,-1.84507753,3.7769719196
H,0,3.1003220344,-2.9104025158,2.0958292328
H,0,4.8153186408,-2.5875940775,1.9149991162
H,0,4.5203694176,-2.6693100636,4.2607575101
H,0,4.606186365,-0.9475854586,3.8990353548
C,0,2.6316612258,-1.66421748,4.4638460792
H,0,2.2239173541,0.4097579192,3.9572650673
H,0,0.8141766351,-0.5203509057,4.4424363609
H,0,2.7957027434,-1.4463173597,5.5238155495
H,0,2.0879353268,-2.6174972879,4.4210707446

Complex 7----8----H-DBU+ in CH2Cl2

/home/biswas/nitrodoc2/DBUfullComplexCH2Cl2
DBU full complex
M062X/6-31+G**
E(RM062X) = -1339.22753350

Zero-point correction= 0.541200 (Hartree/Particle)
Thermal correction to Energy= 0.570241
Thermal correction to Enthalpy= 0.571185
Thermal correction to Gibbs Free Energy= 0.483393
Sum of electronic and ZPE= -1338.686334
Sum of electronic and thermal Energies= -1338.657293
Sum of electronic and thermal Enthalpies= -1338.656349
Sum of electronic and thermal Free Energies= -1338.744140

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.831	112.732	184.773

C,0,-2.7270648599,-0.4744279057,-2.0588951184
C,0,-1.4262919783,-0.2407889363,-2.4578575541
C,0,-0.3670442904,-0.8951023581,-1.8136556162
C,0,-0.6235307954,-1.862626629,-0.7961476403
C,0,-1.9015731099,-2.1171170231,-0.4110940561
C,0,-3.038645043,-1.4455375564,-1.0239379798
C,0,-4.3171739488,-1.6569476325,-0.6009470667
N,0,-3.9036195805,0.9360392557,0.5594903015
C,0,-3.324582277,1.5675381176,-0.4213324166
C,0,-1.8780914741,1.8655575041,-0.5023788349
O,0,-1.6517435512,2.6927069099,-1.5173822958
C,0,-0.2804120288,3.0391683807,-1.7614744984
C,0,-3.1733522046,0.3511935799,1.6919345054
C,0,-5.3648601007,1.0294021182,0.7091068711
O,0,-1.0188862319,1.4623880416,0.2625124607
N,0,0.9580783805,-0.6354406396,-2.2087166302
O,0,1.179390996,0.2507423642,-3.0528092383
O,0,1.8850375105,-1.2825420408,-1.6957703953
H,0,-3.5435554721,-0.0364205505,-2.6261412893
H,0,-1.2105822586,0.4538789164,-3.2630236581
H,0,0.2130823012,-2.3936471415,-0.3569019469
H,0,-2.0988884959,-2.8618796495,0.3555971517
H,0,-5.1554316336,-1.1781136729,-1.0978604617
H,0,-4.5372985226,-2.3670548541,0.1906930054
H,0,-2.3695437455,-0.284916513,1.3184290536
H,0,-3.8814311384,-0.2373074532,2.2719317009
H,0,-2.7509236969,1.1504695421,2.3062056212
H,0,-5.7495116383,0.0721430024,1.0540643789
H,0,-5.5836766804,1.8075976626,1.4463379084
H,0,-5.81502641,1.2889802439,-0.2477372021
H,0,-3.9574535244,2.031627607,-1.1697628148
H,0,0.1538978938,3.4897970241,-0.8661512101
H,0,0.2802856644,2.1477665177,-2.0646276729
H,0,-0.3045104878,3.7611985884,-2.5740860842
H,0,0.9002779122,1.3310036745,0.3439172593
N,0,1.8492615445,0.9621961912,0.3309681652
C,0,2.0772922825,-0.1188973204,1.0622092024
N,0,3.2456482084,-0.735729449,1.0464823512
C,0,3.4924783214,-1.9459048672,1.8486807161
C,0,4.3472626221,-0.2457202989,0.2018504721
C,0,2.8471146161,1.5827892023,-0.541540464
C,0,0.9842393678,-0.5811729096,1.9835936539
C,0,1.3595905938,-0.3739142622,3.4644467223
H,0,0.769580972,-1.6385685233,1.798023772
H,0,0.0801135023,-0.0242009576,1.7295402311
H,0,5.2811136632,-0.4915319606,0.7112552167
H,0,4.3109432568,-0.78063968,-0.7531990071
H,0,2.7241088473,1.2041546533,-1.5615136889
H,0,2.6664078304,2.6597154807,-0.540096508
C,0,4.2296206442,1.2556666578,-0.0030861623
H,0,4.9930895992,1.589132768,-0.7082878952
H,0,4.3927823287,1.7721965087,0.948487976
C,0,3.595393961,-1.6586208137,3.3474200451
H,0,2.7091628585,-2.6827621257,1.6407595051
H,0,4.4270699552,-2.364662997,1.4738006767

H,0,4.1240111492,-2.4962148861,3.8137647434
H,0,4.219276904,-0.767215892,3.4904541169
C,0,2.2405094236,-1.4865555754,4.0366332512
H,0,1.8476080049,0.6015640897,3.5829908536
H,0,0.4294051139,-0.3325978594,4.0385672749
H,0,2.4042888994,-1.2963126035,5.1020922104
H,0,1.6907530501,-2.4350070651,3.9688060323

TS to 23 ----H-DBU+ in CH2Cl2

This is a saddle point for conversion of **7----8** to **3a**.
/home/biswas/nitrodoc2/DBUfull2ndTSto23CH2Cl2
2nd ts with DBU full search
M062X/6-31+G**
E(RM062X) = -1339.22495911

Zero-point correction= 0.541285 (Hartree/Particle)
Thermal correction to Energy= 0.569731
Thermal correction to Enthalpy= 0.570675
Thermal correction to Gibbs Free Energy= 0.483996
Sum of electronic and ZPE= -1338.683675
Sum of electronic and thermal Energies= -1338.655228
Sum of electronic and thermal Enthalpies= -1338.654284
Sum of electronic and thermal Free Energies= -1338.740963

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.512	110.430	182.431

C,0,-3.1085366605,-0.5694571069,1.1982822816
C,0,-2.0391985392,-1.5053546068,1.3231661872
C,0,-0.7795567105,-1.0601533614,1.6233563886
C,0,-0.5124406541,0.3126732088,1.9612809575
C,0,-1.5369220432,1.1957673862,1.9918246053
C,0,-2.9074058929,0.7954443219,1.7002447669
C,0,-3.9356126416,1.6739362068,1.7658273784
N,0,-3.7371617028,1.1118386143,-0.9920112845
C,0,-3.4243964683,-0.1877294524,-0.8448224011
C,0,-2.1500655506,-0.7584278691,-1.3514530196
O,0,-2.2983149017,-2.0625895648,-1.5745512365
C,0,-1.1155106287,-2.7985040235,-1.9174854582
C,0,-2.7292357408,2.1455169858,-1.1925614008
C,0,-5.1261402521,1.4847361527,-1.2436580214
O,0,-1.098906638,-0.162460805,-1.5081062573
N,0,0.3108595977,-1.9985782484,1.6557181019
O,0,0.118442185,-3.1560838182,1.2843114666
O,0,1.4115763802,-1.6012065188,2.0347178557
H,0,-4.1101403183,-0.9783438038,1.3018009739
H,0,-2.2086457542,-2.5594676461,1.129779637
H,0,0.4988260698,0.6002721904,2.2218778162
H,0,-1.3574835328,2.2273483698,2.284105702
H,0,-4.9584235192,1.3569838186,1.587167051
H,0,-3.7727321475,2.7093931225,2.0501734302
H,0,-1.8931001643,1.9855348366,-0.5080743515
H,0,-3.189043404,3.1115032124,-0.9806355181
H,0,-2.3508759897,2.1370954437,-2.2207912278
H,0,-5.3453399743,2.4320735703,-0.7481760267
H,0,-5.3048716039,1.5906352775,-2.32032961
H,0,-5.7911911133,0.7170296265,-0.8454411489
H,0,-4.2591926835,-0.8714609975,-0.9542726849
H,0,-0.6122782044,-2.3323975549,-2.766880552
H,0,-0.4530229792,-2.8501818564,-1.0473451263
H,0,-1.4588516195,-3.7962186827,-2.1805110208
H,0,0.7652377035,-0.6108256105,-1.3212637405
N,0,1.6837506866,-0.7512904147,-0.9029675792
C,0,2.2323276012,0.2970478488,-0.3041396305
N,0,3.3965966078,0.2109941271,0.3149381001
C,0,4.02038059,1.3816961117,0.9570310115
C,0,4.1570284846,-1.0508548863,0.324076688
C,0,2.3282939604,-2.0617621854,-1.0101590939
C,0,1.5286509781,1.619206602,-0.4277545314
C,0,2.3111280722,2.5840849545,-1.3413781958
H,0,1.3992867039,2.0672090692,0.5626693553
H,0,0.5293494413,1.4275093184,-0.8248649776
H,0,5.2167172103,-0.7892293404,0.3425054913
H,0,3.9115263118,-1.5972228116,1.2406762544
H,0,1.9689219347,-2.7183471437,-0.2105566505
H,0,2.0436810348,-2.4937728027,-1.9717338428
C,0,3.8322882935,-1.8711504281,-0.913447492
H,0,4.3281520813,-2.8413572967,-0.8506937331
H,0,4.2008834839,-1.3538433247,-1.8053706679
C,0,4.5434945873,2.4034693742,-0.0535841534
H,0,3.3053062339,1.8400503857,1.6475534794
H,0,4.8359239227,0.9871369201,1.5640767499
H,0,5.2884461581,3.0250002304,0.4534021449
H,0,5.0674168858,1.8673468455,-0.8554356337
C,0,3.4548237096,3.31127179,-0.630475909
H,0,2.6881724841,2.0344373888,-2.2128939482
H,0,1.6039281132,3.3273992118,-1.7204282018
H,0,3.9136331717,4.0173477031,-1.3297646771
H,0,3.030745354,3.9107369351,0.1862781303

Product (3a) ----H-DBU+ in CH2Cl2

/home/biswas/23arom_Doc_first_download/nitro
/DBUfullprodCH2Cl2confbUF
prod with full DBU
M062X/6-31+g**
E(RM062X) = -1339.23484527

Zero-point correction= 0.542486 (Hartree/Particle)
Thermal correction to Energy= 0.571533
Thermal correction to Enthalpy= 0.572477
Thermal correction to Gibbs Free Energy= 0.482314
Sum of electronic and ZPE= -1338.692359
Sum of electronic and thermal Energies= -1338.663312
Sum of electronic and thermal Enthalpies= -1338.662368
Sum of electronic and thermal Free Energies= -1338.752531

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	358.642	111.120	189.764

C,0,-2.9902250639,-0.2368176165,1.2371941492
C,0,-2.0282125879,-1.3880080266,1.3216849267
C,0,-0.7360711347,-1.1612278036,1.593751922
C,0,-0.1914905427,0.1395249916,1.9551679459
C,0,-1.037020355,1.1755177157,2.0921769487
C,0,-2.4814220047,1.0200705444,1.9146077748
C,0,-3.3305458035,1.9522994433,2.3719565864
N,0,-4.0374936145,1.2084700905,-0.5698971115
C,0,-3.4149955933,-0.0672664028,-0.2906920752
C,0,-2.2510212341,-0.4427981108,-1.2098661792
O,0,-2.498320803,-1.5804223908,-1.8545421339

C,0,-1.4268884056,-2.1285827369,-2.6348797353
C,0,-3.1431835305,2.30854334,-0.9255342627
C,0,-5.1242493185,1.1011135827,-1.5396020598
O,0,-1.2098609987,0.1768445563,-1.323184435
N,0,0.2080097442,-2.2834944418,1.5192707556
O,0,-0.185028556,-3.3601043545,1.1007763712
O,0,1.3652388481,-2.0683073258,1.8533736878
H,0,-3.9284091743,-0.5243971999,1.7206600709
H,0,-2.3698073709,-2.3878996175,1.0707201136
H,0,0.8698112843,0.2247873249,2.1520249915
H,0,-0.6647927622,2.1466975618,2.4080834873
H,0,-4.4050569547,1.8226463957,2.2976051559
H,0,-2.9606970516,2.8688475383,2.8229849811
H,0,-2.2724395201,2.328479131,-0.270672437
H,0,-3.6906637779,3.2483094661,-0.8108711179
H,0,-2.7871515322,2.2346201631,-1.9655898514
H,0,-5.6310367284,2.0672460495,-1.6057728909
H,0,-4.7701926606,0.8317584999,-2.5492339286
H,0,-5.8500486071,0.3543569497,-1.2095444307
H,0,-4.1687847237,-0.8403375699,-0.4538623655
H,0,-1.0257208893,-1.3769245436,-3.3162280305
H,0,-0.6473986638,-2.4922242895,-1.9595286451
H,0,-1.8571887968,-2.960461713,-3.1865889277
H,0,0.6550168589,-0.3838917657,-1.3619457625
N,0,1.5661982346,-0.6443958728,-0.9874452842
C,0,2.2303412275,0.3007493716,-0.3343723788
N,0,3.3899150659,0.052793261,0.248657535
C,0,4.1473356566,1.1066161946,0.9479726275
C,0,4.0284263242,-1.2698013022,0.1268158892
C,0,2.0956258839,-1.9821800486,-1.2635287218
C,0,1.6658508128,1.6939219807,-0.3528261048
C,0,2.5311416346,2.6267853954,-1.2255326299
H,0,1.6052638082,2.0877676259,0.6666599954
H,0,0.6434683571,1.6348767659,-0.7324400773
H,0,5.1076195549,-1.107917607,0.1439039013
H,0,3.750019931,-1.8760688256,0.9945877901
H,0,1.6854913594,-2.7039934923,-0.5492903548
H,0,1.7728898739,-2.2643653124,-2.2675038587
C,0,3.6120336419,-1.9363551804,-1.174324574
H,0,4.017770713,-2.948390414,-1.2149942454
H,0,4.0163910901,-1.3705280297,-2.0197131634
C,0,4.7591975743,2.1283877118,-0.0112963886
H,0,3.4972162667,1.5946429566,1.6809554615
H,0,4.9243066795,0.5885432511,1.5111300502
H,0,5.5754367496,2.6350188551,0.5131150567
H,0,5.2074669322,1.5912148334,-0.8568201277
C,0,3.7620430032,3.1801142645,-0.5030173935
H,0,2.8260413405,2.0986589553,-2.1408803879
H,0,1.9008310915,3.4645494559,-1.5362095405
H,0,4.2794131762,3.876239732,-1.1704304406
H,0,3.4228880411,3.7685320388,0.359825877

Ylide (2a) ----H-DBU+ in DMSO

/home/biswas/23arom_Doc_first_download/nitro
/ylideDBUfullconfbDMSOUF
nitrobenzyl SM with DBU actual conf B
M062X/6-31+G**
E(RM062X) = -1339.26216305

Zero-point correction= 0.543903 (Hartree/Particle)
Thermal correction to Energy= 0.572225
Thermal correction to Enthalpy= 0.573169
Thermal correction to Gibbs Free Energy= 0.485425
Sum of electronic and ZPE= -1338.718260
Sum of electronic and thermal Energies= -1338.689938
Sum of electronic and thermal Enthalpies= -1338.688994
Sum of electronic and thermal Free Energies= -1338.776739

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	359.077	110.084	184.675

C,0,2.0738524351,0.7375603852,1.7848081732
C,0,0.7488094159,1.0145468648,2.0948927135
C,0,-0.1270845441,-0.0563604343,2.2410344074
C,0,0.2749779249,-1.3820678286,2.1344894833
C,0,1.6016319974,-1.6358195028,1.8090617721
C,0,2.4968062718,-0.5830324178,1.5987275359
C,0,3.9057810885,-0.877395382,1.1689279774
N,0,4.0863627968,-0.8584690223,-0.3498749161
C,0,3.8535390815,0.4771441847,-0.9259938047
C,0,2.6152953678,0.9567823323,-1.2917095601
O,0,2.7169284598,2.2328023818,-1.8213562653
C,0,1.5090954178,2.9734551716,-1.8638876518
C,0,3.2419370467,-1.9204560207,-0.9902903271
C,0,5.5214141608,-1.2156492568,-0.6054117906
O,0,1.4792655815,0.414498021,-1.2216246655
N,0,-1.547514465,0.2213207217,2.4883451191
O,0,-1.903372398,1.3880708484,2.5522093964
O,0,-2.3114814033,-0.7263669089,2.5881215117
H,0,2.7778985857,1.5527015976,1.6536910009
H,0,0.3952864746,2.0322482197,2.2101259684
H,0,-0.43385888,-2.1860625545,2.2906731566
H,0,1.9361715045,-2.6638775836,1.7078708835
H,0,4.5983727531,-0.124879806,1.5491527158
H,0,4.2194535508,-1.8664838219,1.5138608718
H,0,2.1942737971,-1.6685688129,-0.8544794325
H,0,3.4892775941,-2.8792069434,-0.5315993845
H,0,3.4835405388,-1.9297796524,-2.0526734872
H,0,5.7196674789,-2.2039123615,-0.1908227224
H,0,5.6819164682,-1.2082245818,-1.6821966597
H,0,6.155374592,-0.4700700155,-0.1261983307
H,0,4.7333536207,1.0995514142,-0.9666598942
H,0,0.7627011476,2.4871478391,-2.4996395193
H,0,1.1023217059,3.1083636707,-0.854072206
H,0,1.764607664,3.9470093419,-2.2814662935
H,0,-0.2040798005,0.9752132958,-0.9108699618
N,0,-1.2039688064,1.1060681093,-0.6887139988
C,0,-1.9425844488,0.0127593192,-0.583777346
N,0,-3.225343641,0.0614774706,-0.2553211155
C,0,-4.0292127998,-1.1616509269,-0.0911005904
C,0,-3.9208055389,1.3451654153,-0.0646395747
C,0,-1.7378414052,2.4541767633,-0.4989372122
C,0,-1.2892513898,-1.3049545206,-0.8920028563
C,0,-1.8683905618,-1.9495071815,-2.167336918
H,0,-1.4202096036,-1.9807561834,-0.0388015593
H,0,-0.2187447849,-1.118645291,-1.0031756608
H,0,-4.9428930382,1.2149086121,-0.4265595661
H,0,-3.9561384509,1.565209157,1.0083644516
H,0,-1.5725417754,2.7687688985,0.537508074
H,0,-1.1916002191,3.1293322347,-1.158393556
C,0,-3.2199541949,2.4494798115,-0.8374677514
H,0,-3.6654073729,3.4128174433,-0.5838767752

H,0,-3.3494473122,2.2847554506,-1.9119243958
C,0,-4.335279906,-1.8595347076,-1.416735024
H,0,-3.5169312268,-1.8346479577,0.6040111752
H,0,-4.95040925,-0.8449441547,0.3999964867
H,0,-5.2058382783,-2.5050196168,-1.2626310452
H,0,-4.6249197581,-1.1017282544,-2.1556220698
C,0,-3.1761837737,-2.7100998768,-1.9391699447
H,0,-2.0023836835,-1.1764367326,-2.9340267701
H,0,-1.11870805,-2.6468025835,-2.5518903674
H,0,-3.4769104533,-3.1866638817,-2.8776149235
H,0,-2.9869053079,-3.5203441987,-1.2222899804

TS (6‡) ----H-DBU+ in DMSO

/home/biswas/23arom_Doc_first_download/nitro
/DBUfullTSPSdmsoconfbUF
DBUfullTSPSdmsoconfb UF
M062X/6-31+G**
E(RM062X) = -1339.23180563

Zero-point correction= 0.540952 (Hartree/Particle)
Thermal correction to Energy= 0.569215
Thermal correction to Enthalpy= 0.570159
Thermal correction to Gibbs Free Energy= 0.483523
Sum of electronic and ZPE= -1338.690854
Sum of electronic and thermal Energies= -1338.662591
Sum of electronic and thermal Enthalpies= -1338.661646
Sum of electronic and thermal Free Energies= -1338.748282

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.188	110.346	182.341

C,0,-2.2309621812,-0.6622711616,-1.6627967001
C,0,-0.9295223049,-0.4677829431,-2.1155615683
C,0,0.1094113007,-1.1289052638,-1.4738258042
C,0,-0.1179443246,-2.0484851675,-0.4255996755
C,0,-1.3978944059,-2.2347804908,0.0222152592
C,0,-2.5032051181,-1.5417812981,-0.5721690548
C,0,-3.7704592752,-1.5362283879,0.0089605062
N,0,-3.5121965792,0.5247484442,0.9337383578
C,0,-2.9226393453,1.3380744121,0.0430608079
C,0,-1.5113513601,1.629048987,-0.0320035307
O,0,-1.2679484106,2.510468996,-1.0232042643
C,0,0.1030775895,2.8397832854,-1.2498518819
C,0,-2.790308132,0.1002702791,2.1457907833
C,0,-4.9470347571,0.779729428,1.1671325629
O,0,-0.6102793906,1.191393886,0.6834598648
N,0,1.4630445349,-0.8920237187,-1.9107492366
O,0,1.6652783099,-0.0261481695,-2.7607035795
O,0,2.3716809208,-1.5442647411,-1.4018757204
H,0,-3.0552725991,-0.2076639694,-2.2018330923
H,0,-0.7194617194,0.1994100125,-2.9439078714
H,0,0.7196105056,-2.5849116933,0.0042743118
H,0,-1.5906651835,-2.9243508318,0.8396104183
H,0,-4.6203904257,-1.1711129961,-0.5582204294
H,0,-3.9862514164,-2.1773624224,0.8594112168
H,0,-1.8869406819,-0.4383716207,1.8658939194
H,0,-3.4533395331,-0.5452811341,2.7197899633
H,0,-2.5197012538,0.98234008,2.7334511507
H,0,-5.3963182697,-0.1028835025,1.6200752513
H,0,-5.0497532005,1.6376378674,1.8381350645
H,0,-5.4341453597,0.9955566121,0.2167890212
H,0,-3.5669093018,1.8314024632,-0.6728337165
H,0,0.5512654826,3.2574758423,-0.3448658559
H,0,0.6599232467,1.9540369141,-1.5768087793
H,0,0.0998609457,3.5844196927,-2.0431069747
H,0,1.2564157543,1.0428607313,0.6988669615
N,0,2.209500835,0.6738936475,0.6877072272
C,0,2.4493995152,-0.3823197334,1.4511701807
N,0,3.6290153075,-0.979228119,1.4611628621
C,0,3.8897656046,-2.1648234541,2.2950905789
C,0,4.7513160782,-0.4559503066,0.6648008199
C,0,3.2238147288,1.3218983458,-0.1454681546
C,0,1.3581132082,-0.8381670048,2.3789710393
C,0,1.7279804008,-0.5821694398,3.8542447802
H,0,1.1600425345,-1.9040962073,2.2259714082
H,0,0.449700691,-0.2978861505,2.1068140964
H,0,5.6673054934,-0.66799663,1.2196159128
H,0,4.7849688197,-0.9955426726,-0.2877115301
H,0,3.1601222245,0.941387228,-1.1703519369
H,0,3.0095006105,2.3922332437,-0.1577732422
C,0,4.5935453604,1.0403182393,0.448966849
H,0,5.3743111427,1.3973838588,-0.2245856231
H,0,4.6993055795,1.5625062487,1.4053058944
C,0,3.9842255567,-1.8356924055,3.7854883237
H,0,3.1163483937,-2.9160409487,2.1048531058
H,0,4.8304674734,-2.5810177022,1.9325171592
H,0,4.5224218622,-2.6527872956,4.2763277094
H,0,4.5943203284,-0.9317004372,3.9065144169
C,0,2.6229491384,-1.6643038572,4.4626350718
H,0,2.2008200131,0.4036438739,3.9444957856
H,0,0.7950618086,-0.5370223719,4.4233410028
H,0,2.7780819235,-1.4401838122,5.5227544435
H,0,2.0878513064,-2.6224035584,4.4198981342

TS (6‡) ----H-DBU+ in DMSO, Alternative Conformation A

DBUfullTSPSdmso
nitrobenzyl rearr coord with DBU actual
M062X/6-31+G**
E(RM062X) = -1339.23056733

Zero-point correction= 0.540406 (Hartree/Particle)
Thermal correction to Energy= 0.568844
Thermal correction to Enthalpy= 0.569788
Thermal correction to Gibbs Free Energy= 0.482181
Sum of electronic and ZPE= -1338.690161
Sum of electronic and thermal Energies= -1338.661723
Sum of electronic and thermal Enthalpies= -1338.660779
Sum of electronic and thermal Free Energies= -1338.748387

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	356.955	110.548	184.385

C,0,3.1208567948,0.2224369146,1.5919393087
C,0,1.9286870133,0.7649662367,2.0613171029
C,0,0.7833577093,-0.0206664798,2.0442923177
C,0,0.8095501651,-1.3794111638,1.6612870353
C,0,1.9845178259,-1.9133681819,1.2047207762
C,0,3.176985447,-1.1239669736,1.1248586444

C,0,4.2913312286,-1.5523363884,0.4013942124
N,0,3.79323828,-0.3457106224,-1.4232279092
C,0,3.4429665252,0.8976611292,-1.0501602884
C,0,2.1012922378,1.3876314081,-0.8585064691
O,0,2.1384254255,2.6935729013,-0.5165530858
C,0,0.8827622003,3.311437896,-0.2314585673
C,0,2.7889487249,-1.2477300952,-2.011534418
C,0,5.1196332392,-0.4579139023,-2.0629790092
O,0,1.0337717136,0.7870383577,-0.988253566
N,0,-0.4742836055,0.5621008639,2.447093214
O,0,-0.5136349514,1.7615632169,2.7091241036
O,0,-1.4690695712,-0.1597818535,2.485312961
H,0,4.0322111865,0.8084162893,1.6458394714
H,0,1.879218177,1.7907949854,2.4093433991
H,0,-0.0979798852,-1.9674839068,1.7233168408
H,0,2.0224685213,-2.9528475095,0.8893929918
H,0,5.2328757079,-1.0218577386,0.5009431578
H,0,4.340646928,-2.5705355145,0.0245286435
H,0,1.9823392086,-1.410837388,-1.2993486518
H,0,3.2806138284,-2.1908408502,-2.2458680532
H,0,2.3848638681,-0.7956649218,-2.9217958737
H,0,5.443142294,-1.4976507759,-2.0323934468
H,0,5.0415167162,-0.1208358333,-3.1007789959
H,0,5.8322145787,0.166814126,-1.5254681824
H,0,4.2487296443,1.6000926926,-0.881132241
H,0,0.2102199576,3.22825349,-1.0887390332
H,0,0.4216730615,2.8532630721,0.6504843567
H,0,1.1101180736,4.3567765687,-0.0314657644
H,0,-0.4209643139,-0.3983638904,-0.8613132223
N,0,-1.2801785782,-0.933567723,-0.7350285552
C,0,-2.3534430329,-0.2661980723,-0.3398755809
N,0,-3.5124177212,-0.8687443644,-0.1294787009
C,0,-4.7276476251,-0.103589382,0.2021879205
C,0,-3.6553794841,-2.3223353124,-0.3146429261
C,0,-1.2579393323,-2.3762926954,-0.9636750455
C,0,-2.2205419049,1.2210584485,-0.1859053349
C,0,-2.9638949305,1.996014883,-1.290118162
H,0,-2.5881877502,1.5149053222,0.8035427688
H,0,-1.1524852868,1.4492379075,-0.2230119664
H,0,-4.3919854144,-2.6718593743,0.4104026431
H,0,-4.0457688421,-2.514028299,-1.3207568267
H,0,-1.439093921,-2.5799141905,-2.0240688896
H,0,-0.2600618624,-2.7415032796,-0.7108162415
C,0,-2.324085147,-3.0221456475,-0.0943849523
H,0,-2.4221533188,-4.0805509841,-0.3416333974
H,0,-2.0451582136,-2.9426576858,0.9617210172
H,0,-5.4890471752,-0.8473339573,0.4382624401
H,0,-4.5484838278,0.475936413,1.1150927739
C,0,-5.2135567501,0.796996021,-0.9353411012
H,0,-6.274464088,1.0030899381,-0.7608814656
H,0,-5.1474699529,0.2399763905,-1.8784074536
H,0,-2.5259089307,2.997341127,-1.342501396
H,0,-2.7752025807,1.5182002568,-2.2595884468
C,0,-4.4663232228,2.1269508667,-1.0405211707
H,0,-4.9099697437,2.7232646851,-1.8441789183
H,0,-4.6196183177,2.6893065497,-0.1096287919

Complex 7----8----H-DBU+ in DMSO

/home/biswas/nitrodoc2/DBUfullComplexDMSO
DBU full complex
M062X/6-31+G**
E(RM062X) = -1339.23545664

Zero-point correction= 0.540666 (Hartree/Particle)
Thermal correction to Energy= 0.569931
Thermal correction to Enthalpy= 0.570875
Thermal correction to Gibbs Free Energy= 0.482079
Sum of electronic and ZPE= -1338.694791
Sum of electronic and thermal Energies= -1338.665526
Sum of electronic and thermal Enthalpies= -1338.664582
Sum of electronic and thermal Free Energies= -1338.753377

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.637	113.044	186.886

C,0,-2.7271162987,-0.4906198924,-2.0825658307
C,0,-1.433551121,-0.2426630266,-2.4758651523
C,0,-0.3600638114,-0.8918191972,-1.8331861106
C,0,-0.6151419358,-1.8553798604,-0.8091111657
C,0,-1.8904429609,-2.1162490998,-0.4214348379
C,0,-3.0357285571,-1.4572977775,-1.0381922853
C,0,-4.3125599631,-1.687220355,-0.6251564574
N,0,-3.8936288238,0.9747192614,0.5853535271
C,0,-3.3323992748,1.6041645425,-0.3969327479
C,0,-1.8765419224,1.8801295373,-0.5020353081
O,0,-1.6552613037,2.7011007293,-1.5186878578
C,0,-0.2817912417,3.0357638056,-1.7759143162
C,0,-3.1533254173,0.3688313983,1.7036146218
C,0,-5.3583627242,1.0279070732,0.7339225207
O,0,-1.019759952,1.4640743456,0.2548154634
N,0,0.9515344118,-0.6326535773,-2.2318852534
O,0,1.1721500127,0.2510109231,-3.0875612321
O,0,1.8906315329,-1.2753357638,-1.7226795514
H,0,-3.5485359304,-0.0420192444,-2.6352292445
H,0,-1.224518373,0.4556857558,-3.2796963745
H,0,0.2245486756,-2.3761426068,-0.3631001639
H,0,-2.0808671353,-2.853109638,0.3546718206
H,0,-5.1536084211,-1.2072075972,-1.1167833018
H,0,-4.5273870749,-2.3953769574,0.1696901906
H,0,-2.3710602413,-0.2824012279,1.3115209805
H,0,-3.8639379038,-0.2051464748,2.2941810082
H,0,-2.7044751669,1.1584484406,2.3101735044
H,0,-5.7177865273,0.0505979179,1.0478904419
H,0,-5.5896145139,1.7747938195,1.4983309483
H,0,-5.8125017591,1.3099379348,-0.2141429371
H,0,-3.9719717253,2.0616919886,-1.1442698588
H,0,0.1628177951,3.4835513668,-0.8845744024
H,0,0.2671350292,2.1377992523,-2.0815714985
H,0,-0.3076445164,3.7568580281,-2.5890615957
H,0,0.9013210305,1.3268003394,0.3454800072
N,0,1.8474093336,0.9526639062,0.3292212011
C,0,2.0729150721,-0.1271907703,1.0623582304
N,0,3.2409616091,-0.7450798494,1.049343041
C,0,3.4884839794,-1.947836696,1.8622574118
C,0,4.3451824634,-0.2552000245,0.2086544132
C,0,2.8466379522,1.5728531836,-0.5412844436
C,0,0.9782636459,-0.5865952553,1.9830894502
C,0,1.3484157703,-0.3700954566,3.4637882562
H,0,0.7653987924,-1.6453004343,1.8031604945
H,0,0.074272451,-0.0318208172,1.7244887223
H,0,5.277096217,-0.4994389409,0.7221416223
H,0,4.3135971358,-0.7911439501,-0.7459761954

H,0,2.724477871,1.1931265348,-1.5610935651
H,0,2.665904819,2.6497440822,-0.5403318009
C,0,4.2277735051,1.2459260581,0.0009342612
H,0,4.9935145463,1.5787604605,-0.7021063764
H,0,4.387569679,1.7632282641,0.9525643849
C,0,3.588846278,-1.6473572786,3.3587071724
H,0,2.7055944469,-2.6869754698,1.6613189621
H,0,4.4239717031,-2.3688432471,1.4921982709
H,0,4.1208626181,-2.4787842835,3.8322567365
H,0,4.2078983812,-0.7515309025,3.4947960406
C,0,2.2317414889,-1.4765468051,4.0440393542
H,0,1.8325825785,0.6076735569,3.578107993
H,0,0.4157635482,-0.3296323881,4.0338845724
H,0,2.3922570724,-1.2800717506,5.1089490408
H,0,1.6855261508,-2.4272418896,3.9791571991

TS to 23 ----H-DBU+ in DMSO

This is a saddle point for conversion of **7----8** to **3a**.
/home/biswas/nitrodoc2/DBUfull2ndTSto23DMSO
2nd ts with DBU full search
M062X/6-31+G**
E(RM062X) = -1339.23143231

Zero-point correction= 0.540922 (Hartree/Particle)
Thermal correction to Energy= 0.569478
Thermal correction to Enthalpy= 0.570422
Thermal correction to Gibbs Free Energy= 0.483101
Sum of electronic and ZPE= -1338.690511
Sum of electronic and thermal Energies= -1338.661954
Sum of electronic and thermal Enthalpies= -1338.661010
Sum of electronic and thermal Free Energies= -1338.748331

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.353	110.547	183.783

C,0,-3.107091712,-0.5635826603,1.1900513298
C,0,-2.0544990759,-1.5201154452,1.317213192
C,0,-0.7863656913,-1.0982107688,1.6144539558
C,0,-0.4915745498,0.2716929393,1.9440232632
C,0,-1.4987220978,1.1739759976,1.9754067734
C,0,-2.8786759234,0.7972310926,1.6955273819
C,0,-3.8920696458,1.6910538915,1.7739787138
N,0,-3.7301701315,1.1123032242,-0.9902711842
C,0,-3.4208965526,-0.1881842999,-0.8348499274
C,0,-2.1510197377,-0.7624324786,-1.3533391527
O,0,-2.3033061394,-2.0659308627,-1.5767276684
C,0,-1.1232996224,-2.8017186903,-1.930976032
C,0,-2.7209615514,2.1426858798,-1.2013054718
C,0,-5.1196891015,1.4883734311,-1.2326835358
O,0,-1.1002985941,-0.1687242151,-1.5169250596
N,0,0.2849831958,-2.0568642685,1.6546371741
O,0,0.0745639065,-3.2114025942,1.2819822172
O,0,1.3900728031,-1.6814041074,2.0438223545
H,0,-4.1147287394,-0.9545588278,1.3041022799
H,0,-2.2449702067,-2.5711800315,1.1268784506
H,0,0.5262758457,0.5430400099,2.196413435
H,0,-1.2968483769,2.2042127262,2.2577363523
H,0,-4.9208217055,1.3905851666,1.6010701261
H,0,-3.7096726698,2.724140477,2.0553357132
H,0,-1.8798589564,1.9835922635,-0.5229559282
H,0,-3.1764828933,3.1105004069,-0.9885623752
H,0,-2.3504126804,2.1308705467,-2.2323980357
H,0,-5.3319082203,2.4389689993,-0.7401905729
H,0,-5.3065472121,1.5902237541,-2.3083477623
H,0,-5.7842210262,0.7248633892,-0.8256911263
H,0,-4.2583681954,-0.8685858126,-0.9455799416
H,0,-0.6254793334,-2.3331551915,-2.7818721275
H,0,-0.4544563932,-2.8561410565,-1.0659266475
H,0,-1.468867741,-3.7985230412,-2.194333142
H,0,0.7669152735,-0.6080599006,-1.3197298496
N,0,1.6785385219,-0.747126547,-0.886921391
C,0,2.2234716683,0.3071422897,-0.2950370796
N,0,3.3851005994,0.2269743597,0.3301904779
C,0,4.0067351634,1.4042636733,0.9627721508
C,0,4.1502781466,-1.0320369799,0.3441457273
C,0,2.3297125043,-2.05432185,-0.993791726
C,0,1.5183491941,1.6272055505,-0.4326091383
C,0,2.3034178691,2.5848828094,-1.3513945455
H,0,1.3822518852,2.0841932184,0.5528927634
H,0,0.5219721156,1.4302299331,-0.8341264999
H,0,5.2087654503,-0.7663166355,0.3649780132
H,0,3.9051915764,-1.5776617236,1.261311221
H,0,1.9711453482,-2.7140337372,-0.1961382399
H,0,2.0502168603,-2.4860326655,-1.9568186855
C,0,3.8324669656,-1.8563622645,-0.8924398737
H,0,4.3329966429,-2.8239531934,-0.8267133519
H,0,4.2005333323,-1.3382821669,-1.784020709
C,0,4.5318907375,2.4167597229,-0.0558951045
H,0,3.2892004491,1.8690959333,1.6460986892
H,0,4.8208141165,1.0158036214,1.5756204468
H,0,5.2753141243,3.042788899,0.4478833523
H,0,5.057513263,1.8737647542,-0.8518440113
C,0,3.4438628879,3.3190331816,-0.6426023283
H,0,2.6841848664,2.0279802174,-2.2165978755
H,0,1.5963602696,3.3240825604,-1.7386042546
H,0,3.9039192164,4.020255358,-1.3460967906
H,0,3.0164676775,3.9235867381,0.1686145909

Product (3a) ----H-DBU+ in DMSO

/home/biswas/23arom_Doc_first_download/nitro/
DBUfullprodDMSOconfb
prod with full DBU
M062X/6-31+g**
E(RM062X) = -1339.24578932

Zero-point correction= 0.542164 (Hartree/Particle)
Thermal correction to Energy= 0.571126
Thermal correction to Enthalpy= 0.572070
Thermal correction to Gibbs Free Energy= 0.482113
Sum of electronic and ZPE= -1338.703625
Sum of electronic and thermal Energies= -1338.674664
Sum of electronic and thermal Enthalpies= -1338.673719
Sum of electronic and thermal Free Energies= -1338.763677

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	358.387	111.149	189.331

C,0,-2.8390732532,-0.1834774764,1.2198041163
C,0,-1.7702656318,-1.2084101695,1.4768046847
C,0,-0.5550115696,-0.851005775,1.9091289497

C,0,-0.1530130836,0.5237419752,2.1724409069
C,0,-1.07115434,1.494885201,2.041406102
C,0,-2.4704124116,1.2136664198,1.7041027341
C,0,-3.4053057986,2.1553668992,1.9055593822
N,0,-4.4671095251,0.5334596498,-0.5625439603
C,0,-3.3050183097,-0.2994810962,-0.2661689688
C,0,-2.1758372123,-0.0708693635,-1.2633075237
O,0,-2.5261195287,-0.465416859,-2.4817286455
C,0,-1.5810136367,-0.2144268481,-3.5358844108
C,0,-4.1786786388,1.8086736574,-1.2174867085
C,0,-5.5247607117,-0.180500307,-1.2712818041
O,0,-1.1033098433,0.4418987932,-1.0043827375
N,0,0.4574444832,-1.8959063203,2.0921390938
O,0,0.1318598539,-3.0672204646,1.9730265589
O,0,1.602314123,-1.5355776511,2.3313598582
H,0,-3.7299887213,-0.5078489033,1.7724041398
H,0,-1.9942046584,-2.2526534373,1.2789358498
H,0,0.8630477572,0.7233109628,2.4885568619
H,0,-0.8035038511,2.527221145,2.2513306641
H,0,-4.4567225604,1.9541049073,1.7270491438
H,0,-3.1250943039,3.1501899747,2.2402926737
H,0,-3.3305300966,2.3008185421,-0.7389053312
H,0,-5.0500630424,2.4615338189,-1.1155517932
H,0,-3.9637338428,1.6866955022,-2.2926890793
H,0,-6.4067105288,0.4635073595,-1.3252633986
H,0,-5.232032859,-0.4565544362,-2.2972408243
H,0,-5.7952351737,-1.0859356714,-0.7223845684
H,0,-3.605532834,-1.3453422056,-0.4011758527
H,0,-1.3583631692,0.8525767106,-3.5894301537
H,0,-0.6640364881,-0.7783287191,-3.356853663
H,0,-2.0652701541,-0.5549448464,-4.447736938
H,0,0.6628860627,-0.3119511293,-0.961994624
N,0,1.5666833282,-0.6676032402,-0.657843239
C,0,2.4099765969,0.2151247863,-0.141606873
N,0,3.6010342366,-0.1444752848,0.30192529
C,0,4.5280110333,0.8265313732,0.9089402074
C,0,4.0771558707,-1.5312236277,0.1612111382
C,0,1.8924329434,-2.0766828633,-0.8827123185
C,0,2.0013825245,1.6615065832,-0.1537431648
C,0,2.875100425,2.484393819,-1.1217764033
H,0,2.0714412603,2.0765863431,0.8573355038
H,0,0.9500487341,1.7059087097,-0.4459154273
H,0,5.1575062681,-1.4860388159,0.008614177
H,0,3.8771161624,-2.0654006458,1.096208084
H,0,1.5268588712,-2.6866113314,-0.0500272657
H,0,1.3780381172,-2.3958827214,-1.7904230081
C,0,3.4003462794,-2.2065073236,-1.0207968795
H,0,3.6849469285,-3.2595445096,-1.0523958504
H,0,3.7290445825,-1.7333032441,-1.9517094937
C,0,5.1455830677,1.7800442004,-0.1145527298
H,0,4.0051504523,1.3776177407,1.6973021908
H,0,5.3007112419,0.2318207029,1.3979238677
H,0,6.0525336788,2.2043617972,0.3278576269
H,0,5.4583063899,1.1991494371,-0.9914646584
C,0,4.2149063246,2.9221674198,-0.5266976011
H,0,3.0332568603,1.911879013,-2.0444037713
H,0,2.3060344763,3.3764054705,-1.3985964709
H,0,4.7322116385,3.5583878622,-1.2518680705
H,0,4.0170172057,3.5479725096,0.3538864052

Ylide (2a) ----H-DBU+ in CCl4

/home/biswas/23arom_Doc_first_download/nitro
/ylideDBUfullconfbCCl4UF
nitrobenzyl SM with DBU actual conf B
M062X/6-31+G**
E(RM062X) = -1339.23162300

Zero-point correction= 0.544825 (Hartree/Particle)
Thermal correction to Energy= 0.572846
Thermal correction to Enthalpy= 0.573790
Thermal correction to Gibbs Free Energy= 0.487466
Sum of electronic and ZPE= -1338.686798
Sum of electronic and thermal Energies= -1338.658777
Sum of electronic and thermal Enthalpies= -1338.657833
Sum of electronic and thermal Free Energies= -1338.744157

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	359.466	109.642	181.685

C,0,2.1189644558,0.7057547201,1.8368468735
C,0,0.7885744938,0.9748193303,2.1315991921
C,0,-0.0893610594,-0.098094454,2.2347566151
C,0,0.3163007451,-1.4211846367,2.1131312457
C,0,1.6481270718,-1.667238625,1.8060000892
C,0,2.5434914837,-0.6094773378,1.6251886977
C,0,3.9491708018,-0.8895077006,1.1795831555
N,0,4.1136083722,-0.837924584,-0.341409531
C,0,3.8448360057,0.5000589488,-0.896033231
C,0,2.589257232,0.9567722265,-1.2378530457
O,0,2.6645696532,2.2151126308,-1.7939139944
C,0,1.4500120768,2.9344435497,-1.8635215241
C,0,3.284685014,-1.9038892988,-0.994369154
C,0,5.552142028,-1.1581018031,-0.617806361
O,0,1.4629024354,0.4020013308,-1.1101992513
N,0,-1.5187087307,0.1735083572,2.4439075542
O,0,-1.8747017168,1.3379308943,2.5280026403
O,0,-2.2825134174,-0.7778785353,2.4829272176
H,0,2.8243839791,1.5229164603,1.7272951557
H,0,0.429631162,1.9883794057,2.2659905578
H,0,-0.3959458074,-2.2261351935,2.2477163568
H,0,1.9870585353,-2.6930579853,1.6930756789
H,0,4.641850246,-0.1403337554,1.5668239384
H,0,4.2710909153,-1.884442453,1.5020889122
H,0,2.2338563869,-1.6644469395,-0.8543485186
H,0,3.5456557269,-2.8674170937,-0.5514128653
H,0,3.5232506346,-1.8918330629,-2.0574156896
H,0,5.7812145851,-2.1453634549,-0.2151540577
H,0,5.6998768761,-1.1347419916,-1.6963458968
H,0,6.1743229751,-0.4009655415,-0.1406092705
H,0,4.7199716877,1.1158777866,-1.0248105786
H,0,0.7084658326,2.4119123095,-2.476975463
H,0,1.0438052173,3.105865516,-0.8580700992
H,0,1.6921165051,3.8932169859,-2.3210615923
H,0,-0.2150696241,0.9744446607,-0.8765756141
N,0,-1.220579346,1.1132569331,-0.6727593578
C,0,-1.9709788059,0.0253644189,-0.5937251458
N,0,-3.2570551192,0.0784276411,-0.2787221879
C,0,-4.0707090773,-1.1409668869,-0.1340311677
C,0,-3.9304762939,1.3634988971,-0.0315169604
C,0,-1.7411390268,2.4636792919,-0.4633880213
C,0,-1.3229268053,-1.2923711696,-0.9139448353

C,0,-1.8963564039,-1.9217730481,-2.1995493125
H,0,-1.465795349,-1.9730637543,-0.0657948208
H,0,-0.2506452238,-1.1087918365,-1.0156184476
H,0,-4.9615068943,1.2605715017,-0.3768759998
H,0,-3.9402302616,1.5478550454,1.048873241
H,0,-1.5605429547,2.7648844504,0.5745378576
H,0,-1.1970664007,3.1407184587,-1.123334623
C,0,-3.2274736563,2.4810410795,-0.7837073194
H,0,-3.6596911295,3.442672201,-0.5013619168
H,0,-3.3724600735,2.3464543826,-1.8607156718
C,0,-4.3689163726,-1.8252758109,-1.4685027061
H,0,-3.5712004575,-1.8220932294,0.5624656065
H,0,-4.9940755604,-0.8228286294,0.3521860647
H,0,-5.2441249068,-2.4677773696,-1.3290522859
H,0,-4.6495432115,-1.0603204104,-2.2038364534
C,0,-3.2103972433,-2.676968725,-1.9903167406
H,0,-2.0177845294,-1.1408305735,-2.9603394139
H,0,-1.1483849718,-2.6187839678,-2.5880776165
H,0,-3.5061808201,-3.1429392463,-2.9353357609
H,0,-3.0327478837,-3.4968493101,-1.281126147

TS 6‡ ----H-DBU+ in CCl4

/home/biswas/23arom_Doc_first_download/nitro
/DBUfullTSPSccl4confbUF
DBUfullTSPSccl4confb UF
M062X/6-31+G**
E(RM062X) = -1339.20296644

Zero-point correction= 0.541389 (Hartree/Particle)
Thermal correction to Energy= 0.569680
Thermal correction to Enthalpy= 0.570624
Thermal correction to Gibbs Free Energy= 0.483784
Sum of electronic and ZPE= -1338.661578
Sum of electronic and thermal Energies= -1338.633286
Sum of electronic and thermal Enthalpies= -1338.632342
Sum of electronic and thermal Free Energies= -1338.719182

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.480	110.311	182.770

C,0,-2.2557482952,-0.6730146386,-1.6419040428
C,0,-0.9323931524,-0.507880412,-2.0452661587
C,0,0.0656685905,-1.1946014836,-1.3705864106
C,0,-0.2241332668,-2.1334915146,-0.3528069336
C,0,-1.5228384024,-2.3050210314,0.0366988596
C,0,-2.5923031894,-1.5712093257,-0.581095483
C,0,-3.8750139521,-1.5613282047,-0.0534296693
N,0,-3.5341046545,0.5612096066,0.9163533213
C,0,-2.9095675028,1.3239358064,0.0114874428
C,0,-1.4909264054,1.6069860057,-0.0383100342
O,0,-1.2316130805,2.4660185469,-1.0395773982
C,0,0.1401256878,2.7965438109,-1.2536928054
C,0,-2.8300700426,0.0972590607,2.1195153818
C,0,-4.9630241154,0.8464354095,1.1305836258
O,0,-0.6086770505,1.1781277229,0.7044084776
N,0,1.4431607023,-0.9633218634,-1.7346648728
O,0,1.6912829388,-0.1008913823,-2.5731236639
O,0,2.3190430164,-1.6130534165,-1.1677697804
H,0,-3.0480413567,-0.2075055855,-2.2185026451
H,0,-0.6743776331,0.1611439621,-2.8586455868
H,0,0.5847928937,-2.7032850663,0.0882095548
H,0,-1.7665327536,-3.0213763072,0.8166600038
H,0,-4.6936710166,-1.1351739094,-0.6238677575
H,0,-4.1383335446,-2.2148877359,0.7736901048
H,0,-1.9482986567,-0.4733460785,1.8303418818
H,0,-3.516854707,-0.5294159818,2.6872245427
H,0,-2.520953442,0.9586794217,2.7198610501
H,0,-5.4363053546,-0.0254770841,1.5805960488
H,0,-5.0626734193,1.7109031062,1.7949854905
H,0,-5.4367235573,1.0658073724,0.1739836716
H,0,-3.5293404107,1.8302925974,-0.7174087128
H,0,0.5738934672,3.2252417167,-0.3461163904
H,0,0.702440795,1.9091411084,-1.566844557
H,0,0.1428666192,3.5347470507,-2.0529360587
H,0,1.2787012285,1.0923757108,0.7223826914
N,0,2.2422795574,0.7506524986,0.7212495023
C,0,2.4962499884,-0.3147467936,1.4670744174
N,0,3.6838782452,-0.8955762643,1.4709337453
C,0,3.9468979825,-2.1166561884,2.2509248542
C,0,4.7864983882,-0.373874097,0.6473668257
C,0,3.237409339,1.3934733399,-0.1397796048
C,0,1.4064444019,-0.807237218,2.3774007152
C,0,1.7680765722,-0.6161148557,3.8643689408
H,0,1.2149978778,-1.8664160458,2.175295185
H,0,0.4948332406,-0.263205048,2.1225956119
H,0,5.7162945628,-0.5819862068,1.1810876751
H,0,4.7951785892,-0.9180129129,-0.3035757397
H,0,3.1504306706,1.0001722788,-1.1579706404
H,0,3.0210229422,2.4637652674,-0.1580898783
C,0,4.6204850836,1.1210325802,0.4278115957
H,0,5.3852489494,1.4761314385,-0.2652457651
H,0,4.7473468231,1.6508900863,1.3775817438
C,0,4.0261632088,-1.8616763123,3.7565228525
H,0,3.1838415417,-2.8663029131,2.0142636091
H,0,4.8947490396,-2.5076837593,1.8785662862
H,0,4.560842498,-2.700910393,4.2125689051
H,0,4.6354064973,-0.9652475953,3.9278123387
C,0,2.6597958878,-1.7235779506,4.4300907387
H,0,2.2388605271,0.36541392,4.0016467831
H,0,0.8332412936,-0.5951727655,4.4318993501
H,0,2.8058912389,-1.5497813905,5.5005773313
H,0,2.1271080758,-2.6799386945,4.3400834332

TS (6‡) ----H-DBU+ in CCl4, Alternative Conformation A

DBUfullTSPSccl4
nitrobenzyl rearr coord with DBU actual
M062X/6-31+G**
E(RM062X) = -1339.20131402

Zero-point correction= 0.542124 (Hartree/Particle)
Thermal correction to Energy= 0.570158
Thermal correction to Enthalpy= 0.571102
Thermal correction to Gibbs Free Energy= 0.485551
Sum of electronic and ZPE= -1338.659190
Sum of electronic and thermal Energies= -1338.631156
Sum of electronic and thermal Enthalpies= -1338.630212
Sum of electronic and thermal Free Energies= -1338.715763

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 357.780 110.100 180.057

C,0,3.115617385,0.1896260809,1.5733396199
C,0,1.9006816132,0.7116891175,2.0116107265
C,0,0.7718966554,-0.0919828643,1.9684490589
C,0,0.835916212,-1.4556020909,1.6004239982
C,0,2.0299317017,-1.9735637068,1.1827700923
C,0,3.2146504119,-1.1652780906,1.1279330171
C,0,4.3617306103,-1.5925286283,0.4717294712
N,0,3.8638599715,-0.3196467032,-1.4191114012
C,0,3.464944283,0.891877983,-1.0119031543
C,0,2.0997126805,1.3531222347,-0.8665491458
O,0,2.1083990816,2.6528499304,-0.5224185947
C,0,0.8425197971,3.2693127438,-0.2850325801
C,0,2.9058768965,-1.2487935047,-2.0314237842
C,0,5.2144935781,-0.3918988475,-2.0033621973
O,0,1.0552422824,0.7245340082,-1.0341655187
N,0,-0.5105422558,0.4718227776,2.3217797412
O,0,-0.5818229803,1.6737079231,2.5535384339
O,0,-1.4902361743,-0.2725366891,2.3386952894
H,0,4.0164638416,0.7860978715,1.6723048075
H,0,1.8224112153,1.7373963183,2.3553090787
H,0,-0.0608128091,-2.0600091465,1.65788456
H,0,2.098349639,-3.0192664966,0.8940449665
H,0,5.2878606094,-1.0374076435,0.5807150465
H,0,4.4411095727,-2.612495102,0.1050335995
H,0,2.0628776505,-1.3963759566,-1.3587038391
H,0,3.4194898619,-2.192625196,-2.2114419325
H,0,2.5450742322,-0.8301968109,-2.9766507684
H,0,5.562737237,-1.4238189875,-1.9705142929
H,0,5.1767108933,-0.0429174634,-3.040520243
H,0,5.8920698958,0.2409841468,-1.4306107154
H,0,4.2404654987,1.6215313227,-0.8152626822
H,0,0.1923142027,3.1491181543,-1.1553094496
H,0,0.3681619036,2.8404847757,0.6044841993
H,0,1.0593057085,4.3228698273,-0.1198308486
H,0,-0.4644905221,-0.3789071888,-0.9190177337
N,0,-1.327996356,-0.9072321387,-0.7925687984
C,0,-2.3893397017,-0.2350511014,-0.3710677175
N,0,-3.54240736,-0.8342091227,-0.1245089435
C,0,-4.7423942028,-0.0643576414,0.2523384683
C,0,-3.6808925188,-2.2938271306,-0.2527605166
C,0,-1.3083308484,-2.3547516155,-0.980164077
C,0,-2.2458802314,1.2515236865,-0.2313280153
C,0,-3.0274885564,2.0287352659,-1.3062816667
H,0,-2.566891252,1.5492382294,0.7735894144
H,0,-1.1782198657,1.4700625974,-0.3086467625
H,0,-4.390946471,-2.6216898337,0.508432912
H,0,-4.1033680842,-2.5265611117,-1.2375817509
H,0,-1.5308668301,-2.5928099669,-2.0261150191
H,0,-0.2982799402,-2.7062586144,-0.7566248115
C,0,-2.3377724284,-2.9769646818,-0.0501393106
H,0,-2.4354297975,-4.0456578503,-0.2499368997
H,0,-2.0261644217,-2.8468462171,0.9914122434
H,0,-5.4986938096,-0.8053851616,0.5128696901
H,0,-4.5268399476,0.510151446,1.1608306681
C,0,-5.2661035093,0.8401529908,-0.865218065
H,0,-6.3189297752,1.0510118183,-0.6518471403
H,0,-5.2398347473,0.2840249748,-1.8112023331
H,0,-2.5880340448,3.0284891631,-1.3758139103
H,0,-2.8781956513,1.5513357672,-2.2832120521
C,0,-4.5184052159,2.1666794589,-0.9980998347
H,0,-4.9908376671,2.7668556396,-1.781918662
H,0,-4.6316501463,2.7287410511,-0.0616779341

Complex 7----8 ----H-DBU+ in CCl4

/home/biswas/nitrodoc2/DBUfullComplexCCl4UF
irc of dbu-H coordinated opt to product
M062X/6-31+g**
E(RM062X) = -1339.20348098
(Potential energy of triplet for this geometry: -1339.17322952)

Zero-point correction= 0.541085 (Hartree/Particle)
Thermal correction to Energy= 0.570444
Thermal correction to Enthalpy= 0.571388
Thermal correction to Gibbs Free Energy= 0.481884
Sum of electronic and ZPE= -1338.662396
Sum of electronic and thermal Energies= -1338.633037
Sum of electronic and thermal Enthalpies= -1338.632093
Sum of electronic and thermal Free Energies= -1338.721597

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 357.959 112.865 188.376
C,0,-2.7224261505,-0.4790480139,-1.9995587988
C,0,-1.400233083,-0.2902456347,-2.3970848435
C,0,-0.3820871934,-0.9568686434,-1.729379495
C,0,-0.6643117723,-1.9240461112,-0.7207805906
C,0,-1.9538180994,-2.150606071,-0.3553428911
C,0,-3.0594041299,-1.4464922233,-0.9772645816
C,0,-4.3454933328,-1.5956001218,-0.5407674795
N,0,-3.9375701374,0.8676560374,0.4961292158
C,0,-3.3043652946,1.4779306549,-0.4875734577
C,0,-1.877562381,1.8205256399,-0.5045219494
O,0,-1.6287659284,2.6358016024,-1.5319113852
C,0,-0.2620510545,3.0094652738,-1.7362815418
C,0,-3.2453044298,0.3567623993,1.6813803851
C,0,-5.3867760982,1.0678216132,0.6254689353
O,0,-1.023801645,1.4560746239,0.2917511673
N,0,0.9761479467,-0.701005515,-2.0879916987
O,0,1.2183437393,0.1676774464,-2.9298361567
O,0,1.8698484098,-1.3368195865,-1.5226901199
H,0,-3.5177934288,-0.0683280224,-2.6134370634
H,0,-1.1557052234,0.3895804512,-3.2061786063
H,0,0.156410878,-2.4808690725,-0.2847165564
H,0,-2.182340239,-2.902382548,0.3953211244
H,0,-5.1693742153,-1.1187105875,-1.0617760186
H,0,-4.591845328,-2.2954535641,0.2523568942
H,0,-2.4077458595,-0.2712912462,1.3732845844
H,0,-3.9592973693,-0.2292409371,2.2581999321
H,0,-2.8687883364,1.1897701844,2.2830477124
H,0,-5.8347643824,0.1781110281,1.064947739
H,0,-5.5739825028,1.9349547123,1.2679681076
H,0,-5.8201938099,1.244182265,-0.3588825334
H,0,-3.9117921335,1.9506108771,-1.2501782122
H,0,0.1378226477,3.4780361858,-0.833401079
H,0,0.3292233356,2.1304629868,-2.015836681
H,0,-0.2753372947,3.7241335689,-2.5560227206
H,0,0.9116827591,1.395701424,0.3549791068

N,0,1.8652816916,1.0351949174,0.3403980668
C,0,2.1011515745,-0.0491599798,1.0652228174
N,0,3.2731602011,-0.6588597753,1.0437060853
C,0,3.5040197015,-1.9172623045,1.7727210237
C,0,4.3719271923,-0.1631806068,0.1996008842
C,0,2.855397406,1.6496609656,-0.5466219952
C,0,1.0096567237,-0.5315991825,1.978476809
C,0,1.3970424435,-0.4076353513,3.4658100294
H,0,0.7767123901,-1.5746458087,1.7400943011
H,0,0.1127422132,0.0502160676,1.756922412
H,0,5.3066895099,-0.3994384321,0.7128458746
H,0,4.3427127758,-0.7038262865,-0.7528619787
H,0,2.7300879311,1.256029355,-1.560832124
H,0,2.6691620362,2.7257868136,-0.5588520904
C,0,4.2432224907,1.3365578534,-0.0122105985
H,0,5.0010465024,1.671238467,-0.7227364436
H,0,4.407843643,1.860462284,0.9349849519
C,0,3.6059539306,-1.7271939959,3.2862380795
H,0,2.7151902439,-2.6322554993,1.5134393885
H,0,4.4358069257,-2.321947052,1.3754107929
H,0,4.1143609723,-2.6031503382,3.7014083758
H,0,4.2483673478,-0.8608131358,3.4876089919
C,0,2.2520508585,-1.5679788083,3.9794707587
H,0,1.908252155,0.5487547459,3.6318212597
H,0,0.470842196,-0.3712501151,4.0465716056
H,0,2.4144035568,-1.4412079946,5.0542146033
H,0,1.6838395236,-2.5002338791,3.8583596753

TS to 23 ----H-DBU+ in CCl4

/home/biswas/nitrodoc2/DBUfull2ndTSto23CCl4
trying to find ts2
M062X/6-31+g**
E(RM062X) = -1339.20257288

Zero-point correction= 0.540797 (Hartree/Particle)
Thermal correction to Energy= 0.569639
Thermal correction to Enthalpy= 0.570583
Thermal correction to Gibbs Free Energy= 0.481819
Sum of electronic and ZPE= -1338.661776
Sum of electronic and thermal Energies= -1338.632934
Sum of electronic and thermal Enthalpies= -1338.631990
Sum of electronic and thermal Free Energies= -1338.720754

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	357.454	110.869	186.820

C,0,-3.1129029974,-0.6379871431,1.3928562203
C,0,-2.0127695818,-1.5269926073,1.5480489078
C,0,-0.7915649874,-1.0362283093,1.9291300644
C,0,-0.6096086895,0.3311111536,2.3321027504
C,0,-1.6726551059,1.1687653426,2.3202806523
C,0,-2.9990482446,0.725002698,1.915520803
C,0,-4.0587676413,1.569776398,1.9065875846
N,0,-3.6351521577,1.0993751579,-0.8286566662
C,0,-3.3339285156,-0.2030249369,-0.7091506143
C,0,-2.0347565152,-0.7744111978,-1.1309972718
O,0,-2.1746639312,-2.0777380088,-1.3677204652
C,0,-0.9786333049,-2.8198789598,-1.6386196076
C,0,-2.6133829907,2.1328247036,-0.9440595219
C,0,-5.004479758,1.4838930736,-1.1636589786
O,0,-0.9718569587,-0.1825730168,-1.2212593575
N,0,0.3427813643,-1.9231883819,1.9652999418
O,0,0.2089695311,-3.0792655336,1.5687653165
O,0,1.418016312,-1.4793547544,2.3644003437
H,0,-4.101952934,-1.0872042017,1.408091324
H,0,-2.121105699,-2.581466635,1.3172143731
H,0,0.3647304667,0.6491956418,2.6822647567
H,0,-1.5624369825,2.1929073751,2.6670396566
H,0,-5.0549766473,1.219747852,1.655347639
H,0,-3.9567828898,2.6032587565,2.2237732776
H,0,-1.8299795687,1.9626130769,-0.2018954949
H,0,-3.0857643068,3.0973825951,-0.7560241204
H,0,-2.1616225936,2.1333288816,-1.9421445938
H,0,-5.2533091053,2.4198012037,-0.661459165
H,0,-5.1107405062,1.6141865797,-2.2471725765
H,0,-5.6965549702,0.7100974526,-0.8283729829
H,0,-4.1648112272,-0.8824681545,-0.8617958374
H,0,-0.4225039164,-2.3543874176,-2.4553544884
H,0,-0.3696649804,-2.8791974159,-0.7304648665
H,0,-1.3118978508,-3.8144464295,-1.9256905659
H,0,0.8804740479,-0.6611146337,-0.9843644108
N,0,1.7964071375,-0.7953743356,-0.5570844874
C,0,2.311369889,0.2441819612,0.0848076533
N,0,3.4565549822,0.1586698314,0.7384839479
C,0,4.0093567546,1.3013277334,1.4857374678
C,0,4.2237862697,-1.097856605,0.767165315
C,0,2.4408761836,-2.108734946,-0.6279460164
C,0,1.5878344574,1.5577062601,-0.0175047193
C,0,2.394205118,2.5951934556,-0.8247629019
H,0,1.38640222,1.9430206531,0.9874153081
H,0,0.6185325387,1.3652210221,-0.4821241296
H,0,5.281419399,-0.830053906,0.8172783047
H,0,3.9535722926,-1.6462866108,1.6759107479
H,0,2.0504597955,-2.7535392347,0.1664952376
H,0,2.1899248021,-2.5505979226,-1.5945957977
C,0,3.9414935762,-1.9198129539,-0.4802094054
H,0,4.4336486834,-2.8903575932,-0.397394213
H,0,4.3430890379,-1.4069276513,-1.3602756379
C,0,4.5532825957,2.4049336006,0.577339927
H,0,3.2451650049,1.6898119855,2.1671819086
H,0,4.8042823632,0.890342754,2.1094126106
H,0,5.2450995552,3.0150225349,1.166543463
H,0,5.1418840189,1.9410252273,-0.2243603334
C,0,3.4688984896,3.3132236229,-0.0054822917
H,0,2.8400067761,2.1089963177,-1.7014123094
H,0,1.6882060696,3.338677602,-1.2056380055
H,0,3.9419091262,4.0757296597,-0.6317800418
H,0,2.9790386993,3.8482493327,0.819260373

Product (3a) ----H-DBU+ in CCl4

/home/biswas/23arom_Doc_first_download/nitro
/DBUfullprodCCl4confbUF
prod with full DBU
M062X/6-31+g**
E(RM062X) = -1339.21274613

Zero-point correction= 0.543037 (Hartree/Particle)
Thermal correction to Energy= 0.571824
Thermal correction to Enthalpy= 0.572769
Thermal correction to Gibbs Free Energy= 0.483824
Sum of electronic and ZPE= -1338.669709

Sum of electronic and thermal Energies= -1338.640922
Sum of electronic and thermal Enthalpies= -1338.639978
Sum of electronic and thermal Free Energies= -1338.728922

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	358.825	110.888	187.199

C,0,-3.0121172522,-0.2433014896,1.2072977056
C,0,-2.0184253547,-1.363947106,1.3236511669
C,0,-0.7380115138,-1.0910164679,1.6103388888
C,0,-0.2476033429,0.2240535571,1.9952827342
C,0,-1.1359925223,1.2238463468,2.1350768323
C,0,-2.5671962727,1.0216510066,1.9134192316
C,0,-3.460060465,1.9296545007,2.3329785674
N,0,-3.8640729151,1.273590922,-0.6563199969
C,0,-3.3782724461,-0.0465171309,-0.3499309538
C,0,-2.2264441829,-0.5646594552,-1.2121570537
O,0,-2.465770348,-1.8104836089,-1.6155709658
C,0,-1.3907288537,-2.5047380746,-2.2619475859
C,0,-2.8706303741,2.3086730449,-0.9307074875
C,0,-4.9082580948,1.2750605686,-1.675776027
O,0,-1.1937857095,0.0292771619,-1.4617998
N,0,0.2502125403,-2.1743896574,1.5242118566
O,0,-0.0911339214,-3.244997824,1.0479213597
O,0,1.3898317853,-1.9286726915,1.8938600049
H,0,-3.961001873,-0.5599904869,1.6480239014
H,0,-2.3192070104,-2.3761881614,1.071381821
H,0,0.8053211481,0.3434121087,2.2191124691
H,0,-0.8094198941,2.2018105134,2.4799618703
H,0,-4.52662211,1.7715017396,2.2149894903
H,0,-3.1370197168,2.8560079242,2.7995167437
H,0,-2.0307708834,2.2329650998,-0.2392335478
H,0,-3.3455579454,3.2850397148,-0.798230918
H,0,-2.4734695787,2.2443948307,-1.9552522654
H,0,-5.3268205855,2.2820520743,-1.7473591799
H,0,-4.5324090495,0.9903515888,-2.6733627749
H,0,-5.7116986501,0.5910578662,-1.3928172723
H,0,-4.1984718758,-0.7448131496,-0.5285842197
H,0,-0.9889209238,-1.9072429939,-3.0821130934
H,0,-0.6144287726,-2.7258064638,-1.5222836254
H,0,-1.8196183584,-3.4315567791,-2.6350132599
H,0,0.6472735979,-0.5251144321,-1.4007701333
N,0,1.5609955939,-0.7329448194,-0.9983102701
C,0,2.173395333,0.2660205156,-0.3751677342
N,0,3.3353172639,0.0932910058,0.2305260935
C,0,4.0256930047,1.2028363403,0.9119660985
C,0,4.0394971835,-1.1999757952,0.1665637309
C,0,2.1492145953,-2.0608749638,-1.1956927088
C,0,1.5499402793,1.6318243801,-0.4581274887
C,0,2.3936874497,2.5717481277,-1.3446835222
H,0,1.4475982661,2.0572689016,0.5450641253
H,0,0.5394685418,1.5141250043,-0.8557744925
H,0,5.1098392548,-0.9829837739,0.1780380284
H,0,3.7871978239,-1.7811510566,1.0593031523
H,0,1.7695821984,-2.7570039949,-0.4402918307
H,0,1.8403615453,-2.4152551002,-2.1815356817
C,0,3.6619305291,-1.9420383235,-1.1058295049
H,0,4.1134485657,-2.9354204604,-1.09956071
H,0,4.0453541658,-1.3980247214,-1.9754154896
C,0,4.6132452452,2.2213022165,-0.0657687346
H,0,3.3348151488,1.6828395178,1.6125364761
H,0,4.8104635616,0.7405996009,1.512208748
H,0,5.3928211214,2.7828805738,0.458435801
H,0,5.1069059695,1.678342629,-0.8821113692
C,0,3.5802996308,3.207375888,-0.6159871966
H,0,2.7346955983,2.0260685543,-2.2334484933
H,0,1.7343851348,3.3675894981,-1.7020153229
H,0,4.0801636125,3.904537259,-1.295185151
H,0,3.194447108,3.8091804003,0.2176839638

Nitro(benzyl anion){8}----H-DBU+ in CCl4

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionfulldbu
m062xpsccl4
Free Nirto tol
opt
E(RM062X) = -937.783659412

Zero-point correction= 0.381235 (Hartree/Particle)
Thermal correction to Energy= 0.400784
Thermal correction to Enthalpy= 0.401728
Thermal correction to Gibbs Free Energy= 0.331458
Sum of electronic and ZPE= -937.402424
Sum of electronic and thermal Energies= -937.382876
Sum of electronic and thermal Enthalpies= -937.381931
Sum of electronic and thermal Free Energies= -937.452202

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	251.496	76.053	147.896

H,0,-1.1141690844,1.4922191564,-0.1393454747
N,0,-1.9488383323,1.8123332489,-0.6937042521
C,0,-2.3896037759,3.1890303643,-0.487771874
H,0,-1.5034473202,3.7891738619,-0.268253843
C,0,-3.1139975594,3.6595243301,-1.736854238
H,0,-2.4064426927,3.7378800947,-2.5687616625
H,0,-3.5564388783,4.6442865416,-1.5735916803
C,0,-4.2104141298,2.6633825475,-2.0866645347
H,0,-5.0237728,2.7004063624,-1.3514153714
H,0,-4.6302058983,2.8889407562,-3.0695545058
N,0,-3.6779235889,1.2911506351,-2.1414362656
C,0,-2.5932840376,0.9504618998,-1.4433519239
C,0,-2.0815148254,-0.4639551408,-1.4629086997
C,0,-3.0237566339,-1.4459414936,-0.7398140327
C,0,-4.2268434613,-1.8876980628,-1.5712538745
C,0,-5.149068768,-0.7474043723,-2.0021319798
C,0,-4.4634859011,0.2959584893,-2.8866462521
H,0,-3.3627137959,-0.9899950436,0.1982881487
H,0,-2.4348613382,-2.3267894903,-0.4674811273
H,0,-1.9215641377,-0.7811760042,-2.4999955166
H,0,-1.1055369455,-0.4568110915,-0.9710359473
H,0,-3.8688338544,-2.4103229567,-2.469104418
H,0,-4.8051379036,-2.6180486356,-0.9962542384
H,0,-5.9881097589,-1.1655661497,-2.5682864694
H,0,-5.5746186666,-0.242682355,-1.1252503703
H,0,-5.2133691915,0.8651113498,-3.4382919683
H,0,-3.8222736765,-0.1904871502,-3.6313673315
O,0,0.0185149452,1.3572368281,1.040531452
N,0,-0.4660359232,2.239096845,1.854116165
O,0,0.1532534242,3.3155454746,2.0289713875
C,0,-1.6598753414,2.0033924452,2.4469382324
C,0,-2.3091448527,3.0380097381,3.2056688963

C,0,-3.5665516747,2.8589946987,3.6761557018
C,0,-4.3129812564,1.61799294,3.4637804036
C,0,-3.5958058869,0.5698665689,2.7377807263
C,0,-2.3419520543,0.7527702721,2.2587407766
H,0,-1.771518216,3.9653549204,3.3687226326
H,0,-4.0534558601,3.6526046005,4.2369576696
C,0,-5.578866251,1.4467385415,3.9181255819
H,0,-4.0928466267,-0.388949743,2.6083887862
H,0,-1.8155511675,-0.0441721232,1.7436591804
H,0,-6.111565474,0.5147069086,3.7571268011
H,0,-6.0915461684,2.2318096794,4.4646509417
H,0,-3.0460686598,3.2222147135,0.3913053682

Nitro(benzyl anion){8}----H-DBU+ in MeOH

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionfulldbu
m062xpsmeoh
Free Nirto tol
opt
E(RM062X) = -937.801924294

Zero-point correction= 0.381262 (Hartree/Particle)
Thermal correction to Energy= 0.400953
Thermal correction to Enthalpy= 0.401898
Thermal correction to Gibbs Free Energy= 0.330905
Sum of electronic and ZPE= -937.420663
Sum of electronic and thermal Energies= -937.400971
Sum of electronic and thermal Enthalpies= -937.400027
Sum of electronic and thermal Free Energies= -937.471019

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	251.602	76.439	149.416

H,0,-1.1511317944,1.4737304625,-0.16884306
N,0,-1.9707799374,1.787673352,-0.7100078138
C,0,-2.400271688,3.1723328315,-0.5362510045
H,0,-1.5147456287,3.7672546443,-0.3013472454
C,0,-3.0782087796,3.6298402048,-1.8158691876
H,0,-2.3428157404,3.6826137913,-2.6246615037
H,0,-3.5123730275,4.622293484,-1.6828592469
C,0,-4.177314833,2.6442006365,-2.1821732988
H,0,-5.0145689108,2.7043113602,-1.4769627925
H,0,-4.5588481106,2.8539892129,-3.1831479537
N,0,-3.6663262492,1.2612057866,-2.1903651565
C,0,-2.6060841441,0.9175025115,-1.4707430386
C,0,-2.1090366113,-0.500990794,-1.4585377023
C,0,-3.0754459146,-1.4559379126,-0.7312883198
C,0,-4.2661922168,-1.8980794409,-1.5801777344
C,0,-5.163668812,-0.755892844,-2.0546919938
C,0,-4.4491690366,0.2642376167,-2.9427347223
H,0,-3.4273110706,-0.9791227223,0.1922050955
H,0,-2.5023099334,-2.338398526,-0.4324299841
H,0,-1.9424581002,-0.8383018167,-2.4873932134
H,0,-1.1382102314,-0.5003741134,-0.9569379612
H,0,-3.8932897703,-2.441731416,-2.4586517204
H,0,-4.8661822478,-2.6091802504,-1.0033083702
H,0,-5.991815612,-1.1756091016,-2.6348574023
H,0,-5.606339929,-0.2304363098,-1.1988627337
H,0,-5.1797557366,0.8362385725,-3.5152689011
H,0,-3.7961287859,-0.2367844274,-3.6663589078
O,0,0.073821946,1.460567024,1.1444630929
N,0,-0.4690358798,2.3384482712,1.9180877081
O,0,0.1250674328,3.4417093081,2.0990243949
C,0,-1.6651170445,2.0847647791,2.485654008
C,0,-2.3423550722,3.1056085961,3.2434563779
C,0,-3.5820463156,2.8853090146,3.7403002662
C,0,-4.2840394674,1.6141802561,3.5533203253
C,0,-3.549971216,0.5891439833,2.8100695611
C,0,-2.313667674,0.811086454,2.3056395412
H,0,-1.8410203853,4.0558309993,3.3874217734
H,0,-4.0896270739,3.6677994437,4.2984474094
C,0,-5.5297580649,1.3983814483,4.0419559258
H,0,-4.0239913927,-0.3803939949,2.6775662691
H,0,-1.7815621041,0.0311304604,1.7707846524
H,0,-6.0332271543,0.4481210979,3.8933869352
H,0,-6.0577402507,2.1691782171,4.5947913956
H,0,-3.0871714308,3.2287448496,0.3175372371

Nitro(benzyl anion){8}----H-DBU+ in DMSO

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionfulldbu
m062xpsdmso
Free Nirto tol
opt
E(RM062X) = -937.802473789

Zero-point correction= 0.381249 (Hartree/Particle)
Thermal correction to Energy= 0.400947
Thermal correction to Enthalpy= 0.401891
Thermal correction to Gibbs Free Energy= 0.330880
Sum of electronic and ZPE= -937.421225
Sum of electronic and thermal Energies= -937.401527
Sum of electronic and thermal Enthalpies= -937.400583
Sum of electronic and thermal Free Energies= -937.471594

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	251.598	76.452	149.456

H,0,-1.1508902802,1.4716814377,-0.168271332
N,0,-1.9697970841,1.7867336307,-0.7093553693
C,0,-2.3975238189,3.1719461325,-0.535746891
H,0,-1.511362171,3.7657227548,-0.3003047845
C,0,-3.0738071031,3.6305536279,-1.8158421706
H,0,-2.3376660402,3.6825145611,-2.6239935239
H,0,-3.5068286758,4.6235214912,-1.6829886585
C,0,-4.1738892389,2.6464910022,-2.1832967808
H,0,-5.0117691157,2.7075949551,-1.4789557441
H,0,-4.5540555434,2.856924331,-3.1846296807
N,0,-3.6648477177,1.2627470022,-2.1911367978
C,0,-2.6056975815,0.9174725783,-1.4710079637
C,0,-2.1104645913,-0.5016384571,-1.4588339394
C,0,-3.0788108113,-1.4555859871,-0.7328283571
C,0,-4.2691244714,-1.8960338851,-1.5832147294
C,0,-5.1647874076,-0.7525916698,-2.0581251901
C,0,-4.44820507,0.2671281848,-2.9449093428
H,0,-3.4312149948,-0.9785716752,0.1903665011
H,0,-2.50704757,-2.3388008418,-0.4335752962
H,0,-1.9433971309,-0.838795639,-2.4876486705
H,0,-1.140037879,-0.5025169876,-0.9564535257
H,0,-3.8957863502,-2.4395809223,-2.4615561067

H,0,-4.8705171149,-2.6067398133,-1.0073203865
H,0,-5.9927170349,-1.1710497986,-2.639494433
H,0,-5.6078456452,-0.2270770172,-1.2025432754
H,0,-5.1775410442,0.8403921514,-3.5177365521
H,0,-3.7950389564,-0.2342195239,-3.6681509007
O,0,0.0747974133,1.4596345213,1.1488714565
N,0,-0.4691238116,2.3368791469,1.9226173044
O,0,0.1256028627,3.4399571837,2.1056474995
C,0,-1.6658066804,2.0833084295,2.488214157
C,0,-2.3434799,3.1036343595,3.2466019752
C,0,-3.5832538851,2.8828336929,3.7428882812
C,0,-4.2850010895,1.6117177938,3.5547015548
C,0,-3.5508551874,0.5873560565,2.8105346318
C,0,-2.314474325,0.8097224093,2.3066502532
H,0,-1.8425058274,4.0539231443,3.3913009995
H,0,-4.0912175385,3.6649347813,4.3012281531
C,0,-5.5306901877,1.3953570842,4.0430284614
H,0,-4.0250789925,-0.3818680549,2.6765709352
H,0,-1.782460863,0.0303070464,1.7709411246
H,0,-6.0341048466,0.4452427542,3.893331961
H,0,-6.0588614456,2.1657002903,4.5963276795
H,0,-3.0850392532,3.2293327381,0.3174784739

Nitro(benzyl anion){8}----H-DBU+ in CH2Cl2

/home/biswas/nitrodoc2/dissociation/nitrobenzylanionfulldbu
m062xpsdcm
Free Nirto tol
opt
E(RM062X) = -937.797475308

Zero-point correction= 0.381345 (Hartree/Particle)
Thermal correction to Energy= 0.400990
Thermal correction to Enthalpy= 0.401934
Thermal correction to Gibbs Free Energy= 0.330918
Sum of electronic and ZPE= -937.416130
Sum of electronic and thermal Energies= -937.396486
Sum of electronic and thermal Enthalpies= -937.395541
Sum of electronic and thermal Free Energies= -937.466557

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	251.625	76.335	149.466

H,0,-1.1420464144,1.4770887272,-0.1649910492
N,0,-1.9648216498,1.7898768738,-0.7078063097
C,0,-2.3993028693,3.1721310527,-0.5271058047
H,0,-1.5149691895,3.7692548101,-0.2934531212
C,0,-3.0858633378,3.6312414118,-1.8014897796
H,0,-2.3553259896,3.6887737263,-2.6144797097
H,0,-3.5220819234,4.6221844678,-1.6635212507
C,0,-4.1839576879,2.6427753809,-2.1641634627
H,0,-5.0173635119,2.6994638791,-1.453871413
H,0,-4.5721570761,2.8537928147,-3.162546265
N,0,-3.6686077377,1.2616736077,-2.1785412201
C,0,-2.6018959262,0.9200714025,-1.4646379285
C,0,-2.0999073414,-0.4969123399,-1.4596928971
C,0,-3.0569062301,-1.458316964,-0.7284234367
C,0,-4.2542618537,-1.9014044853,-1.5674167596
C,0,-5.1589089835,-0.7603216128,-2.0311446132
C,0,-4.4545995135,0.2629639122,-2.92390075
H,0,-3.4016744957,-0.9860851203,0.1999330671
H,0,-2.478310595,-2.339983578,-0.4378622607
H,0,-1.9382717132,-0.8303938978,-2.4907659643
H,0,-1.1259926251,-0.4933632464,-0.964097968
H,0,-3.8887954488,-2.4428988445,-2.4504460465
H,0,-4.8474084799,-2.6151866728,-0.986797311
H,0,-5.9920013943,-1.1808836595,-2.6037024134
H,0,-5.5943085084,-0.2373716425,-1.1699894147
H,0,-5.1919199853,0.8327299072,-3.4903778146
H,0,-3.8068859656,-0.2364667461,-3.6535903387
O,0,0.0648282126,1.4453713589,1.1253685548
N,0,-0.4688662846,2.3266816258,1.9012900583
O,0,0.1254048204,3.4273609837,2.0749289179
C,0,-1.6649537669,2.07607742,2.4751619266
C,0,-2.3398614303,3.1019253895,3.2263980469
C,0,-3.5846022292,2.8906405961,3.7153838942
C,0,-4.2938467958,1.6239903581,3.5268551003
C,0,-3.5591444987,0.5919802608,2.7944261889
C,0,-2.3177197193,0.8055720374,2.2978526532
H,0,-1.8322424053,4.0486286027,3.3719839449
H,0,-4.0901329121,3.6771666987,4.2697122157
C,0,-5.5454308113,1.417902853,4.0054294077
H,0,-4.0356090528,-0.3770597993,2.6662759549
H,0,-1.7837678939,0.0202593885,1.7727259129
H,0,-6.0531813472,0.4698319444,3.8576027137
H,0,-6.0729207423,2.1934165206,4.5519783247
H,0,-3.0816306958,3.2220165971,0.3308874199

Geometry of 6‡ with different methods

6‡ B3LYPD3 IN DMSO

home/biswas/quiver/tdb3lypd3
Nitro TS
b3lyp/6-31+G**
E(RB3LYP) = -877.250602126

Zero-point correction= 0.273409 (Hartree/Particle)
Thermal correction to Energy= 0.290932
Thermal correction to Enthalpy= 0.291876
Thermal correction to Gibbs Free Energy= 0.227162
Sum of electronic and ZPE= -876.977193
Sum of electronic and thermal Energies= -876.959670
Sum of electronic and thermal Enthalpies= -876.958726
Sum of electronic and thermal Free Energies= -877.023440

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.563	65.840	136.202

C,0,-1.1335881879,-0.464536678,2.0781237071
C,0,-1.0358322865,-0.7287418892,3.4392357402
C,0,0.2054687744,-0.5929709788,4.0635252034
C,0,1.3464613083,-0.152429946,3.3661278462
C,0,1.2428568975,0.0853666346,2.009938159
C,0,0.0083400998,-0.0828211713,1.3286518778
C,0,-0.0715324581,-0.0844626839,-0.0989232353
N,0,-0.048758551,-2.0444256807,-0.5419381253
C,0,-0.876369562,-2.8018034052,0.2756203657
C,0,-0.4952569619,-3.3974341724,1.5126833191
O,0,-1.5935866839,-3.9954179483,2.0999825252
C,0,-1.3741998064,-4.5707609569,3.3965567838

C,0,1.4094949318,-2.3481737885,-0.5009964047
C,0,-0.5372621641,-1.9958300125,-1.949424647
O,0,0.618927479,-3.4486978142,2.0523264178
N,0,0.3198531553,-0.9163430957,5.4737512564
O,0,-0.6649582451,-1.3979136822,6.0562716803
O,0,1.4028791674,-0.7113001183,6.0438769737
H,0,-2.0957652813,-0.5466349695,1.5864937149
H,0,-1.8981040804,-1.0504270403,4.0090933182
H,0,2.287166305,-0.0348406694,3.8882991114
H,0,2.1210014473,0.3909466935,1.4494355338
H,0,-1.0415316862,0.1115124377,-0.5446283116
H,0,0.7740260332,0.2964616857,-0.6649397359
H,0,1.789472521,-2.1688654271,0.5002719031
H,0,1.9141838891,-1.7114399747,-1.2270574632
H,0,1.5559774066,-3.3999590729,-0.7583667337
H,0,0.0197802218,-1.2358737828,-2.4976839543
H,0,-0.3861143402,-2.9749523915,-2.4109173502
H,0,-1.5986351724,-1.7480227346,-1.9560303727
H,0,-1.9253409544,-2.7893232682,0.0160130221
H,0,-0.6047158516,-5.3469466966,3.3600306926
H,0,-1.0751715253,-3.8024776907,4.1166298341
H,0,-2.3308768386,-5.0044747112,3.6895563481

6‡ PBEPBED2 IN DMSO

home/biswas/quiver/tdPBEPBE-D2
Nitro TS
PBEPBE/6-31+G**
E(RPBE-PBE) = -876.238062942

Zero-point correction= 0.265313 (Hartree/Particle)
Thermal correction to Energy= 0.283227
Thermal correction to Enthalpy= 0.284171
Thermal correction to Gibbs Free Energy= 0.218908
Sum of electronic and ZPE= -875.972750
Sum of electronic and thermal Energies= -875.954836
Sum of electronic and thermal Enthalpies= -875.953892
Sum of electronic and thermal Free Energies= -876.019155

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.727	67.734	137.358

C,0,-1.1359126153,-0.5047050043,2.1052737125
C,0,-1.0121064438,-0.7435137334,3.4747043215
C,0,0.24321462,-0.5699779984,4.0802911722
C,0,1.3705996775,-0.1231762886,3.3536242783
C,0,1.2413043189,0.0833625909,1.9856960343
C,0,-0.0060748972,-0.1165091278,1.3300343169
C,0,-0.1152433202,-0.1473498389,-0.1033122266
N,0,-0.0487165037,-2.0237558309,-0.5396866636
C,0,-0.890305979,-2.8187185474,0.2458940821
C,0,-0.5280718636,-3.406451144,1.4981450202
O,0,-1.6501187512,-4.0168617764,2.0597207732
C,0,-1.4308277129,-4.5975993779,3.3591455083
C,0,1.4127583869,-2.3157929089,-0.4622185827
C,0,-0.4920697179,-1.9868161553,-1.9653572936
O,0,0.5811932081,-3.4520721121,2.0674110982
N,0,0.3835395408,-0.856118919,5.5012030988
O,0,-0.5996210635,-1.3289362394,6.1177427538
O,0,1.4872624587,-0.6294328092,6.0488726703
H,0,-2.1087340799,-0.6152090016,1.6202930667
H,0,-1.8637726529,-1.0701711788,4.0744723195
H,0,2.3223346683,0.0234532594,3.8670943392
H,0,2.1101894707,0.3941989786,1.3973866732
H,0,-1.1077801932,0.0460813761,-0.5252531234
H,0,0.7162418864,0.2599021226,-0.6899105596
H,0,1.7521499488,-2.1647985919,0.5689628968
H,0,1.9317469148,-1.6408683082,-1.1573533306
H,0,1.573521952,-3.3656643137,-0.7523095574
H,0,0.0852133331,-1.2158514727,-2.495844938
H,0,-0.3134131275,-2.9756707172,-2.4151933263
H,0,-1.5635726775,-1.7452819184,-2.0018528694
H,0,-1.9410929795,-2.8013709396,-0.0437922447
H,0,-0.6417752882,-5.3677316332,3.3232495099
H,0,-1.1416790338,-3.8218415744,4.0904765801
H,0,-2.3920924844,-5.0487658662,3.6439794897

6‡ PBEPBED3 IN DMSO

/home/biswas/quiver/tdPBE0
Nitro TS
pbe1pbe/6-31+G**
C,0,-1.1308935553,-0.4577835354,2.0038841625
C,0,-1.0484594262,-0.7724927625,3.3531769892
C,0,0.1816518532,-0.6677685359,3.9931288393
C,0,1.3286566784,-0.1936649865,3.3311424877
C,0,1.2420421627,0.1055126175,1.9924786799
C,0,0.0172619176,-0.0360207244,1.2855204837
C,0,-0.0425541782,-0.0031775981,-0.1253084427
N,0,-0.0544884429,-2.0566827707,-0.5072767466
C,0,-0.8725113994,-2.7384873897,0.3475026108
C,0,-0.4769015961,-3.3534284878,1.5776029726
O,0,-1.5657627583,-3.9222684953,2.1724212281
C,0,-1.3302526738,-4.5119857608,3.4473026959
C,0,1.3910351189,-2.3366491617,-0.4601380747
C,0,-0.5575834544,-2.0179982706,-1.8926002842
O,0,0.6412388461,-3.4289328328,2.0858852755
N,0,0.2808522641,-1.0573440803,5.3766900675
O,0,-0.7020120801,-1.5649632736,5.9173832312
O,0,1.3497178726,-0.8806928029,5.9601425389
H,0,-2.0920848161,-0.500700959,1.5030574475
H,0,-1.9171995196,-1.1149883499,3.9030195758
H,0,2.2620010621,-0.0994312681,3.8730364453
H,0,2.1251071613,0.4428623831,1.4569723182
H,0,-1.007076286,0.1589616752,-0.597219954
H,0,0.8206164421,0.3426372049,-0.688535023
H,0,1.7750828704,-2.1157773546,0.5330462714
H,0,1.8852159858,-1.7192372211,-1.2101637537
H,0,1.5573162314,-3.3951592777,-0.6798199755
H,0,-0.0028682067,-1.2678675326,-2.4574703863
H,0,-0.4228789667,-3.0020935167,-2.351319048
H,0,-1.6171991526,-1.7612253625,-1.8880216883
H,0,-1.924192643,-2.7455932832,0.0936901902
H,0,-0.5665371044,-5.2919995081,3.3868462995
H,0,-1.0145139383,-3.7555757434,4.1730315468
H,0,-2.2835372688,-4.9439980349,3.7525000195

6‡ M11L IN DMSO

home/biswas/quiver/tdM11L
Nitro TS
m11l/6-31+G**
E(RM11L) = -876.925441220

Zero-point correction= 0.267483 (Hartree/Particle)
Thermal correction to Energy= 0.284975
Thermal correction to Enthalpy= 0.285919
Thermal correction to Gibbs Free Energy= 0.222253
Sum of electronic and ZPE= -876.657958
Sum of electronic and thermal Energies= -876.640467
Sum of electronic and thermal Enthalpies= -876.639522
Sum of electronic and thermal Free Energies= -876.703189

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	178.824	66.508	133.997

C,0,-1.133591421,-0.4701180496,2.075838161
C,0,-1.058749034,-0.730486061,3.4274120567
C,0,0.1734019915,-0.6273894072,4.0577379322
C,0,1.325847791,-0.2293607321,3.3770819473
C,0,1.2437006867,-0.000688729,2.0272795736
C,0,0.0198809727,-0.1330836217,1.3391521826
C,0,-0.0478458857,-0.1346635524,-0.0782786737
N,0,-0.0624420642,-2.0605726909,-0.5306737444
C,0,-0.8732623467,-2.8250263737,0.2589610156
C,0,-0.479998334,-3.3795472953,1.506976741
O,0,-1.5504000895,-3.942004352,2.1065154167
C,0,-1.2851744575,-4.4583537598,3.3789765533
C,0,1.3648936668,-2.3637644484,-0.5165958992
C,0,-0.5529196096,-1.9752678072,-1.9004295309
O,0,0.6203733489,-3.4178591369,2.0194315163
N,0,0.2620748774,-0.9392024401,5.4458699161
O,0,-0.7260207759,-1.3798895834,6.0010014221
O,0,1.3258058435,-0.7642743247,6.0070455388
H,0,-2.0998163794,-0.5251398017,1.5653549358
H,0,-1.941347822,-1.0196748278,4.001731532
H,0,2.2687500137,-0.1342065739,3.9174706081
H,0,2.1418910373,0.2823547317,1.4673781018
H,0,-1.018597144,0.0934211539,-0.5344486799
H,0,0.8157628399,0.2427393086,-0.6403228374
H,0,1.7841600029,-2.1873730107,0.4792980201
H,0,1.8605185184,-1.7257509304,-1.260742812
H,0,1.5129810166,-3.422517227,-0.7812734608
H,0,-0.0044435787,-1.189665606,-2.437945277
H,0,-0.4020219247,-2.9428942825,-2.4041431501
H,0,-1.624000495,-1.7346165123,-1.8948771626
H,0,-1.935454712,-2.7795751702,0.0200672728
H,0,-0.4928998716,-5.2235584279,3.3549258181
H,0,-0.9781395663,-3.6595849639,4.0793714857
H,0,-2.2246280954,-4.9064204946,3.7264424804

6‡ BP86D2 IN DMSO

home/biswas/quiver/tdBP86-D2
Nitro TS
BP86/6-31+G**
E(RB-P86) = -877.284243343

Zero-point correction= 0.264668 (Hartree/Particle)
Thermal correction to Energy= 0.282413
Thermal correction to Enthalpy= 0.283357
Thermal correction to Gibbs Free Energy= 0.219039
Sum of electronic and ZPE= -877.019575
Sum of electronic and thermal Energies= -877.001830
Sum of electronic and thermal Enthalpies= -877.000886
Sum of electronic and thermal Free Energies= -877.065204

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.217	67.720	135.368

C,0,-1.1577317107,-0.5327397048,2.0881633751
C,0,-1.0316177316,-0.8037153477,3.452955113
C,0,0.2268940859,-0.6437387287,4.0588641445
C,0,1.3520018164,-0.1676435115,3.3443755819
C,0,1.2202967459,0.0679207511,1.979345662
C,0,-0.0269187423,-0.1287777978,1.3214124078
C,0,-0.1328055442,-0.1618712114,-0.116456604
N,0,-0.0407947953,-2.0092823576,-0.547166375
C,0,-0.8762417994,-2.8235449777,0.2378397038
C,0,-0.5108872289,-3.3716058546,1.506428137
O,0,-1.6278769508,-3.9820116853,2.0881669268
C,0,-1.410185768,-4.4633944531,3.4320958849
C,0,1.4277227398,-2.2891425009,-0.467476274
C,0,-0.4797932791,-1.9898083634,-1.9789916349
O,0,0.5987634415,-3.3869273706,2.080569842
N,0,0.3729908021,-0.9820925799,5.4697946776
O,0,-0.5991625693,-1.5114620246,6.0639184338
O,0,1.4704918659,-0.7468979831,6.0325212314
H,0,-2.1289940536,-0.640341591,1.5987031251
H,0,-1.8811323103,-1.1490443743,4.0458867316
H,0,2.3040629389,-0.0308067697,3.8609451849
H,0,2.0878275263,0.3924067743,1.395329398
H,0,-1.1271683611,0.0322283297,-0.5369236255
H,0,0.6960318181,0.2592171189,-0.698782867
H,0,1.7610885123,-2.1262533088,0.5647628203
H,0,1.9381926922,-1.6117370662,-1.1681940643
H,0,1.5936352266,-3.3406085177,-0.7510265164
H,0,0.0912476602,-1.2133096357,-2.5103484496
H,0,-0.2846000298,-2.9809983829,-2.4182518177
H,0,-1.5552261708,-1.7620248929,-2.0176610513
H,0,-1.9275587384,-2.8109512951,-0.0523026317
H,0,-0.5861167558,-5.1974010011,3.4635334265
H,0,-1.1697272962,-3.6221875223,4.1088922777
H,0,-2.3584190365,-4.935467164,3.7306668257

6‡ BLYPD2 IN DMSO

home/biswas/quiver/tdBLYP-D2
Nitro TS
BLYP/6-31+G**
E(RB-LYP) = -876.994800740

Zero-point correction= 0.264159 (Hartree/Particle)
Thermal correction to Energy= 0.282111
Thermal correction to Enthalpy= 0.283056
Thermal correction to Gibbs Free Energy= 0.217527
Sum of electronic and ZPE= -876.730642
Sum of electronic and thermal Energies= -876.712689

Sum of electronic and thermal Enthalpies= -876.711745
Sum of electronic and thermal Free Energies= -876.777273

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.028	67.928	137.916

C,0,-1.1224342345,-0.5244481378,2.1795342936
C,0,-0.9866612516,-0.6786061626,3.5634909272
C,0,0.2761709761,-0.454693254,4.1504153066
C,0,1.4002829599,-0.0603298453,3.3819998769
C,0,1.2544394297,0.0664402948,2.0003571403
C,0,-0.0026769191,-0.1676332171,1.3736492092
C,0,-0.137333902,-0.2149822675,-0.0723449965
N,0,-0.0472539305,-0.2178676011,-0.5571626798
C,0,-0.9050138327,-2.8672635817,0.1906369268
C,0,-0.5578792873,-3.480137427,1.4310105716
O,0,-1.6947792336,-4.1179917789,1.971515632
C,0,-1.4880577226,-4.7461229384,3.2658975954
C,0,1.4285481188,-2.327953487,-0.4814804599
C,0,-0.4763258482,-1.9576741501,-2.0045660866
O,0,0.5486201404,-3.5389230655,2.0186832286
N,0,0.4269862468,-0.6294862189,5.5980042934
O,0,-0.5752883854,-0.99549913,6.275325347
O,0,1.5584304126,-0.4146598757,6.1184353226
H,0,-2.0938876695,-0.6788736798,1.7085421968
H,0,-1.8313838859,-0.972004237,4.1858708871
H,0,2.3566431847,0.1193247437,3.8714959695
H,0,2.1142673567,0.3443358625,1.3863034739
H,0,-1.1368565528,-0.0020520744,-0.4639364744
H,0,0.6738622935,0.2283865756,-0.658808425
H,0,1.7578917323,-2.2099716337,0.5544090632
H,0,1.9503328416,-1.6326738473,-1.1524997968
H,0,1.5751119618,-3.3683480052,-0.8048069762
H,0,0.1107836422,-1.179754266,-2.5117241162
H,0,-0.292698216,-2.9411929346,-2.459831146
H,0,-1.5459462155,-1.7128105737,-2.0434130273
H,0,-1.9508552447,-2.8202186309,-0.1061525526
H,0,-0.7117858809,-5.5269374357,3.2056374911
H,0,-1.1880443747,-3.9951163576,4.0163226023
H,0,-2.4589197095,-5.1882766622,3.5307783822

6‡ N12SX IN DMSO

home/biswas/quiver/tdN12SX
Nitro TS
N12SX/6-31+G**
E(RN12SX) = -876.763523451

Zero-point correction= 0.277068 (Hartree/Particle)
Thermal correction to Energy= 0.294634
Thermal correction to Enthalpy= 0.295578
Thermal correction to Gibbs Free Energy= 0.230909
Sum of electronic and ZPE= -876.486455
Sum of electronic and thermal Energies= -876.468890
Sum of electronic and thermal Enthalpies= -876.467946
Sum of electronic and thermal Free Energies= -876.532614

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.885	65.464	136.106

C,0,-1.090237939,-0.4283357277,2.0573717124
C,0,-1.013114833,-0.6704636027,3.4166381426
C,0,0.2108003081,-0.525176859,4.0617199798
C,0,1.3628517131,-0.1121250013,3.3711104023
C,0,1.2826289706,0.11328428,2.0212669636
C,0,0.0569345628,-0.0405385435,1.3192890728
C,0,-0.0124475677,0.0062008834,-0.0830036006
N,0,-0.068183704,-2.1007861413,-0.5138910675
C,0,-0.8906656448,-2.7711518843,0.3309808525
C,0,-0.5033195407,-3.4473567999,1.5314146114
O,0,-1.5896984505,-4.0302861884,2.0995655016
C,0,-1.3725356996,-4.7433678338,3.3081104097
C,0,1.3725728373,-2.3895906657,-0.4829942527
C,0,-0.5828685335,-1.9948822772,-1.8884700017
O,0,0.6153150912,-3.5626070529,2.0258435106
N,0,0.2931593332,-0.7840367101,5.4657095914
O,0,-0.7183206131,-1.1612468838,6.0638803697
O,0,1.37746189,-0.6252360629,6.0331351277
H,0,-2.0467357707,-0.4931147292,1.5600209341
H,0,-1.883280386,-0.9697359238,3.9799084652
H,0,2.2910347021,0.0105287892,3.9066973674
H,0,2.1652506182,0.4191938796,1.4758712622
H,0,-0.9741910311,0.1580854591,-0.5512942505
H,0,0.8481411517,0.3348675391,-0.6501754331
H,0,1.7628207326,-2.2117338889,0.5106796126
H,0,1.8667625337,-1.7527396405,-1.2088423431
H,0,1.5325603918,-3.4354059416,-0.7435545493
H,0,-0.016004979,-1.2447445823,-2.4304608196
H,0,-0.4800506097,-2.9603872377,-2.3831933095
H,0,-1.6305495531,-1.7126088051,-1.8654168451
H,0,-1.9389529561,-2.7599417046,0.0825652224
H,0,-0.6505063076,-5.5447909631,3.1622657255
H,0,-1.0123220386,-4.0769690543,4.0905437207
H,0,-2.3360196785,-5.1568151249,3.5882969145

6‡ BP86 IN DMSO

home/biswas/quiver/tdBP86
Nitro TS
BP86/6-31+G**
E(RB-P86) = -877.232413505

Zero-point correction= 0.264289 (Hartree/Particle)
Thermal correction to Energy= 0.282578
Thermal correction to Enthalpy= 0.283523
Thermal correction to Gibbs Free Energy= 0.216916
Sum of electronic and ZPE= -876.968124
Sum of electronic and thermal Energies= -876.949835
Sum of electronic and thermal Enthalpies= -876.948891
Sum of electronic and thermal Free Energies= -877.015497

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.321	68.330	140.185

C,0,-1.0743732676,-0.3905458835,2.233316883
C,0,-0.9607241437,-0.4528265133,3.6232585155
C,0,0.2963663965,-0.2250726977,4.2149709081
C,0,1.4406862562,0.0709942614,3.4371564099
C,0,1.317801662,0.1172674565,2.0527690286
C,0,0.0606386278,-0.1087587115,1.414419047
C,0,-0.0677199926,-0.1613100723,-0.0172240662
N,0,-0.0756116639,-2.0853775811,-0.5281706127

C,0,-0.9376319648,-2.8823689051,0.2262478266
C,0,-0.5814907183,-3.6208258078,1.4004819201
O,0,-1.7102934732,-4.290301518,1.8765054196
C,0,-1.4880344195,-5.1187974993,3.0383061603
C,0,1.3793638965,-2.4320209165,-0.4836211146
C,0,-0.5405483018,-1.9555115806,-1.9464166946
O,0,0.5280979339,-3.7463119726,1.9606404101
N,0,0.4170779514,-0.2792847111,5.6629025826
O,0,-0.6077921734,-0.5345157511,6.34502691
O,0,1.5452057824,-0.0716940637,6.1776855968
H,0,-2.0531128316,-0.5315213938,1.7661790001
H,0,-1.8254527884,-0.6661683004,4.2551428615
H,0,2.3969816224,0.2556733177,3.9304385589
H,0,2.1973460931,0.3424224418,1.4407560185
H,0,-1.0595346586,0.0500881033,-0.4301073592
H,0,0.7640713509,0.2230965391,-0.6182769855
H,0,1.7403941623,-2.3582611906,0.5480823043
H,0,1.9195282073,-1.7401476365,-1.143981753
H,0,1.505336064,-3.4671927372,-0.8384872791
H,0,0.0506345042,-1.1787811047,-2.4514622089
H,0,-0.4047435494,-2.9233792781,-2.4541917933
H,0,-1.6040596865,-1.6798134416,-1.9559474878
H,0,-1.9886904773,-2.8308582567,-0.0595204102
H,0,-0.7355901553,-5.8977004955,2.8312678855
H,0,-1.1544362162,-4.5140460154,3.8978232743
H,0,-2.4614010291,-5.5801630844,3.2556192437

6‡ wB97 IN DMSO

home/biswas/quiver/tdwB97
Nitro TS
wB97/6-31+G**
E(RwB97) = -877.044276862

Zero-point correction= 0.277126 (Hartree/Particle)
Thermal correction to Energy= 0.294279
Thermal correction to Enthalpy= 0.295223
Thermal correction to Gibbs Free Energy= 0.232728
Sum of electronic and ZPE= -876.767151
Sum of electronic and thermal Energies= -876.749998
Sum of electronic and thermal Enthalpies= -876.749053
Sum of electronic and thermal Free Energies= -876.811549

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.663	65.336	131.533

C,0,-1.1206193559,-0.4516844103,1.9281171063
C,0,-1.0559175353,-0.807970015,3.2783993216
C,0,0.1630038729,-0.7423977174,3.9314121203
C,0,1.3307243506,-0.2490546624,3.3002756835
C,0,1.2629145014,0.1116234482,1.9812372506
C,0,0.0365959837,0.0135830307,1.2415085209
C,0,0.0029028034,0.1124213917,-0.1546288105
N,0,-0.063965513,-2.0893941421,-0.4956455383
C,0,-0.8754512931,-2.6688115913,0.4130411902
C,0,-0.4612232388,-3.3167901666,1.6425295376
O,0,-1.5459731579,-3.8605574336,2.2560950949
C,0,-1.3016281703,-4.4664793543,3.533337889
C,0,1.3846682397,-2.3564329341,-0.4584357692
C,0,-0.6021005865,-2.0453227101,-1.8688549548
O,0,0.6670792123,-3.4135873587,2.1186420625
N,0,0.2412321965,-1.1758219289,5.3146937291
O,0,-0.7356439748,-1.7290822285,5.8156338004
O,0,1.2862366166,-0.986066716,5.9303505159
H,0,-2.0866681823,-0.4328833466,1.4284620824
H,0,-1.9392652766,-1.1578285558,3.8067205694
H,0,2.2591662099,-0.183906492,3.8604028937
H,0,2.1546186318,0.4775560748,1.4727886914
H,0,-0.9546798785,0.2454625438,-0.6550822072
H,0,0.8854352692,0.4490510328,-0.6992376352
H,0,1.7901849168,-2.0630147389,0.5105329762
H,0,1.8560573852,-1.782003378,-1.2588359513
H,0,1.5603818217,-3.4274664984,-0.6132071975
H,0,-0.0404281487,-1.3117125905,-2.4516303892
H,0,-0.5048752619,-3.0375573042,-2.3254590321
H,0,-1.6556426766,-1.7578366304,-1.8374576205
H,0,-1.9316452633,-2.7053147654,0.1666193598
H,0,-0.5419652489,-5.2496604015,3.45050569
H,0,-0.9773404523,-3.7105225371,4.2590279857
H,0,-2.2578797971,-4.8945519138,3.8397300345

6‡ SOGGA11X IN DMSO

home/biswas/quiver/tdSOGGA11X
Nitro TS
SOGGA11X/6-31+G**
E(RSOGGA11X) = -876.925136810

Zero-point correction= 0.277851 (Hartree/Particle)
Thermal correction to Energy= 0.295356
Thermal correction to Enthalpy= 0.296300
Thermal correction to Gibbs Free Energy= 0.231690
Sum of electronic and ZPE= -876.647286
Sum of electronic and thermal Energies= -876.629781
Sum of electronic and thermal Enthalpies= -876.628837
Sum of electronic and thermal Free Energies= -876.693447

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.339	65.266	135.983

C,0,-1.1086661373,-0.4310663209,2.0158058156
C,0,-1.0368261654,-0.7214280226,3.374502355
C,0,0.1905149294,-0.6091529131,4.0254640115
C,0,1.3531581307,-0.1693693115,3.354538841
C,0,1.2771938334,0.1113853185,2.0110607077
C,0,0.0471662492,-0.0162642789,1.2941132073
C,0,-0.0084202707,0.0573594991,-0.1100376905
N,0,-0.0649992748,-2.1009296846,-0.5142390048
C,0,-0.8830150498,-2.74966388,0.3481085744
C,0,-0.4852276051,-3.4021337359,1.5710795427
O,0,-1.5733584492,-3.9750628781,2.1487227614
C,0,-1.3432580747,-4.6476663833,3.3875537965
C,0,1.3825891637,-2.3765758955,-0.4802812248
C,0,-0.5879632935,-2.0121644497,-1.8911069923
O,0,0.6358019066,-3.5001600852,2.0634363264
N,0,0.2691632134,-0.9282189437,5.4276653509
O,0,-0.7397674391,-1.3348029482,5.999342806
O,0,1.3469709172,-0.7871828757,6.0003010467
H,0,-2.0702208221,-0.4649439411,1.5151565967
H,0,-1.9148516706,-1.0354437738,3.9264609836
H,0,2.283957647,-0.0713231917,3.8997713225
H,0,2.1659781037,0.4396663562,1.4791354082

H,0,-0.9704482335,0.1985154735,-0.5918904793
H,0,0.8627637622,0.3903974819,-0.6680777884
H,0,1.7765344747,-2.1590601487,0.5095154043
H,0,1.8638846985,-1.7525281266,-1.2326920916
H,0,1.5530133774,-3.43313908,-0.710028065
H,0,-0.0236861608,-1.2589002403,-2.4408514177
H,0,-0.4806554327,-2.9858934682,-2.3798549891
H,0,-1.6415365522,-1.73356462,-1.8626056794
H,0,-1.9364844511,-2.7505821399,0.1016987278
H,0,-0.6198831267,-5.4566154183,3.2624521216
H,0,-0.9794849665,-3.9474842525,4.1441836731
H,0,-2.3116482308,-5.0500181212,3.6831850422

6‡ lc-B97D IN DMSO

home/biswas/quiver/tdlc-B97D
Nitro TS
lc-B97D/6-31+G**
E(RB97D) = -875.044816416

Zero-point correction= 0.278877 (Hartree/Particle)
Thermal correction to Energy= 0.295406
Thermal correction to Enthalpy= 0.296351
Thermal correction to Gibbs Free Energy= 0.235529
Sum of electronic and ZPE= -874.765940
Sum of electronic and thermal Energies= -874.749410
Sum of electronic and thermal Enthalpies= -874.748466
Sum of electronic and thermal Free Energies= -874.809287

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.370	63.923	128.010

C,0,-1.1951229566,-0.4615371422,1.9228299279
C,0,-1.0916686405,-0.8653441619,3.2471924555
C,0,0.1447121184,-0.8270368094,3.8575202777
C,0,1.2866694894,-0.3054799691,3.2138395069
C,0,1.1759343004,0.1152581251,1.9248612608
C,0,-0.0648360064,0.024646791,1.2242924285
C,0,-0.1179319386,0.0971180634,-0.1641735586
N,0,-0.0324587964,-2.0758198596,-0.4639780066
C,0,-0.835112507,-2.7044150219,0.4113779335
C,0,-0.438666797,-3.2609430242,1.6742413216
O,0,-1.5080030549,-3.8113527984,2.2942825397
C,0,-1.2890256795,-4.3196006578,3.6151523887
C,0,1.4263924715,-2.2431570428,-0.371587547
C,0,-0.5135093459,-2.0701030295,-1.8555209805
O,0,0.6700298426,-3.2731620868,2.1941205828
N,0,0.2818469187,-1.3592571275,5.192742379
O,0,-0.7111369816,-1.7931977796,5.7641203143
O,0,1.3905669085,-1.3788727692,5.7076824529
H,0,-2.1583768227,-0.4874770175,1.4236666043
H,0,-1.9479854242,-1.2744648964,3.7722057694
H,0,2.233077224,-0.2752634468,3.7412251267
H,0,2.0471873336,0.4895907993,1.3925101828
H,0,-1.0835694138,0.1606273568,-0.6584484829
H,0,0.7526477696,0.4222152747,-0.7293311268
H,0,1.7695310056,-1.9263113373,0.6119540035
H,0,1.8812103852,-1.6315641805,-1.1532351285
H,0,1.6713914749,-3.3011042318,-0.5170836182
H,0,0.0349763441,-1.3067526962,-2.4112429827
H,0,-0.3391181967,-3.0589725111,-2.2950345737
H,0,-1.5809401818,-1.8371718115,-1.8630281421
H,0,-1.8803815858,-2.783688181,0.1389045896
H,0,-0.4681169931,-5.0425217642,3.6138598497
H,0,-1.0565722679,-3.4994307805,4.3020192896
H,0,-2.2253509962,-4.7994692755,3.9036519621

6‡ B97D IN DMSO

home/biswas/quiver/tdb97d
Nitro TS
b97d/6-31+G**
E(RB97D) = -876.651803836

Zero-point correction= 0.266770 (Hartree/Particle)
Thermal correction to Energy= 0.284568
Thermal correction to Enthalpy= 0.285513
Thermal correction to Gibbs Free Energy= 0.220154
Sum of electronic and ZPE= -876.385034
Sum of electronic and thermal Energies= -876.367235
Sum of electronic and thermal Enthalpies= -876.366291
Sum of electronic and thermal Free Energies= -876.431650

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	178.569	67.265	137.560

C,0,-1.1134107729,-0.5097414179,2.1784996635
C,0,-0.980784999,-0.6560657082,3.5604533064
C,0,0.2773456008,-0.4332227718,4.147933189
C,0,1.4003264641,-0.0474766023,3.3804311738
C,0,1.2575675648,0.0748767427,2.0016912947
C,0,0.0044315798,-0.1577650226,1.3743904805
C,0,-0.1283071259,-0.2078410587,-0.0666834479
N,0,-0.048404333,-2.0208714295,-0.5429632166
C,0,-0.9014641325,-2.857936446,0.2090581267
C,0,-0.5522287072,-3.4949343072,1.435121091
O,0,-1.6884338465,-4.1162133433,1.9694338769
C,0,-1.490019582,-4.7847641977,3.232266062
C,0,1.4186174554,-2.3319468889,-0.4745315937
C,0,-0.4833815552,-1.9648273018,-1.9805170501
O,0,0.5528350545,-3.5843318883,2.0057825082
N,0,0.4248067299,-0.599309135,5.5954018782
O,0,-0.5689900127,-0.9546980227,6.2619675036
O,0,1.5428186702,-0.3851294348,6.1075607742
H,0,-2.0839562402,-0.661474995,1.7099838244
H,0,-1.8275910172,-0.9426626555,4.1790953937
H,0,2.3555075978,0.132176011,3.8671488475
H,0,2.1179492378,0.3491440529,1.3910298244
H,0,-1.1245692971,0.0065050992,-0.4591785543
H,0,0.6833038395,0.2294354245,-0.6528356852
H,0,1.7580218436,-2.2038248964,0.5539898475
H,0,1.9385552238,-1.6471165777,-1.1532713881
H,0,1.5627091519,-3.3730767102,-0.7872528143
H,0,0.1015159911,-1.1940030766,-2.495330489
H,0,-0.3074121394,-2.9482154555,-2.4328714634
H,0,-1.5494057964,-1.7163610773,-2.017181255
H,0,-1.9474700277,-2.8001542536,-0.0766449854
H,0,-0.7388612418,-5.5835030244,3.1431011024
H,0,-1.1661442185,-4.0700042669,4.0039402894
H,0,-2.4671879599,-5.2086803643,3.4925708847

6‡ wb97xd IN DMSO

home/biswas/quiver/tdwb97xd
Nitro TS
wb97xd/6-31+G**
E(RwB97XD) = -876.919262363

Zero-point correction= 0.276338 (Hartree/Particle)
Thermal correction to Energy= 0.293539
Thermal correction to Enthalpy= 0.294483
Thermal correction to Gibbs Free Energy= 0.231323
Sum of electronic and ZPE= -876.642925
Sum of electronic and thermal Energies= -876.625723
Sum of electronic and thermal Enthalpies= -876.624779
Sum of electronic and thermal Free Energies= -876.687939

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.199	65.314	132.932

C,0,-1.1334027661,-0.4499018599,1.9644646509
C,0,-1.0602841437,-0.7937460135,3.3100913411
C,0,0.1637417286,-0.7153719991,3.9574848141
C,0,1.3200689297,-0.2321407094,3.3116165567
C,0,1.2419249289,0.1105750386,1.9872599685
C,0,0.0173116049,-0.0015565487,1.2631085113
C,0,-0.0278340157,0.0801909408,-0.1368137546
N,0,-0.0519092919,-2.0836069385,-0.5032670591
C,0,-0.8602438922,-2.7113200081,0.3846806925
C,0,-0.4540582554,-3.3414220656,1.6132445948
O,0,-1.5394856432,-3.8880039397,2.222241565
C,0,-1.3097507335,-4.4797277631,3.5005015366
C,0,1.3985190067,-2.3389030192,-0.4638768346
C,0,-0.580463441,-2.0387261337,-1.8799377
O,0,0.6699835368,-3.4335274063,2.0989582958
N,0,0.2528425269,-1.1332940442,5.337116342
O,0,-0.7397875411,-1.6300258261,5.8708016916
O,0,1.3229035667,-0.9894163967,5.9274004893
H,0,-2.0949905889,-0.4656545191,1.4645084248
H,0,-1.9367787874,-1.1439516418,3.8407745979
H,0,2.2520684313,-0.1588266292,3.8572807218
H,0,2.1289322846,0.4629978734,1.4696155196
H,0,-0.9865325311,0.2153413381,-0.6263009759
H,0,0.8443486424,0.4205769912,-0.6877105686
H,0,1.7903379185,-2.0830671589,0.5175059359
H,0,1.8725083182,-1.73203584,-1.2341418776
H,0,1.5840350138,-3.3988736685,-0.6587946265
H,0,-0.0268927472,-1.2960316895,-2.453669255
H,0,-0.4672798557,-3.0242218306,-2.3408455586
H,0,-1.6352076225,-1.7663552713,-1.8556557551
H,0,-1.9131102521,-2.7340196889,0.1396716391
H,0,-0.5912998437,-5.2994289796,3.4287844468
H,0,-0.9436456964,-3.733051353,4.2104977665
H,0,-2.2782797892,-4.8574882396,3.8249928631

6‡ PBEPBE IN DMSO

home/biswas/quiver/tdpbepbe
Nitro TS
pbepbe/6-31+G**
E(RPBE-PBE) = -876.201031323

Zero-point correction= 0.265314 (Hartree/Particle)
Thermal correction to Energy= 0.283474
Thermal correction to Enthalpy= 0.284418
Thermal correction to Gibbs Free Energy= 0.218256
Sum of electronic and ZPE= -875.935717
Sum of electronic and thermal Energies= -875.917557
Sum of electronic and thermal Enthalpies= -875.916613
Sum of electronic and thermal Free Energies= -875.982775

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.883	68.036	139.249

C,0,-1.0855909465,-0.4086811799,2.1965112877
C,0,-0.9856170248,-0.5088515176,3.5840538829
C,0,0.2656975747,-0.3075551585,4.1921633409
C,0,1.4171145178,0.0050142353,3.434429992
C,0,1.3083561551,0.0866946586,2.0520272279
C,0,0.0583026385,-0.117104585,1.3968937145
C,0,-0.0548126482,-0.1557359929,-0.0346835286
N,0,-0.0725840493,-2.0751410057,-0.5404984333
C,0,-0.9240954472,-2.8638497884,0.2302246731
C,0,-0.5549533429,-3.5709450028,1.4186197905
O,0,-1.675536475,-4.2234259335,1.9282136611
C,0,-1.4419574015,-4.9895483958,3.1249445662
C,0,1.3793714604,-2.4207512443,-0.5112507512
C,0,-0.5522008472,-1.9534604273,-1.9501439413
O,0,0.560202655,-3.6799427699,1.967546806
N,0,0.373244724,-0.4072324694,5.6378607406
O,0,-0.6547945942,-0.6864718297,6.2991707503
O,0,1.4934379658,-0.2137574207,6.1667783412
H,0,-2.0601874504,-0.5304061337,1.7167429591
H,0,-1.8570524224,-0.7345844555,4.2015715966
H,0,2.3691615157,0.1708210252,3.9414699919
H,0,2.1948268864,0.3202561383,1.454188625
H,0,-1.0399630351,0.0673304856,-0.4562790508
H,0,0.7864134761,0.223984889,-0.6243194046
H,0,1.7537129225,-2.3387095835,0.5143876332
H,0,1.9119274813,-1.7354383786,-1.1835835897
H,0,1.5008714561,-3.4584665409,-0.8583935583
H,0,0.029478406,-1.1767872598,-2.4651626845
H,0,-0.417418504,-2.921804174,-2.4559568418
H,0,-1.6165019724,-1.6832362325,-1.950501343
H,0,-1.9780312134,-2.8174887448,-0.0435865894
H,0,-0.6860854012,-5.7733823037,2.9548651553
H,0,-1.1064013133,-4.3401998698,3.9503639532
H,0,-2.4100467465,-5.4451580337,3.3729200272

6‡ MN12L IN DMSO

home/biswas/quiver/tdMN12L
Nitro TS
MN12L/6-31+G**
E(RMN12L) = -876.380845793

Zero-point correction= 0.275873 (Hartree/Particle)
Thermal correction to Energy= 0.292761
Thermal correction to Enthalpy= 0.293705
Thermal correction to Gibbs Free Energy= 0.231978
Sum of electronic and ZPE= -876.104973
Sum of electronic and thermal Energies= -876.088085
Sum of electronic and thermal Enthalpies= -876.087141

Sum of electronic and thermal Free Energies= -876.148868

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.710	64.982	129.915

C,0,-1.1665033538,-0.4768442902,2.0543049805
C,0,-1.067335681,-0.7900662943,3.3982257359
C,0,0.1836925447,-0.7120665996,4.0095421855
C,0,1.3275265417,-0.2663980844,3.3278943051
C,0,1.220197386,0.0242319093,1.9886927347
C,0,-0.0187181894,-0.1043164205,1.3108811791
C,0,-0.0977424401,-0.087286022,-0.1053353505
N,0,-0.046675802,-2.0595297412,-0.5321225224
C,0,-0.863984688,-2.8179559348,0.2738322484
C,0,-0.4845891587,-3.3297352387,1.5464056161
O,0,-1.5550184167,-3.9065555496,2.1539594885
C,0,-1.3228288741,-4.3712096277,3.4714377163
C,0,1.4063835124,-2.3072310737,-0.4753449386
C,0,-0.5201232874,-2.0008960462,-1.9269402959
O,0,0.6186548104,-3.3179746038,2.0899595954
N,0,0.3022012123,-1.0973579745,5.3814411652
O,0,-0.6861332011,-1.5762920883,5.9532236041
O,0,1.393466659,-0.9550819986,5.9460363061
H,0,-2.130232151,-0.5266830839,1.5537787424
H,0,-1.9320563333,-1.1075351412,3.9718630482
H,0,2.2717433721,-0.1896766866,3.8543882697
H,0,2.0980608698,0.3376575445,1.4272806474
H,0,-1.0716059325,0.0761839464,-0.5632255332
H,0,0.7552903231,0.2737565818,-0.6795569346
H,0,1.7884034591,-2.0669656958,0.5162731856
H,0,1.8840625723,-1.6859698134,-1.2355770046
H,0,1.5949519695,-3.3653578025,-0.6829813493
H,0,0.0190731572,-1.2122932748,-2.4561766943
H,0,-0.3349703375,-2.9653009579,-2.410162868
H,0,-1.5902233941,-1.7871590431,-1.9366068987
H,0,-1.9140860653,-2.819924659,0.0046756946
H,0,-0.534485589,-5.1292853378,3.4922523334
H,0,-1.0323876539,-3.5423370909,4.1303943163
H,0,-2.2657188409,-4.8005588069,3.8088762918

6‡ M11 IN DMSO

home/biswas/quiver/tdM11
Nitro TS
M11/6-31+G**
E(RM11) = -876.740360678

Zero-point correction= 0.273446 (Hartree/Particle)
Thermal correction to Energy= 0.290667
Thermal correction to Enthalpy= 0.291611
Thermal correction to Gibbs Free Energy= 0.229147
Sum of electronic and ZPE= -876.466915
Sum of electronic and thermal Energies= -876.449694
Sum of electronic and thermal Enthalpies= -876.448750
Sum of electronic and thermal Free Energies= -876.511214

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.396	65.765	131.467

C,0,-1.1384489049,-0.5078815365,1.9224563671
C,0,-1.061195569,-0.8690389485,3.2677588368
C,0,0.1607720626,-0.782617463,3.912387668
C,0,1.3176664549,-0.271489505,3.2809779783
C,0,1.2350362751,0.1023072508,1.9682650959
C,0,0.0065804817,-0.0082382748,1.2359538199
C,0,-0.0386538142,0.119156303,-0.1524343772
N,0,-0.0581340011,-2.1046924156,-0.4978663639
C,0,-0.8764723145,-2.6764325464,0.3969433656
C,0,-0.4684239065,-3.290505319,1.6456808855
O,0,-1.5469213989,-3.8307133241,2.2656948458
C,0,-1.2935902371,-4.4202490862,3.54731351
C,0,1.3976106549,-2.3187821763,-0.4170078901
C,0,-0.5668238178,-2.0450998553,-1.881948277
O,0,0.654737651,-3.3621391948,2.1325127948
N,0,0.2517342229,-1.2082346733,5.2913041254
O,0,-0.7431497865,-1.6900565375,5.8299662249
O,0,1.3255287877,-1.081246662,5.8741677008
H,0,-2.107740052,-0.5038517176,1.4232575668
H,0,-1.9344733754,-1.2422803059,3.8025943481
H,0,2.247991886,-0.1971648377,3.8407902949
H,0,2.1173540815,0.4909991384,1.455513013
H,0,-1.0039160121,0.218129159,-0.6509402515
H,0,0.8379364043,0.4691446912,-0.7024914436
H,0,1.7642108812,-1.9927590864,0.5601250468
H,0,1.8679473043,-1.7408516593,-1.2187751058
H,0,1.6141204976,-3.3884849458,-0.5439981135
H,0,-0.000111297,-1.2918387353,-2.438596004
H,0,-0.4430000753,-3.0302112046,-2.3525451083
H,0,-1.6271859413,-1.772808307,-1.8667931223
H,0,-1.9306743671,-2.7355663345,0.1367090798
H,0,-0.5467613306,-5.2187699688,3.4596360244
H,0,-0.9335529878,-3.6564285715,4.250561975
H,0,-2.2517094566,-4.8253183498,3.8844144897

6‡ N12 IN DMSO

home/biswas/quiver/tdN12
Nitro TS
N12/6-31+G**
E(RN12) = -877.063939794

Zero-point correction= 0.271978 (Hartree/Particle)
Thermal correction to Energy= 0.289830
Thermal correction to Enthalpy= 0.290774
Thermal correction to Gibbs Free Energy= 0.225168
Sum of electronic and ZPE= -876.791962
Sum of electronic and thermal Energies= -876.774110
Sum of electronic and thermal Enthalpies= -876.773166
Sum of electronic and thermal Free Energies= -876.838771

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	181.871	66.669	138.079

C,0,-1.0662536845,-0.3928300737,2.2028606293
C,0,-0.9691301649,-0.4688502121,3.5785459789
C,0,0.2698466214,-0.2575622384,4.1822566963
C,0,1.4129154743,0.0358480221,3.4255908929
C,0,1.3075870584,0.0978519995,2.0555267785
C,0,0.0678193651,-0.1109519905,1.40626358
C,0,-0.0454192147,-0.1523392393,-0.0081609161
N,0,-0.0767259493,-2.0917309749,-0.5095143151

C,0,-0.9221160568,-2.8555646134,0.2592154425
C,0,-0.5564722942,-3.596969401,1.4147715266
O,0,-1.6545095547,-4.2361667514,1.9151151878
C,0,-1.4428126686,-5.0637535608,3.0457089853
C,0,1.357497686,-2.4318764729,-0.4798375388
C,0,-0.5562083483,-1.9554148041,-1.8987435769
O,0,0.5510123123,-3.7335239286,1.9365645758
N,0,0.3729233209,-0.329067249,5.6059144719
O,0,-0.6474039976,-0.574352195,6.2688029087
O,0,1.4827919926,-0.1460342229,6.1307211225
H,0,-2.0271427773,-0.5216962574,1.7306323983
H,0,-1.8304480388,-0.6808894386,4.1894138236
H,0,2.3514329735,0.2061173051,3.9253792995
H,0,2.1835425625,0.3193648329,1.4644653379
H,0,-1.018111552,0.0504853528,-0.4297627613
H,0,0.7860885123,0.205562591,-0.5976398698
H,0,1.72840689,-2.3583477623,0.5319668291
H,0,1.8853684902,-1.7523564758,-1.1375086094
H,0,1.4824292936,-3.4536050633,-0.8283160809
H,0,0.0172397691,-1.1881442788,-2.405767677
H,0,-0.4309963092,-2.906174337,-2.4099093145
H,0,-1.6054157244,-1.6846059575,-1.8943074169
H,0,-1.9630959048,-2.8036546124,-0.0057160942
H,0,-0.7655297513,-5.8820012671,2.809617389
H,0,-1.0327427549,-4.4947055428,3.8767932351
H,0,-2.4180785761,-5.4560761822,3.3106460816

6‡ B3LYP IN DMSO

home/biswas/quiver/tdb3lyp
Nitro TS
b3lyp/6-31+G**
E(RB3LYP) = -877.211171489

Zero-point correction= 0.272537 (Hartree/Particle)
Thermal correction to Energy= 0.290384
Thermal correction to Enthalpy= 0.291328
Thermal correction to Gibbs Free Energy= 0.225662
Sum of electronic and ZPE= -876.938635
Sum of electronic and thermal Energies= -876.920787
Sum of electronic and thermal Enthalpies= -876.919843
Sum of electronic and thermal Free Energies= -876.985510

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.219	66.379	138.207

C,0,-1.0808483729,-0.3725374146,2.1559026633
C,0,-0.9972605276,-0.5122182633,3.5354914391
C,0,0.2418269108,-0.3399550846,4.1614789989
C,0,1.4006413515,-0.0143916192,3.4280442045
C,0,1.3095689252,0.1121742989,2.0568095078
C,0,0.0688474358,-0.0621126243,1.3794165339
C,0,-0.0209401444,-0.0636030153,-0.0399578643
N,0,-0.073370787,-2.1076034171,-0.5319635418
C,0,-0.9102791393,-2.8441331952,0.2735273667
C,0,-0.5318265823,-3.5661534383,1.4497688504
O,0,-1.6385817641,-4.186023621,1.9843800476
C,0,-1.4144308802,-4.9750281669,3.162971459
C,0,1.3769575876,-2.4352332123,-0.5208470133
C,0,-0.5826603842,-1.974389722,-1.9242645275
O,0,0.5869767421,-3.7013788844,1.9611840351
N,0,0.3317513363,-0.4828214456,5.5971629317
O,0,-0.6951989856,-0.7678639444,6.236730675
O,0,1.4362306021,-0.3181954006,6.1427625937
H,0,-2.0448161614,-0.4674706802,1.6688046323
H,0,-1.8729172162,-0.7479051546,4.1271339687
H,0,2.3419698203,0.1269340985,3.9435208781
H,0,2.1978856181,0.3565458644,1.4821324222
H,0,-0.9909604198,0.1274032535,-0.4856731628
H,0,0.8324392134,0.2767890064,-0.6185165863
H,0,1.7707233538,-2.3258691646,0.4850091359
H,0,1.8853665872,-1.7632564734,-1.2112088319
H,0,1.5080933839,-3.470940365,-0.8470462504
H,0,-0.0102345211,-1.2078932447,-2.4463137326
H,0,-0.4706593285,-2.9343270687,-2.4362877448
H,0,-1.6359249385,-1.6958685798,-1.9011266659
H,0,-1.9610838146,-2.8010239477,0.0227528753
H,0,-0.7122408982,-5.7884152874,2.9613099061
H,0,-1.0264484327,-4.3573150217,3.9772569592
H,0,-2.3903065696,-5.3799340647,3.4312428368

6‡ B971 IN DMSO

home/biswas/quiver/tdB971
Nitro TS
B971/6-31+G**
E(RB971) = -876.953613758

Zero-point correction= 0.271946 (Hartree/Particle)
Thermal correction to Energy= 0.289815
Thermal correction to Enthalpy= 0.290759
Thermal correction to Gibbs Free Energy= 0.225323
Sum of electronic and ZPE= -876.681668
Sum of electronic and thermal Energies= -876.663799
Sum of electronic and thermal Enthalpies= -876.662854
Sum of electronic and thermal Free Energies= -876.728291

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	181.862	66.610	137.722

C,0,-1.089893258,-0.4062375304,2.1079001083
C,0,-1.009572898,-0.6002441731,3.4847653808
C,0,0.2262309241,-0.4328047629,4.1240880111
C,0,1.3861738453,-0.0529073392,3.409879865
C,0,1.3003378973,0.1253276253,2.0420868239
C,0,0.0625508737,-0.0458134914,1.3480600784
C,0,-0.0164093387,-0.0234027205,-0.0702791897
N,0,-0.0695891038,-2.1062572591,-0.5345581702
C,0,-0.9024649418,-2.8161227303,0.2917100294
C,0,-0.5154132666,-3.5252808871,1.4838006159
O,0,-1.6239261959,-4.1068756607,2.0458912269
C,0,-1.3974280341,-4.8459776297,3.2538326666
C,0,1.3821731289,-2.4187507852,-0.5156223769
C,0,-0.5837029621,-1.9867425608,-1.9248570469
O,0,0.6092738419,-3.6731294758,1.9742290277
N,0,0.3127509749,-0.6377234396,5.5517708674
O,0,-0.7072422579,-0.9902120935,6.16981362
O,0,1.4081403953,-0.4579104737,6.1120703314
H,0,-2.0529360909,-0.491346401,1.613065255
H,0,-1.8843967631,-0.8757351604,4.0640049118

H,0,2.3227143445,0.08503363,3.9389076417
H,0,2.1881017104,0.4075208171,1.4805532111
H,0,-0.9868822699,0.1496654044,-0.5274132217
H,0,0.8431211358,0.3180218892,-0.6432611377
H,0,1.7727316532,-2.2863654538,0.4913367157
H,0,1.8851358002,-1.7520354313,-1.2180061295
H,0,1.5254244144,-3.4606190655,-0.8234441994
H,0,-0.0119571385,-1.2235333863,-2.4564895425
H,0,-0.4733831109,-2.9532908142,-2.4290516187
H,0,-1.6384719156,-1.7066889312,-1.9001114794
H,0,-1.9574879698,-2.7743452583,0.0489243536
H,0,-0.6867632881,-5.6619127031,3.0871252325
H,0,-1.0163251599,-4.1899962812,4.0441570345
H,0,-2.3723259764,-5.2473224668,3.5367101038

6‡ APFD IN DMSO

home/biswas/quiver/tdAPFD
Nitro TS
APFD/6-31+G**
E(RAPFD) = -876.519182271

Zero-point correction= 0.274957 (Hartree/Particle)
Thermal correction to Energy= 0.292256
Thermal correction to Enthalpy= 0.293201
Thermal correction to Gibbs Free Energy= 0.230034
Sum of electronic and ZPE= -876.244225
Sum of electronic and thermal Energies= -876.226926
Sum of electronic and thermal Enthalpies= -876.225982
Sum of electronic and thermal Free Energies= -876.289148

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.394	65.531	132.945

C,0,-1.1518065918,-0.4515019913,2.0114856903
C,0,-1.0579653732,-0.7805573839,3.3567391329
C,0,0.1830064846,-0.6968765294,3.9812379893
C,0,1.3254821615,-0.2200221372,3.3137499984
C,0,1.226020477,0.0940554265,1.9778636077
C,0,-0.0060496,-0.0402515935,1.2853600334
C,0,-0.0736724071,-0.026602385,-0.1297858662
N,0,-0.0464164536,-2.0428842538,-0.507850729
C,0,-0.8604843055,-2.7553846881,0.335352025
C,0,-0.4690197903,-3.3212339701,1.5891952978
O,0,-1.5577941452,-3.908371757,2.1782344182
C,0,-1.3355976636,-4.4584810771,3.4740481597
C,0,1.4031697868,-2.3148493653,-0.4527661033
C,0,-0.5363725523,-2.0249072157,-1.8997312691
O,0,0.6419362106,-3.3452326139,2.1252985497
N,0,0.2979934742,-1.1149280815,5.3558713536
O,0,-0.6847260255,-1.6299609021,5.8971803179
O,0,1.3789936581,-0.955206585,5.9282600825
H,0,-2.1153845158,-0.4938795271,1.5143369046
H,0,-1.9234704796,-1.1229277155,3.9122573219
H,0,2.2661856904,-0.1395637915,3.8458124661
H,0,2.1054836815,0.4291729999,1.4342605582
H,0,-1.0415233188,0.1370566273,-0.5950383647
H,0,0.7809926074,0.3326086819,-0.6978086787
H,0,1.7755817267,-2.0929583796,0.544076782
H,0,1.8991177965,-1.6936477923,-1.1981054889
H,0,1.5734618905,-3.3718906201,-0.6730302676
H,0,0.0120530302,-1.271479869,-2.465823722
H,0,-0.3806946694,-3.0106745839,-2.3464712298
H,0,-1.5996380483,-1.7852404468,-1.908424977
H,0,-1.9082299462,-2.7822188517,0.0677990371
H,0,-0.5452838357,-5.2139373161,3.4536623667
H,0,-1.0654768775,-3.6755496677,4.1895053425
H,0,-2.2815830767,-4.9156876445,3.7648382606

6‡ B98 IN DMSO

home/biswas/quiver/tdB98
Nitro TS
B98/6-31+G**
E(RB98) = -876.863204208

Zero-point correction= 0.272350 (Hartree/Particle)
Thermal correction to Energy= 0.290161
Thermal correction to Enthalpy= 0.291105
Thermal correction to Gibbs Free Energy= 0.225932
Sum of electronic and ZPE= -876.590855
Sum of electronic and thermal Energies= -876.573043
Sum of electronic and thermal Enthalpies= -876.572099
Sum of electronic and thermal Free Energies= -876.637272

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.079	66.474	137.168

C,0,-1.0870624322,-0.3965925174,2.1139567476
C,0,-1.0077320365,-0.5823990058,3.4909983571
C,0,0.2277391239,-0.4151897021,4.1298986812
C,0,1.3887846248,-0.0451911614,3.4133585302
C,0,1.3038895136,0.1259770691,2.0457225109
C,0,0.0658470989,-0.0433957593,1.3522688591
C,0,-0.0134003277,-0.0203058181,-0.0646359117
N,0,-0.0712123432,-2.112409175,-0.5331704321
C,0,-0.9036675073,-2.8204663386,0.2919702825
C,0,-0.5168061357,-3.5362275157,1.4800622004
O,0,-1.6228920477,-4.1206388687,2.0382262416
C,0,-1.3987188603,-4.8735328769,3.2367393396
C,0,1.3801477019,-2.4250216098,-0.5165588238
C,0,-0.5869054539,-1.9861295607,-1.921929996
O,0,0.6069377008,-3.685848703,1.9685648339
N,0,0.31272461,-0.6094999348,5.5573204941
O,0,-0.7086332035,-0.9496454349,6.1782593821
O,0,1.4082440036,-0.4330890018,6.1165203439
H,0,-2.0500275302,-0.4807061635,1.6201688967
H,0,-1.8834768655,-0.8507022237,4.0710178076
H,0,2.3255113813,0.0920254169,3.9409357641
H,0,2.1924750539,0.4018843448,1.4835856195
H,0,-0.9831516102,0.1516443522,-0.5219008917
H,0,0.8461343313,0.3180484746,-0.6380683165
H,0,1.7715242431,-2.2978072215,0.4899721047
H,0,1.8826419223,-1.7556302558,-1.2156954997
H,0,1.5230043891,-3.4648982158,-0.8294940251
H,0,-0.0151342751,-1.2221313205,-2.4510491984
H,0,-0.4786273757,-2.9502329351,-2.4301357803
H,0,-1.6407239062,-1.705064238,-1.8950749058
H,0,-1.9582545437,-2.7780427775,0.0502010496
H,0,-0.6973236305,-5.6942470289,3.0582441027
H,0,-1.0080067608,-4.2301103431,4.0315968834

H,0,-2.3755598525,-5.26843895,3.5197137487

6‡ B972 IN DMSO

home/biswas/quiver/tdB972
Nitro TS
B972/6-31+G**
E(RB972) = -876.893771677

Zero-point correction= 0.275027 (Hartree/Particle)
Thermal correction to Energy= 0.292722
Thermal correction to Enthalpy= 0.293667
Thermal correction to Gibbs Free Energy= 0.228533
Sum of electronic and ZPE= -876.618745
Sum of electronic and thermal Energies= -876.601049
Sum of electronic and thermal Enthalpies= -876.600105
Sum of electronic and thermal Free Energies= -876.665239

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.686	65.949	137.086

C,0,-1.0762146813,-0.380007967,2.1203188788
C,0,-1.0034208121,-0.5447394702,3.4957258282
C,0,0.2257207897,-0.3794159079,4.1349468583
C,0,1.3871022844,-0.0343896491,3.4187048577
C,0,1.3082163795,0.1186051571,2.0528322265
C,0,0.0761755374,-0.0466239562,1.3604061229
C,0,-0.000733818,-0.0290663692,-0.052329847
N,0,-0.073349101,-2.1115933453,-0.5208193904
C,0,-0.8998265385,-2.815891984,0.3060768274
C,0,-0.5122518395,-3.549827442,1.4750368779
O,0,-1.6174939694,-4.1383848814,2.0236208139
C,0,-1.392784103,-4.9296068573,3.1900630434
C,0,1.3681297826,-2.432197601,-0.5172278994
C,0,-0.597073782,-1.9843665198,-1.8980601955
O,0,0.6088285716,-3.7120956927,1.9573355141
N,0,0.303622417,-0.5499330495,5.5646230381
O,0,-0.718331616,-0.8580169478,6.1805129622
O,0,1.3926895575,-0.3838388077,6.1166391485
H,0,-2.0362619615,-0.4629819866,1.6265781773
H,0,-1.8825729515,-0.7948266351,4.0736019492
H,0,2.3223035749,0.101178558,3.9438869634
H,0,2.1994205959,0.3786906359,1.4926823783
H,0,-0.9657230131,0.1537492852,-0.5086388397
H,0,0.8592790838,0.3025639871,-0.6234732879
H,0,1.7726001089,-2.301521983,0.4800203721
H,0,1.8679665666,-1.7732447827,-1.2230764548
H,0,1.5025702802,-3.4713603465,-0.8244523742
H,0,-0.0279524481,-1.2271897518,-2.4332481867
H,0,-0.4998864333,-2.9463282985,-2.4056497087
H,0,-1.6459550931,-1.6981752213,-1.865158274
H,0,-1.9524736486,-2.7686220558,0.0702870298
H,0,-0.7189918973,-5.7607367549,2.9756108858
H,0,-0.9737207924,-4.3255679871,3.9964416189
H,0,-2.3713180304,-5.3082503716,3.4777710854

6‡ MN12SX IN DMSO

home/biswas/quiver/tdMN12SX
Nitro TS
MN12SX/6-31+G**
E(RMN12SX) = -876.505223838

Zero-point correction= 0.274467 (Hartree/Particle)
Thermal correction to Energy= 0.291727
Thermal correction to Enthalpy= 0.292671
Thermal correction to Gibbs Free Energy= 0.229848
Sum of electronic and ZPE= -876.230757
Sum of electronic and thermal Energies= -876.213497
Sum of electronic and thermal Enthalpies= -876.212553
Sum of electronic and thermal Free Energies= -876.275376

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.061	65.633	132.222

C,0,-1.1448017133,-0.459572263,2.0430183093
C,0,-1.0530887236,-0.7702425579,3.3899586808
C,0,0.1903578025,-0.6836365285,4.01241842
C,0,1.337761616,-0.233819561,3.3363378528
C,0,1.2385306772,0.0571602901,1.9967201137
C,0,0.0040685451,-0.0741532037,1.3057154787
C,0,-0.0684285296,-0.0420483717,-0.1078706076
N,0,-0.0513316497,-2.0726732142,-0.5289161835
C,0,-0.8699478439,-2.7931306855,0.2959663893
C,0,-0.4862719962,-3.3546189387,1.552444788
O,0,-1.5651877845,-3.9285288875,2.1514731536
C,0,-1.3408002022,-4.4450908523,3.4534407501
C,0,1.3994409127,-2.3293017779,-0.479377049
C,0,-0.541542803,-2.0055256655,-1.9176075412
O,0,0.6234584569,-3.3829124225,2.0830716951
N,0,0.2990580238,-1.0610075715,5.3926987041
O,0,-0.6915177952,-1.5384888449,5.9588348788
O,0,1.3839803247,-0.9095931014,5.9649078444
H,0,-2.1125231008,-0.5038070272,1.5446732313
H,0,-1.9258312504,-1.0893466636,3.9560581387
H,0,2.2820247024,-0.1486551042,3.868052121
H,0,2.1226225708,0.3804490095,1.4456395334
H,0,-1.0409633186,0.1200927716,-0.5729419672
H,0,0.7912576953,0.311960683,-0.679645083
H,0,1.7909675418,-2.0903524644,0.5113256163
H,0,1.8815756516,-1.7114667279,-1.2424885582
H,0,1.5833142054,-3.3908978993,-0.6896588111
H,0,0.0040468316,-1.2262440849,-2.4584488567
H,0,-0.3797202568,-2.9760248915,-2.404601721
H,0,-1.6105463607,-1.773266797,-1.9164997579
H,0,-1.9227076607,-2.8022643678,0.0313398851
H,0,-0.5686860377,-5.2240503577,3.4455141398
H,0,-1.0343443172,-3.6451837215,4.1435855956
H,0,-2.2959352137,-4.8677731994,3.7764498167

6‡ wB97X IN DMSO

home/biswas/quiver/tdwB97X
Nitro TS
wB97X/6-31+G**
E(RwB97X) = -876.971748349

Zero-point correction= 0.277305 (Hartree/Particle)
Thermal correction to Energy= 0.294431
Thermal correction to Enthalpy= 0.295375
Thermal correction to Gibbs Free Energy= 0.232756

Sum of electronic and ZPE= -876.694443
Sum of electronic and thermal Energies= -876.677317
Sum of electronic and thermal Enthalpies= -876.676373
Sum of electronic and thermal Free Energies= -876.738993

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.758	65.137	131.794

C,0,-1.1133039754,-0.440839874,1.9425259096
C,0,-1.0529487634,-0.7851007258,3.2919320998
C,0,0.1633970299,-0.714874762,3.9486148939
C,0,1.3306642003,-0.2355802428,3.3144253301
C,0,1.2671670533,0.1100025165,1.9918910406
C,0,0.045279092,0.0096888494,1.2531175828
C,0,0.0109234602,0.1062781203,-0.14256395
N,0,-0.065910799,-2.0932983222,-0.4988891411
C,0,-0.8747081315,-2.6814257147,0.4066946631
C,0,-0.460933154,-3.3342337809,1.6280898145
O,0,-1.5433458277,-3.8780351129,2.2411406868
C,0,-1.2998298907,-4.4996623818,3.5063335073
C,0,1.3805385893,-2.3670072874,-0.4724266679
C,0,-0.6109704543,-2.0378706486,-1.8677300138
O,0,0.667078612,-3.4387651296,2.0986960405
N,0,0.2365405155,-1.1315078899,5.3329108925
O,0,-0.7486120646,-1.6599883689,5.8430396602
O,0,1.2859705748,-0.9531761745,5.9441189831
H,0,-2.0753020189,-0.4299988269,1.4399491118
H,0,-1.9370929609,-1.1264683393,3.8194346668
H,0,2.2569660258,-0.1672532038,3.8733160976
H,0,2.1603429524,0.4649535385,1.483261136
H,0,-0.9440082635,0.2464080179,-0.6407256247
H,0,0.8924795403,0.4379986835,-0.6867972733
H,0,1.7913134751,-2.0919595178,0.49712773
H,0,1.8510958314,-1.7846054082,-1.26465587
H,0,1.5507873984,-3.4344794248,-0.6441287729
H,0,-0.0505977025,-1.3052520266,-2.4490627525
H,0,-0.5219856116,-3.0258019902,-2.3307503399
H,0,-1.6610703862,-1.7465924689,-1.8294378937
H,0,-1.9302457659,-2.7069874584,0.1667029081
H,0,-0.5622301063,-5.2996911761,3.4099092204
H,0,-0.9487726422,-3.7620526263,4.2349683391
H,0,-2.2603868319,-4.9068358431,3.8205569851

6‡ B3LYPD2 IN DMSO

home/biswas/quiver/tdb3lypd2
Nitro TS
b3lyp/6-31+G**
E(RB3LYP) = -877.263539919

Zero-point correction= 0.273043 (Hartree/Particle)
Thermal correction to Energy= 0.290382
Thermal correction to Enthalpy= 0.291327
Thermal correction to Gibbs Free Energy= 0.227895
Sum of electronic and ZPE= -876.990497
Sum of electronic and thermal Energies= -876.973157
Sum of electronic and thermal Enthalpies= -876.972213
Sum of electronic and thermal Free Energies= -877.035645

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.218	65.773	133.502

C,0,-1.1549491543,-0.4765755152,2.0403701143
C,0,-1.0526303134,-0.7892901695,3.3909478799
C,0,0.192400772,-0.6787886023,4.0136853946
C,0,1.3300267575,-0.2016383486,3.3317146261
C,0,1.2221366874,0.0848049189,1.9856671932
C,0,-0.0139739615,-0.06898082,1.3028268946
C,0,-0.0918598709,-0.0674274847,-0.1203107342
N,0,-0.043111992,-2.0340776439,-0.5271643537
C,0,-0.8616416264,-2.7882192502,0.2967462981
C,0,-0.4808775577,-3.3520678074,1.5503850145
O,0,-1.5764244326,-3.9426326245,2.1474720479
C,0,-1.3596681912,-4.4559092724,3.4711245922
C,0,1.4194868576,-2.2976634584,-0.4719774122
C,0,-0.5218711513,-2.0102101492,-1.9357404878
O,0,0.6310193314,-3.3818599224,2.0943333009
N,0,0.3159406703,-1.0756097861,5.4021669706
O,0,-0.6555526496,-1.6167496808,5.9556035042
O,0,1.3936306398,-0.8767027734,5.9851388214
H,0,-2.1150719047,-0.5480213222,1.5431981392
H,0,-1.9111537465,-1.1365145848,3.9514977883
H,0,2.2718726121,-0.1035439867,3.8561795373
H,0,2.0963987241,0.4106480219,1.430436405
H,0,-1.0641086354,0.1066096062,-0.5717806656
H,0,0.7589754586,0.2978161739,-0.689003865
H,0,1.781868034,-2.0875000631,0.5310317363
H,0,1.9045630821,-1.6534352793,-1.2063983104
H,0,1.5936450858,-3.3501053615,-0.7124997099
H,0,0.0314072968,-1.2447427894,-2.4822666844
H,0,-0.3495733175,-2.9934059313,-2.3830378719
H,0,-1.5878317456,-1.7778708324,-1.9450075668
H,0,-1.9081317529,-2.7956940146,0.0253215931
H,0,-0.5614267168,-5.2045361372,3.4751805202
H,0,-1.0978091626,-3.6442342642,4.1591280171
H,0,-2.3074151268,-4.909885845,3.766620273

6‡ PBE0 IN DMSO

home/biswas/quiver/tdPBE1PBE
Nitro TS
PBE1PBE/6-31+G**
E(RPBE1PBE) = -876.214648000

Zero-point correction= 0.274932 (Hartree/Particle)
Thermal correction to Energy= 0.292553
Thermal correction to Enthalpy= 0.293497
Thermal correction to Gibbs Free Energy= 0.228901
Sum of electronic and ZPE= -875.939716
Sum of electronic and thermal Energies= -875.922095
Sum of electronic and thermal Enthalpies= -875.921151
Sum of electronic and thermal Free Energies= -875.985747

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.580	65.866	135.953

C,0,-1.0869492893,-0.4314798058,2.0386334655
C,0,-1.0167271336,-0.6794469928,3.4021838315
C,0,0.2044418534,-0.532901447,4.0541666759
C,0,1.3622739944,-0.1108934098,3.372941679
C,0,1.2887204267,0.1230386175,2.0211561139
C,0,0.0646274517,-0.029317693,1.3096360256

C,0,0.0025492801,0.0240596426,-0.0951842772
N,0,-0.0711896744,-2.0953583953,-0.5083704773
C,0,-0.8943682772,-2.7502349191,0.3496542653
C,0,-0.49913853,-3.4441946003,1.5432389834
O,0,-1.5963495792,-4.0085498583,2.1188381851
C,0,-1.3596414335,-4.7410055314,3.3174588867
C,0,1.3681714271,-2.3968740549,-0.4820789696
C,0,-0.5927898156,-2.0010241738,-1.8825887813
O,0,0.6249317652,-3.5880745683,2.0194893407
N,0,0.2795964814,-0.8019447455,5.4643081495
O,0,-0.7325178975,-1.1936143758,6.0473041566
O,0,1.3578473764,-0.6348469782,6.0359268307
H,0,-2.046824763,-0.4865812758,1.5361181349
H,0,-1.8927832988,-0.9851331802,3.9623543534
H,0,2.2906989864,0.0119316645,3.9178418766
H,0,2.1770919598,0.4375936368,1.4803319431
H,0,-0.9613596245,0.1808985884,-0.5689944463
H,0,0.8706956955,0.35531592,-0.6589958048
H,0,1.7660111575,-2.2118229182,0.5128548377
H,0,1.8645230387,-1.7663159697,-1.2192517812
H,0,1.519447938,-3.4508382517,-0.7354506982
H,0,-0.0210233572,-1.2554842405,-2.435712173
H,0,-0.4976739805,-2.9764208787,-2.3702895132
H,0,-1.6431925592,-1.7105780205,-1.856447961
H,0,-1.9492579565,-2.7275934856,0.1089110192
H,0,-0.6542109355,-5.5581041579,3.1447502208
H,0,-0.9679063924,-4.0881150221,4.1026053251
H,0,-2.3294353344,-5.1401041198,3.6142495828

6‡ M062XD3 23 IN DMSO

home/biswas/quiver/tdm062xd3
Nitro TS
m062x/6-31+G**
E(RM062X) = -876.824570553

Zero-point correction= 0.275768 (Hartree/Particle)
Thermal correction to Energy= 0.293008
Thermal correction to Enthalpy= 0.293952
Thermal correction to Gibbs Free Energy= 0.231054
Sum of electronic and ZPE= -876.548802
Sum of electronic and thermal Energies= -876.531562
Sum of electronic and thermal Enthalpies= -876.530618
Sum of electronic and thermal Free Energies= -876.593517

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.865	65.422	132.382

C,0,-1.1350913442,-0.4659555781,1.9542508634
C,0,-1.0594110013,-0.8255239441,3.2966923945
C,0,0.1700126911,-0.7597260033,3.9362435033
C,0,1.3280809572,-0.2692005583,3.2979777862
C,0,1.2465402018,0.0913609868,1.9779366977
C,0,0.0182959297,-0.0138493786,1.2550870531
C,0,-0.0284032739,0.0749668143,-0.1433111227
N,0,-0.0615237822,-2.080953086,-0.5021415026
C,0,-0.8766803074,-2.700982704,0.3776723526
C,0,-0.4700206198,-3.3000088105,1.6272300021
O,0,-1.5502557323,-3.8522645025,2.2393335966
C,0,-1.3063900827,-4.4184022141,3.5271823927
C,0,1.3904647537,-2.3350236119,-0.4441482071
C,0,-0.5740138441,-2.0321784687,-1.8858884437
O,0,0.6489777666,-3.3585881452,2.12297345
N,0,0.2625238589,-1.1940372095,5.3137878408
O,0,-0.7352393225,-1.6679338129,5.8502476836
O,0,1.3397764184,-1.083187598,5.889943848
H,0,-2.0977877936,-0.4673831913,1.4539526262
H,0,-1.9331994845,-1.1774374686,3.8332881493
H,0,2.2586910103,-0.2040533419,3.8480501483
H,0,2.1307468212,0.4535635214,1.4605931527
H,0,-0.9884098941,0.2022099075,-0.6339872468
H,0,0.8457368151,0.4107824052,-0.6952991667
H,0,1.7742081404,-2.0491650366,0.5327570406
H,0,1.8652997851,-1.7510073705,-1.2316233488
H,0,1.57189547,-3.4017136917,-0.6056622413
H,0,-0.0168751166,-1.2813600245,-2.4455192844
H,0,-0.4458798076,-3.015529118,-2.3475608227
H,0,-1.6313664333,-1.7689294442,-1.8681189431
H,0,-1.9277816353,-2.7387685011,0.1237735788
H,0,-0.5426992104,-5.196613075,3.469175298
H,0,-0.9852729142,-3.6439101445,4.2302336293
H,0,-2.2566600194,-4.8432126015,3.846466242

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