Stereoselectivities of Histidine-Catalyzed Asymmetric Aldol Additions and Contrasts with Proline Catalysis: A Quantum Mechanical Analysis

Yu-hong Lam, K. N. Houk, Ulf Scheffler and Rainer Mahrwald

Department of Chemistry, University of California, Los Angeles, California 90095-1569 and

Institute of Chemistry, Humboldt-University, Brook-Taylor Str. 2, 12489 Berlin, Germany

Experimental Procedures and Characterization of the Products

The aldehydes were freshly distilled before use. Ethyl glyoxylate **1c** (50% in toluene - FLUKA), 2.2-dimethoxy-acetaldehyde **1b** (60% aqueous solution - FLUKA) and chloroacetaldehyde **1a** (50% aqueous solution - FLUKA) were used as purchased. Aldehyde **1d**, protected lactaldehyde **1f** and glyceraldehyde **1g** were prepared by procedures from literature.

^{1}H-NMR spectra were recorded at 500 or 300 MHz and ^{13}C-NMR spectra were recorded at 75 or 125 MHz in $CDCl_3$ (unless stated otherwise), respectively, using an AC-300 or a BRUKER AV500 spectrometer. Chemical shifts are given in ppm, and coupling constants are given in Hz. High-resolution mass spectrometry was performed on an LTQ-FT-ICR machine (Finnigan). Optical rotation values were measured with a JASCO DIP-370 polarimeter. Angles of rotations refer to the enantiomeric excess. Purification of products was accomplished by flash chromatography (Merck silica gel 60, particle size 0.04 -0.063 mm). Thin layer chromatography was performed with Merck Silica Gel 60 F_{254} TLC plates.

A varying mixture of aldol adducts **2d** and **2e** and their corresponding acetales was observed.[1] In order to obtain defined reaction products, the reaction mixtures were treated with ethylene glycol to yield the corresponding 1,3-dioxolanes. No racemization was observed in this process – the enantioselectivities of the 1,3-dioxolane products were found to be the same as those found in the corresponding aldol adducts **2d** and **2e** isolated. The formation of acetals in these reactions is

consistent with reported observations in chiral imidazolidinones-catalyzed aldol additions[2] and tertiary amine-catalyzed aldol additions.[3]

General aldol-procedure **A**

Isolation of aldehydes **2d** abd **2e** as their corresponging 1,3-dioxolanes

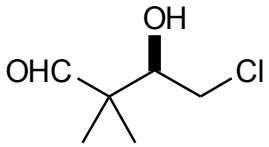
In a typical experiment, 78 mg L-histidine (0.5 mmol) was added to a mixture of isobutyraldehyde (10 mmol) and 5 mmol of aldehydes **1d** or **1e** and 200 mg water. The reaction mixture was stirred vigorously at room temperature and monitored by TLC. After completion of the reaction (5-7 days) the mixture was quenched with acetone, dried ($MgSO_4$) and filtered. The filtrate was removed in vacuo. The remaining residue was dissolved in 1.0 ml glycol and 5 ml THF. 0.5 mmol of toluenesulfonic acid was then added. The reaction was monitored by TLC (~ 12 h, room temperature). After completion of the reaction, the mixture was neutralized, filtered, absorbed to Celite® and purified by column chromatography (hexane / acetone 19/1 - 4/1).

General aldol-procedure **B**

78 mg L-histidine was added to a mixture of isobutyraldehyde (5.5 mmol), 5 mmol of aldehydes **1f**[4] or **1g**[5] and 200 mg water. The reaction mixture was stirred vigorously at room temperature and monitored by TLC. After completion of the reaction (12 h-2 days), the mixture was quenched with acetone, dried ($MgSO_4$) and filtered. The filtrate was absorbed to Celite®, evaporated in vacuo, and the remaining residue was purified by column chromatography.

(*R*)-4-Chloro-3-hydroxy -2,2-dimethylbutanal (**2a**)

78 mg L-histidine (0.5 mmol) was added to a mixture of isobutyraldehyde (5.5 mmol) and 5 mmol of chloroacetaldehyde **1a**. The reaction mixture was stirred vigorously at room temperature and monitored by TLC. After completion of the reaction (20 h), the mixture was quenched with acetone, dried ($MgSO_4$) and filtrated. The filtrate was absorbed to Celite®, evaporated in vacuo, and the remaining residue was purified by column chromatography.



^{1}H-NMR ($CDCl_3$, 300 MHz): δ = 1.15 (s, 3H), 1.16 (s, 3H), 3.49 (dd, 1H, *J* = 9.6, 11.4), 3.71 (dd, 1H, *J* = 2.4, 11.4), 3.97 (dd, 1H, *J* = 2.2, 9.6), 9.57 (s, 1H).

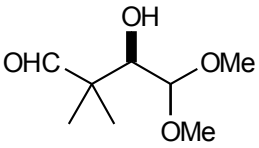
^{13}C-NMR (75 MHz): δ = 17.1, 19.1, 46.9, 49.6, 75.3, 204.7.

HRMS(ESI): calc. for $C_{12}H_{22}Cl_2O_4 + Na^+$: 323.0787 found: 323.0787

[α] = -12.2° (c = 1, $CHCl_3$)

(*R*)-3-hydroxy-4,4-dimethoxy-2,2-dimethylbutanal (**2b**)

78 mg L-histidine (0.5 mmol) was added to a mixture of isobutyraldehyde (5.5 mmol) and 5 mmol of dimethoxyacetaldehyde **1b** and 200 mg water. The reaction mixture was stirred vigorously at room temperature and monitored by TLC. After completion of the reaction (20 h), the mixture was quenched with acetone, dried ($MgSO_4$) and filtrated. The filtrate was absorbed to Celite®, evaporated in vacuo, and the remaining residue was purified by column chromatography.



^{1}H-NMR ($CDCl_3$, 300 MHz): δ = 1.05 (s, 3H), 1.08 (s, 3H), 3.33 (s, 3H) , 3.41 (s, 3H), 3.68 (1H, d, *J* = 6.2), 4.18 (1H, d, *J* = 6.2), 9.42 (s, 1H).

^{13}C-NMR (75 MHz): δ = 16.6, 19.5, 48.4, 54.9, 55.8, 74.2, 104.8, 203.1.

HRMS (ESI):

calc. for $C_{14}H_{28}O_8 + NH_4^+$: 342.2122 found: 342.2129 $2[M - CH_2] + NH_4^+$

calc. for $C_{14}H_{28}O_8 + Na^+$: 347.1676 found: 347.1683 $2[M - CH_2] + Na^+$

calc. for $C_{14}H_{28}O_8 + K^+$: 363.1416 found: 363.1423 $2[M - CH_2] + K^+$

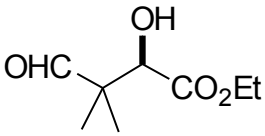
EIMS: calc. for $C_7H_{13}O_4^+$: 161.081 found: 161.088 $[M - CH_3]^+$

calc. for $C_7H_{13}O_3^+$: 145.086 found: 145.097 $[M - OCH_3]^+$

[α] = +5.3° (c = 1, $CHCl_3$)

2(*R*)-Hydroxy-3,3-dimethyl-4-oxo-butxyric acid ethyl ester (**2c**) [6]

155 mg L-histidine (1.0 mmol) was added to a mixture of ethyl glyoxylate **1c** (10 mmol, 50% in toluene), 11 mmol of isobutyraldehyde and 1.0 ml glycol. The reaction mixture was stirred vigorously at room temperature and monitored by TLC. After completion of the reaction (12 h), the mixture was quenched with acetone, dried ($MgSO_4$) and filtered. The filtrate was evaporated in vacuo with toluene (3 times), absorbed to Celite® and the remaining residue was purified by column chromatography.



^{1}H-NMR ($CDCl_3$, 300 MHz): δ = 1.06 (s, 3H), 1.14 (s, 3H), 1.27 (t, 3H, *J* = 7.2), 4.25 (m, 2H), 4.32 (s, 1H), 9.57 (s, 1H).

^{13}C-NMR (75 MHz): δ = 14.1, 16.9, 18.2, 50.4, 62.3, 73.5, 172.8, 202.5.

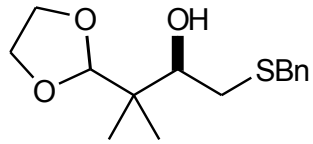
HRMS(ESI): calc. for $C_8H_{14}O_4 + H^+$: 175.0965 found: 175.0963

calc. for $C_{16}H_{28}O_8 + NH_4^+$: 366.2122 found: 366.2122

[α] = -15.4° (c = 1, $CHCl_3$)

(*R*)-1-Benzylthio-3-(1,3-dioxolan-2-yl)-3-methylbutan-2-ol

general procedure **A**



^{1}H-NMR ($CDCl_3$, 300 MHz): δ = 0.84 (s, 3H), 0.92 (s, 3H), 2.43 (dd, 1H, *J* = 8.8, 13.6), 2.60 (dd, 1H, *J* = 1.2, 13.7), 3.71 (dd, 1H, *J* = 1.3, 8.7), 3.72-3.79 (m, 2H), 3.81-3.98 (m, 4H), 4.69 (s, 1H), 7.23-7.36 (m, 5H).

^{13}C-NMR (75 MHz): δ = 16.9, 19.1, 33.8, 35.9, 41.0, 64.9, 65.1, 73.7, 108.6, 127.0, 128.4, 129.0, 138.2.

HRMS (ESI): calc. for $C_{15}H_{22}O_3S + NH_4^+$: 300.1628 found: 300.1626

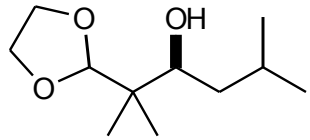
calc. for $C_{15}H_{22}O_3S + Na^+$: 305.1182 found: 305.1182

calc. for $C_{15}H_{22}O_3S + K^+$: 321.0921 found: 321.0921

[α] = -45.9° (c = 1, $CHCl_3$)

(*S*)-2-(1,3-dioxolan-2-yl)-2,5-dimethylhexan-3-ol

general procedure **A**



^{1}H-NMR ($CDCl_3$, 300 MHz): *δ* = 0.85 (s, 3H), 0.88 (d, 3H, *J* = 6.6), 0.91 (s, 3H), 0.92 (d, 3H, *J* = 6.5), 1.11 (ddd, 1H, *J* = 1.8, 10.3, 13.7), 1.35 (ddd, 1H, *J* = 3.6, 10.9, 13.6), 1.84 (ddsept, 1H, *J* = 3.5, 6.6, 10.2) , 3.63 (dd, 1H, *J* = 1.9, 10.8), 3.81-3.99 (m, 4H), 4.65 (s, 1H).

^{13}C-NMR (75 MHz): *δ* = 16.5, 20.2, 21.2, 24.2, 24.4, 40.1, 40.6, 64.8, 65.1, 73.3, 110.0.

HRMS (ESI): calc. for $C_{11}H_{22}O_3 + NH_4^+$: 220.1907 found: 220.1907

calc. for $C_{11}H_{22}O_3 + Na^+$: 225.1461 found: 225.1462

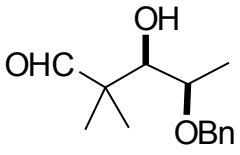
calc. for $C_{22}H_{44}O_6 + H^+$: 405.3211 found: 405.3212

calc. for $C_{22}H_{44}O_6 + Na^+$: 427.3030 found: 427.3030

[α] = -31.6° (c = 1, $CHCl_3$)

3,4(*R*,*R*)-4-Benzyloxy-3-hydroxy-2,2-dimethyl-pentanal **2f**

general aldol-procedure **B**



^{1}H-NMR ($CDCl_3$, 300 MHz): *δ* = 1.05 (s, 3H), 1.15 (s, 3H), 1.28 (d, 3H, *J* = 6.2 Hz), 3.39 (d, 1H, *J* = 2.0 Hz), 3.69 (dq, 1H, *J* = 2.0, 6.2 Hz), 4.33 (d, 1H, *J* = 11.1 Hz), 4.56 (d, 1H, *J* = 11.1 Hz), 7.27-7.37 (m, 5H), 9.62 (s, 1H).

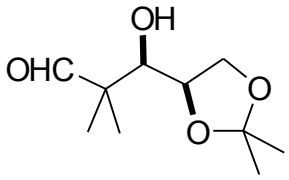
^{13}C-NMR (75 MHz): δ = 16.4, 18.9, 20.3, 49.2, 70.4, 72.5, 81.1, 127.9, 128.2, 128.4, 137.4, 205.3.

HRMS (ESI): calc. for $C_{14}H_{20}O_3 + NH_4^+$: 254.1751 found: 254.1752
calc. for $C_{14}H_{20}O_3 + Na^+$: 259.1305 found: 259.1306
calc. for $C_{14}H_{20}O_3 + K^+$: 275.1044 found: 275.1044

[α] = -34.0° (c = 1, $CHCl_3$)

3,4-(*R,R*)-3-[2,2-Dimethyl-(1,3)dioxolan-4-yl]-3-hydroxy-2,2-dimethyl-propionaldehyde **2g**

general aldol-procedure **B**



^{1}H-NMR ($CDCl_3$, 300 MHz): δ = 1.09 (s, 3H), 1.11(s, 3H), 1.32 (s, 3H), 1.38 (s, 3H), 2.62 (d, 1H, *J* = 7.6, OH), 3.54 (dd, 1H, *J* =2.6, 7.6), 3.81 (dd, 1H, *J* =7.0, 8.1) , 4.01 (dd, 1H, *J* =7.0, 8.1), 4.19 (ddd, 1H, *J* =2.6, 7.0, 7.0), 9.59 (s, 1H).

^{13}C-NMR (75 MHz): δ = 18.2, 19.5, 25.3, 26.1, 49.6, 66.8, 74.3, 74.8, 109.6, 205.6.

HRMS(ESI): calc. for $C_{10}H_{18}O_4 + NH_4^+$: 220.1543 found: 220.1543
calc. for $C_{10}H_{18}O_4 + Na^+$: 225.1097 found: 225.1097
calc. for $C_{20}H_{36}O_8 + Na^+$: 427.2302 found: 427.2304

[α] = +0.5° (c = 1, $CHCl_3$)

Proof of configuration

The absolute and relative configurations of the aldol adducts were determined by single-crystal X-ray analysis and NMR correlations.[1]

The **relative configuration** was determined by analysis of the vicinal ^{1}H-coupling constants and comparison with literature.

To determine the **absolute configuration,** the (*R*)- and (*S*)-Mosher esters were prepared and the anisotropic ^{1}H chemical shifts were used to establish the absolute configuration of the hydroxyl stereocenter.[7]

Determination of enantiomeric excess

The aldol adducts were converted into the corresponding (*S*)-MTPA-esters as follows:

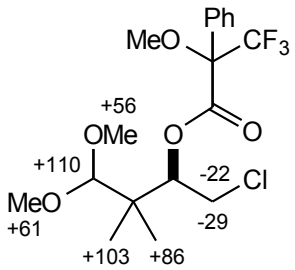
1.0 ml (0.01 mmol) of a CH_2Cl_2-solution of (*R*)-MTPA-Cl (0.01 mol / l) was added to a solution of the corresponding aldol adduct (0.01 mmol) and a catalytic amount of DMAP in 1.0 ml abs. CH_2Cl_2. After 10 h at r.t., the reaction mixture was diluted with diethyl ether and extracted with aq. NH_4Cl-solution. The organic layer was separated, dried (Na_2SO_4), and filtered. The filtrate was evaporated in vacuo. The remaining crude residue was used for ^{1}H-NMR experiments.

The enantiomeric excess of the products was determined by integration of corresponding signals in the ^{1}H NMR spectra.

Proof of absolute configuration

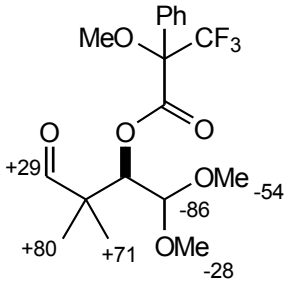
The calculated differences of chemical shifts in the ^{1}H NMR spectra of corresponding Mosher esters indicate the assigned configuration of aldol-products.

The indicated chemical shift differences ($\Delta\delta$(*S*-*R*), ppb) established the absolute stereochemistry at the C3 for aldol adducts (stereogenic center formed by aldol addition).



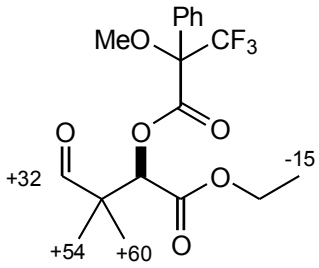
(*S*)-Mosher-ester of **2a** (dimethylacetal): **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 0.94 (s, 3H), 0.97 (s, 3H), 3.51 (m, 3H), 3.52 (s, 3H), 3.53 (s, 3H), 3.59 (dd, 1H, *J* = 9.8, 12.3), 3.88 (s, 1H), 3.93 (dd, 1H, *J* = 2.3, 12.3), 5.46 (dd, 1H, *J* = 2.3, 9.8), 7.38-7.71 (m, 5H).

(*R*)-Mosher-ester of **2a** (dimethylacetal): **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 0.87 (s, 3H), 0.87 (s, 3H), 3.40 (s, 3H), 3.41 (s, 3H), 3.62 (dd, 1H, *J* = 9.4, 12.3), 3.63 (m, 3H), 3.77 (s, 1H), 3.96 (dd, 1H, *J* = 2.1, 12.3), 5.44 (dd, 1H, *J* = 2.1, 9.4), 7.39-7.71 (m, 5H).



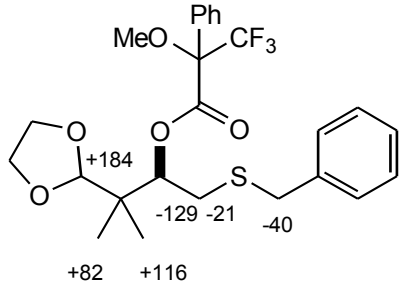
(*S*)-Mosher-ester of **2b**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 1.04 (s, 3H), 1.10 (s, 3H), 3.27 (s, 3H), 3.33 (s, 3H), 3.51 (m, 3H), 4.32 (d, 1H, *J* = 6.8), 5.42 (d, 1H, *J* = 6.8), 7.44-7.39 (m, 3H), 7.54-7.59 (m, 2H), 9.44 (s, 1H).

(*R*)-Mosher-ester of **2b**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 0.97 (s, 3H), 1.02 (s, 3H), 3.32 (s, 3H), 3.36 (s, 3H), 3.59 (m, 3H), 4.40 (d, 1H, *J* = 6.8), 5.46 (d, 1H, *J* = 6.8), 7.44-7.39 (m, 3H), 7.54-7.59 (m, 2H), 9.41 (s, 1H).



(*S*)-Mosher-ester of **2c**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 1.14 (s, 3H), 1.17 (s, 3H), 1.27 (t, 3H, *J* = 7.2), 3.51 (q, 3H, *J* = 1.0), 4.20-4.29 (m, 2H), 5.33 (s, 1H), 7.38-7.66 (m, 5H), 9.51 (s, 1H).

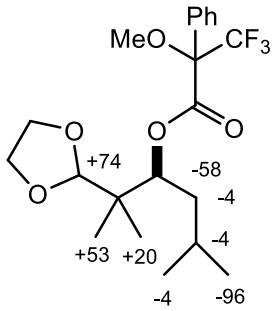
(*R*)-Mosher-ester of **2c**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 1.09 (s, 3H), 1.11 (s, 3H), 1.28 (t, 3H, *J* = 7.2), 3.62 (q, 3H, *J* = 1.2), 4.20-4.29 (m, 2H), 5.31 (s, 1H), 7.38-7.66 (m, 5H), 9.58 (s, 1H).



(*S*)-Mosher-ester of **2d**: **^{1}H-NMR** ($CDCl_3$, 500 MHz): δ= 0.90 (s, 3H), 0.93 (s, 3H), 2.48 (dd, 1H, *J* = 10.6, 14.6), 2.78 (dd, 1H, *J* = 2.4, 14.6), 3.53 (m, 3H), 3.73 (m, 2H),

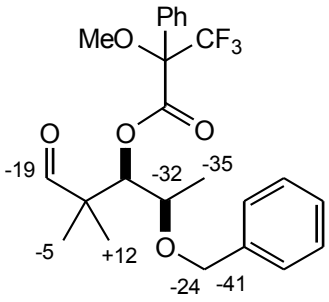
3.74-3.94 (m, 4H), 3.56 (m, 3H), 4.55 (s, 1H), 5.41 (dd, 1H, *J* = 2.4, 10.5), 7.23-7.71 (m, 10H).

(*R*)-Mosher-ester of **2d**: **^{1}H-NMR** ($CDCl_3$, 500 MHz): *δ*= 0.81 (s, 3H), 0.82 (s, 3H), 2.50 (dd, 1H, *J* = 10.6, 14.6), 2.81 (dd, 1H, *J* = 2.3, 14.6), 3.63 (m, 3H), 3.77 (m, 2H), 3.78-3.95 (m, 4H), 3.63 (m, 3H), 4.36 (s, 1H), 5.39 (dd, 1H, *J* = 2.3, 10.5), 7.23-7.71 (m, 10H).



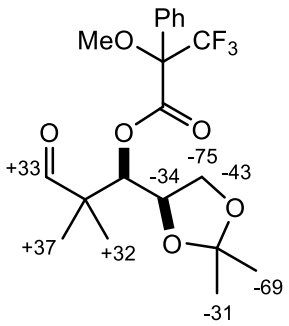
(*S*)-Mosher-ester of **2e**: **^{1}H-NMR** ($CDCl_3$, 500 MHz): *δ*= 0.81 (d, 3H, *J* = 6.3), 0.89 (s, 3H), 0.93 (s, 3H), 0.94 (d, 3H, *J* = 6.7), 1.13 (ddd, 1H, *J* = 1.8, 10.4, 13.6), 1.52 (m, 1H), 1.86 (m, 1H), 3.52 (m, 3H), 3.74-3.99 (m, 4H), 4.51 (s, 1H), 5.30 (dd, 1H, *J* = 1.6, 10.6), 7.31-7.71 (m, 5H).

(*R*)-Mosher-ester of **2e**: **^{1}H-NMR** ($CDCl_3$, 500 MHz): *δ*= 0.87 (s, 3H), 0.87 (s, 3H), 0.90 (d, 3H, *J* = 6.4), 0.94 (d, 3H, *J* = 6.3), 1.13 (ddd, 1H, *J* = 1.8, 10.1, 13.6), 1.58 (m, 1H), 1.86 (m, 1H), 3.57 (m, 3H), 3.74-4.01 (m, 4H), 4.44 (s, 1H), 5.31 (dd, 1H, *J* = 1.5, 10.3), 7.34-7.73 (m, 5H).



(*S*)-Mosher-ester of **2f**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): *δ* = 0.96 (s, 3H), 1.05 (s, 3H), 1.07 (d, 3H, *J* = 6.4), 3.49 (m, 3H), 3.80 (dq, 1H, *J* = 2.1, 6.4), 4.29 (d, 1H, *J* = 11.7), 4.46 (d, 1H, *J* = 11.7), 5.15 (d, 1H, 2.1), 7.20-7.68 (m, 10H), 9.57 (s, 1H).

(*R*)-Mosher-ester of **2f**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): *δ* = 0.94 (s, 3H), 1.06 (s, 3H), 1.11 (d, 3H, *J* = 6.4), 3.60 (m, 3H), 3.82 (dq, 1H, *J* = 2.0, 6.4), 4.32 (d, 1H, *J* = 11.5), 4.49 (d, 1H, 11.5), 5.15 (d, 1H, 2.0), 7.23–7.68 (m, 10H), 9.59 (s, 1H).



(*S*)-Mosher-ester of **2g**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 1.06 (s, 3H), 1.19 (s, 3H), 1.26 (s, 3H), 1.27 (s, 3H), 3.50 (m, 3H), 3.54 (dd, 1H, *J* = 6.8, 8.5), 3.94 (dd, 1H, *J* = 6.8, 8.5), 4.34 (ddd, 1H, *J* = 3.6, 6.8, 6.8), 5.27 (d, 1H, *J* = 3.4), 7.37-7.45 (m, 3H), 7.53-7.60 (m, 2H), 9.57 (s, 1H).

(*R*)-Mosher-ester of **2g**: **^{1}H-NMR** ($CDCl_3$, 300 MHz): δ = 1.02 (s, 3H), 1.15 (s, 3H), 1.30 (s, 3H), 1.34 (s, 3H), 3.58 (m, 3H), 3.61 (dd, 1H, *J* = 6.6, 8.7), 3.99 (dd, 1H, *J* = 6.6, 8.7), 4.37 (ddd, 1H, *J* = 4.0, 6.6, 6.6), 5.32 (d, 1H, *J* = 4.0), 7.36-7.47 (m, 3H), 7.61-7.68 (m, 2H), 9.54 (s, 1H).

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Computational Section

Full citation for ref. 54 in main text
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

TS-4a
 SCF Energy=   -819.047712337
 Zero-point correction (ZPE)= -818.76625
 Internal Energy (U)= -818.74905
 Enthalpy (H)= -818.74811
 Gibbs Free Energy (G)= -818.81130
H,0.5831741328,-0.081529716,1.3110493499
C,2.1380974516,-1.6872162092,1.2596995791
O,0.9056924217,-1.5912279701,1.1646216853
C,3.1030540201,-1.2208550657,-0.9853961957
C,2.4363310215,-0.0463973199,-0.8441347374
N,1.1026519704,0.126196588,-1.1082974542
C,0.4149858366,1.3622587605,-0.8174408761
C,-1.0489367004,1.2742380975,-1.3012357115
C,0.3959254525,1.7913071208,0.6551206725
O,0.5090499023,0.8884279,1.6091590556
O,0.2362241054,2.9699428152,0.9433938092
H,0.9034719885,2.1872793051,-1.3456074889
H,-1.5366918504,2.2289550102,-1.0891155947
H,-1.0347631198,1.1343530696,-2.3859776751
H,0.5219817272,-0.7038834595,-1.1904709755
C,-1.7939059983,0.1582791649,-0.6399697543
C,-2.5956228916,0.2196506273,0.4714941986
N,-1.6614654289,-1.1566755862,-1.0495392695
H,-2.9288682686,1.0501352349,1.075623335
C,-2.3674285081,-1.8659268687,-0.1894690187
H,-2.4926070594,-2.9390793416,-0.2019431871
N,-2.9499440326,-1.0785792858,0.7427135003
H,2.954842737,0.8419342507,-0.4841355829
H,2.6395900128,-2.6364333998,1.0373476673
H,2.7321118889,-0.8972965557,1.7375726952
H,-3.5507672468,-1.3938944839,1.4940137636
C,2.4486866248,-2.4254992311,-1.6129846055
H,1.4227679058,-2.5849954511,-1.2582646258
H,2.4026244849,-2.3215294291,-2.7047552072
H,3.0188288706,-3.3325104056,-1.3904938663
C,4.5768262893,-1.2972335141,-0.6989922765
H,4.791503766,-2.0689047039,0.0524415869
H,5.1380521062,-1.5693140671,-1.6014332058
H,4.963532078,-0.3430636706,-0.32934077

TS-4b
 SCF Energy=   -819.035508621
 Zero-point correction (ZPE)= -818.75478
 Internal Energy (U)= -818.73769
 Enthalpy (H)= -818.73675
 Gibbs Free Energy (G)= -818.80076
C,-2.8266452244,-1.9298065033,0.7848869052
C,-2.0724783277,-0.8253365015,1.0941384746
N,-0.8607082589,-0.5092717032,0.6037344751
C,-0.19627952,0.7566852611,0.8384354623
C,-0.1433885187,1.6465966612,-0.4185233089
O,0.8172371007,2.3789237193,-0.6249065117
O,-1.163407765,1.6417654927,-1.2442263856
H,-0.3060334976,-1.2104788429,0.1187675224
H,-2.057286722,1.1326081173,-0.9857317523
C,-3.4465371543,-0.6301196044,-0.9275315557
O,-3.3711269857,0.6307950824,-0.8262521604
H,-4.4302241863,-1.1063250124,-0.8466652259
H,-2.5234003594,-0.0518722476,1.7147850714
H,-2.6740279308,-1.160336288,-1.4993183664
C,1.2047088368,0.5482726231,1.4306116055
H,1.0793350111,-0.0124702107,2.3626210969
H,1.6290712746,1.5212184852,1.6873709873
C,2.1474694112,-0.1670077856,0.5118512452
C,3.3733671981,0.2581498631,0.0702654798
N,1.8649897104,-1.4102454275,-0.0278179457
H,3.9317460359,1.1628217508,0.2569092932
C,2.9074566652,-1.7167000852,-0.7775266637
H,3.0312865566,-2.6220109903,-1.354461801
N,3.8433654026,-0.7427346958,-0.7452493124
H,4.728005198,-0.7526598536,-1.2374962346

H,-0.8010400286,1.3197917894,1.5599960745
C,-2.2967912065,-3.0919305033,-0.0074404712
H,-1.3881599367,-2.8555241025,-0.5689437226
H,-2.074936654,-3.9377689258,0.6539517576
H,-3.0543475997,-3.4330725711,-0.7254807379
C,-4.1030718584,-2.1786807938,1.5441600146
H,-4.8847579986,-2.5525366979,0.8716231931
H,-3.9563384291,-2.9404871526,2.3195835045
H,-4.4706238188,-1.2674345061,2.0256681129

TS-4c
 SCF Energy=   -819.034121014
 Zero-point correction (ZPE)= -818.75316
 Internal Energy (U)= -818.73621
 Enthalpy (H)= -818.73527
 Gibbs Free Energy (G)= -818.79814
H,2.456074209,1.0850159721,0.0853370316
C,1.6106963146,-2.4369677146,0.3779080564
C,0.8250294229,-1.316588065,0.2605732966
N,0.5910359843,-0.5944967363,-0.8503629958
C,0.04789388,0.7564232998,-0.8940606974
C,-0.5685299287,1.2309508706,0.4242774703
C,1.107185733,1.7857094531,-1.3142210286
O,2.2631019667,1.7934674822,-0.7008916031
O,0.8466666467,2.6072513493,-2.1878410931
H,-0.7155513597,0.7885252956,-1.6770344831
H,0.186911412,1.2286969058,1.2192604868
H,0.9071916923,-0.9573557256,-1.7430940869
H,0.4098209692,-0.9053236122,1.1765223018
C,3.1917108074,-0.9004962303,0.6754226233
O,2.8964072978,0.2600600405,1.1018457351
H,3.6494864772,-1.6109904331,1.3718113706
H,3.4144070207,-1.0244819253,-0.3921139368
C,-1.7654142945,0.4380473767,0.8506859375
C,-2.5236399898,-0.4468281653,0.1269688137
N,-2.2707427082,0.5541696943,2.1295427259
H,-2.4550858737,-0.80768588,-0.8879026927
C,-3.3198354628,-0.2451918789,2.1672349253
H,-4.2470636231,-1.5327770039,0.774274807
H,-3.9658279423,-0.4049871177,3.0180670516
N,-3.512076752,-0.8687887157,0.9843201374
H,-0.8564027366,2.278647268,0.2767200127
C,1.588682965,-3.1982218521,1.6775989786
H,2.5915491486,-3.5656128264,1.925332507
H,1.2361619454,-2.5725564624,2.5033601335
H,0.9334020139,-4.0747750004,1.6067522978
C,2.2122499617,-3.1599849395,-0.7934909441
H,1.6307507256,-4.0590151166,-1.0290198804
H,2.2716053512,-2.5489539516,-1.6983172462
H,3.2297615265,-3.4876697952,-0.5446143121

TS-4d
 SCF Energy=   -819.042615508
 Zero-point correction (ZPE)= -818.76195
 Internal Energy (U)= -818.74439
 Enthalpy (H)= -818.74345
 Gibbs Free Energy (G)= -818.80850
C,1.7236050558,-2.1674216738,1.0241257174
C,1.2203838478,-0.9070148298,0.9105596168
N,0.6693676734,-0.3979419716,-0.2274911819
C,0.1138295066,0.9354356464,-0.2910018759
C,1.1882831689,2.0266632227,-0.2072420676
O,0.8999193882,3.1744479514,0.0967574063
O,2.4335721712,1.7222589245,-0.5242955972
H,0.3900049668,-1.0401595959,-0.956506773
H,2.6306238146,0.753550722,-0.7608234602
C,3.655524654,-1.1207383813,0.0908889109
O,3.3551078785,-0.6245949429,-1.0114729713
H,3.8279739094,-0.4835800289,0.9682959787
H,1.3258439908,-0.2012306618,1.7341253748
H,4.0058242386,-2.1583084044,0.1521294029
C,-1.0094105851,1.1963377309,0.7325724471
H,-0.595714567,1.1624482299,1.7456264951
H,-1.3920013859,2.2056579199,0.5671405292
C,-2.1160259989,0.1965849554,0.6128664748
C,-3.1233007335,0.161391458,-0.3197829795
N,-2.2317606726,-0.8852414898,1.4641853609
H,-3.3741032283,0.8208337768,-1.1368498425
C,-3.2900951666,-1.5535541833,1.0460760773
H,-3.6853265285,-2.4585949193,1.4839647396
N,-3.8594453222,-0.9609402826,-0.0280160889
H,-4.6882187667,-1.2815937673,-0.5131624942
H,-0.3092811316,1.0482224695,-1.2961963793
C,2.2782408385,-2.6496149438,2.334925327
H,3.2848016574,-3.0673586764,2.2020955597
H,2.3342991614,-1.841719861,3.0701699439
H,1.6551754374,-3.4504763746,2.75132437
C,1.5250137408,-3.1796631989,-0.0733435185
H,0.4948401886,-3.5589786598,-0.0820943504
H,1.7295598307,-2.7565822851,-1.0647967034
H,2.1916019674,-4.035434875,0.0689675514

TS-4e
 SCF Energy=   -819.048552975

Zero-point correction (ZPE)= -818.76649
Internal Energy (U)= -818.74935
Enthalpy (H)= -818.74840
Gibbs Free Energy (G)= -818.81128
C,-2.0933976589,2.0961386098,-0.4238064398
O,-1.2193505225,2.3074408593,0.4329764754
C,-2.9888079816,-0.1020776733,-0.0319151665
C,-1.823440141,-0.5163343833,-0.6048119737
N,-0.6386502809,-0.7180861395,0.0336907924
C,0.5091580449,-1.2454077009,-0.6800328452
C,1.2021685445,-0.1719560973,-1.5498485374
C,1.533487632,-1.8470235741,0.3001711709
O,1.338246447,-1.6900601978,1.5339659306
O,2.5146060197,-2.4354128115,-0.2278838295
H,0.189330539,-2.0496480267,-1.3542135717
H,1.8995654589,-0.6645542065,-2.2308118157
H,-0.6096779606,-0.8149438579,1.0417157192
H,-1.7876839836,-0.6718736275,-1.6829054123
H,-3.1439844847,2.3214252114,-0.204735194
H,-1.8263505845,1.9330832486,-1.4761095246
C,1.9643039668,0.8205102294,-0.7403965303
C,2.2941361235,2.502496284,0.6597190072
H,0.3268122675,1.9926793519,0.0949268866
H,2.1219800504,3.3383223833,1.3203976982
N,1.3640516061,1.816949137,0.0060123593
H,0.4417630198,0.3348308493,-2.1539739546
N,3.4801641977,1.9785548434,0.3592224774
C,3.3062375901,0.9247231811,-0.5114105685
H,4.1356339769,0.3505563407,-0.8925066192
H,4.3656108264,2.316571269,0.7222142227
C,-4.2496984492,-0.0477575938,-0.8510511194
H,-4.9482433384,-0.8383367578,-0.5490771382
H,-4.774510058,0.9059623933,-0.7095502798
H,-4.0417661936,-0.1712233887,-1.9182644406
C,-3.1225510082,0.0539039956,1.4575281551
H,-2.1931234668,0.4017959075,1.9221933547
H,-3.908016283,0.7792121135,1.697289866
H,-3.3982223957,-0.8961685711,1.9331409254

TS-4f
SCF Energy= -819.042637745
Zero-point correction (ZPE)= -818.76019
Internal Energy (U)= -818.74337
Enthalpy (H)= -818.74243
Gibbs Free Energy (G)= -818.80449
C,-4.391393791,0.3858561983,1.8532475586
O,-3.6564034324,-0.1969436626,2.6930092386
C,-4.1308733269,2.5778759884,1.4885705115
C,-2.7753316539,2.3661979517,1.4270507371
N,-2.0515387987,2.0236779314,0.3456120649
C,-0.6098048933,1.840684348,0.3907043953
C,-0.1859452336,0.6432715702,1.2644298232
C,-0.0591357521,1.6760503053,-1.0415427261
O,1.1874200108,1.5242872457,-1.1328613991
O,-0.8765175469,1.7013899998,-1.9984252707
H,-0.1344876648,2.7346119282,0.8140469603
H,0.9037611569,0.6409355142,1.3332300908
H,-2.4495450703,2.0791556853,-0.5859157644
H,-2.2079297631,2.4044203847,2.3567953656
H,-4.212409679,0.2284905798,0.7776294145
H,-5.4057289069,0.6855816532,2.1457871573
C,-0.648401855,-0.6661313753,0.7189944098
C,-2.0060676257,-2.3907213727,0.4434785351
H,-2.5155597182,-0.8583249945,1.8296849053
H,-2.8400360378,-3.0688462655,0.5414256693
N,-1.8287104428,-1.2619577496,1.1180711049
H,-0.5806835532,0.7739089919,2.2768410669
N,-0.9708893993,-2.5450394776,-0.3800177918
C,-0.1047366858,-1.4841809383,-0.2306149172
H,0.8100038486,-1.4065737747,-0.7965111758
H,-0.8481564494,-3.3316065943,-1.0092970492
C,-4.9848907835,2.6522531474,0.2530325628
H,-5.1006305946,3.6900393105,-0.0827816725
H,-5.9900183527,2.2663627608,0.4652248367
H,-4.5780884336,2.073482951,-0.5822261242
C,-4.7197351686,3.1602680354,2.7476831064
H,-4.0752832137,2.9776728565,3.6133888437
H,-5.7053775012,2.7258971234,2.9551922516
H,-4.8619261083,4.2441982939,2.654097711

TS-4g
SCF Energy= -819.044220046
Zero-point correction (ZPE)= -818.76247
Internal Energy (U)= -818.74505
Enthalpy (H)= -818.74411
Gibbs Free Energy (G)= -818.80818
C,1.0147864891,-2.6172444133,0.7091193438
O,0.1732242573,-2.7315800876,-0.1997503137
C,2.5733694173,-0.9164022643,0.1334340408
C,1.5132588804,-0.0850122052,0.3377906857
N,0.5709700254,0.2389730435,-0.5966965169
C,-0.3869426003,1.3053804269,-0.3485712629
C,-1.376853668,0.93700216,0.7751760285
C,0.2428819393,2.6969339104,-0.0583928906

O,1.4904972251,2.7981181747,0.0462343592
O,-0.585634034,3.6455712654,0.0356356754
H,-0.9598204121,1.4321653333,-1.2722735007
H,-1.9114933082,1.8384858221,1.0794955963
H,0.8393484334,0.1208560144,-1.5659336637
H,1.343942253,0.3220555623,1.3322637026
H,1.9510800122,-3.1869919618,0.6645249381
H,0.7423182768,-2.1824446119,1.6803567067
C,-2.4008424732,-0.0640651568,0.3615764267
C,-3.2408224822,-1.9996309735,-0.3097207508
H,-1.166604382,-1.8313158265,-0.0328520951
H,-3.3252393351,-3.0281572001,-0.6253335526
N,-2.1156772783,-1.3710822875,0.0111348014
H,-0.8280045424,0.5708286169,1.6501612487
N,-4.246815478,-1.1384923598,-0.1786290621
C,-3.7528598648,0.0777237901,0.2396571235
H,-4.3922102174,0.9276495406,0.4172092877
H,-5.221407314,-1.3553472843,-0.3606824587
C,2.9025872589,-1.4375707718,-1.2397188739
H,3.3758711696,-0.6652812672,-1.859808329
H,3.5993103063,-2.2790456807,-1.1724208771
H,2.0073395915,-1.7845737329,-1.7706070471
C,3.5917796958,-1.112847257,1.2231902493
H,3.2487736459,-0.6917674973,2.1730762572
H,3.8108255906,-2.1775365195,1.3768602402
H,4.5415906822,-0.6300107419,0.961870963

TS-4h
 SCF Energy=   -819.038731864
 Zero-point correction (ZPE)= -818.75630
 Internal Energy (U)= -818.73925
 Enthalpy (H)= -818.73831
 Gibbs Free Energy (G)= -818.80151
C,-2.1329578373,1.6084065808,-0.4086485691
O,-1.6589312712,2.2049590435,0.5946866936
C,-2.8399086207,-0.4859893474,-0.1497108407
C,-1.6293193479,-0.7640967374,0.433163835
N,-0.4931214834,-1.149172231,-0.1899391566
C,0.6881695027,-1.5455621409,0.5600217146
C,1.2623500381,-0.3969907118,1.4159057364
C,0.4682478157,-2.7961967752,1.4544432835
O,-0.689169623,-3.2736133527,1.557639951
O,1.5065510572,-3.242531702,2.0167450686
H,1.4468946788,-1.8221866969,-0.1774005651
H,2.1116043702,-0.7926421224,1.9754596492
H,-0.5756420041,-1.542564023,-1.1197926284
H,-1.5215284703,-0.5738482312,1.499645093
H,-1.4565499191,1.2636424532,-1.2067626477
H,-3.1750001324,1.7963028493,-0.6990639688
C,1.7348462152,0.7625714142,0.6051850977
C,1.6269600165,2.6825964702,-0.4891627684
H,-0.0992552851,1.9687451536,0.499412584
H,1.2615583622,3.6079563334,-0.9075833088
N,0.9309952306,1.8307580227,0.2537532514
H,0.5197618662,-0.0578084258,2.1455641938
N,2.8615843955,2.2015917365,-0.6223670269
C,2.9594744239,1.0048960662,0.0519596384
H,3.8746011586,0.4353934955,0.0858423772
H,3.6054043716,2.6602876721,-1.1383902951
C,-3.1134216489,-0.7878569447,-1.5975821116
H,-3.4992302746,-1.8067324218,-1.7248197022
H,-3.8726096938,-0.1004032568,-1.9888639514
H,-2.220993179,-0.6874158543,-2.2248272073
C,-4.0383293555,-0.2646515605,0.7372427255
H,-3.739138179,0.0478757898,1.7426802152
H,-4.6983287773,0.5051520769,0.3193728843
H,-4.6335221103,-1.1814275618,0.8310306157

TS-5a
 SCF Energy=   -1317.92345660
 Zero-point correction (ZPE)= -1317.62139
 Internal Energy (U)= -1317.60191
 Enthalpy (H)= -1317.60097
 Gibbs Free Energy (G)= -1317.67034
C,-1.0530887984,-1.6423935222,-0.5673784983
C,-2.1909824786,-1.8707770254,0.160983444
C,-3.497005582,-2.1119124375,-0.5466357606
O,3.7040551831,-1.8087520503,-0.8116662835
C,-2.2738132323,0.4217953761,0.6253051751
O,-1.3020584425,0.6889337107,1.3563301838
H,-1.1291466828,-1.4801534365,-1.6429464184
H,1.2822003144,-2.1065797842,-1.7609013199
H,2.268110347,-0.0230261756,-2.308821182
H,-4.2952485739,-1.4796516148,-0.1337153722
H,-3.422088007,-1.9136473685,-1.6198811768
H,-3.819864403,-3.1521570873,-0.4161779812
N,0.1971638808,-1.5364750589,-0.066053837
C,1.5125264546,0.0087439871,-1.5204652766
C,1.364407346,-1.4063378648,-0.9216337725
C,2.640373223,-1.7722692508,-0.1382614469
O,2.5351573192,-1.980754404,1.0985346643
H,0.3925195994,-1.7978162826,0.8942866623
H,0.562648488,0.2981195918,-1.9817136461
C,1.940319382,1.0248997445,-0.5175700871

C,3.1402976724,1.6593152902,-0.3735479362
N,1.1438679102,1.4631428417,0.524996886
H,4.0404910957,1.6091456553,-0.9651345778
C,1.8235436397,2.3251867967,1.2717539153
H,0.1653138727,1.1512044783,0.7388993128
H,3.7611449536,3.0669213475,1.1128622817
H,1.4584291279,2.8308415788,2.1526503371
N,3.0370489483,2.4597908567,0.742956395
C,-2.1211575511,-2.2726314728,1.6102517257
H,-1.3513700774,-1.7232436549,2.1621179044
H,-3.0822494408,-2.0898037078,2.1030425455
H,-1.9027071485,-3.3440391887,1.7059451136
C,-2.361339722,0.9853596123,-0.7727016588
H,-1.3735054429,1.0922827108,-1.2205060607
H,-3.0370049391,0.4231867339,-1.4147663569
H,-3.223512227,0.0975510917,1.0741436899
Cl,-3.0553870088,2.6593809833,-0.633542587

TS-5b
 SCF Energy=   -1317.91954313
 Zero-point correction (ZPE)= -1317.61742
 Internal Energy (U)= -1317.59814
 Enthalpy (H)= -1317.59719
 Gibbs Free Energy (G)= -1317.66631
C,-0.6742349203,-1.8136382179,-0.4802295425
C,-1.8571835233,-1.9040537203,0.2211512081
C,-3.0144397632,-2.627927668,-0.4213752301
O,4.0630464132,-1.6190027772,-0.5106250811
C,-1.96169236,0.3856617426,-0.2434031921
O,-1.3033792343,0.9077043841,0.6895369849
H,-0.6724761368,-1.9986715281,-1.5544427934
H,1.7225721468,-2.159994624,-1.5164683574
H,2.5755295385,-0.0825692613,-2.2909238425
H,-3.9743523519,-2.2786935734,-0.0286618869
H,-3.0163182586,-2.5081188589,-1.5095399768
H,-2.9575169746,-3.702115182,-0.201896641
N,0.5177076536,-1.480685286,0.0370134353
C,1.7844572179,-0.0153846693,-1.5404775265
C,1.7159428494,-1.3562890085,-0.7733171511
C,2.971649268,-1.499896301,0.1062121995
O,2.8226191115,-1.4458297197,1.3547864183
H,0.6411841281,-1.3648480737,1.0376676484
H,0.8333790065,0.1377427308,-2.0619712396
C,2.0829592184,1.1404880728,-0.6487851801
C,3.2427018671,1.8384279453,-0.4689111005
N,1.1680318009,1.6617008629,0.2459654253
H,4.2013455438,1.7547673805,-0.9557904417
C,1.7393705437,2.6382398006,0.9398339452
H,0.1637043687,1.325309204,0.3902836698
H,3.6602443713,3.4402032431,0.8855580202
H,1.2689656366,3.2310735074,1.709253958
N,2.9976951337,2.763230926,0.5221793166
C,-1.8430248369,-1.8342463999,1.7222953637
H,-1.2327371931,-1.0017375584,2.0893853699
H,-2.8573930375,-1.7095697603,2.1142040646
H,-1.43449946,-2.7596444028,2.1499259708
C,-3.4660965966,0.3638340275,-0.1769766248
H,-3.8316261712,0.1097612014,0.8185215611
H,-3.906659381,-0.2671396426,-0.944185127
Cl,-4.0454797988,2.0527627449,-0.5300570698
H,-1.5403418199,0.3502904591,-1.2571845549

TS-5c
 SCF Energy=   -1317.92128210
 Zero-point correction (ZPE)= -1317.61962
 Internal Energy (U)= -1317.60008
 Enthalpy (H)= -1317.59914
 Gibbs Free Energy (G)= -1317.66904
H,0.0194111822,-0.9708309753,-0.5418570132
C,2.0804974386,0.2057326319,-0.9943277048
O,0.9352908382,0.0038313401,-1.4271176104
C,1.8399588915,1.9676214318,0.6892598421
C,1.0355524804,1.061286724,1.3139067892
N,-0.2657628825,0.827336788,0.9937037428
C,-1.0735062561,-0.1739185325,1.6468926884
C,-2.5643108646,0.2227029331,1.5888486608
C,-0.9602646777,-1.5900652676,1.0690063625
O,-0.4153297006,-1.7765955693,-0.1172966052
O,-1.4232626746,-2.5377904608,1.6877054169
H,-0.7702683951,-0.2541654412,2.6957212848
H,-3.1371303997,-0.5002168081,2.1739782935
H,-2.6682577379,1.2034947843,2.0621982532
H,-0.7115153488,1.3675666539,0.257982809
C,-3.0783433306,0.2514374708,0.1840084803
C,-3.8549701478,-0.6863145482,-0.4475337464
N,-2.7298501136,1.2492065477,-0.7090256523
H,-4.3142761236,-1.5974735476,-0.0952110517
C,-3.2941372084,0.9104760255,-1.852991146
H,-3.2383993166,1.4661761464,-2.7778406742
N,-3.9823837571,-0.2479364692,-1.7423605705
H,1.4299563182,0.4337657475,2.1123158882
H,2.7034176763,0.9951150802,-1.4375319023
H,-4.5056599942,-0.7006336901,-2.4817960871
C,1.2861938047,2.9495093227,-0.3096569376

H,0.5449931075,2.4993722287,-0.9799403471
H,0.8013827996,3.7913554687,0.2014267767
H,2.0901262387,3.358956715,-0.9295751061
C,3.2399325607,2.2119839544,1.1795848797
H,3.9646449765,2.1105941449,0.3601725103
H,3.3410561871,3.2337832052,1.5660264592
H,3.5216544284,1.5171151999,1.9763424297
C,2.8011401048,-0.8187631855,-0.1529060904
H,3.5949289528,-0.3758189552,0.4453051366
H,2.1160633741,-1.4066701414,0.4567781797
Cl,3.6025125691,-1.9686059525,-1.3089096384

TS-5d
 SCF Energy=   -1317.91804624
 Zero-point correction (ZPE)= -1317.61680
 Internal Energy (U)= -1317.59744
 Enthalpy (H)= -1317.59649
 Gibbs Free Energy (G)= -1317.66596
H,-0.2402297049,-0.5089243962,1.0356061324
C,1.8034025066,-0.5017285668,0.2035591416
O,0.6524336972,-0.9557809887,-0.013705106
C,1.843881499,1.6693423677,-0.7716168288
C,0.765380825,1.8938619575,0.0476366064
N,-0.5026671569,1.5426983057,-0.2424957839
C,-1.5977286445,1.6727742393,0.6973941296
C,-2.9299896824,1.347508586,-0.0098725262
C,-1.4979040181,0.7848031884,1.9426372856
O,-0.7474357112,-0.2901233699,1.9220462388
O,-2.1572278354,1.073535752,2.9345144411
H,-1.6380044265,2.700518373,1.0714470355
H,-3.7406541661,1.498597757,0.7066112488
H,-3.0623775842,2.0617860528,-0.8277662184
H,-0.68809613,1.0174094693,-1.0935769143
C,-2.9536867456,-0.0547765396,-0.5287290272
C,-3.475961932,-1.1704731641,0.074432255
N,-2.3139181404,-0.4121982943,-1.7018047683
H,-4.031093832,-1.3022432244,0.9910552224
C,-2.4500301727,-1.7214526194,-1.7921529048
H,-2.0762161837,-2.3468939958,-2.5899476254
N,-3.145592169,-2.2207355503,-0.74540214
H,0.9072702441,2.3488285453,1.0280377884
H,-3.3888179272,-3.1936413644,-0.6051096063
C,1.6310033797,1.2625280376,-2.2080343112
H,0.9478571471,0.4100479077,-2.3092356059
H,1.2047312919,2.0937757277,-2.785070278
H,2.580082366,0.9880009981,-2.6774860815
C,3.1548684897,2.3221347674,-0.4156043652
H,4.0134592995,1.7051702987,-0.6982600657
H,3.2654241627,3.2722482308,-0.9542742323
H,3.2187116602,2.5326973325,0.6560603673
C,2.9437678712,-0.9827286527,-0.6530746052
H,2.6165508997,-1.1945413567,-1.6699007418
H,3.8078296062,-0.3239809224,-0.6330040967
Cl,3.4949794677,-2.5592357139,0.0589267513
H,2.0683477494,-0.1114381749,1.194007189

Table 2 Entry 2 Type a TS
 SCF Energy=   -1087.32302281
 Zero-point correction (ZPE)= -1086.94458
 Internal Energy (U)= -1086.92151
 Enthalpy (H)= -1086.92057
 Gibbs Free Energy (G)= -1086.99661
C,0.7033650202,-0.8975679015,-2.018386112
C,0.0017062407,0.4697494636,-2.1485922196
C,2.1750435412,-0.7709003252,-2.460086866
C,0.7380627481,1.5723202186,-1.4665433372
H,-0.0688143642,0.7227490671,-3.208625829
H,-1.0140037613,0.3803417494,-1.7539101046
N,0.63605946,-1.4460036686,-0.6727105887
H,0.2083635706,-1.5837338954,-2.7151436444
O,2.3594182839,-0.4083414979,-3.6516964948
O,3.0703982911,-1.0096162694,-1.6078861595
N,0.9137269564,1.6618534729,-0.0982888978
C,1.4172938173,2.6260682257,-2.0078545865
C,-0.4886427195,-1.9685026349,-0.1511672922
H,1.5359089578,-1.6301468108,-0.2413188985
C,1.6589881239,2.7221625543,0.18587234
H,0.5350388514,1.0020223887,0.6238485522
N,1.9748551132,3.3237647178,-0.9595542327
H,1.5471085511,2.9271627804,-3.0352189078
C,-0.5694262834,-2.619916494,1.0569496958
H,-1.393247011,-1.7987675116,-0.7361292381
H,1.9568699529,3.0437490437,1.172048119
H,2.5367485384,4.1653123301,-1.0333236861
C,-1.8434576088,-3.3291424076,1.434371295
C,0.681621223,-3.0675534812,1.7702790333
H,-1.7013640421,-4.41621393,1.3972409552
H,-2.147637531,-3.0835875643,2.4614523512
H,-2.667891833,-3.0753276143,0.7618542304
H,0.4498931221,-3.3475996766,2.8032902957
H,1.1138997875,-3.9478509948,1.2777121113
H,1.4507878929,-2.2889257719,1.8012229914
O,-1.7939699364,0.729186704,0.5255335517
C,-2.0654394049,-0.0873396694,1.6194466096

C,-2.9640875136,1.2107977678,-0.1266484848
C,-0.7344673356,-0.6446088251,2.1224088689
O,-2.7054505509,0.6140553916,2.6699604914
H,-2.7706019822,-0.884538107,1.3583523017
H,-3.5800464802,1.8009067315,0.5592310545
H,-3.5529505002,0.3737601102,-0.5216722258
H,-2.6298348102,1.8469515676,-0.9481384149
O,0.3281821293,-0.0083161563,1.9444817651
H,-0.8370076569,-1.3090504788,2.9936746007
C,-1.9936075771,1.7521224226,3.1602345429
H,-1.6801614934,2.4030904836,2.3380775665
H,-1.1170294616,1.4501520769,3.743128436
H,-2.6870932157,2.2913974184,3.8063494619

Table 2 Entry 2 Type b TS
 SCF Energy=   -1087.31692447
 Zero-point correction (ZPE)= -1086.93873
 Internal Energy (U)= -1086.91600
 Enthalpy (H)= -1086.91505
 Gibbs Free Energy (G)= -1086.99041
C,2.1360343534,-1.4966089077,-0.6730236282
C,2.1789628796,-0.244686098,-1.5798869655
C,3.3881531348,-1.5139373853,0.2229785577
C,2.4443652901,1.0082858391,-0.8172884792
H,2.9788738999,-0.373361004,-2.312647184
H,1.2299165252,-0.1718890309,-2.1221927932
N,0.9347754346,-1.5561996291,0.1417460817
H,2.1631785016,-2.3770564066,-1.3226695233
O,4.4845801653,-1.6928860284,-0.3692565278
O,3.2298025794,-1.3062066013,1.4542844551
N,1.5179700801,1.6030287691,0.0180088889
C,3.5893787903,1.7451485286,-0.7176971729
C,-0.2530390052,-1.9276419,-0.3493621082
H,1.0441894817,-1.3130075075,1.1216985042
C,2.0709005616,2.659444343,0.6010911047
H,0.5075227154,1.2690951253,0.1936406662
N,3.3270592298,2.7650563495,0.1693524176
H,4.5497510673,1.6270814528,-1.1939141152
C,-1.4454816384,-1.9125850918,0.3492798758
H,-0.2446349581,-2.2315132197,-1.3961588119
H,1.5908680991,3.3220428332,1.3049037654
H,3.9764827699,3.4902421125,0.4549128686
C,-1.4102829045,-1.7026151655,1.8384820299
C,-2.6069901508,-2.6997063194,-0.206019695
H,-0.9527844001,-0.7409548221,2.1008423278
H,-0.8234318987,-2.4919517379,2.327582725
H,-2.4189516144,-1.725145046,2.2579227606
H,-3.563454851,-2.283995738,0.1284758346
H,-2.5681611585,-3.7352505082,0.1559090222
H,-2.5971173246,-2.727460363,-1.3004334506
C,-1.5330611487,0.2260227553,-0.4047383788
C,-3.0514108797,0.2943481527,-0.5112704785
O,-0.9332354758,0.8863081489,0.4888491946
H,-1.0566548625,0.0859262313,-1.3857586691
O,-3.4143318086,1.4394425614,-1.2622642829
O,-3.5957028865,0.3033112055,0.7708115969
H,-3.4420544893,-0.5360430071,-1.1072985316
C,-3.0849349629,2.7014243314,-0.6801272702
C,-5.0206862767,0.3044351846,0.7712730401
H,-3.3993298527,2.7483333396,0.3666963504
H,-2.0116349313,2.9034840076,-0.7501510862
H,-3.6311014419,3.4505372887,-1.2547726241
H,-5.4131504503,1.2652381093,0.4220318671
H,-5.405974186,-0.4992277272,0.1320206047
H,-5.335565052,0.1354245255,1.8014764368

Table 2 Entry 2 Type c TS
 SCF Energy=   -1087.31991088
 Zero-point correction (ZPE)= -1086.94271
 Internal Energy (U)= -1086.91947
 Enthalpy (H)= -1086.91853
 Gibbs Free Energy (G)= -1086.99564
C,0.1252677675,1.558620212,-0.2120663422
C,1.1695893208,2.6651558864,0.0565644312
C,0.4619260595,0.9364040788,-1.5756285682
C,2.5661006018,2.1275322833,0.0970648184
H,1.0960558524,3.4155821584,-0.7335303747
H,0.9086016034,3.1445553827,1.004756598
N,0.0717115656,0.6192738582,0.8818249246
H,-0.8627372551,2.0190458062,-0.3193406404
O,0.7873454371,-0.3384283254,-1.6540356396
O,0.4993669048,1.6475566662,-2.5706949508
C,3.5802492718,2.3518628995,-0.7986044488
N,2.9954933394,1.2483156052,1.0772148434
C,-1.0881567015,0.2233427387,1.4583868349
H,0.9615098574,0.3255639823,1.2724710309
H,0.4328886328,-0.9095483293,-0.89317759
N,4.642427217,1.6051780527,-0.3508800472
H,3.6348001542,2.9639071632,-1.6860778992
C,4.2461521817,0.9615696364,0.7696959108
C,-1.2081037528,-0.7656955883,2.3941141373
H,-1.9798943088,0.7196654641,1.0798419283
H,5.5592172928,1.5466504849,-0.7763505233
H,4.9011076768,0.3030252654,1.3216136517

C,-2.5397263663,-1.0263325148,3.0436035302
C,-0.0036295806,-1.3993642205,3.0363106603
H,-2.5110057142,-0.756968805,4.1066197443
H,-2.7990371603,-2.0924209683,2.9936448601
H,-3.343370216,-0.4525656334,2.5724710685
H,0.8247389419,-1.531870809,2.332315918
H,0.3598827611,-0.7860346336,3.8704966417
H,-0.261668729,-2.3841137671,3.4404329586
O,-1.9659239723,-0.6268989103,-1.1364716394
C,-2.4031245342,-1.6449751384,-0.2955876613
C,-3.0231759106,0.109981424,-1.7397937372
C,-1.1972582167,-2.1574638777,0.4905283363
O,-2.9937850722,-2.7165104986,-1.0050539064
H,-3.1913000549,-1.2998432696,0.3838340409
H,-3.6347630071,-0.531759907,-2.3824617813
H,-3.6562121763,0.569754696,-0.9708374307
H,-2.5560101621,0.8885641008,-2.3453645234
O,-0.041331886,-2.0929773755,0.0300551621
H,-1.4424407251,-2.9013933511,1.2619009058
C,-2.1576121981,-3.3207253368,-1.995014326
H,-1.7291486488,-2.5649821705,-2.6599153097
H,-1.353095951,-3.902363027,-1.5327283227
H,-2.7994391395,-3.9888533882,-2.5698262736

Table 2 Entry 2 Type d TS
 SCF Energy=   -1087.31521255
 Zero-point correction (ZPE)= -1086.93753
 Internal Energy (U)= -1086.91459
 Enthalpy (H)= -1086.91365
 Gibbs Free Energy (G)= -1086.99114
C,2.1109639998,-1.8726729251,0.2642813541
C,3.2847699834,-1.0959400784,-0.3739171487
C,2.0063860733,-1.4581903133,1.7360694228
C,2.9612375646,0.3554368472,-0.5381658159
H,4.1640937845,-1.2284171486,0.2606570976
H,3.4986885304,-1.5437394844,-1.3484678191
N,0.9087923847,-1.6541776515,-0.5165415122
H,2.3589299949,-2.93841153,0.2770397983
O,1.1131194563,-0.5747747261,2.1048743599
O,2.7919562177,-1.9394473428,2.5453852892
C,3.1710825604,1.385348417,0.3436495214
N,2.2506602079,0.8143633276,-1.6326859549
C,-0.2835464107,-2.1961955738,-0.2227374364
H,0.9538496944,-0.9256151218,-1.2251670893
H,0.5218482599,-0.1325736147,1.3514051377
N,2.5772348444,2.4843458024,-0.226146097
H,3.6737239018,1.4265444595,1.2983323541
C,2.0366214609,2.0955595322,-1.4029674847
C,-1.4641136063,-1.8586314318,-0.8445987078
H,-0.2863035903,-2.8947996768,0.6139674377
H,2.5545293843,3.4218080659,0.1564191012
H,1.5087247172,2.779679322,-2.051694143
C,-2.6792616093,-2.7017816371,-0.5526257345
C,-1.4382370838,-1.1031831377,-2.1513519058
H,-3.5962572192,-2.1036398477,-0.5149610325
H,-2.8252933218,-3.4474359372,-1.344405551
H,-2.5798751931,-3.2325546693,0.3988933843
H,-0.780201376,-0.2273183569,-2.1189305911
H,-1.089218809,-1.7550493354,-2.9628252289
H,-2.4397142139,-0.7512723668,-2.4192046243
C,-1.5364154543,-0.0681175089,0.6039174407
C,-2.7805980891,0.5951778253,0.007748553
O,-0.4267537681,0.5245302655,0.5261341401
H,-1.7548911371,-0.7302323849,1.4520024295
O,-3.5658114785,1.1090103571,1.0661288224
O,-2.3669482194,1.585388157,-0.8801581463
H,-3.4417447609,-0.1226015096,-0.487528458
C,-2.9357265841,2.1315976275,1.8403524995
C,-3.4524434543,2.17780056,-1.5879461719
H,-2.6077190757,2.9597865412,1.2054785379
H,-2.079910806,1.736535896,2.3988141637
H,-3.6881205128,2.4894491525,2.5433081312
H,-4.097819411,2.7469693855,-0.9110235281
H,-4.0450984777,1.4066849806,-2.0949359075
H,-3.0163324086,2.8502746888,-2.3269623873

Table 2 Entry 3 Type a TS
 SCF Energy=   -1046.85799954
 Zero-point correction (ZPE)= -1046.53152
 Internal Energy (U)= -1046.51020
 Enthalpy (H)= -1046.50925
 Gibbs Free Energy (G)= -1046.58207
C,-1.0476945982,-1.5544562531,-0.5740833962
C,-2.1695170407,-1.8828639559,0.1322046162
C,-3.4531140226,-2.1984324825,-0.5839068849
O,3.6841580785,-1.8064289779,-0.7677993236
C,-2.3454111354,0.5395475086,0.6673060504
O,-1.4036703288,0.8173028344,1.4058890722
H,-1.1154399447,-1.3928590968,-1.6507854789
H,1.2735228038,-2.0122193978,-1.7166149235
H,2.3382775601,0.0396868048,-2.2882648423
H,-4.2967687749,-1.6457496593,-0.1510593143
H,-3.3948421706,-1.9587830829,-1.6496013248
H,-3.6889168318,-3.2657468539,-0.4841318196

N,0.1897409525,-1.3615307473,-0.043199613
C,1.5612985703,0.1028358306,-1.5233670042
C,1.3676522421,-1.29379245,-0.8941425367
C,2.6296967984,-1.6685612683,-0.0929645331
O,2.5269291195,-1.7776507243,1.1568789896
H,0.3757773687,-1.6744077855,0.9039141734
H,0.627581333,0.4040823805,-2.0074439931
C,1.9828318076,1.1220039132,-0.5209863194
C,3.2014493027,1.7034378778,-0.320484421
N,1.1616688388,1.6010973442,0.4829491273
H,4.1263844413,1.6062325887,-0.866262447
C,1.8402061436,2.4374882786,1.2596268525
H,0.1745602994,1.3397341275,0.6328359988
H,3.8150988471,3.0883442608,1.1902781633
H,1.4552872796,2.9645959553,2.119274946
N,3.0814951976,2.5136909579,0.7873373039
C,-2.0931076892,-2.2410765347,1.5918216567
H,-1.3792308036,-1.6163828064,2.1399964704
H,-3.0731071735,-2.1274872364,2.0666907631
H,-1.7845891296,-3.2869559328,1.7185304319
H,-3.3005520639,0.1460503203,1.0371629974
C,-2.3053976894,1.0133642633,-0.77269053
O,-1.3337420278,1.5656516323,-1.251865085
O,-3.4432274361,0.7812543302,-1.4084676659
C,-3.4686351098,1.1215185702,-2.8068012516
H,-4.456351331,0.8327373349,-3.1592100491
H,-3.3135654367,2.1944619806,-2.9313091992
H,-2.6921705563,0.5624856711,-3.333710807

Table 2 Entry 3 Type c TS
 SCF Energy=   -1046.85517532
 Zero-point correction (ZPE)= -1046.52946
 Internal Energy (U)= -1046.50825
 Enthalpy (H)= -1046.50731
 Gibbs Free Energy (G)= -1046.58000
H,0.2783768353,-1.2283233031,-0.7978009829
C,2.5955477097,-0.0691466887,-0.9521066635
O,1.5917663148,-0.4508428369,-1.5675765948
C,1.9714041965,1.9453408642,0.180473505
C,1.1836297706,1.1009156581,0.9182936923
N,-0.0174375625,0.6189960517,0.5226281172
C,-0.782346675,-0.3213917167,1.3112583939
C,-2.2131458124,0.1987306329,1.5708803002
C,-0.9021317683,-1.7115794894,0.6733912417
O,-0.3768968019,-1.9253817485,-0.5207876492
O,-1.5247833647,-2.5962278561,1.2383432886
H,-0.2709636365,-0.4677920354,2.2686437626
H,-2.7153248506,-0.4868766612,2.2566785694
H,-2.1283465227,1.1723476373,2.0624819467
H,-0.5164436046,1.0745787925,-0.2379140599
C,-3.0028816777,0.3060631877,0.3045297552
C,-4.0564061827,-0.4722635754,-0.1023860711
N,-2.6879697662,1.2211545732,-0.6855490196
H,-4.5803289021,-1.2849793485,0.3774374917
C,-3.5452421105,0.9927329212,-1.6622641722
H,-3.5977989336,1.5265416756,-2.6001903892
N,-4.3897069656,-0.0169017738,-1.3545672671
H,1.54324074,0.7183885278,1.8732664574
H,3.3339045941,0.6127532963,-1.3927725368
H,-5.1392506267,-0.3633791313,-1.9406867198
C,1.4569594052,2.6041103019,-1.0697194108
H,0.8505781924,1.9274162607,-1.6816789097
H,0.833848575,3.4715869722,-0.8176012329
H,2.2900511533,2.9610889391,-1.6831813499
C,3.239211657,2.4917614917,0.7739643
H,4.0732607965,2.3927983338,0.068167402
H,3.1303673213,3.5612769759,0.9920437073
H,3.5060121422,1.9788739267,1.7020043796
C,3.0803430117,-0.7885895461,0.2894675665
O,4.1757732165,-0.5929859835,0.7839623758
O,2.1776388238,-1.6406016575,0.7551696796
C,2.4764460801,-2.2725149649,2.0113834264
H,1.6113336601,-2.8944216402,2.2356118553
H,3.3751576898,-2.8847865083,1.9187822913
H,2.6142015584,-1.5102610353,2.7819796937

Table 2 Entry 4 TS type a
 SCF Energy=   -1295.80749069
 Zero-point correction (ZPE)= -1295.46730
 Internal Energy (U)= -1295.44632
 Enthalpy (H)= -1295.44538
 Gibbs Free Energy (G)= -1295.51683
C,-0.9988844854,-1.6385804734,-0.5855200427
C,-2.1255467206,-1.8689296504,0.180329824
C,-3.4442079153,-2.0812461642,-0.518401383
O,3.7682690715,-1.5571662053,-0.9027721754
C,-2.1720764519,0.2017199581,0.7927152644
O,-1.153044806,0.4093901948,1.5214547056
H,-1.1155595429,-1.3887212976,-1.6401914998
H,1.3593917365,-1.9999007295,-1.8579789061
H,2.1776109018,0.1673323565,-2.3188072566
H,-4.2494645473,-1.5318078648,-0.0124914876
H,-3.4116174442,-1.7584134114,-1.5630418255
H,-3.7223950662,-3.1420484272,-0.5019927222

N,0.2573543168,-1.6008981628,-0.1301780324
C,1.440208104,0.1107397444,-1.5152191194
C,1.4046860324,-1.3369000175,-0.986921333
C,2.7090812731,-1.6563463641,-0.2300227368
O,2.6243525957,-1.966512312,0.9866575035
H,0.4782967643,-1.8768077405,0.8216313134
H,0.4639327304,0.3508785928,-1.9503942207
C,1.8158775008,1.1239864751,-0.4857926899
C,2.9065697159,1.94476339,-0.4403038939
N,1.0730051337,1.3913787023,0.6489059956
H,3.7352975547,2.0566802678,-1.1213213355
C,1.6749277712,2.3441290649,1.3487994437
H,0.1238655132,0.9509421747,0.9337264665
H,3.4426256525,3.4015465362,1.0312076583
H,1.3282150739,2.7659218935,2.2800969888
N,2.7909415476,2.693661189,0.7095029861
C,-2.0070180888,-2.4738534135,1.5563904525
H,-1.1955460681,-2.0336779731,2.1430699988
H,-2.9384302374,-2.3254116829,2.1136075584
H,-1.8293434903,-3.5541072134,1.4863033266
C,-2.3601792924,0.9888232933,-0.4829676274
H,-1.410688334,1.1215618716,-1.0115592646
H,-3.0815228796,0.5033206686,-1.1441981434
H,-3.108979849,-0.0918969822,1.2896629462
S,-3.0664468035,2.6292854826,-0.1030118501
C,-1.6224842646,3.4513375538,0.6256941428
H,-0.7867256069,3.4486786846,-0.0787005246
H,-1.9143075053,4.4845580768,0.8270078993
H,-1.3278555504,2.9751776844,1.563175516

Table 2 Entry 4 TS type b
 SCF Energy=   -1295.80192088
 Zero-point correction (ZPE)= -1295.46270
 Internal Energy (U)= -1295.44147
 Enthalpy (H)= -1295.44052
 Gibbs Free Energy (G)= -1295.51406
C,-0.6110901315,-1.8200749261,-0.4394807796
C,-1.8173163236,-1.871768168,0.2383536283
C,-2.9700496368,-2.5504204171,-0.4639032045
O,4.1302414394,-1.5045219914,-0.4497759184
C,-1.9090236309,0.3083282782,-0.087812261
O,-1.2129993829,0.791499514,0.8644686371
H,-0.6070240507,-1.9677141156,-1.5198360942
H,1.8268134165,-2.1803939279,-1.4493079672
H,2.5481107881,-0.0788672199,-2.272693875
H,-3.9304738643,-2.2301530517,-0.0493334848
H,-2.9686211154,-2.3459894776,-1.5396940505
H,-2.9115929925,-3.6377768924,-0.3272523744
N,0.5813828603,-1.5410903498,0.0910845155
C,1.7652468147,-0.0354486747,-1.5120088435
C,1.7745001998,-1.3643321284,-0.722256872
C,3.0332456074,-1.418845093,0.1618970686
O,2.877570624,-1.3294368906,1.4077171054
H,0.6991216161,-1.4117258579,1.0915370868
H,0.8012982287,0.0599638842,-2.0240351536
C,2.0213504554,1.1541276231,-0.6509763418
C,3.1359077111,1.9374633282,-0.5579207328
N,1.121148524,1.6252561266,0.285515367
H,4.0664350398,1.9126876769,-1.1025295442
C,1.6624873344,2.6553318399,0.9220196464
H,0.1158372982,1.2221451219,0.506812957
H,3.5154689447,3.595399035,0.7386715874
H,1.1990128404,3.2303409449,1.7092951643
N,2.8835730174,2.8649297608,0.4284584231
C,-1.8348547742,-1.920542129,1.7421457918
H,-1.1513028938,-1.1941968024,2.1912901648
H,-2.8410380405,-1.712245492,2.1203894353
H,-1.5481768668,-2.9193267598,2.0961279779
C,-3.4090061719,0.4349338706,-0.0326992127
H,-3.8877218072,-0.1853277711,-0.7906450333
H,-3.8001952269,0.18331621,0.9582847237
H,-1.4945569324,0.3451620822,-1.1059401172
S,-3.8885611103,2.1461998337,-0.4588365768
C,-3.3663368928,3.0403759352,1.0303030086
H,-3.7908516955,4.0442619272,0.9607269021
H,-3.7576841919,2.5487685018,1.9239934512
H,-2.2797388878,3.1132173224,1.092859355

Table 2 Entry 4 TS type c
 SCF Energy=   -1295.80542544
 Zero-point correction (ZPE)= -1295.46585
 Internal Energy (U)= -1295.44505
 Enthalpy (H)= -1295.44411
 Gibbs Free Energy (G)= -1295.51585
H,0.1790986962,-0.9375492658,-0.5666871679
C,2.0662555557,0.2486543233,-0.9397370793
O,0.9100931478,-0.0605713663,-1.3704213909
C,1.8058050892,1.9722048623,0.409471241
C,1.0241713314,1.1539573396,1.1941125049
N,-0.2707556994,0.8912149325,0.955574716
C,-1.0259212258,-0.1270319092,1.6540425975
C,-2.5257976396,0.2342019737,1.6430389369
C,-0.8881196943,-1.547167161,1.0852300793
O,-0.3158647998,-1.7451021624,-0.0715688735

O,-1.3676212782,-2.4816200743,1.7225386266
H,-0.6747395773,-0.1764063543,2.689358961
H,-3.0574966897,-0.4769455206,2.2785994361
H,-2.6350135299,1.2312422598,2.0805288557
H,-0.7384006815,1.342049203,0.1721118711
C,-3.0938890478,0.19197399,0.2595377914
C,-3.9372071976,-0.7448834611,-0.2801232002
N,-2.7380479506,1.1144198759,-0.7089507804
H,-4.4196228041,-1.6115308506,0.1458366801
C,-3.363686489,0.7323586831,-1.8059467904
H,-3.3195778336,1.2240331528,-2.767074148
N,-4.1004344545,-0.3809047674,-1.5945273405
H,1.4642641548,0.6094760175,2.0289160787
H,2.6538659982,0.9644977691,-1.5304363877
H,-4.6697314688,-0.8546743519,-2.2849281229
C,1.1805583814,2.8968395134,-0.6046246921
H,0.399974844,2.4093103655,-1.1975141112
H,0.7328199032,3.7667995664,-0.1082670002
H,1.9441304421,3.2669084952,-1.2965003749
C,3.1932719079,2.3359797083,0.8662355613
H,3.9130228359,2.2315040373,0.0436020685
H,3.2259262317,3.3840319805,1.1878003785
H,3.5288881129,1.7139837465,1.7008221067
C,2.8812947465,-0.7425155542,-0.1467428701
H,3.6626553753,-0.2379185982,0.4248870364
H,2.255927122,-1.3346367768,0.5278480979
S,3.753488242,-1.858831026,-1.2985725909
C,2.3772175938,-2.9013249207,-1.8538961285
H,2.8033197007,-3.6599888964,-2.5140481759
H,1.905229594,-3.3952589761,-1.001688992
H,1.6369424348,-2.3214780223,-2.407983638

Table 2 Entry 4 TS type d
SCF Energy=   -1295.80178545
 Zero-point correction (ZPE)= -1295.46340
 Internal Energy (U)= -1295.44210
 Enthalpy (H)= -1295.44115
 Gibbs Free Energy (G)= -1295.51530
H,0.2265188794,0.1704502324,1.1886036142
C,-1.8186357374,-0.0057336571,0.6353182117
O,-0.7669010021,0.7019679789,0.4895078638
C,-1.7120165989,-1.6313602455,-0.9159528845
C,-0.4879476202,-1.95661238,-0.3696037
N,0.6613319243,-1.3400039496,-0.6789965539
C,1.8985524164,-1.5329062093,0.0549827193
C,3.0380484363,-0.7690745176,-0.6527675313
C,1.8579707178,-1.0767974902,1.5200179029
O,0.9484502518,-0.2318549109,1.9133640049
O,2.7222161117,-1.4983168113,2.2868939313
H,2.1450049804,-2.5984843532,0.0785813324
H,3.9620642161,-0.9464908004,-0.0979471698
H,3.1577001904,-1.1883013208,-1.6559652436
H,0.6355061893,-0.5544233135,-1.3264810431
C,2.7517995732,0.6971638472,-0.7288071142
C,3.1578638831,1.6861675062,0.1302759876
N,1.8905948278,1.22309502,-1.6750988543
H,3.815724083,1.6728569893,0.9861015985
C,1.7818120398,2.5043963629,-1.3790182646
H,1.1883047797,3.2324062363,-1.9127984289
N,2.5305616035,2.8286561873,-0.3008283311
H,-0.4193775442,-2.7107141061,0.4142253131
H,2.6212465721,3.7531633086,0.1025689034
C,-1.7655606366,-0.7902941069,-2.1680990624
H,-1.2189501563,0.1548401833,-2.0609585918
H,-1.3261741744,-1.3309538103,-3.0163424459
H,-2.8001191575,-0.5495864663,-2.4269644655
C,-2.8636475327,-2.5709067731,-0.6590065996
H,-3.8256843865,-2.0523034454,-0.7002149323
H,-2.8974240236,-3.3558975514,-1.4249242766
H,-2.7741169483,-3.0570106165,0.3174265654
C,-3.1276259557,0.5801555968,0.1871205085
H,-3.0111686101,1.1394059155,-0.7444571233
H,-3.899587519,-0.1814412129,0.0745637561
H,-1.8740226793,-0.7071178811,1.4768886873
S,-3.7504181315,1.7050050862,1.4862275028
C,-2.5856710741,3.0858215944,1.328269604
H,-2.5250501368,3.4142784563,0.2880658105
H,-2.9819794378,3.9016835981,1.936409582
H,-1.5932417733,2.8169027396,1.6920089369

TS-6a
 SCF Energy=   -976.242564688
 Zero-point correction (ZPE)= -975.84766
 Internal Energy (U)= -975.82560
 Enthalpy (H)= -975.82465
 Gibbs Free Energy (G)= -975.89850
C,1.2184590494,-1.5942407244,0.4657612117
C,2.3361663256,-1.7692619633,-0.3291826348
C,3.6692542674,-1.9883746024,0.339875494
O,-3.5476655334,-1.5399387054,0.8371548517
C,2.3260635961,0.3103730305,-0.8506320453
O,1.2883802422,0.5098101534,-1.5654075157
H,1.349188897,-1.3812880383,1.5269456753
H,-1.1414746869,-2.0299173063,1.7482072371

H,-1.9280524955,0.1146256007,2.3169732088
H,4.4582919419,-1.4130690001,-0.1628016895
H,3.6506570878,-1.6979292389,1.3939563237
H,3.9595271588,-3.0446968691,0.285441969
N,-0.0444353996,-1.5668557819,0.0330155479
C,-1.2027338541,0.0942683749,1.5004932796
C,-1.1838657397,-1.3285901288,0.9079076351
C,-2.4972395057,-1.592380315,0.1456699915
O,-2.4280549253,-1.8104498244,-1.0917669421
H,-0.2715482,-1.7896370974,-0.9313009437
H,-0.2196622102,0.3120963969,1.9312975959
C,-1.5909383604,1.1552845765,0.5258124488
C,-2.6943951727,1.9603563557,0.5289463875
N,-0.8520127463,1.4959836887,-0.5918842954
H,-3.5230347155,2.0205594008,1.2165355346
C,-1.4706849338,2.4769016994,-1.2346601575
H,0.1003929403,1.0532896231,-0.9355581761
H,-3.2542033016,3.4908171691,-0.8553405454
H,-1.1340049651,2.9537239951,-2.1428611806
N,-2.5915681808,2.7754995012,-0.575856336
C,2.2036983011,-2.332037836,-1.7222423771
H,1.3746513232,-1.8865256182,-2.2793566
H,3.1225011957,-2.1506475846,-2.2907472756
H,2.0446726331,-3.4169384446,-1.6862152361
C,2.5326783081,1.0879682338,0.4289914721
H,3.2523029474,0.5575346107,1.0613163245
H,3.2542984052,0.050573935,-1.3834392861
C,3.0724478548,2.5048164771,0.1478698966
H,3.9405959382,2.4077558874,-0.5199160172
H,1.5843567825,1.1646008366,0.9774696037
C,3.5445092265,3.1362667322,1.4579466499
H,4.3273040667,2.5348099126,1.9311478027
H,3.9429986245,4.1415046426,1.2860132254
H,2.7085238372,3.2210185177,2.1631899276
C,2.0342556652,3.403205908,-0.5253222933
H,1.6986404563,3.0010730761,-1.4854274347
H,1.153520992,3.5163940047,0.120081313
H,2.4504569926,4.4002960586,-0.7040097155

TS-6b
 SCF Energy=   -976.238882736
 Zero-point correction (ZPE)= -975.84423
 Internal Energy (U)= -975.82214
 Enthalpy (H)= -975.82119
 Gibbs Free Energy (G)= -975.89532
C,-0.7285311999,-1.7456402298,-0.5022814438
C,-1.9972719901,-1.5979367086,0.027055865
C,-3.1411382516,-2.2286269201,-0.7293264496
O,3.9988935691,-1.8776719175,0.0200809228
C,-1.8255574739,0.5323997841,-0.5696526779
O,-1.1811903442,1.0743868969,0.3902114124
H,-0.6243060355,-2.0167095461,-1.5531203724
H,1.7522848782,-2.4634804581,-1.1690572223
H,2.7912843883,-0.5502974269,-2.107563937
H,-4.0877457799,-1.7286937259,-0.5041064891
H,-2.9788734877,-2.1968903194,-1.8116731155
H,-3.2574321707,-3.2802728691,-0.4371625915
N,0.4249623387,-1.5285190716,0.1361738051
C,1.9404498133,-0.3433159812,-1.4545403197
C,1.7116211916,-1.568474828,-0.5402250315
C,2.8528329104,-1.6511667661,0.4898757025
O,2.5690218151,-1.4507303407,1.6994571305
H,0.448503377,-1.323223488,1.1301061763
H,1.0558532752,-0.2075621314,-2.086618476
C,2.2320373905,0.9012988091,-0.6876071256
C,3.4204274258,1.5461394574,-0.4944389466
N,1.2804451063,1.5833691729,0.0464461731
H,4.4067492053,1.3440293532,-0.8809563683
C,1.8633299086,2.6051979265,0.6587934249
H,0.2059118134,1.3185326344,0.1629409319
H,3.8343698133,3.2875497774,0.6764712991
H,1.3769694528,3.3229061974,1.3014994628
N,3.160206109,2.6055436834,0.3459558465
C,-2.1847117847,-1.4425492676,1.5117087166
H,-1.4800300153,-0.7265449092,1.9458875674
H,-3.1982729436,-1.0937513679,1.7355048444
H,-2.0463440545,-2.4050384134,2.0210688022
C,-3.2998114596,0.8193678294,-0.7024336628
H,-3.7195067381,0.2360118954,-1.5287370314
H,-1.290526335,0.373808024,-1.5167135032
C,-3.5296610251,2.3188784729,-0.9818526029
H,-3.1386390804,2.8807662703,-0.1237282186
H,-3.8202369823,0.5426683422,0.2224838946
C,-5.0277082159,2.5906574041,-1.1001370761
H,-5.2196362581,3.6587275656,-1.2466825261
H,-5.4490820723,2.0509396018,-1.9568000294
H,-5.5630494428,2.2692293251,-0.2005397645
C,-2.7964317376,2.7815597452,-2.2414943068
H,-1.7092501724,2.6925460683,-2.1424184541
H,-3.1084464422,2.1853501882,-3.1079725446
H,-3.0248464182,3.8308029415,-2.4548048707

TS-6c
 SCF Energy=   -976.241350874

Zero-point correction (ZPE)= -975.84650
Internal Energy (U)= -975.82464
Enthalpy (H)= -975.82370
Gibbs Free Energy (G)= -975.89735
H,-0.1184625628,-0.4072706608,1.0320091725
C,1.8668775273,0.3876078289,0.424480105
O,0.9772163937,-0.4965829205,0.2064171202
C,1.3461178463,2.1332198094,-0.8595336349
C,0.1922538268,2.2174884686,-0.119035296
N,-0.9102163242,1.4726828266,-0.3202270409
C,-2.0112783757,1.4218447374,0.6184487104
C,-3.3083504173,1.0146749917,-0.1103914546
C,-1.8298745963,0.4583167546,1.8021554508
O,-0.8881766041,-0.4447580846,1.7856816262
O,-2.6264119744,0.5278985074,2.7360715224
H,-2.1441256789,2.4164463858,1.0548020946
H,-4.142174507,1.1178892934,0.5873137227
H,-3.4670549764,1.7150429243,-0.9358990877
H,-0.9353472964,0.8036710821,-1.0859224456
C,-3.2468604544,-0.3946609597,-0.6081703294
C,-3.8798675191,-1.4965547444,-0.0927486057
N,-2.4240628978,-0.773694335,-1.65414172
H,-4.5833309644,-1.6099163164,0.7180904696
C,-2.5708812511,-2.0810084428,-1.7615382064
H,-2.0769495771,-2.7191853996,-2.4798876857
N,-3.4388146972,-2.5594386838,-0.8421024411
H,0.1503811761,2.875992902,0.7471148162
H,-3.7135781726,-3.5277012312,-0.7323227134
C,1.3768123223,1.4016364178,-2.1768158885
H,0.8141392872,0.4626902657,-2.1546380561
H,0.9557549076,2.0274751162,-2.9733999547
H,2.4097231461,1.16516065,-2.4530970533
C,2.4523033716,3.1258983578,-0.6218851169
H,3.4227017975,2.6168035215,-0.5493509691
H,2.5238677016,3.8320812222,-1.458035603
H,2.2942669285,3.6993150823,0.2958448783
H,2.7456057581,0.3792809091,-0.2332191483
C,2.0684281042,0.9322605247,1.8173072187
C,2.7218275746,-0.1309769622,2.7236289333
H,1.1024821356,1.2174999529,2.2478304732
C,2.8266972226,0.4087375616,4.1481441053
H,1.8427830694,0.6807889963,4.5442932048
H,3.267324697,-0.3390230428,4.8156479904
H,3.4631116031,1.3015614069,4.1749069274
H,2.7103230592,1.8200943366,1.7804708742
H,2.0627402052,-1.0097749663,2.7314480699
C,4.09490791,-0.5544719842,2.2022600524
H,4.7539285902,0.3180819989,2.1112323477
H,4.5666418092,-1.2623043712,2.8913212625
H,4.0342360661,-1.0370120875,1.2212820125

TS-6d
SCF Energy= -976.238186613
Zero-point correction (ZPE)= -975.84466
Internal Energy (U)= -975.82256
Enthalpy (H)= -975.82161
Gibbs Free Energy (G)= -975.89645
H,-0.0764430366,-0.4158719843,1.2948174361
C,-2.1207885527,-0.2258048098,0.7171507192
O,-1.0146530905,0.3764467151,0.9300950139
C,-2.0066220422,-0.9445195286,-1.4381345037
C,-0.8570068309,-1.6037934675,-1.0663591752
N,0.360814589,-1.044430381,-1.0034521735
C,1.5140891621,-1.7127582905,-0.4351499473
C,2.8044003984,-1.0181007923,-0.9114066532
C,1.5347447212,-1.7748894299,1.1000779731
O,0.6835793511,-1.0811449862,1.7925611835
O,2.3897157251,-2.4813312814,1.6379402939
H,1.5239261659,-2.7525439161,-0.7771574362
H,3.6571572279,-1.5686480419,-0.5087922324
H,2.843043601,-1.0823314138,-2.0027145747
H,0.4777559293,-0.0651367381,-1.2547328182
C,2.8634614872,0.4095974385,-0.4682031132
C,3.5416957465,0.9384802343,0.6002809226
N,2.1212012434,1.3997299825,-1.088016351
H,4.2138510337,0.4956912843,1.3196971896
C,2.3592521787,2.5006918905,-0.4005895458
H,1.9467520947,3.4781153973,-0.6048728413
N,3.2095323113,2.2710198042,0.6245429086
H,-0.9064946545,-2.6397925119,-0.7317746168
H,3.5530866963,2.9651571375,1.276785946
C,-1.92198127,0.4026699233,-2.1094478518
H,-1.2889467444,1.1054546863,-1.5537664851
H,-1.5037479997,0.3090208839,-3.1202482843
H,-2.9160460114,0.84902554,-2.2030414887
C,-3.2299272873,-1.781483674,-1.7113231257
H,-4.1533975551,-1.2498903352,-1.4616979896
H,-3.2912363961,-2.0319434792,-2.7781919518
H,-3.2083542739,-2.7182128106,-1.1457943566
C,-3.3651819779,0.6056695286,0.598190288
H,-4.0853723964,0.1503792857,-0.0849062263
H,-2.2442170709,-1.2429239547,1.1105217635
C,-4.0502646613,0.7584662686,1.9748435998
H,-4.3270476364,-0.2454579335,2.3238154747

C,-5.3290342231,1.5776143866,1.8007249565
H,-5.8656510485,1.6654566111,2.7508070978
H,-5.0890512482,2.5901518778,1.4546096669
H,-6.0010259772,1.1184167858,1.0685377181
C,-3.1366424986,1.4026821605,3.0163433145
H,-2.7801275743,2.377980316,2.6625767566
H,-3.6803387267,1.5605776271,3.9534178445
H,-2.2621823549,0.7832313758,3.2368895754
H,-3.0897564728,1.5943316094,0.2113226794

TS-8a (chelated)
 SCF Energy=   -1012.13244424
 Zero-point correction (ZPE)= -1011.76033
 Internal Energy (U)= -1011.73834
 Enthalpy (H)= -1011.73739
 Gibbs Free Energy (G)= -1011.81155
C,-1.1315832739,-1.3421782767,-0.7243915134
C,-2.3305637152,-1.407449933,-0.0446800006
C,-3.6182918314,-1.3214488566,-0.8224219524
O,3.4968961408,-2.5142698665,-0.7630704235
C,-2.0811870888,0.5992285162,0.7661283449
O,-1.0483687474,0.6088871564,1.4941720994
H,-1.1112949964,-0.9879632508,-1.7558638155
H,1.1532754494,-2.1943553712,-1.8813267855
H,2.5716491645,-0.3005162162,-2.0786383808
H,-4.3395595539,-0.6589076424,-0.324265147
H,-3.458383964,-0.9523400881,-1.8395748485
H,-4.0890807112,-2.3098270397,-0.8918725344
N,0.0639651555,-1.6248926351,-0.1905785016
C,1.7610924274,-0.2112267012,-1.3521301241
C,1.301708038,-1.6276564593,-0.9554871467
C,2.4132767849,-2.3280684521,-0.1499364201
O,2.1722724444,-2.6316873425,1.0476796052
H,0.1294050523,-2.0339336821,0.7363848666
H,0.9265634128,0.3018055482,-1.8368974477
C,2.2629007986,0.5853105443,-0.1964020928
C,3.539011817,0.9619014906,0.1112065532
N,1.4625643461,1.0363714504,0.8365152207
H,4.466325978,0.811799067,-0.4183848425
C,2.213116681,1.6631166953,1.7324509585
H,0.4126371943,0.8919910858,0.9452692748
H,4.260059622,2.0448911407,1.8090614339
H,1.8640243227,2.1218400542,2.6448741844
N,3.4770436143,1.6332976278,1.3121358167
C,-2.4056036512,-2.1257371334,1.2808809789
H,-1.6013210808,-1.8295764702,1.9622532177
H,-3.3580331647,-1.9069205751,1.7750776695
H,-2.347763153,-3.2123180848,1.1388728806
C,-2.1841569843,1.5422973943,-0.4177032787
H,-2.8662979398,1.1247243064,-1.1688512482
H,-3.0539037868,0.376293166,1.2324711102
O,-0.889237282,1.6990382663,-0.9743684028
C,-0.9192182582,2.0721960381,-2.3434577887
H,-1.4992932133,2.98928548,-2.4984668093
H,0.1114595282,2.2539932358,-2.6546809783
H,-1.3498499947,1.2669739788,-2.9536245888
C,-2.7326510768,2.8798018045,0.0826527747
H,-2.0748065268,3.2909779356,0.8546934892
H,-2.8014711203,3.594892547,-0.7418345159
H,-3.733791817,2.7492724171,0.5033375587

TS-8a (Felkin-Anh)
 SCF Energy=   -1012.12701427
 Zero-point correction (ZPE)= -1011.75469
 Internal Energy (U)= -1011.73316
 Enthalpy (H)= -1011.73221
 Gibbs Free Energy (G)= -1011.80443
C,-1.0294788929,-1.8470158685,-0.5893882906
C,-2.1501557082,-2.1248785355,0.1720982695
C,-3.4445452397,-2.4717457156,-0.5200814459
O,3.7382547069,-1.3231753285,-0.6468311298
C,-2.2122327212,-0.0286773673,0.8272949803
O,-1.2044247361,0.1008806851,1.5816750861
H,-1.1424739157,-1.6505670443,-1.6554235571
H,1.4755696807,-2.1497014077,-1.7085410265
H,2.0833552203,0.0251054912,-2.3602756573
H,-4.2893678957,-1.9304416736,-0.0751227124
H,-3.4159151429,-2.2516504218,-1.5903175767
H,-3.6539840666,-3.5423017923,-0.4024751382
N,0.2083287526,-1.7083880967,-0.1046439783
C,1.3047402736,-0.0228148662,-1.5956941642
C,1.3787000715,-1.4005816466,-0.9147472704
C,2.6477864936,-1.4904231336,-0.041810892
O,2.5017323399,-1.7014664053,1.190147697
H,0.4047763515,-1.9032658128,0.8720065584
H,0.3423662561,0.0664181918,-2.1121320023
C,1.5077647909,1.1373556095,-0.6765816893
C,2.3763180459,2.185012334,-0.7967760553
N,0.7884411911,1.3557890641,0.4846351672
H,3.1188975831,2.4042998315,-1.5475934048
C,1.180852348,2.4978376476,1.0329951304
H,-0.0238900597,0.7713652954,0.8954422891
H,2.6377960884,3.8813803481,0.4790344221
H,0.7877761965,2.9332967955,1.9396854335

N,2.1483303639,3.0156374914,0.2774795525
C,-2.0157307653,-2.6981934079,1.5615744156
H,-1.187104092,-2.2687913249,2.1288923906
H,-2.9358123904,-2.523561373,2.1309307563
H,-1.8660934387,-3.7832953782,1.5018355622
C,-2.3083650152,0.9033354564,-0.3892463945
H,-1.4598061976,0.7153107101,-1.0617506256
H,-3.1709871406,-0.3423789289,1.2679648335
O,-2.1442093678,2.2131379252,0.1661656237
C,-1.6575278447,3.1647051011,-0.7684576636
H,-2.3906538162,3.3697433883,-1.5571425246
H,-1.4631752023,4.0854511983,-0.2150351928
H,-0.7241981155,2.8140537929,-1.231736337
C,-3.6206272253,0.7950048964,-1.1448075472
H,-4.4653481578,0.8359796534,-0.449494284
H,-3.7131487005,1.6202093132,-1.8557684387
H,-3.6727299962,-0.1368350115,-1.7101114886

TS-8c (chelated)
 SCF Energy=   -1012.12674884
 Zero-point correction (ZPE)= -1011.75565
 Internal Energy (U)= -1011.73397
 Enthalpy (H)= -1011.73302
 Gibbs Free Energy (G)= -1011.80646
H,0.4114574351,0.6073419186,1.2380559376
C,2.499818849,-0.4238783678,1.0548667988
O,1.3846316594,-0.3364828763,1.6527588302
C,2.1274709359,-1.9216203656,-0.5651343533
C,1.3890762495,-0.9130960206,-1.1429944597
N,0.1155705299,-0.6204468851,-0.8244720281
C,-0.5501747433,0.5985514095,-1.2208997258
C,-1.9840486054,0.2982095189,-1.7115497809
C,-0.6659647734,1.6560670413,-0.109524397
O,-0.3256701134,1.3602195049,1.1199295034
O,-1.1652009167,2.7439833558,-0.3826623906
H,0.0215847438,1.0550974736,-2.0343232446
H,-2.4081558758,1.2140834181,-2.1286430535
H,-1.9169468597,-0.4415432505,-2.5145978047
H,-0.4082639637,-1.2397375075,-0.2126281751
C,-2.8624427137,-0.1891744607,-0.6025755801
C,-3.8904975593,0.483495667,0.006344165
N,-2.6745275454,-1.4143685674,0.0141453805
H,-4.3274487927,1.4529588596,-0.1796966722
C,-3.5828010515,-1.4690043635,0.9706992853
H,-3.7338316601,-2.2897305443,1.6569107695
N,-4.3389937128,-0.3490382034,1.0024225122
H,1.8478088533,-0.2584950989,-1.8808457817
H,3.2115460294,-1.1932874885,1.3849932287
H,-5.1035438249,-0.1662182898,1.6408420174
C,1.479427923,-2.9613084849,0.3119707391
H,0.6721887375,-2.5598512558,0.9291112173
H,1.0671031572,-3.7675600863,-0.3074175488
H,2.2236115834,-3.4085277221,0.9803500476
C,3.4428270807,-2.3405470844,-1.169767853
H,4.2338445872,-2.3811470265,-0.410459031
H,3.34781298,-3.3508226424,-1.5866224173
H,3.7637861358,-1.6762250093,-1.9748108715
C,3.1475457362,0.8490256247,0.5286558218
H,3.4074675259,1.3754291575,1.4639398683
O,2.1827789813,1.6181133133,-0.1734780151
C,2.2603637943,3.010629596,0.0954880065
H,3.2703696266,3.3957484727,-0.0889416788
H,1.561163627,3.5073578138,-0.580153352
H,1.9765020516,3.2209571637,1.1341833419
C,4.4112423097,0.6693664336,-0.2922705666
H,4.1774854795,0.2696905795,-1.2806253746
H,4.9020117106,1.6380852202,-0.419995902
H,5.1108748587,-0.0039052106,0.211788427

TS-8c (Felkin-Anh)
 SCF Energy=   -1012.12603246
 Zero-point correction (ZPE)= -1011.75487
 Internal Energy (U)= -1011.73292
 Enthalpy (H)= -1011.73198
 Gibbs Free Energy (G)= -1011.80672
H,-0.0096421606,-1.2420600714,-0.620737143
C,2.1436164527,-0.1140090103,-0.9362683551
O,1.0412573646,-0.5359539326,-1.3893481153
C,1.747836301,1.75142427,0.1723579943
C,0.9316868986,1.0056593122,0.9916485256
N,-0.3406814345,0.6933097779,0.6977730344
C,-1.1597192089,-0.204183298,1.4810820483
C,-2.5600629399,0.4012022532,1.7088866364
C,-1.3384729545,-1.5960362802,0.8557026621
O,-0.7474556619,-1.8869935297,-0.2776964587
O,-2.0617710718,-2.4143144789,1.4115541361
H,-0.6708916517,-0.3631182203,2.4483609295
H,-3.1154900224,-0.2493856667,2.3870422031
H,-2.4298002676,1.3706717062,2.1988221967
H,-0.8040165339,1.1548485568,-0.0820094838
C,-3.3195902675,0.5472145139,0.427286189
C,-4.4179957864,-0.1627383336,0.0154523299
N,-2.9349233272,1.4314272228,-0.5667031861
H,-5.0018391281,-0.9313651664,0.4986804228

C,-3.7969668921,1.2527838852,-1.5499624393
H,-3.8038573582,1.781592157,-2.492200322
N,-4.7088003464,0.303336806,-1.2434309923
H,1.3268732009,0.5656219793,1.9063080689
H,2.7317625931,0.5688710829,-1.5668398203
H,-5.4735508655,0.0016461584,-1.8347913405
C,1.1679653878,2.5301982924,-0.9819017298
H,0.4750376426,1.9344574315,-1.5860888911
H,0.6263948064,3.4125217401,-0.6187038969
H,1.9705084444,2.879358906,-1.6391980319
C,3.0910916958,2.2084249465,0.6736623997
H,3.8756043762,2.0055179846,-0.0681421649
H,3.0835800291,3.2916756476,0.8436592317
H,3.3679182147,1.7224049503,1.6133318719
C,3.0169605095,-0.9656593806,-0.0135068239
H,3.5243868498,-0.3141739082,0.7080741131
O,4.0087089203,-1.5076945046,-0.8940662158
C,5.2470133514,-1.7664221498,-0.2466198402
H,5.1311196761,-2.4897178944,0.5687831473
H,5.9206225417,-2.1822510326,-0.9975786815
H,5.674023011,-0.8373013803,0.150727913
C,2.2705144555,-2.0800604089,0.6974387075
H,2.9704204855,-2.673757446,1.2913800055
H,1.5092940717,-1.6844939663,1.3768001349
H,1.7834503186,-2.7343537608,-0.030494259

TS-9a
 SCF Energy=   -1164.73921617
 Zero-point correction (ZPE)= -1164.32682
 Internal Energy (U)= -1164.30286
 Enthalpy (H)= -1164.30191
 Gibbs Free Energy (G)= -1164.37967
C,-0.5028519011,0.1461035629,-1.5294891081
C,0.3355539711,-0.6503894937,-0.7841497078
C,0.5212843954,-2.0938463577,-1.1723361138
O,-1.6014167314,4.5669855974,-2.9630658233
C,-1.1711448828,-0.7474432673,0.8694339425
O,-1.3340037853,0.4142185927,1.3166852081
H,-1.1809150859,-0.3113583046,-2.249711074
H,-1.2380605288,1.9883511001,-3.3389109378
H,-3.4791920747,2.6194584094,-2.8594912371
H,0.4810618886,-2.7506490277,-0.2923704522
H,-0.238270629,-2.427537496,-1.8854882127
H,1.5060098761,-2.2407628509,-1.6331611636
N,-0.6122722567,1.480189942,-1.4090312923
C,-2.9364285998,2.1324121151,-2.0463622789
C,-1.4259153675,2.2908492898,-2.3021478539
C,-1.0210323854,3.7733662596,-2.1765750967
O,-0.1695988695,4.0812572324,-1.3021812707
H,0.0499099083,2.003058368,-0.8446350301
H,-3.1875556595,1.0670638393,-2.0616463587
C,-3.3867049979,2.7446387373,-0.763942607
C,-4.2152893138,3.8086320191,-0.5495204221
N,-2.9896794767,2.3035597672,0.4838353439
H,-4.7368401472,4.4473688809,-1.2445975147
C,-3.5616053666,3.0499729606,1.419769875
H,-2.3696281497,1.472130707,0.6959014419
H,-4.8509257918,4.6824856947,1.2962691834
H,-3.4439168923,2.9338946081,2.4865130846
N,-4.3069179809,3.9738269376,0.814897983
C,1.4356559266,-0.0367416831,0.0451875513
H,1.0941574116,0.8279470618,0.6235655818
H,1.8331499534,-0.7732078041,0.7514603352
H,2.2660496031,0.2927040469,-0.5923057699
H,-0.3907089788,-1.3889479298,1.3068810137
C,-2.3334938277,-1.525982308,0.2899215465
C,-3.1995191822,-2.1416882772,1.4277016284
O,-3.2277447081,-0.6513986446,-0.3812121162
O,-4.4551750639,-1.4818775544,1.296183097
H,-2.808686955,-1.9337099264,2.4260111798
H,-3.3074113772,-3.2220788947,1.2944863107
C,-4.5568623501,-1.0660087699,-0.0614589442
C,-5.4910340061,0.1180514814,-0.1496042362
C,-4.9819303403,-2.2208304851,-0.9576789675
H,-5.4510487569,0.5461605485,-1.1551225141
H,-6.5150320246,-0.2066371333,0.0509392759
H,-5.2077608405,0.8788292643,0.5816044558
H,-5.9694312129,-2.5781885029,-0.6547633876
H,-5.0327625752,-1.8803778081,-1.9953110889
H,-4.2733939755,-3.0520134133,-0.8977356299
H,-1.9720434246,-2.3130998716,-0.3786863284

TS-9b
 SCF Energy=   -1164.73272429
 Zero-point correction (ZPE)= -1164.31983
 Internal Energy (U)= -1164.29630
 Enthalpy (H)= -1164.29536
 Gibbs Free Energy (G)= -1164.37253
H,1.2538138135,1.670606243,0.3418634743
C,2.0144250434,-0.7177233773,0.3658823672
O,1.6066247032,0.3110391064,0.9590789819
C,0.2285871394,-1.6380422856,-0.7079317319
C,0.0997497935,-0.4305167001,-1.346011768
N,-0.5097012235,0.6410442059,-0.7997966757

C,-0.6109989484,1.9390033432,-1.4269923553
C,-2.0499270376,2.4841865773,-1.3085932735
C,0.3437027493,2.9946786604,-0.8487754588
O,1.1785181185,2.6650421431,0.1128318254
O,0.3099679339,4.1409646723,-1.2748857212
H,-0.3476585517,1.8373497933,-2.4853151872
H,-2.1259989761,3.4053927651,-1.8893900239
H,-2.7233826645,1.744839454,-1.7523257839
H,-1.0208025015,0.5331235875,0.0733573626
C,-2.4209868565,2.7605059756,0.1148347738
C,-2.6262915769,3.9764364987,0.7143950551
N,-2.5341467579,1.7509889166,1.0562679537
H,-2.615337554,4.9831249735,0.3248619573
C,-2.8082897042,2.3593239423,2.1946748117
H,-2.9681170831,1.8795480185,3.1494150205
N,-2.8769909529,3.6997259266,2.0361574709
H,0.5531455917,-0.269636259,-2.3237851398
H,1.9760247028,-1.6799793939,0.8994937732
H,-3.082472404,4.3731980824,2.7639164086
C,-0.5595261149,-1.9270168149,0.5453673273
H,-0.4989279262,-1.1139975738,1.2778479173
H,-1.6194110901,-2.0854090185,0.3086458913
H,-0.1870297438,-2.8367358312,1.0260005124
C,0.7737128381,-2.8294743281,-1.4468112331
H,1.5362183715,-3.3456490786,-0.8482294565
H,-0.0257148969,-3.5553239113,-1.6397981587
H,1.2172877666,-2.5487969339,-2.4064054066
C,3.0998934881,-0.6776418477,-0.7062682722
C,3.2725782489,0.6442906962,-1.4366460001
O,4.3471210222,-0.8043983793,-0.0078603796
O,4.0680876094,1.3962322309,-0.5260801117
H,2.3475855541,1.1894115902,-1.6213488389
H,3.7983988442,0.4927340742,-2.3862373943
C,4.9801949728,0.4879747196,0.0829358826
C,5.1517386831,0.8801560294,1.534151801
C,6.2884171671,0.4346674297,-0.6855173325
H,5.8320900042,0.1828107321,2.0294721565
H,5.5746690054,1.8861524985,1.5988468396
H,4.1822258654,0.8616345045,2.0386785404
H,6.7996232086,1.3984094055,-0.6146573368
H,6.9362165263,-0.3382150728,-0.2635836489
H,6.1005047252,0.2032600972,-1.7376911987
H,3.0039809841,-1.5292256078,-1.3815030471