catalysts

Protonated Chiral 1,2-Diamine Organocatalysts for *N*-Selective Nitroso-Aldol Reaction

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Supporting Information

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Additional test results for optimization conditions

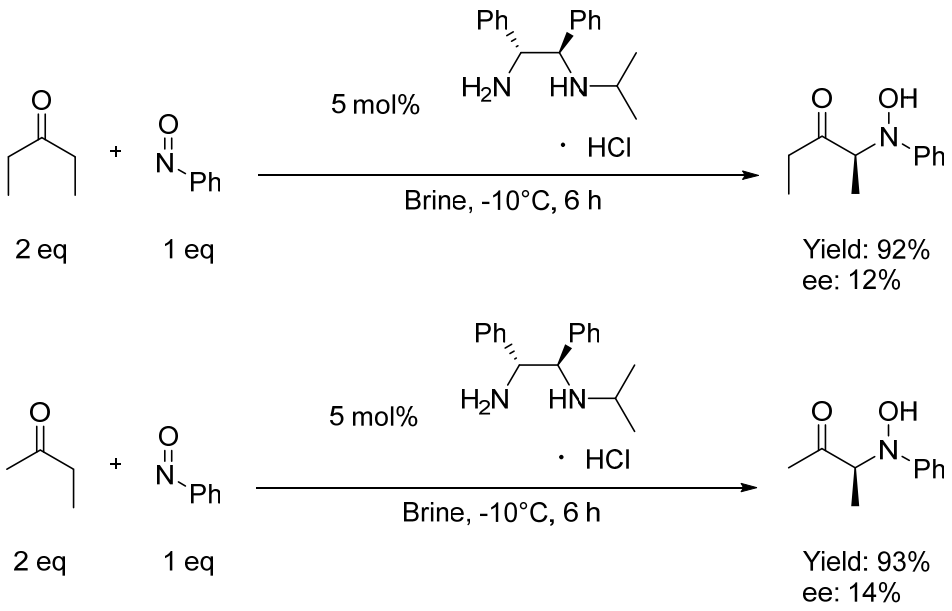
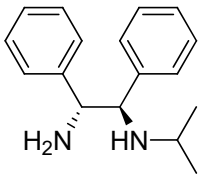


Figure S1. Results to changes in ketone types under optimized experimental conditions.

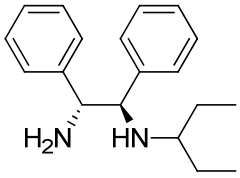
Compound characterization data

(1*R*,2*R*)-*N*-isopropyl-1,2-diphenyl ethylenediamine(1a)[1]



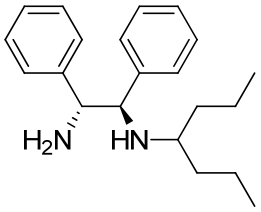
$[\alpha]_D$ ^{25} +24.5° (c = 5.1, $CHCl_3$), IR (KBr): 3378, 3023, 2958, 1609, 1454, 767, 718 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 – 7.07 (m, 10H), 3.96 (d, 1H, *J* = 7.5 Hz), 3.79 (d, 1H, *J* = 7.2 Hz), 2.60 – 2.47 (m, 1H), 1.74 (s, 3H), 0.95 (d, 3H, *J* = 2.7 Hz), 0.93 (d, 3H, *J* = 2.7 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ143.3, 141.9, 127.7 (2C), 127.7 (2C), 127.5 (2C), 126.9 (2C), 126.6, 126.5, 66.8, 61.8, 45.6, 24.3, 21.7, HRMS (FAB+) for $C_{17}H_{23}N_2$ $[M+H]^+$, Calcd: 255.1861, Found: 255.1863

(1*R*,2*R*)-*N*-(3-pentyl)-1,2-diphenyl ethylenediamine(1b)[1]



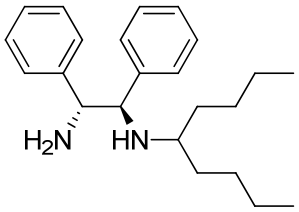
$[\alpha]_D$ ^{25} +9.4 (c = 6.3, $CHCl_3$), IR (KBr): 3374, 3031, 2953, 1605, 1458, 767, 702 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.09 (m, 10H), 3.95 (d, 1H, *J* = 6.8 Hz), 3.77 (d, 1H, *J* = 6.4 Hz), 2.21 – 2.16 (m, 1H), 1.71 (s, 3H), 1.37 – 1.19 (m, 4H), 0.76 (t, 3H, *J* = 7.6 Hz), 0.68 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ143.5, 142.1, 127.8 (2C), 127.7 (2C), 126.9 (2C), 126.6 (2C), 126.5 (2C), 66.6, 62.0, 56.1, 26.6, 24.1, 10.2, 8.2; HRMS (FAB+) for $C_{19}H_{27}N_2$ $[M+H]^+$, Calcd: 283.2174, Found: 283.2176

(1*R*,2*R*)-*N*-(4-heptyl)-1,2-diphenyl ethylenediamine(1c)[1]



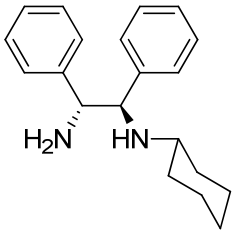
$[\alpha]_D^{25}$ +16.7 (c = 17.3, $CHCl_3$), IR (KBr): 3382, 3023, 2953, 1597, 1450, 759, 710 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.10 (m, 10H), 3.95 (d, 1H, *J* = 7.2 Hz), 3.78 (d, 1H, *J* = 7.2 Hz), 2.30 – 2.24 (m, 1H), 1.69 (s, 3H), 1.33 – 1.07 (m, 8H), 0.80 (t, 3H, *J* = 6.8 Hz), 0.74 (t, 3H, *J* = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ143.6, 142.3, 127.9 (2C), 127.8 (2C), 127.7 (2C), 126.9 (2C), 126.7, 126.6, 66.8, 62.0, 53.6, 37.2, 35.2, 18.9, 17.6, 14.4, 14.1; HRMS (FAB+) for $C_{21}H_{31}N_2$ $[M+H]^+$, Calcd: 311.2487, Found: 311.2480

(1*R*,2*R*)-*N*-(5-nonyl)-1,2-diphenyl ethylenediamine(1d)[1]



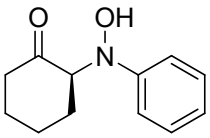
$[\alpha]_D^{25}$ -4.1 (c = 8.5 , $CHCl_3$), IR (KBr): 3370, 3031, 2925, 1601, 1458, 767, 702 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.10 (m, 10H), 3.96 (d, 1H, *J* = 6.8 Hz), 3.78 (d, 1H, *J* = 6.8 Hz), 2.29 – 2.23 (m, 1H), 1.74 (s, 3H), 1.31 – 0.99 (m, 12H), 0.83 (t, 3H, *J* = 6.8 Hz), 0.80 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ143.5, 142.2, /126.6, 126.6, 66.6, 61.9, 53.8, 34.4, 32.2, 27.9, 26.3, 23.0, 22.7, 14.0, 13.9; HRMS (FAB+) for $C_{23}H_{35}N_2$ $[M+H]^+$, Calcd: 339.2800, Found: 339.2806

(1*R*,2*R*)-*N*-(cyclohexyl)-1,2-diphenyl ethylenediamine(1e)[1]



$[\alpha]_D^{25}$ +14.8 (c = 31.8, $CHCl_3$), IR (KBr): 3362, 3027, 2933, 2847, 1609, 1458, 751, 706 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.23 – 7.10 (m, 10H), 3.95 (d, 1H, *J* = 6.9 Hz), 3.85 (d, 1H, *J* =6.9 Hz), 2.23 – 2.16 (m, 1H), 1.69 (s, 3H), 1.88 – 1.47 (m, 5H), 1.10 – 0.90 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ143.4, 142.2, 127.8 (2C), 127.7 (2C), 127.5 (2C), 126.9 (2C), 126.6, 126.5, 66.1, 61.9, 53.3, 34.7, 32.4, 26.0, 24.9, 24.4; HRMS (FAB+) for $C_{20}H_{27}N_2$ $[M+H]^+$, Calcd: 295.2174, Found: 295.2178

(*S*)-2-(*N*-Phenyl hydroxyamino)-cyclohexanone(2a)[2]



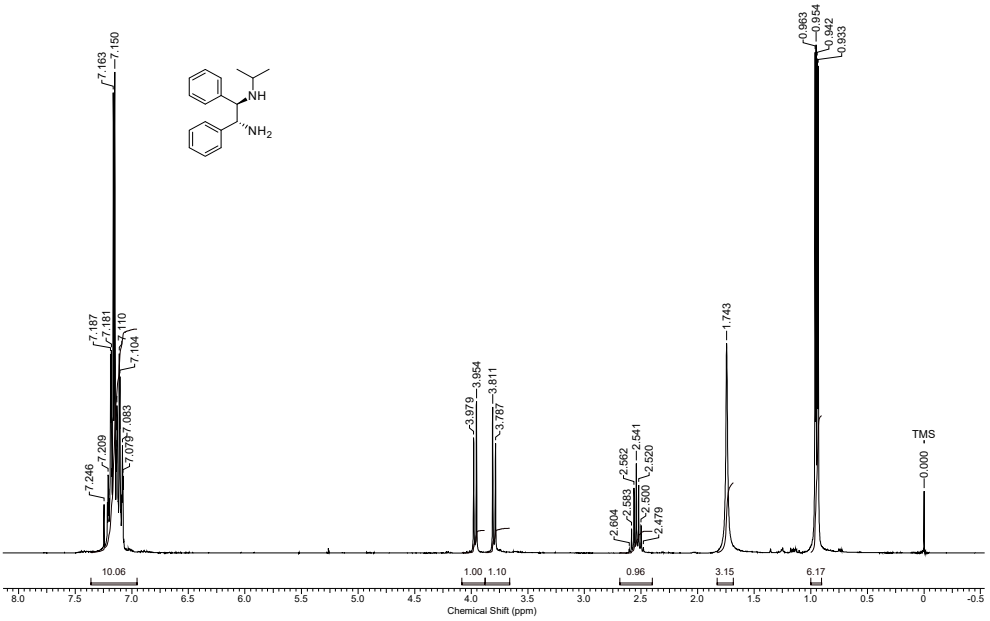
$[\alpha]_D^{25}$ +189.2 (c = 9.8, $CHCl_3$), IR (KBr) : 3398, 3058, 2937, 1712, 1598, 1492, 1448, 1400, 1290, 1122, 935 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.26 (t, 2H, *J* = 8.4 Hz, Ar-*H*), 7.05 (d, 2H, *J* =7.5 Hz, Ar-*H*), 6.94 (t, 1H, *J* = 7.2 Hz, Ar-*H*), 6.27 (s, 1H, O*H*), 4.23 (t, 1H, *J* = 9.6 Hz, C*H*), 1.63 – 2.58 (m, 8H, eight proton of CH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.7, 150.1, 128.6 (2C), 121.6, 115.9 (2C), 72.5, 42.0, 27.8, 27.2, 24.3; HRMS (FAB+) for $C_{12}H_{15}NO_2$ $[M]^+$, Calcd 205.1103, Found 205.1106; Enantiomeric excess was determined by HPLC with a Chiralpak AD-H column (97.6:2.4 hexane:2-propanol), 1.0 mL/min; major enantiomer t_r = 42.5 min, minor enantiomer t_r = 50.3 min.

References

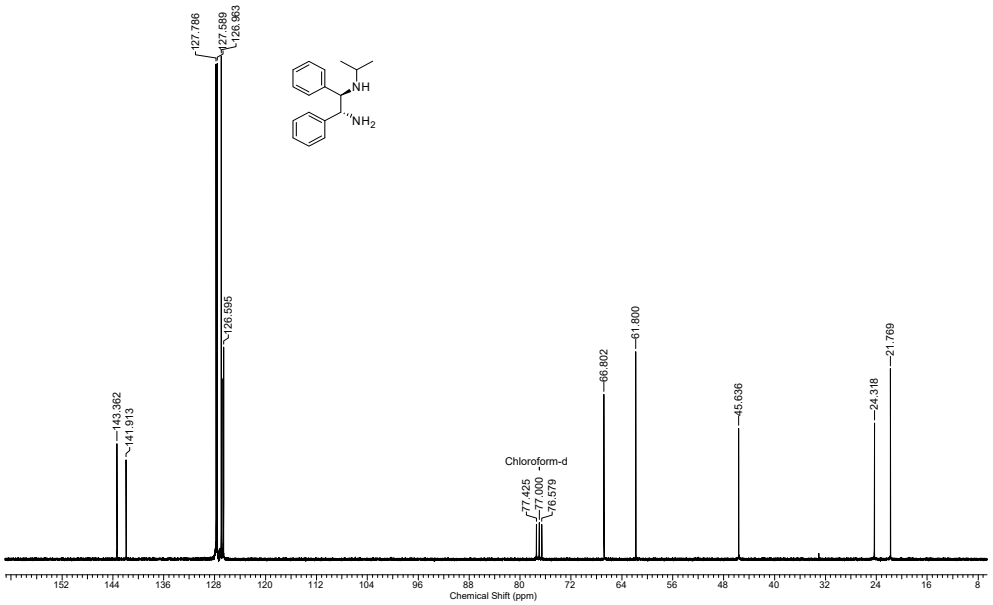
1. Shim, J.H.; Kim, M.J.; Lee, J.Y.; Kim, K.H.; Ha, D.C. Organocatalytic Asymmetric Aldol Reaction Using Protonated Chiral 1,2-Diamines. *Tetrahedron Lett*. **2020**, *61*, 152295.
2. Momiyama, N.; Yamamoto, H. Brønsted Acid Catalysis of Achiral Enamine for Regio- and Enantioselective Nitroso Aldol Synthesis. *J. Am. Chem. Soc*. **2005**, *127*, 4, 1080–1081.
3. Li, Y.; Zhang, L.; Yan, N.; Meng, X.; Zhao. Y. Acid/Base-Co-catalyzed Direct Oxidativea-Amination of CyclicKetones: Using Molecular Oxygen as the Oxidant. *Adv. Synth. Catal.* **2018**, *360*, 455–461.

Copy of catalysts and products data (^{1}H, ^{13}C NMR, HR-MS)

^{1}H NMR(1a)



^{13}C NMR(1a)

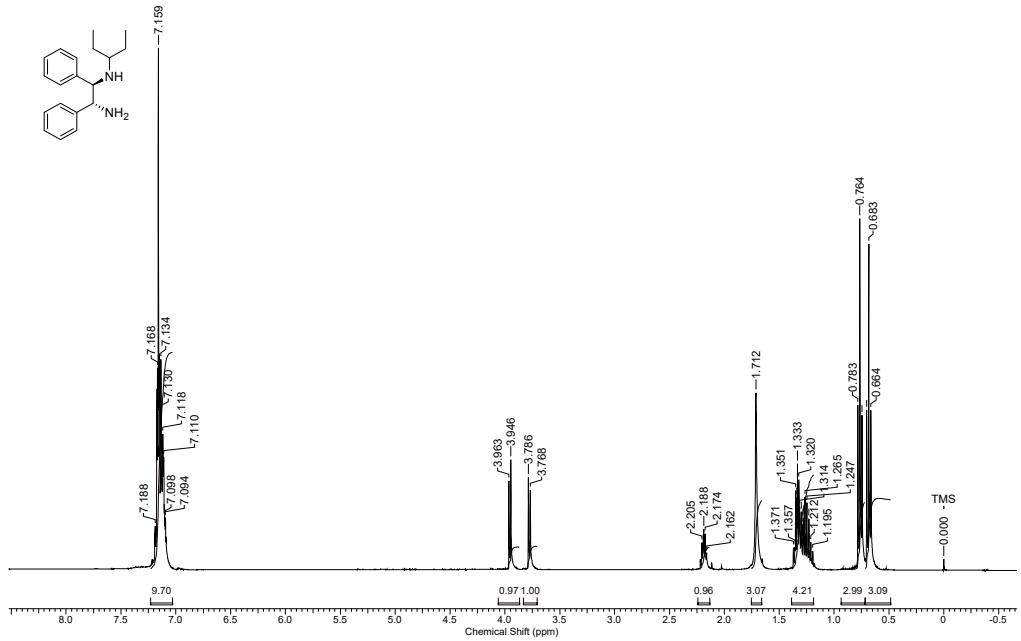


HR-MS(1a)

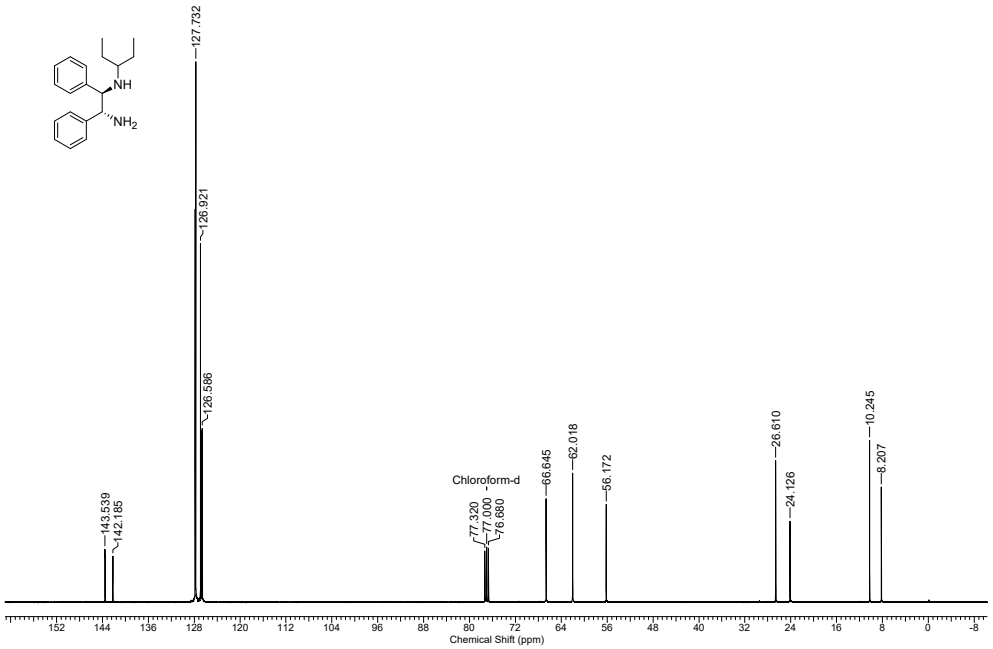
```
Note : in MC with NBA
Inlet : Direct                          Ion Mode : FAB+
RT : 2.52 min                           Scan#: 28
Elements : C 17/0, H 23/0, N 2/0
Mass Tolerance      : 5ppm, 5mmu if m/z > 1000
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z Int%   Err[ppm / mmu]    U.S.  Composition
  255.1863    58.9     +0.8 /  +0.2    7.5  C 17 H 23 N 2
```

^{1}H NMR(1b)



^{13}C NMR(1b)

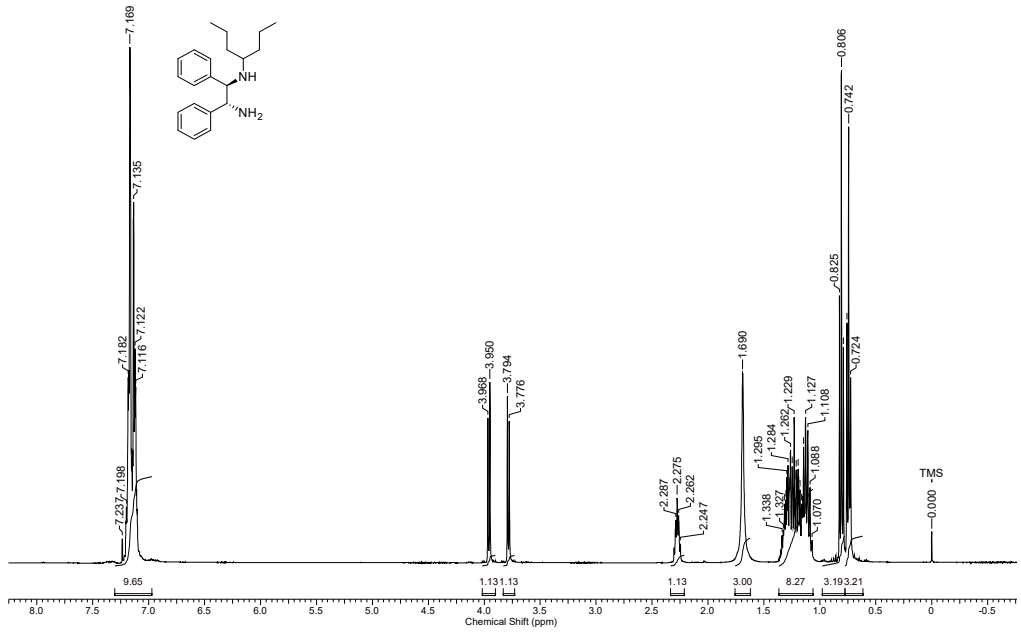


HR-MS(1b)

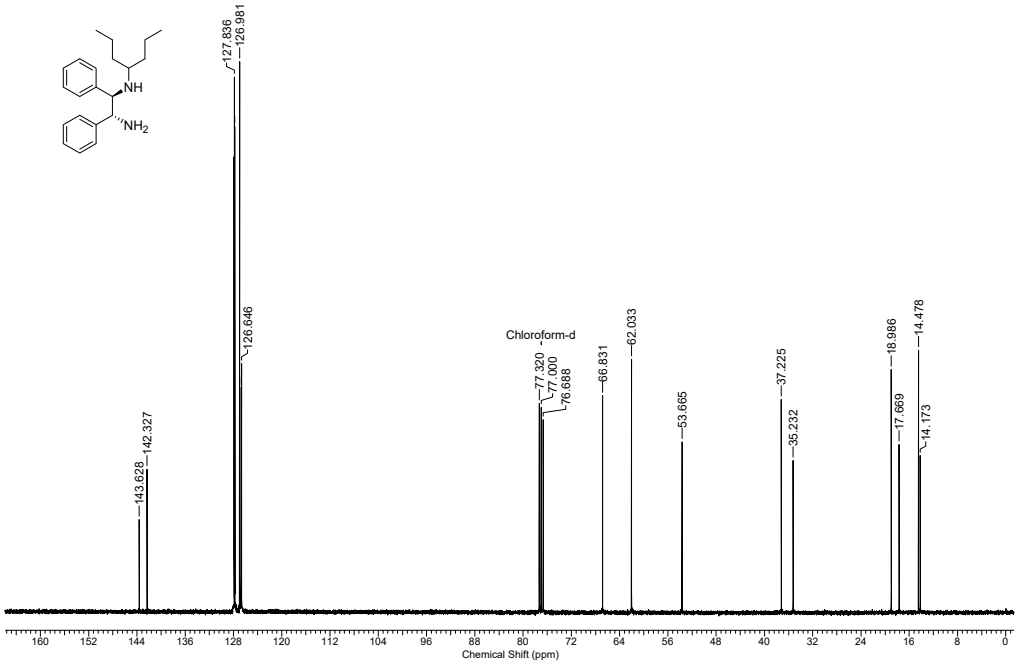
Note : in MC with NBA
Inlet : Direct Ion Mode : FAB+
RT : 0.75 min Scan#: 10
Elements : C 19/0, H 27/0, N 2/0
Mass Tolerance : 20ppm, 5mmu if m/z > 250
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
283.2176	100.0	+0.5 / +0.1	7.5	C 19 H 27 N 2

^{1}H NMR(1c)



^{13}C NMR(1c)

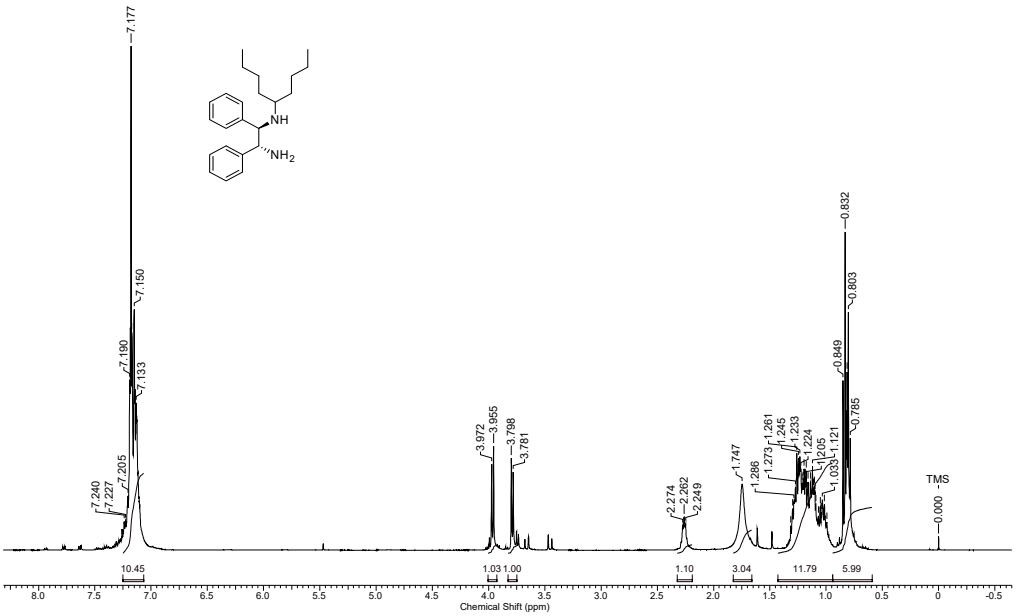


HR-MS(1c)

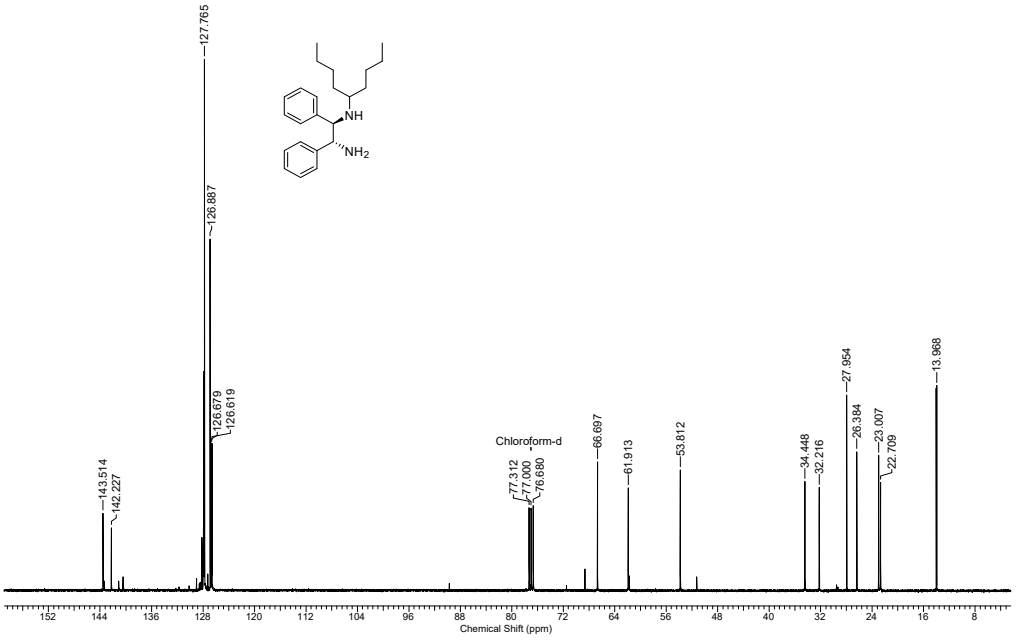
Note : in MC with NBA
Inlet : Direct Ion Mode : FAB+
RT : 1.75 min Scan#: 22
Elements : C 20/0, H 27/0, N 2/0
Mass Tolerance : 5ppm, 5mmu if m/z > 1000
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
295.2178	100.0	+1.4 / +0.4	8.5	C 20 H 27 N 2

^{1}H NMR(1d)



^{13}C NMR(1d)

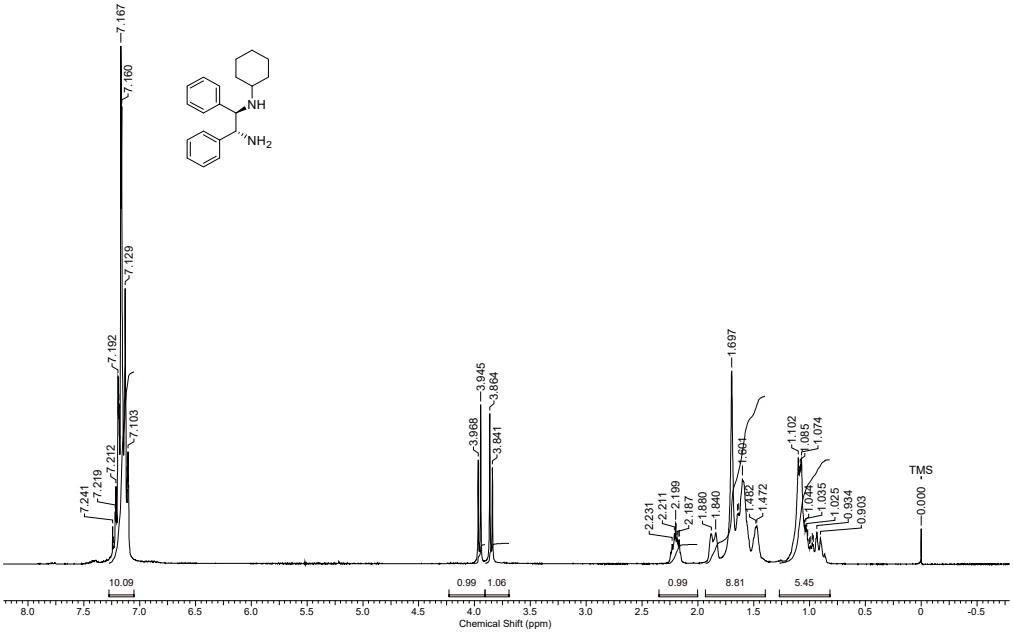


HR-MS(1d)

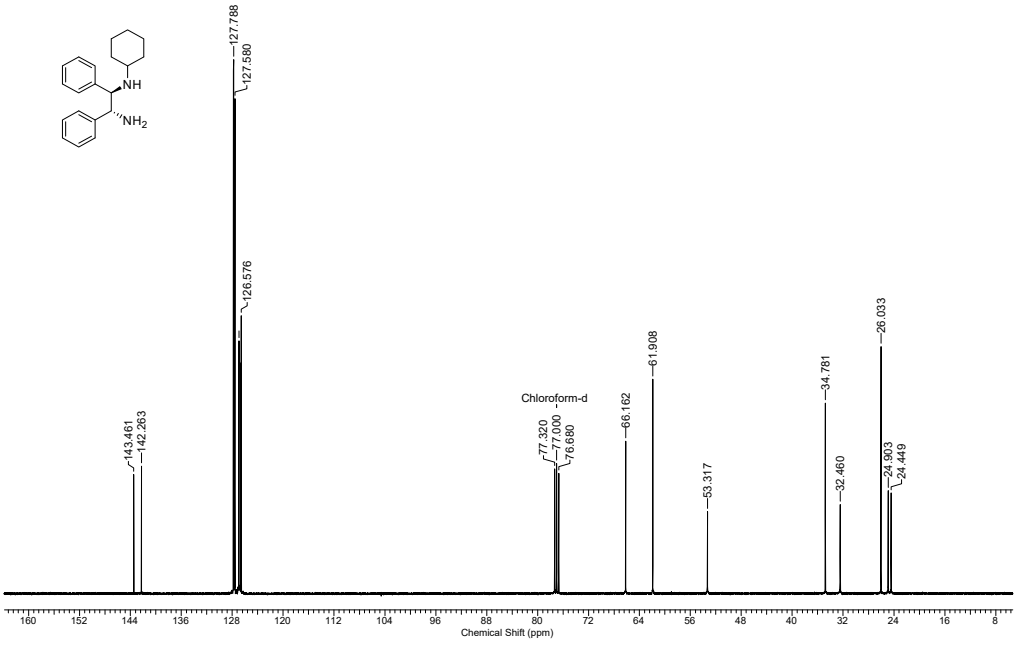
Note : in MC with NBA
Inlet : Direct
RT : 1.96 min
Ion Mode : FAB+
Scan#: 26
Elements : C 23/0, H 35/0, N 2/0
Mass Tolerance : 20ppm, 50mmu if m/z > 2500
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
339.2806	100.0	+1.6 / +0.6	7.5	C 23 H 35 N 2

^{1}H NMR(1e)



^{13}C NMR(1e)

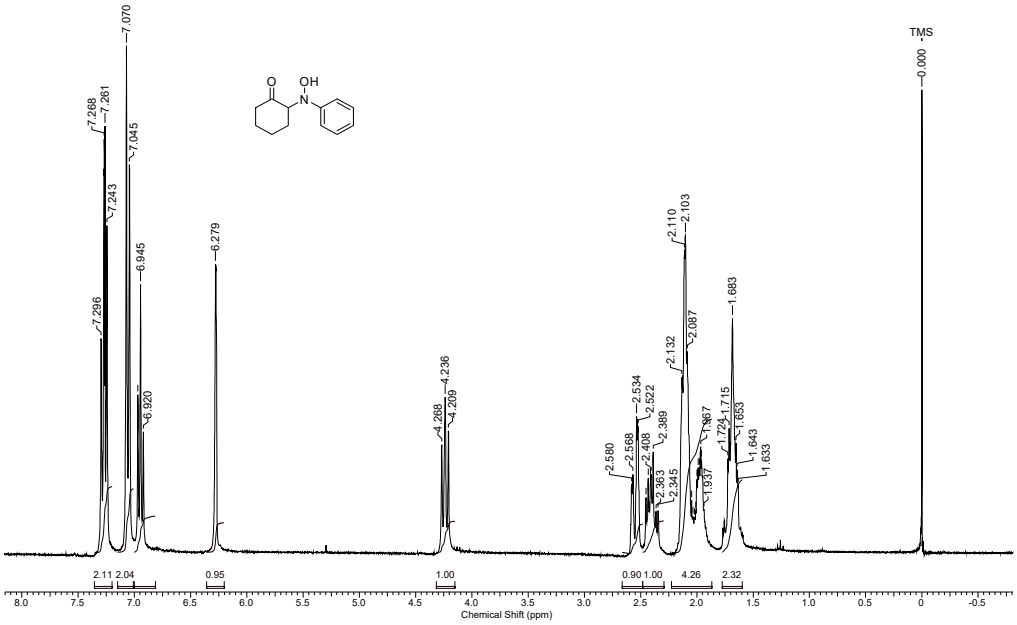


HR-MS(1e)

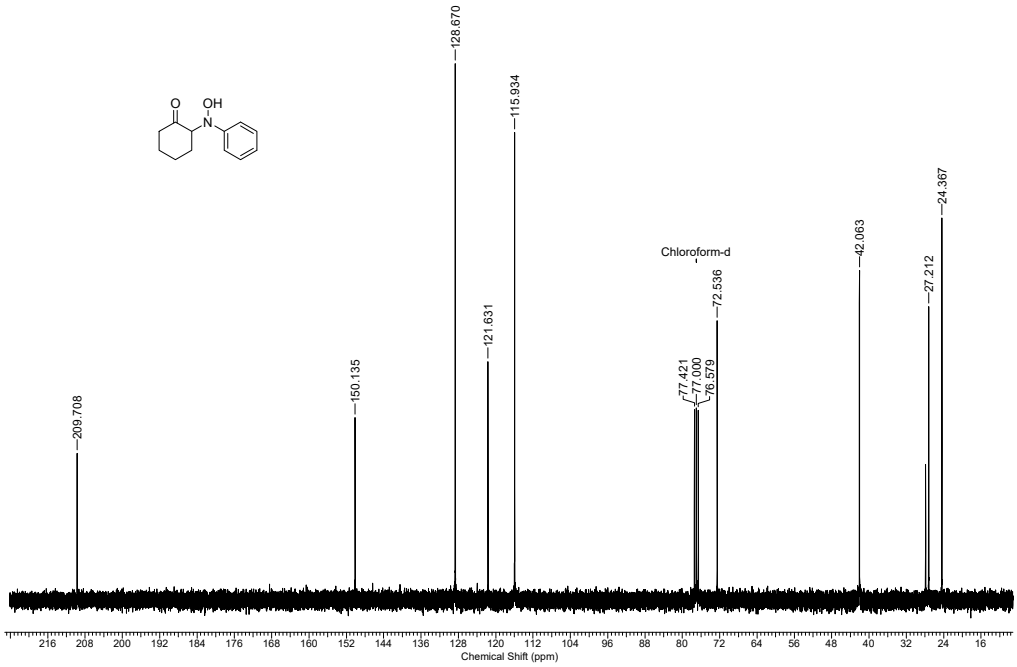
Note : in MC with NBA
Inlet : Direct Ion Mode : FAB+
RT : 1.75 min Scan#: 22
Elements : C 20/0, H 27/0, N 2/0
Mass Tolerance : 5ppm, 5mmu if m/z > 1000
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
295.2178	100.0	+1.4 / +0.4	8.5	C 20 H 27 N 2

^{1}H NMR(2a)



^{13}C NMR(2a)



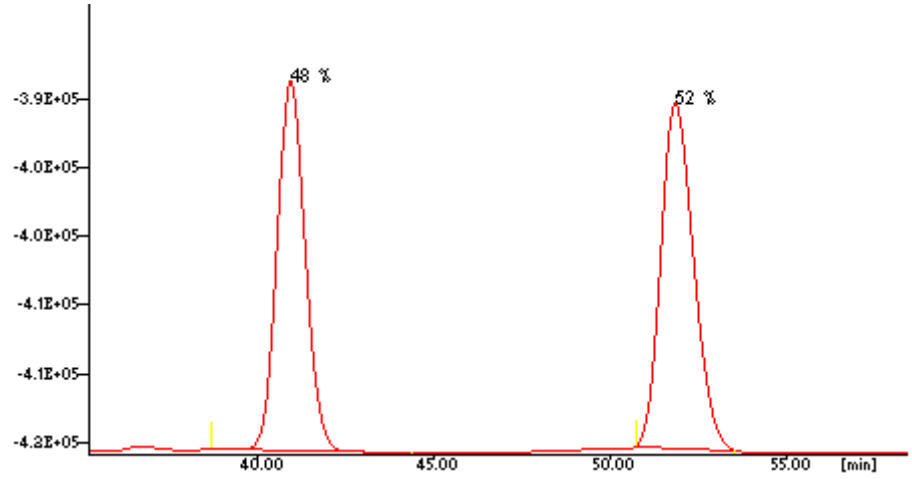
HR-MS(2a)

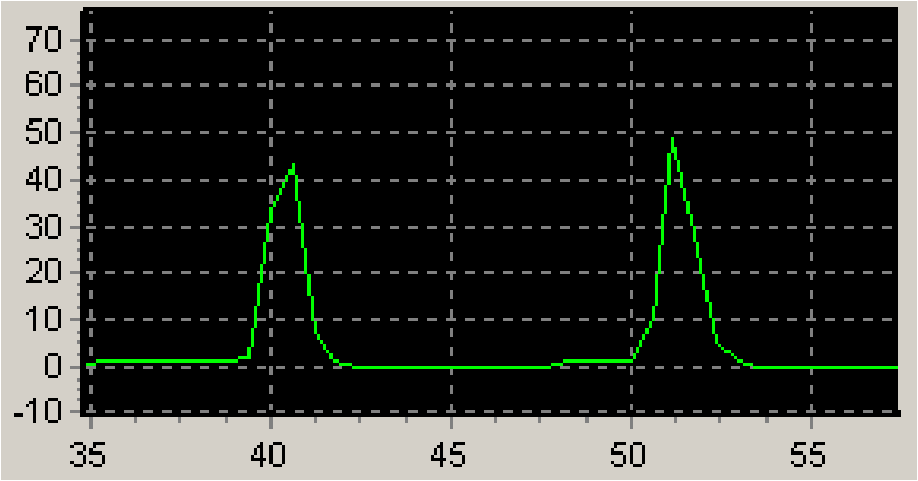
Note : in with MC
Inlet : Direct Ion Mode : FAB+
RT : 3.10 min Scan#: 33
Elements : C 12/0, H 15/0, O 2/0, N 1/0
Mass Tolerance : 20ppm, 50mmu if m/z > 2500
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%					
205.1106	18.2					
Estimated m/z	Error[ppm]	U.S.	C	H	O	N
205.1103	+1.7	6.0	12	15	2	1

Copy of table data (HPLC Chromatograms)

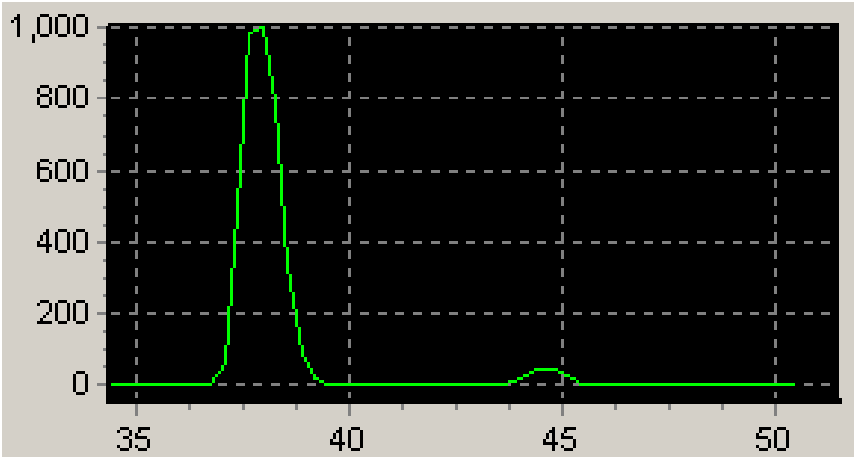
2-(*N*-Phenyl hydroxyamino)-cyclohexanone (racemic)





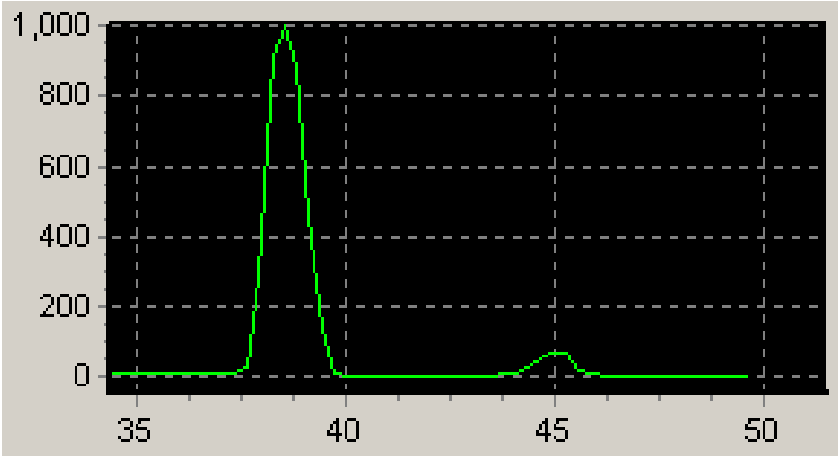
Peak Name	RT (min)	% Area	ee (%)
(*S*)	40.95	48	-
(*R*)	51.85	52	

(Table 1, entry 1)



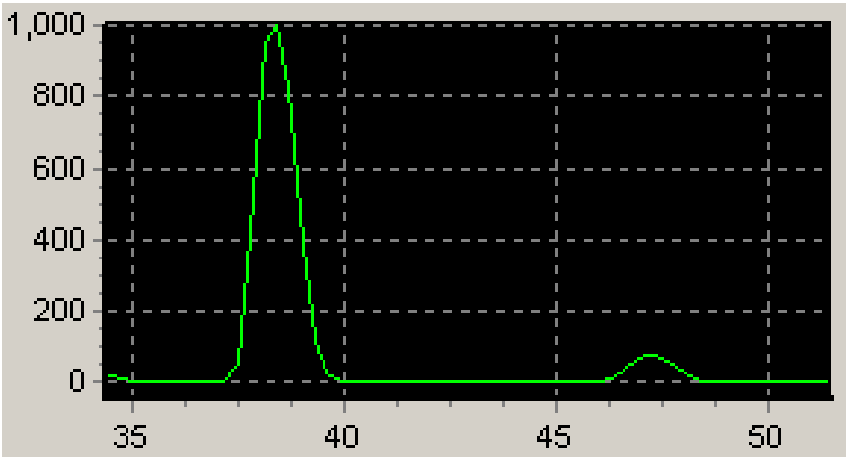
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.29	97	94
(*R*)	44.60	3	

(Table 1, entry 2)



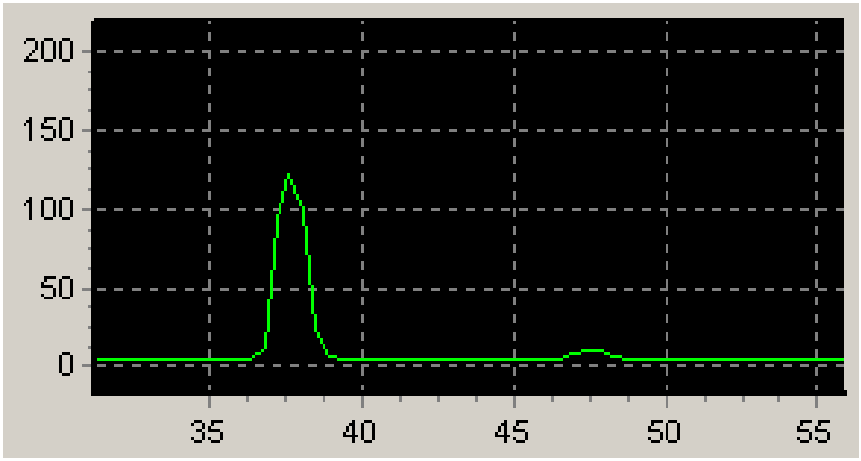
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.87	95.5	91
(*R*)	45.38	4.5	

(Table 1, entry 3)



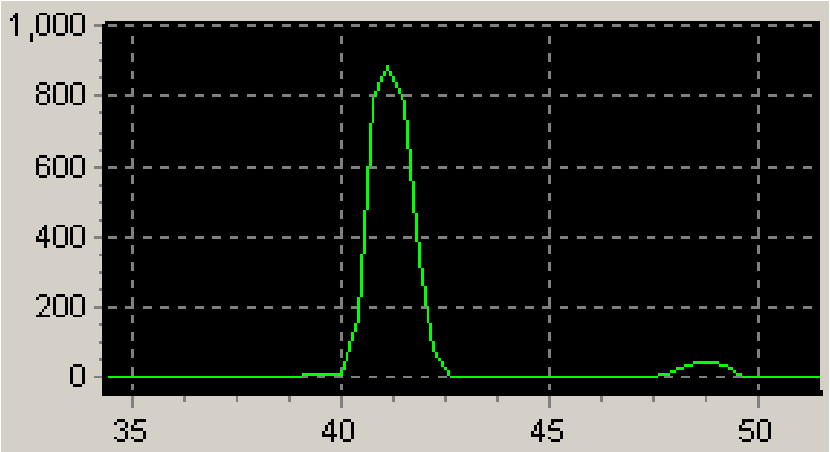
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.95	95	90
(*R*)	47.56	5	

(Table 1, entry 4)



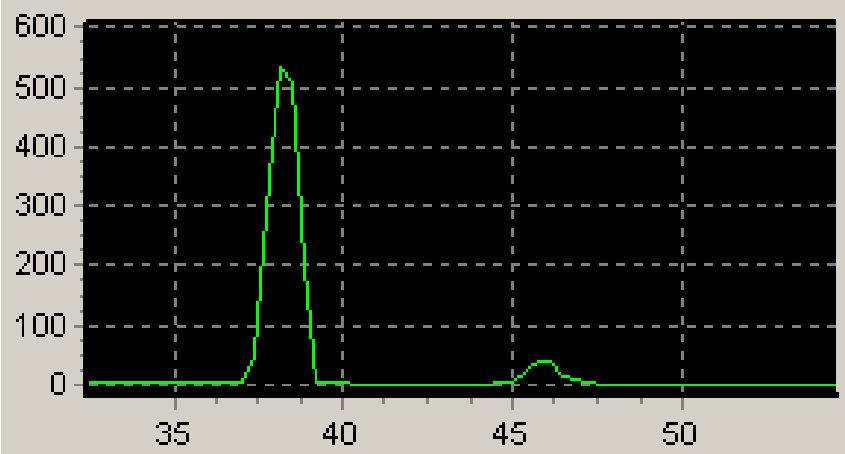
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.19	95	90
(*R*)	48.14	5	

(Table 1, entry 5)



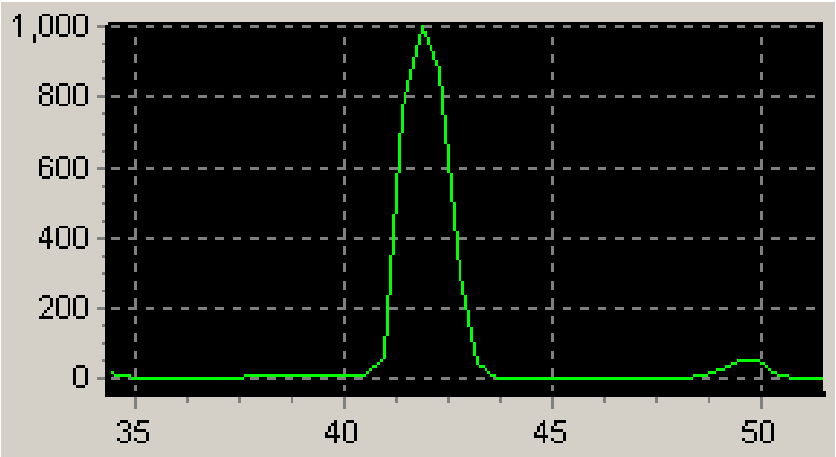
Peak Name	RT (min)	% Area	ee (%)
(*S*)	41.23	96	92
(*R*)	49.12	4	

(Table 1, entry 6)



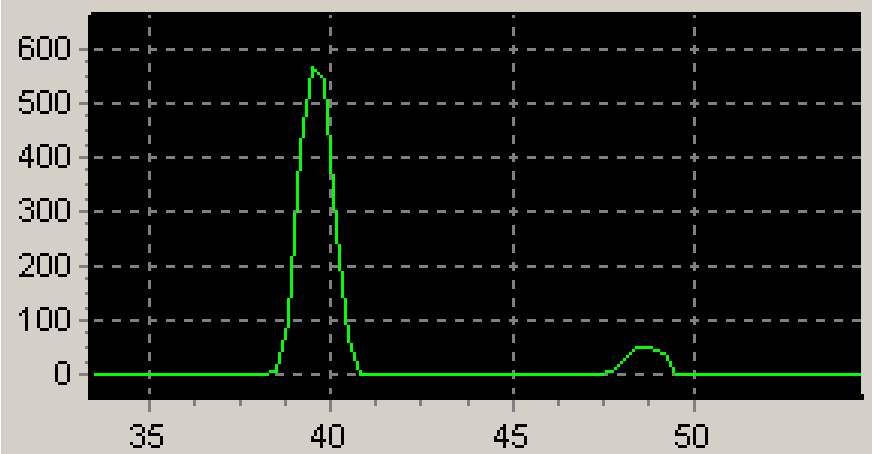
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.86	90.5	81
(*R*)	46.05	9.5	

(Table 1, entry 7)



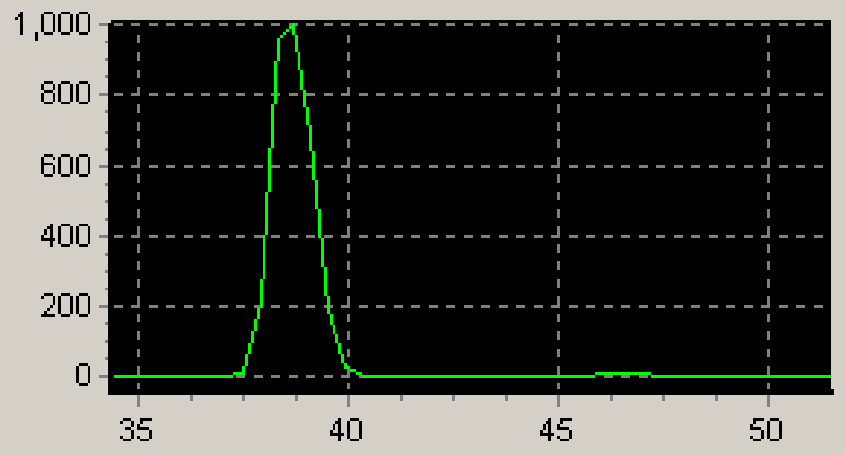
Peak Name	RT (min)	% Area	ee (%)
(*S*)	42.53	97	94
(*R*)	49.24	3	

(Table 1, entry 8)



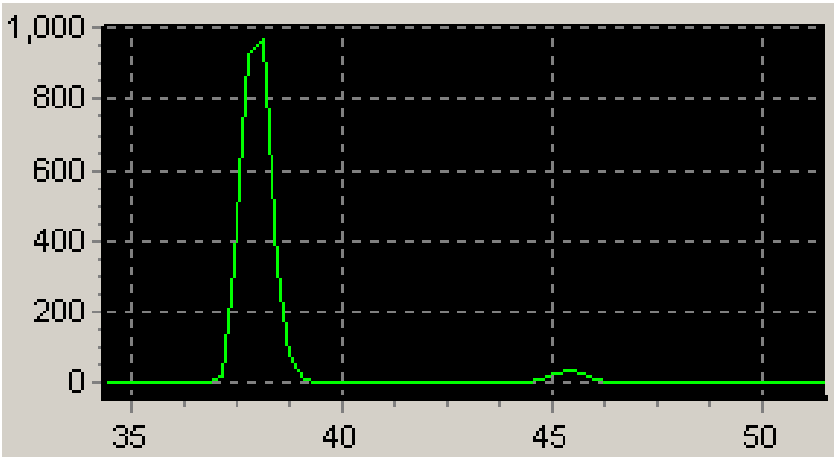
Peak Name	RT (min)	% Area	ee (%)
(*S*)	39.19	93	86
(*R*)	48.86	7	

(Table 2, entry 1)



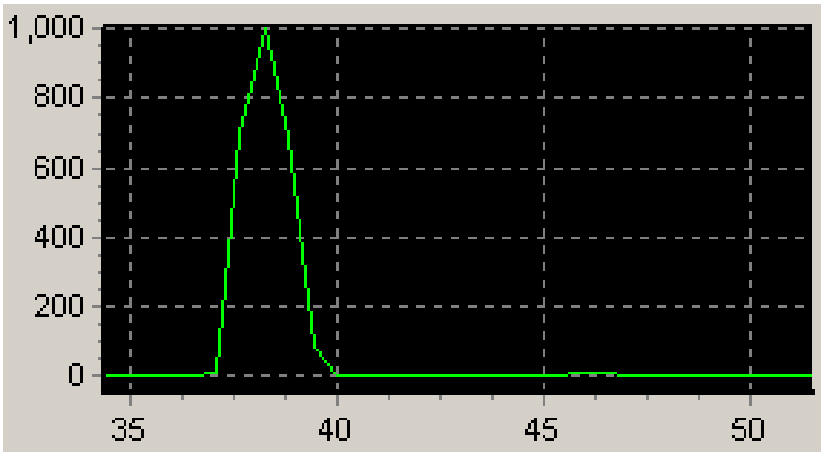
Peak Name	RT (min)	% Area	ee (%)
(*S*)	39.18	99.5	99
(*R*)	46.84	0.5	

(Table 2, entry 3)



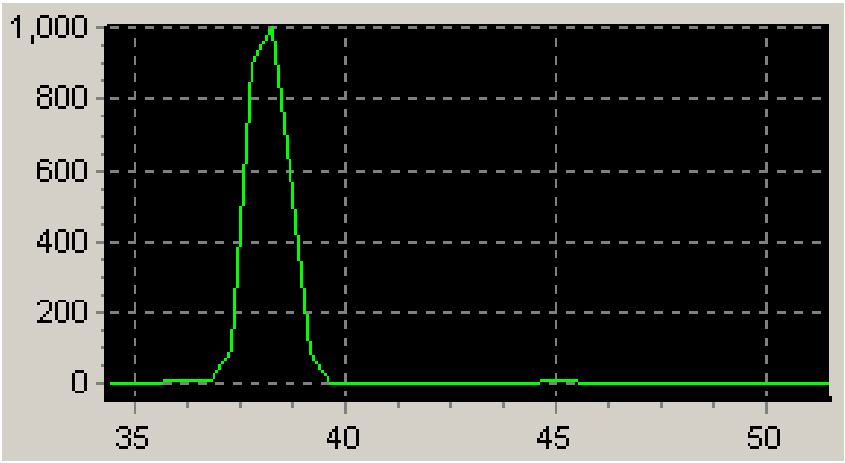
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.82	98	96
(*R*)	45.34	2	

(Table 2, entry 4)



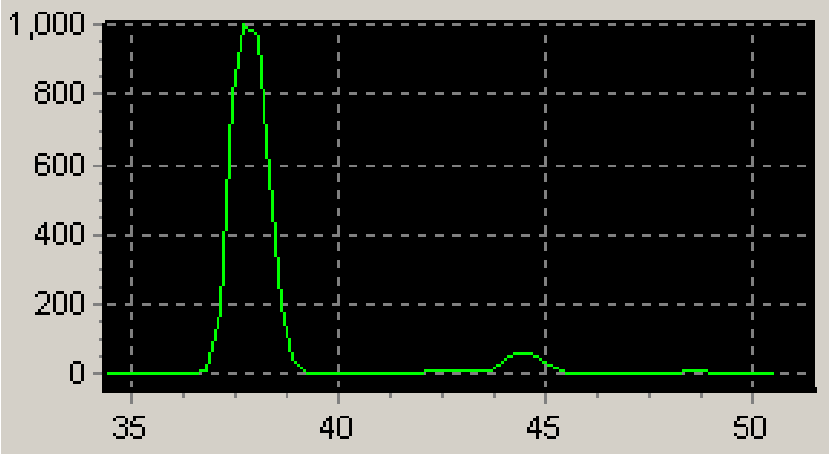
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.81	99	98
(*R*)	46.51	1	

(Table 2, entry 5)



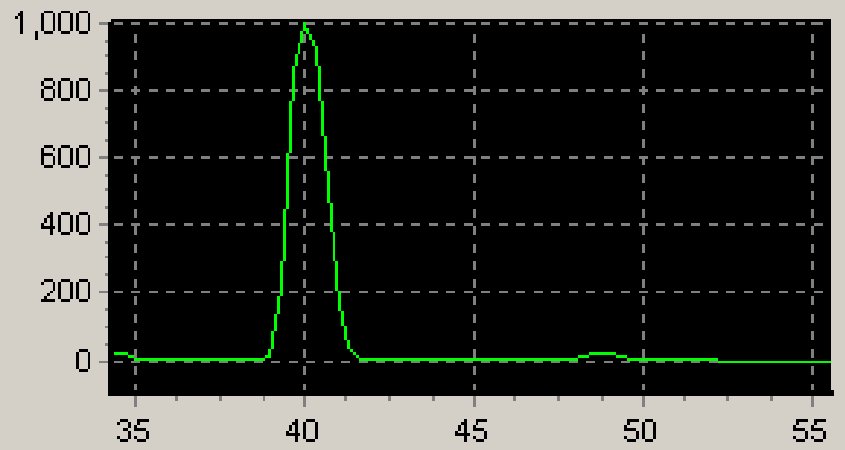
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.88	99	98
(*R*)	45.02	1	

(Table 3, entry 1)



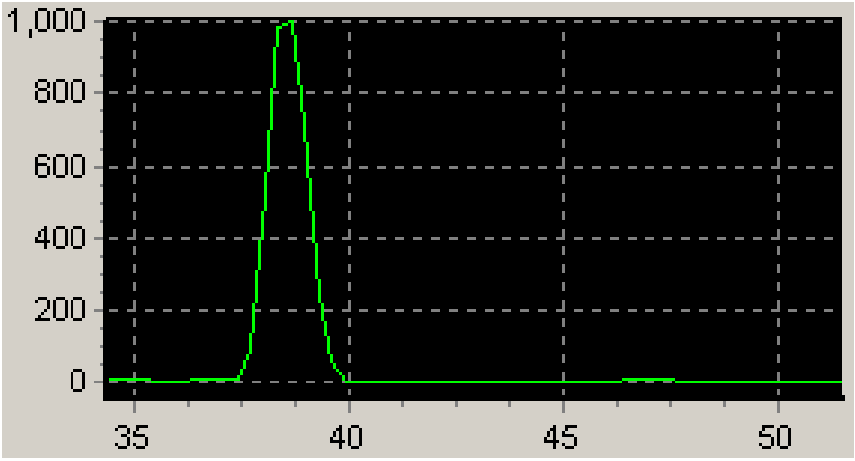
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.11	96	92
(*R*)	44.74	4	

(Table 3, entry 2)



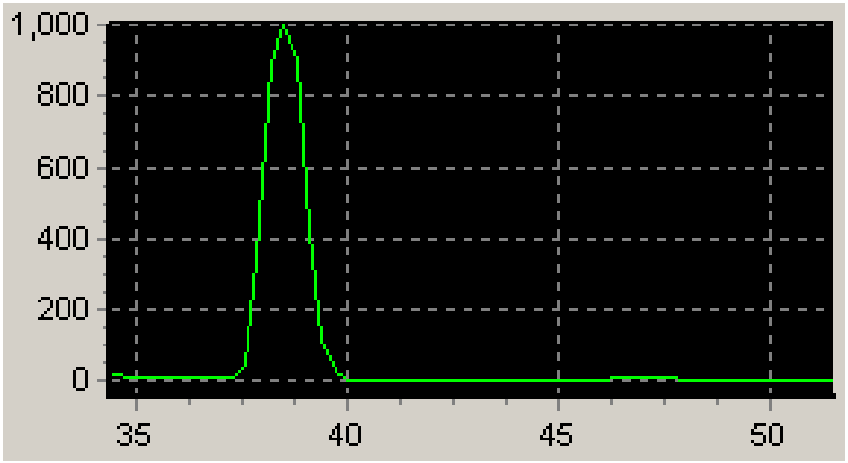
Peak Name	RT (min)	% Area	ee (%)
(*S*)	40.03	99	98
(*R*)	49.02	1	

(Table 3, entry 3)



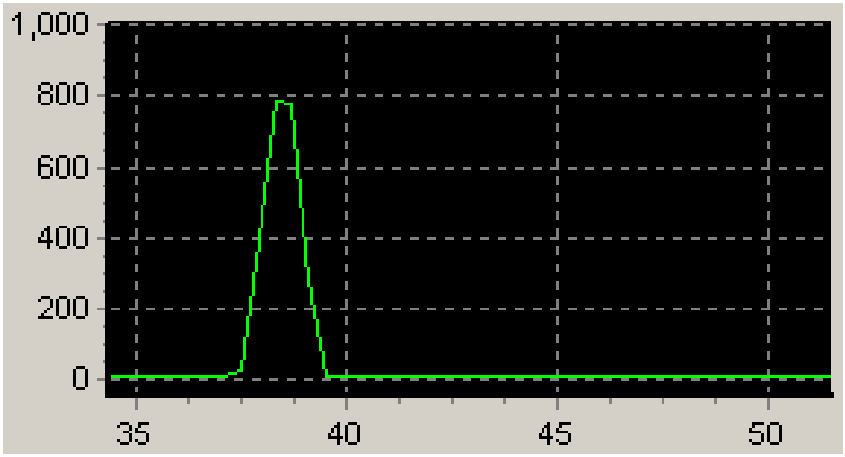
Peak Name	RT (min)	% Area	ee (%)
(*S*)	39.10	99.5	99
(*R*)	47.12	0.5	

(Table 3, entry 4)



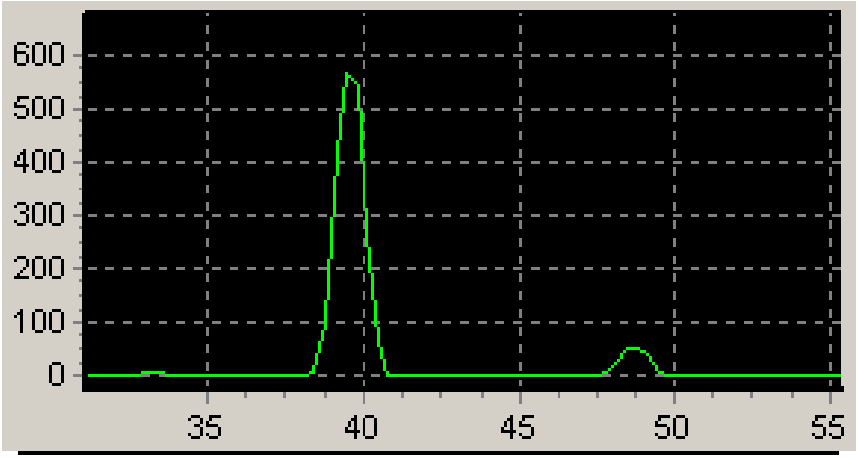
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.84	99.5	99
(*R*)	46.24	0.5	

(Table 3, entry 5)



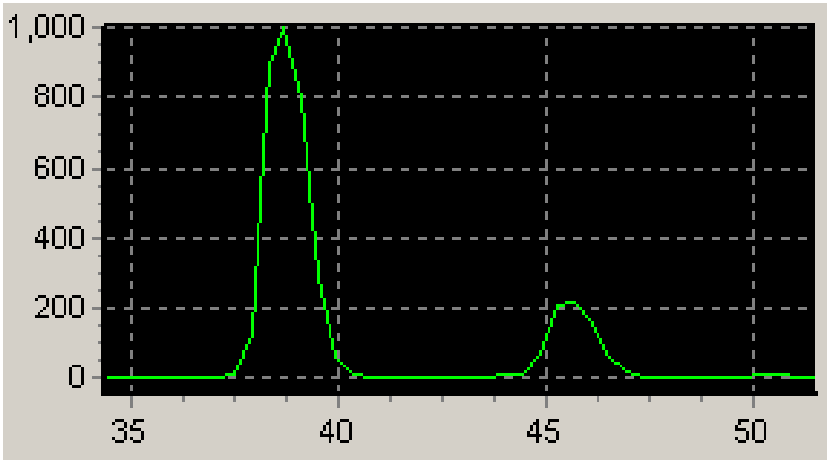
Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.75	>99.5	>99.5
(*R*)			

(Table 3, entry 6)



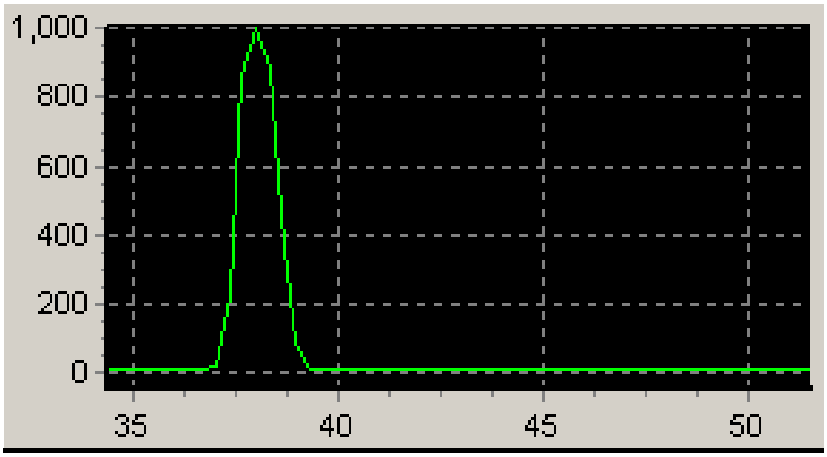
Peak Name	RT (min)	% Area	ee (%)
(*S*)	39.29	91	82
(*R*)	48.85	9	

(Table 3, entry 7)



Peak Name	RT (min)	% Area	ee (%)
(*S*)	39.01	90	80
(*R*)	45.65	10	

(Table 3, entry 8)

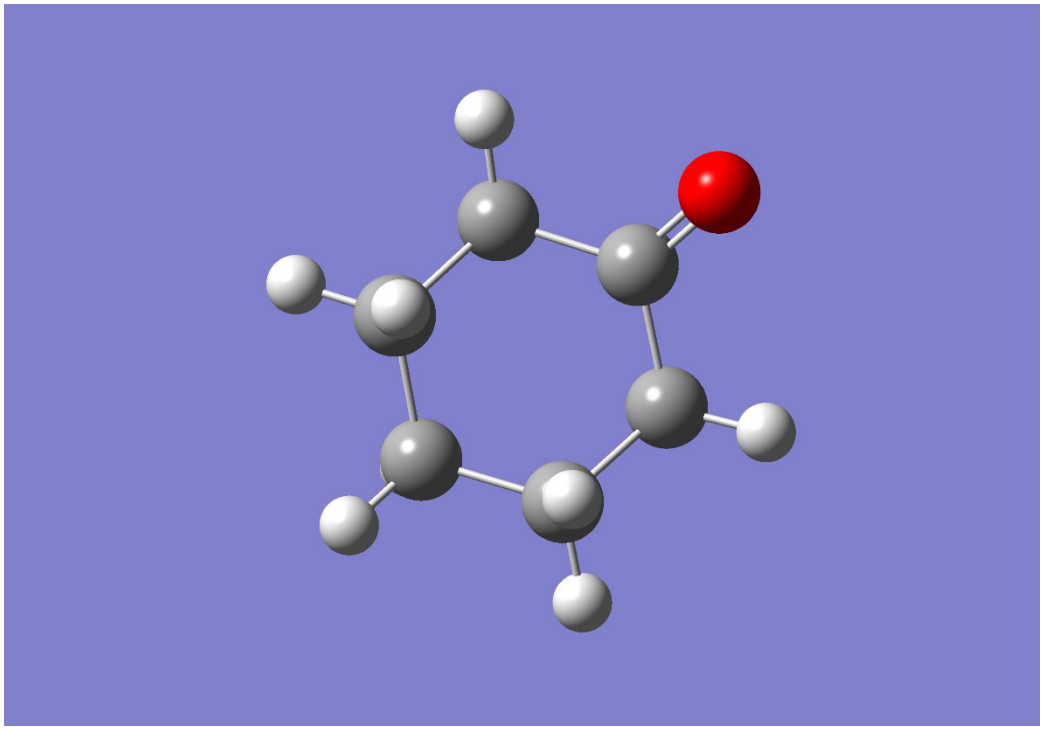


Peak Name	RT (min)	% Area	ee (%)
(*S*)	38.45	>99.5	>99.5
(*R*)			

Computational results of DFT Calculations for all calculated

structures.

Figure 4.



Cyclohexanone-gas(1)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -308.19162 Hartree

Zero-point Energy Correction = 0.162365 Hartree

Thermal Correction to Energy = 0.168434 Hartree

Thermal Correction to Enthalpy = 0.169378 Hartree

Thermal Correction to Free Energy = 0.132343 Hartree

EE + Zero-point Energy = -308.02926 Hartree

EE + Thermal Energy Correction = -308.02319 Hartree

EE + Thermal Enthalpy Correction = -308.02224 Hartree

EE + Thermal Free Energy Correction = -308.05928 Hartree

E (Thermal) = 105.694 kcal/mol

Heat Capacity (Cv) = 22.782 cal/mol-kelvin

Entropy (S) = 77.947 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.18033	1.02034	1.26399
C	-0.87411	1.5609	0.
C	-0.18033	1.02034	-1.26399
C	-0.18033	-0.52675	-1.26995
C	0.44993	-1.06087	0.
C	-0.18033	-0.52675	1.26995
H	-0.67881	1.38437	-2.1547
H	-1.9161	1.25379	0.
H	-0.85159	2.64511	0.
H	0.84421	1.37736	1.29194
H	-0.67881	1.38437	2.1547
H	-1.20747	-0.87863	-1.31895
H	0.36312	-0.91763	-2.11915
H	-1.20747	-0.87863	1.31895
H	0.36312	-0.91763	2.11915
H	0.84421	1.37736	-1.29194
O	1.37483	-1.84414	0.

Cyclohexanone-water(1)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -308.19847 Hartree

Zero-point Energy Correction = 0.162138 Hartree

Thermal Correction to Energy = 0.168209 Hartree

Thermal Correction to Enthalpy = 0.169153 Hartree

Thermal Correction to Free Energy = 0.132108 Hartree

EE + Zero-point Energy = -308.03634 Hartree

EE + Thermal Energy Correction = -308.03026 Hartree

EE + Thermal Enthalpy Correction = -308.02932 Hartree

EE + Thermal Free Energy Correction = -308.06637 Hartree

E (Thermal) = 105.553 kcal/mol

Heat Capacity (Cv) = 22.803 cal/mol-kelvin

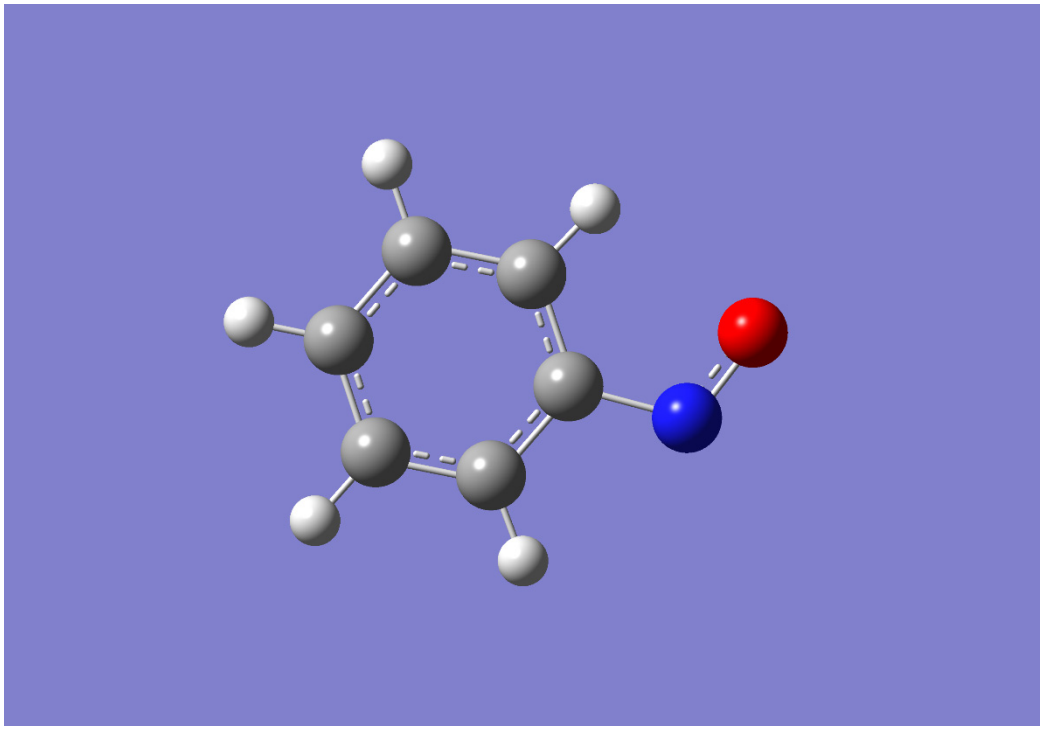
Entropy (S) = 77.967 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.18033	1.02034	1.26399
C	-0.87411	1.5609	0.
C	-0.18033	1.02034	-1.26399
C	-0.18033	-0.52675	-1.26995
C	0.44993	-1.06087	0.
C	-0.18033	-0.52675	1.26995
H	-0.67881	1.38437	-2.1547
H	-1.9161	1.25379	0.
H	-0.85159	2.64511	0.

H	0.84421	1.37736	1.29194
H	-0.67881	1.38437	2.1547
H	-1.20747	-0.87863	-1.31895
H	0.36312	-0.91763	-2.11915
H	-1.20747	-0.87863	1.31895
H	0.36312	-0.91763	2.11915
H	0.84421	1.37736	-1.29194
O	1.37483	-1.84414	0.



Nitrosobenzene-gas(2)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -359.53313 Hartree

Zero-point Energy Correction = 0.097794 Hartree

Thermal Correction to Energy = 0.103841 Hartree

Thermal Correction to Enthalpy = 0.104785 Hartree

Thermal Correction to Free Energy = 0.067536 Hartree

EE + Zero-point Energy = -359.43533 Hartree

EE + Thermal Energy Correction = -359.42929 Hartree

EE + Thermal Enthalpy Correction = -359.42834 Hartree

EE + Thermal Free Energy Correction = -359.46559 Hartree

E (Thermal) = 65.161 kcal/mol

Heat Capacity (Cv) = 22.921 cal/mol-kelvin

Entropy (S) = 78.398 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	2.74053	0.37856	-0.00008
C	0.55208	-0.25309	-0.00001
C	-0.36713	-1.30821	0.00002
C	0.11304	1.07824	-0.00001
C	-1.73353	-1.03397	0.00005
H	0.00617	-2.32465	0.00001
C	-1.24751	1.35223	0.00003
H	0.86379	1.85631	-0.00003
C	-2.172	0.29466	0.00006
H	-2.45182	-1.84403	0.00008
H	-1.59825	2.37688	0.00003
H	-3.2337	0.51064	0.00009
N	1.9457	-0.6261	-0.00005

Nitrosobenzene-water(2)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -359.5391 Hartree

Zero-point Energy Correction = 0.097803 Hartree

Thermal Correction to Energy = 0.103851 Hartree

Thermal Correction to Enthalpy = 0.104795 Hartree

Thermal Correction to Free Energy = 0.06754 Hartree

EE + Zero-point Energy = -359.4413 Hartree

EE + Thermal Energy Correction = -359.43525 Hartree

EE + Thermal Enthalpy Correction = -359.43431 Hartree

EE + Thermal Free Energy Correction = -359.47156 Hartree

E (Thermal) = 65.167 kcal/mol

Heat Capacity (Cv) = 22.923 cal/mol-kelvin

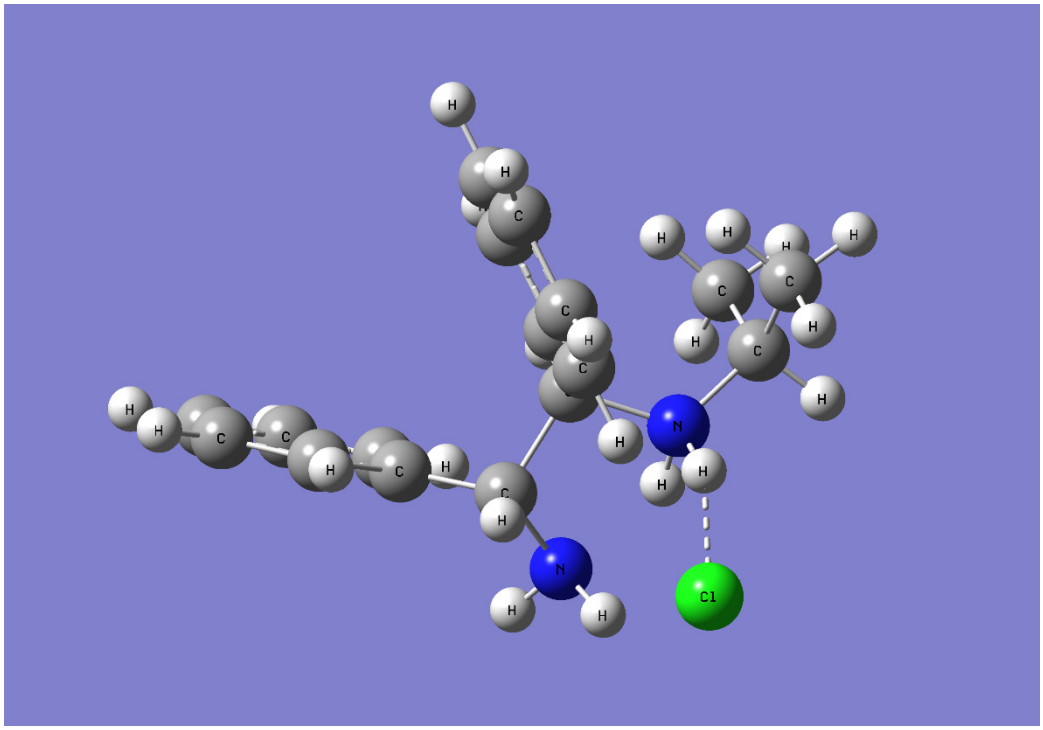
Entropy (S) = 78.41 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	2.74053	0.37856	-0.00008
C	0.55208	-0.25309	-0.00001
C	-0.36713	-1.30821	0.00002
C	0.11304	1.07824	-0.00001
C	-1.73353	-1.03397	0.00005
H	0.00617	-2.32465	0.00001
C	-1.24751	1.35223	0.00003
H	0.86379	1.85631	-0.00003

C	-2.172	0.29466	0.00006
H	-2.45182	-1.84403	0.00008
H	-1.59825	2.37688	0.00003
H	-3.2337	0.51064	0.00009
N	1.9457	-0.6261	-0.00005



1a cat.-gas(3)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1224.9946 Hartree

Zero-point Energy Correction = 0.375214 Hartree

Thermal Correction to Energy = 0.394746 Hartree

Thermal Correction to Enthalpy = 0.395691 Hartree

Thermal Correction to Free Energy = 0.325221 Hartree

EE + Zero-point Energy = -1224.6194 Hartree

EE + Thermal Energy Correction = -1224.5999 Hartree

EE + Thermal Enthalpy Correction = -1224.599 Hartree

EE + Thermal Free Energy Correction = -1224.6694 Hartree

E (Thermal) = 247.707 kcal/mol

Heat Capacity (Cv) = 74.696 cal/mol-kelvin

Entropy (S) = 148.317 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.63346	-0.98793	0.89695
C	0.29211	-0.50444	-0.28498
N	1.62729	-1.19101	-0.01139
N	-0.29163	-2.42775	1.13926
H	-0.86115	-3.06466	0.57262
H	-0.33839	-0.43525	1.79239
H	-0.08851	-0.93515	-1.21245
C	0.33749	1.00418	-0.39667
C	-0.38065	1.62391	-1.43022
C	1.014	1.80085	0.53985
C	-0.42464	3.01623	-1.52998
H	-0.90973	1.01539	-2.15537
C	0.97302	3.19337	0.43303
H	1.60236	1.34576	1.33053
C	0.25292	3.80516	-0.59708
H	-0.98349	3.48079	-2.3338
H	1.5064	3.80001	1.15576
H	0.22336	4.88573	-0.6737
C	-2.09896	-0.72142	0.59461
C	-2.82463	0.18975	1.37243
C	-2.74726	-1.38616	-0.45795

C	-4.17461	0.43425	1.10593
H	-2.33211	0.70905	2.18717
C	-4.09622	-1.14413	-0.72358
H	-2.20521	-2.09397	-1.0771
C	-4.81349	-0.23266	0.0579
H	-4.72403	1.14189	1.71566
H	-4.58569	-1.66412	-1.53867
H	-5.86035	-0.04497	-0.1495
C	2.52351	-1.54653	-1.20242
C	3.02007	-0.27519	-1.90367
C	1.81059	-2.51664	-2.15457
H	2.19129	0.2637	-2.37057
H	3.51833	0.3877	-1.1897
H	0.99691	-2.02419	-2.69563
H	2.53493	-2.876	-2.8921
H	3.3711	-2.05663	-0.73359
Cl	3.59864	-0.09687	2.20182
H	2.21708	-0.67685	0.70155
H	1.24181	-2.07747	0.48897
H	3.7381	-0.55682	-2.68035
H	1.41219	-3.38145	-1.61399
H	-0.37044	-2.68005	2.12842

1a cat.-water(3)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1225.0267 Hartree

Zero-point Energy Correction = 0.374478 Hartree

Thermal Correction to Energy = 0.394565 Hartree

Thermal Correction to Enthalpy = 0.395509 Hartree

Thermal Correction to Free Energy = 0.32271 Hartree

EE + Zero-point Energy = -1224.6522 Hartree

EE + Thermal Energy Correction = -1224.6321 Hartree

EE + Thermal Enthalpy Correction = -1224.6312 Hartree

EE + Thermal Free Energy Correction = -1224.704 Hartree

E (Thermal) = 247.593 kcal/mol

Heat Capacity (Cv) = 75.543 cal/mol-kelvin

Entropy (S) = 153.22 cal/mol-kelvin

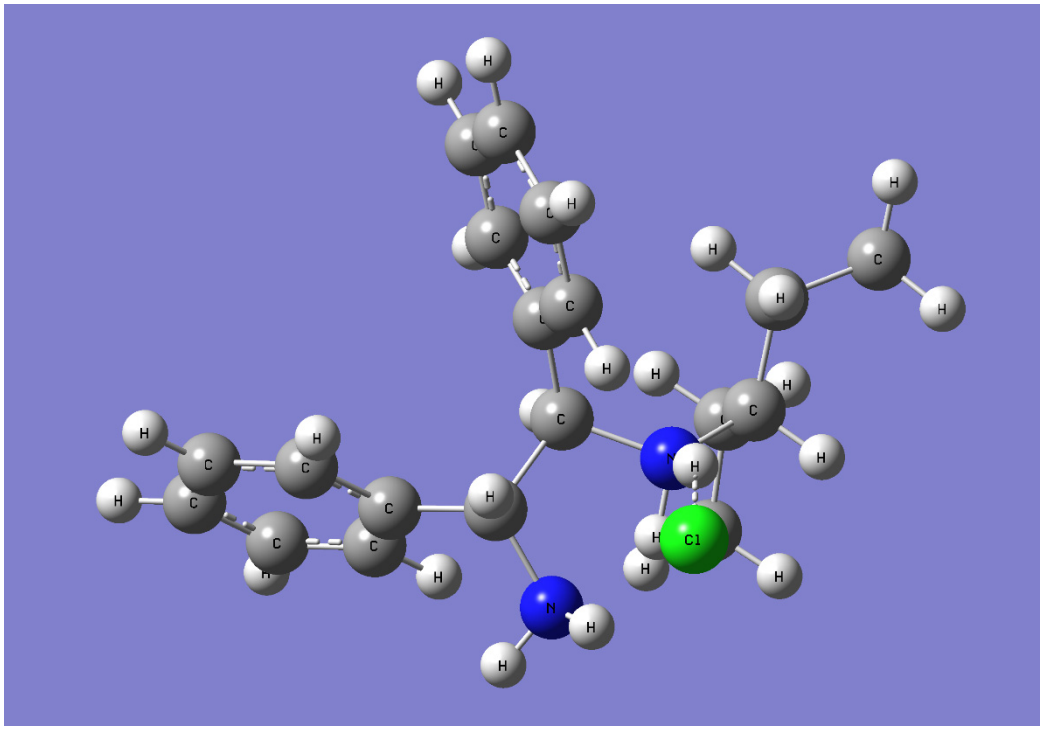
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.26638	1.01429	-1.75936
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
H	-0.35098	-1.26416	-0.83323
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524
H	-1.06811	1.23509	-0.24



1b cat.-gas(3)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1303.1972 Hartree

Zero-point Energy Correction = 0.433132 Hartree

Thermal Correction to Energy = 0.455341 Hartree

Thermal Correction to Enthalpy = 0.456285 Hartree

Thermal Correction to Free Energy = 0.379938 Hartree

EE + Zero-point Energy = -1302.7641 Hartree

EE + Thermal Energy Correction = -1302.7419 Hartree

EE + Thermal Enthalpy Correction = -1302.7409 Hartree

EE + Thermal Free Energy Correction = -1302.8173 Hartree

E (Thermal) = 285.731 kcal/mol

Heat Capacity (Cv) = 84.367 cal/mol-kelvin

Entropy (S) = 160.685 cal/mol-kelvin

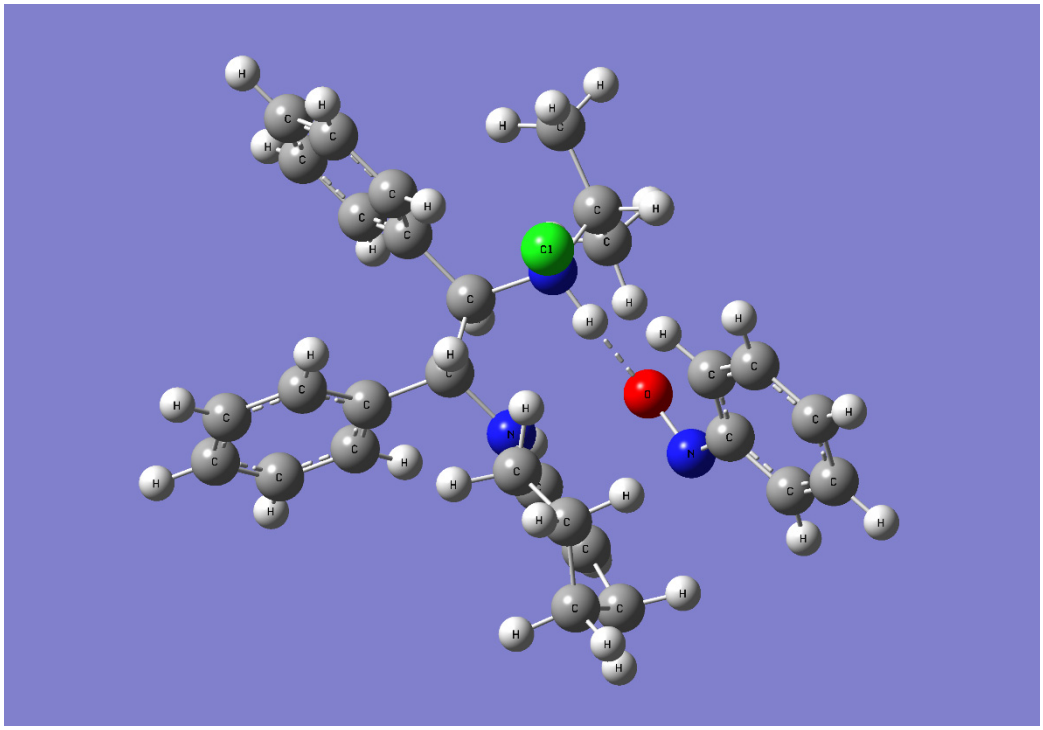
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.85086	1.03343	0.02132
C	-1.53034	-0.28093	0.54253
N	-0.5443	-1.42629	0.29236
N	0.41073	1.24449	0.75526
H	0.20834	1.46725	1.70889
H	-0.61627	0.87978	-1.03479
H	-1.65453	-0.19807	1.62598
C	-2.88659	-0.50285	-0.1045
C	-4.04035	-0.4246	0.68555
C	-3.01155	-0.73356	-1.48366
C	-5.3047	-0.58644	0.11577
H	-3.95166	-0.22335	1.74815
C	-4.27733	-0.89718	-2.04851
H	-2.12347	-0.80714	-2.10701
C	-5.425	-0.82582	-1.254
H	-6.18919	-0.52229	0.73866
H	-4.36371	-1.08331	-3.1127
H	-6.40473	-0.95394	-1.69956
C	-1.79461	2.22546	0.18364
C	-2.5125	2.71034	-0.91535
C	-1.95183	2.84764	1.42824

C	-3.3819	3.79322	-0.77025
H	-2.39789	2.23295	-1.88154
C	-2.8227	3.92758	1.57579
H	-1.37898	2.50199	2.28162
C	-3.54103	4.40289	0.47562
H	-3.93155	4.1599	-1.62927
H	-2.93471	4.40219	2.54389
H	-4.21412	5.24479	0.5882
C	-0.90412	-2.86362	0.73429
C	-1.74059	-3.57809	-0.35137
C	-1.5459	-2.89072	2.13456
C	-1.67713	-5.11341	-0.19189
C	-0.56771	-2.53774	3.27961
H	-2.24633	-5.59524	-0.9934
H	-0.64073	-5.46534	-0.25299
H	-2.09912	-5.44137	0.76422
H	0.17477	-3.33621	3.39336
H	-0.01428	-1.61445	3.08627
H	-1.10706	-2.44045	4.228
H	-2.77658	-3.23224	-0.30805
H	-1.33643	-3.30471	-1.33332
H	-2.42108	-2.2329	2.13924
H	-1.92417	-3.90647	2.29438
H	0.078	-3.3514	0.78295
Cl	0.28769	-1.18537	-2.62995
H	-0.31418	-1.43892	-0.75926

H	0.36911	-1.16123	0.76779
H	0.91749	1.9984	0.33715



TS of 1a cat.-Gas

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7336 Hartree

Zero-point Energy Correction = 0.602506 Hartree

Thermal Correction to Energy = 0.635968 Hartree

Thermal Correction to Enthalpy = 0.636912 Hartree

Thermal Correction to Free Energy = 0.532796 Hartree

EE + Zero-point Energy = -1816.1311 Hartree

EE + Thermal Energy Correction = -1816.0976 Hartree

EE + Thermal Enthalpy Correction = -1816.0967 Hartree

EE + Thermal Free Energy Correction = -1816.2008 Hartree

E (Thermal) = 399.076 kcal/mol

Heat Capacity (Cv) = 126.268 cal/mol-kelvin

Entropy (S) = 219.131 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.68632	0.99979	-0.13589
C	-1.73002	-0.44464	0.46951
N	-0.27694	-0.90569	0.52539
N	-0.70165	1.80172	0.63573
H	-1.15017	2.43208	1.30008
H	-1.3486	0.93159	-1.17344
H	-2.05968	-0.35338	1.50588
C	-2.67072	-1.36982	-0.27644
C	-3.8657	-1.7538	0.34975
C	-2.42156	-1.79157	-1.5911
C	-4.7984	-2.54714	-0.31905
H	-4.07195	-1.42051	1.36147
C	-3.35529	-2.59043	-2.25448
H	-1.48253	-1.54739	-2.0795
C	-4.54405	-2.96768	-1.62598
H	-5.71787	-2.83411	0.17792
H	-3.14423	-2.92226	-3.26435
H	-5.26438	-3.58694	-2.1481
C	-3.06484	1.64286	-0.0865
C	-3.73263	1.98699	-1.26685
C	-3.67686	1.92241	1.14548

C	-4.9849	2.60309	-1.22005
H	-3.27239	1.76658	-2.22309
C	-4.92655	2.54104	1.19352
H	-3.18147	1.65335	2.07382
C	-5.58396	2.88361	0.0092
H	-5.49058	2.86288	-2.14264
H	-5.38762	2.7523	2.15153
H	-6.55526	3.36269	0.04552
C	0.10009	-2.08181	1.44383
C	-0.36594	-3.41472	0.82703
C	-0.38156	-1.83646	2.88545
H	-1.42922	-3.49595	0.91495
H	-0.09013	-3.44527	-0.20636
H	-1.45038	-1.87636	2.91606
H	0.02206	-2.58967	3.5294
H	1.19465	-2.04134	1.4208
Cl	0.95882	-1.51997	-2.20269
H	0.10589	-1.13835	-0.45946
C	0.46965	2.3728	0.04513
C	1.0147	3.52966	0.87406
C	1.07448	1.92348	-1.06482
C	2.48682	3.83419	0.53093
C	2.32948	2.55692	-1.63692
C	2.65229	3.92552	-0.99955
H	2.79344	4.76853	1.01522
H	2.21456	2.66603	-2.72342

H	1.9651	4.68718	-1.39093
H	3.17681	1.87423	-1.48067
H	3.67344	4.22789	-1.25962
H	3.11502	3.02347	0.91955
H	0.26367	-0.0755	0.84595
O	2.30587	0.08852	1.16412
N	3.53347	0.42962	1.35714
H	0.39552	4.42396	0.70614
C	4.44319	-0.15422	0.41658
C	4.04347	-0.89597	-0.70652
C	5.80185	0.08339	0.67396
C	5.01481	-1.4025	-1.56169
H	2.99037	-1.04424	-0.92461
C	6.76908	-0.43755	-0.17834
H	6.06638	0.67166	1.54388
C	6.37357	-1.18122	-1.29732
H	4.70706	-1.96134	-2.43691
H	7.8202	-0.26474	0.01762
H	7.12486	-1.58121	-1.96873
H	0.9321	3.26098	1.93618
H	0.73297	1.0356	-1.58985
H	0.09792	-4.22853	1.34419
H	-0.05109	-0.87285	3.21278

TS of 1a cat.-Water

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7688 Hartree

Zero-point Energy Correction = 0.603687 Hartree

Thermal Correction to Energy = 0.636367 Hartree

Thermal Correction to Enthalpy = 0.637311 Hartree

Thermal Correction to Free Energy = 0.537745 Hartree

EE + Zero-point Energy = -1816.1651 Hartree

EE + Thermal Energy Correction = -1816.1324 Hartree

EE + Thermal Enthalpy Correction = -1816.1315 Hartree

EE + Thermal Free Energy Correction = -1816.2311 Hartree

E (Thermal) = 399.326 kcal/mol

Heat Capacity (Cv) = 125.929 cal/mol-kelvin

Entropy (S) = 209.554 cal/mol-kelvin

Symbolic Z-matrix:

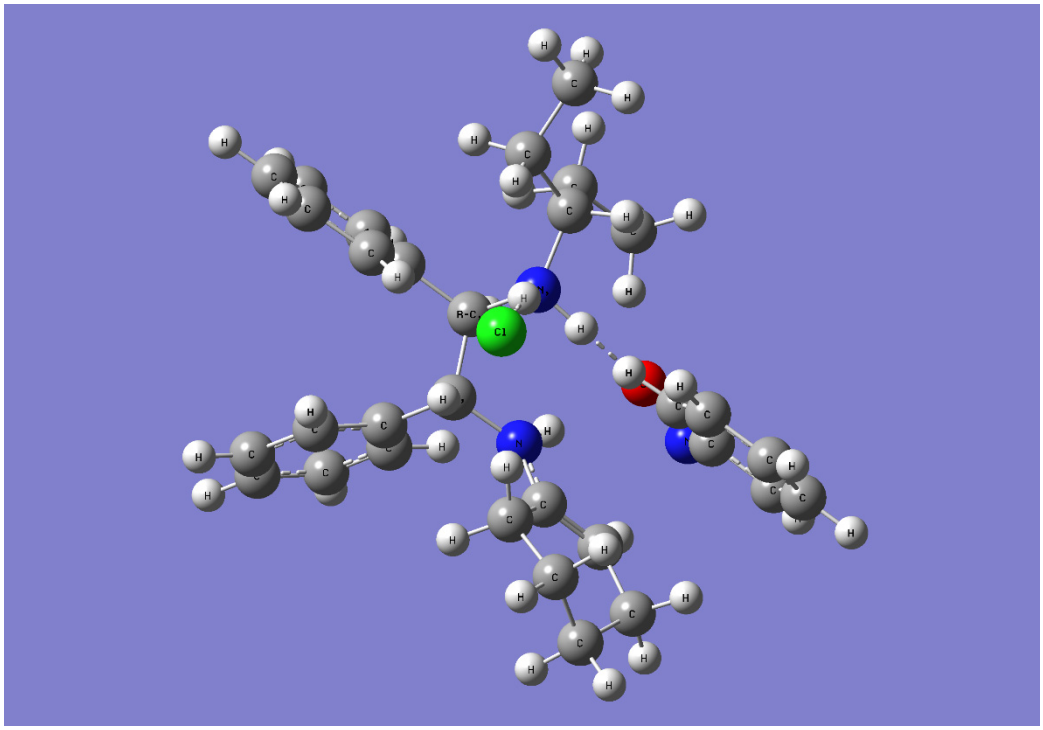
Charge = 0 Multiplicity = 1

C	1.01914	0.71901	-0.04951
C	1.6276	-0.59086	-0.64984
N	0.56383	-1.6828	-0.4991
N	-0.24104	1.02342	-0.75802
H	-0.20661	0.99881	-1.77584
H	0.78038	0.52363	0.99711
H	1.77481	-0.44802	-1.72226
C	2.9507	-0.94987	0.00208

C	4.12573	-0.88073	-0.75883
C	3.02853	-1.30951	1.35617
C	5.36352	-1.17079	-0.1802
H	4.07419	-0.59738	-1.8044
C	4.26774	-1.60162	1.93073
H	2.12647	-1.38221	1.95651
C	5.43674	-1.53322	1.16707
H	6.26438	-1.11469	-0.77969
H	4.31903	-1.88403	2.97584
H	6.39552	-1.76096	1.61785
C	2.01515	1.8754	-0.13605
C	2.65308	2.3389	1.02107
C	2.29397	2.49143	-1.36375
C	3.56259	3.39784	0.95288
H	2.44281	1.86858	1.97511
C	3.20431	3.54755	-1.43335
H	1.79886	2.15776	-2.26887
C	3.84113	4.00354	-0.27474
H	4.04887	3.74846	1.85564
H	3.41305	4.01578	-2.38813
H	4.54504	4.82559	-0.32926
C	0.72667	-2.98705	-1.31115
C	1.8884	-3.84779	-0.803
C	0.81608	-2.66233	-2.81012
H	2.85071	-3.3795	-1.01643
H	1.80841	-4.01992	0.2747

H	1.78637	-2.22712	-3.06866
H	0.70193	-3.59217	-3.37589
H	-0.21845	-3.50451	-1.11632
Cl	-0.32578	-1.9188	2.50664
H	0.41785	-1.90325	0.52543
C	-1.3483	1.6301	-0.20362
C	-2.33449	2.11047	-1.01967
C	-1.45389	1.6577	1.31201
C	-3.5925	2.76039	-0.49996
C	-2.8737	2.02993	1.79671
H	-1.18147	0.6726	1.71353
C	-3.44904	3.19905	0.97446
H	-3.8533	3.61806	-1.13216
H	-2.82909	2.28718	2.86061
H	-2.77481	4.06245	1.03992
H	-3.52826	1.15779	1.68683
H	-4.42579	3.49985	1.36967
H	-4.42538	2.04146	-0.57074
H	-0.35218	-1.26355	-0.83244
O	-1.59135	-0.79873	-1.84734
N	-2.79476	-0.25299	-1.87166
H	-0.72824	2.38702	1.70029
H	-2.16303	2.13915	-2.08888
C	-3.67207	-0.7058	-0.82484
C	-3.29033	-1.45607	0.29723
C	-5.02112	-0.35828	-1.00554

C	-4.25103	-1.84964	1.22327
H	-2.25219	-1.70281	0.46675
C	-5.98311	-0.76416	-0.08124
H	-5.29438	0.2041	-1.88978
C	-5.59929	-1.50996	1.03706
H	-3.94931	-2.41608	2.09636
H	-7.02338	-0.50244	-0.23183
H	-6.34161	-1.82403	1.76108
H	1.84508	-4.81592	-1.31271
H	0.01328	-1.97528	-3.09369



TS of 1b cat.-Gas

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1894.9424 Hartree

Zero-point Energy Correction = 0.661461 Hartree

Thermal Correction to Energy = 0.696676 Hartree

Thermal Correction to Enthalpy = 0.697621 Hartree

Thermal Correction to Free Energy = 0.592772 Hartree

EE + Zero-point Energy = -1894.2809 Hartree

EE + Thermal Energy Correction = -1894.2457 Hartree

EE + Thermal Enthalpy Correction = -1894.2447 Hartree

EE + Thermal Free Energy Correction = -1894.3496 Hartree

E (Thermal) = 437.171 kcal/mol

Heat Capacity (Cv) = 135.388 cal/mol-kelvin

Entropy (S) = 220.672 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.71111	0.82245	-0.15845
C	1.692	-0.74115	-0.34045
N	0.21384	-1.13099	-0.40158
N	0.69183	1.41569	-1.08208
H	1.03291	1.48442	-2.04737
H	1.37395	1.03915	0.85659
H	2.09878	-0.98146	-1.3267
C	2.51099	-1.43188	0.73345
C	3.74182	-1.99729	0.3706
C	2.11067	-1.46586	2.07845
C	4.56222	-2.59305	1.3294
H	4.0642	-1.96132	-0.66477
C	2.93286	-2.06946	3.03236
H	1.14964	-1.05841	2.3798
C	4.15738	-2.63149	2.66451
H	5.51162	-3.02429	1.03397
H	2.60802	-2.10158	4.06577
H	4.78991	-3.09718	3.41151
C	3.11786	1.36219	-0.36712
C	3.81622	1.94437	0.69663
C	3.73266	1.29782	-1.62629

C	5.1021	2.45501	0.50789
H	3.35382	1.99001	1.6763
C	5.01652	1.80821	-1.81767
H	3.21305	0.8464	-2.46683
C	5.70474	2.38958	-0.74938
H	5.63095	2.90206	1.34144
H	5.47924	1.75335	-2.79631
H	6.70194	2.78696	-0.8973
C	-0.14804	-2.4674	-1.07146
C	0.2655	-3.61832	-0.13234
C	0.43743	-2.50852	-2.50592
C	-0.32286	-4.98632	-0.5425
C	-0.43053	-3.32003	-3.50018
H	-0.12036	-5.72258	0.24254
H	-1.40828	-4.91884	-0.67533
H	0.11877	-5.35596	-1.47199
H	-0.39993	-4.38874	-3.27601
H	-1.46959	-2.98509	-3.44546
H	-0.06051	-3.17665	-4.52157
H	1.35768	-3.67697	-0.08229
H	-0.0969	-3.36782	0.87214
H	0.49445	-1.47776	-2.88394
H	1.45951	-2.90712	-2.47939
H	-1.23816	-2.41928	-1.13416
Cl	-1.45336	-0.66157	2.0949
H	-0.2857	-1.0786	0.5549

C	0.03605	2.63697	-0.67538
C	-0.2428	3.59112	-1.5744
C	-0.36669	2.73912	0.78726
C	-1.012	4.85843	-1.25506
C	-1.4717	3.79646	0.99696
H	-0.70702	1.76705	1.16625
C	-1.1041	5.10525	0.26827
H	-0.52518	5.71417	-1.74172
H	-1.60046	3.97393	2.07021
H	-0.13192	5.4588	0.63506
H	-2.41955	3.40983	0.61192
H	-1.84719	5.88377	0.4768
H	-2.0276	4.79114	-1.67545
H	-0.18486	-0.30761	-0.93307
O	-3.53435	-1.65673	-1.63336
N	-4.74945	-1.25477	-1.62656
H	0.51365	3.03023	1.38049
H	0.06488	3.45863	-2.61076
C	-5.12347	-0.58052	-0.41911
C	-4.26248	-0.36476	0.66749
C	-6.44771	-0.12114	-0.38329
C	-4.72952	0.3148	1.78242
H	-3.2405	-0.71871	0.64641
C	-6.91345	0.55644	0.73598
H	-7.08119	-0.30756	-1.24151
C	-6.05287	0.77513	1.81802

H	-4.05329	0.47827	2.60796
H	-7.93508	0.91422	0.77134
H	-6.41483	1.30515	2.6915

TS of 1b cat.-Water

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1894.9692 Hartree

Zero-point Energy Correction = 0.661552 Hartree

Thermal Correction to Energy = 0.696912 Hartree

Thermal Correction to Enthalpy = 0.697856 Hartree

Thermal Correction to Free Energy = 0.592423 Hartree

EE + Zero-point Energy = -1894.3077 Hartree

EE + Thermal Energy Correction = -1894.2723 Hartree

EE + Thermal Enthalpy Correction = -1894.2714 Hartree

EE + Thermal Free Energy Correction = -1894.3768 Hartree

E (Thermal) = 437.319 kcal/mol

Heat Capacity (Cv) = 135.57 cal/mol-kelvin

Entropy (S) = 221.902 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

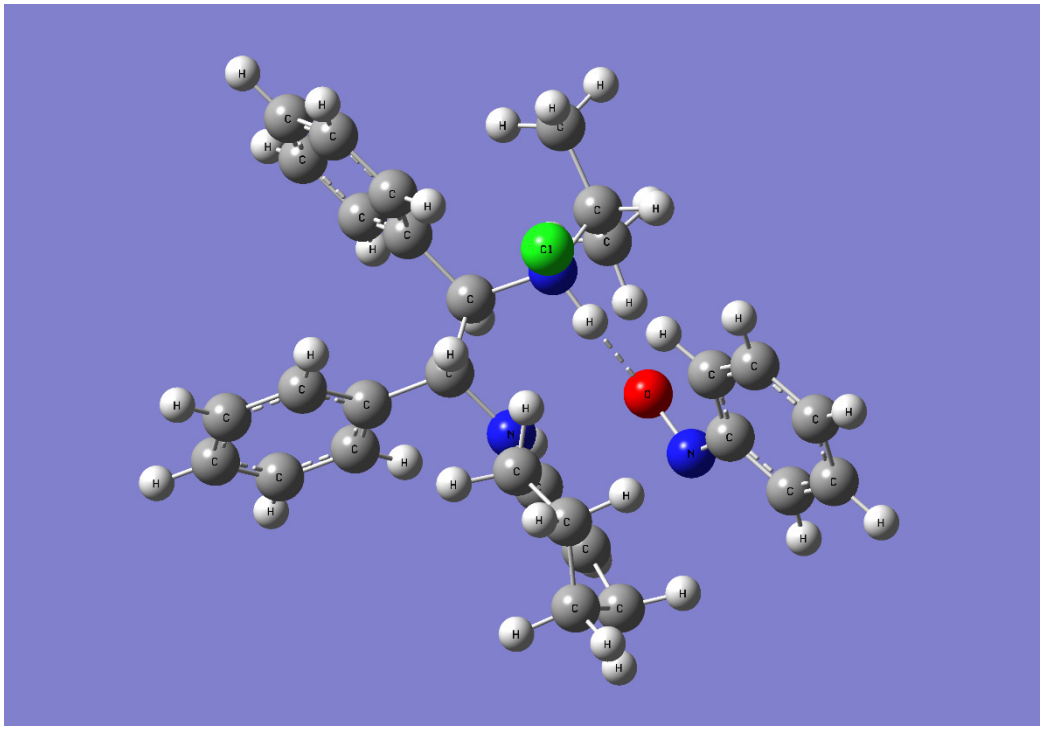
C	-0.85086	1.03343	0.02132
C	-1.53034	-0.28093	0.54253
N	-0.5443	-1.42629	0.29236
N	0.41073	1.24449	0.75526
H	0.4194	1.01839	1.7483
H	-0.61627	0.87978	-1.03479
H	-1.65453	-0.19807	1.62598
C	-2.88659	-0.50285	-0.1045

C	-4.04035	-0.4246	0.68555
C	-3.01155	-0.73356	-1.48366
C	-5.3047	-0.58644	0.11577
H	-3.95166	-0.22335	1.74815
C	-4.27733	-0.89718	-2.04851
H	-2.12347	-0.80714	-2.10701
C	-5.425	-0.82582	-1.254
H	-6.18919	-0.52229	0.73866
H	-4.36371	-1.08331	-3.1127
H	-6.40473	-0.95394	-1.69956
C	-1.79461	2.22546	0.18364
C	-2.5125	2.71034	-0.91535
C	-1.95183	2.84764	1.42824
C	-3.3819	3.79322	-0.77025
H	-2.39789	2.23295	-1.88154
C	-2.8227	3.92758	1.57579
H	-1.37898	2.50199	2.28162
C	-3.54103	4.40289	0.47562
H	-3.93155	4.1599	-1.62927
H	-2.93471	4.40219	2.54389
H	-4.21412	5.24479	0.5882
C	-0.90412	-2.86362	0.73429
C	-1.74059	-3.57809	-0.35137
C	-1.5459	-2.89072	2.13456
C	-1.67713	-5.11341	-0.19189
C	-0.56771	-2.53774	3.27961

H	-2.24633	-5.59524	-0.9934
H	-0.64073	-5.46534	-0.25299
H	-2.09912	-5.44137	0.76422
H	0.17477	-3.33621	3.39336
H	-0.01428	-1.61445	3.08627
H	-1.10706	-2.44045	4.228
H	-2.77658	-3.23224	-0.30805
H	-1.33643	-3.30471	-1.33332
H	-2.42108	-2.2329	2.13924
H	-1.92417	-3.90647	2.29438
H	0.078	-3.3514	0.78295
Cl	0.28769	-1.18537	-2.62995
H	-0.31418	-1.43892	-0.75926
C	1.56653	1.79163	0.25535
C	2.5907	2.08578	1.12034
C	1.68468	1.9704	-1.24789
C	3.91417	2.64866	0.66591
C	3.13572	2.26146	-1.69464
H	1.32906	1.06468	-1.75868
C	3.82232	3.26477	-0.74835
H	4.26521	3.3964	1.38787
H	3.11864	2.6426	-2.72141
H	3.24004	4.19421	-0.70823
H	3.70079	1.32263	-1.69645
H	4.82669	3.50857	-1.11326
H	4.66202	1.8386	0.64692

H	0.36911	-1.16123	0.76779
O	1.55952	-0.69999	1.78166
N	2.81945	-0.2743	1.79878
H	1.02934	2.80197	-1.54704
H	2.40279	2.0549	2.18589
C	3.62768	-0.77298	0.71642
C	3.15853	-1.33019	-0.48117
C	5.01049	-0.65004	0.93158
C	4.06407	-1.7594	-1.44609
H	2.10384	-1.38203	-0.70853
C	5.9154	-1.10023	-0.02808
H	5.34593	-0.22516	1.86959
C	5.44326	-1.65501	-1.22086
H	3.68256	-2.15559	-2.37947
H	6.98081	-1.01634	0.15079
H	6.14279	-1.99509	-1.9755

Figure 5.



TS of 1a cat.-Heptane

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7499 Hartree

Zero-point Energy Correction = 0.603464 Hartree

Thermal Correction to Energy = 0.636088 Hartree

Thermal Correction to Enthalpy = 0.637032 Hartree

Thermal Correction to Free Energy = 0.537404 Hartree

EE + Zero-point Energy = -1816.1464 Hartree

EE + Thermal Energy Correction = -1816.1138 Hartree

EE + Thermal Enthalpy Correction = -1816.1129 Hartree

EE + Thermal Free Energy Correction = -1816.2125 Hartree

E (Thermal) = 399.151 kcal/mol

Heat Capacity (Cv) = 125.83 cal/mol-kelvin

Entropy (S) = 209.685 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.96217	0.73486	-0.04304
C	1.5532	-0.5817	-0.66155
N	0.47154	-1.66349	-0.55229
N	-0.2511	1.12223	-0.79019
H	-0.21027	1.03493	-1.80312
H	0.68618	0.51125	0.98956
H	1.72533	-0.4094	-1.72766
C	2.86476	-0.98088	-0.00771
C	4.04568	-0.90289	-0.75842
C	2.92762	-1.39505	1.33146
C	5.27432	-1.23908	-0.18727
H	4.00596	-0.57014	-1.79035
C	4.15851	-1.73343	1.89765
H	2.0192	-1.47844	1.92184
C	5.33249	-1.65747	1.14373
H	6.17996	-1.17336	-0.77882
H	4.19621	-2.06063	2.93017
H	6.28435	-1.92237	1.58928
C	2.00463	1.85419	-0.07423
C	2.70426	2.19647	1.08854

C	2.2776	2.544	-1.2624
C	3.66775	3.20729	1.06308
H	2.50209	1.66465	2.01119
C	3.24151	3.55263	-1.29002
H	1.72831	2.30662	-2.16691
C	3.93985	3.88652	-0.12627
H	4.20267	3.46294	1.97022
H	3.44283	4.08099	-2.21481
H	4.68587	4.67233	-0.14646
C	0.63961	-2.96273	-1.35856
C	1.76584	-3.84828	-0.81282
C	0.78206	-2.64056	-2.85452
H	2.74464	-3.40058	-0.99465
H	1.64606	-4.01171	0.26221
H	1.76781	-2.21899	-3.07728
H	0.6747	-3.56674	-3.42796
H	-0.32101	-3.46367	-1.19516
Cl	-0.4355	-1.71805	2.37407
H	0.29077	-1.86485	0.4807
C	-1.36692	1.75602	-0.28715
C	-2.33751	2.18544	-1.15092
C	-1.49802	1.87594	1.22205
C	-3.61643	2.84356	-0.69425
C	-2.92713	2.27313	1.65838
H	-1.23282	0.9213	1.69615
C	-3.50137	3.3782	0.75106

H	-3.87954	3.65719	-1.38161
H	-2.89944	2.60176	2.70297
H	-2.83802	4.25232	0.76841
H	-3.57386	1.39012	1.6009
H	-4.48738	3.69281	1.11171
H	-4.43575	2.10616	-0.73674
H	-0.42953	-1.23256	-0.91195
O	-1.57455	-0.63353	-1.87404
N	-2.82978	-0.23505	-1.833
H	-0.77774	2.6307	1.57029
H	-2.14271	2.16611	-2.21579
C	-3.56842	-0.81234	-0.74571
C	-3.02159	-1.42413	0.39397
C	-4.96064	-0.66482	-0.85887
C	-3.86598	-1.88629	1.3998
H	-1.95102	-1.50804	0.53756
C	-5.80296	-1.14967	0.13987
H	-5.35411	-0.18074	-1.7441
C	-5.25639	-1.75853	1.27401
H	-3.42992	-2.35107	2.27585
H	-6.87678	-1.04654	0.04012
H	-5.9069	-2.12581	2.05902
H	1.7191	-4.81833	-1.31945
H	-0.00085	-1.94136	-3.1631

TS of 1a cat.-Cyclohexane

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.766 Hartree

Zero-point Energy Correction = 0.603813 Hartree

Thermal Correction to Energy = 0.636422 Hartree

Thermal Correction to Enthalpy = 0.637366 Hartree

Thermal Correction to Free Energy = 0.538254 Hartree

EE + Zero-point Energy = -1816.1622 Hartree

EE + Thermal Energy Correction = -1816.1295 Hartree

EE + Thermal Enthalpy Correction = -1816.1286 Hartree

EE + Thermal Free Energy Correction = -1816.2277 Hartree

E (Thermal) = 399.361 kcal/mol

Heat Capacity (Cv) = 125.859 cal/mol-kelvin

Entropy (S) = 208.599 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.20533	0.99883	-1.77758
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
C	-1.34786	1.6292	-0.20539
C	-2.33372	2.11032	-1.02126
C	-1.45348	1.65645	1.31028
C	-3.59098	2.76154	-0.50137
C	-2.87274	2.0305	1.79524
H	-1.18233	0.67076	1.71126
C	-3.44674	3.20025	0.97294
H	-3.85104	3.61938	-1.13364
H	-2.8276	2.28788	2.85909
H	-2.77142	4.0628	1.03821
H	-3.52854	1.15926	1.68556
H	-4.42304	3.50231	1.3683
H	-4.42465	2.0435	-0.57187
H	-0.35098	-1.26416	-0.83323
O	-1.59288	-0.80111	-1.84696
N	-2.79578	-0.25456	-1.87144
H	-0.72684	2.38454	1.69895
H	-2.16244	2.1386	-2.09053
C	-3.67306	-0.70595	-0.8239
C	-3.29144	-1.45765	0.29725
C	-5.02168	-0.35608	-1.00302

C	-4.25174	-1.84991	1.22425
H	-2.25352	-1.7067	0.46473
C	-5.98334	-0.76055	-0.07772
H	-5.29507	0.20706	-1.88675
C	-5.59959	-1.50751	1.03984
H	-3.95031	-2.41781	2.09651
H	-7.0233	-0.4969	-0.22702
H	-6.34167	-1.82059	1.76453
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524

TS of 1a cat.-CCl_4

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7518 Hartree

Zero-point Energy Correction = 0.603494 Hartree

Thermal Correction to Energy = 0.636146 Hartree

Thermal Correction to Enthalpy = 0.63709 Hartree

Thermal Correction to Free Energy = 0.537178 Hartree

EE + Zero-point Energy = -1816.1483 Hartree

EE + Thermal Energy Correction = -1816.1157 Hartree

EE + Thermal Enthalpy Correction = -1816.1147 Hartree

EE + Thermal Free Energy Correction = -1816.2147 Hartree

E (Thermal) = 399.188 kcal/mol

Heat Capacity (Cv) = 125.819 cal/mol-kelvin

Entropy (S) = 210.283 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.00289	0.72657	-0.03914
C	1.60065	-0.5894	-0.64163
N	0.53851	-1.67635	-0.46784
N	-0.25202	1.04204	-0.75002
H	-0.24028	0.95718	-1.76445
H	0.76278	0.52819	1.00745
H	1.73203	-0.44792	-1.71747
C	2.93413	-0.95058	-0.0124

C	4.09516	-0.89212	-0.79447
C	3.03264	-1.30999	1.34045
C	5.34044	-1.1942	-0.23976
H	4.0275	-0.60236	-1.83775
C	4.27951	-1.61409	1.89029
H	2.1395	-1.37328	1.95627
C	5.43437	-1.55806	1.10524
H	6.23113	-1.14438	-0.85504
H	4.34568	-1.89764	2.9342
H	6.39914	-1.79572	1.5381
C	2.01089	1.87108	-0.13526
C	2.70392	2.29484	1.00441
C	2.25226	2.51075	-1.35806
C	3.63007	3.33732	0.92261
H	2.52497	1.80313	1.95383
C	3.17916	3.55049	-1.44193
H	1.7093	2.20828	-2.24709
C	3.87073	3.96652	-0.30055
H	4.15987	3.65676	1.81235
H	3.35725	4.03886	-2.39303
H	4.58766	4.77666	-0.36456
C	0.70253	-3.00694	-1.22552
C	1.84178	-3.86599	-0.66503
C	0.82238	-2.73896	-2.7341
H	2.81495	-3.41968	-0.8759
H	1.73865	-3.9937	0.41658

H	1.80203	-2.32007	-2.98611
H	0.71337	-3.68648	-3.27105
H	-0.25289	-3.5061	-1.03059
Cl	-0.30391	-1.7141	2.49336
H	0.37932	-1.85118	0.57277
C	-1.36721	1.64085	-0.20793
C	-2.36152	2.08265	-1.03867
C	-1.47265	1.70798	1.30574
C	-3.63492	2.71582	-0.53609
C	-2.89836	2.07014	1.78063
H	-1.18587	0.73989	1.73812
C	-3.49944	3.20133	0.92458
H	-3.91801	3.54817	-1.1924
H	-2.85617	2.36004	2.83607
H	-2.8443	4.08104	0.96178
H	-3.53492	1.18167	1.70215
H	-4.48234	3.49286	1.31196
H	-4.44901	1.97357	-0.58362
H	-0.37636	-1.269	-0.82484
O	-1.56078	-0.78497	-1.8586
N	-2.77869	-0.26474	-1.87169
H	-0.75801	2.46099	1.66943
H	-2.18645	2.09635	-2.10734
C	-3.63931	-0.73549	-0.81921
C	-3.23714	-1.4258	0.33375
C	-5.00052	-0.45338	-1.02339

C	-4.19032	-1.82955	1.26332
H	-2.19319	-1.61067	0.54338
C	-5.95407	-0.87338	-0.09766
H	-5.28497	0.06958	-1.92812
C	-5.5499	-1.56235	1.04931
H	-3.86684	-2.34015	2.1623
H	-7.00348	-0.66465	-0.26791
H	-6.28569	-1.88392	1.77694
H	1.79326	-4.85277	-1.138
H	0.0297	-2.05704	-3.05722

TS of 1a cat.-Benzen

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7521 Hartree

Zero-point Energy Correction = 0.603506 Hartree

Thermal Correction to Energy = 0.636155 Hartree

Thermal Correction to Enthalpy = 0.637099 Hartree

Thermal Correction to Free Energy = 0.537233 Hartree

EE + Zero-point Energy = -1816.1486 Hartree

EE + Thermal Energy Correction = -1816.1159 Hartree

EE + Thermal Enthalpy Correction = -1816.115 Hartree

EE + Thermal Free Energy Correction = -1816.2148 Hartree

E (Thermal) = 399.193 kcal/mol

Heat Capacity (Cv) = 125.816 cal/mol-kelvin

Entropy (S) = 210.186 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.00933	0.7233	-0.04085
C	1.61165	-0.59018	-0.64259
N	0.55003	-1.68009	-0.47739
N	-0.24814	1.03376	-0.75036
H	-0.22664	0.97399	-1.76655
H	0.77042	0.52655	1.00593
H	1.74838	-0.44768	-1.71718
C	2.94199	-0.94984	-0.00579

C	4.10796	-0.88558	-0.78036
C	3.03368	-1.31107	1.34697
C	5.35096	-1.18284	-0.21767
H	4.04566	-0.59718	-1.82419
C	4.27821	-1.61038	1.90517
H	2.13761	-1.37983	1.9573
C	5.43804	-1.54769	1.12774
H	6.2452	-1.12909	-0.82736
H	4.33935	-1.89494	2.9491
H	6.401	-1.78136	1.56664
C	2.01253	1.8724	-0.13523
C	2.68666	2.3121	1.00997
C	2.26656	2.50167	-1.36115
C	3.60678	3.36049	0.93107
H	2.49744	1.82936	1.96207
C	3.18733	3.54737	-1.44186
H	1.74068	2.18615	-2.25578
C	3.86004	3.97955	-0.29494
H	4.12177	3.69234	1.82496
H	3.37579	4.02708	-2.39531
H	4.57224	4.79396	-0.35703
C	0.71362	-2.99964	-1.25835
C	1.86504	-3.85827	-0.72322
C	0.81613	-2.70795	-2.76369
H	2.83248	-3.4011	-0.93738
H	1.77465	-4.00539	0.3571

H	1.79099	-2.28204	-3.02192
H	0.70379	-3.64833	-3.31226
H	-0.23629	-3.50772	-1.06075
Cl	-0.31092	-1.79156	2.50146
H	0.39739	-1.87399	0.55702
C	-1.36024	1.63698	-0.20463
C	-2.35108	2.09274	-1.03071
C	-1.46584	1.69183	1.30974
C	-3.61929	2.73239	-0.52315
C	-2.89	2.05665	1.78721
H	-1.18333	0.71859	1.73252
C	-3.482	3.20125	0.94269
H	-3.89381	3.57398	-1.17119
H	-2.84776	2.33481	2.84582
H	-2.82047	4.07564	0.99048
H	-3.53226	1.17335	1.69694
H	-4.46313	3.49562	1.33221
H	-4.44023	1.99842	-0.57977
H	-0.36617	-1.26854	-0.82327
O	-1.572	-0.79211	-1.84981
N	-2.78455	-0.26281	-1.86989
H	-0.74813	2.43782	1.68137
H	-2.17742	2.11007	-2.09968
C	-3.65328	-0.72524	-0.82051
C	-3.26066	-1.43516	0.32389
C	-5.01005	-0.41998	-1.02038

C	-4.21913	-1.83451	1.24991
H	-2.21875	-1.64207	0.52253
C	-5.96912	-0.83411	-0.09738
H	-5.28845	0.11607	-1.91931
C	-5.57467	-1.54212	1.04144
H	-3.9054	-2.36347	2.1418
H	-7.01519	-0.60681	-0.26385
H	-6.3146	-1.8604	1.76622
H	1.81897	-4.8372	-1.21214
H	0.01773	-2.02435	-3.06805

TS of 1a cat.-Toluene

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7526 Hartree

Zero-point Energy Correction = 0.603537 Hartree

Thermal Correction to Energy = 0.636176 Hartree

Thermal Correction to Enthalpy = 0.63712 Hartree

Thermal Correction to Free Energy = 0.537369 Hartree

EE + Zero-point Energy = -1816.1491 Hartree

EE + Thermal Energy Correction = -1816.1164 Hartree

EE + Thermal Enthalpy Correction = -1816.1155 Hartree

EE + Thermal Free Energy Correction = -1816.2152 Hartree

E (Thermal) = 399.206 kcal/mol

Heat Capacity (Cv) = 125.81 cal/mol-kelvin

Entropy (S) = 209.943 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.20533	0.99883	-1.77758
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
C	-1.34786	1.6292	-0.20539
C	-2.33372	2.11032	-1.02126
C	-1.45348	1.65645	1.31028
C	-3.59098	2.76154	-0.50137
C	-2.87274	2.0305	1.79524
H	-1.18233	0.67076	1.71126
C	-3.44674	3.20025	0.97294
H	-3.85104	3.61938	-1.13364
H	-2.8276	2.28788	2.85909
H	-2.77142	4.0628	1.03821
H	-3.52854	1.15926	1.68556
H	-4.42304	3.50231	1.3683
H	-4.42465	2.0435	-0.57187
H	-0.35098	-1.26416	-0.83323
O	-1.59288	-0.80111	-1.84696
N	-2.79578	-0.25456	-1.87144
H	-0.72684	2.38454	1.69895
H	-2.16244	2.1386	-2.09053
C	-3.67306	-0.70595	-0.8239
C	-3.29144	-1.45765	0.29725
C	-5.02168	-0.35608	-1.00302

C	-4.25174	-1.84991	1.22425
H	-2.25352	-1.7067	0.46473
C	-5.98334	-0.76055	-0.07772
H	-5.29507	0.20706	-1.88675
C	-5.59959	-1.50751	1.03984
H	-3.95031	-2.41781	2.09651
H	-7.0233	-0.4969	-0.22702
H	-6.34167	-1.82059	1.76453
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524

TS of 1a cat.-Toluene

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7585 Hartree

Zero-point Energy Correction = 0.603768 Hartree

Thermal Correction to Energy = 0.636359 Hartree

Thermal Correction to Enthalpy = 0.637303 Hartree

Thermal Correction to Free Energy = 0.538111 Hartree

EE + Zero-point Energy = -1816.1548 Hartree

EE + Thermal Energy Correction = -1816.1222 Hartree

EE + Thermal Enthalpy Correction = -1816.1212 Hartree

EE + Thermal Free Energy Correction = -1816.2204 Hartree

E (Thermal) = 399.321 kcal/mol

Heat Capacity (Cv) = 125.793 cal/mol-kelvin

Entropy (S) = 208.766 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01078	0.72351	-0.04094
C	1.61298	-0.58984	-0.64283
N	0.55073	-1.67957	-0.47936
N	-0.24715	1.03392	-0.74975
H	-0.2248	0.97783	-1.76616
H	0.77235	0.52714	1.00595
H	1.75075	-0.44699	-1.71718
C	2.94249	-0.95036	-0.0048

C	4.10927	-0.88631	-0.77822
C	3.03279	-1.31187	1.34797
C	5.35166	-1.18387	-0.21428
H	4.048	-0.5982	-1.82216
C	4.2767	-1.61149	1.90748
H	2.13619	-1.38077	1.95742
C	5.43735	-1.54884	1.13123
H	6.24648	-1.13039	-0.82312
H	4.33683	-1.89621	2.95143
H	6.39981	-1.78271	1.57108
C	2.01381	1.87283	-0.13529
C	2.6864	2.31379	1.01038
C	2.26897	2.50122	-1.36147
C	3.60616	3.36257	0.93174
H	2.49621	1.8319	1.96272
C	3.18936	3.54732	-1.44188
H	1.74459	2.18473	-2.2566
C	3.86056	3.98076	-0.2945
H	4.11991	3.69541	1.82597
H	3.37877	4.02625	-2.39551
H	4.57248	4.79543	-0.35644
C	0.71376	-2.99745	-1.26385
C	1.86572	-3.85703	-0.73152
C	0.81523	-2.70211	-2.76853
H	2.83292	-3.39924	-0.94543
H	1.77618	-4.00676	0.34852

H	1.78988	-2.27573	-3.02672
H	0.70225	-3.64126	-3.31905
H	-0.23593	-3.50608	-1.06677
Cl	-0.31319	-1.80417	2.50203
H	0.39864	-1.87643	0.55405
C	-1.35869	1.63723	-0.20271
C	-2.3492	2.09579	-1.0275
C	-1.46411	1.68877	1.31183
C	-3.61659	2.73584	-0.51837
C	-2.88807	2.05315	1.7902
H	-1.18191	0.71444	1.73222
C	-3.47896	3.20059	0.94874
H	-3.88987	3.5795	-1.16421
H	-2.84583	2.32836	2.84958
H	-2.81659	4.07419	0.99903
H	-3.53101	1.17062	1.69718
H	-4.45982	3.49482	1.339
H	-4.43853	2.00318	-0.5771
H	-0.3653	-1.26685	-0.82395
O	-1.57351	-0.79049	-1.84971
N	-2.78523	-0.25962	-1.87011
H	-0.74611	2.43356	1.68528
H	-2.17581	2.11493	-2.0965
C	-3.65517	-0.72216	-0.82179
C	-3.26398	-1.43663	0.32027
C	-5.01126	-0.41315	-1.02046

C	-4.22314	-1.83666	1.24526
H	-2.2224	-1.647	0.51686
C	-5.97107	-0.82769	-0.09835
H	-5.28881	0.12609	-1.91773
C	-5.57804	-1.54018	1.03817
H	-3.91079	-2.36968	2.13523
H	-7.01662	-0.59735	-0.26383
H	-6.31855	-1.85899	1.76211
H	1.81942	-4.83481	-1.22269
H	0.01672	-2.0177	-3.0707

TS of 1a cat.-$CHCl_3$

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7594 Hartree

Zero-point Energy Correction = 0.603782 Hartree

Thermal Correction to Energy = 0.636373 Hartree

Thermal Correction to Enthalpy = 0.637317 Hartree

Thermal Correction to Free Energy = 0.538128 Hartree

EE + Zero-point Energy = -1816.1556 Hartree

EE + Thermal Energy Correction = -1816.123 Hartree

EE + Thermal Enthalpy Correction = -1816.1221 Hartree

EE + Thermal Free Energy Correction = -1816.2213 Hartree

E (Thermal) = 399.33 kcal/mol

Heat Capacity (Cv) = 125.796 cal/mol-kelvin

Entropy (S) = 208.761 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01734	0.72436	-0.04214
C	1.61894	-0.58843	-0.64476
N	0.5537	-1.67713	-0.4887
N	-0.24276	1.03442	-0.74762
H	-0.21653	0.99562	-1.76495
H	0.78116	0.52953	1.00528
H	1.76122	-0.44436	-1.71803
C	2.94477	-0.95243	-0.00111

C	4.11518	-0.88907	-0.76928
C	3.02887	-1.31461	1.3519
C	5.35487	-1.18728	-0.19944
H	4.05861	-0.60257	-1.81382
C	4.27003	-1.61486	1.91752
H	2.12984	-1.38405	1.9574
C	5.43439	-1.55224	1.14661
H	6.25235	-1.13487	-0.8044
H	4.32571	-1.89974	2.9617
H	6.3947	-1.78644	1.59089
C	2.01936	1.8749	-0.13588
C	2.68357	2.32217	1.01249
C	2.28047	2.49924	-1.36305
C	3.6012	3.37319	0.93576
H	2.4881	1.84432	1.96585
C	3.19873	3.54761	-1.44137
H	1.76384	2.17807	-2.26085
C	3.86172	3.98731	-0.29143
H	4.10822	3.71102	1.83196
H	3.39309	4.02294	-2.39576
H	4.57196	4.8035	-0.35216
C	0.7144	-2.98793	-1.28807
C	1.86817	-3.85164	-0.76679
C	0.81251	-2.67702	-2.78965
H	2.83456	-3.39147	-0.97933
H	1.78158	-4.01211	0.31204

H	1.78634	-2.24843	-3.04676
H	0.69736	-3.6109	-3.34857
H	-0.23459	-3.4987	-1.0938
Cl	-0.32248	-1.86394	2.50472
H	0.40392	-1.88678	0.54013
C	-1.35171	1.63742	-0.19391
C	-2.34058	2.10988	-1.01218
C	-1.45652	1.67148	1.3214
C	-3.6039	2.75148	-0.49495
C	-2.87936	2.03412	1.8043
H	-1.17652	0.6912	1.72918
C	-3.46447	3.19568	0.97829
H	-3.87127	3.60533	-1.12971
H	-2.83692	2.2947	2.8674
H	-2.79776	4.06515	1.04092
H	-3.52601	1.15575	1.69782
H	-4.44395	3.48939	1.37226
H	-4.43076	2.02534	-0.56403
H	-0.36131	-1.25917	-0.82802
O	-1.5806	-0.78313	-1.85049
N	-2.78818	-0.24438	-1.87217
H	-0.73673	2.40945	1.70453
H	-2.16832	2.13865	-2.0812
C	-3.66382	-0.7073	-0.82873
C	-3.27946	-1.44406	0.30141
C	-5.01637	-0.37942	-1.0206

C	-4.24157	-1.84645	1.22218
H	-2.23964	-1.67185	0.4869
C	-5.97942	-0.7951	-0.10209
H	-5.28996	0.1753	-1.90959
C	-5.59318	-1.52924	1.02297
H	-3.93596	-2.39943	2.10237
H	-7.02229	-0.54942	-0.26193
H	-6.33622	-1.84998	1.74338
H	1.82096	-4.82454	-1.26723
H	0.01379	-1.98923	-3.0831

TS of 1a cat.-Chlorobenzene

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7609 Hartree

Zero-point Energy Correction = 0.60381 Hartree

Thermal Correction to Energy = 0.636397 Hartree

Thermal Correction to Enthalpy = 0.637341 Hartree

Thermal Correction to Free Energy = 0.53822 Hartree

EE + Zero-point Energy = -1816.1571 Hartree

EE + Thermal Energy Correction = -1816.1245 Hartree

EE + Thermal Enthalpy Correction = -1816.1235 Hartree

EE + Thermal Free Energy Correction = -1816.2226 Hartree

E (Thermal) = 399.345 kcal/mol

Heat Capacity (Cv) = 125.802 cal/mol-kelvin

Entropy (S) = 208.616 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01784	0.72399	-0.04275
C	1.61991	-0.58855	-0.64524
N	0.55464	-1.67746	-0.48991
N	-0.2424	1.03359	-0.74827
H	-0.21532	0.99686	-1.76568
H	0.7816	0.52921	1.00464
H	1.76274	-0.44453	-1.7184
C	2.94537	-0.95233	-0.00073

C	4.11628	-0.88861	-0.76815
C	3.02875	-1.3143	1.35238
C	5.35573	-1.18621	-0.19739
H	4.06027	-0.60251	-1.81281
C	4.26966	-1.61393	1.91896
H	2.12941	-1.38398	1.95735
C	5.43452	-1.55091	1.14879
H	6.25356	-1.13361	-0.80178
H	4.32484	-1.89858	2.96322
H	6.39463	-1.78461	1.59376
C	2.01934	1.87504	-0.13593
C	2.68127	2.32378	1.01323
C	2.28197	2.49864	-1.36319
C	3.59819	3.3755	0.93724
H	2.48449	1.84665	1.96669
C	3.19954	3.5477	-1.44074
H	1.76727	2.17636	-2.26167
C	3.86028	3.98885	-0.29003
H	4.10341	3.71448	1.83402
H	3.39515	4.02237	-2.39519
H	4.56996	4.80556	-0.35024
C	0.7154	-2.9874	-1.29103
C	1.86998	-3.85102	-0.77141
C	0.81255	-2.67463	-2.79225
H	2.83597	-3.39008	-0.98411
H	1.78419	-4.01288	0.30728

H	1.78603	-2.24538	-3.0495
H	0.69736	-3.60794	-3.35211
H	-0.23321	-3.49886	-1.09678
Cl	-0.32319	-1.87116	2.50532
H	0.40534	-1.8886	0.53833
C	-1.35108	1.63683	-0.19412
C	-2.33965	2.11067	-1.01186
C	-1.45593	1.66938	1.32124
C	-3.60236	2.75296	-0.49399
C	-2.87852	2.03254	1.80451
H	-1.17657	0.68842	1.72783
C	-3.46259	3.1955	0.9797
H	-3.86887	3.60771	-1.12789
H	-2.83597	2.29198	2.86789
H	-2.79509	4.06428	1.04333
H	-3.52592	1.15486	1.69691
H	-4.4418	3.48966	1.37397
H	-4.42995	2.02775	-0.56385
H	-0.36041	-1.25915	-0.82848
O	-1.58179	-0.78393	-1.85023
N	-2.78881	-0.24417	-1.87224
H	-0.73566	2.40635	1.70533
H	-2.16749	2.14002	-2.08089
C	-3.66496	-0.70632	-0.82887
C	-3.28124	-1.44539	0.29998
C	-5.01703	-0.37587	-1.01955

C	-4.24348	-1.84725	1.22086
H	-2.24165	-1.67561	0.48364
C	-5.98025	-0.79086	-0.10086
H	-5.29033	0.18032	-1.90771
C	-5.59464	-1.52713	1.02303
H	-3.93861	-2.4024	2.09995
H	-7.02276	-0.54308	-0.25972
H	-6.33781	-1.84748	1.74348
H	1.82299	-4.82333	-1.27298
H	0.01345	-1.98676	-3.08445

TS of 1a cat.-Aniline

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7621 Hartree

Zero-point Energy Correction = 0.603839 Hartree

Thermal Correction to Energy = 0.636418 Hartree

Thermal Correction to Enthalpy = 0.637362 Hartree

Thermal Correction to Free Energy = 0.538352 Hartree

EE + Zero-point Energy = -1816.1583 Hartree

EE + Thermal Energy Correction = -1816.1257 Hartree

EE + Thermal Enthalpy Correction = -1816.1248 Hartree

EE + Thermal Free Energy Correction = -1816.2238 Hartree

E (Thermal) = 399.358 kcal/mol

Heat Capacity (Cv) = 125.808 cal/mol-kelvin

Entropy (S) = 208.384 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01356	0.72431	-0.04093
C	1.61502	-0.58901	-0.64328
N	0.55131	-1.67801	-0.4829
N	-0.2453	1.03499	-0.74808
H	-0.22185	0.98541	-1.76487
H	0.77627	0.52865	1.00625
H	1.75458	-0.44545	-1.71719
C	2.94302	-0.95152	-0.00323

C	4.11117	-0.88816	-0.77469
C	3.03084	-1.31367	1.34954
C	5.35241	-1.18673	-0.20866
H	4.05176	-0.6004	-1.81879
C	4.27358	-1.61428	1.91122
H	2.1333	-1.38263	1.95749
C	5.43564	-1.55204	1.13696
H	6.24825	-1.13396	-0.81606
H	4.33189	-1.89939	2.95518
H	6.39719	-1.78663	1.5784
C	2.01661	1.87371	-0.13551
C	2.68728	2.31636	1.01071
C	2.27324	2.50082	-1.3621
C	3.60668	3.36555	0.9323
H	2.49577	1.83575	1.96345
C	3.19326	3.54735	-1.44223
H	1.7508	2.18309	-2.25788
C	3.8626	3.98246	-0.29434
H	4.11888	3.69972	1.82692
H	3.38391	4.02514	-2.39617
H	4.57423	4.79738	-0.3562
C	0.71309	-2.99316	-1.27315
C	1.86513	-3.85497	-0.74474
C	0.81384	-2.69181	-2.77663
H	2.83234	-3.39675	-0.95773
H	1.77623	-4.0088	0.3348

H	1.78845	-2.26501	-3.03415
H	0.69977	-3.62886	-3.33048
H	-0.23664	-3.50217	-1.07749
Cl	-0.31732	-1.82666	2.50253
H	0.39986	-1.87984	0.54882
C	-1.35582	1.63799	-0.19821
C	-2.34581	2.10201	-1.02035
C	-1.46087	1.68254	1.31666
C	-3.61179	2.7422	-0.50789
C	-2.88452	2.04559	1.7969
H	-1.17913	0.70598	1.7321
C	-3.4736	3.19857	0.96177
H	-3.883	3.58997	-1.14919
H	-2.84228	2.31478	2.85784
H	-2.80986	4.07082	1.0171
H	-3.52854	1.16442	1.6984
H	-4.45403	3.49214	1.35357
H	-4.43545	2.01183	-0.5709
H	-0.36418	-1.263	-0.82556
O	-1.57589	-0.7861	-1.85034
N	-2.78613	-0.25238	-1.87101
H	-0.74246	2.42499	1.69385
H	-2.17292	2.12521	-2.08936
C	-3.65831	-0.71587	-0.82498
C	-3.26978	-1.43898	0.31254
C	-5.01315	-0.40016	-1.02146

C	-4.23024	-1.84072	1.23539
H	-2.22883	-1.65547	0.50554
C	-5.97436	-0.81595	-0.10127
H	-5.28909	0.14523	-1.9155
C	-5.58398	-1.53696	1.03081
H	-3.92041	-2.38137	2.12167
H	-7.01896	-0.58018	-0.26494
H	-6.32558	-1.85712	1.753
H	1.81816	-4.83085	-1.23953
H	0.01561	-2.00575	-3.07565

TS of 1a cat.-THF

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7626 Hartree

Zero-point Energy Correction = 0.603847 Hartree

Thermal Correction to Energy = 0.636424 Hartree

Thermal Correction to Enthalpy = 0.637368 Hartree

Thermal Correction to Free Energy = 0.538388 Hartree

EE + Zero-point Energy = -1816.1588 Hartree

EE + Thermal Energy Correction = -1816.1262 Hartree

EE + Thermal Enthalpy Correction = -1816.1252 Hartree

EE + Thermal Free Energy Correction = -1816.2242 Hartree

E (Thermal) = 399.362 kcal/mol

Heat Capacity (Cv) = 125.811 cal/mol-kelvin

Entropy (S) = 208.322 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.20533	0.99883	-1.77758
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
C	-1.34786	1.6292	-0.20539
C	-2.33372	2.11032	-1.02126
C	-1.45348	1.65645	1.31028
C	-3.59098	2.76154	-0.50137
C	-2.87274	2.0305	1.79524
H	-1.18233	0.67076	1.71126
C	-3.44674	3.20025	0.97294
H	-3.85104	3.61938	-1.13364
H	-2.8276	2.28788	2.85909
H	-2.77142	4.0628	1.03821
H	-3.52854	1.15926	1.68556
H	-4.42304	3.50231	1.3683
H	-4.42465	2.0435	-0.57187
H	-0.35098	-1.26416	-0.83323
O	-1.59288	-0.80111	-1.84696
N	-2.79578	-0.25456	-1.87144
H	-0.72684	2.38454	1.69895
H	-2.16244	2.1386	-2.09053
C	-3.67306	-0.70595	-0.8239
C	-3.29144	-1.45765	0.29725
C	-5.02168	-0.35608	-1.00302

C	-4.25174	-1.84991	1.22425
H	-2.25352	-1.7067	0.46473
C	-5.98334	-0.76055	-0.07772
H	-5.29507	0.20706	-1.88675
C	-5.59959	-1.50751	1.03984
H	-3.95031	-2.41781	2.09651
H	-7.0233	-0.4969	-0.22702
H	-6.34167	-1.82059	1.76453
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524

TS of 1a cat.-CH_2Cl_2

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7636 Hartree

Zero-point Energy Correction = 0.603855 Hartree

Thermal Correction to Energy = 0.636433 Hartree

Thermal Correction to Enthalpy = 0.637377 Hartree

Thermal Correction to Free Energy = 0.538427 Hartree

EE + Zero-point Energy = -1816.1598 Hartree

EE + Thermal Energy Correction = -1816.1272 Hartree

EE + Thermal Enthalpy Correction = -1816.1263 Hartree

EE + Thermal Free Energy Correction = -1816.2252 Hartree

E (Thermal) = 399.368 kcal/mol

Heat Capacity (Cv) = 125.82 cal/mol-kelvin

Entropy (S) = 208.259 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01906	0.7196	-0.04868
C	1.62677	-0.59056	-0.6493
N	0.56283	-1.68219	-0.49803
N	-0.24118	1.02458	-0.75677
H	-0.20754	0.99883	-1.77457
H	0.78067	0.52433	0.99804
H	1.77344	-0.44758	-1.7218
C	2.95015	-0.95014	0.00174

C	4.12468	-0.88166	-0.75998
C	3.02868	-1.31004	1.35572
C	5.36269	-1.17258	-0.1823
H	4.07257	-0.59807	-1.80547
C	4.26811	-1.603	1.92932
H	2.12696	-1.38239	1.95663
C	5.43661	-1.53522	1.16486
H	6.26317	-1.11691	-0.7824
H	4.31991	-1.88563	2.97434
H	6.39556	-1.76364	1.61494
C	2.01567	1.87541	-0.13604
C	2.65657	2.3371	1.02014
C	2.29243	2.49244	-1.36368
C	3.56694	3.3952	0.95103
H	2.44798	1.86592	1.97412
C	3.2036	3.54776	-1.43422
H	1.79491	2.16018	-2.26802
C	3.84338	4.00191	-0.27656
H	4.05556	3.7444	1.85308
H	3.41066	4.01682	-2.38896
H	4.54796	4.82335	-0.33174
C	0.72546	-2.98703	-1.30899
C	1.88652	-3.84803	-0.79972
C	0.81559	-2.66353	-2.8082
H	2.84918	-3.38052	-1.01324
H	1.80607	-4.019	0.27811

H	1.78619	-2.22892	-3.06667
H	0.70132	-3.59374	-3.37334
H	-0.21999	-3.50391	-1.11416
Cl	-0.32555	-1.9138	2.50688
H	0.41656	-1.90169	0.52686
C	-1.34858	1.63082	-0.2023
C	-2.33501	2.11065	-1.01846
C	-1.4541	1.65868	1.3133
C	-3.59355	2.75963	-0.49885
C	-2.87428	2.02964	1.79786
H	-1.18079	0.674	1.71521
C	-3.4506	3.19829	0.97563
H	-3.8549	3.61717	-1.13101
H	-2.83002	2.2868	2.86178
H	-2.77716	4.06231	1.0412
H	-3.52797	1.15685	1.68788
H	-4.42767	3.4982	1.37076
H	-4.42587	2.04006	-0.56981
H	-0.35308	-1.26304	-0.83191
O	-1.59027	-0.79691	-1.84763
N	-2.79404	-0.25173	-1.87179
H	-0.72915	2.38888	1.70128
H	-2.16345	2.13962	-2.08764
C	-3.67138	-0.70563	-0.8255
C	-3.28956	-1.45491	0.2972
C	-5.02072	-0.35983	-1.00735

C	-4.25055	-1.84949	1.22251
H	-2.25126	-1.69997	0.46823
C	-5.98297	-0.76679	-0.08381
H	-5.29388	0.20206	-1.89195
C	-5.5991	-1.51179	1.03498
H	-3.94862	-2.41491	2.09617
H	-7.02346	-0.50646	-0.23535
H	-6.3416	-1.82663	1.75849
H	1.84275	-4.81664	-1.3085
H	0.01315	-1.9764	-3.09262

TS of 1a cat.-$EtCl_2$(chloroethane)

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7642 Hartree

Zero-point Energy Correction = 0.603852 Hartree

Thermal Correction to Energy = 0.636435 Hartree

Thermal Correction to Enthalpy = 0.637379 Hartree

Thermal Correction to Free Energy = 0.538416 Hartree

EE + Zero-point Energy = -1816.1604 Hartree

EE + Thermal Energy Correction = -1816.1278 Hartree

EE + Thermal Enthalpy Correction = -1816.1269 Hartree

EE + Thermal Free Energy Correction = -1816.2258 Hartree

E (Thermal) = 399.369 kcal/mol

Heat Capacity (Cv) = 125.828 cal/mol-kelvin

Entropy (S) = 208.285 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01886	0.72132	-0.0462
C	1.62446	-0.58963	-0.64768
N	0.55993	-1.68026	-0.49531
N	-0.24141	1.02811	-0.75324
H	-0.20994	0.99918	-1.77094
H	0.78131	0.52619	1.00076
H	1.76986	-0.44609	-1.72037
C	2.94849	-0.95101	0.00106

C	4.12177	-0.88435	-0.76266
C	3.02865	-1.31181	1.35469
C	5.36024	-1.17787	-0.18742
H	4.06832	-0.59987	-1.80785
C	4.26855	-1.60736	1.92582
H	2.12775	-1.38318	1.95701
C	5.4358	-1.54136	1.15937
H	6.2598	-1.12341	-0.78903
H	4.3215	-1.89083	2.97055
H	6.39513	-1.77183	1.60765
C	2.01729	1.87541	-0.13552
C	2.66612	2.33198	1.01819
C	2.28869	2.49519	-1.36291
C	3.57896	3.38772	0.94675
H	2.46194	1.85841	1.97191
C	3.20225	3.54822	-1.43581
H	1.78474	2.1669	-2.26519
C	3.84997	3.99722	-0.28062
H	4.07383	3.7329	1.84694
H	3.40498	4.0196	-2.39036
H	4.55648	4.8169	-0.3375
C	0.72192	-2.98668	-1.3033
C	1.88072	-3.84873	-0.79067
C	0.81453	-2.66643	-2.80312
H	2.84455	-3.38354	-1.00395
H	1.79851	-4.01668	0.28746

H	1.78615	-2.23364	-3.06105
H	0.69991	-3.59756	-3.36668
H	-0.22463	-3.50174	-1.10884
Cl	-0.32524	-1.90011	2.50675
H	0.4126	-1.89723	0.53059
C	-1.34925	1.63305	-0.19864
C	-2.33633	2.11137	-1.01515
C	-1.45474	1.66158	1.31689
C	-3.59637	2.75773	-0.4959
C	-2.87595	2.02912	1.80097
H	-1.1791	0.67801	1.71986
C	-3.4549	3.19646	0.97873
H	-3.85928	3.61486	-1.12801
H	-2.83262	2.28613	2.86494
H	-2.78361	4.06214	1.04455
H	-3.52726	1.1546	1.69081
H	-4.43283	3.49394	1.37359
H	-4.42711	2.03633	-0.56732
H	-0.35561	-1.26124	-0.83079
O	-1.58706	-0.79139	-1.84886
N	-2.79186	-0.24787	-1.87245
H	-0.73168	2.39409	1.7041
H	-2.1644	2.14119	-2.08423
C	-3.66926	-0.70506	-0.82775
C	-3.28727	-1.45169	0.29667
C	-5.01944	-0.36416	-1.01286

C	-4.24909	-1.84929	1.21982
H	-2.24857	-1.69195	0.47208
C	-5.98242	-0.77436	-0.09159
H	-5.29229	0.19642	-1.89838
C	-5.59845	-1.51725	1.02854
H	-3.94657	-2.41191	2.09505
H	-7.02353	-0.51804	-0.24581
H	-6.34148	-1.83439	1.75051
H	1.83572	-4.81856	-1.29707
H	0.01329	-1.97893	-3.09006

TS of 1a cat.-Cyclohexanone

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.766 Hartree

Zero-point Energy Correction = 0.603813 Hartree

Thermal Correction to Energy = 0.636422 Hartree

Thermal Correction to Enthalpy = 0.637366 Hartree

Thermal Correction to Free Energy = 0.538254 Hartree

EE + Zero-point Energy = -1816.1622 Hartree

EE + Thermal Energy Correction = -1816.1295 Hartree

EE + Thermal Enthalpy Correction = -1816.1286 Hartree

EE + Thermal Free Energy Correction = -1816.2277 Hartree

E (Thermal) = 399.361 kcal/mol

Heat Capacity (Cv) = 125.859 cal/mol-kelvin

Entropy (S) = 208.599 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.20533	0.99883	-1.77758
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
C	-1.34786	1.6292	-0.20539
C	-2.33372	2.11032	-1.02126
C	-1.45348	1.65645	1.31028
C	-3.59098	2.76154	-0.50137
C	-2.87274	2.0305	1.79524
H	-1.18233	0.67076	1.71126
C	-3.44674	3.20025	0.97294
H	-3.85104	3.61938	-1.13364
H	-2.8276	2.28788	2.85909
H	-2.77142	4.0628	1.03821
H	-3.52854	1.15926	1.68556
H	-4.42304	3.50231	1.3683
H	-4.42465	2.0435	-0.57187
H	-0.35098	-1.26416	-0.83323
O	-1.59288	-0.80111	-1.84696
N	-2.79578	-0.25456	-1.87144
H	-0.72684	2.38454	1.69895
H	-2.16244	2.1386	-2.09053
C	-3.67306	-0.70595	-0.8239
C	-3.29144	-1.45765	0.29725
C	-5.02168	-0.35608	-1.00302

C	-4.25174	-1.84991	1.22425
H	-2.25352	-1.7067	0.46473
C	-5.98334	-0.76055	-0.07772
H	-5.29507	0.20706	-1.88675
C	-5.59959	-1.50751	1.03984
H	-3.95031	-2.41781	2.09651
H	-7.0233	-0.4969	-0.22702
H	-6.34167	-1.82059	1.76453
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524

TS of 1a cat.-Aceton

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7668 Hartree

Zero-point Energy Correction = 0.603786 Hartree

Thermal Correction to Energy = 0.636411 Hartree

Thermal Correction to Enthalpy = 0.637356 Hartree

Thermal Correction to Free Energy = 0.538139 Hartree

EE + Zero-point Energy = -1816.163 Hartree

EE + Thermal Energy Correction = -1816.1304 Hartree

EE + Thermal Enthalpy Correction = -1816.1294 Hartree

EE + Thermal Free Energy Correction = -1816.2286 Hartree

E (Thermal) = 399.354 kcal/mol

Heat Capacity (Cv) = 125.876 cal/mol-kelvin

Entropy (S) = 208.818 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01894	0.72063	-0.04729
C	1.62533	-0.59006	-0.64838
N	0.56105	-1.68108	-0.49626
N	-0.24138	1.02664	-0.75468
H	-0.20912	0.99889	-1.77241
H	0.78115	0.52553	0.99961
H	1.77113	-0.44683	-1.72101
C	2.94916	-0.95066	0.00118

C	4.12286	-0.88333	-0.76186
C	3.0288	-1.311	1.35497
C	5.36121	-1.17577	-0.18575
H	4.06984	-0.5993	-1.80719
C	4.26858	-1.60547	1.92699
H	2.12764	-1.38272	1.95683
C	5.43625	-1.53881	1.16121
H	6.26108	-1.12087	-0.78685
H	4.32117	-1.88852	2.97185
H	6.39547	-1.76842	1.61013
C	2.01664	1.87539	-0.13602
C	2.66248	2.33405	1.01857
C	2.29001	2.49402	-1.36358
C	3.57434	3.39072	0.94789
H	2.45666	1.86149	1.97245
C	3.20263	3.54795	-1.43571
H	1.78849	2.16412	-2.26661
C	3.84736	3.99904	-0.27964
H	4.06685	3.73753	1.84874
H	3.40695	4.01836	-2.39039
H	4.5531	4.81941	-0.33598
C	0.72325	-2.98694	-1.30533
C	1.88304	-3.8485	-0.79409
C	0.81471	-2.66552	-2.80495
H	2.84636	-3.38238	-1.00764
H	1.80167	-4.01754	0.28394

H	1.78589	-2.23202	-3.06324
H	0.70019	-3.59634	-3.36904
H	-0.22282	-3.50274	-1.11059
Cl	-0.32518	-1.90528	2.50708
H	0.41423	-1.89897	0.52927
C	-1.349	1.63214	-0.20009
C	-2.33588	2.111	-1.01643
C	-1.45439	1.66052	1.31548
C	-3.59529	2.75843	-0.49699
C	-2.87518	2.0294	1.7998
H	-1.17962	0.67655	1.71808
C	-3.45315	3.19721	0.97754
H	-3.85762	3.61568	-1.12916
H	-2.83143	2.28652	2.86374
H	-2.78103	4.06224	1.04318
H	-3.52741	1.15554	1.68979
H	-4.43073	3.49565	1.37255
H	-4.42666	2.03775	-0.56815
H	-0.35467	-1.26205	-0.83106
O	-1.58845	-0.79372	-1.84816
N	-2.79284	-0.24953	-1.87197
H	-0.73058	2.39217	1.70288
H	-2.16416	2.14041	-2.08556
C	-3.67017	-0.70533	-0.82657
C	-3.2882	-1.45293	0.29721
C	-5.02003	-0.3625	-1.01035

C	-4.24965	-1.84927	1.22128
H	-2.24964	-1.69507	0.47085
C	-5.98269	-0.77135	-0.08811
H	-5.29305	0.19853	-1.89553
C	-5.59871	-1.515	1.03153
H	-3.94734	-2.41293	2.09592
H	-7.02356	-0.51345	-0.24124
H	-6.3415	-1.83117	1.75416
H	1.83848	-4.81789	-1.30134
H	0.01295	-1.97821	-3.09087

TS of 1a cat.-EtOH

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7672 Hartree

Zero-point Energy Correction = 0.603765 Hartree

Thermal Correction to Energy = 0.636402 Hartree

Thermal Correction to Enthalpy = 0.637347 Hartree

Thermal Correction to Free Energy = 0.538055 Hartree

EE + Zero-point Energy = -1816.1635 Hartree

EE + Thermal Energy Correction = -1816.1308 Hartree

EE + Thermal Enthalpy Correction = -1816.1299 Hartree

EE + Thermal Free Energy Correction = -1816.2292 Hartree

E (Thermal) = 399.349 kcal/mol

Heat Capacity (Cv) = 125.888 cal/mol-kelvin

Entropy (S) = 208.976 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.01903	0.71983	-0.04837
C	1.62645	-0.59045	-0.64909
N	0.56244	-1.68194	-0.49762
N	-0.24123	1.02504	-0.7563
H	-0.2079	0.99885	-1.77408
H	0.78078	0.5246	0.9984
H	1.77292	-0.44741	-1.72162
C	2.94994	-0.95025	0.00161

C	4.12427	-0.88203	-0.76041
C	3.02872	-1.31024	1.35555
C	5.36236	-1.17328	-0.18309
H	4.07195	-0.59834	-1.80586
C	4.26823	-1.60354	1.92879
H	2.12713	-1.38246	1.95668
C	5.43654	-1.53601	1.16403
H	6.2627	-1.11778	-0.78342
H	4.32021	-1.88627	2.97377
H	6.39556	-1.76469	1.61384
C	2.01588	1.87541	-0.13603
C	2.65791	2.33641	1.01979
C	2.29186	2.49281	-1.36366
C	3.56861	3.39419	0.95032
H	2.44995	1.86491	1.97375
C	3.20336	3.54782	-1.43455
H	1.79343	2.16109	-2.2677
C	3.84427	4.00127	-0.27725
H	4.05811	3.74285	1.8521
H	3.40979	4.01719	-2.38928
H	4.54911	4.82247	-0.3327
C	0.72498	-2.98702	-1.30816
C	1.88576	-3.84813	-0.79846
C	0.81539	-2.66398	-2.80747
H	2.84857	-3.38092	-1.012
H	1.80512	-4.01866	0.27941

H	1.78612	-2.22961	-3.0659
H	0.70107	-3.59432	-3.37237
H	-0.2206	-3.50366	-1.11335
Cl	-0.32547	-1.91189	2.50696
H	0.41605	-1.90109	0.52741
C	-1.34867	1.63111	-0.2018
C	-2.33521	2.11073	-1.01799
C	-1.45417	1.65908	1.3138
C	-3.59394	2.75936	-0.49842
C	-2.8745	2.02956	1.7983
H	-1.18053	0.67455	1.71586
C	-3.45118	3.19803	0.97607
H	-3.85551	3.61684	-1.13058
H	-2.83035	2.28669	2.86222
H	-2.77804	4.06227	1.04167
H	-3.52785	1.15652	1.6883
H	-4.42837	3.4976	1.37118
H	-4.42605	2.03954	-0.56944
H	-0.35343	-1.26283	-0.83171
O	-1.58986	-0.7962	-1.84775
N	-2.79377	-0.25124	-1.87184
H	-0.72948	2.3896	1.70165
H	-2.16361	2.1398	-2.08717
C	-3.67111	-0.70556	-0.82575
C	-3.28927	-1.45447	0.2972
C	-5.02057	-0.36042	-1.00804

C	-4.25036	-1.84943	1.22222
H	-2.25091	-1.69887	0.46881
C	-5.98291	-0.7678	-0.08479
H	-5.29369	0.20127	-1.89276
C	-5.59902	-1.5125	1.03419
H	-3.94835	-2.41446	2.09611
H	-7.02349	-0.50801	-0.23669
H	-6.34159	-1.82764	1.7575
H	1.84182	-4.81691	-1.3069
H	0.0131	-1.97681	-3.09222

TS of 1a cat.-MeOH

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7678 Hartree

Zero-point Energy Correction = 0.603739 Hartree

Thermal Correction to Energy = 0.636391 Hartree

Thermal Correction to Enthalpy = 0.637335 Hartree

Thermal Correction to Free Energy = 0.537951 Hartree

EE + Zero-point Energy = -1816.164 Hartree

EE + Thermal Energy Correction = -1816.1314 Hartree

EE + Thermal Enthalpy Correction = -1816.1304 Hartree

EE + Thermal Free Energy Correction = -1816.2298 Hartree

E (Thermal) = 399.342 kcal/mol

Heat Capacity (Cv) = 125.901 cal/mol-kelvin

Entropy (S) = 209.172 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.20533	0.99883	-1.77758
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
C	-1.34786	1.6292	-0.20539
C	-2.33372	2.11032	-1.02126
C	-1.45348	1.65645	1.31028
C	-3.59098	2.76154	-0.50137
C	-2.87274	2.0305	1.79524
H	-1.18233	0.67076	1.71126
C	-3.44674	3.20025	0.97294
H	-3.85104	3.61938	-1.13364
H	-2.8276	2.28788	2.85909
H	-2.77142	4.0628	1.03821
H	-3.52854	1.15926	1.68556
H	-4.42304	3.50231	1.3683
H	-4.42465	2.0435	-0.57187
H	-0.35098	-1.26416	-0.83323
O	-1.59288	-0.80111	-1.84696
N	-2.79578	-0.25456	-1.87144
H	-0.72684	2.38454	1.69895
H	-2.16244	2.1386	-2.09053
C	-3.67306	-0.70595	-0.8239
C	-3.29144	-1.45765	0.29725
C	-5.02168	-0.35608	-1.00302

C	-4.25174	-1.84991	1.22425
H	-2.25352	-1.7067	0.46473
C	-5.98334	-0.76055	-0.07772
H	-5.29507	0.20706	-1.88675
C	-5.59959	-1.50751	1.03984
H	-3.95031	-2.41781	2.09651
H	-7.0233	-0.4969	-0.22702
H	-6.34167	-1.82059	1.76453
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524

TS of 1a cat.-Acetonitrile

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7679 Hartree

Zero-point Energy Correction = 0.603732 Hartree

Thermal Correction to Energy = 0.636388 Hartree

Thermal Correction to Enthalpy = 0.637332 Hartree

Thermal Correction to Free Energy = 0.537922 Hartree

EE + Zero-point Energy = -1816.1642 Hartree

EE + Thermal Energy Correction = -1816.1315 Hartree

EE + Thermal Enthalpy Correction = -1816.1306 Hartree

EE + Thermal Free Energy Correction = -1816.23 Hartree

E (Thermal) = 399.34 kcal/mol

Heat Capacity (Cv) = 125.905 cal/mol-kelvin

Entropy (S) = 209.226 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.0193	0.7182	-0.05066
C	1.62873	-0.59129	-0.65061
N	0.56513	-1.6836	-0.50061
N	-0.2408	1.02191	-0.75972
H	-0.20533	0.99883	-1.77758
H	0.78004	0.5227	0.99581
H	1.7767	-0.44864	-1.72292
C	2.95141	-0.94957	0.00258

C	4.12716	-0.87954	-0.75716
C	3.0282	-1.3089	1.35682
C	5.36461	-1.16848	-0.17718
H	4.07647	-0.59646	-1.80284
C	4.26706	-1.5999	1.93274
H	2.12563	-1.38207	1.95632
C	5.43679	-1.53065	1.17024
H	6.26602	-1.11178	-0.77578
H	4.31759	-1.88202	2.97797
H	6.39529	-1.75752	1.62203
C	2.01453	1.87535	-0.13611
C	2.64834	2.3414	1.0223
C	2.29629	2.48993	-1.36389
C	3.5567	3.40143	0.95535
H	2.43571	1.87229	1.97642
C	3.20554	3.5471	-1.43223
H	1.80452	2.15428	-2.27007
C	3.83822	4.00566	-0.27234
H	4.03975	3.75404	1.85908
H	3.41665	4.01412	-2.38707
H	4.54124	4.82852	-0.32594
C	0.72819	-2.98704	-1.31416
C	1.89075	-3.84752	-0.80747
C	0.81671	-2.66067	-2.8128
H	2.85261	-3.37822	-1.0207
H	1.8113	-4.02125	0.27003

H	1.78662	-2.22471	-3.07139
H	0.7027	-3.59001	-3.37941
H	-0.21653	-3.50522	-1.11935
Cl	-0.32617	-1.9257	2.50613
H	0.4195	-1.90534	0.52342
C	-1.34786	1.6292	-0.20539
C	-2.33372	2.11032	-1.02126
C	-1.45348	1.65645	1.31028
C	-3.59098	2.76154	-0.50137
C	-2.87274	2.0305	1.79524
H	-1.18233	0.67076	1.71126
C	-3.44674	3.20025	0.97294
H	-3.85104	3.61938	-1.13364
H	-2.8276	2.28788	2.85909
H	-2.77142	4.0628	1.03821
H	-3.52854	1.15926	1.68556
H	-4.42304	3.50231	1.3683
H	-4.42465	2.0435	-0.57187
H	-0.35098	-1.26416	-0.83323
O	-1.59288	-0.80111	-1.84696
N	-2.79578	-0.25456	-1.87144
H	-0.72684	2.38454	1.69895
H	-2.16244	2.1386	-2.09053
C	-3.67306	-0.70595	-0.8239
C	-3.29144	-1.45765	0.29725
C	-5.02168	-0.35608	-1.00302

C	-4.25174	-1.84991	1.22425
H	-2.25352	-1.7067	0.46473
C	-5.98334	-0.76055	-0.07772
H	-5.29507	0.20706	-1.88675
C	-5.59959	-1.50751	1.03984
H	-3.95031	-2.41781	2.09651
H	-7.0233	-0.4969	-0.22702
H	-6.34167	-1.82059	1.76453
H	1.84801	-4.81497	-1.31848
H	0.01347	-1.97369	-3.09524

TS of 1a cat.-Nitromethane

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.768 Hartree

Zero-point Energy Correction = 0.603731 Hartree

Thermal Correction to Energy = 0.636387 Hartree

Thermal Correction to Enthalpy = 0.637332 Hartree

Thermal Correction to Free Energy = 0.537915 Hartree

EE + Zero-point Energy = -1816.1642 Hartree

EE + Thermal Energy Correction = -1816.1316 Hartree

EE + Thermal Enthalpy Correction = -1816.1306 Hartree

EE + Thermal Free Energy Correction = -1816.23 Hartree

E (Thermal) = 399.339 kcal/mol

Heat Capacity (Cv) = 125.906 cal/mol-kelvin

Entropy (S) = 209.24 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.99971	0.7278	-0.03852
C	1.5959	-0.58908	-0.64119
N	0.534	-1.67533	-0.46323
N	-0.25379	1.04506	-0.75083
H	-0.24661	0.94681	-1.76411
H	0.7586	0.5286	1.00786
H	1.72455	-0.4483	-1.71759
C	2.93107	-0.95067	-0.01586

C	4.0891	-0.89628	-0.80252
C	3.03383	-1.30779	1.33732
C	5.33583	-1.20024	-0.25223
H	4.01783	-0.60787	-1.846
C	4.28216	-1.61373	1.88263
H	2.14262	-1.36766	1.95652
C	5.43406	-1.56193	1.09298
H	6.22429	-1.15346	-0.87099
H	4.35165	-1.89555	2.92679
H	6.39995	-1.80111	1.52251
C	2.00944	1.8707	-0.13459
C	2.71068	2.28651	1.00294
C	2.24488	2.51635	-1.35528
C	3.63918	3.32675	0.9208
H	2.53624	1.79006	1.9507
C	3.1742	3.55381	-1.43956
H	1.69434	2.22059	-2.2419
C	3.87406	3.96172	-0.30042
H	4.17537	3.64004	1.80892
H	3.34749	4.04702	-2.38908
H	4.59284	4.77022	-0.36457
C	0.69867	-3.01021	-1.21171
C	1.83314	-3.86901	-0.64101
C	0.82574	-2.75148	-2.72136
H	2.8085	-3.42711	-0.85094
H	1.72524	-3.98858	0.44107

H	1.8071	-2.3348	-2.97054
H	0.71865	-3.70186	-3.25369
H	-0.25881	-3.50613	-1.0182
Cl	-0.29912	-1.67963	2.49308
H	0.37308	-1.84216	0.57969
C	-1.3703	1.64232	-0.2111
C	-2.36632	2.07668	-1.04448
C	-1.47579	1.7169	1.30212
C	-3.64181	2.70796	-0.54484
C	-2.90231	2.07812	1.7753
H	-1.18677	0.75176	1.73991
C	-3.50721	3.20243	0.91293
H	-3.92835	3.53547	-1.20577
H	-2.86042	2.3743	2.829
H	-2.85481	4.08441	0.9446
H	-3.53632	1.18732	1.70266
H	-4.49087	3.49322	1.29898
H	-4.45312	1.96238	-0.58752
H	-0.38068	-1.27019	-0.82454
O	-1.55668	-0.78336	-1.86076
N	-2.77671	-0.2662	-1.87083
H	-0.76274	2.47359	1.66139
H	-2.19011	2.08835	-2.11292
C	-3.63398	-0.74053	-0.81704
C	-3.22777	-1.42376	0.33868
C	-4.99693	-0.46785	-1.02243

C	-4.17858	-1.83033	1.26948
H	-2.18297	-1.59961	0.55185
C	-5.948	-0.89091	-0.0956
H	-5.28417	0.05021	-1.92909
C	-5.53974	-1.57314	1.05391
H	-3.85122	-2.33478	2.17055
H	-6.9987	-0.68961	-0.26694
H	-6.2737	-1.89678	1.78251
H	1.78349	-4.85899	-1.10721
H	0.03513	-2.07068	-3.05208

TS of 1a cat.-DMSO

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -1816.7683 Hartree

Zero-point Energy Correction = 0.603713 Hartree

Thermal Correction to Energy = 0.636379 Hartree

Thermal Correction to Enthalpy = 0.637323 Hartree

Thermal Correction to Free Energy = 0.537847 Hartree

EE + Zero-point Energy = -1816.1646 Hartree

EE + Thermal Energy Correction = -1816.1319 Hartree

EE + Thermal Enthalpy Correction = -1816.131 Hartree

EE + Thermal Free Energy Correction = -1816.2304 Hartree

E (Thermal) = 399.334 kcal/mol

Heat Capacity (Cv) = 125.915 cal/mol-kelvin

Entropy (S) = 209.366 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

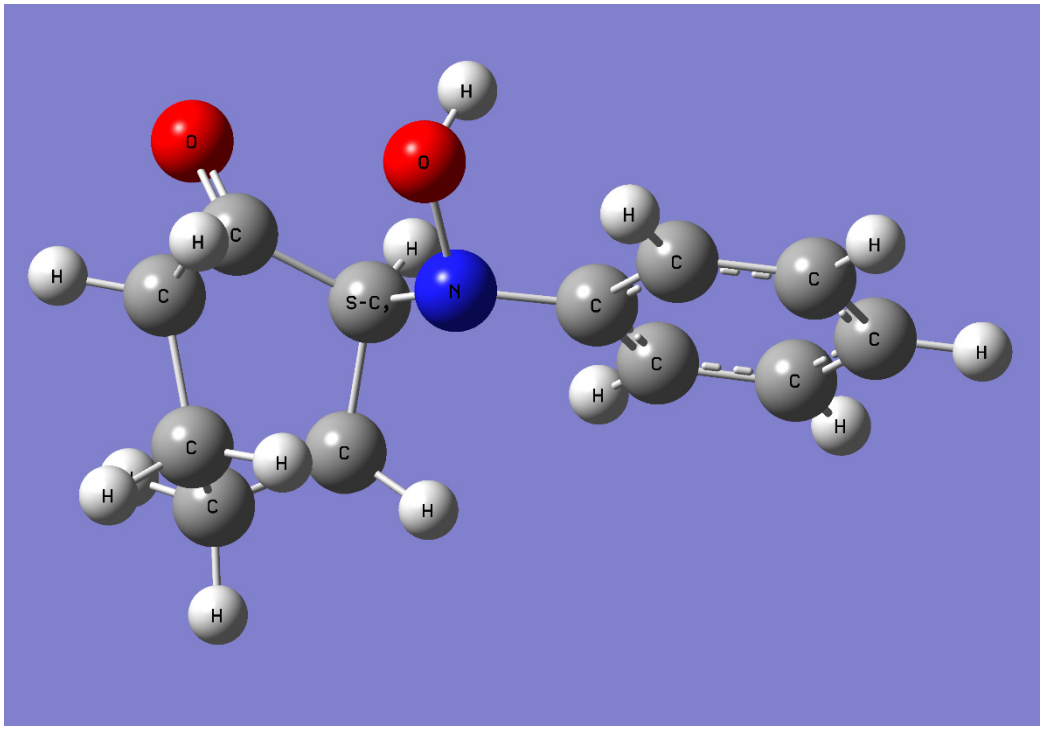
C	-0.8622	1.02987	0.03712
C	-1.56313	-0.27844	0.532
N	-0.59032	-1.44055	0.28331
N	0.40683	1.20936	0.77103
H	0.36469	1.10597	1.78318
H	-0.62725	0.90214	-1.02063
H	-1.69987	-0.21328	1.61306
C	-2.91111	-0.47389	-0.13989

C	-4.07546	-0.434	0.63849
C	-3.0187	-0.64506	-1.52885
C	-5.33219	-0.57207	0.04351
H	-4.00252	-0.28895	1.71092
C	-4.27557	-0.78467	-2.12029
H	-2.12442	-0.69625	-2.14254
C	-5.43442	-0.74893	-1.33813
H	-6.22459	-0.54074	0.65722
H	-4.34975	-0.92321	-3.19262
H	-6.40766	-0.85789	-1.8021
C	-1.7819	2.23964	0.2108
C	-2.34655	2.85774	-0.91151
C	-2.0567	2.75472	1.48518
C	-3.1818	3.96858	-0.76384
H	-2.13836	2.46709	-1.90119
C	-2.89332	3.86231	1.634
H	-1.61712	2.30132	2.3667
C	-3.45839	4.47218	0.50938
H	-3.61204	4.43849	-1.64046
H	-3.10048	4.25071	2.62428
H	-4.10521	5.33376	0.62573
C	-0.9762	-2.8656	0.76768
C	-1.89867	-3.56034	-0.25907
C	-1.55033	-2.85508	2.19689
H	-2.89961	-3.20164	-0.13928
H	-1.55781	-3.34231	-1.24961

H	-2.3559	-2.15304	2.25249
H	-1.91079	-3.83185	2.44365
H	-0.01099	-3.38607	0.77157
Cl	0.2956	-1.34844	-2.73893
H	-0.37929	-1.48879	-0.75446
C	1.55928	1.764	0.26713
C	2.5755	2.09374	1.12487
C	1.68237	1.90664	-1.24018
C	3.8855	2.68199	0.6633
C	3.1317	2.20386	-1.68801
H	1.33629	0.98415	-1.72461
C	3.79038	3.25119	-0.76997
H	4.20808	3.46062	1.36527
H	3.11705	2.55138	-2.72678
H	3.18736	4.16807	-0.76501
H	3.71423	1.27622	-1.65025
H	4.79151	3.50491	-1.13617
H	4.65786	1.89546	0.67545
H	0.32992	-1.17858	0.74315
O	1.58421	-0.7514	1.7341
N	2.83138	-0.3045	1.78428
H	1.02096	2.72213	-1.56727
H	2.38874	2.0681	2.19122
C	3.6731	-0.77632	0.7151
C	3.23669	-1.41844	-0.45281
C	5.04668	-0.56754	0.92272

C	4.16656	-1.84187	-1.39744
H	2.18271	-1.55643	-0.64366
C	5.97683	-1.00329	-0.02057
H	5.36199	-0.08899	1.84165
C	5.53817	-1.64043	-1.18489
H	3.82239	-2.3226	-2.30559
H	7.03511	-0.84856	0.15133
H	6.25592	-1.97659	-1.92363
H	-1.87734	-4.61812	-0.09928
H	-0.78314	-2.57304	2.88738

Figure 6.



Product

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -667.77052 Hartree

Zero-point Energy Correction = 0.253318 Hartree

Thermal Correction to Energy = 0.266508 Hartree

Thermal Correction to Enthalpy = 0.267452 Hartree

Thermal Correction to Free Energy = 0.213275 Hartree

EE + Zero-point Energy = -667.51721 Hartree

EE + Thermal Energy Correction = -667.50402 Hartree

EE + Thermal Enthalpy Correction = -667.50307 Hartree

EE + Thermal Free Energy Correction = -667.55725 Hartree

E (Thermal) = 167.236 kcal/mol

Heat Capacity (Cv) = 52.181 cal/mol-kelvin

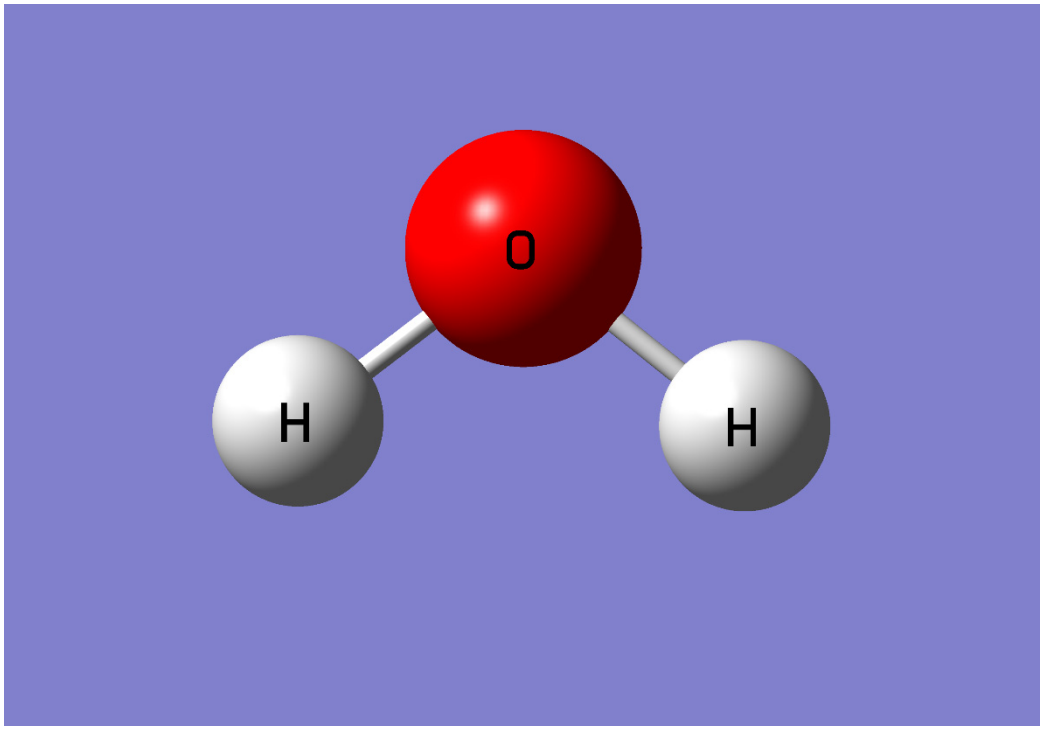
Entropy (S) = 114.026 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.2262	-0.59145	0.73242
C	-0.94088	0.25452	0.7442
C	-2.87112	-0.74782	-0.6359
C	-1.2497	1.69383	0.21642
C	-2.61827	0.48463	-1.54335
H	-2.44336	-1.65319	-1.08
C	-2.53033	1.74419	-0.6565
H	-1.34432	2.3717	1.07054
H	-3.42731	0.57604	-2.27475
H	-3.42038	1.79247	-0.01492
H	-1.67406	0.35901	-2.08066
H	-2.51144	2.65389	-1.26596
H	-0.40023	2.02403	-0.38729
O	-0.20987	-1.90814	-0.08327
N	0.01581	-0.42968	-0.17175
H	-3.94214	-0.90975	-0.47637
H	-0.56222	0.27319	1.77459
C	1.41495	-0.15311	-0.06907
C	2.31591	-1.03622	-0.69403
C	1.92005	0.9722	0.60227

C	3.68327	-0.78245	-0.66871
H	1.91818	-1.91516	-1.18023
C	3.29528	1.22305	0.61217
H	1.25712	1.65204	1.11871
C	4.18403	0.35346	-0.02117
H	4.36157	-1.47423	-1.15484
H	3.66749	2.09877	1.13134
H	5.24906	0.55041	-0.00501
O	-2.7017	-1.05418	1.77246
H	0.19189	-2.18192	0.80097



H_2O

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -75.981704 Hartree

Zero-point Energy Correction = 0.019853 Hartree

Thermal Correction to Energy = 0.022688 Hartree

Thermal Correction to Enthalpy = 0.023632 Hartree

Thermal Correction to Free Energy = 0.002108 Hartree

EE + Zero-point Energy = -75.961851 Hartree

EE + Thermal Energy Correction = -75.959016 Hartree

EE + Thermal Enthalpy Correction = -75.958072 Hartree

EE + Thermal Free Energy Correction = -75.979596 Hartree

E (Thermal) = 14.237 kcal/mol

Heat Capacity (Cv) = 5.998 cal/mol-kelvin

Entropy (S) = 45.3 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1			
O	0.	0.	0.12313
H	0.	0.78232	-0.49254
H	0.	-0.78232	-0.49254