# Enantioselective Organocatalyzed Michael Addition of Isobutyraldehydes to Maleimides in Aqueous Media

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# Supporting Information

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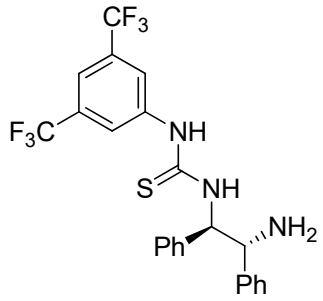
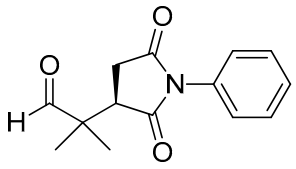
# 1. Compound Characterization Data

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-[3,5-bis(trifluoromethyl)phenyl]thiourea(1a)**



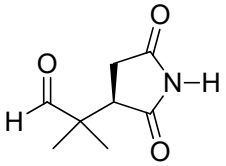

$[\alpha]_D^{25}$ +13.5 (*c* 1.0, $CH_3Cl$); $^1H$ NMR (500 MHz, DMSO-$d_6$) δ 8.25 (s, 2H), 7.78 (s, 1H),7.32~7.15 (m, 13H), 5.99 (d, *J* = 3 Hz, 1H), 4.77 (d, *J* = 3 Hz, 1H) ppm; $^{13}C$ NMR (125 MHz, DMSO-$d_6$) δ 180.5, 143.2, 142.4, 130.8, 130.5, 128.5, 128.2, 127.6, 127.5, 127.3, 124.7, 122.6, 121.3, 116.0, 63.6, 59.9 ppm; IR (KBr) 3305, 3032, 2963, 1652,1601, 1557, 1383, 1277, 1262, 803, 700 $cm^{-1}$; HRMS (FAB+) for $C_{23}H_{19}F_6N_3S$ $[M+H]^+$ Calcd: 484.1282, Found: 484.1254;

**(*R*)-2-(2,5-Dioxo-1-phenylpyrrolidin-3-yl)-2-methylpropanal (2a)[1,2]**



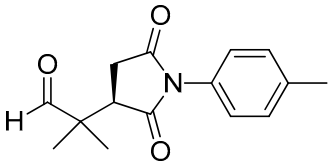

$[\alpha]_D^{25}$ +6.2 (*c* 0.2, $CH_2Cl_2$); $^1H$ NMR (300 MHz, $CDCl_3$) δ 9.51 (s, 1H), 7.26~7.50 (m, 5H), 3.14 (dd, *J* = 6.0, 12 Hz, 1H), 2.96 (dd, *J* = 9.0, 18 Hz, 1H), 2.60 (dd, *J* = 6.0, 12 Hz, 1H), 1.32 (s, 3H), 1.27 (s, 3H) ppm; $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 203.0, 177.1, 175.0, 132.0, 129.4, 128.9, 126.7, 48.8, 45.2, 32.1, 20.6, 19.8 ppm; LRMS ($EI^+$) Calcd. for $[C_{14}H_{15}NO_3]^+$: 245, found: 245; HPLC [Chiralcel OD-H, hexane/2-propanol = 75/25, flow rate = 0.7 mL/min, λ = 210nm, retention times: (major) 38.8 min, (minor) 32.3 min].

**(*R*)-2-(2,5-Dioxopyrrolidin-3-yl)-2-methylpropanal (2b)**[7]



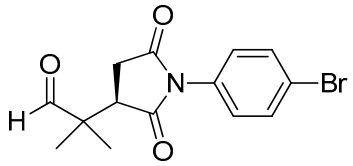
$[\alpha]_D^{21}$ –9.00 (*c* 0.2, $CH_2Cl_2$); $^1H$ NMR (300 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.57 (br. s, 1H), 3.09 (dd, *J* = 6.0, 9.0 Hz, 1H), 2.85 (dd, *J* = 12, 18 Hz, 1H), 2.51 (dd, *J* = 6.0, 18 Hz, 1H), 1.26 (s, 3H), 1.24 (s, 3H) ppm; $^{13}C$ NMR (100 MHz, DMSO) δ 185.4, 183.3, 182.8, 53.3, 48.8, 38.8, 29.5, 28.4 ppm; LRMS ($EI^+$) Calcd. for $[C_8H_{11}NO_3]^+$: 169, found: 169; HPLC [Chiralcel AD-H, hexane/2-propanol = 85/15, flow rate = 0.7 mL/min, λ = 210nm, retention times: (major) 25.3 min, (minor) 33.7 min].

**(*R*)-2-(2,5-Dioxo-1-p-tolylpyrrolidin-3-yl)-2-methylpropanal (2c)**[7]



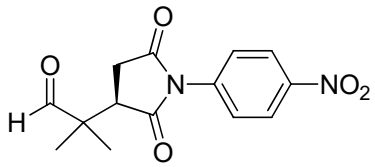
$[\alpha]_D^{21}$ –6.5 (*c* 0.2, $CH_2Cl_2$); $^1H$ NMR (300 MHz, $CDCl_3$) δ 9.52 (s, 1H), 7.26 (t, 3H), 7.15 (d , *J* = 9.0 Hz, 2H), 3.14 (dd, *J* = 6.0, 9.0 Hz, 1H), 2.96 (dd, *J* = 9.0, 18 Hz, 1H), 2.56~2.64 (dd, *J* = 6.0, 18 Hz, 1H), 2.37 (s, 3H), 1.31 (s, 3H), 1.28 (s, 3H) ppm; $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 203.0, 177.2, 175.2, 139.0, 130.1, 129.3, 126.5, 48.7, 45.2, 32.0, 21.4, 20.5, 19.8 ppm; LRMS ($EI^+$) Calcd. for $[C_{15}H_{17}NO_3]^+$: 259, found: 259; HPLC [Chiralcel OD-H, hexane/2-propanol = 75/25, flow rate = 0.6 mL/min, λ = 210nm, retention times: (major) 37.7 min, (minor) 31.3 min].

**(*R*)-2-[1-(4-Bromophenyl)-2,5-dioxopyrrolidin-3-yl]-2-methylpropanal (2d)[3,4]**



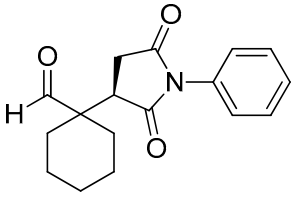

$[\alpha]_D^{20}$ +5.7 (*c* 0.2, $CH_2Cl_2$); $^1$H NMR (300 MHz, $CDCl_3$) δ 9.48 (s, 1H), 7.60 (d, *J* = 9.0 Hz, 2H), 7.19 (d, *J* = 6.0 Hz, 2H), 3.11 (dd, *J* = 6.0, 9.0 Hz, 1H), 2.97 (dd, *J* = 9.0, 18 Hz, 1H), 2.60 (dd, *J* = 6.0, 18 Hz, 1H), 1.36 (s, 3H), 1.28 (s, 3H) ppm; $^{13}$C NMR (100 MHz, $CDCl_3$) δ 203.0, 176.8, 174.6, 132.6, 131.0, 128.3, 122.8, 48.9, 45.1, 32.2, 20.7, 20.1 ppm; LRMS ($EI^+$) Calcd. for $[C_{14}H_{14}BrNO_3]^+$: 323, found: 323; HPLC [Chiralcel OD-H, hexane/2-propanol = 75/25, flow rate = 0.6 mL/min, λ = 210nm, retention times: (major) 58.6 min, (minor) 31.5 min].

**(*R*)-2-[1-(4-Nitrophenyl)-2,5-dioxopyrrolidin-3-yl]-2-methylpropanal (2e)[1]**



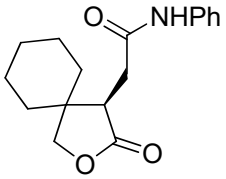

$[\alpha]_D^{20}$ +2.7 (*c* 0.1, $CH_2Cl_2$); $^1$H NMR (300 MHz, $CDCl_3$) δ 9.47 (s, 1H), 8.33 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 9.0 Hz, 2H), 3.13 (dd, *J* = 6.0, 12 Hz, 1H), 3.02 (dd, *J* = 12, 18 Hz, 1H), 2.68 (dd, *J* = 6.0, 18 Hz, 1H), 1.42 (s, 3H), 1.31 (s, 3H) ppm; $^{13}$C NMR (100 MHz, $CDCl_3$) δ 203.0, 176.5, 174.1, 147.2, 137.6, 127.3, 124.6, 49.2, 45.2, 32.4, 21.0, 20.5 ppm; LRMS ($EI^+$) Calcd. for $[C_{14}H_{14}N2O_5]^+$: 290, found: 290; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 210nm, retention times: (major) 72.6 min, (minor) 44.4 min].

**(*R*)-1-(2,5-Dioxo-1-phenylpyrrolidin-3-yl)cyclohexanecarbaldehyde (2f)**[1,5]



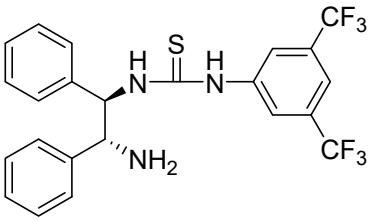
$[\alpha]_D^{20}$ +5.2 (*c* 0.1, $CH_2Cl_2$); $^1$H NMR (300 MHz, $CDCl_3$) δ 9.54 (s, 1H), 7.26~7.50 (m, 5H), 3.25 (dd, *J* = 6.0, 9.0 Hz, 1H), 2.88 (dd, *J* = 9.0, 18 Hz, 1H), 2.67 (dd, *J* = 6.0, 18 Hz, 1H), 1.82~2.04 (m, 3H), 1.53~1.64 (m, 7H) ppm; $^{13}$C NMR (100 MHz, $CDCl_3$) δ 204.9, 177.4, 175.2, 132.3, 129.5, 129.0, 127.0, 52.6, 43.0, 31.9, 29.0, 28.5, 25.5, 21.8, 21.6 ppm; LRMS ($FAB^+$) Calcd. for $[C_{17}H_{19}NO_3]^+$: 285, found: 285; HPLC [Chiralcel OD-H, hexane/2-propanol = 75/25, flow rate = 1.0 mL/min, λ = 210nm, retention times: (major) 53.2 min, (minor) 42.4 min].

**(*R*)-2-(3-Oxo-2-oxaspiro[4.5]decan-4-yl)-*N*-phenylacetamide (3a)**[6]



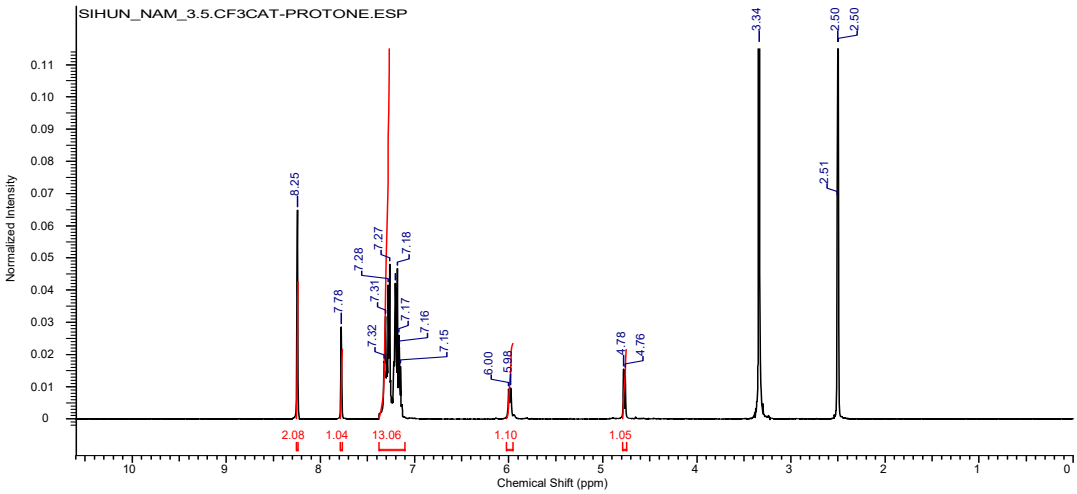
$[\alpha]_D^{20}$ –4.2 (*c* 0.1, $CH_2Cl_2$); $^1$H NMR (300 MHz, $CDCl_3$) δ 8.78 (s, 1H), 7.55 (d, *J* = 6.0, Hz, 2H), 7.32 (t, *J* = 6.0 Hz, 2H), 7.10 (t, *J* = 9.0 Hz, 1H), 3.85 (m, 1H), 3.54 (m, 1H), 3.06 (dd, *J* = 3.0, 9.0 Hz, 1H), 2.59 (dd, *J* = 9.0, 15 Hz, 1H), 2.29 (dd, *J* = 3.0, 15 Hz, 1H), 1.60 (m, 4H), 1.39 (m, 4H), 1.25 (m, 2H) ppm; $^{13}$C NMR (100 MHz, $CDCl_3$) δ 180.2, 170.0, 138.9, 129.5, 124.7, 120.5, 70.3, 47.3, 46.1, 33.2, 32.0, 28.9, 25.8, 23.1, 19.9 ppm; LRMS ($FAB^+$) Calcd. for $[C_{17}H_{21}NO_3]^+$: 287, found: 287; HPLC [Chiralcel OD-H, hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254nm, retention times: (major) 9.9 min, (minor) 14.9 min].

## 2. Copy of HPLC, NMR and MASS Spectra

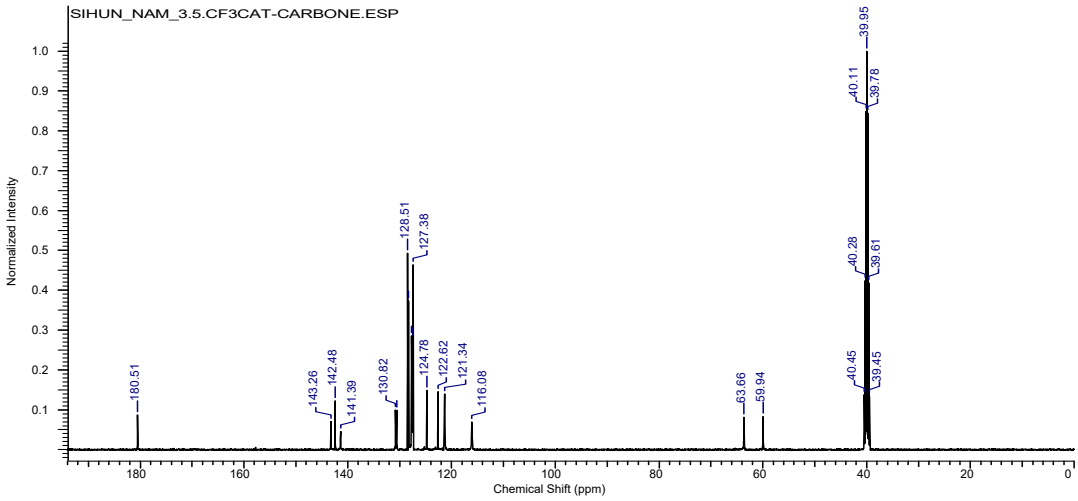



**1a**

**$^{1}$H NMR**




**$^{13}$C NMR**

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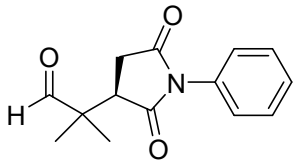
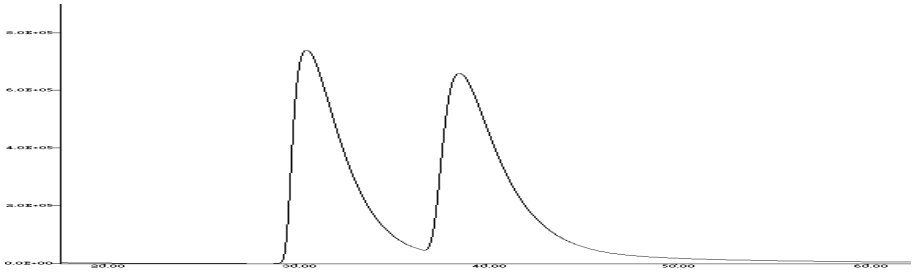


**2a**

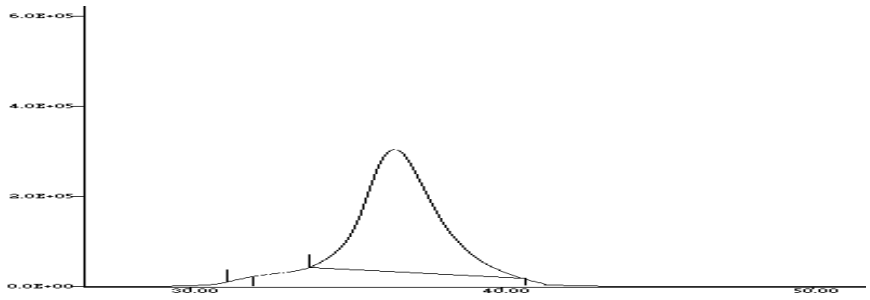
Racemic



| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 30.533128147734.660 | | 0.000 |
| 2 | | 38.567130363968.160 | | 0.000 |

Total Area of Peak = 258511702.830 [uV.Sec]

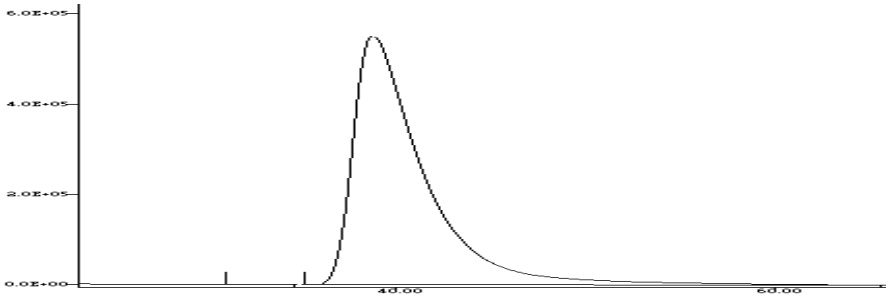
**Table 1, entry 1**




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 32.017 | 2618451.000 | 0.000 |
| 2 | | 36.525 | 46704778.000 | 0.000 |

Total Area of Peak = 49323229.000 [uV.Sec]

**Table 1, entry 2**




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 32.308 | 116686.528 | 0.000 |
| 2 | | 38.767139045145.770 | | 0.000 |

Total Area of Peak = 139161832.300 [uV.Sec]

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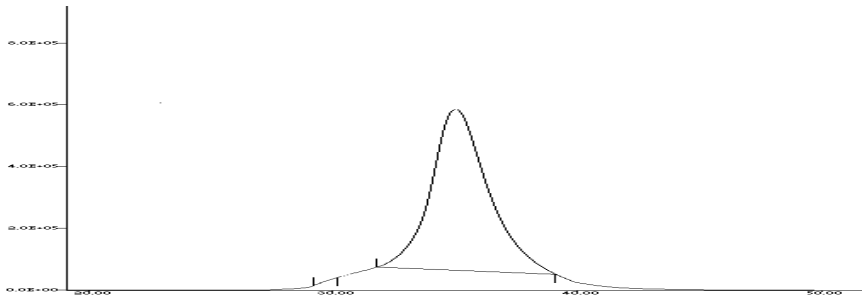

| # | Name | RT | Area[uV.Sec] | Quantity |
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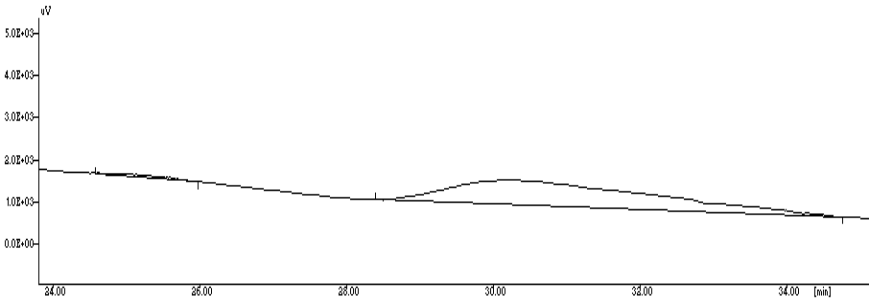
| 1 | | 30.208 | 4499914.000 | 0.000 |
| 2 | | 34.992 | 93686806.678 | 0.000 |

Total Area of Peak = 98186720.678 [uV.Sec]

**Table 1, entry 4**




| # | Name | RT | Area[uV.Sec] | Quantity |
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| 1 | | 24.608 | 2552.000 | 0.000 |
| 2 | | 30.225 | 113965.381 | 0.000 |

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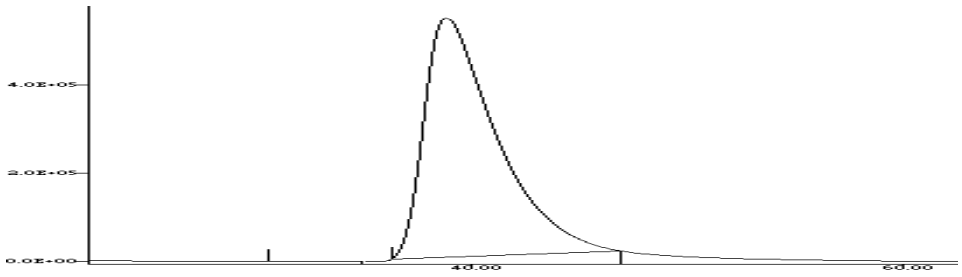


| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 32.308 | 151709.253 | 0.000 |
| 2 | | 38.767127118381.700 | | 0.000 |

Total Area of Peak = 127270090.950 [uV.Sec]

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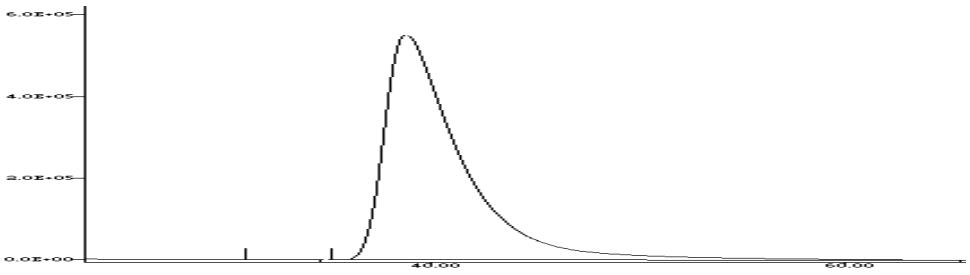
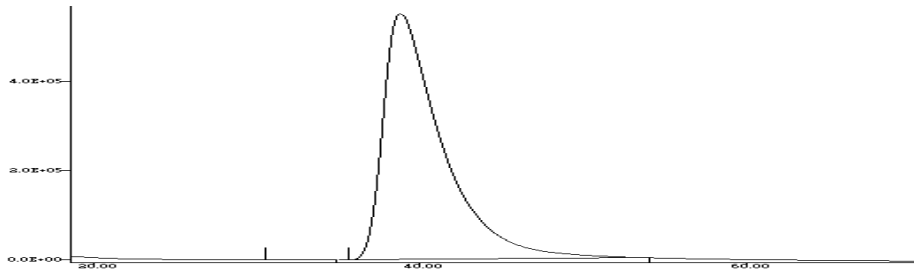



| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 32.308 | 116686.528 | 0.000 |
| 2 | | 38.767139045145.770 | | 0.000 |

Total Area of Peak = 139161832.300 [uV.Sec]

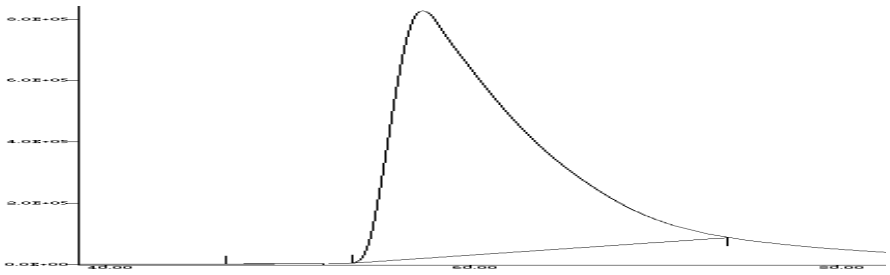
**Table 1, entry 7**




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 32.308 | 151709.253 | 0.000 |
| 2 | | 38.767134498855.210 | | 0.000 |

Total Area of Peak = 134650564.460 [uV.Sec]

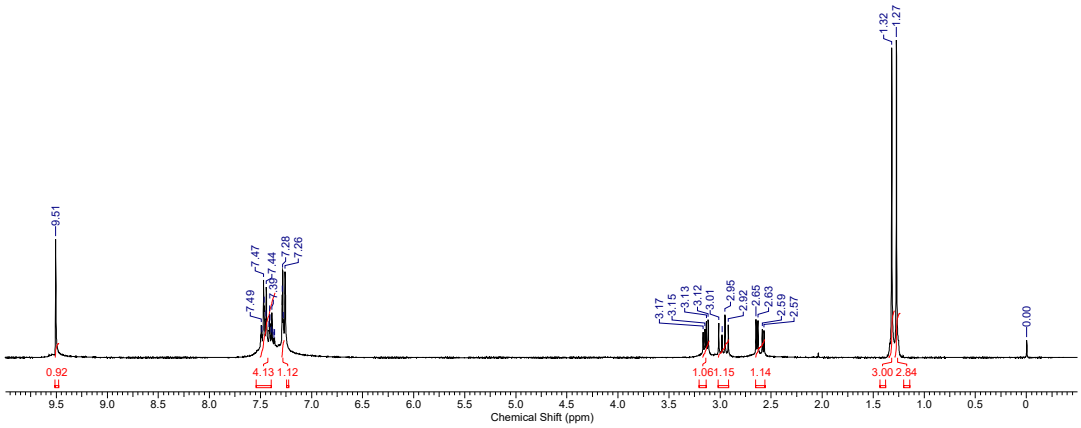
**Table 1, entry 8**



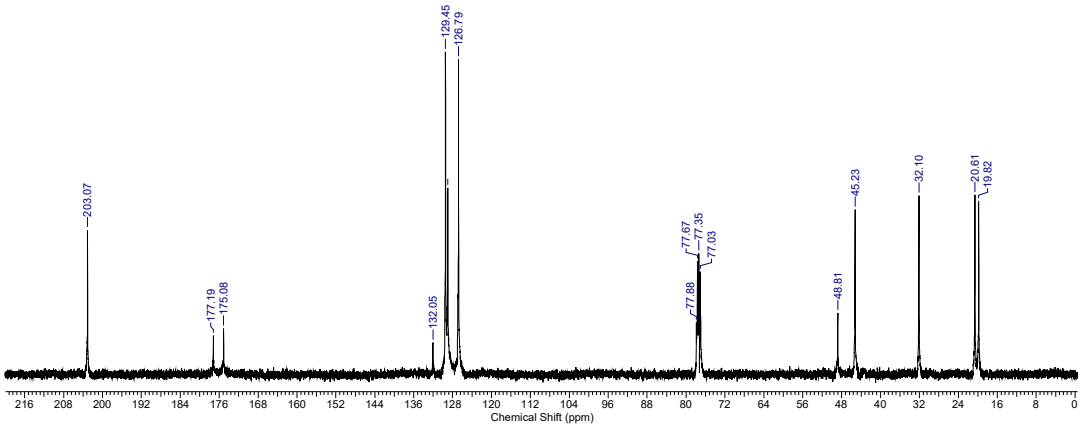

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 49.375 | 191950.470 | 0.000 |
| 2 | | 57.308384251931.500 | | 0.000 |

Total Area of Peak = 384443881.970 [uV.Sec]

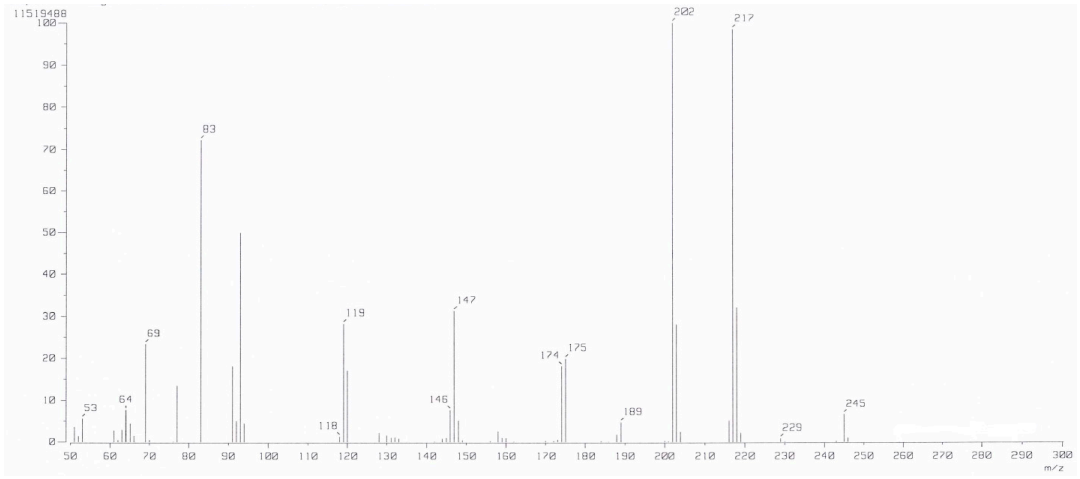
**$^{1}$H NMR**




**$^{13}$C NMR**




**Mass**

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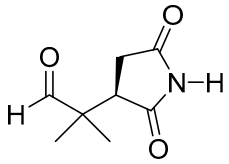
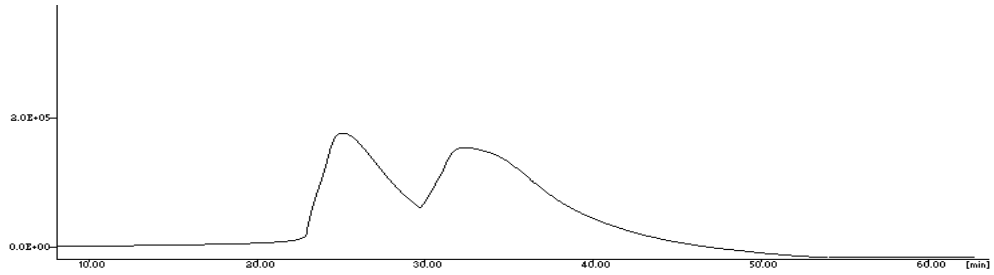



**2b**

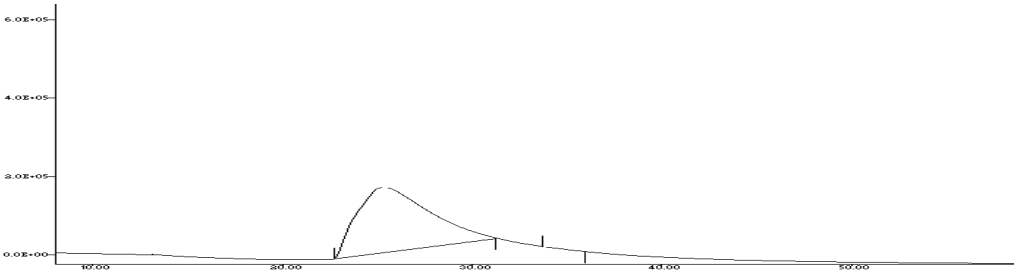
Racemic




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 25.008 | 36453687.573 | 0.000 |
| 2 | | 32.308 | 34838408.000 | 0.000 |

Total Area of Peak = 71292095.573 [uV.Sec]

Asymmetric

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|---|---|---|---|---|
| 1 | | 25.300 | 43443193.250 | 0.000 |
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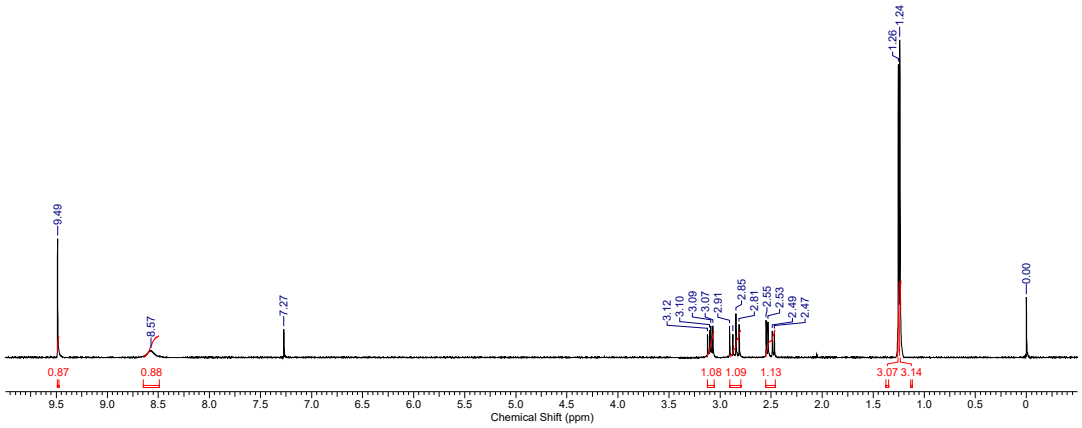
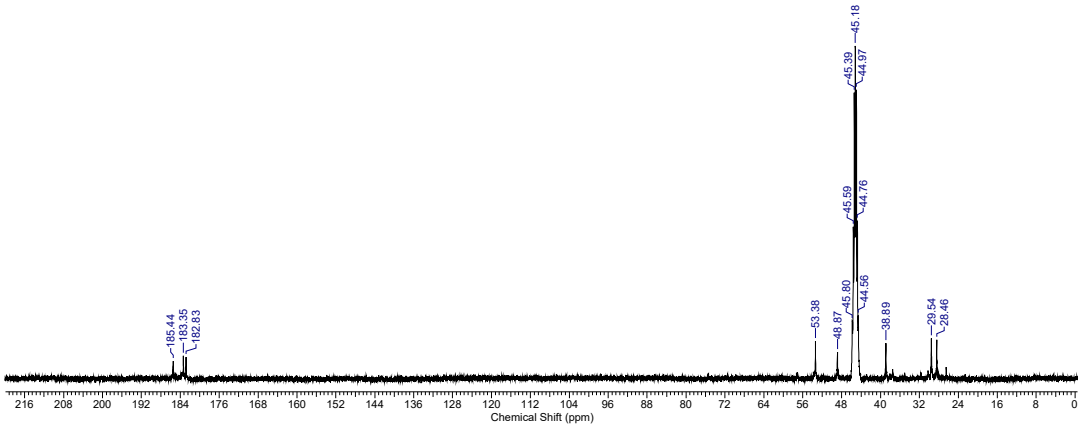
Total Area of Peak = 45235764.250 [uV.Sec]

**$^{1}$H NMR**




**$^{13}$C NMR**




**Mass**

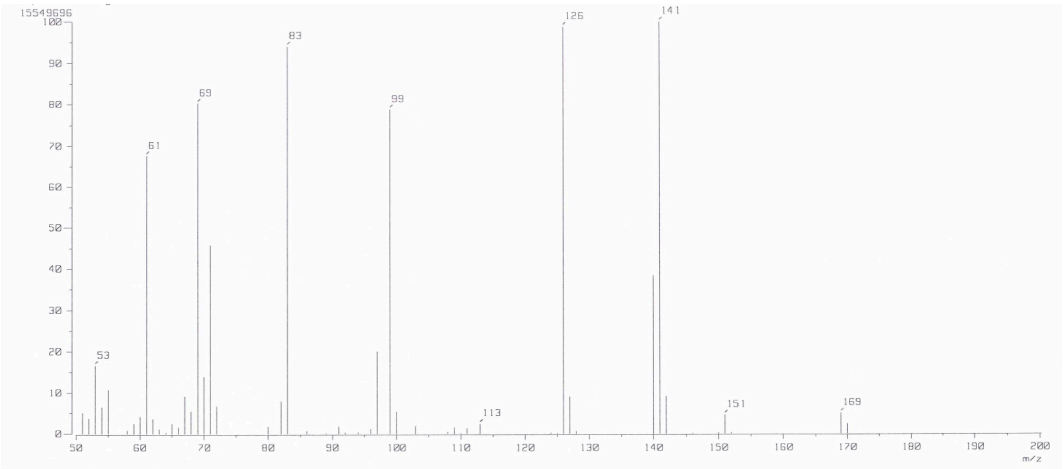
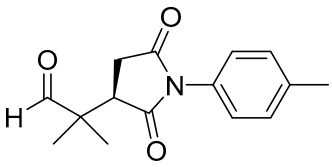
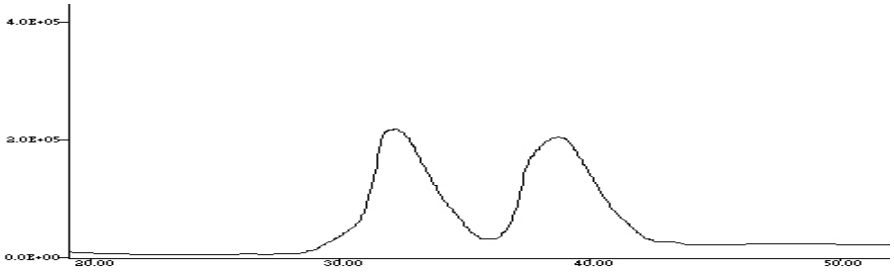



**Table 2, entry 2**



**2c**

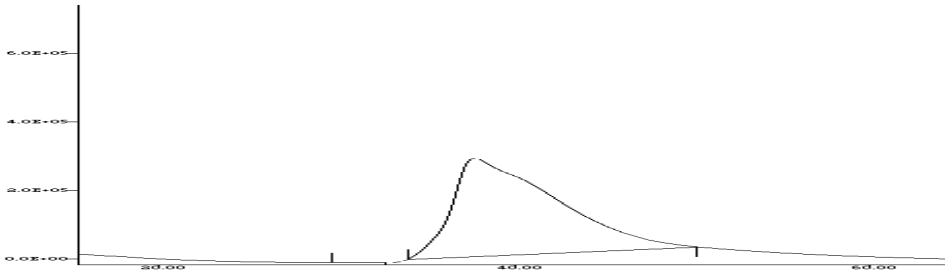
Racemic




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 31.358 | 48994375.503 | 0.000 |
| 2 | | 38.958 | 52721832.569 | 0.000 |

Total Area of Peak = 101716208.070 [uV.Sec]

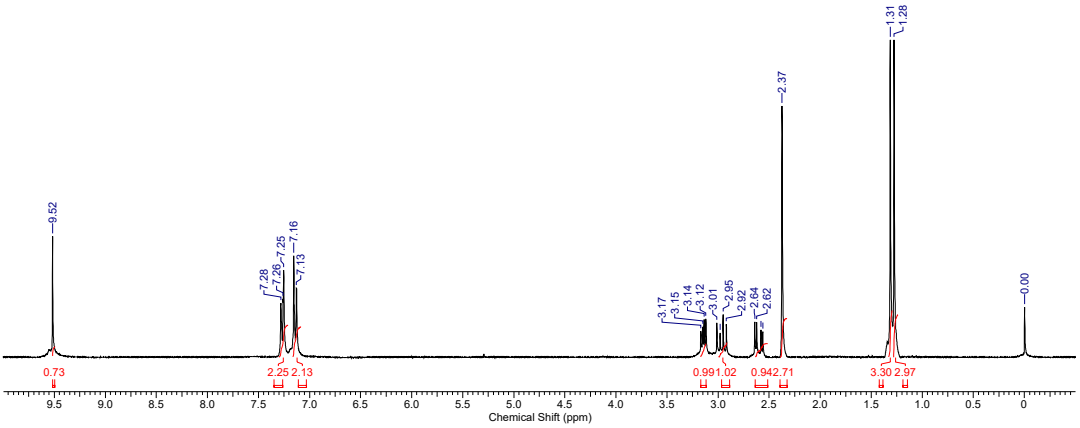
Asymmetric



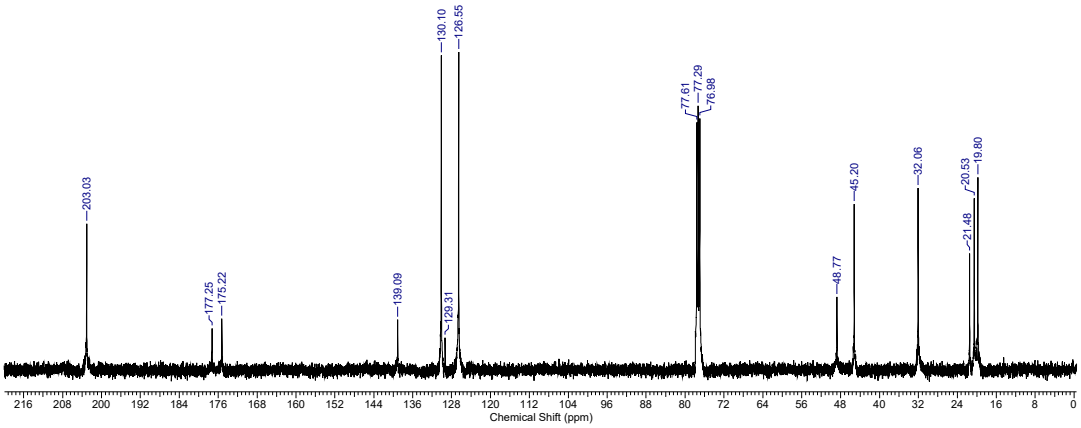

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 31.292 | 37762.205 | 0.000 |
| 2 | | 37.742 | 114516169.000 | 0.000 |

Total Area of Peak = 114553931.210 [uV.Sec]

**$^{1}$H NMR**




**$^{13}$C NMR**




**Mass**

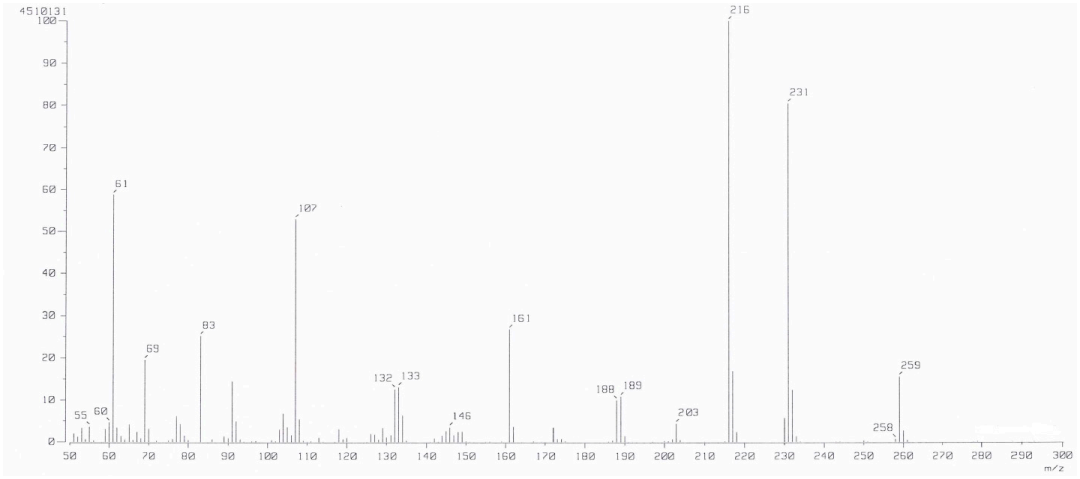
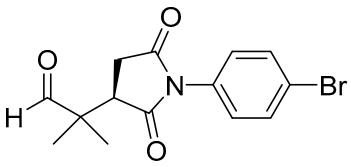
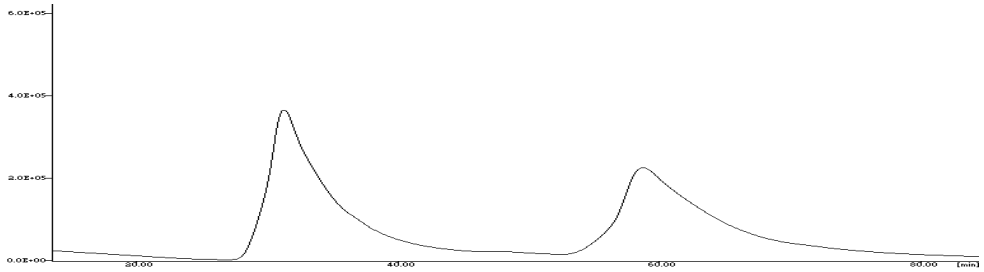



**Table 2, entry 3**




**2d**

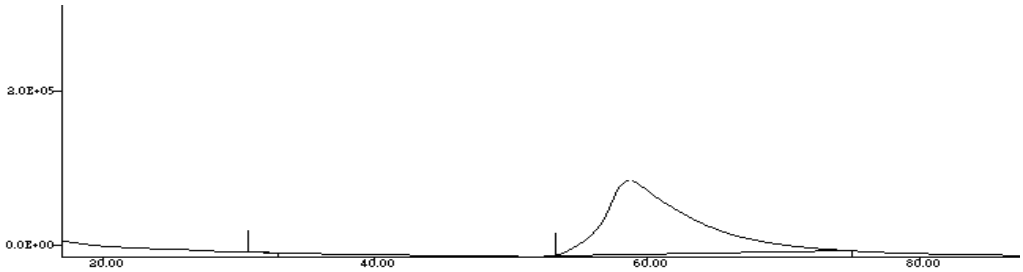
Racemic




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 31.242 | 86766751.250 | 0.000 |
| 2 | | 58.717 | 93286295.875 | 0.000 |

Total Area of Peak = 180053047.130 [uV.Sec]

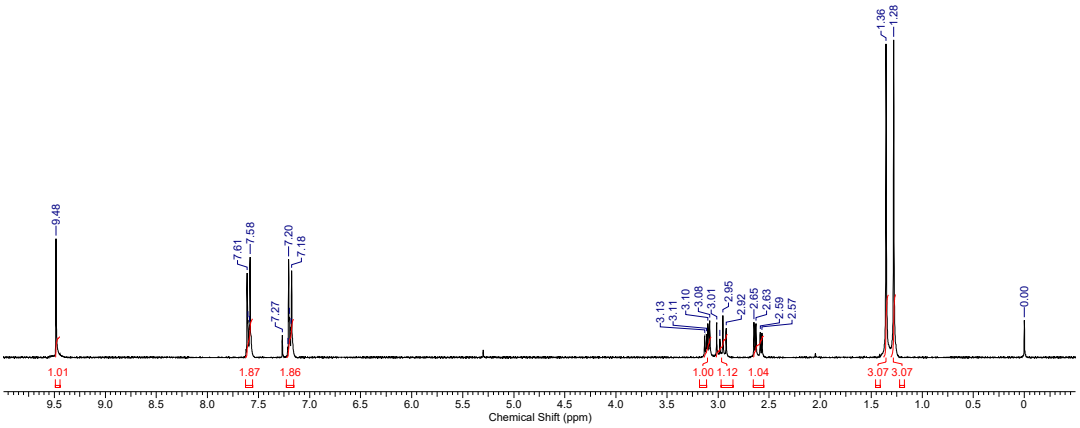
Asymmetic



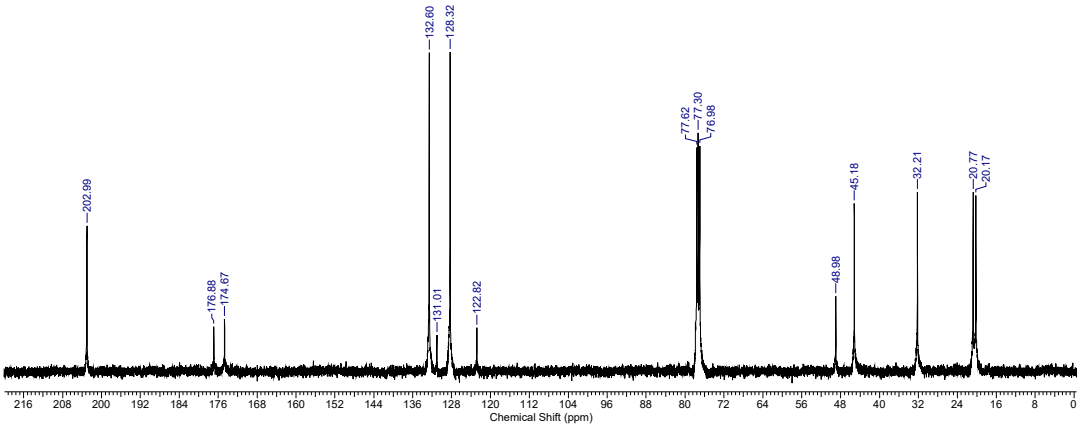

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 31.467 | 34118.000 | 0.000 |
| 2 | | 58.600 | 41605038.775 | 0.000 |

Total Area of Peak = 41639156.775 [uV.Sec]

**$^{1}$H NMR**




**$^{13}$C NMR**




**Mass**

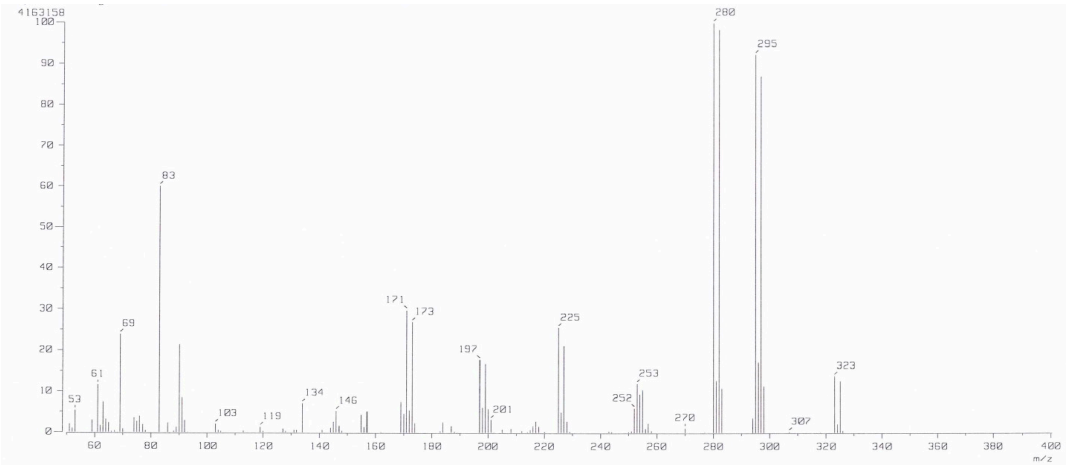
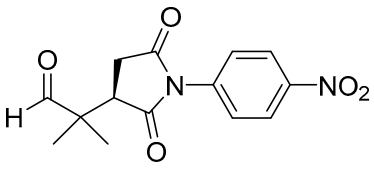
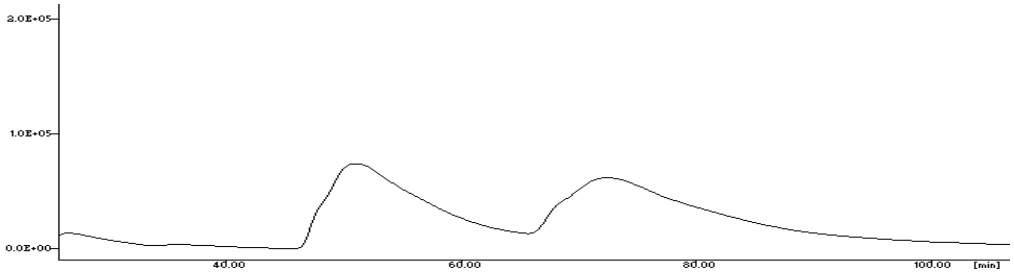



**Table 2, entry 4**



**2e**

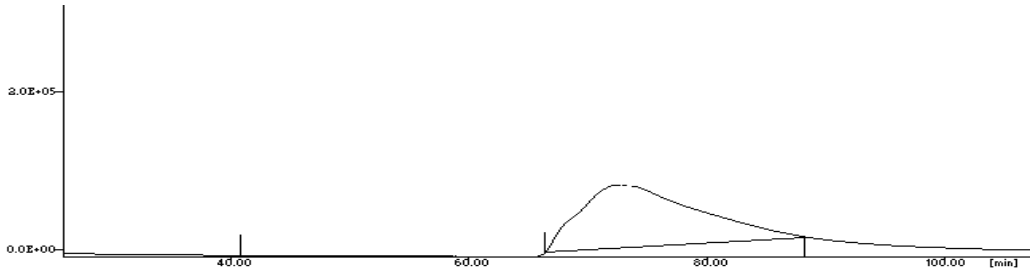
Racemic




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 50.975 | 32694061.500 | 0.000 |
| 2 | | 72.325 | 34471650.877 | 0.000 |

Total Area of Peak = 67165712.377 [uV.Sec]

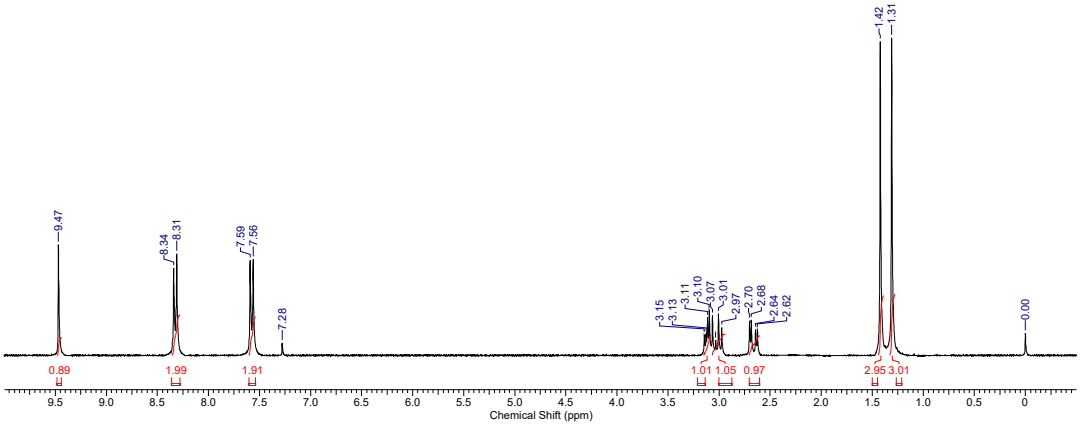
Asymmetric



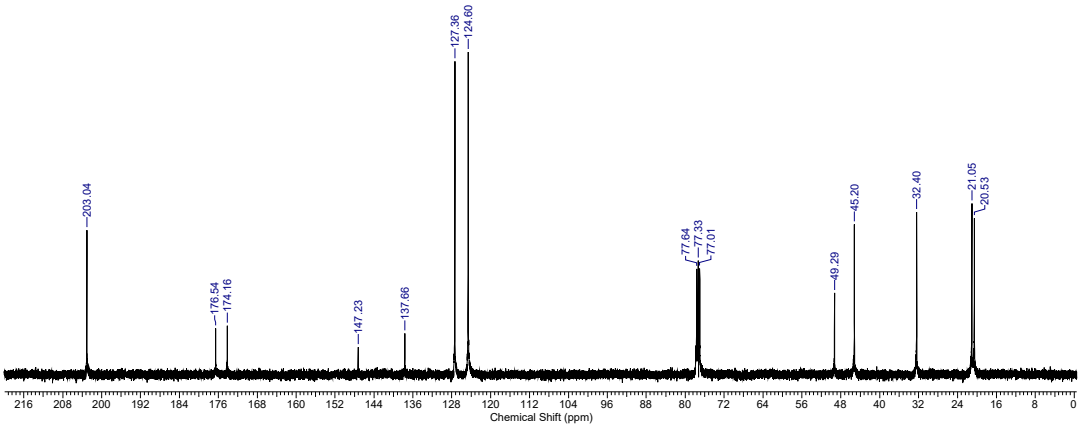

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 44.442 | 312501.490 | 0.000 |
| 2 | | 72.600 | 53641693.000 | 0.000 |

Total Area of Peak = 53954194.490 [uV.Sec]

**$^{1}$H NMR**




**$^{13}$C NMR**




**Mass**

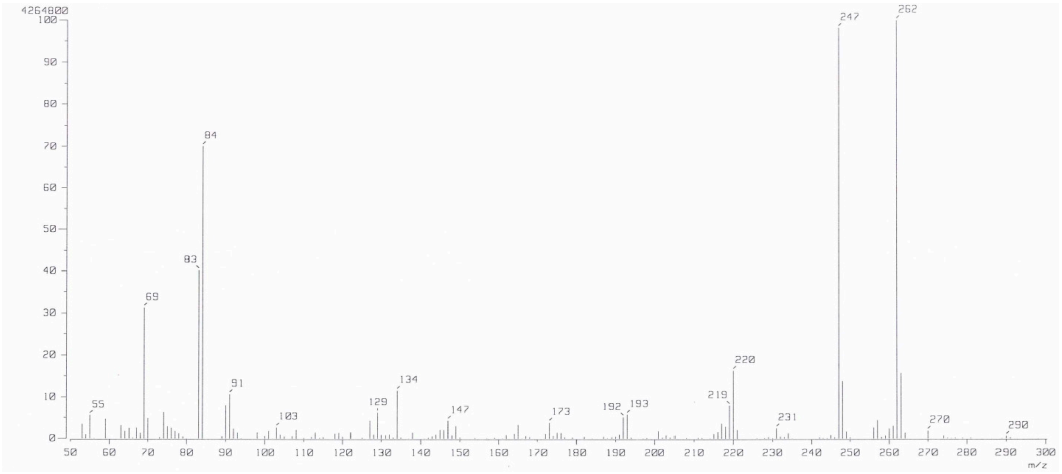
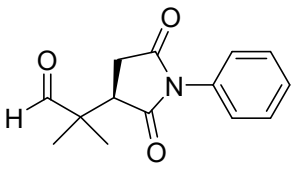
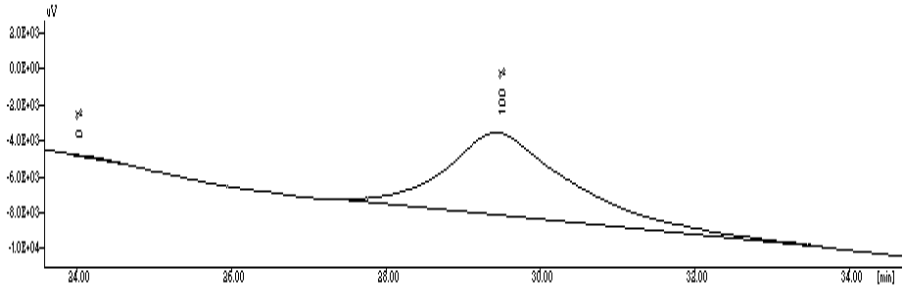



**Figure 6. 1st**



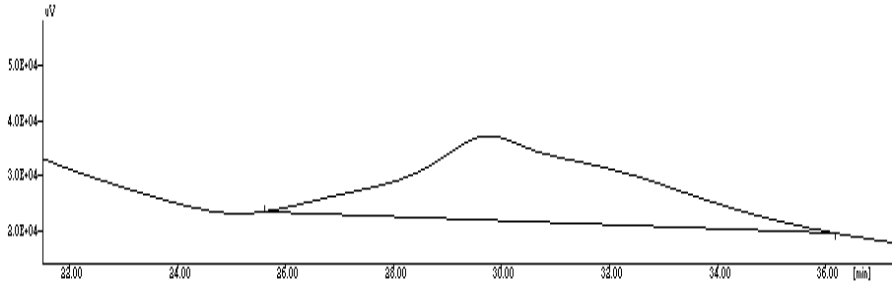
**2a**

Asymmetric



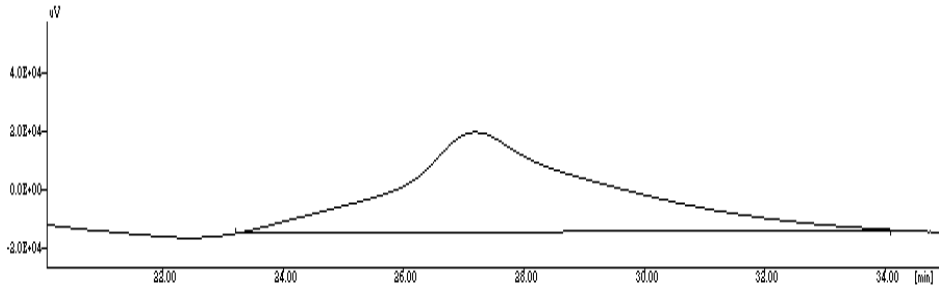

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 25.117 | 16883.500 | 0.000 |
| 2 | | 30.267 | 976364.631 | 0.000 |

**Figure 6. 2nd**



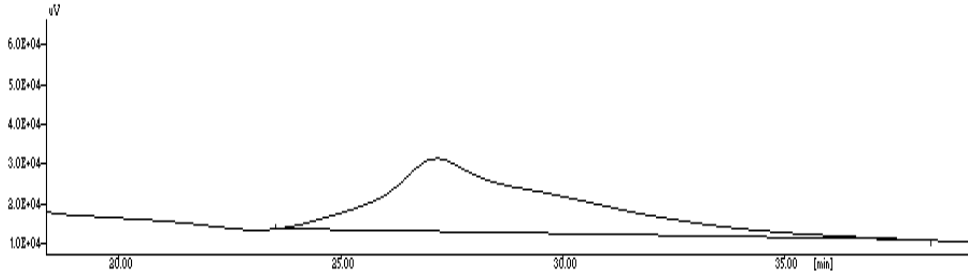

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 29.808 | 4406342.000 | 0.000 |

**Figure 6. 3rd**



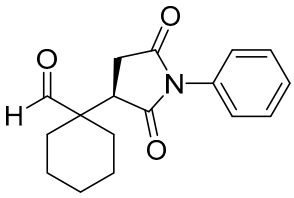

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 27.175 | 7898467.500 | 0.000 |

**Figure 6. 4th**



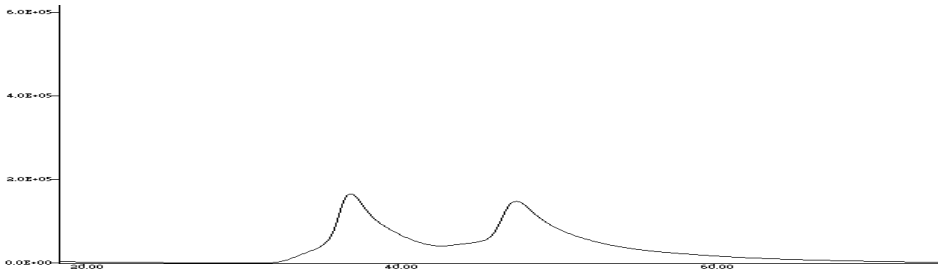

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 29.808 | 4406342.000 | 0.000 |

**Figure 7.**




**2f**

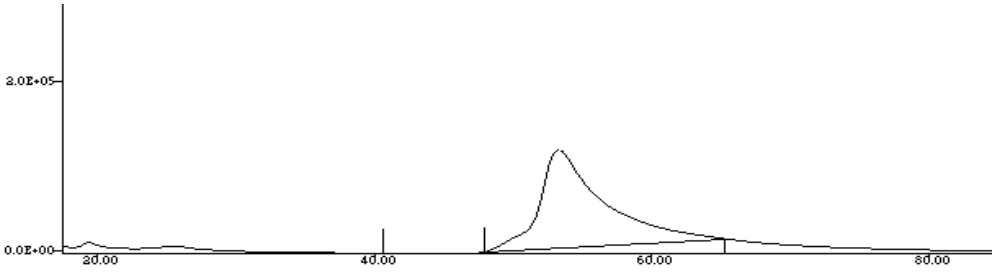
Racemic




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 36.900 | 24715311.000 | 0.000 |
| 2 | | 47.400 | 24489120.000 | 0.000 |

Total Area of Peak = 49204431.000 [uV.Sec]

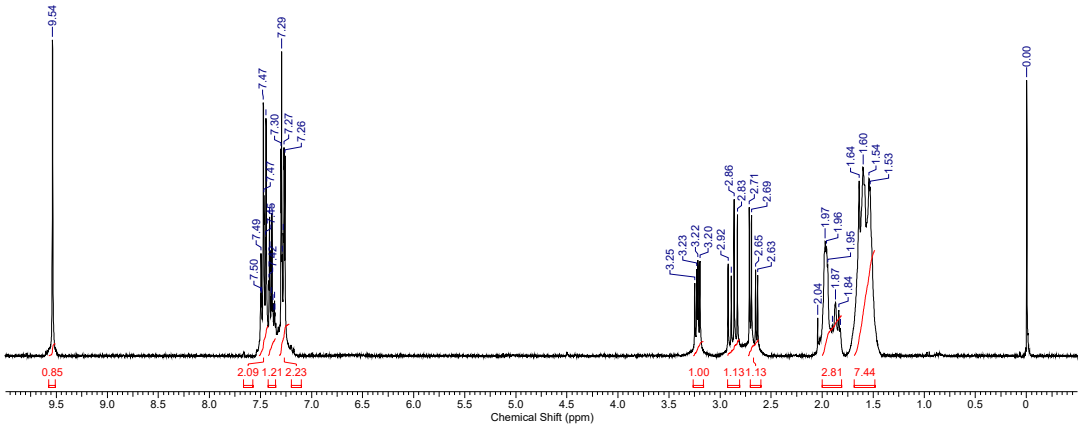
Asymmetric



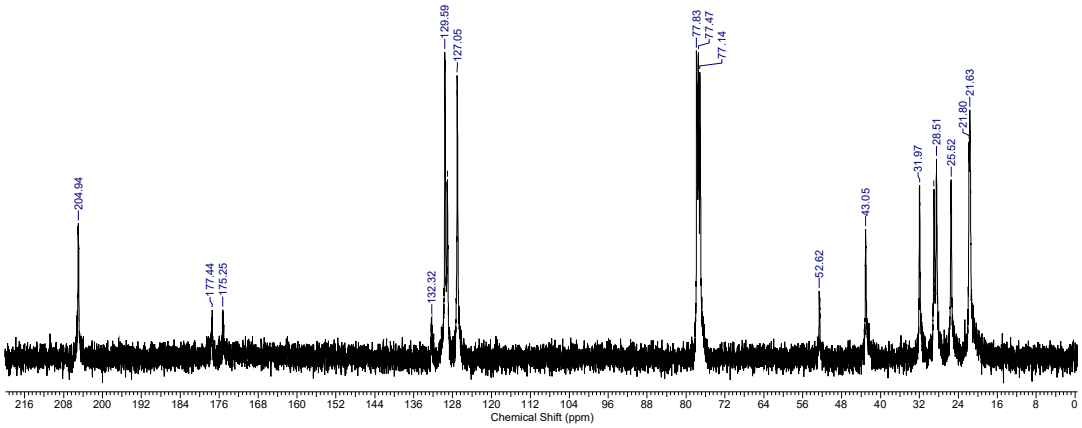

| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 42.400 | 2822.259 | 0.000 |
| 2 | | 53.233 | 36830060.500 | 0.000 |

Total Area of Peak = 36832882.759 [uV.Sec]

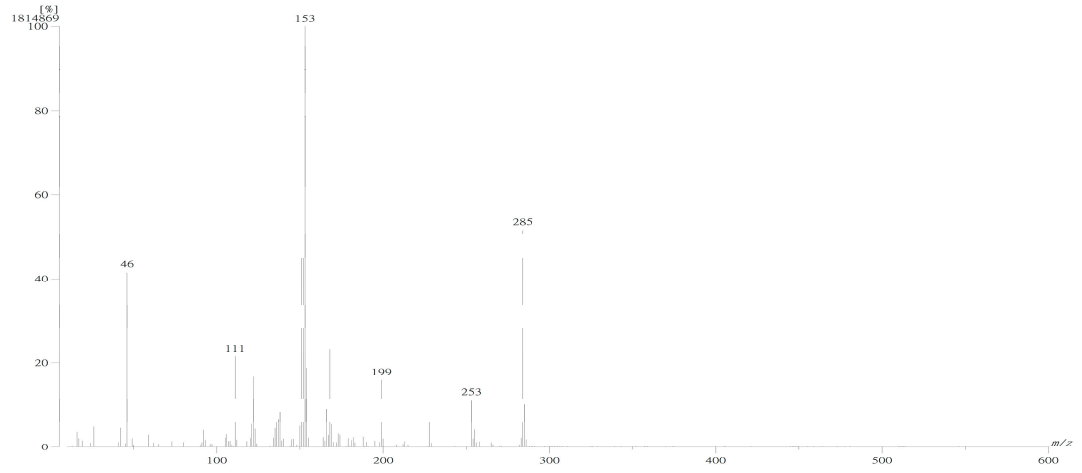
**$^{1}$H NMR**

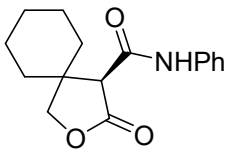

9.54
7.29
7.47
7.30
7.27
7.26
7.41
7.49
7.50
3.25
3.23
3.22
3.20
2.92
2.86
2.83
2.71
2.69
2.65
2.63
2.04
1.97
1.96
1.95
1.87
1.84
1.64
1.60
1.54
1.53
0.00
0.85
2.09
1.21
2.23
1.00
1.13
1.13
2.81
7.44
Chemical Shift (ppm)

## $^{13}$C NMR


204.94
177.44
175.25
132.32
129.59
127.05
77.83
77.47
77.14
52.62
43.05
31.97
28.51
25.52
21.80
21.63
Chemical Shift (ppm)

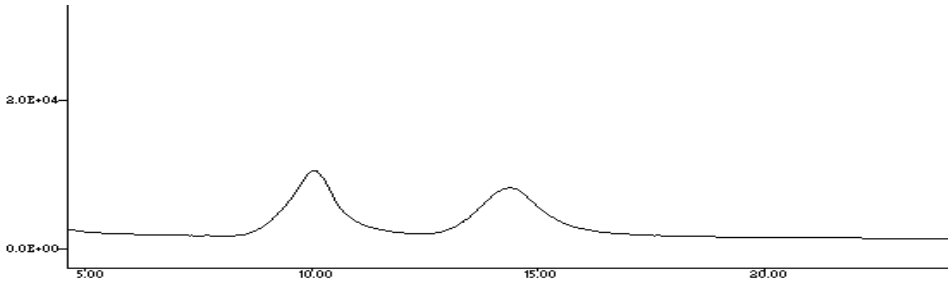
## Mass


[%]
1814869
153
285
46
111
199
253
m/z




**3a**

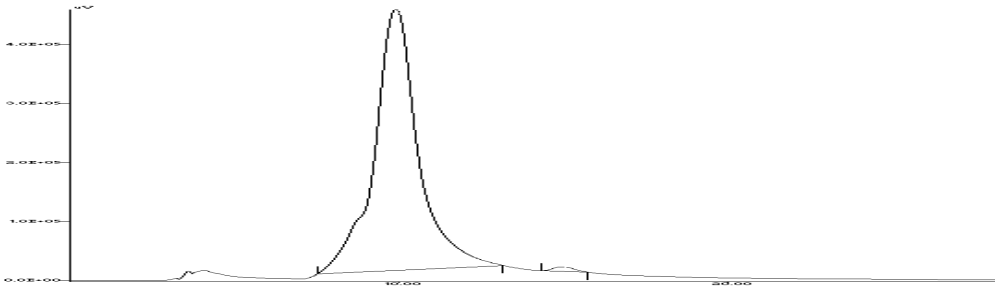
Racemic




| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 10.050 | 631497.500 | 0.000 |
| 2 | | 14.342 | 586048.000 | 0.000 |

Total Area of Peak = 1217545.500 [uV.Sec]

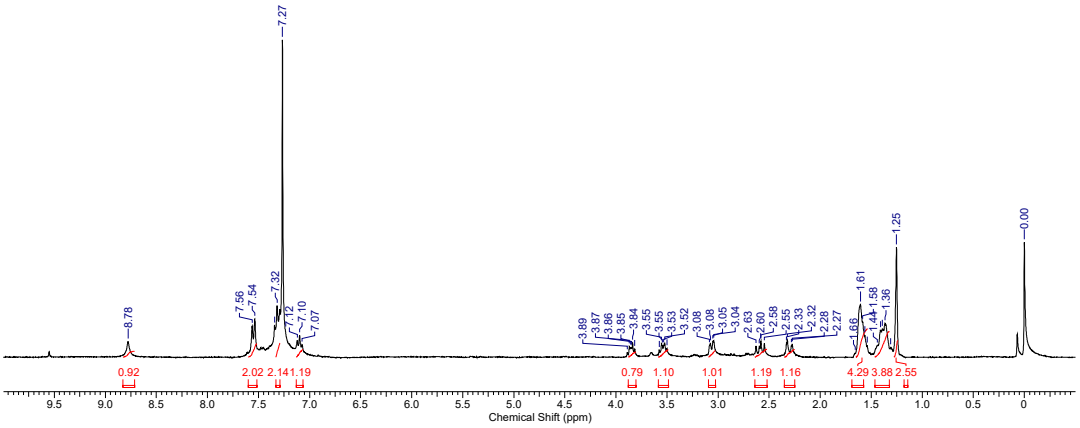
Asymmetric



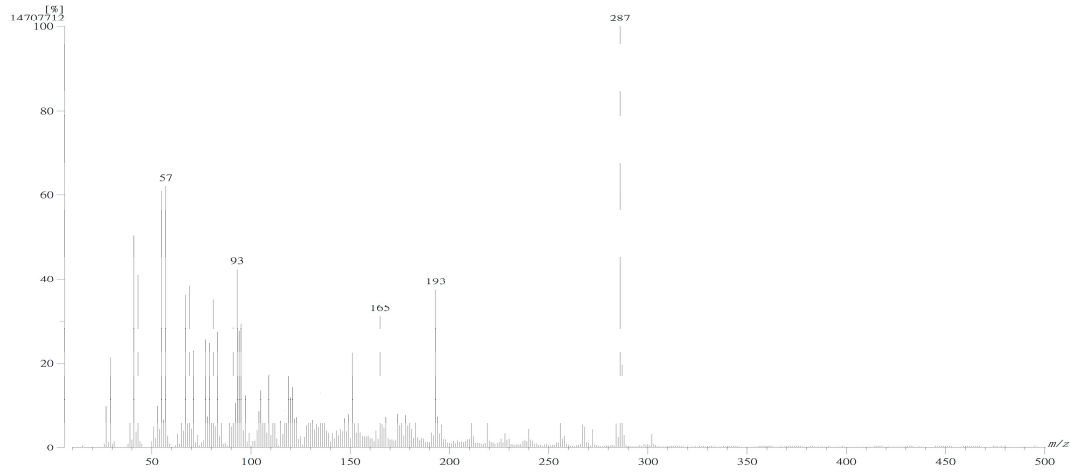
| # | Name | RT | Area[uV.Sec] | Quantity |
|---|---|---|---|---|
| 1 | | 9.875 | 39721216.000 | 0.000 |
| 2 | | 14.933 | 316721.500 | 0.000 |

Total Area of Peak = 40037937.500 [uV.Sec]

**$^{1}$H NMR**



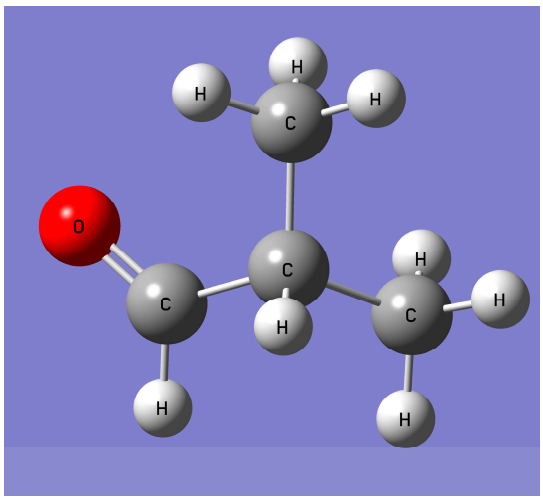

**Mass**




# 3. DFT Calculations for all Calculated Structures

**Figure 2.**

**Isobutyraldehyde(1)**




Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -231.1863 Hartree

RMS Gradient Norm = 1.149e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -231.1863 Hartree

Zero-point Energy Correction = 0.113857 Hartree

Thermal Correction to Energy = 0.120107 Hartree

Thermal Correction to Enthalpy = 0.121051 Hartree

Thermal Correction to Free Energy = 0.084517 Hartree

EE + Zero-point Energy = -231.07245 Hartree

EE + Thermal Energy Correction = -231.0662 Hartree

EE + Thermal Enthalpy Correction = -231.06525 Hartree

EE + Thermal Free Energy Correction = -231.10179 Hartree

E (Thermal) = 75.368 kcal/mol

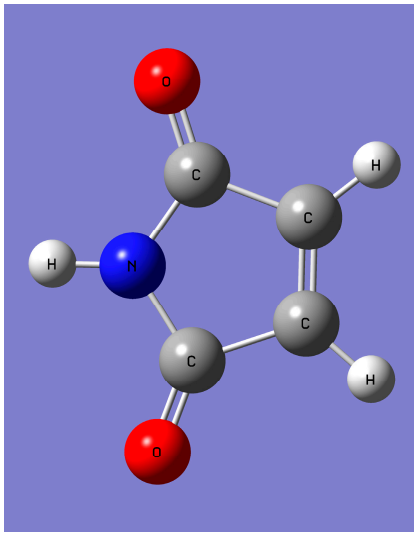
Heat Capacity (Cv) = 20.996 cal/mol-kelvin

Entropy (S) = 76.892 cal/mol-kelvin

Symbolic Z-matrix:

| Charge = 0 Multiplicity = 1 | | | |
|---|---|---|---|
| O | -1.93772 | -0.01911 | -0.18662 |
| H | -0.98241 | -1.73615 | 0.18648 |
| C | 0.40553 | -0.0029 | 0.40549 |
| C | 1.50957 | -0.84953 | -0.20595 |
| H | 0.50964 | -0.02487 | 1.51893 |
| H | 1.44892 | -0.86091 | -1.30238 |
| H | 2.49975 | -0.45869 | 0.06243 |
| H | 1.46195 | -1.89091 | 0.13935 |
| C | -0.94117 | -0.63596 | 0.10753 |
| C | 0.51426 | 1.43524 | -0.06485 |
| H | -0.27004 | 2.06351 | 0.37674 |
| H | 1.48383 | 1.86805 | 0.21441 |
| H | 0.421 | 1.51168 | -1.15631 |

**Maleimide(2)**




Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -357.44052 Hartree

RMS Gradient Norm = 1.933e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -357.44052 Hartree

Zero-point Energy Correction = 0.068699 Hartree

Thermal Correction to Energy = 0.073931 Hartree

Thermal Correction to Enthalpy = 0.074875 Hartree

Thermal Correction to Free Energy = 0.040319 Hartree

EE + Zero-point Energy = -357.37182 Hartree

EE + Thermal Energy Correction = -357.36659 Hartree

EE + Thermal Enthalpy Correction = -357.36564 Hartree

EE + Thermal Free Energy Correction = -357.4002 Hartree

E (Thermal) = 46.392 kcal/mol

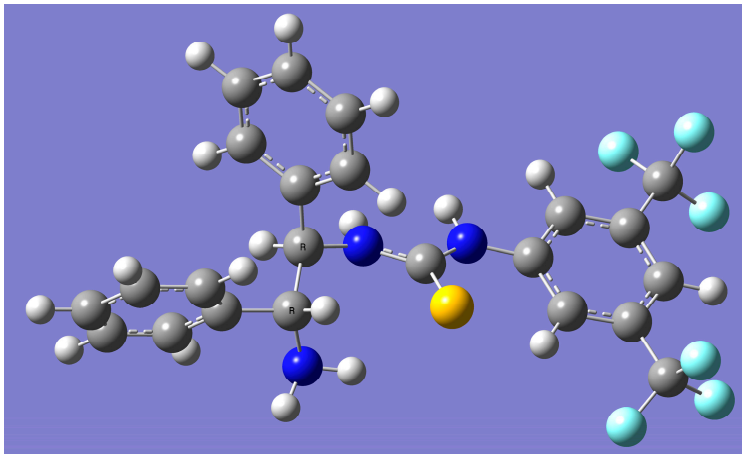
Heat Capacity (Cv) = 19.398 cal/mol-kelvin

Entropy (S) = 72.729 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 1.59514 | 1.16029 | 0. |
| C | 3.01303 | 0.66578 | 0. |
| C | 3.01303 | -0.66578 | 0. |
| C | 1.59514 | -1.16029 | 0. |
| H | 3.84575 | 1.34874 | 0. |
| H | 3.84574 | -1.34874 | 0. |
| O | 1.22636 | 2.33376 | 0.00001 |
| O | 1.22636 | -2.33376 | -0.00001 |
| N | 0.7628 | 0. | 0. |
| H | -0.2372 | 0. | 0. |

## 1b Cat.(3)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2038.4342 Hartree

RMS Gradient Norm = 2.73e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2038.4342 Hartree

Zero-point Energy Correction = 0.390498 Hartree

Thermal Correction to Energy = 0.419537 Hartree

Thermal Correction to Enthalpy = 0.420482 Hartree

Thermal Correction to Free Energy = 0.325242 Hartree

EE + Zero-point Energy = -2038.0437 Hartree

EE + Thermal Energy Correction = -2038.0147 Hartree

EE + Thermal Enthalpy Correction = -2038.0138 Hartree

EE + Thermal Free Energy Correction = -2038.109 Hartree

E (Thermal) = 263.264 kcal/mol

Heat Capacity (Cv) = 110.445 cal/mol-kelvin

Entropy (S) = 200.448 cal/mol-kelvin

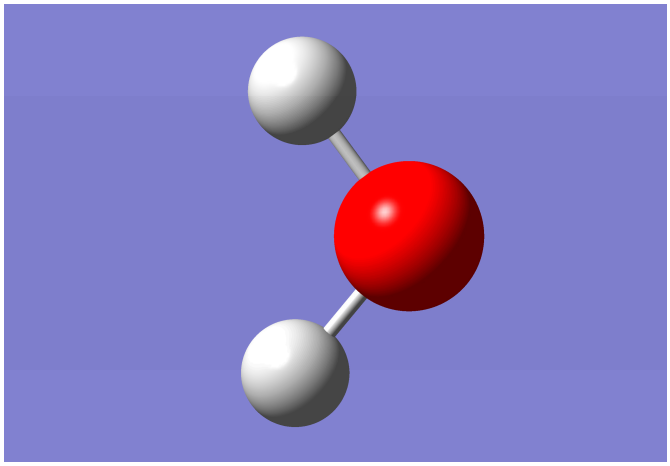
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 5.35849 | 1.33787 | -1.80781 |
| C | 4.82708 | 1.14638 | -0.52483 |
| C | 5.69825 | 0.95831 | 0.5539 |
| C | 7.08048 | 0.9594 | 0.3547 |
| C | 7.60459 | 1.1496 | -0.92613 |
| C | 6.73965 | 1.33999 | -2.00723 |
| H | 4.67012 | 1.50429 | -2.62759 |
| H | 5.29272 | 0.8047 | 1.54752 |
| H | 7.74614 | 0.81433 | 1.19782 |
| H | 8.67773 | 1.1541 | -1.07954 |
| H | 7.1414 | 1.49523 | -3.00239 |
| C | 3.29335 | -1.35884 | 0.35108 |
| C | 4.2752 | -2.28379 | -0.02492 |
| C | 4.73342 | -3.24351 | 0.88009 |
| C | 4.21062 | -3.28913 | 2.17354 |
| C | 3.23141 | -2.36846 | 2.55692 |
| C | 2.77436 | -1.40784 | 1.65364 |
| H | 4.69377 | -2.24224 | -1.0248 |
| H | 5.49665 | -3.95033 | 0.57561 |
| H | 4.56373 | -4.03365 | 2.87769 |
| H | 2.82295 | -2.39699 | 3.56063 |
| H | 2.01493 | -0.69495 | 1.95103 |
| C | 3.3155 | 1.12842 | -0.32606 |
| C | 2.81394 | -0.3166 | -0.65186 |
| N | 1.33778 | -0.45595 | -0.89719 |

| | | | |
|---|---|---|---|
| N | 2.68733 | 2.05148 | -1.30251 |
| H | 3.24995 | -0.54539 | -1.62815 |
| H | 3.07939 | 1.35208 | 0.7202 |
| H | 3.151 | 2.9666 | -1.25754 |
| H | 1.69517 | 2.17017 | -1.06525 |
| H | 1.14702 | -1.08786 | -1.67474 |
| C | 0.25972 | 0.03025 | -0.23611 |
| C | -2.73205 | 0.98572 | 0.09707 |
| C | -4.09709 | 1.1922 | 0.26486 |
| C | -5.03531 | 0.22018 | -0.05727 |
| C | -4.57426 | -0.9948 | -0.54801 |
| C | -3.217 | -1.22889 | -0.71787 |
| C | -2.27072 | -0.24091 | -0.40093 |
| H | -2.03806 | 1.77115 | 0.34469 |
| H | -6.0936 | 0.41447 | 0.04014 |
| H | -2.90295 | -2.18378 | -1.12204 |
| N | -0.92225 | -0.55008 | -0.67028 |
| S | 0.33444 | 1.23285 | 1.01256 |
| H | -0.81622 | -1.3929 | -1.23506 |
| F | -5.79041 | -2.88065 | 0.25434 |
| F | -5.05699 | -2.91949 | -1.82873 |
| F | -6.75108 | -1.57598 | -1.24681 |
| F | -3.69111 | 3.50442 | 0.54004 |
| F | -5.8118 | 2.80855 | 0.3756 |
| F | -4.65299 | 2.43695 | 2.21884 |
| C | -5.54204 | -2.08849 | -0.84265 |
| C | -4.55983 | 2.48514 | 0.84774 |

**$H_2O$**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -75.973965 Hartree

RMS Gradient Norm = 0.000115305 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -75.973965 Hartree

Zero-point Energy Correction = 0.019746 Hartree

Thermal Correction to Energy = 0.022581 Hartree

Thermal Correction to Enthalpy = 0.023525 Hartree

Thermal Correction to Free Energy = 0.002 Hartree

EE + Zero-point Energy = -75.954218 Hartree

EE + Thermal Energy Correction = -75.951384 Hartree

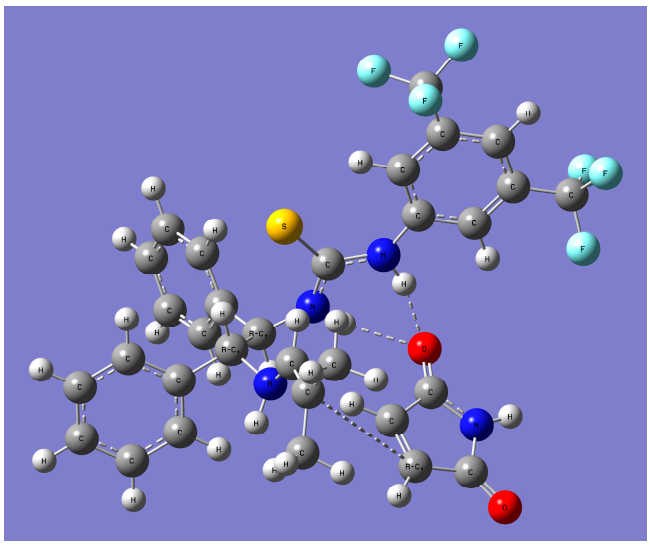
EE + Thermal Enthalpy Correction = -75.95044 Hartree

EE + Thermal Free Energy Correction = -75.971965 Hartree

E (Thermal) = 14.17 kcal/mol
Heat Capacity (Cv) = 5.999 cal/mol-kelvin
Entropy (S) = 45.304 cal/mol-kelvin

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
O -0.0579 2.33917 -0.16269
H 0.9021 2.33917 -0.16269
H -0.37836 3.24411 -0.16269

**TS**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2551.0871 Hartree

RMS Gradient Norm = 4.11e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2551.0871 Hartree

Zero-point Energy Correction = 0.551515 Hartree

Thermal Correction to Energy = 0.592901 Hartree

Thermal Correction to Enthalpy = 0.593846 Hartree

Thermal Correction to Free Energy = 0.468285 Hartree

EE + Zero-point Energy = -2550.5356 Hartree

EE + Thermal Energy Correction = -2550.4942 Hartree

EE + Thermal Enthalpy Correction = -2550.4933 Hartree

EE + Thermal Free Energy Correction = -2550.6188 Hartree

E (Thermal) = 372.051 kcal/mol

Heat Capacity (Cv) = 153.154 cal/mol-kelvin

Entropy (S) = 264.265 cal/mol-kelvin

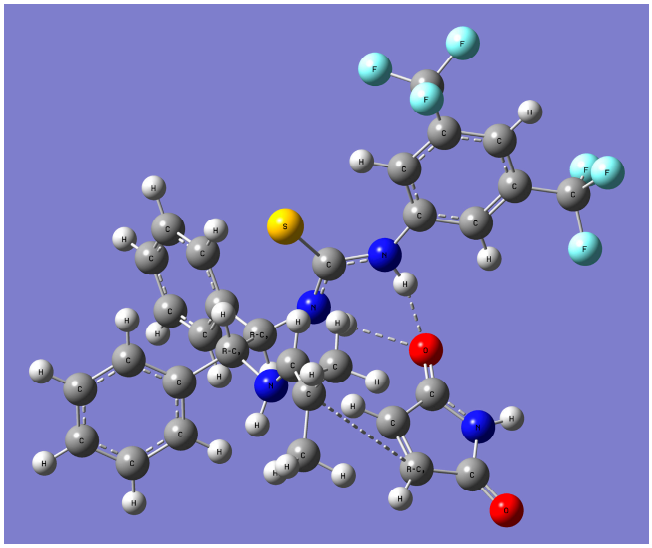
Symbolic Z-matrix:

| Charge = 0 Multiplicity = 1 | | | |
|---|---|---|---|
| C | 5.37602 | 0.57255 | 0.13239 |
| C | 4.58852 | -0.4647 | 0.65675 |
| C | 5.22523 | -1.57803 | 1.21612 |
| C | 6.61882 | -1.6545 | 1.25587 |
| C | 7.3942 | -0.61565 | 0.73765 |
| C | 6.76879 | 0.49963 | 0.1748 |
| H | 4.90214 | 1.44068 | -0.31631 |
| H | 4.62603 | -2.38756 | 1.61669 |
| H | 7.09726 | -2.52375 | 1.69171 |
| H | 8.47578 | -0.67426 | 0.76986 |
| H | 7.36469 | 1.30805 | -0.23329 |
| C | 3.07802 | -1.57727 | -1.66749 |
| C | 4.00068 | -1.29683 | -2.68556 |
| C | 4.53106 | -2.31758 | -3.47533 |
| C | 4.13998 | -3.63987 | -3.25913 |
| C | 3.21847 | -3.92887 | -2.25035 |
| C | 2.69023 | -2.90824 | -1.45784 |
| H | 4.31385 | -0.27221 | -2.85649 |
| H | 5.24493 | -2.08024 | -4.25573 |
| H | 4.54756 | -4.4361 | -3.87133 |
| H | 2.90592 | -4.95255 | -2.07824 |

| | | | |
|---|---|---|---|
| H | 1.96749 | -3.1348 | -0.68589 |
| C | 3.06977 | -0.37141 | 0.63869 |
| C | 2.54146 | -0.41496 | -0.83161 |
| N | 1.06486 | -0.23863 | -0.93127 |
| N | 2.6361 | 0.91997 | 1.27578 |
| H | 2.92913 | 0.50072 | -1.29052 |
| H | 2.63788 | -1.2062 | 1.19017 |
| H | 0.78975 | 0.506 | -1.57595 |
| C | 0.03522 | -0.85826 | -0.29362 |
| C | -2.96022 | -1.70535 | 0.39432 |
| C | -4.32442 | -1.86924 | 0.61564 |
| C | -5.26805 | -0.98264 | 0.11442 |
| C | -4.81312 | 0.10339 | -0.62528 |
| C | -3.45975 | 0.30004 | -0.84787 |
| C | -2.50395 | -0.6033 | -0.34361 |
| H | -2.25995 | -2.42436 | 0.78613 |
| H | -6.32295 | -1.13153 | 0.29326 |
| H | -3.13638 | 1.16903 | -1.40831 |
| N | -1.1721 | -0.30019 | -0.65779 |
| S | 0.20123 | -2.14907 | 0.8641 |
| H | -1.08496 | 0.54178 | -1.23937 |
| F | -6.9374 | 1.12313 | -0.49143 |
| F | -6.17629 | 0.63918 | -2.50724 |
| F | -5.25227 | 2.29816 | -1.38078 |
| F | -3.92513 | -4.07187 | 1.37743 |
| F | -4.82966 | -2.65282 | 2.80856 |
| F | -6.04535 | -3.4028 | 1.12405 |
| C | -5.79221 | 1.03675 | -1.2464 |
| C | -4.77712 | -2.99896 | 1.477 |
| C | -0.08855 | 3.1443 | -1.35866 |
| C | 0.09261 | 5.37327 | -0.74436 |

| | | | |
|---|---|---|---|
| C | 1.00825 | 4.54202 | 0.11701 |
| O | -0.45908 | 2.1194 | -1.96482 |
| H | 1.4294 | 2.39401 | 0.1837 |
| H | 3.43346 | 1.53357 | 1.45189 |
| C | 1.70364 | 0.87334 | 2.34793 |
| C | 1.59899 | 1.75253 | 3.35788 |
| C | 2.52885 | 2.93284 | 3.55985 |
| C | 0.48255 | 1.62411 | 4.37553 |
| H | 1.00075 | 0.05123 | 2.26528 |
| H | 2.02982 | 3.87886 | 3.29957 |
| H | 2.82585 | 3.00533 | 4.61401 |
| H | 3.44684 | 2.86017 | 2.96515 |
| H | 0.89082 | 1.52648 | 5.39111 |
| H | -0.16261 | 2.51466 | 4.36818 |
| H | -0.14253 | 0.74903 | 4.17088 |
| C | 0.90833 | 3.25372 | -0.23067 |
| H | 1.61847 | 4.98031 | 0.88925 |
| O | -0.1085 | 6.57853 | -0.74394 |
| N | -0.53034 | 4.4275 | -1.61151 |
| H | -1.21607 | 4.67095 | -2.31721 |

**TS(Gas)**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2551.0871 Hartree

RMS Gradient Norm = 4.11e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2551.0871 Hartree

Zero-point Energy Correction = 0.551515 Hartree

Thermal Correction to Energy = 0.592901 Hartree

Thermal Correction to Enthalpy = 0.593846 Hartree

Thermal Correction to Free Energy = 0.468285 Hartree

EE + Zero-point Energy = -2550.5356 Hartree

EE + Thermal Energy Correction = -2550.4942 Hartree

EE + Thermal Enthalpy Correction = -2550.4933 Hartree

EE + Thermal Free Energy Correction = -2550.6188 Hartree

E (Thermal) = 372.051 kcal/mol

Heat Capacity (Cv) = 153.154 cal/mol-kelvin

Entropy (S) = 264.265 cal/mol-kelvin

Symbolic Z-matrix:

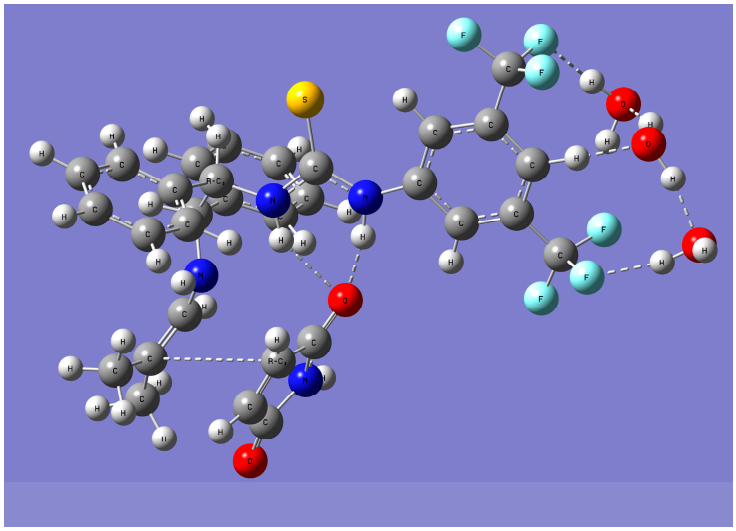
Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 5.37602 | 0.57255 | 0.13239 |
| C | 4.58852 | -0.4647 | 0.65675 |
| C | 5.22523 | -1.57803 | 1.21612 |
| C | 6.61882 | -1.6545 | 1.25587 |
| C | 7.3942 | -0.61565 | 0.73765 |
| C | 6.76879 | 0.49963 | 0.1748 |
| H | 4.90214 | 1.44068 | -0.31631 |
| H | 4.62603 | -2.38756 | 1.61669 |
| H | 7.09726 | -2.52375 | 1.69171 |
| H | 8.47578 | -0.67426 | 0.76986 |
| H | 7.36469 | 1.30805 | -0.23329 |
| C | 3.07802 | -1.57727 | -1.66749 |
| C | 4.00068 | -1.29683 | -2.68556 |
| C | 4.53106 | -2.31758 | -3.47533 |
| C | 4.13998 | -3.63987 | -3.25913 |
| C | 3.21847 | -3.92887 | -2.25035 |
| C | 2.69023 | -2.90824 | -1.45784 |
| H | 4.31385 | -0.27221 | -2.85649 |
| H | 5.24493 | -2.08024 | -4.25573 |
| H | 4.54756 | -4.4361 | -3.87133 |
| H | 2.90592 | -4.95255 | -2.07824 |
| H | 1.96749 | -3.1348 | -0.68589 |

| | | | |
|---|---|---|---|
| C | 3.06977 | -0.37141 | 0.63869 |
| C | 2.54146 | -0.41496 | -0.83161 |
| N | 1.06486 | -0.23863 | -0.93127 |
| N | 2.6361 | 0.91997 | 1.27578 |
| H | 2.92913 | 0.50072 | -1.29052 |
| H | 2.63788 | -1.2062 | 1.19017 |
| H | 0.78975 | 0.506 | -1.57595 |
| C | 0.03522 | -0.85826 | -0.29362 |
| C | -2.96022 | -1.70535 | 0.39432 |
| C | -4.32442 | -1.86924 | 0.61564 |
| C | -5.26805 | -0.98264 | 0.11442 |
| C | -4.81312 | 0.10339 | -0.62528 |
| C | -3.45975 | 0.30004 | -0.84787 |
| C | -2.50395 | -0.6033 | -0.34361 |
| H | -2.25995 | -2.42436 | 0.78613 |
| H | -6.32295 | -1.13153 | 0.29326 |
| H | -3.13638 | 1.16903 | -1.40831 |
| N | -1.1721 | -0.30019 | -0.65779 |
| S | 0.20123 | -2.14907 | 0.8641 |
| H | -1.08496 | 0.54178 | -1.23937 |
| F | -6.9374 | 1.12313 | -0.49143 |
| F | -6.17629 | 0.63918 | -2.50724 |
| F | -5.25227 | 2.29816 | -1.38078 |
| F | -3.92513 | -4.07187 | 1.37743 |
| F | -4.82966 | -2.65282 | 2.80856 |
| F | -6.04535 | -3.4028 | 1.12405 |
| C | -5.79221 | 1.03675 | -1.2464 |
| C | -4.77712 | -2.99896 | 1.477 |
| C | -0.08855 | 3.1443 | -1.35866 |
| C | 0.09261 | 5.37327 | -0.74436 |
| C | 1.00825 | 4.54202 | 0.11701 |

| | | | |
|---|---|---|---|
| O | -0.45908 | 2.1194 | -1.96482 |
| H | 1.4294 | 2.39401 | 0.1837 |
| H | 3.43346 | 1.53357 | 1.45189 |
| C | 1.70364 | 0.87334 | 2.34793 |
| C | 1.59899 | 1.75253 | 3.35788 |
| C | 2.52885 | 2.93284 | 3.55985 |
| C | 0.48255 | 1.62411 | 4.37553 |
| H | 1.00075 | 0.05123 | 2.26528 |
| H | 2.02982 | 3.87886 | 3.29957 |
| H | 2.82585 | 3.00533 | 4.61401 |
| H | 3.44684 | 2.86017 | 2.96515 |
| H | 0.89082 | 1.52648 | 5.39111 |
| H | -0.16261 | 2.51466 | 4.36818 |
| H | -0.14253 | 0.74903 | 4.17088 |
| C | 0.90833 | 3.25372 | -0.23067 |
| H | 1.61847 | 4.98031 | 0.88925 |
| O | -0.1085 | 6.57853 | -0.74394 |
| N | -0.53034 | 4.4275 | -1.61151 |
| H | -1.21607 | 4.67095 | -2.31721 |

**TS(Gas)+3$H_2O$**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2779.1179 Hartree

RMS Gradient Norm = 2.45e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2779.1179 Hartree

Zero-point Energy Correction = 0.626939 Hartree

Thermal Correction to Energy = 0.675005 Hartree

Thermal Correction to Enthalpy = 0.675949 Hartree

Thermal Correction to Free Energy = 0.539008 Hartree

EE + Zero-point Energy = -2778.4909 Hartree

EE + Thermal Energy Correction = -2778.4429 Hartree

EE + Thermal Enthalpy Correction = -2778.4419 Hartree

EE + Thermal Free Energy Correction = -2778.5789 Hartree

E (Thermal) = 423.572 kcal/mol

Heat Capacity (Cv) = 178.166 cal/mol-kelvin

Entropy (S) = 288.218 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -2.31938 | 0.37882 | 2.66547 |
| C | -3.31181 | -0.58515 | 2.42974 |
| C | -3.89683 | -1.23303 | 3.52691 |
| C | -3.49912 | -0.93829 | 4.83143 |
| C | -2.50971 | 0.01964 | 5.05749 |
| C | -1.9255 | 0.67573 | 3.97201 |
| H | -1.84194 | 0.8968 | 1.84508 |
| H | -4.67206 | -1.97326 | 3.35695 |
| H | -3.96179 | -1.4522 | 5.66585 |
| H | -2.19617 | 0.25231 | 6.06834 |
| H | -1.15222 | 1.41643 | 4.1411 |
| C | -3.38857 | -2.54405 | -0.92274 |
| C | -4.36022 | -3.5409 | -0.7552 |
| C | -5.03558 | -4.06732 | -1.85587 |
| C | -4.74826 | -3.603 | -3.14291 |
| C | -3.77294 | -2.62082 | -3.31971 |
| C | -3.09469 | -2.0968 | -2.21529 |
| H | -4.57735 | -3.91709 | 0.23961 |
| H | -5.77763 | -4.84414 | -1.71236 |
| H | -5.27 | -4.01422 | -3.99898 |
| H | -3.52791 | -2.27336 | -4.31698 |
| H | -2.30668 | -1.3666 | -2.35207 |
| C | -3.75747 | -0.99895 | 1.03466 |
| C | -2.72449 | -1.93348 | 0.31619 |

| | | | |
|---|---|---|---|
| N | -1.5568 | -1.11951 | -0.00133 |
| N | -3.99603 | 0.17174 | 0.12485 |
| H | -2.4152 | -2.73186 | 0.99655 |
| H | -4.68468 | -1.57904 | 1.13908 |
| H | -1.7527 | -0.12376 | -0.09662 |
| C | -0.26252 | -1.55888 | 0.00278 |
| C | 2.87814 | -1.56139 | -0.30529 |
| C | 4.24714 | -1.35356 | -0.44264 |
| C | 4.79316 | -0.08384 | -0.57731 |
| C | 3.92731 | 1.00423 | -0.55688 |
| C | 2.5595 | 0.82805 | -0.41936 |
| C | 2.00705 | -0.46152 | -0.29611 |
| H | 2.48574 | -2.56262 | -0.22306 |
| H | 5.85461 | 0.05294 | -0.72381 |
| H | 1.90901 | 1.69442 | -0.42692 |
| N | 0.61223 | -0.51564 | -0.19573 |
| S | 0.13163 | -3.22474 | 0.23546 |
| H | 0.16527 | 0.41036 | -0.23629 |
| F | 5.63957 | 2.41502 | -1.36285 |
| F | 4.78111 | 2.899 | 0.61328 |
| F | 3.5699 | 3.2508 | -1.19867 |
| F | 4.54523 | -3.66009 | -0.87544 |
| F | 6.30097 | -2.29632 | -1.12504 |
| F | 5.56954 | -2.8198 | 0.89203 |
| C | 4.47774 | 2.38513 | -0.62791 |
| C | 5.15943 | -2.5316 | -0.39018 |
| C | -1.90819 | 2.42179 | -0.64265 |
| C | -3.56717 | 2.8898 | -2.18279 |
| C | -3.71101 | 3.83217 | -1.02093 |
| O | -0.94361 | 1.8759 | -0.06898 |
| C | -2.52144 | 2.0814 | -1.96805 |

| | | | |
|---|---|---|---|
| O | -4.52373 | 4.7308 | -0.83442 |
| N | -2.64252 | 3.47957 | -0.14791 |
| H | -2.48105 | 3.91511 | 0.75255 |
| H | -2.1336 | 1.29717 | -2.59659 |
| H | -4.19477 | -0.16628 | -0.82146 |
| C | -4.89222 | 1.17144 | 0.57129 |
| C | -5.93286 | 1.69974 | -0.10337 |
| C | -6.44758 | 1.18882 | -1.43649 |
| C | -6.70218 | 2.86538 | 0.48213 |
| H | -4.65616 | 1.53938 | 1.56423 |
| H | -7.47707 | 0.82573 | -1.31338 |
| H | -6.47934 | 1.99301 | -2.18216 |
| H | -5.85078 | 0.36678 | -1.84324 |
| H | -6.45344 | 3.78979 | -0.05872 |
| H | -7.78351 | 2.69933 | 0.40122 |
| H | -6.45176 | 3.01745 | 1.5376 |
| H | -4.23361 | 2.91908 | -3.02779 |
| O | 8.13333 | -0.78187 | 1.99614 |
| H | 7.17861 | -0.69147 | 2.04028 |
| H | 8.36615 | -1.71281 | 1.96878 |
| O | 8.25845 | 1.26837 | 0.73659 |
| H | 7.30374 | 1.35877 | 0.78073 |
| H | 8.49127 | 0.33743 | 0.70923 |
| O | 7.66637 | 3.37291 | -0.68953 |
| H | 6.71166 | 3.46331 | -0.64538 |
| H | 7.89919 | 2.44198 | -0.71689 |

**TS(Water) +3$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2779.171 Hartree

RMS Gradient Norm = 3.9e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2779.171 Hartree

Zero-point Energy Correction = 0.626631 Hartree

Thermal Correction to Energy = 0.674753 Hartree

Thermal Correction to Enthalpy = 0.675697 Hartree

Thermal Correction to Free Energy = 0.539009 Hartree

EE + Zero-point Energy = -2778.5444 Hartree

EE + Thermal Energy Correction = -2778.4963 Hartree

EE + Thermal Enthalpy Correction = -2778.4953 Hartree

EE + Thermal Free Energy Correction = -2778.632 Hartree

E (Thermal) = 423.414 kcal/mol

Heat Capacity (Cv) = 177.86 cal/mol-kelvin

Entropy (S) = 287.685 cal/mol-kelvin

Symbolic Z-matrix:

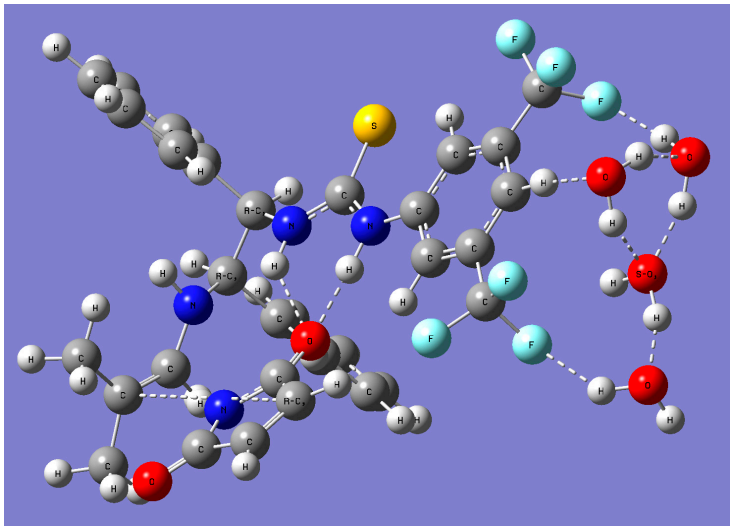
| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | -2.73659 | 0.12686 | 2.5497 |
| C | -3.7398 | -0.78489 | 2.18601 |
| C | -4.40162 | -1.5037 | 3.19167 |
| C | -4.06692 | -1.32521 | 4.53593 |

| | | | |
|---|---|---|---|
| C | -3.0669 | -0.41648 | 4.89136 |
| C | -2.40685 | 0.30889 | 3.89517 |
| H | -2.21735 | 0.6985 | 1.79189 |
| H | -5.18469 | -2.20415 | 2.92017 |
| H | -4.58888 | -1.88829 | 5.30084 |
| H | -2.80746 | -0.27136 | 5.93355 |
| H | -1.6328 | 1.01815 | 4.16514 |
| C | -3.62157 | -2.59368 | -1.24001 |
| C | -4.62985 | -3.56852 | -1.19778 |
| C | -5.21026 | -4.03928 | -2.37627 |
| C | -4.79014 | -3.5396 | -3.61389 |
| C | -3.78231 | -2.5745 | -3.66309 |
| C | -3.19775 | -2.10525 | -2.48175 |
| H | -4.95685 | -3.96381 | -0.24127 |
| H | -5.98498 | -4.79584 | -2.33044 |
| H | -5.24095 | -3.90442 | -4.52928 |
| H | -3.44556 | -2.18852 | -4.61829 |
| H | -2.40019 | -1.37374 | -2.52581 |
| C | -4.09942 | -1.07401 | 0.73402 |
| C | -3.05912 | -2.05723 | 0.0782 |
| N | -1.82315 | -1.29462 | -0.09544 |
| N | -4.11027 | 0.14436 | -0.11205 |
| H | -2.86965 | -2.8871 | 0.76265 |
| H | -5.07056 | -1.58722 | 0.71698 |
| H | -1.98178 | -0.28518 | -0.21422 |
| C | -0.56307 | -1.78222 | -0.02469 |
| C | 2.63732 | -1.86873 | -0.12341 |
| C | 4.01142 | -1.65104 | -0.22008 |
| C | 4.57606 | -0.38658 | -0.35953 |
| C | 3.69374 | 0.69474 | -0.33753 |
| C | 2.32695 | 0.51765 | -0.23573 |

| | | | |
|---|---|---|---|
| C | 1.7671 | -0.77173 | -0.15977 |
| H | 2.24809 | -2.86793 | -0.0149 |
| H | 5.67039 | -0.247 | -0.45861 |
| H | 1.66878 | 1.37229 | -0.20065 |
| N | 0.37115 | -0.78723 | -0.10632 |
| S | -0.22475 | -3.4884 | 0.16155 |
| H | -0.02433 | 0.16508 | -0.12554 |
| F | 4.97022 | 2.37496 | -1.46876 |
| F | 5.15501 | 2.22915 | 0.72009 |
| F | 3.28126 | 3.03864 | -0.18235 |
| F | 4.28591 | -4.00347 | -0.03387 |
| F | 5.93034 | -2.83701 | -0.97782 |
| F | 5.59274 | -2.69726 | 1.20028 |
| C | 4.24309 | 2.07103 | -0.31916 |
| C | 4.93658 | -2.79902 | -0.03664 |
| C | -1.09748 | 2.85369 | -0.27946 |
| C | -0.73421 | 5.09489 | -0.69915 |
| C | -2.22229 | 4.83231 | -0.60882 |
| O | -0.88777 | 1.6474 | -0.05512 |
| C | -0.08 | 3.94517 | -0.50767 |
| O | -3.1588 | 5.61844 | -0.72249 |
| N | -2.33594 | 3.44849 | -0.35391 |
| H | -3.22592 | 2.94463 | -0.23966 |
| H | 0.98267 | 3.76161 | -0.49544 |
| H | -4.19964 | -0.08033 | -1.10506 |
| C | -4.77266 | 1.313 | 0.3046 |
| C | -5.25614 | 2.2977 | -0.48416 |
| C | -5.25876 | 2.24753 | -2.00172 |
| C | -5.82986 | 3.56785 | 0.12179 |
| H | -4.82096 | 1.42012 | 1.3831 |
| H | -6.25785 | 2.4976 | -2.38122 |

| | | | |
|---|---|---|---|
| H | -4.55872 | 2.9837 | -2.4212 |
| H | -4.98751 | 1.26391 | -2.39796 |
| H | -5.2237 | 4.43914 | -0.16522 |
| H | -6.85211 | 3.73984 | -0.24102 |
| H | -5.85585 | 3.51163 | 1.21558 |
| H | -0.33287 | 6.07658 | -0.88637 |
| O | 6.4475 | -0.07721 | 2.13977 |
| H | 5.77729 | 0.62394 | 1.91901 |
| H | 5.99788 | -0.95168 | 1.97726 |
| O | 7.48507 | 0.03124 | -0.32121 |
| H | 7.65191 | 1.00733 | -0.56035 |
| H | 7.30818 | 0.00937 | 0.67684 |
| O | 7.73605 | 2.6156 | -1.01964 |
| H | 6.77041 | 2.74508 | -1.22158 |
| H | 8.20129 | 2.64861 | -1.89737 |

**TS(Water) +4$H_2O$**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2855.1919 Hartree

RMS Gradient Norm = 3.93e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2855.1919 Hartree

Zero-point Energy Correction = 0.652279 Hartree

Thermal Correction to Energy = 0.702153 Hartree

Thermal Correction to Enthalpy = 0.703097 Hartree

Thermal Correction to Free Energy = 0.563221 Hartree

EE + Zero-point Energy = -2854.5396 Hartree

EE + Thermal Energy Correction = -2854.4897 Hartree

EE + Thermal Enthalpy Correction = -2854.4888 Hartree

EE + Thermal Free Energy Correction = -2854.6287 Hartree

E (Thermal) = 440.608 kcal/mol

Heat Capacity (Cv) = 184.729 cal/mol-kelvin

Entropy (S) = 294.394 cal/mol-kelvin

Symbolic Z-matrix:

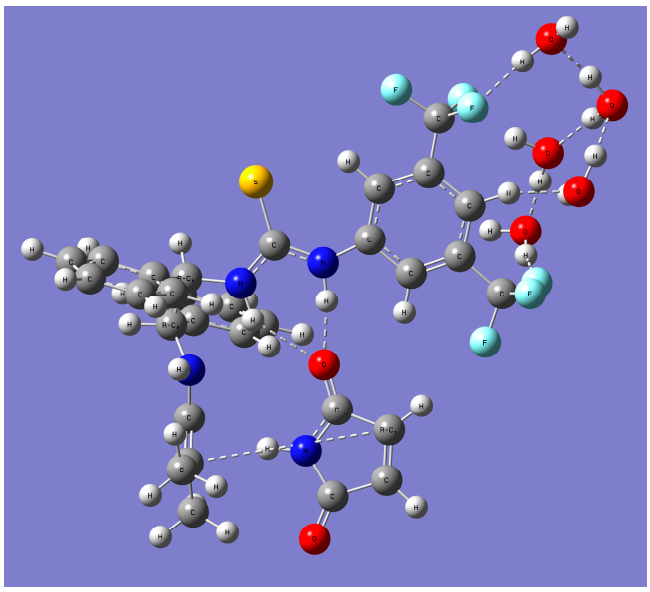
Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -2.82374 | 0.34655 | 2.59229 |
| C | -3.86205 | -0.56515 | 2.34542 |
| C | -4.49101 | -1.18894 | 3.43239 |
| C | -4.0898 | -0.9175 | 4.74248 |
| C | -3.05517 | -0.00945 | 4.98146 |
| C | -2.42747 | 0.6217 | 3.90359 |
| H | -2.32836 | 0.8465 | 1.77046 |
| H | -5.30079 | -1.88823 | 3.25135 |
| H | -4.58717 | -1.40783 | 5.57121 |
| H | -2.744 | 0.2079 | 5.9966 |
| H | -1.62675 | 1.3301 | 4.08294 |
| C | -3.94657 | -2.62976 | -0.93577 |
| C | -4.97517 | -3.57062 | -0.77565 |
| C | -5.61971 | -4.11263 | -1.88833 |
| C | -5.2442 | -3.71921 | -3.17753 |
| C | -4.21636 | -2.78889 | -3.34394 |
| C | -3.56751 | -2.24834 | -2.22845 |
| H | -5.26773 | -3.88414 | 0.22143 |
| H | -6.40951 | -4.84205 | -1.75115 |
| H | -5.74472 | -4.13932 | -4.04196 |
| H | -3.91375 | -2.48576 | -4.33959 |
| H | -2.75441 | -1.5455 | -2.36305 |
| C | -4.29688 | -0.95399 | 0.93775 |
| C | -3.31195 | -2.01203 | 0.3122 |

| | | | |
|---|---|---|---|
| N | -2.06718 | -1.29831 | 0.02921 |
| N | -4.31891 | 0.19587 | 0.00115 |
| H | -3.11223 | -2.79378 | 1.04851 |
| H | -5.2795 | -1.44069 | 1.00512 |
| H | -2.20588 | -0.29555 | -0.15227 |
| C | -0.81687 | -1.81376 | 0.08017 |
| C | 2.35915 | -2.00569 | -0.2531 |
| C | 3.73675 | -1.83622 | -0.40419 |
| C | 4.34917 | -0.58669 | -0.50519 |
| C | 3.50119 | 0.5225 | -0.44336 |
| C | 2.13153 | 0.38906 | -0.29778 |
| C | 1.53167 | -0.87918 | -0.20082 |
| H | 1.93067 | -2.99349 | -0.19644 |
| H | 5.44256 | -0.47349 | -0.68999 |
| H | 1.5 | 1.26451 | -0.26215 |
| N | 0.13723 | -0.85189 | -0.09456 |
| S | -0.51412 | -3.51399 | 0.36511 |
| H | -0.2333 | 0.10887 | -0.15046 |
| F | 5.14555 | 1.95852 | -1.36659 |
| F | 4.50604 | 2.39121 | 0.70471 |
| F | 3.12744 | 2.82031 | -0.95637 |
| F | 3.88063 | -4.17216 | -0.82175 |
| F | 5.67901 | -2.9147 | -1.24386 |
| F | 5.10644 | -3.37338 | 0.83363 |
| C | 4.06125 | 1.89479 | -0.53426 |
| C | 4.5789 | -3.05959 | -0.43955 |
| C | -1.24962 | 2.78255 | -0.53884 |
| C | -0.85404 | 4.93435 | -1.27489 |
| C | -2.34062 | 4.73634 | -1.06687 |
| O | -1.05909 | 1.6103 | -0.16539 |
| C | -0.21946 | 3.79833 | -0.9687 |

| | | | |
|---|---|---|---|
| O | -3.26281 | 5.53031 | -1.23185 |
| N | -2.47432 | 3.40269 | -0.62405 |
| H | -3.36947 | 2.94538 | -0.40358 |
| H | 0.83624 | 3.57827 | -0.99652 |
| H | -4.46149 | -0.1023 | -0.96576 |
| C | -4.92908 | 1.41331 | 0.35215 |
| C | -5.42519 | 2.34421 | -0.49231 |
| C | -5.50563 | 2.17055 | -1.99858 |
| C | -5.93244 | 3.67829 | 0.02925 |
| H | -4.92011 | 1.60948 | 1.41913 |
| H | -6.51978 | 2.40509 | -2.34707 |
| H | -4.81965 | 2.86014 | -2.51032 |
| H | -5.26627 | 1.15428 | -2.32715 |
| H | -5.32438 | 4.50192 | -0.37203 |
| H | -6.97022 | 3.84683 | -0.28844 |
| H | -5.89403 | 3.72089 | 1.12323 |
| H | -0.43941 | 5.86817 | -1.61536 |
| O | 7.88566 | -1.91377 | 1.39852 |
| H | 7.72367 | -1.38615 | 2.22463 |
| H | 7.12341 | -2.55219 | 1.33998 |
| O | 7.46651 | -0.21406 | -0.64777 |
| H | 7.48662 | 0.69207 | -0.17292 |
| H | 7.69162 | -0.86306 | 0.10849 |
| O | 7.28255 | 1.92869 | 0.92393 |
| H | 6.97062 | 2.79559 | 0.49167 |
| H | 6.44551 | 1.56962 | 1.32158 |
| O | 6.45065 | 4.35166 | 0.46941 |
| H | 6.76208 | 4.39931 | 1.41606 |
| H | 5.45978 | 4.33143 | 0.5609 |

**TS(Water) +5$H_2O$**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2931.2015 Hartree

RMS Gradient Norm = 6.94e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2931.2015 Hartree

Zero-point Energy Correction = 0.677019 Hartree

Thermal Correction to Energy = 0.729465 Hartree

Thermal Correction to Enthalpy = 0.730409 Hartree

Thermal Correction to Free Energy = 0.584429 Hartree

EE + Zero-point Energy = -2930.5245 Hartree

EE + Thermal Energy Correction = -2930.472 Hartree

EE + Thermal Enthalpy Correction = -2930.4711 Hartree

EE + Thermal Free Energy Correction = -2930.6171 Hartree

E (Thermal) = 457.746 kcal/mol

Heat Capacity (Cv) = 192.946 cal/mol-kelvin

Entropy (S) = 307.243 cal/mol-kelvin

Symbolic Z-matrix:

| Charge = 0 Multiplicity = 1 | | | |
|---|---|---|---|
| C | -2.85292 | 0.35827 | 2.63683 |
| C | -3.85632 | -0.58871 | 2.37822 |
| C | -4.47943 | -1.23081 | 3.45797 |
| C | -4.10643 | -0.94326 | 4.77282 |
| C | -3.10644 | -0.00029 | 5.02383 |
| C | -2.48524 | 0.64922 | 3.9532 |
| H | -2.36141 | 0.87383 | 1.82202 |
| H | -5.26261 | -1.95736 | 3.26724 |
| H | -4.59881 | -1.44827 | 5.59567 |
| H | -2.81723 | 0.22975 | 6.04266 |
| H | -1.71154 | 1.38467 | 4.14204 |
| C | -3.83861 | -2.67278 | -0.89168 |
| C | -4.841 | -3.64369 | -0.74627 |
| C | -5.45626 | -4.20092 | -1.86808 |
| C | -5.07719 | -3.793 | -3.15166 |
| C | -4.07515 | -2.83253 | -3.30344 |
| C | -3.4557 | -2.27651 | -2.17892 |
| H | -5.13616 | -3.96852 | 0.24641 |
| H | -6.22606 | -4.95339 | -1.74228 |
| H | -5.55498 | -4.22491 | -4.0231 |
| H | -3.76982 | -2.51765 | -4.29459 |
| H | -2.6622 | -1.54972 | -2.30259 |

| | | | |
|---|---|---|---|
| C | -4.25898 | -0.99777 | 0.96682 |
| C | -3.23982 | -2.03757 | 0.36529 |
| N | -2.00761 | -1.29565 | 0.1013 |
| N | -4.29415 | 0.14433 | 0.01966 |
| H | -3.03658 | -2.8116 | 1.10875 |
| H | -5.23096 | -1.50672 | 1.02173 |
| H | -2.17118 | -0.29734 | -0.08132 |
| C | -0.74629 | -1.78167 | 0.15334 |
| C | 2.42697 | -1.89155 | -0.25461 |
| C | 3.78501 | -1.68502 | -0.49409 |
| C | 4.34589 | -0.42145 | -0.6662 |
| C | 3.48379 | 0.66895 | -0.53903 |
| C | 2.13314 | 0.49897 | -0.28973 |
| C | 1.57178 | -0.78525 | -0.16968 |
| H | 2.0336 | -2.89013 | -0.15071 |
| H | 5.41238 | -0.29736 | -0.91474 |
| H | 1.48329 | 1.35724 | -0.19833 |
| N | 0.18416 | -0.79233 | -0.00247 |
| S | -0.4019 | -3.4766 | 0.41216 |
| H | -0.20848 | 0.16112 | -0.02563 |
| F | 5.14173 | 2.16842 | -1.34938 |
| F | 4.35301 | 2.52086 | 0.68788 |
| F | 3.07069 | 2.95458 | -1.06305 |
| F | 4.02334 | -4.03352 | -0.76349 |
| F | 5.71918 | -2.72339 | -1.39576 |
| F | 5.3037 | -3.04547 | 0.74667 |
| C | 4.00733 | 2.05747 | -0.59668 |
| C | 4.68864 | -2.86551 | -0.50198 |
| C | -1.26025 | 2.77906 | -0.55089 |
| C | -0.97981 | 4.81936 | -1.5956 |
| C | -2.45326 | 4.57419 | -1.34893 |

| | | | |
|---|---|---|---|
| O | -1.00804 | 1.67885 | -0.02407 |
| C | -0.28551 | 3.77441 | -1.13337 |
| O | -3.42208 | 5.27412 | -1.63351 |
| N | -2.51381 | 3.32045 | -0.70516 |
| H | -3.38907 | 2.85694 | -0.42485 |
| H | 0.77972 | 3.60511 | -1.14323 |
| H | -4.42806 | -0.16885 | -0.94382 |
| C | -4.94605 | 1.34602 | 0.35706 |
| C | -5.42875 | 2.27622 | -0.4951 |
| C | -5.44044 | 2.13733 | -2.00727 |
| C | -6.0051 | 3.58343 | 0.021 |
| H | -4.98213 | 1.53197 | 1.42518 |
| H | -6.47423 | 2.13158 | -2.37851 |
| H | -4.93679 | 2.99922 | -2.46588 |
| H | -4.94757 | 1.2279 | -2.36389 |
| H | -5.43504 | 4.42845 | -0.39012 |
| H | -7.0486 | 3.70043 | -0.30223 |
| H | -5.97376 | 3.63493 | 1.11451 |
| H | -0.61573 | 5.7125 | -2.07475 |
| O | 7.65068 | -1.37927 | 1.01536 |
| H | 7.32021 | -0.4732 | 1.37224 |
| H | 6.86961 | -1.99351 | 1.05601 |
| O | 7.2328 | 0.04668 | -1.14458 |
| H | 7.02767 | 0.76326 | -0.47071 |
| H | 7.51959 | -0.69758 | -0.49498 |
| O | 6.62367 | 0.98424 | 1.37894 |
| H | 6.87655 | 1.97523 | 1.57484 |
| H | 5.64483 | 0.92634 | 1.5151 |
| O | 6.80736 | 3.50844 | 1.65478 |
| H | 6.76881 | 3.867 | 2.57993 |
| H | 5.90749 | 3.65099 | 1.25385 |

| | | | |
|---|---|---|---|
| O | 6.40225 | -4.56686 | -0.53906 |
| H | 7.36225 | -4.56686 | -0.53906 |
| H | 6.0818 | -3.66192 | -0.53906 |

**TS($CH_2Cl_2$) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=dichloromethane

E(RB3LYP) = -2931.1925 Hartree

RMS Gradient Norm = 1.293e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2931.1925 Hartree

Zero-point Energy Correction = 0.67728 Hartree

Thermal Correction to Energy = 0.729695 Hartree

Thermal Correction to Enthalpy = 0.730639 Hartree

Thermal Correction to Free Energy = 0.584691 Hartree

EE + Zero-point Energy = -2930.5152 Hartree

EE + Thermal Energy Correction = -2930.4628 Hartree

EE + Thermal Enthalpy Correction = -2930.4618 Hartree

EE + Thermal Free Energy Correction = -2930.6078 Hartree

E (Thermal) = 457.89 kcal/mol

Heat Capacity (Cv) = 192.928 cal/mol-kelvin

Entropy (S) = 307.172 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -3.12237 | 0.21549 | 2.56869 |
| C | -4.02674 | -0.82673 | 2.31271 |
| C | -4.6002 | -1.50913 | 3.39487 |
| C | -4.27494 | -1.1673 | 4.70921 |
| C | -3.37401 | -0.12898 | 4.95721 |
| C | -2.80283 | 0.56073 | 3.8841 |
| H | -2.67237 | 0.76188 | 1.75033 |
| H | -5.30746 | -2.31036 | 3.20641 |
| H | -4.72764 | -1.70505 | 5.53406 |
| H | -3.12263 | 0.14308 | 5.97569 |
| H | -2.10596 | 1.36986 | 4.07099 |
| C | -3.77053 | -2.92878 | -0.93502 |
| C | -4.6699 | -3.99436 | -0.78125 |
| C | -5.22138 | -4.62367 | -1.89775 |
| C | -4.88117 | -4.19385 | -3.18486 |
| C | -3.98127 | -3.13863 | -3.34514 |
| C | -3.42555 | -2.51035 | -2.22565 |
| H | -4.93211 | -4.33763 | 0.21454 |
| H | -5.91024 | -5.44986 | -1.76527 |
| H | -5.30855 | -4.68261 | -4.05243 |
| H | -3.70441 | -2.80715 | -4.33929 |
| H | -2.70659 | -1.71061 | -2.35496 |
| C | -4.37045 | -1.28988 | 0.90291 |
| C | -3.24445 | -2.22152 | 0.31594 |
| N | -2.09645 | -1.35794 | 0.04528 |
| N | -4.51826 | -0.16641 | -0.05544 |
| H | -2.96162 | -2.96288 | 1.06669 |
| H | -5.28459 | -1.897 | 0.95581 |
| H | -2.35857 | -0.383 | -0.14776 |

| | | | |
|---|---|---|---|
| C | -0.79195 | -1.71608 | 0.10495 |
| C | 2.3812 | -1.5075 | -0.24877 |
| C | 3.71768 | -1.16206 | -0.45637 |
| C | 4.14989 | 0.14589 | -0.65378 |
| C | 3.17478 | 1.14306 | -0.58794 |
| C | 1.84354 | 0.8381 | -0.37143 |
| C | 1.41474 | -0.49477 | -0.22374 |
| H | 2.0923 | -2.53722 | -0.11087 |
| H | 5.20789 | 0.41528 | -0.82925 |
| H | 1.10767 | 1.62582 | -0.31955 |
| N | 0.03343 | -0.63892 | -0.07698 |
| S | -0.27942 | -3.35754 | 0.39774 |
| H | -0.45475 | 0.26686 | -0.12747 |
| F | 4.24932 | 2.85176 | -1.86084 |
| F | 4.41648 | 2.962 | 0.33312 |
| F | 2.47502 | 3.41596 | -0.65005 |
| F | 4.22439 | -3.48673 | -0.4178 |
| F | 5.68165 | -2.10926 | -1.40803 |
| F | 5.50906 | -2.13703 | 0.78521 |
| C | 3.56841 | 2.57205 | -0.71523 |
| C | 4.74367 | -2.22844 | -0.38107 |
| C | -1.78804 | 2.81248 | -0.54317 |
| C | -1.67648 | 4.99213 | -1.29771 |
| C | -3.12585 | 4.59127 | -1.12274 |
| O | -1.4431 | 1.68118 | -0.15344 |
| C | -0.89854 | 3.9583 | -0.96174 |
| O | -4.14477 | 5.24597 | -1.3232 |
| N | -3.08413 | 3.25646 | -0.6624 |
| H | -3.91536 | 2.68384 | -0.45815 |
| H | 0.1778 | 3.8871 | -0.96041 |
| H | -4.60743 | -0.50018 | -1.01727 |

| | | | |
|---|---|---|---|
| C | -5.29007 | 0.96571 | 0.26363 |
| C | -5.8631 | 1.82904 | -0.60343 |
| C | -5.85758 | 1.65588 | -2.11184 |
| C | -6.57167 | 3.07796 | -0.10666 |
| H | -5.3516 | 1.15968 | 1.32925 |
| H | -6.88739 | 1.65654 | -2.49268 |
| H | -5.33435 | 2.49263 | -2.5953 |
| H | -5.3799 | 0.72702 | -2.43841 |
| H | -6.07319 | 3.97834 | -0.49306 |
| H | -7.61151 | 3.09694 | -0.45991 |
| H | -6.57818 | 3.12616 | 0.98767 |
| H | -1.38737 | 5.97126 | -1.64085 |
| O | 8.72488 | 0.10311 | 0.29812 |
| H | 8.09547 | 0.2106 | 1.08851 |
| H | 8.66537 | -0.87553 | 0.00872 |
| O | 6.74511 | 1.39203 | -0.74668 |
| H | 6.46087 | 1.44625 | 0.21386 |
| H | 7.63602 | 0.8738 | -0.59199 |
| O | 6.56884 | 0.4029 | 1.81587 |
| H | 5.94014 | 0.98249 | 2.39802 |
| H | 6.08279 | -0.41947 | 1.55286 |
| O | 4.81444 | 1.92497 | 2.91551 |
| H | 4.03252 | 1.4398 | 3.28657 |
| H | 4.5115 | 2.36794 | 2.07597 |
| O | 8.38874 | -2.37376 | -0.595 |
| H | 8.93514 | -2.47995 | -1.41764 |
| H | 7.4415 | -2.33431 | -0.8979 |

**TS(THF) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=thf

E(RB3LYP) = -2931.1907 Hartree

RMS Gradient Norm = 1.46e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2931.1907 Hartree

Zero-point Energy Correction = 0.677318 Hartree

Thermal Correction to Energy = 0.729724 Hartree

Thermal Correction to Enthalpy = 0.730668 Hartree

Thermal Correction to Free Energy = 0.585007 Hartree

EE + Zero-point Energy = -2930.5134 Hartree

EE + Thermal Energy Correction = -2930.461 Hartree

EE + Thermal Enthalpy Correction = -2930.46 Hartree

EE + Thermal Free Energy Correction = -2930.6057 Hartree

E (Thermal) = 457.909 kcal/mol

Heat Capacity (Cv) = 192.946 cal/mol-kelvin

Entropy (S) = 306.568 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | -3.13167 | 0.21987 | 2.56732 |
| C | -4.03515 | -0.82283 | 2.31028 |
| C | -4.61319 | -1.50222 | 3.39186 |
| C | -4.29329 | -1.15712 | 4.7066 |

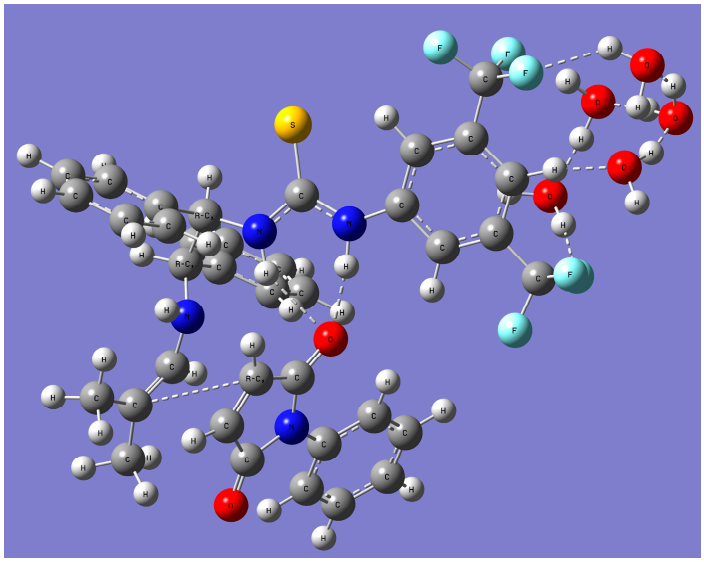
| | | | |
|---|---|---|---|
| C | -3.39325 | -0.11834 | 4.95563 |
| C | -2.81758 | 0.56846 | 3.88311 |
| H | -2.67808 | 0.76403 | 1.74948 |
| H | -5.31984 | -2.3038 | 3.2026 |
| H | -4.74942 | -1.69271 | 5.53096 |
| H | -3.14599 | 0.15626 | 5.97442 |
| H | -2.12131 | 1.37792 | 4.07085 |
| C | -3.76821 | -2.93182 | -0.93215 |
| C | -4.66871 | -3.99646 | -0.77895 |
| C | -5.2175 | -4.62749 | -1.89575 |
| C | -4.87341 | -4.20033 | -3.18267 |
| C | -3.97225 | -3.14616 | -3.34241 |
| C | -3.41931 | -2.51616 | -2.22256 |
| H | -4.93352 | -4.338 | 0.21676 |
| H | -5.90709 | -5.45312 | -1.76368 |
| H | -5.29854 | -4.69055 | -4.05052 |
| H | -3.69201 | -2.81711 | -4.33642 |
| H | -2.69879 | -1.7177 | -2.35115 |
| C | -4.37347 | -1.28952 | 0.9004 |
| C | -3.24542 | -2.22221 | 0.31891 |
| N | -2.09706 | -1.35887 | 0.04986 |
| N | -4.51868 | -0.16841 | -0.06133 |
| H | -2.96439 | -2.9621 | 1.07183 |
| H | -5.28772 | -1.89666 | 0.9515 |
| H | -2.3591 | -0.38446 | -0.14514 |
| C | -0.79235 | -1.71677 | 0.11361 |
| C | 2.38008 | -1.50677 | -0.24316 |
| C | 3.71622 | -1.16068 | -0.45187 |
| C | 4.14836 | 0.14778 | -0.64646 |
| C | 3.17336 | 1.14475 | -0.5767 |
| C | 1.84233 | 0.83925 | -0.35914 |

| | | | |
|---|---|---|---|
| C | 1.41367 | -0.49396 | -0.21437 |
| H | 2.09112 | -2.5368 | -0.10744 |
| H | 5.20639 | 0.41814 | -0.82357 |
| H | 1.10635 | 1.62674 | -0.30483 |
| N | 0.03255 | -0.63865 | -0.06749 |
| S | -0.27955 | -3.35654 | 0.40991 |
| H | -0.45591 | 0.26675 | -0.11746 |
| F | 4.24449 | 2.8578 | -1.84729 |
| F | 4.41634 | 2.96153 | 0.34683 |
| F | 2.47271 | 3.41752 | -0.63081 |
| F | 4.22292 | -3.48548 | -0.41832 |
| F | 5.67527 | -2.10728 | -1.41441 |
| F | 5.51392 | -2.13718 | 0.7796 |
| C | 3.56679 | 2.5741 | -0.70123 |
| C | 4.74243 | -2.22735 | -0.38277 |
| C | -1.78554 | 2.81473 | -0.54136 |
| C | -1.67297 | 4.99166 | -1.30374 |
| C | -3.12272 | 4.58971 | -1.13418 |
| O | -1.44074 | 1.68526 | -0.14617 |
| C | -0.89539 | 3.96007 | -0.96004 |
| O | -4.14147 | 5.24207 | -1.34243 |
| N | -3.08152 | 3.25671 | -0.66813 |
| H | -3.91334 | 2.68399 | -0.46588 |
| H | 0.18102 | 3.88999 | -0.95338 |
| H | -4.60595 | -0.50532 | -1.02224 |
| C | -5.29097 | 0.96473 | 0.25278 |
| C | -5.85774 | 1.82869 | -0.61779 |
| C | -5.84314 | 1.65591 | -2.12622 |
| C | -6.5708 | 3.07679 | -0.12545 |
| H | -5.35887 | 1.15889 | 1.31799 |
| H | -6.87107 | 1.64291 | -2.51201 |

| | | | |
|---|---|---|---|
| H | -5.32918 | 2.50014 | -2.60654 |
| H | -5.35126 | 0.73389 | -2.45111 |
| H | -6.07247 | 3.97766 | -0.51082 |
| H | -7.60914 | 3.09338 | -0.48326 |
| H | -6.58244 | 3.12609 | 0.96879 |
| H | -1.38347 | 5.96979 | -1.64941 |
| O | 8.72994 | 0.10329 | 0.27787 |
| H | 8.11025 | 0.20888 | 1.07578 |
| H | 8.66892 | -0.875 | -0.01166 |
| O | 6.73951 | 1.39173 | -0.74472 |
| H | 6.46577 | 1.44511 | 0.21884 |
| H | 7.63344 | 0.87546 | -0.6 |
| O | 6.58666 | 0.39481 | 1.81733 |
| H | 5.95717 | 0.97089 | 2.40129 |
| H | 6.10097 | -0.42646 | 1.55012 |
| O | 4.82394 | 1.90684 | 2.92025 |
| H | 4.04274 | 1.41729 | 3.28696 |
| H | 4.52166 | 2.35458 | 2.08299 |
| O | 8.38672 | -2.37232 | -0.6177 |
| H | 8.92869 | -2.47593 | -1.44356 |
| H | 7.4378 | -2.33142 | -0.91511 |

**Figure 3.**

**TS(Gas) +5$H_2O$**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -3160.9475 Hartree

RMS Gradient Norm = 1.42e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9475 Hartree

Zero-point Energy Correction = 0.75884 Hartree

Thermal Correction to Energy = 0.814779 Hartree

Thermal Correction to Enthalpy = 0.815723 Hartree

Thermal Correction to Free Energy = 0.660379 Hartree

EE + Zero-point Energy = -3160.1886 Hartree

EE + Thermal Energy Correction = -3160.1327 Hartree

EE + Thermal Enthalpy Correction = -3160.1317 Hartree

EE + Thermal Free Energy Correction = -3160.2871 Hartree

E (Thermal) = 511.282 kcal/mol

Heat Capacity (Cv) = 209.304 cal/mol-kelvin

Entropy (S) = 326.949 cal/mol-kelvin

Symbolic Z-matrix:

| Charge = 0 Multiplicity = 1 | | | |
|---|---|---|---|
| C | 2.67135 | -0.37866 | 2.27695 |
| C | 3.46932 | 0.7741 | 2.32576 |
| C | 4.01466 | 1.16863 | 3.55649 |
| C | 3.76706 | 0.43327 | 4.71773 |
| C | 2.97651 | -0.71749 | 4.66011 |
| C | 2.43376 | -1.12065 | 3.43705 |
| H | 2.23258 | -0.70878 | 1.34584 |
| H | 4.64036 | 2.05392 | 3.60405 |
| H | 4.19706 | 0.75284 | 5.65985 |
| H | 2.78972 | -1.29634 | 5.5571 |
| H | 1.82883 | -2.01824 | 3.37907 |
| C | 2.97449 | 3.69365 | -0.1753 |
| C | 3.74277 | 4.75668 | 0.32284 |
| C | 4.22791 | 5.74413 | -0.53557 |
| C | 3.95166 | 5.68035 | -1.9057 |
| C | 3.18164 | 4.62889 | -2.40687 |
| C | 2.69178 | 3.64124 | -1.54538 |
| H | 3.95657 | 4.81431 | 1.38547 |
| H | 4.81625 | 6.5626 | -0.13738 |
| H | 4.32856 | 6.44641 | -2.573 |
| H | 2.95575 | 4.57715 | -3.46564 |
| H | 2.07471 | 2.84179 | -1.93635 |

| | | | |
|---|---|---|---|
| C | 3.73623 | 1.64744 | 1.10737 |
| C | 2.52633 | 2.59581 | 0.79248 |
| N | 1.4668 | 1.74626 | 0.24901 |
| N | 4.00052 | 0.84791 | -0.13506 |
| H | 2.175 | 3.04869 | 1.72236 |
| H | 4.59319 | 2.29492 | 1.33384 |
| H | 1.82661 | 0.89845 | -0.19711 |
| C | 0.1343 | 1.94905 | 0.36347 |
| C | -2.98852 | 1.60667 | 0.00795 |
| C | -4.32 | 1.25505 | -0.21104 |
| C | -4.69608 | 0.02995 | -0.75013 |
| C | -3.66877 | -0.86185 | -1.06217 |
| C | -2.33406 | -0.54837 | -0.85315 |
| C | -1.9686 | 0.70173 | -0.31486 |
| H | -2.74146 | 2.57397 | 0.414 |
| H | -5.74605 | -0.23964 | -0.95571 |
| H | -1.5656 | -1.26447 | -1.11491 |
| N | -0.59247 | 0.91882 | -0.17128 |
| S | -0.50681 | 3.38302 | 1.13564 |
| H | -0.01959 | 0.12482 | -0.50294 |
| F | -5.00827 | -2.15595 | -2.5483 |
| F | -4.52801 | -3.04714 | -0.5919 |
| F | -2.93743 | -2.85411 | -2.12265 |
| F | -4.91467 | 3.50705 | 0.24341 |
| F | -6.47204 | 2.16958 | -0.63433 |
| F | -5.86997 | 1.9532 | 1.48192 |
| C | -4.019 | -2.20461 | -1.59459 |
| C | -5.37239 | 2.21924 | 0.20243 |
| C | 2.12938 | -1.47314 | -1.46164 |
| C | 3.68678 | -1.28128 | -3.14593 |
| C | 4.03995 | -2.4621 | -2.29753 |

| | | | |
|---|---|---|---|
| O | 1.15575 | -1.20941 | -0.72425 |
| C | 2.57708 | -0.71421 | -2.66633 |
| O | 4.98727 | -3.23266 | -2.42183 |
| N | 3.01586 | -2.53797 | -1.28167 |
| H | 2.04071 | 0.14572 | -3.02994 |
| H | 4.07898 | 1.47879 | -0.93913 |
| C | 5.05025 | -0.10902 | -0.07585 |
| C | 6.07951 | -0.24033 | -0.93432 |
| C | 6.38763 | 0.71708 | -2.07009 |
| C | 7.04461 | -1.4 | -0.79066 |
| H | 4.94762 | -0.80391 | 0.75057 |
| H | 7.39575 | 1.13153 | -1.93467 |
| H | 6.38028 | 0.19772 | -3.03634 |
| H | 5.68601 | 1.55415 | -2.12948 |
| H | 6.90336 | -2.11293 | -1.61476 |
| H | 8.08295 | -1.04648 | -0.8205 |
| H | 6.88369 | -1.93856 | 0.14951 |
| H | 4.28026 | -0.99785 | -3.99798 |
| O | -8.51282 | -1.27177 | 0.74586 |
| H | -7.80545 | -1.02147 | 1.49375 |
| H | -8.9445 | -0.39523 | 0.4263 |
| O | -7.35031 | -0.95339 | -1.38066 |
| H | -7.17521 | -1.65982 | -2.05026 |
| H | -7.78112 | -1.33992 | -0.43332 |
| O | -6.69572 | -0.62583 | 2.40492 |
| H | -5.89955 | -1.28357 | 2.30299 |
| H | -6.37643 | 0.27083 | 2.12687 |
| O | -4.70943 | -2.23599 | 2.06595 |
| H | -3.83727 | -1.84166 | 2.32264 |
| H | -4.62985 | -2.53607 | 1.12016 |
| O | -9.03486 | 0.83283 | -0.73073 |

| | | | |
|---|---|---|---|
| H | -8.4381 | 0.2015 | -1.2972 |
| H | -8.38917 | 1.52306 | -0.41957 |
| C | 2.93846 | -3.53536 | -0.25208 |
| C | 1.72242 | -3.78625 | 0.40676 |
| C | 4.07623 | -4.27906 | 0.10316 |
| C | 1.65584 | -4.75644 | 1.40703 |
| H | 0.84636 | -3.21365 | 0.15208 |
| C | 3.99335 | -5.24841 | 1.10283 |
| H | 5.00522 | -4.11738 | -0.41731 |
| C | 2.78786 | -5.49248 | 1.76309 |
| H | 0.70976 | -4.93605 | 1.90397 |
| H | 4.88099 | -5.81299 | 1.36274 |
| H | 2.73047 | -6.24493 | 2.54016 |

**TS(Toluene) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=toluene

E(RB3LYP) = -3160.9659 Hartree

RMS Gradient Norm = 3.53e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9659 Hartree

Zero-point Energy Correction = 0.759077 Hartree

Thermal Correction to Energy = 0.814822 Hartree

Thermal Correction to Enthalpy = 0.815766 Hartree

Thermal Correction to Free Energy = 0.662255 Hartree

EE + Zero-point Energy = -3160.2069 Hartree

EE + Thermal Energy Correction = -3160.1511 Hartree

EE + Thermal Enthalpy Correction = -3160.1502 Hartree

EE + Thermal Free Energy Correction = -3160.3037 Hartree

E (Thermal) = 511.308 kcal/mol

Heat Capacity (Cv) = 209.089 cal/mol-kelvin

Entropy (S) = 323.092 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.75062 | -0.45199 | 2.23246 |
| C | 3.49809 | 0.72989 | 2.33721 |
| C | 4.00745 | 1.09906 | 3.59048 |
| C | 3.77365 | 0.31151 | 4.71877 |

| | | | |
|---|---|---|---|
| C | 3.03523 | -0.86833 | 4.60472 |
| C | 2.52903 | -1.24707 | 3.35929 |
| H | 2.33948 | -0.76473 | 1.28285 |
| H | 4.59563 | 2.00657 | 3.68166 |
| H | 4.17419 | 0.61338 | 5.67947 |
| H | 2.86027 | -1.48829 | 5.47617 |
| H | 1.96561 | -2.1673 | 3.25752 |
| C | 2.99138 | 3.69755 | -0.10376 |
| C | 3.75229 | 4.74873 | 0.42799 |
| C | 4.25444 | 5.75193 | -0.40069 |
| C | 4.00235 | 5.71732 | -1.77579 |
| C | 3.23636 | 4.68064 | -2.31092 |
| C | 2.73071 | 3.67719 | -1.47834 |
| H | 3.94097 | 4.78794 | 1.49626 |
| H | 4.8341 | 6.56279 | 0.02479 |
| H | 4.38989 | 6.49771 | -2.41991 |
| H | 3.02073 | 4.65787 | -3.37302 |
| H | 2.10572 | 2.89465 | -1.88999 |
| C | 3.75566 | 1.65485 | 1.15646 |
| C | 2.53067 | 2.57604 | 0.83118 |
| N | 1.50181 | 1.71933 | 0.24405 |
| N | 4.08011 | 0.9167 | -0.11053 |
| H | 2.13899 | 3.00615 | 1.75633 |
| H | 4.58694 | 2.3202 | 1.42472 |
| H | 1.87846 | 0.87145 | -0.1973 |
| C | 0.16063 | 1.90524 | 0.37088 |
| C | -2.94169 | 1.5997 | -0.10294 |
| C | -4.27507 | 1.2446 | -0.30251 |
| C | -4.66453 | -0.02818 | -0.70804 |
| C | -3.64578 | -0.95959 | -0.91501 |
| C | -2.30814 | -0.64314 | -0.72269 |

| | | | |
|---|---|---|---|
| C | -1.93102 | 0.64963 | -0.31025 |
| H | -2.68389 | 2.60092 | 0.20317 |
| H | -5.71881 | -0.30879 | -0.89995 |
| H | -1.54677 | -1.39136 | -0.90434 |
| N | -0.55563 | 0.86997 | -0.17726 |
| S | -0.49275 | 3.30792 | 1.15791 |
| H | 0.01584 | 0.07575 | -0.49175 |
| F | -4.97945 | -2.39943 | -2.27112 |
| F | -4.53859 | -3.06583 | -0.21545 |
| F | -2.92478 | -3.06581 | -1.7334 |
| F | -4.83616 | 3.54397 | -0.13793 |
| F | -6.40114 | 2.13424 | -0.87675 |
| F | -5.84158 | 2.16915 | 1.26254 |
| C | -4.00873 | -2.34756 | -1.30312 |
| C | -5.31777 | 2.27005 | -0.03098 |
| C | 2.19113 | -1.50967 | -1.45341 |
| C | 3.82789 | -1.23462 | -3.04691 |
| C | 4.11689 | -2.47951 | -2.2695 |
| O | 1.1969 | -1.27679 | -0.74662 |
| C | 2.7084 | -0.67944 | -2.57906 |
| O | 5.06437 | -3.26114 | -2.4211 |
| N | 3.03708 | -2.60041 | -1.30681 |
| H | 2.20184 | 0.21318 | -2.90495 |
| H | 4.15726 | 1.58786 | -0.88165 |
| C | 5.1537 | -0.00641 | -0.06999 |
| C | 6.20031 | -0.06126 | -0.91519 |
| C | 6.49822 | 0.96454 | -1.99245 |
| C | 7.20584 | -1.18776 | -0.80914 |
| H | 5.06124 | -0.73845 | 0.72472 |
| H | 7.481 | 1.41684 | -1.80291 |
| H | 6.54847 | 0.4933 | -2.98196 |

| | | | |
|---|---|---|---|
| H | 5.76175 | 1.77275 | -2.03391 |
| H | 7.1138 | -1.85717 | -1.67543 |
| H | 8.2297 | -0.79333 | -0.79268 |
| H | 7.04471 | -1.78266 | 0.09601 |
| H | 4.46792 | -0.9092 | -3.84868 |
| O | -8.75774 | -1.01476 | 0.66872 |
| H | -8.12943 | -0.68078 | 1.45037 |
| H | -9.13684 | -0.18321 | 0.19355 |
| O | -7.29773 | -1.00876 | -1.2722 |
| H | -7.17896 | -1.77656 | -1.8844 |
| H | -7.91129 | -1.25287 | -0.34714 |
| O | -7.04314 | -0.18818 | 2.35096 |
| H | -6.24763 | -0.84546 | 2.34414 |
| H | -6.69539 | 0.68065 | 2.0243 |
| O | -4.97307 | -1.73539 | 2.19348 |
| H | -4.12201 | -1.26046 | 2.36808 |
| H | -4.86969 | -2.2286 | 1.33629 |
| O | -8.99831 | 0.88706 | -1.09287 |
| H | -8.33835 | 0.18632 | -1.48075 |
| H | -8.39764 | 1.62386 | -0.80066 |
| C | 2.85973 | -3.65845 | -0.34672 |
| C | 1.61939 | -3.813 | 0.29243 |
| C | 3.9003 | -4.55415 | -0.04149 |
| C | 1.43038 | -4.83477 | 1.22123 |
| H | 0.81718 | -3.12659 | 0.07441 |
| C | 3.695 | -5.57221 | 0.88941 |
| H | 4.84475 | -4.4698 | -0.54722 |
| C | 2.46398 | -5.71985 | 1.52883 |
| H | 0.46408 | -4.93684 | 1.70113 |
| H | 4.50862 | -6.25321 | 1.1098 |
| H | 2.31138 | -6.51231 | 2.2513 |

**TS(Diethyl ether) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=diethylether

E(RB3LYP) = -3160.9752 Hartree

RMS Gradient Norm = 1.034e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9752 Hartree

Zero-point Energy Correction = 0.758779 Hartree

Thermal Correction to Energy = 0.814619 Hartree

Thermal Correction to Enthalpy = 0.815564 Hartree

Thermal Correction to Free Energy = 0.661501 Hartree

EE + Zero-point Energy = -3160.2164 Hartree

EE + Thermal Energy Correction = -3160.1606 Hartree

EE + Thermal Enthalpy Correction = -3160.1597 Hartree

EE + Thermal Free Energy Correction = -3160.3137 Hartree

E (Thermal) = 511.181 kcal/mol

Heat Capacity (Cv) = 209.223 cal/mol-kelvin

Entropy (S) = 324.253 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.55028 | -0.28891 | 2.33655 |
| C | 3.3537 | 0.85963 | 2.375 |
| C | 3.86078 | 1.28859 | 3.61008 |
| C | 3.57033 | 0.59166 | 4.7844 |

| | | | |
|---|---|---|---|
| C | 2.77585 | -0.55636 | 4.73613 |
| C | 2.27092 | -0.99414 | 3.50945 |
| H | 2.13933 | -0.64465 | 1.40316 |
| H | 4.4917 | 2.17063 | 3.65103 |
| H | 3.97058 | 0.93841 | 5.72999 |
| H | 2.55681 | -1.10644 | 5.6438 |
| H | 1.66397 | -1.89074 | 3.45835 |
| C | 2.98659 | 3.687 | -0.26185 |
| C | 3.80593 | 4.73315 | 0.18728 |
| C | 4.32923 | 5.66128 | -0.71304 |
| C | 4.03994 | 5.55523 | -2.07754 |
| C | 3.21651 | 4.52295 | -2.53035 |
| C | 2.68948 | 3.5947 | -1.62628 |
| H | 4.02591 | 4.82708 | 1.24606 |
| H | 4.95531 | 6.46875 | -0.35171 |
| H | 4.44475 | 6.27676 | -2.77729 |
| H | 2.97445 | 4.4441 | -3.58398 |
| H | 2.0234 | 2.81517 | -1.97622 |
| C | 3.67504 | 1.68807 | 1.13964 |
| C | 2.49562 | 2.64905 | 0.7508 |
| N | 1.43019 | 1.79774 | 0.22627 |
| N | 3.97168 | 0.83766 | -0.06279 |
| H | 2.13431 | 3.15661 | 1.64823 |
| H | 4.53804 | 2.32558 | 1.37288 |
| H | 1.78133 | 0.93405 | -0.17616 |
| C | 0.09598 | 2.00381 | 0.34065 |
| C | -3.02495 | 1.58891 | 0.03257 |
| C | -4.35047 | 1.22066 | -0.19481 |
| C | -4.71018 | -0.00736 | -0.73877 |
| C | -3.66979 | -0.88353 | -1.05136 |
| C | -2.33946 | -0.55209 | -0.84016 |

| | | | |
|---|---|---|---|
| C | -1.99081 | 0.70006 | -0.29469 |
| H | -2.79054 | 2.55949 | 0.43938 |
| H | -5.75764 | -0.29147 | -0.95229 |
| H | -1.56121 | -1.25592 | -1.10691 |
| N | -0.61815 | 0.9309 | -0.1403 |
| S | -0.55048 | 3.46355 | 1.03687 |
| H | -0.03409 | 0.12704 | -0.43481 |
| F | -4.9717 | -2.18751 | -2.56443 |
| F | -4.5222 | -3.07304 | -0.5978 |
| F | -2.90394 | -2.86913 | -2.09905 |
| F | -4.98908 | 3.46532 | 0.23656 |
| F | -6.52884 | 2.07877 | -0.59597 |
| F | -5.88555 | 1.90697 | 1.51327 |
| C | -4.00218 | -2.22676 | -1.59352 |
| C | -5.41803 | 2.1685 | 0.21977 |
| C | 2.1858 | -1.419 | -1.42362 |
| C | 3.78467 | -1.10504 | -3.05311 |
| C | 4.15531 | -2.30789 | -2.24659 |
| O | 1.16366 | -1.19103 | -0.72016 |
| C | 2.64312 | -0.59724 | -2.58305 |
| O | 5.12053 | -3.03139 | -2.38242 |
| N | 3.11148 | -2.46799 | -1.26117 |
| H | 2.08596 | 0.25733 | -2.92782 |
| H | 4.08882 | 1.43848 | -0.88469 |
| C | 5.00422 | -0.13194 | 0.07415 |
| C | 6.06944 | -0.31609 | -0.73111 |
| C | 6.45282 | 0.59242 | -1.88369 |
| C | 7.0046 | -1.48534 | -0.49232 |
| H | 4.85597 | -0.7911 | 0.92273 |
| H | 7.45149 | 1.01144 | -1.70086 |
| H | 6.50752 | 0.03184 | -2.82563 |

| | | | |
|---|---|---|---|
| H | 5.7607 | 1.42803 | -2.02286 |
| H | 6.89076 | -2.23232 | -1.29105 |
| H | 8.04968 | -1.15129 | -0.48781 |
| H | 6.79017 | -1.97869 | 0.46145 |
| H | 4.39214 | -0.76822 | -3.87524 |
| O | -8.60079 | -1.35811 | 0.66694 |
| H | -7.93256 | -1.08644 | 1.44112 |
| H | -9.05709 | -0.49699 | 0.33674 |
| O | -7.33014 | -1.0056 | -1.38014 |
| H | -7.18826 | -1.69058 | -2.07955 |
| H | -7.82746 | -1.40613 | -0.45365 |
| O | -6.83622 | -0.65371 | 2.35543 |
| H | -6.03202 | -1.2985 | 2.27793 |
| H | -6.51637 | 0.24904 | 2.09994 |
| O | -4.79226 | -2.20355 | 2.03249 |
| H | -3.9305 | -1.79257 | 2.29579 |
| H | -4.69844 | -2.52421 | 1.09519 |
| O | -9.08873 | 0.74686 | -0.80048 |
| H | -8.44002 | 0.14023 | -1.33647 |
| H | -8.48986 | 1.4607 | -0.45212 |
| C | 3.07084 | -3.52854 | -0.28856 |
| C | 1.88588 | -3.85699 | 0.397 |
| C | 4.23651 | -4.26351 | -0.02364 |
| C | 1.88294 | -4.8926 | 1.33225 |
| H | 0.98743 | -3.29682 | 0.21293 |
| C | 4.21697 | -5.29681 | 0.9117 |
| H | 5.14086 | -4.04366 | -0.56806 |
| C | 3.04542 | -5.61786 | 1.59805 |
| H | 0.96115 | -5.13205 | 1.84951 |
| H | 5.12827 | -5.85204 | 1.09954 |
| H | 3.03724 | -6.4211 | 2.32469 |

**TS(THF) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=thf

E(RB3LYP) = -3160.9817 Hartree

RMS Gradient Norm = 1.18e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9817 Hartree

Zero-point Energy Correction = 0.758585 Hartree

Thermal Correction to Energy = 0.814441 Hartree

Thermal Correction to Enthalpy = 0.815385 Hartree

Thermal Correction to Free Energy = 0.661171 Hartree

EE + Zero-point Energy = -3160.2231 Hartree

EE + Thermal Energy Correction = -3160.1672 Hartree

EE + Thermal Enthalpy Correction = -3160.1663 Hartree

EE + Thermal Free Energy Correction = -3160.3205 Hartree

E (Thermal) = 511.069 kcal/mol

Heat Capacity (Cv) = 209.254 cal/mol-kelvin

Entropy (S) = 324.57 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.65968 | -0.38054 | 2.27692 |
| C | 3.45798 | 0.77176 | 2.33033 |
| C | 3.99762 | 1.1651 | 3.56394 |
| C | 3.74416 | 0.42899 | 4.72342 |

| | | | |
|---|---|---|---|
| C | 2.95349 | -0.72143 | 4.66116 |
| C | 2.41637 | -1.12338 | 3.43526 |
| H | 2.22513 | -0.7098 | 1.34355 |
| H | 4.6236 | 2.04998 | 3.61516 |
| H | 4.16981 | 0.74767 | 5.66782 |
| H | 2.76231 | -1.30094 | 5.55678 |
| H | 1.81147 | -2.02075 | 3.37366 |
| C | 2.98046 | 3.69132 | -0.17466 |
| C | 3.75093 | 4.75188 | 0.32534 |
| C | 4.24229 | 5.73714 | -0.532 |
| C | 3.97008 | 5.6737 | -1.90295 |
| C | 3.19777 | 4.62484 | -2.40599 |
| C | 2.70174 | 3.63937 | -1.54554 |
| H | 3.96142 | 4.80939 | 1.38863 |
| H | 4.83221 | 6.55375 | -0.13236 |
| H | 4.35173 | 6.43813 | -2.56942 |
| H | 2.97473 | 4.57361 | -3.46539 |
| H | 2.08259 | 2.84223 | -1.93794 |
| C | 3.73201 | 1.64533 | 1.11373 |
| C | 2.52542 | 2.59558 | 0.79232 |
| N | 1.46643 | 1.74779 | 0.24516 |
| N | 4.00237 | 0.84613 | -0.12773 |
| H | 2.17068 | 3.05031 | 1.72001 |
| H | 4.58869 | 2.29152 | 1.3449 |
| H | 1.82567 | 0.89853 | -0.19841 |
| C | 0.13375 | 1.95224 | 0.35672 |
| C | -2.98873 | 1.61032 | -0.00151 |
| C | -4.32024 | 1.25771 | -0.21865 |
| C | -4.69646 | 0.03091 | -0.7539 |
| C | -3.66907 | -0.86124 | -1.06463 |
| C | -2.33426 | -0.54675 | -0.85742 |

| | | | |
|---|---|---|---|
| C | -1.96874 | 0.70468 | -0.32234 |
| H | -2.74162 | 2.57877 | 0.40182 |
| H | -5.74667 | -0.23994 | -0.95726 |
| H | -1.56575 | -1.26325 | -1.118 |
| N | -0.59267 | 0.92215 | -0.17921 |
| S | -0.50766 | 3.387 | 1.12622 |
| H | -0.01959 | 0.12804 | -0.51005 |
| F | -5.01143 | -2.16223 | -2.54231 |
| F | -4.52202 | -3.04671 | -0.58486 |
| F | -2.93769 | -2.85501 | -2.12211 |
| F | -4.91533 | 3.51093 | 0.22917 |
| F | -6.47338 | 2.16986 | -0.6419 |
| F | -5.86812 | 1.96064 | 1.47413 |
| C | -4.01877 | -2.20606 | -1.59215 |
| C | -5.37252 | 2.22288 | 0.19298 |
| C | 2.13565 | -1.46794 | -1.46245 |
| C | 3.70458 | -1.26917 | -3.13518 |
| C | 4.05012 | -2.4553 | -2.29137 |
| O | 1.15708 | -1.20644 | -0.7306 |
| C | 2.59266 | -0.70297 | -2.65962 |
| O | 4.99661 | -3.2271 | -2.41461 |
| N | 3.01925 | -2.53511 | -1.28232 |
| H | 2.06005 | 0.15983 | -3.02196 |
| H | 4.08622 | 1.47761 | -0.93081 |
| C | 5.04996 | -0.11252 | -0.06331 |
| C | 6.08466 | -0.24399 | -0.91535 |
| C | 6.40264 | 0.71593 | -2.04627 |
| C | 7.04671 | -1.40556 | -0.76746 |
| H | 4.94096 | -0.8086 | 0.76127 |
| H | 7.40979 | 1.12953 | -1.90131 |
| H | 6.40329 | 0.199 | -3.01383 |

| | | | |
|---|---|---|---|
| H | 5.70201 | 1.55357 | -2.10932 |
| H | 6.90917 | -2.11693 | -1.59356 |
| H | 8.08584 | -1.05392 | -0.7903 |
| H | 6.87888 | -1.9453 | 0.1708 |
| H | 4.30405 | -0.98213 | -3.98179 |
| O | -8.51131 | -1.2693 | 0.75221 |
| H | -7.8028 | -1.01668 | 1.49815 |
| H | -8.94452 | -0.39389 | 0.43148 |
| O | -7.35081 | -0.95519 | -1.37566 |
| H | -7.1787 | -1.66283 | -2.04474 |
| H | -7.78152 | -1.33976 | -0.42688 |
| O | -6.69062 | -0.61651 | 2.40434 |
| H | -5.89299 | -1.27246 | 2.30412 |
| H | -6.37364 | 0.28023 | 2.12406 |
| O | -4.69868 | -2.22098 | 2.06911 |
| H | -3.82757 | -1.8224 | 2.32266 |
| H | -4.6195 | -2.52648 | 1.12505 |
| O | -9.03614 | 0.83146 | -0.72792 |
| H | -8.43947 | 0.19942 | -1.29369 |
| H | -8.39111 | 1.52375 | -0.42 |
| C | 2.93355 | -3.53836 | -0.25891 |
| C | 1.71444 | -3.78673 | 0.39526 |
| C | 4.06623 | -4.29057 | 0.09475 |
| C | 1.63989 | -4.76283 | 1.38917 |
| H | 0.84225 | -3.20779 | 0.14181 |
| C | 3.97533 | -5.26569 | 1.08806 |
| H | 4.99743 | -4.13083 | -0.42228 |
| C | 2.76682 | -5.50734 | 1.7436 |
| H | 0.6915 | -4.94036 | 1.88247 |
| H | 4.85919 | -5.83677 | 1.34668 |
| H | 2.70323 | -6.26435 | 2.51573 |

**TS(Cabon tetrachloride) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=ccl4

E(RB3LYP) = -3160.9648 Hartree

RMS Gradient Norm = 3.97e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9648 Hartree

Zero-point Energy Correction = 0.759043 Hartree

Thermal Correction to Energy = 0.814809 Hartree

Thermal Correction to Enthalpy = 0.815753 Hartree

Thermal Correction to Free Energy = 0.66209 Hartree

EE + Zero-point Energy = -3160.2057 Hartree

EE + Thermal Energy Correction = -3160.15 Hartree

EE + Thermal Enthalpy Correction = -3160.149 Hartree

EE + Thermal Free Energy Correction = -3160.3027 Hartree

E (Thermal) = 511.3 kcal/mol

Heat Capacity (Cv) = 209.11 cal/mol-kelvin

Entropy (S) = 323.411 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.62899 | -0.40703 | 2.27324 |
| C | 3.39931 | 0.76144 | 2.357 |
| C | 3.9051 | 1.14994 | 3.60581 |
| C | 3.64545 | 0.39404 | 4.74997 |

| | | | |
|---|---|---|---|
| C | 2.88526 | -0.77381 | 4.65644 |
| C | 2.38259 | -1.17172 | 3.41565 |
| H | 2.21884 | -0.73266 | 1.328 |
| H | 4.51082 | 2.04732 | 3.68116 |
| H | 4.0432 | 0.71061 | 5.70709 |
| H | 2.69091 | -1.36992 | 5.54031 |
| H | 1.80434 | -2.08418 | 3.32892 |
| C | 2.96528 | 3.67871 | -0.16294 |
| C | 3.75152 | 4.72695 | 0.33669 |
| C | 4.27114 | 5.69599 | -0.52136 |
| C | 4.01135 | 5.62959 | -1.89392 |
| C | 3.22002 | 4.59594 | -2.39715 |
| C | 2.69696 | 3.62682 | -1.53516 |
| H | 3.9462 | 4.79127 | 1.40267 |
| H | 4.87039 | 6.50529 | -0.12079 |
| H | 4.4125 | 6.38356 | -2.56077 |
| H | 2.99808 | 4.54942 | -3.45717 |
| H | 2.05211 | 2.84725 | -1.92137 |
| C | 3.6876 | 1.6517 | 1.15751 |
| C | 2.48421 | 2.59228 | 0.80288 |
| N | 1.43896 | 1.74137 | 0.23913 |
| N | 4.01321 | 0.87241 | -0.08566 |
| H | 2.10358 | 3.05602 | 1.71636 |
| H | 4.53086 | 2.30529 | 1.41729 |
| H | 1.79638 | 0.88124 | -0.17904 |
| C | 0.09994 | 1.9449 | 0.35211 |
| C | -3.01069 | 1.5934 | -0.05488 |
| C | -4.34014 | 1.23171 | -0.27018 |
| C | -4.71453 | -0.01644 | -0.75751 |
| C | -3.68377 | -0.91817 | -1.0276 |
| C | -2.3497 | -0.59575 | -0.8211 |

| | | | |
|---|---|---|---|
| C | -1.9871 | 0.67466 | -0.3306 |
| H | -2.76446 | 2.57741 | 0.31146 |
| H | -5.76641 | -0.30202 | -0.95871 |
| H | -1.57916 | -1.3203 | -1.05323 |
| N | -0.61428 | 0.90031 | -0.18676 |
| S | -0.54896 | 3.36672 | 1.10665 |
| H | -0.03472 | 0.10907 | -0.50515 |
| F | -5.01078 | -2.29108 | -2.45734 |
| F | -4.52918 | -3.08194 | -0.45608 |
| F | -2.93641 | -2.95199 | -1.992 |
| F | -4.94154 | 3.50602 | 0.03698 |
| F | -6.49996 | 2.10587 | -0.73534 |
| F | -5.87925 | 2.03539 | 1.3857 |
| C | -4.02772 | -2.28464 | -1.50149 |
| C | -5.39513 | 2.21844 | 0.08522 |
| C | 2.20269 | -1.42773 | -1.46139 |
| C | 3.84584 | -1.1267 | -3.04567 |
| C | 4.16853 | -2.3485 | -2.24775 |
| O | 1.18026 | -1.21032 | -0.7739 |
| C | 2.70398 | -0.59924 | -2.59588 |
| O | 5.12659 | -3.10486 | -2.37732 |
| N | 3.09323 | -2.489 | -1.28897 |
| H | 2.17251 | 0.27091 | -2.94255 |
| H | 4.10984 | 1.51858 | -0.87526 |
| C | 5.06438 | -0.07443 | -0.00375 |
| C | 6.12416 | -0.18668 | -0.83006 |
| C | 6.47444 | 0.80191 | -1.92658 |
| C | 7.09575 | -1.33612 | -0.6636 |
| H | 4.94287 | -0.77801 | 0.81262 |
| H | 7.45267 | 1.25226 | -1.71027 |
| H | 6.56123 | 0.30075 | -2.89863 |

| | | | |
|---|---|---|---|
| H | 5.74794 | 1.61419 | -2.02367 |
| H | 6.98559 | -2.04755 | -1.49416 |
| H | 8.13069 | -0.97208 | -0.66025 |
| H | 6.91263 | -1.87996 | 0.26919 |
| H | 4.47961 | -0.79478 | -3.84965 |
| O | -8.5656 | -1.25223 | 0.76528 |
| H | -7.89179 | -0.96177 | 1.525 |
| H | -9.026 | -0.40344 | 0.40779 |
| O | -7.33277 | -1.02204 | -1.3139 |
| H | -7.22638 | -1.74373 | -1.98196 |
| H | -7.82535 | -1.36514 | -0.34815 |
| O | -6.77828 | -0.48288 | 2.40137 |
| H | -5.94884 | -1.09168 | 2.33429 |
| H | -6.4962 | 0.42412 | 2.11888 |
| O | -4.63673 | -1.91021 | 2.06908 |
| H | -3.81641 | -1.35657 | 2.11674 |
| H | -4.62983 | -2.36882 | 1.18601 |
| O | -9.07444 | 0.7693 | -0.79596 |
| H | -8.44231 | 0.13074 | -1.3136 |
| H | -8.46825 | 1.50703 | -0.51736 |
| C | 2.97794 | -3.544 | -0.31794 |
| C | 1.75623 | -3.78488 | 0.33386 |
| C | 4.08471 | -4.35484 | -0.01684 |
| C | 1.6544 | -4.81086 | 1.27279 |
| H | 0.90435 | -3.16294 | 0.1186 |
| C | 3.96613 | -5.37753 | 0.92326 |
| H | 5.0156 | -4.20172 | -0.53589 |
| C | 2.7557 | -5.61235 | 1.57605 |
| H | 0.7033 | -4.98321 | 1.76301 |
| H | 4.83081 | -5.99334 | 1.14073 |
| H | 2.67083 | -6.40829 | 2.3058 |

**TS(Dichloromethane) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=dichloromethane

E(RB3LYP) = -3160.9699 Hartree

RMS Gradient Norm = 1.382e-06 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9699 Hartree

Zero-point Energy Correction = 0.758 Hartree

Thermal Correction to Energy = 0.814663 Hartree

Thermal Correction to Enthalpy = 0.815607 Hartree

Thermal Correction to Free Energy = 0.659533 Hartree

EE + Zero-point Energy = -3160.2119 Hartree

EE + Thermal Energy Correction = -3160.1552 Hartree

EE + Thermal Enthalpy Correction = -3160.1543 Hartree

EE + Thermal Free Energy Correction = -3160.3104 Hartree

E (Thermal) = 511.209 kcal/mol

Heat Capacity (Cv) = 211.428 cal/mol-kelvin

Entropy (S) = 328.485 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | -3.12235 | 0.21549 | 2.56868 |
| C | -4.02673 | -0.82673 | 2.31271 |
| C | -4.60018 | -1.50913 | 3.39487 |
| C | -4.27491 | -1.1673 | 4.70921 |

| | | | |
|---|---|---|---|
| C | -3.37397 | -0.12898 | 4.95721 |
| C | -2.8028 | 0.56073 | 3.88409 |
| H | -2.67236 | 0.76188 | 1.75032 |
| H | -5.30744 | -2.31035 | 3.20642 |
| H | -4.7276 | -1.70505 | 5.53406 |
| H | -3.12259 | 0.14308 | 5.97568 |
| H | -2.10593 | 1.36986 | 4.07098 |
| C | -3.77053 | -2.92878 | -0.93502 |
| C | -4.66991 | -3.99435 | -0.78125 |
| C | -5.2214 | -4.62367 | -1.89774 |
| C | -4.8812 | -4.19385 | -3.18485 |
| C | -3.98129 | -3.13863 | -3.34514 |
| C | -3.42556 | -2.51035 | -2.22565 |
| H | -4.93211 | -4.33763 | 0.21454 |
| H | -5.91026 | -5.44985 | -1.76526 |
| H | -5.30858 | -4.6826 | -4.05242 |
| H | -3.70443 | -2.80716 | -4.33929 |
| H | -2.7066 | -1.71061 | -2.35497 |
| C | -4.37044 | -1.28988 | 0.90291 |
| C | -3.24445 | -2.22152 | 0.31593 |
| N | -2.09645 | -1.35794 | 0.04527 |
| N | -4.51826 | -0.16641 | -0.05544 |
| H | -2.96162 | -2.96288 | 1.06669 |
| H | -5.28458 | -1.897 | 0.95582 |
| H | -2.35857 | -0.38301 | -0.14777 |
| C | -0.79194 | -1.71608 | 0.10493 |
| C | 2.3812 | -1.5075 | -0.24879 |
| C | 3.71768 | -1.16206 | -0.45638 |
| C | 4.1499 | 0.14589 | -0.65379 |
| C | 3.17478 | 1.14306 | -0.58795 |
| C | 1.84354 | 0.83809 | -0.37144 |

| | | | |
|---|---|---|---|
| C | 1.41474 | -0.49477 | -0.22375 |
| H | 2.09231 | -2.53722 | -0.11088 |
| H | 5.2079 | 0.41528 | -0.82924 |
| H | 1.10767 | 1.62582 | -0.31957 |
| N | 0.03343 | -0.63892 | -0.07701 |
| S | -0.27942 | -3.35754 | 0.39772 |
| H | -0.45475 | 0.26686 | -0.12749 |
| F | 4.24934 | 2.85176 | -1.86085 |
| F | 4.41647 | 2.962 | 0.33312 |
| F | 2.47503 | 3.41596 | -0.65008 |
| F | 4.22439 | -3.48673 | -0.41781 |
| F | 5.68166 | -2.10926 | -1.40802 |
| F | 5.50906 | -2.13704 | 0.78522 |
| C | 3.56842 | 2.57205 | -0.71524 |
| C | 4.74367 | -2.22844 | -0.38107 |
| C | -2.69432 | 3.05603 | -0.80583 |
| C | -3.57889 | 4.74432 | -2.10961 |
| C | -3.70529 | 5.11578 | -0.64742 |
| O | -2.14563 | 1.98901 | -0.47246 |
| C | -2.99208 | 3.54684 | -2.20216 |
| O | -4.18438 | 6.1251 | -0.13874 |
| N | -3.14029 | 4.02955 | 0.05704 |
| H | -2.74076 | 2.97699 | -3.08289 |
| H | -4.60743 | -0.50018 | -1.01726 |
| C | -5.29007 | 0.96571 | 0.26363 |
| C | -5.86311 | 1.82904 | -0.60342 |
| C | -5.8576 | 1.65587 | -2.11183 |
| C | -6.57166 | 3.07796 | -0.10665 |
| H | -5.35158 | 1.15968 | 1.32926 |
| H | -6.88742 | 1.65656 | -2.49266 |
| H | -5.33435 | 2.4926 | -2.5953 |

| | | | |
|---|---|---|---|
| H | -5.37995 | 0.72699 | -2.43839 |
| H | -6.07319 | 3.97834 | -0.49305 |
| H | -7.61151 | 3.09694 | -0.45989 |
| H | -6.57817 | 3.12617 | 0.98768 |
| H | -3.92609 | 5.389 | -2.89947 |
| O | 8.72487 | 0.10311 | 0.29816 |
| H | 8.09545 | 0.21061 | 1.08855 |
| H | 8.66536 | -0.87553 | 0.00876 |
| O | 6.74511 | 1.39203 | -0.74666 |
| H | 6.46086 | 1.44625 | 0.21388 |
| H | 7.63602 | 0.8738 | -0.59196 |
| O | 6.56881 | 0.4029 | 1.81589 |
| H | 5.9401 | 0.98249 | 2.39804 |
| H | 6.08277 | -0.41947 | 1.55287 |
| O | 4.8144 | 1.92497 | 2.91552 |
| H | 4.03247 | 1.4398 | 3.28656 |
| H | 4.51147 | 2.36795 | 2.07597 |
| O | 8.38874 | -2.37376 | -0.59497 |
| H | 8.93516 | -2.47994 | -1.4176 |
| H | 7.44151 | -2.33431 | -0.89787 |
| C | -3.05997 | 3.93904 | 1.52205 |
| C | -1.93905 | 4.4316 | 2.19092 |
| C | -4.10438 | 3.36085 | 2.24347 |
| C | -1.86234 | 4.34534 | 3.58085 |
| H | -1.11548 | 4.88668 | 1.62182 |
| C | -4.02824 | 3.27537 | 3.63391 |
| H | -4.98799 | 2.97274 | 1.71647 |
| C | -2.90741 | 3.76736 | 4.30265 |
| H | -0.97857 | 4.73299 | 4.10808 |
| H | -4.85205 | 2.81981 | 4.20249 |
| H | -2.84673 | 3.69951 | 5.39855 |

**TS(DMSO) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=dmso

E(RB3LYP) = -3160.991 Hartree

RMS Gradient Norm = 8.9e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.991 Hartree

Zero-point Energy Correction = 0.757961 Hartree

Thermal Correction to Energy = 0.814018 Hartree

Thermal Correction to Enthalpy = 0.814962 Hartree

Thermal Correction to Free Energy = 0.659777 Hartree

EE + Zero-point Energy = -3160.233 Hartree

EE + Thermal Energy Correction = -3160.177 Hartree

EE + Thermal Enthalpy Correction = -3160.176 Hartree

EE + Thermal Free Energy Correction = -3160.3312 Hartree

E (Thermal) = 510.804 kcal/mol

Heat Capacity (Cv) = 209.505 cal/mol-kelvin

Entropy (S) = 326.615 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.67135 | -0.37866 | 2.27695 |
| C | 3.46932 | 0.7741 | 2.32576 |
| C | 4.01466 | 1.16863 | 3.55649 |
| C | 3.76706 | 0.43327 | 4.71773 |

| | | | |
|---|---|---|---|
| C | 2.97651 | -0.7175 | 4.66011 |
| C | 2.43377 | -1.12065 | 3.43705 |
| H | 2.23258 | -0.70878 | 1.34585 |
| H | 4.64036 | 2.05392 | 3.60405 |
| H | 4.19706 | 0.75284 | 5.65986 |
| H | 2.78972 | -1.29634 | 5.5571 |
| H | 1.82883 | -2.01824 | 3.37907 |
| C | 2.97449 | 3.69365 | -0.1753 |
| C | 3.74276 | 4.75669 | 0.32285 |
| C | 4.2279 | 5.74414 | -0.53556 |
| C | 3.95165 | 5.68036 | -1.90569 |
| C | 3.18164 | 4.62889 | -2.40687 |
| C | 2.69178 | 3.64124 | -1.54537 |
| H | 3.95655 | 4.81432 | 1.38548 |
| H | 4.81623 | 6.56261 | -0.13737 |
| H | 4.32855 | 6.44642 | -2.57299 |
| H | 2.95575 | 4.57715 | -3.46564 |
| H | 2.07471 | 2.84178 | -1.93635 |
| C | 3.73623 | 1.64744 | 1.10737 |
| C | 2.52633 | 2.59581 | 0.79248 |
| N | 1.4668 | 1.74626 | 0.24902 |
| N | 4.00052 | 0.84791 | -0.13505 |
| H | 2.175 | 3.04869 | 1.72237 |
| H | 4.59319 | 2.29492 | 1.33384 |
| H | 1.82661 | 0.89845 | -0.1971 |
| C | 0.1343 | 1.94905 | 0.36347 |
| C | -2.98853 | 1.60667 | 0.00794 |
| C | -4.32 | 1.25505 | -0.21106 |
| C | -4.69608 | 0.02994 | -0.75014 |
| C | -3.66877 | -0.86186 | -1.06217 |
| C | -2.33406 | -0.54838 | -0.85315 |

| | | | |
|---|---|---|---|
| C | -1.9686 | 0.70173 | -0.31487 |
| H | -2.74146 | 2.57398 | 0.41398 |
| H | -5.74605 | -0.23965 | -0.95571 |
| H | -1.5656 | -1.26448 | -1.1149 |
| N | -0.59247 | 0.91882 | -0.17129 |
| S | -0.50681 | 3.38302 | 1.13564 |
| H | -0.01959 | 0.12482 | -0.50294 |
| F | -5.00827 | -2.15597 | -2.54829 |
| F | -4.52801 | -3.04714 | -0.59188 |
| F | -2.93742 | -2.85412 | -2.12264 |
| F | -4.91467 | 3.50705 | 0.24338 |
| F | -6.47205 | 2.16957 | -0.63435 |
| F | -5.86997 | 1.95321 | 1.4819 |
| C | -4.019 | -2.20462 | -1.59457 |
| C | -5.37239 | 2.21924 | 0.20241 |
| C | 2.12938 | -1.47314 | -1.46164 |
| C | 3.68678 | -1.28127 | -3.14594 |
| C | 4.03995 | -2.4621 | -2.29754 |
| O | 1.15576 | -1.20941 | -0.72426 |
| C | 2.57707 | -0.71421 | -2.66633 |
| O | 4.98727 | -3.23265 | -2.42184 |
| N | 3.01587 | -2.53797 | -1.28168 |
| H | 2.04071 | 0.14573 | -3.02994 |
| H | 4.07897 | 1.4788 | -0.93913 |
| C | 5.05025 | -0.10902 | -0.07585 |
| C | 6.07951 | -0.24033 | -0.93432 |
| C | 6.38763 | 0.71708 | -2.07009 |
| C | 7.04461 | -1.39999 | -0.79066 |
| H | 4.94762 | -0.8039 | 0.75057 |
| H | 7.39575 | 1.13154 | -1.93466 |
| H | 6.38027 | 0.19773 | -3.03634 |

| | | | |
|---|---|---|---|
| H | 5.68601 | 1.55416 | -2.12947 |
| H | 6.90336 | -2.11292 | -1.61476 |
| H | 8.08295 | -1.04647 | -0.8205 |
| H | 6.88369 | -1.93856 | 0.14951 |
| H | 4.28026 | -0.99785 | -3.99799 |
| O | -8.51281 | -1.27177 | 0.74587 |
| H | -7.80544 | -1.02146 | 1.49376 |
| H | -8.94449 | -0.39523 | 0.42631 |
| O | -7.35031 | -0.95341 | -1.38066 |
| H | -7.17521 | -1.65984 | -2.05025 |
| H | -7.78111 | -1.33993 | -0.43331 |
| O | -6.69571 | -0.62582 | 2.40492 |
| H | -5.89954 | -1.28355 | 2.303 |
| H | -6.37642 | 0.27084 | 2.12687 |
| O | -4.70941 | -2.23597 | 2.06596 |
| H | -3.83725 | -1.84163 | 2.32265 |
| H | -4.62983 | -2.53607 | 1.12017 |
| O | -9.03486 | 0.83282 | -0.73073 |
| H | -8.43811 | 0.20148 | -1.2972 |
| H | -8.38917 | 1.52305 | -0.41958 |
| C | 2.93847 | -3.53535 | -0.25209 |
| C | 1.72243 | -3.78625 | 0.40675 |
| C | 4.07623 | -4.27906 | 0.10315 |
| C | 1.65585 | -4.75644 | 1.40702 |
| H | 0.84636 | -3.21365 | 0.15208 |
| C | 3.99336 | -5.24841 | 1.10282 |
| H | 5.00522 | -4.11738 | -0.41731 |
| C | 2.78787 | -5.49249 | 1.76308 |
| H | 0.70977 | -4.93605 | 1.90397 |
| H | 4.881 | -5.81299 | 1.36273 |
| H | 2.73048 | -6.24494 | 2.54015 |

**TS(EtOH) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=ethanol

E(RB3LYP) = -3160.9892 Hartree

RMS Gradient Norm = 9.13e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9892 Hartree

Zero-point Energy Correction = 0.758137 Hartree

Thermal Correction to Energy = 0.814152 Hartree

Thermal Correction to Enthalpy = 0.815096 Hartree

Thermal Correction to Free Energy = 0.660088 Hartree

EE + Zero-point Energy = -3160.2311 Hartree

EE + Thermal Energy Correction = -3160.175 Hartree

EE + Thermal Enthalpy Correction = -3160.1741 Hartree

EE + Thermal Free Energy Correction = -3160.3291 Hartree

E (Thermal) = 510.888 kcal/mol

Heat Capacity (Cv) = 209.442 cal/mol-kelvin

Entropy (S) = 326.241 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.65968 | -0.38054 | 2.27692 |
| C | 3.45798 | 0.77176 | 2.33033 |
| C | 3.99762 | 1.1651 | 3.56394 |
| C | 3.74416 | 0.42899 | 4.72342 |

| | | | |
|---|---|---|---|
| C | 2.95349 | -0.72143 | 4.66116 |
| C | 2.41637 | -1.12338 | 3.43526 |
| H | 2.22513 | -0.7098 | 1.34355 |
| H | 4.6236 | 2.04998 | 3.61516 |
| H | 4.16981 | 0.74767 | 5.66782 |
| H | 2.76231 | -1.30094 | 5.55678 |
| H | 1.81147 | -2.02075 | 3.37366 |
| C | 2.98046 | 3.69132 | -0.17466 |
| C | 3.75093 | 4.75188 | 0.32534 |
| C | 4.24229 | 5.73714 | -0.532 |
| C | 3.97008 | 5.6737 | -1.90295 |
| C | 3.19777 | 4.62484 | -2.40599 |
| C | 2.70174 | 3.63937 | -1.54554 |
| H | 3.96142 | 4.80939 | 1.38863 |
| H | 4.83221 | 6.55375 | -0.13236 |
| H | 4.35173 | 6.43813 | -2.56942 |
| H | 2.97473 | 4.57361 | -3.46539 |
| H | 2.08259 | 2.84223 | -1.93794 |
| C | 3.73201 | 1.64533 | 1.11373 |
| C | 2.52542 | 2.59558 | 0.79232 |
| N | 1.46643 | 1.74779 | 0.24516 |
| N | 4.00237 | 0.84613 | -0.12773 |
| H | 2.17068 | 3.05031 | 1.72001 |
| H | 4.58869 | 2.29152 | 1.3449 |
| H | 1.82567 | 0.89853 | -0.19841 |
| C | 0.13375 | 1.95224 | 0.35672 |
| C | -2.98873 | 1.61032 | -0.00151 |
| C | -4.32024 | 1.25771 | -0.21865 |
| C | -4.69646 | 0.03091 | -0.7539 |
| C | -3.66907 | -0.86124 | -1.06463 |
| C | -2.33426 | -0.54675 | -0.85742 |

| | | | |
|---|---|---|---|
| C | -1.96874 | 0.70468 | -0.32234 |
| H | -2.74162 | 2.57877 | 0.40182 |
| H | -5.74667 | -0.23994 | -0.95726 |
| H | -1.56575 | -1.26325 | -1.118 |
| N | -0.59267 | 0.92215 | -0.17921 |
| S | -0.50766 | 3.387 | 1.12622 |
| H | -0.01959 | 0.12804 | -0.51005 |
| F | -5.01143 | -2.16223 | -2.54231 |
| F | -4.52202 | -3.04671 | -0.58486 |
| F | -2.93769 | -2.85501 | -2.12211 |
| F | -4.91533 | 3.51093 | 0.22917 |
| F | -6.47338 | 2.16986 | -0.6419 |
| F | -5.86812 | 1.96064 | 1.47413 |
| C | -4.01877 | -2.20606 | -1.59215 |
| C | -5.37252 | 2.22288 | 0.19298 |
| C | 2.13565 | -1.46794 | -1.46245 |
| C | 3.70458 | -1.26917 | -3.13518 |
| C | 4.05012 | -2.4553 | -2.29137 |
| O | 1.15708 | -1.20644 | -0.7306 |
| C | 2.59266 | -0.70297 | -2.65962 |
| O | 4.99661 | -3.2271 | -2.41461 |
| N | 3.01925 | -2.53511 | -1.28232 |
| H | 2.06005 | 0.15983 | -3.02196 |
| H | 4.08622 | 1.47761 | -0.93081 |
| C | 5.04996 | -0.11252 | -0.06331 |
| C | 6.08466 | -0.24399 | -0.91535 |
| C | 6.40264 | 0.71593 | -2.04627 |
| C | 7.04671 | -1.40556 | -0.76746 |
| H | 4.94096 | -0.8086 | 0.76127 |
| H | 7.40979 | 1.12953 | -1.90131 |
| H | 6.40329 | 0.199 | -3.01383 |

| | | | |
|---|---|---|---|
| H | 5.70201 | 1.55357 | -2.10932 |
| H | 6.90917 | -2.11693 | -1.59356 |
| H | 8.08584 | -1.05392 | -0.7903 |
| H | 6.87888 | -1.9453 | 0.1708 |
| H | 4.30405 | -0.98213 | -3.98179 |
| O | -8.51131 | -1.2693 | 0.75221 |
| H | -7.8028 | -1.01668 | 1.49815 |
| H | -8.94452 | -0.39389 | 0.43148 |
| O | -7.35081 | -0.95519 | -1.37566 |
| H | -7.1787 | -1.66283 | -2.04474 |
| H | -7.78152 | -1.33976 | -0.42688 |
| O | -6.69062 | -0.61651 | 2.40434 |
| H | -5.89299 | -1.27246 | 2.30412 |
| H | -6.37364 | 0.28023 | 2.12406 |
| O | -4.69868 | -2.22098 | 2.06911 |
| H | -3.82757 | -1.8224 | 2.32266 |
| H | -4.6195 | -2.52648 | 1.12505 |
| O | -9.03614 | 0.83146 | -0.72792 |
| H | -8.43947 | 0.19942 | -1.29369 |
| H | -8.39111 | 1.52375 | -0.42 |
| C | 2.93355 | -3.53836 | -0.25891 |
| C | 1.71444 | -3.78673 | 0.39526 |
| C | 4.06623 | -4.29057 | 0.09475 |
| C | 1.63989 | -4.76283 | 1.38917 |
| H | 0.84225 | -3.20779 | 0.14181 |
| C | 3.97533 | -5.26569 | 1.08806 |
| H | 4.99743 | -4.13083 | -0.42228 |
| C | 2.76682 | -5.50734 | 1.7436 |
| H | 0.6915 | -4.94036 | 1.88247 |
| H | 4.85919 | -5.83677 | 1.34668 |
| H | 2.70323 | -6.26435 | 2.5157 |

**TS(Formic acid) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=formicacid

E(RB3LYP) = -3160.9911 Hartree

RMS Gradient Norm = 8.77e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9911 Hartree

Zero-point Energy Correction = 0.757932 Hartree

Thermal Correction to Energy = 0.813998 Hartree

Thermal Correction to Enthalpy = 0.814942 Hartree

Thermal Correction to Free Energy = 0.659706 Hartree

EE + Zero-point Energy = -3160.2332 Hartree

EE + Thermal Energy Correction = -3160.1772 Hartree

EE + Thermal Enthalpy Correction = -3160.1762 Hartree

EE + Thermal Free Energy Correction = -3160.3314 Hartree

E (Thermal) = 510.791 kcal/mol

Heat Capacity (Cv) = 209.516 cal/mol-kelvin

Entropy (S) = 326.722 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| C | 2.67135 | -0.37866 | 2.27695 |
| C | 3.46932 | 0.7741 | 2.32576 |
| C | 4.01466 | 1.16863 | 3.55649 |
| C | 3.76706 | 0.43327 | 4.71773 |

| | | | |
|---|---|---|---|
| C | 2.97651 | -0.7175 | 4.66011 |
| C | 2.43377 | -1.12065 | 3.43705 |
| H | 2.23258 | -0.70878 | 1.34585 |
| H | 4.64036 | 2.05392 | 3.60405 |
| H | 4.19706 | 0.75284 | 5.65986 |
| H | 2.78972 | -1.29634 | 5.5571 |
| H | 1.82883 | -2.01824 | 3.37907 |
| C | 2.97449 | 3.69365 | -0.1753 |
| C | 3.74276 | 4.75669 | 0.32285 |
| C | 4.2279 | 5.74414 | -0.53556 |
| C | 3.95165 | 5.68036 | -1.90569 |
| C | 3.18164 | 4.62889 | -2.40687 |
| C | 2.69178 | 3.64124 | -1.54537 |
| H | 3.95655 | 4.81432 | 1.38548 |
| H | 4.81623 | 6.56261 | -0.13737 |
| H | 4.32855 | 6.44642 | -2.57299 |
| H | 2.95575 | 4.57715 | -3.46564 |
| H | 2.07471 | 2.84178 | -1.93635 |
| C | 3.73623 | 1.64744 | 1.10737 |
| C | 2.52633 | 2.59581 | 0.79248 |
| N | 1.4668 | 1.74626 | 0.24902 |
| N | 4.00052 | 0.84791 | -0.13505 |
| H | 2.175 | 3.04869 | 1.72237 |
| H | 4.59319 | 2.29492 | 1.33384 |
| H | 1.82661 | 0.89845 | -0.1971 |
| C | 0.1343 | 1.94905 | 0.36347 |
| C | -2.98853 | 1.60667 | 0.00794 |
| C | -4.32 | 1.25505 | -0.21106 |
| C | -4.69608 | 0.02994 | -0.75014 |
| C | -3.66877 | -0.86186 | -1.06217 |
| C | -2.33406 | -0.54838 | -0.85315 |

| | | | |
|---|---|---|---|
| C | -1.9686 | 0.70173 | -0.31487 |
| H | -2.74146 | 2.57398 | 0.41398 |
| H | -5.74605 | -0.23965 | -0.95571 |
| H | -1.5656 | -1.26448 | -1.1149 |
| N | -0.59247 | 0.91882 | -0.17129 |
| S | -0.50681 | 3.38302 | 1.13564 |
| H | -0.01959 | 0.12482 | -0.50294 |
| F | -5.00827 | -2.15597 | -2.54829 |
| F | -4.52801 | -3.04714 | -0.59188 |
| F | -2.93742 | -2.85412 | -2.12264 |
| F | -4.91467 | 3.50705 | 0.24338 |
| F | -6.47205 | 2.16957 | -0.63435 |
| F | -5.86997 | 1.95321 | 1.4819 |
| C | -4.019 | -2.20462 | -1.59457 |
| C | -5.37239 | 2.21924 | 0.20241 |
| C | 2.12938 | -1.47314 | -1.46164 |
| C | 3.68678 | -1.28127 | -3.14594 |
| C | 4.03995 | -2.4621 | -2.29754 |
| O | 1.15576 | -1.20941 | -0.72426 |
| C | 2.57707 | -0.71421 | -2.66633 |
| O | 4.98727 | -3.23265 | -2.42184 |
| N | 3.01587 | -2.53797 | -1.28168 |
| H | 2.04071 | 0.14573 | -3.02994 |
| H | 4.07897 | 1.4788 | -0.93913 |
| C | 5.05025 | -0.10902 | -0.07585 |
| C | 6.07951 | -0.24033 | -0.93432 |
| C | 6.38763 | 0.71708 | -2.07009 |
| C | 7.04461 | -1.39999 | -0.79066 |
| H | 4.94762 | -0.8039 | 0.75057 |
| H | 7.39575 | 1.13154 | -1.93466 |
| H | 6.38027 | 0.19773 | -3.03634 |

| | | | |
|---|---|---|---|
| H | 5.68601 | 1.55416 | -2.12947 |
| H | 6.90336 | -2.11292 | -1.61476 |
| H | 8.08295 | -1.04647 | -0.8205 |
| H | 6.88369 | -1.93856 | 0.14951 |
| H | 4.28026 | -0.99785 | -3.99799 |
| O | -8.51281 | -1.27177 | 0.74587 |
| H | -7.80544 | -1.02146 | 1.49376 |
| H | -8.94449 | -0.39523 | 0.42631 |
| O | -7.35031 | -0.95341 | -1.38066 |
| H | -7.17521 | -1.65984 | -2.05025 |
| H | -7.78111 | -1.33993 | -0.43331 |
| O | -6.69571 | -0.62582 | 2.40492 |
| H | -5.89954 | -1.28355 | 2.303 |
| H | -6.37642 | 0.27084 | 2.12687 |
| O | -4.70941 | -2.23597 | 2.06596 |
| H | -3.83725 | -1.84163 | 2.32265 |
| H | -4.62983 | -2.53607 | 1.12017 |
| O | -9.03486 | 0.83282 | -0.73073 |
| H | -8.43811 | 0.20148 | -1.2972 |
| H | -8.38917 | 1.52305 | -0.41958 |
| C | 2.93847 | -3.53535 | -0.25209 |
| C | 1.72243 | -3.78625 | 0.40675 |
| C | 4.07623 | -4.27906 | 0.10315 |
| C | 1.65585 | -4.75644 | 1.40702 |
| H | 0.84636 | -3.21365 | 0.15208 |
| C | 3.99336 | -5.24841 | 1.10282 |
| H | 5.00522 | -4.11738 | -0.41731 |
| C | 2.78787 | -5.49249 | 1.76308 |
| H | 0.70977 | -4.93605 | 1.90397 |
| H | 4.881 | -5.81299 | 1.36273 |
| H | 2.73048 | -6.24494 | 2.54015 |

**TS(Water) +5$H_2O$**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -3160.9918 Hartree

RMS Gradient Norm = 8.18e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9918 Hartree

Zero-point Energy Correction = 0.757812 Hartree

Thermal Correction to Energy = 0.813916 Hartree

Thermal Correction to Enthalpy = 0.81486 Hartree

Thermal Correction to Free Energy = 0.659441 Hartree

EE + Zero-point Energy = -3160.234 Hartree

EE + Thermal Energy Correction = -3160.1779 Hartree

EE + Thermal Enthalpy Correction = -3160.177 Hartree

EE + Thermal Free Energy Correction = -3160.3324 Hartree

E (Thermal) = 510.74 kcal/mol

Heat Capacity (Cv) = 209.564 cal/mol-kelvin

Entropy (S) = 327.108 cal/mol-kelvin

Symbolic Z-matrix:

| | | | | |
|---|---|---|---|---|
| Charge = | 0 Multiplicity = 1 | | | |
| C | | 2.67135 | -0.37866 | 2.27695 |
| C | | 3.46932 | 0.7741 | 2.32576 |
| C | | 4.01466 | 1.16863 | 3.55649 |
| C | | 3.76706 | 0.43327 | 4.71773 |

| | | | |
|---|---|---|---|
| C | 2.97651 | -0.71749 | 4.66011 |
| C | 2.43376 | -1.12065 | 3.43705 |
| H | 2.23258 | -0.70878 | 1.34584 |
| H | 4.64036 | 2.05392 | 3.60405 |
| H | 4.19706 | 0.75284 | 5.65985 |
| H | 2.78972 | -1.29634 | 5.5571 |
| H | 1.82883 | -2.01824 | 3.37907 |
| C | 2.97449 | 3.69365 | -0.1753 |
| C | 3.74277 | 4.75668 | 0.32284 |
| C | 4.22791 | 5.74413 | -0.53557 |
| C | 3.95166 | 5.68035 | -1.9057 |
| C | 3.18164 | 4.62889 | -2.40687 |
| C | 2.69178 | 3.64124 | -1.54538 |
| H | 3.95657 | 4.81431 | 1.38547 |
| H | 4.81625 | 6.5626 | -0.13738 |
| H | 4.32856 | 6.44641 | -2.573 |
| H | 2.95575 | 4.57715 | -3.46564 |
| H | 2.07471 | 2.84179 | -1.93635 |
| C | 3.73623 | 1.64744 | 1.10737 |
| C | 2.52633 | 2.59581 | 0.79248 |
| N | 1.4668 | 1.74626 | 0.24901 |
| N | 4.00052 | 0.84791 | -0.13506 |
| H | 2.175 | 3.04869 | 1.72236 |
| H | 4.59319 | 2.29492 | 1.33384 |
| H | 1.82661 | 0.89845 | -0.19711 |
| C | 0.1343 | 1.94905 | 0.36347 |
| C | -2.98852 | 1.60667 | 0.00795 |
| C | -4.32 | 1.25505 | -0.21104 |
| C | -4.69608 | 0.02995 | -0.75013 |
| C | -3.66877 | -0.86185 | -1.06217 |
| C | -2.33406 | -0.54837 | -0.85315 |

| | | | |
|---|---|---|---|
| C | -1.9686 | 0.70173 | -0.31486 |
| H | -2.74146 | 2.57397 | 0.414 |
| H | -5.74605 | -0.23964 | -0.95571 |
| H | -1.5656 | -1.26447 | -1.11491 |
| N | -0.59247 | 0.91882 | -0.17128 |
| S | -0.50681 | 3.38302 | 1.13564 |
| H | -0.01959 | 0.12482 | -0.50294 |
| F | -5.00827 | -2.15595 | -2.5483 |
| F | -4.52801 | -3.04714 | -0.5919 |
| F | -2.93743 | -2.85411 | -2.12265 |
| F | -4.91467 | 3.50705 | 0.24341 |
| F | -6.47204 | 2.16958 | -0.63433 |
| F | -5.86997 | 1.9532 | 1.48192 |
| C | -4.019 | -2.20461 | -1.59459 |
| C | -5.37239 | 2.21924 | 0.20243 |
| C | 2.12938 | -1.47314 | -1.46164 |
| C | 3.68678 | -1.28128 | -3.14593 |
| C | 4.03995 | -2.4621 | -2.29753 |
| O | 1.15575 | -1.20941 | -0.72425 |
| C | 2.57708 | -0.71421 | -2.66633 |
| O | 4.98727 | -3.23266 | -2.42183 |
| N | 3.01586 | -2.53797 | -1.28167 |
| H | 2.04071 | 0.14572 | -3.02994 |
| H | 4.07898 | 1.47879 | -0.93913 |
| C | 5.05025 | -0.10902 | -0.07585 |
| C | 6.07951 | -0.24033 | -0.93432 |
| C | 6.38763 | 0.71708 | -2.07009 |
| C | 7.04461 | -1.4 | -0.79066 |
| H | 4.94762 | -0.80391 | 0.75057 |
| H | 7.39575 | 1.13153 | -1.93467 |
| H | 6.38028 | 0.19772 | -3.03634 |

| | | | |
|---|---|---|---|
| H | 5.68601 | 1.55415 | -2.12948 |
| H | 6.90336 | -2.11293 | -1.61476 |
| H | 8.08295 | -1.04648 | -0.8205 |
| H | 6.88369 | -1.93856 | 0.14951 |
| H | 4.28026 | -0.99785 | -3.99798 |
| O | -8.51282 | -1.27177 | 0.74586 |
| H | -7.80545 | -1.02147 | 1.49375 |
| H | -8.9445 | -0.39523 | 0.4263 |
| O | -7.35031 | -0.95339 | -1.38066 |
| H | -7.17521 | -1.65982 | -2.05026 |
| H | -7.78112 | -1.33992 | -0.43332 |
| O | -6.69572 | -0.62583 | 2.40492 |
| H | -5.89955 | -1.28357 | 2.30299 |
| H | -6.37643 | 0.27083 | 2.12687 |
| O | -4.70943 | -2.23599 | 2.06595 |
| H | -3.83727 | -1.84166 | 2.32264 |
| H | -4.62985 | -2.53607 | 1.12016 |
| O | -9.03486 | 0.83283 | -0.73073 |
| H | -8.4381 | 0.2015 | -1.2972 |
| H | -8.38917 | 1.52306 | -0.41957 |
| C | 2.93846 | -3.53536 | -0.25208 |
| C | 1.72242 | -3.78625 | 0.40676 |
| C | 4.07623 | -4.27906 | 0.10316 |
| C | 1.65584 | -4.75644 | 1.40703 |
| H | 0.84636 | -3.21365 | 0.15208 |
| C | 3.99335 | -5.24841 | 1.10283 |
| H | 5.00522 | -4.11738 | -0.41731 |
| C | 2.78786 | -5.49248 | 1.76309 |
| H | 0.70976 | -4.93605 | 1.90397 |
| H | 4.88099 | -5.81299 | 1.36274 |
| H | 2.73047 | -6.24493 | 2.54016 |

**Figure 7.**

**Isobutyraldehyde(1)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -231.19058 Hartree

RMS Gradient Norm = 1.3092e-05 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -231.19058 Hartree

Zero-point Energy Correction = 0.113758 Hartree

Thermal Correction to Energy = 0.119987 Hartree

Thermal Correction to Enthalpy = 0.120931 Hartree

Thermal Correction to Free Energy = 0.084489 Hartree

EE + Zero-point Energy = -231.07683 Hartree

EE + Thermal Energy Correction = -231.0706 Hartree

EE + Thermal Enthalpy Correction = -231.06965 Hartree

EE + Thermal Free Energy Correction = -231.10609 Hartree

E (Thermal) = 75.293 kcal/mol

Heat Capacity (Cv) = 21.001 cal/mol-kelvin

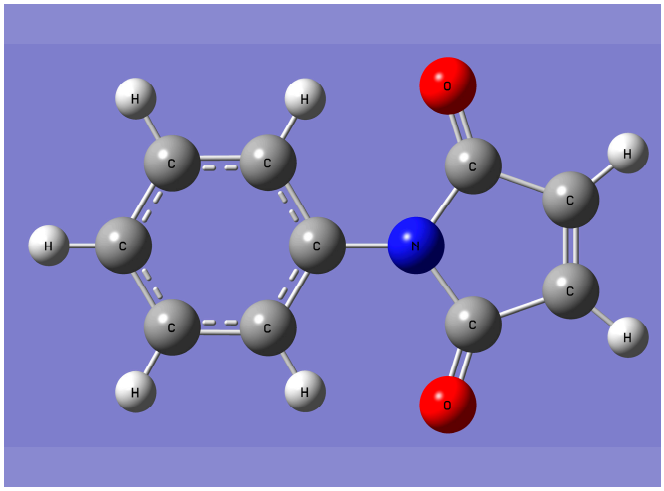
Entropy (S) = 76.699 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| O | -1.8992 | -0.10315 | -0.26595 |
| H | -0.91113 | -1.73269 | 0.47759 |
| C | 0.43632 | 0.01567 | 0.43676 |

| | | | |
|---|---|---|---|
| C | 1.54479 | -0.81135 | -0.26368 |
| H | 0.61992 | -0.02198 | 1.52255 |
| H | 1.40682 | -0.78259 | -1.35008 |
| H | 2.52952 | -0.39606 | -0.02739 |
| H | 1.5247 | -1.85767 | 0.06339 |
| C | -0.90422 | -0.65864 | 0.19693 |
| C | 0.40064 | 1.47363 | -0.04454 |
| H | -0.41764 | 2.01768 | 0.43591 |
| H | 1.34567 | 1.97845 | 0.17845 |
| H | 0.23052 | 1.50422 | -1.12573 |

**_N_-Phenylmaleimide(2)**




Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -587.23576 Hartree

RMS Gradient Norm = 6.6e-08 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -587.23576 Hartree

Zero-point Energy Correction = 0.150857 Hartree

Thermal Correction to Energy = 0.160386 Hartree

Thermal Correction to Enthalpy = 0.16133 Hartree

Thermal Correction to Free Energy = 0.114807 Hartree

EE + Zero-point Energy = -587.08491 Hartree

EE + Thermal Energy Correction = -587.07538 Hartree

EE + Thermal Enthalpy Correction = -587.07443 Hartree

EE + Thermal Free Energy Correction = -587.12095 Hartree

E (Thermal) = 100.644 kcal/mol

Heat Capacity (Cv) = 37.562 cal/mol-kelvin

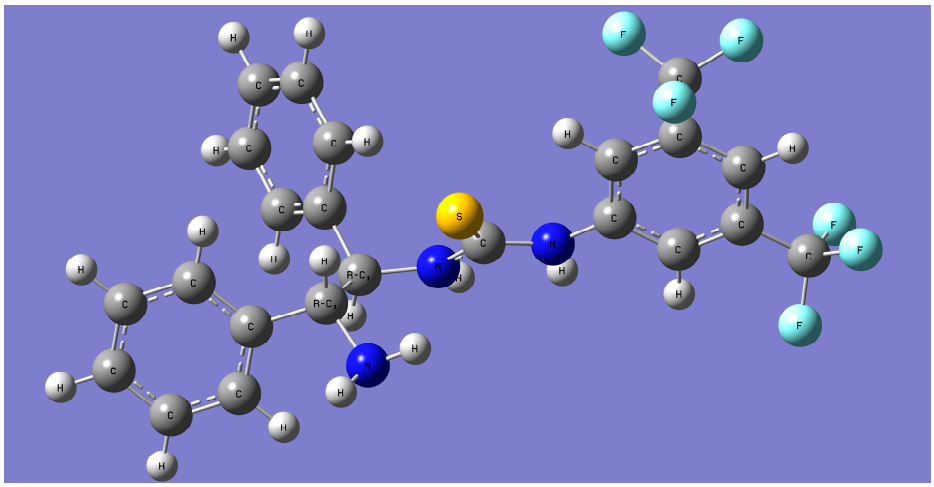
Entropy (S) = 97.917 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.59603 | -1.15994 | -0.01622 |
| C | 3.01362 | -0.66487 | -0.00952 |
| C | 3.01305 | 0.66641 | 0.01062 |
| C | 1.59507 | 1.16022 | 0.01577 |
| H | 3.84643 | -1.34763 | -0.0194 |
| H | 3.84529 | 1.34985 | 0.02159 |
| O | 1.2295 | -2.33409 | -0.02985 |
| O | 1.22711 | 2.33387 | 0.0299 |
| N | 0.7625 | -0.00029 | -0.00113 |
| C | -0.67254 | -0.00045 | -0.00018 |
| C | -1.38986 | -1.21078 | 0.03381 |
| C | -1.38954 | 1.21009 | -0.03432 |
| C | -2.78428 | -1.20165 | 0.03416 |
| H | -0.85001 | -2.14195 | 0.05294 |
| C | -2.78395 | 1.20138 | -0.03373 |
| H | -0.84971 | 2.14123 | -0.05437 |
| C | -3.49376 | -0.00004 | 0.00054 |
| H | -3.31439 | -2.1468 | 0.06073 |
| H | -3.3138 | 2.14668 | -0.06036 |
| H | -4.57709 | 0.00013 | 0.00086 |

**1b Cat. (3)**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2038.4563 Hartree

RMS Gradient Norm = 4.83e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2038.4563 Hartree

Zero-point Energy Correction = 0.389951 Hartree

Thermal Correction to Energy = 0.419074 Hartree

Thermal Correction to Enthalpy = 0.420018 Hartree

Thermal Correction to Free Energy = 0.324348 Hartree

EE + Zero-point Energy = -2038.0664 Hartree

EE + Thermal Energy Correction = -2038.0373 Hartree

EE + Thermal Enthalpy Correction = -2038.0363 Hartree

EE + Thermal Free Energy Correction = -2038.132 Hartree

E (Thermal) = 262.973 kcal/mol

Heat Capacity (Cv) = 110.61 cal/mol-kelvin

Entropy (S) = 201.355 cal/mol-kelvin

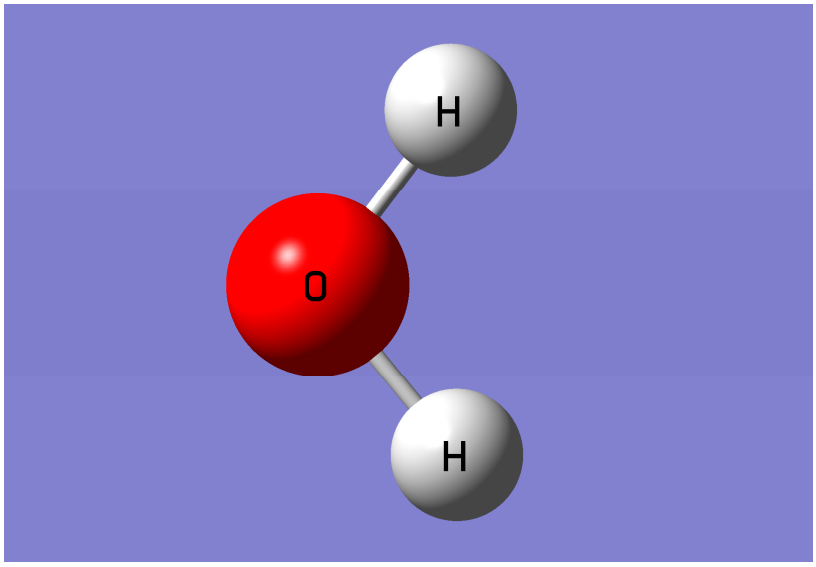
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 5.95702 | -2.0257 | -0.99747 |
| C | 5.31343 | -0.78977 | -1.15311 |
| C | 6.08417 | 0.35455 | -1.3923 |
| C | 7.4772 | 0.26852 | -1.46758 |
| C | 8.11327 | -0.96582 | -1.30522 |
| C | 7.34877 | -2.11364 | -1.07154 |
| H | 5.34877 | -2.90778 | -0.84029 |
| H | 5.59286 | 1.31319 | -1.51709 |
| H | 8.06328 | 1.16099 | -1.65527 |
| H | 9.19349 | -1.03345 | -1.36527 |
| H | 7.83615 | -3.07477 | -0.95197 |
| C | 3.89545 | 0.58264 | 1.1739 |
| C | 4.94237 | 0.48821 | 2.10013 |
| C | 5.41299 | 1.6259 | 2.76155 |
| C | 4.83664 | 2.8724 | 2.50476 |
| C | 3.78736 | 2.97356 | 1.5853 |
| C | 3.31822 | 1.83683 | 0.92364 |
| H | 5.39328 | -0.47753 | 2.30146 |
| H | 6.22394 | 1.53746 | 3.47528 |
| H | 5.19895 | 3.75603 | 3.01732 |
| H | 3.33395 | 3.93758 | 1.38433 |
| H | 2.50024 | 1.91008 | 0.21708 |
| C | 3.79434 | -0.70344 | -1.05643 |
| C | 3.40676 | -0.67122 | 0.45678 |
| N | 1.9588 | -0.92522 | 0.7652 |

| | | | |
|---|---|---|---|
| N | 3.20105 | -1.93013 | -1.64968 |
| H | 3.90898 | -1.5372 | 0.89565 |
| H | 3.45423 | 0.22643 | -1.5242 |
| H | 3.5871 | -2.07576 | -2.59057 |
| H | 1.85504 | -1.45948 | 1.62979 |
| C | 0.82062 | -0.50323 | 0.18225 |
| C | -2.09556 | 0.64191 | 0.19432 |
| C | -3.45486 | 0.89091 | 0.02454 |
| C | -4.42239 | -0.08562 | 0.23553 |
| C | -3.98211 | -1.35313 | 0.6043 |
| C | -2.63084 | -1.6402 | 0.76007 |
| C | -1.66918 | -0.63958 | 0.56089 |
| H | -1.38016 | 1.43301 | 0.04259 |
| H | -5.49698 | 0.11274 | 0.11464 |
| H | -2.32892 | -2.64378 | 1.02737 |
| N | -0.31601 | -0.96901 | 0.80595 |
| H | -0.18708 | -1.68947 | 1.51789 |
| F | -5.87206 | -2.51813 | -0.24276 |
| F | -5.77538 | -2.18874 | 1.9346 |
| F | -4.40485 | -3.65399 | 0.98784 |
| F | -2.95742 | 3.20037 | -0.2284 |
| F | -4.0937 | 2.21453 | -1.85513 |
| F | -5.0932 | 2.6085 | 0.07102 |
| C | -4.99283 | -2.42396 | 0.82923 |
| C | -3.88315 | 2.22416 | -0.46421 |
| S | 0.74853 | 0.4812 | -1.26775 |
| H | 2.18444 | -1.80902 | -1.73222 |

**$H_2O$**




Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -75.981704 Hartree

RMS Gradient Norm = 0.000103805 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -75.981704 Hartree

Zero-point Energy Correction = 0.019862 Hartree

Thermal Correction to Energy = 0.022697 Hartree

Thermal Correction to Enthalpy = 0.023641 Hartree

Thermal Correction to Free Energy = 0.002118 Hartree

EE + Zero-point Energy = -75.961842 Hartree

EE + Thermal Energy Correction = -75.959007 Hartree

EE + Thermal Enthalpy Correction = -75.958063 Hartree

EE + Thermal Free Energy Correction = -75.979586 Hartree

E (Thermal) = 14.243 kcal/mol

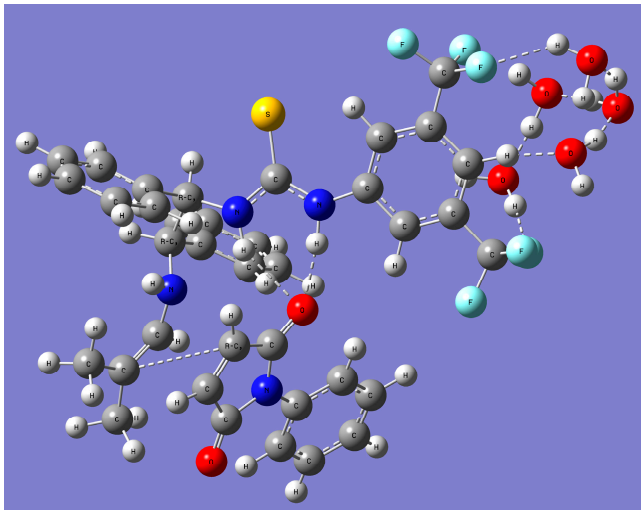
Heat Capacity (Cv) = 5.998 cal/mol-kelvin

Entropy (S) = 45.3 cal/mol-kelvin

Symbolic Z-matrix:

| | | | |
|---|---|---|---|
| Charge = 0 Multiplicity = 1 | | | |
| O | -2.30435 | 1.26087 | 0. |
| H | -1.34435 | 1.26087 | 0. |
| H | -2.6248 | 2.16581 | 0. |

**TS**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -3160.9918 Hartree

RMS Gradient Norm = 8.18e-07 Hartree/Bohr

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3160.9918 Hartree

Zero-point Energy Correction = 0.757812 Hartree

Thermal Correction to Energy = 0.813916 Hartree

Thermal Correction to Enthalpy = 0.81486 Hartree

Thermal Correction to Free Energy = 0.659441 Hartree

EE + Zero-point Energy = -3160.234 Hartree

EE + Thermal Energy Correction = -3160.1779 Hartree

EE + Thermal Enthalpy Correction = -3160.177 Hartree

EE + Thermal Free Energy Correction = -3160.3324 Hartree

E (Thermal) = 510.74 kcal/mol

Heat Capacity (Cv) = 209.564 cal/mol-kelvin

Entropy (S) = 327.108 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 2.67135 | -0.37866 | 2.27695 |
| C | 3.46932 | 0.7741 | 2.32576 |
| C | 4.01466 | 1.16863 | 3.55649 |
| C | 3.76706 | 0.43327 | 4.71773 |
| C | 2.97651 | -0.71749 | 4.66011 |
| C | 2.43376 | -1.12065 | 3.43705 |
| H | 2.23258 | -0.70878 | 1.34584 |
| H | 4.64036 | 2.05392 | 3.60405 |
| H | 4.19706 | 0.75284 | 5.65985 |
| H | 2.78972 | -1.29634 | 5.5571 |
| H | 1.82883 | -2.01824 | 3.37907 |
| C | 2.97449 | 3.69365 | -0.1753 |
| C | 3.74277 | 4.75668 | 0.32284 |
| C | 4.22791 | 5.74413 | -0.53557 |
| C | 3.95166 | 5.68035 | -1.9057 |
| C | 3.18164 | 4.62889 | -2.40687 |
| C | 2.69178 | 3.64124 | -1.54538 |
| H | 3.95657 | 4.81431 | 1.38547 |
| H | 4.81625 | 6.5626 | -0.13738 |
| H | 4.32856 | 6.44641 | -2.573 |
| H | 2.95575 | 4.57715 | -3.46564 |
| H | 2.07471 | 2.84179 | -1.93635 |
| C | 3.73623 | 1.64744 | 1.10737 |
| C | 2.52633 | 2.59581 | 0.79248 |

| | | | |
|---|---|---|---|
| N | 1.4668 | 1.74626 | 0.24901 |
| N | 4.00052 | 0.84791 | -0.13506 |
| H | 2.175 | 3.04869 | 1.72236 |
| H | 4.59319 | 2.29492 | 1.33384 |
| H | 1.82661 | 0.89845 | -0.19711 |
| C | 0.1343 | 1.94905 | 0.36347 |
| C | -2.98852 | 1.60667 | 0.00795 |
| C | -4.32 | 1.25505 | -0.21104 |
| C | -4.69608 | 0.02995 | -0.75013 |
| C | -3.66877 | -0.86185 | -1.06217 |
| C | -2.33406 | -0.54837 | -0.85315 |
| C | -1.9686 | 0.70173 | -0.31486 |
| H | -2.74146 | 2.57397 | 0.414 |
| H | -5.74605 | -0.23964 | -0.95571 |
| H | -1.5656 | -1.26447 | -1.11491 |
| N | -0.59247 | 0.91882 | -0.17128 |
| S | -0.50681 | 3.38302 | 1.13564 |
| H | -0.01959 | 0.12482 | -0.50294 |
| F | -5.00827 | -2.15595 | -2.5483 |
| F | -4.52801 | -3.04714 | -0.5919 |
| F | -2.93743 | -2.85411 | -2.12265 |
| F | -4.91467 | 3.50705 | 0.24341 |
| F | -6.47204 | 2.16958 | -0.63433 |
| F | -5.86997 | 1.9532 | 1.48192 |
| C | -4.019 | -2.20461 | -1.59459 |
| C | -5.37239 | 2.21924 | 0.20243 |
| C | 2.12938 | -1.47314 | -1.46164 |
| C | 3.68678 | -1.28128 | -3.14593 |
| C | 4.03995 | -2.4621 | -2.29753 |
| O | 1.15575 | -1.20941 | -0.72425 |
| C | 2.57708 | -0.71421 | -2.66633 |

| | | | |
|---|---|---|---|
| O | 4.98727 | -3.23266 | -2.42183 |
| N | 3.01586 | -2.53797 | -1.28167 |
| H | 2.04071 | 0.14572 | -3.02994 |
| H | 4.07898 | 1.47879 | -0.93913 |
| C | 5.05025 | -0.10902 | -0.07585 |
| C | 6.07951 | -0.24033 | -0.93432 |
| C | 6.38763 | 0.71708 | -2.07009 |
| C | 7.04461 | -1.4 | -0.79066 |
| H | 4.94762 | -0.80391 | 0.75057 |
| H | 7.39575 | 1.13153 | -1.93467 |
| H | 6.38028 | 0.19772 | -3.03634 |
| H | 5.68601 | 1.55415 | -2.12948 |
| H | 6.90336 | -2.11293 | -1.61476 |
| H | 8.08295 | -1.04648 | -0.8205 |
| H | 6.88369 | -1.93856 | 0.14951 |
| H | 4.28026 | -0.99785 | -3.99798 |
| O | -8.51282 | -1.27177 | 0.74586 |
| H | -7.80545 | -1.02147 | 1.49375 |
| H | -8.9445 | -0.39523 | 0.4263 |
| O | -7.35031 | -0.95339 | -1.38066 |
| H | -7.17521 | -1.65982 | -2.05026 |
| H | -7.78112 | -1.33992 | -0.43332 |
| O | -6.69572 | -0.62583 | 2.40492 |
| H | -5.89955 | -1.28357 | 2.30299 |
| H | -6.37643 | 0.27083 | 2.12687 |
| O | -4.70943 | -2.23599 | 2.06595 |
| H | -3.83727 | -1.84166 | 2.32264 |
| H | -4.62985 | -2.53607 | 1.12016 |
| O | -9.03486 | 0.83283 | -0.73073 |
| H | -8.4381 | 0.2015 | -1.2972 |
| H | -8.38917 | 1.52306 | -0.41957 |

| | | | |
|---|---|---|---|
| C | 2.93846 | -3.53536 | -0.25208 |
| C | 1.72242 | -3.78625 | 0.40676 |
| C | 4.07623 | -4.27906 | 0.10316 |
| C | 1.65584 | -4.75644 | 1.40703 |
| H | 0.84636 | -3.21365 | 0.15208 |
| C | 3.99335 | -5.24841 | 1.10283 |
| H | 5.00522 | -4.11738 | -0.41731 |
| C | 2.78786 | -5.49248 | 1.76309 |
| H | 0.70976 | -4.93605 | 1.90397 |
| H | 4.88099 | -5.81299 | 1.36274 |
| H | 2.73047 | -6.24493 | 2.54016 |

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