Supporting information

Catalytic Regeneration of Metal-Hydrides From Their Corresponding Metal-Alkoxides via The Hydroboration of Carbonates to Obtain Methanol and Diols.

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1. Table 1: Crystallographic data for complexes Th-2, Th-3 and Th-4.

	Th-2	**Th-3**	**Th-4**
Formulae	$C_{39}H_{80}N_6Si_6Th$	$C_{40}H_{82}N_6Si_6Th$	$C_{41}H_{84}N_6Si_6Th \cdot 0.5(C_6H_{14})$
Molecular weight	1033.67	1047.70	1104.81
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P21/c	P21/c	P21/c
Temperature/K	200	200	200
Wavelength	0.71073	0.71073	0.71073
a/Å	21.6196(19)	20.597(11)	20.8858(18)
b/Å	12.2443(10)	12.447(8)	12.2278(11)
c/Å	19.8455(16)	21.000(11)	24.084(2)
α/°	90	90	90
β/°	99.296(3)	98.366(15)	112.951(2)
γ/°	90	90	90
V/ $Å^3$	5184.4(8)	5327(5)	5663.9(9)
Z	4	4	4
Density/gcm^{-1}	1.324	1.306	1.296
Absorption Coefficient	3.046	2.965	2.792
Absorption Correction	Multi-scan	Multi-scan	Multi-scan
F(000)	2120	2152	2284
Total no of reflections	9269	9401	10035
Reflections, *I>2σ(I)*	6797	5819	6030
Max. 2θ/°	25.173	25.308	25.107
Complete to 2θ(%)	99.6	97.0	99.0
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Goof (F^2)	0.971	0.869	0.981
R indices [*I>2σ(I)*]	0.0304	0.0406	0.0482
R Indices (all data)	0.0578	0.0872	0.1136
wR2	0.0500	0.0898	0.0805

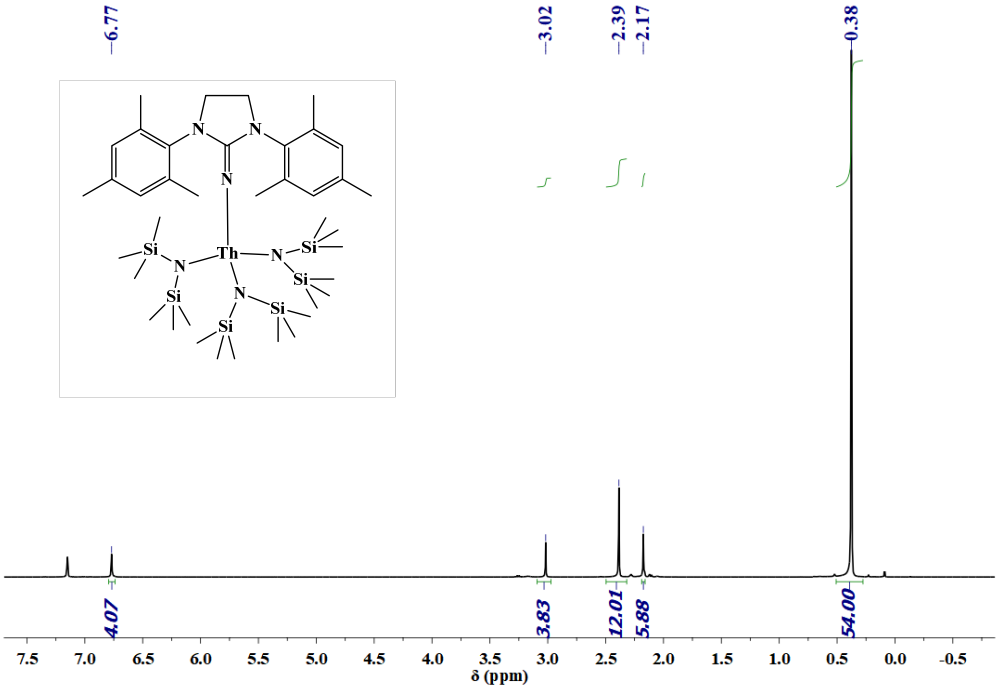


Figure S1. ^{13}C NMR spectrum of **Th-2** in C_6D_6.

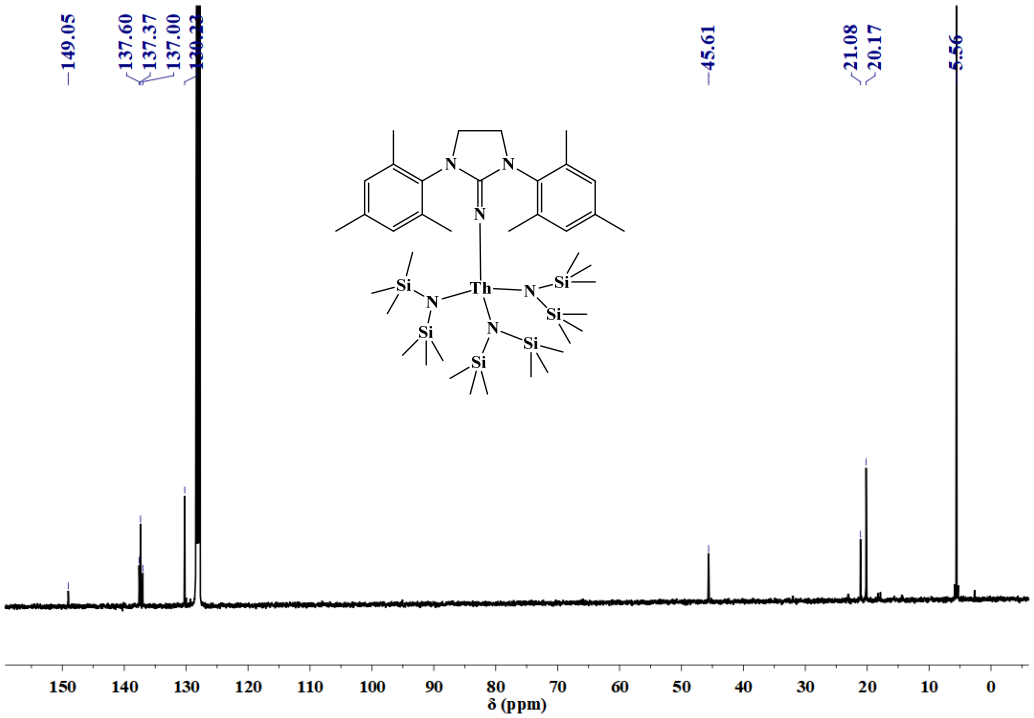


Figure S2. ^{13}C NMR spectrum of **Th-2** in C_6D_6.

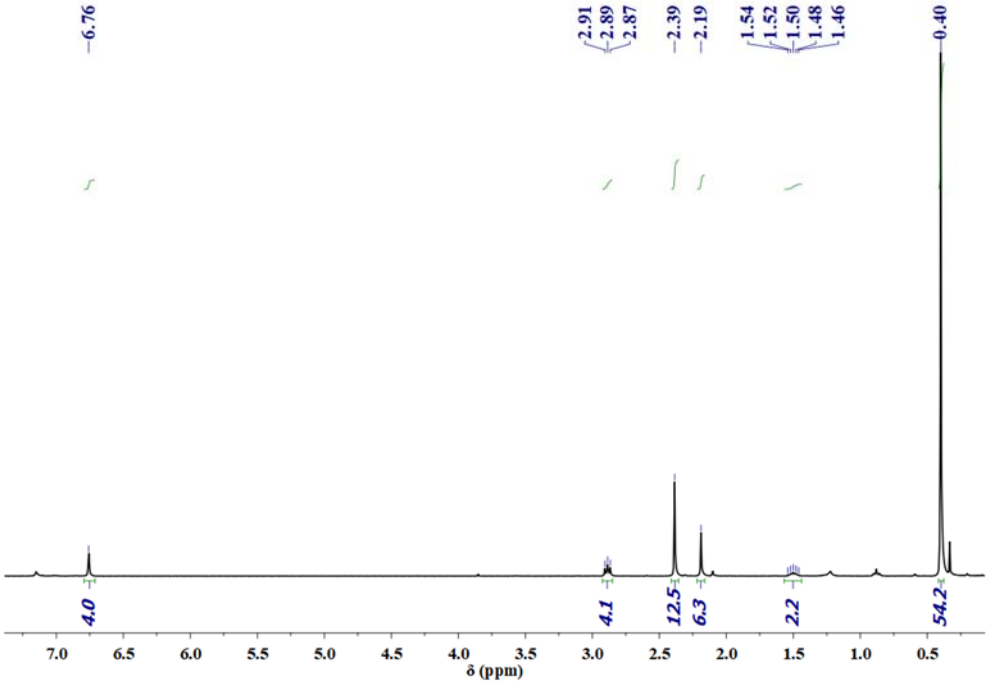


Figure S3. ^{1}H NMR spectrum of **Th-3** in C_6D_6.

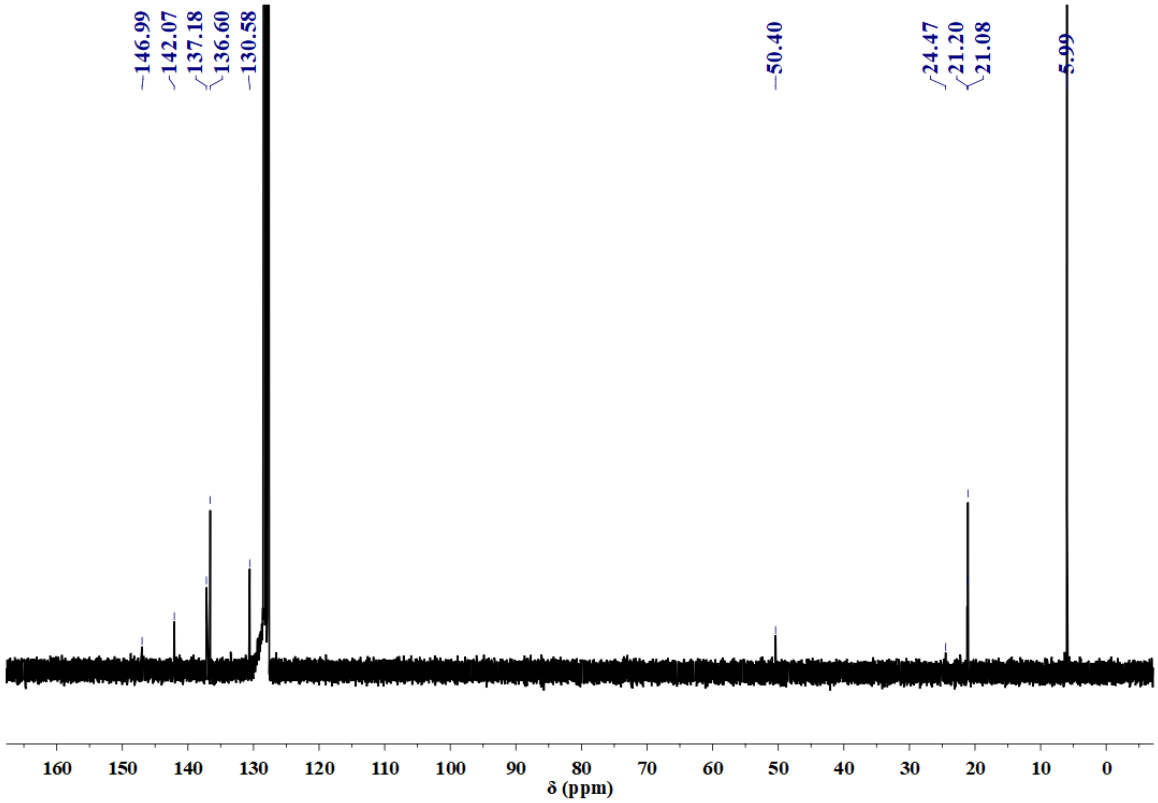


Figure S4. ^{13}C NMR spectrum of **Th-3** in C_6D_6.

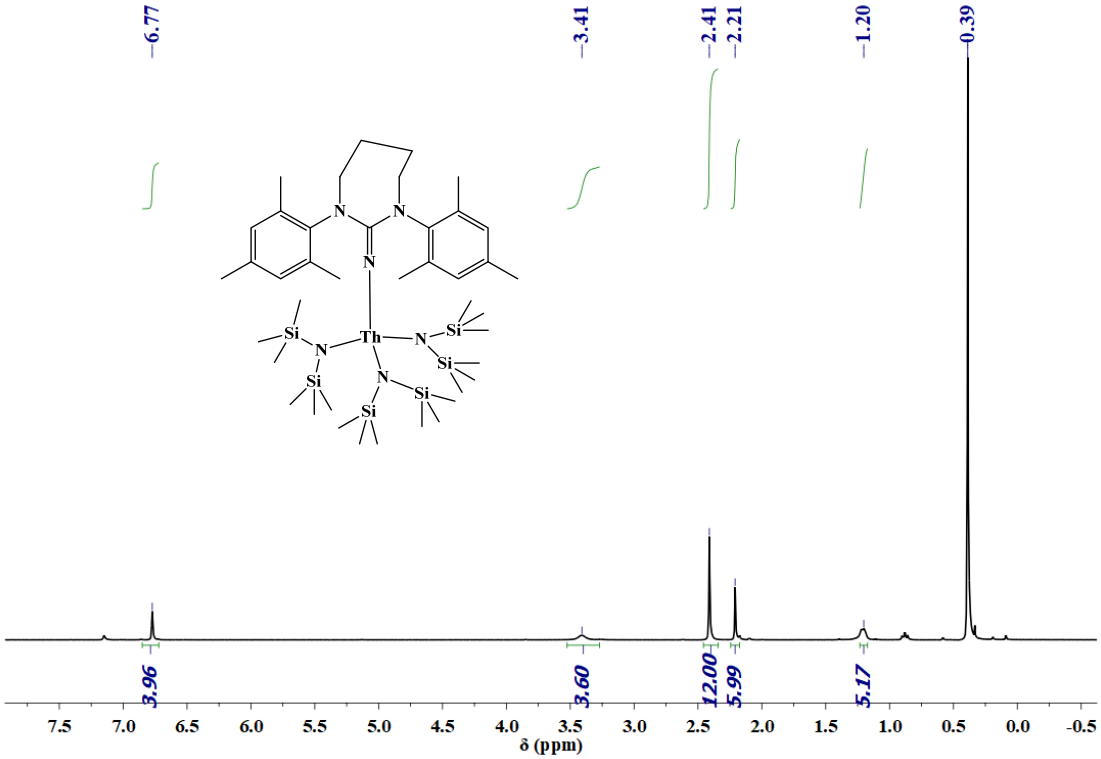


Figure S5. ^{1}H NMR spectrum of **Th-4** in C_6D_6.

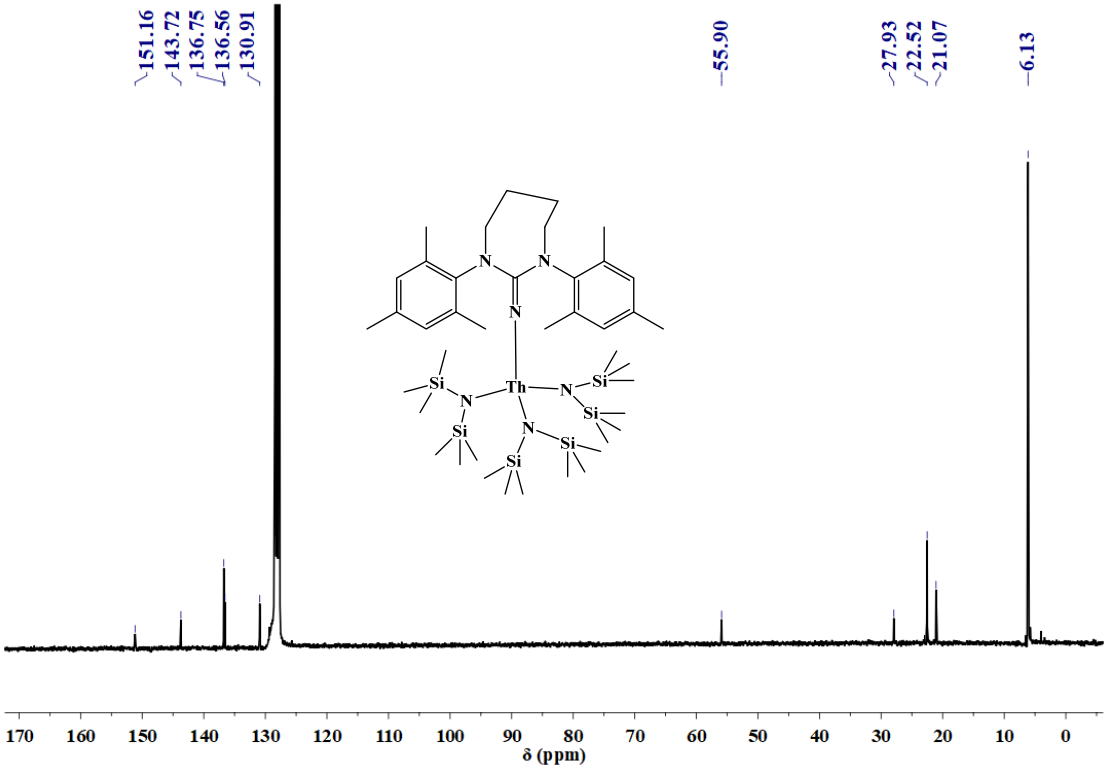


Figure S6. ^{13}C NMR spectrum of **Th-4** in C_6D_6.

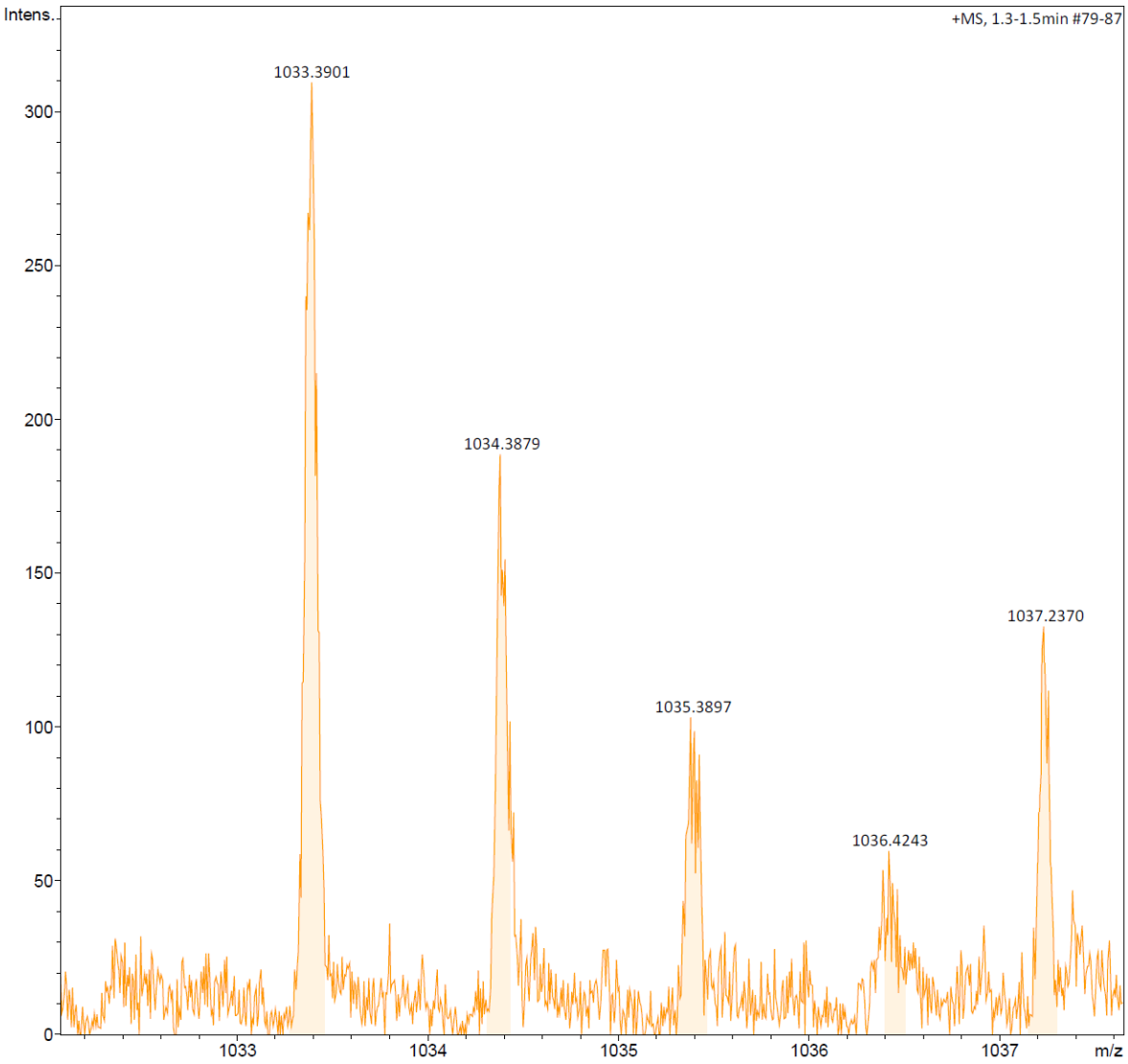


Figure S7. APCI mass spectrum of **Th-2**.

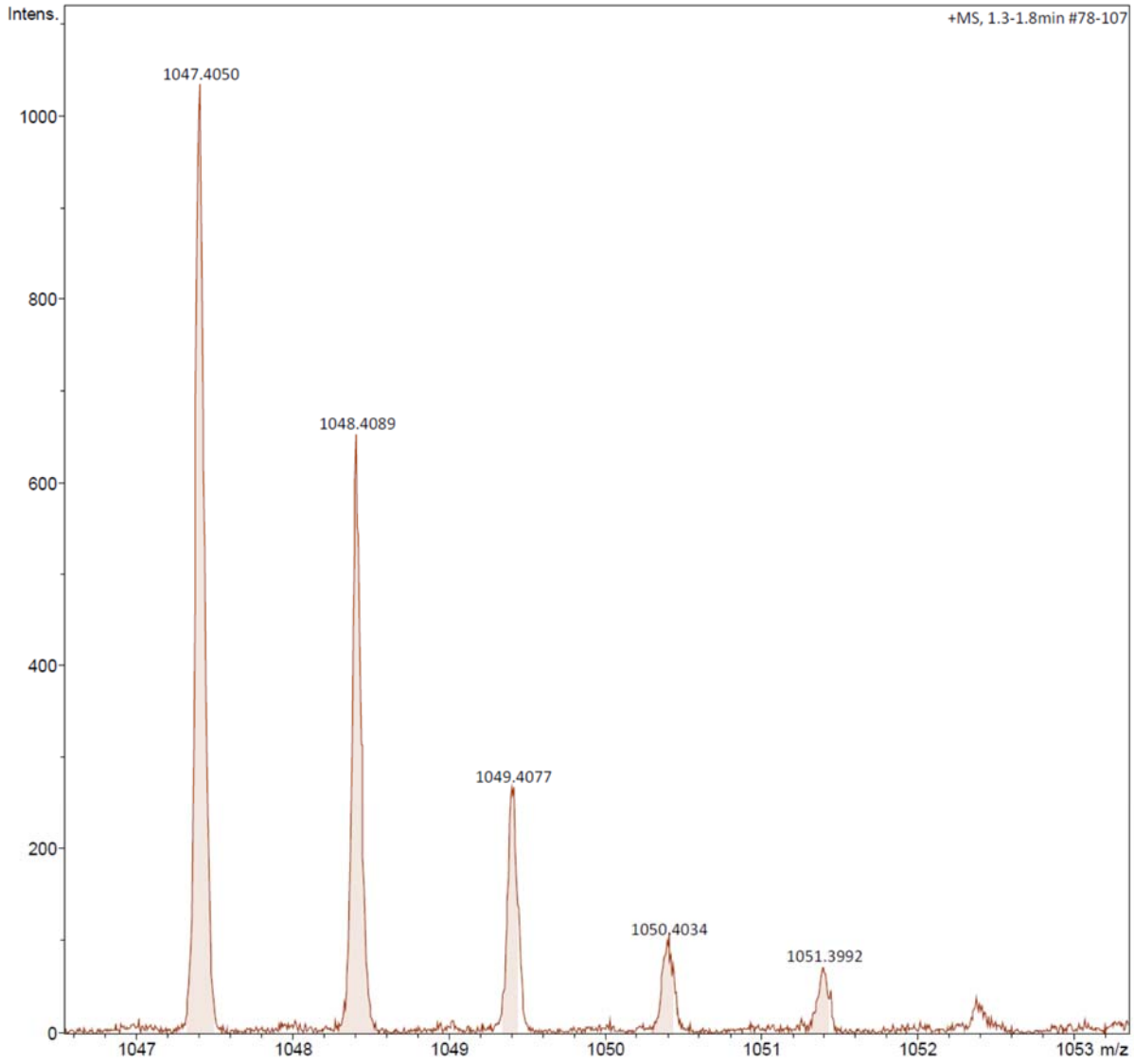


Figure S8. APCI mass spectrum of **Th-3**.

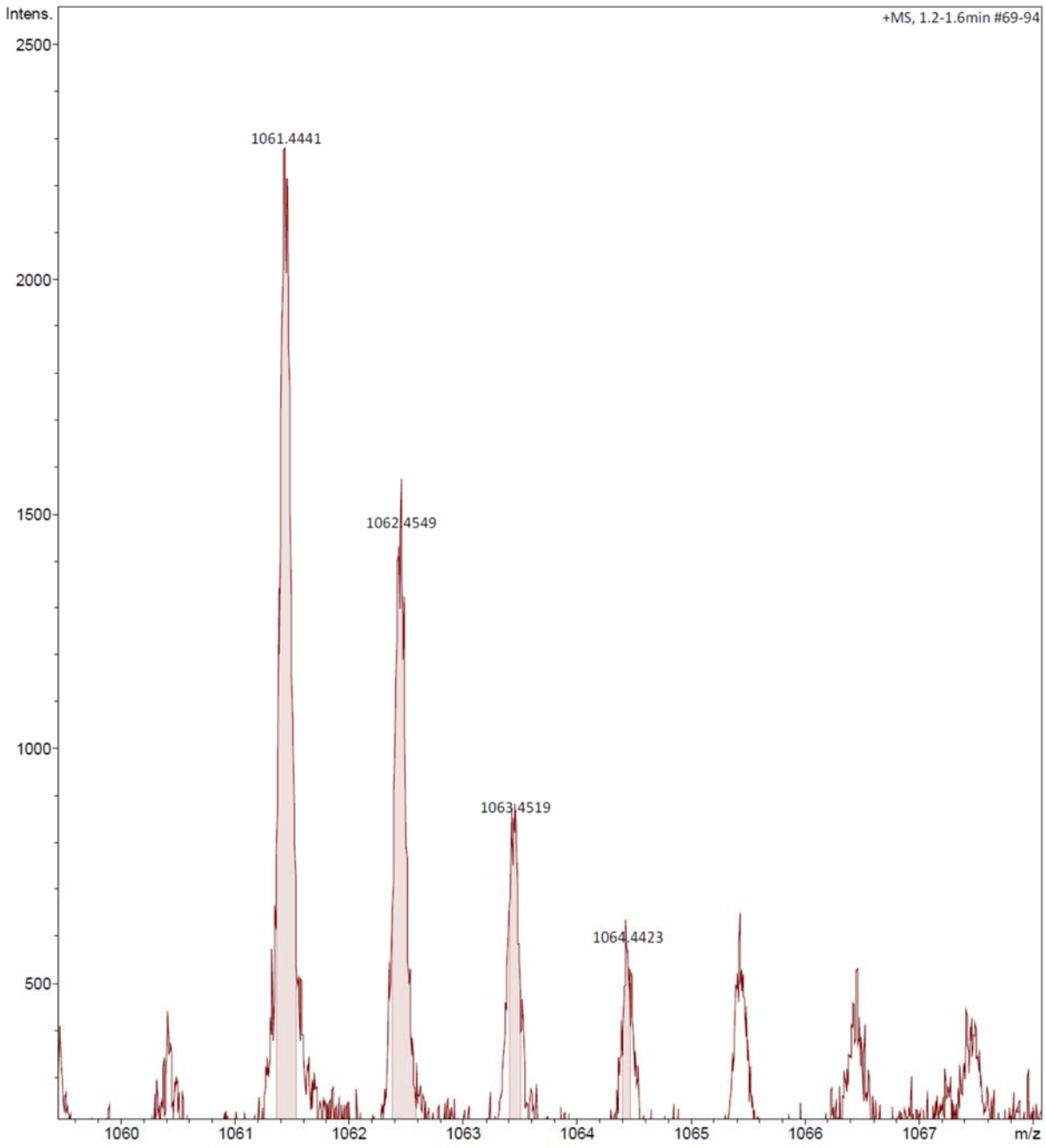
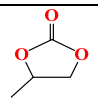
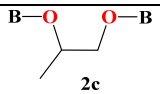
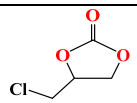
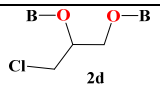
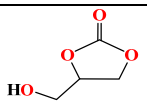
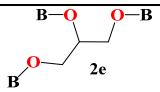
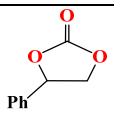
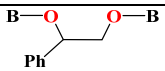
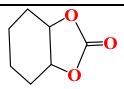
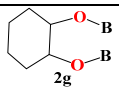
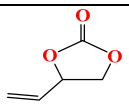
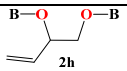
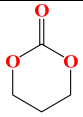
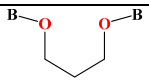
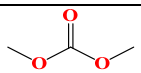
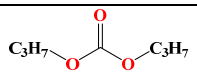
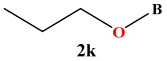
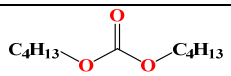
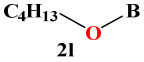
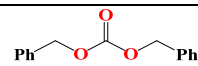
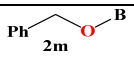
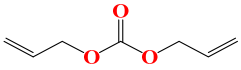
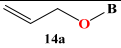
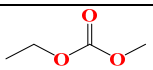
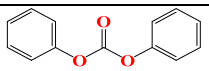
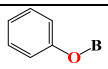
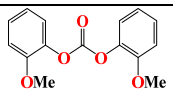
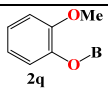
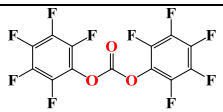
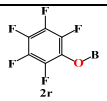
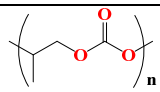
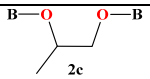
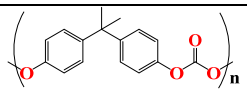
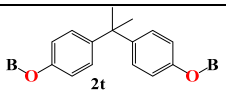


Figure S9. APCI mass spectrum of **Th-4**.

2. Table S2: List of substrates and products.[a]

Entry	Carbonate	Product	Time(h)	Yield[b]
1		 **2c**	1	99
2		 **2d**	1	99
3[b]		 **2e**	1	99
4		 **2f**	1	99
5		 **2g**	1	99
6		 **2h**	1	99
7		 **2i**	1	99
8		 **2j**	1	99
9		 **2k**	5	99
10		 **2l**	5	99
11		 **2m**	12	99
12		 **14a**	12	99
13		 **2a**	1	99
14		 **2p**	24	99
15		 **2q**	24	50
16		 **2r**	24	Trace

17			48	99
18			48	99
19	CO_2		48	76

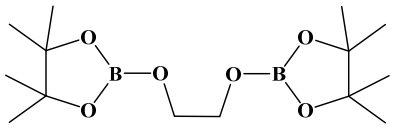
[a]Reaction condition: Carbonate (0.1 mmol), HBpin (0.33 mmol), and precatalyst **Th-4** (0.001 mmol, 1mol%) at 80 °C in C_6D_6 (0.6 mL); yields were determined by ^{1}H NMR spectroscopy of the crude reaction mixture. Corresponding hydroboration products are shown in Table S2. [b]4 mmol of HBpin was used.

3. Typical NMR-scale reaction procedure for the catalytic hydroboration of carbonates.

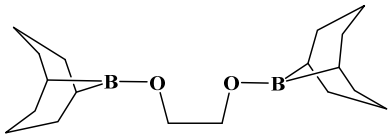
In a typical experiment, into a J. Young Teflon sealed NMR tube was added organic carbonate (0.1 mmol, 1equiv) and HBpin (0.44 mmol, 4.2equiv), followed by adding desired amount of catalyst (0.1-1µmol) in C_6D_6. The reaction was diluted to 550 µL with C_6D_6 and sealed, and placed in an oil bath preheated to 80 °C. The crude reactions mixtures were analyzed using ^{1}H NMR, ^{13}C NMR, ^{11}B NMR the values of known compounds were compared to previous literature. The yield was calculated from the ratio of Carbonate and product from the crude ^{1}H NMR spectra.

4. Spectroscopic data of the carbonate hydroboration products:

4.1 Hydroboration of ethylene carbonate [**1a**]



[**2a**]

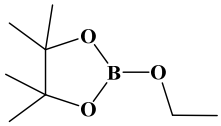


[**4a**]

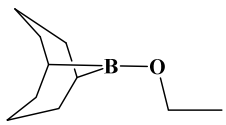
2a) ^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.94 (*s*, 4H), 1.08 (*s*, 24H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.6, 65.5, 24.7. Spectroscopic data agrees with those previously reported.[1]

4a) ^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.90 (*s*, 4H), 1.93-1.79 (*m*, 20H, merges with MeOBBN), 1.42-1.31 (*m*, 8H, merges with MeOBBN). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 66.4, 33.8, 33.6, 33.5, 23.7. Spectroscopic data agree with those previously reported.[1]

4.2 Hydroboration of diethyl carbonate [**1b**]



[**2b**]

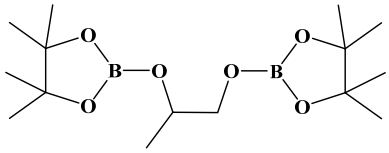


[**4b**]

2a) ^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.89 (*q*, *J* = 8.0 Hz, 2H), 1.10 (*t*, *J* = 8.0 Hz, 3H), 1.05 (*s*, 12H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.4, 60.7, 24.7, 17.5. Spectroscopic data agree with those previously reported.[1]

1b) ^{1}H NMR (300 MHz, C_6D_6): (δ ppm 3.79 (*q*, *J* = 6.8 Hz, 2H), 1.92-1.82 (*m*, 10H, merges with MeOBBN), 1.38-1.34 (*m*, 4H, merges with MeOBBN) 1.09 (*t*, *J* = 6.8 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 61.4, 33.6, 33.5, 24.3, 23.7, 17.9. ^{11}B{^{1}H} NMR (133 MHz, C_6D_6): (δ ppm) 56.4. Spectroscopic data is in agreement with those previously reported.[1]

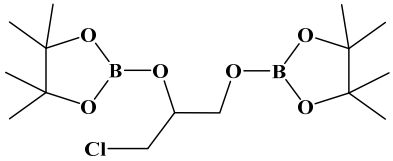
4.3 Hydroboration of propylene carbonate [**1c**].



[**2c**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 4.50 – 4.44 (*m*, 1H), 3.84 – 3.80 (*m*, 2H), 1.10 (*s*, 6H), 1.08 (*s*, 18H), 1.06 – 1.04 (*m*, 3H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.6, 82.4, 70.7, 69.6, 24.8, 24.8, 24.7, 18.6. Spectroscopic data agrees with those previously reported.[1]

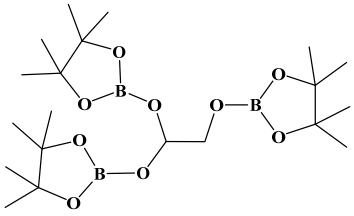
4.4 Hydroboration of 4-(chloromethyl)-1,3-dioxolan-2-one [**1d**].



[**2d**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 4.48 – 4.43 (*m*, 1H), 4.02 – 3.89 (*m*, 2H), 3.34-2.28 (*m*. 2H), 1.07,1.06 (*s*, 24H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.9, 82.8, 74.3, 65.7, 44.7, 24.7, 24.7, 24.7, 24.6. Mass(m/z, +ESI) Calculated: 362.18 Found:363.17

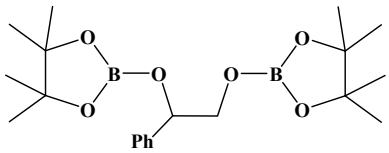
4.5 Hydroboration of 4-(hydroxymethyl)-1,3-dioxolan-2-one [**1e**].



[**2e**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 4.62-4.57 (*m*, 1H), 4.10-3.99 (*m*, 4H), 1.10 (*s*, 12H), 1.05 (s, 24H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.6, 82.6, 74.5, 65.6, 24.7, 24.7 . Spectroscopic data is in agreement with those previously reported.[1]

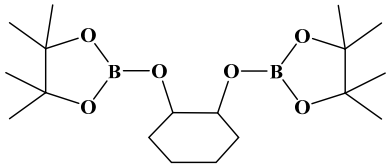
4.6 Hydroboration of styrene carbonate [**1f**].



[**2f**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 7.34 (*d*, *J* = 6 Hz, 2H), 7.07 – 7.00 (*m*, 3H), 5.53 (*m*, 1H), 4.16 – 4.05 (*m*, 2H), 1.10 (*s*, 6H), 1.09 (*s*, 6H), 1.08 (*s*, 6H), 1.05 (*s*, 6H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 140.1, 128.5, 126.7, 82.8, 82.7, 77.0, 70.2, 24.8, 24.8, 24.6. Spectroscopic data is in agreement with those previously reported.[1]

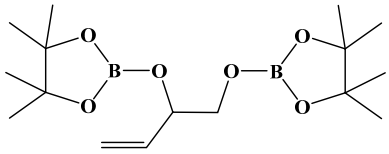
4.7 Hydroboration of hexahydro-1,3-benzodioxol-2-one [**1g**].



[**2g**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 4.41 (*d*, *J* = 8 Hz, 2H), 1.95 – 1.88 (*m*, 2H), 1.59 – 1.53 (*m*, 2H), 1.42 – 1.37 (*m*, 2H), 1.16 (s, 12H), 1.12 (s, 12H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.4, 73.5, 29.9, 24.9, 24.7, 21.9. Spectroscopic datais in agreement with those previously reported.[1]

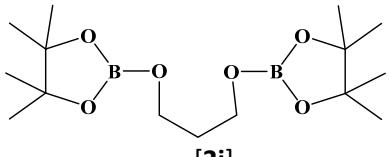
4.8 Hydroboration of 4-vinyl-1,3-dioxolan-2-one [**1h**].



[**2h**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 5.78 – 5.67 (*m*, 1H), 5.36 – 5.30 (*m*, 1H), 4.98 – 4.90 (*m*, 2H), 3.91 (*d*, *J* = 6.0 Hz, 2H), 1.10 (*s*, 6H), 1.08 (*s*, 12H), 1.07 (*s*, 6H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 136.0, 116.3, 82.7, 82.7, 75.5, 68.4, 25.1, 24.8, 24.7. Spectroscopic data agrees with those previously reported.[1]

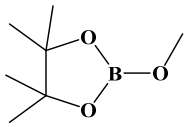
4.9 Hydroboration of trimethylene carbonate [**1i**].



[**2i**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.98 (*t*, *J* = 6 Hz, 4H), 1.76 (*p*, *J* = 6 Hz, 2H), 1.04 (s, 24H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 82.4, 61.8, 33.9, 24.7. Spectroscopic data is in agreement with those previously reported.[1]

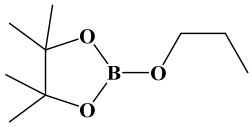
4.10 Hydroboration of dimethyl carbonate [**1j**].



[**MeOBPin**] **(2j)**

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.50 (*s*, 3H), 1.04 (s, 12H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 82.5, 24.7. Spectroscopic data is in agreement with those previously reported.[1]

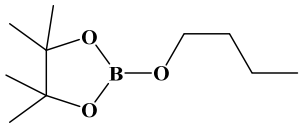
4.11 Hydroboration of dipropyl carbonate [**1k**].



[**2k**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.84 (*t*, *J* = 6.6 Hz, 2H), 1.53-1.46 (*m*, 2H) 1.06 (*s*, 12H), 0.81 (*t*, *J* = 6.0 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 82.4, 66.6, 25.21, 24.7, 10.3. Spectroscopic data agrees with those previously reported.[1]

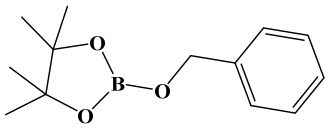
4.12 Hydroboration of dibutyl carbonate [**1l**].



[**2l**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.90 (*t*, *J* = 6 Hz, 2H), 1.52-1.45 (*m*, 2H), 1.34-1.25 (*m*, 2H) 1.06 (*s*, 12H), 0.81 (*t*, *J* = 6.0 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 82.4, 64.8, 34.0 24.7, 19.2 13.9. Spectroscopic data is in agreement with those previously reported.[1]

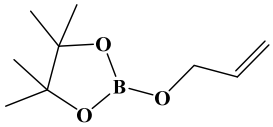
4.13 Hydroboration of dibenzyl carbonate [**1m**].



[**2m**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 7.31 (*d*, *J* = 6 Hz, 2H), 7.15 – 7.11 (*m*, 2H), 7.07-7.04 (*m*, 1H), 4.95 (*s*, 2H), 1.03 (s, 12H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 140.1, 128.6, 127.6, 127.0, 82.7, 66.9, 24.7. Spectroscopic data agrees with those previously reported.[1]

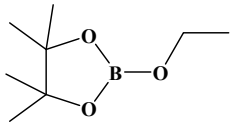
4.14 Hydroboration of diallyl carbonate [**1n**].



[**2n**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 5.86 – 5.76 (*m*, 1H), 5.32-5.27 (*m*, 1H), 5.00-4.97 (*m*, 1H), 4.38-4.36 (*m*, 2H), 1.04 (s, 12H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 136.2, 114.7, 82.6, 65.7 127.0, 82.7, 66.9, 24.7. Spectroscopic data agrees with those previously reported.[1]

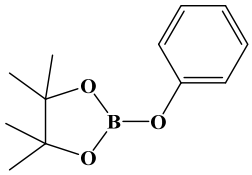
4.15 Hydroboration of ethyl methyl carbonate [**1o**].



[**2b**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.89 (*q*, *J* = 8.0 Hz, 2H), 1.10 (*t*, *J* = 8.0 Hz, 3H), 1.05 (*s*, 12H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 82.4, 60.7, 24.7, 17.5. Spectroscopic data agrees with those previously reported.[1]

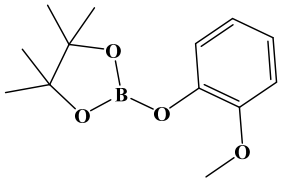
4.16 Hydroboration of diphenyl carbonate [**1p**].



[**2p**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 7.18 – 7.16 (*m*, 2H), 7.09 – 7.05 (*m*, 2H), 6.87 – 6.83 (*m*, 1H), 1.05 (*s*, 12H). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): (δ ppm) 154.3, 129.6, 123.3, 120.0, 83.3, 24.61. Spectroscopic data is in agreement with those previously reported.[1]

4.17 Hydroboration of bis(2-methoxyphenyl) carbonate [**1q**].

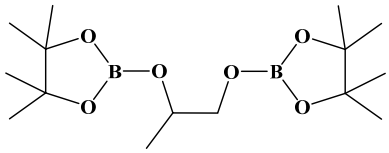


[**2q**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 7.15 – 7.13 (*dd*, J = 7.8 Hz, J = 1.6 Hz, 1H), 6.84 – 6.80 (*td*, J = 7.8 Hz, J = 1.6 Hz, 1H), 6.73 – 6.69 (*td*, J = 7.8 Hz, J = 1.6 Hz, 1H), 6.57 – 6.55 (*dd*, J = 7.8 Hz, J = 1.6

Hz, 1H), 3.35 (*s*, 3H), 1.07 (*s*, 12H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 151.0, 144.1, 123.9, 121.1, 121.1 112.6, 83.2, 55.3, 24.6. Spectroscopic data is in agreement with those previously reported.[1]

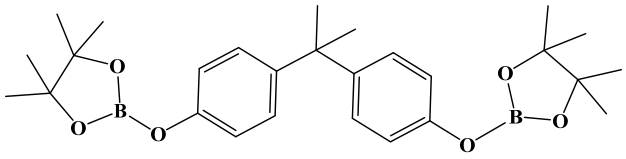
4.18 Hydroboration of poly(propylene carbonate) [**1s**].



[**2c**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 4.50 – 4.44 (*m*, 1H), 3.84 – 3.80 (*m*, 2H), 1.10 (*s*, 6H), 1.08 (*s*, 18H), 1.06 – 1.04 (*m*, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 82.6, 82.4, 70.7, 69.6, 24.8, 24.8, 24.7, 18.6. Spectroscopic data agrees with those previously reported.[1]

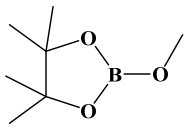
4.19 Hydroboration of poly(bisphenol-A carbonate) [**1t**].



[**2t**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 7.12 – 7.10 (*d*, *J* = 6Hz, 4H), 6.99 – 6.97 (*d*, *J* = 6 Hz, 4H), 1.42 (*s*, 6H), 1.03 (*s*, 24H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 154.3, 129.6, 123.3, 120.0, 83.3, 24.61.

4.20 Hydroboration of carbon dioxide [**1u**].



[**MeOBpin**]

^{1}H NMR (300 MHz, C_6D_6): (δ ppm) 3.50 (*s*, 3H), 1.04 (s, 12H). $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6): (δ ppm) 82.5, 24.7. Spectroscopic data agrees with those previously reported.[1,2]

^{1}H & ^{13}C NMR spectra of hydroborated products in the reaction mixtures

- Peaks for residual HBpin *- Peaks of MeOBpin

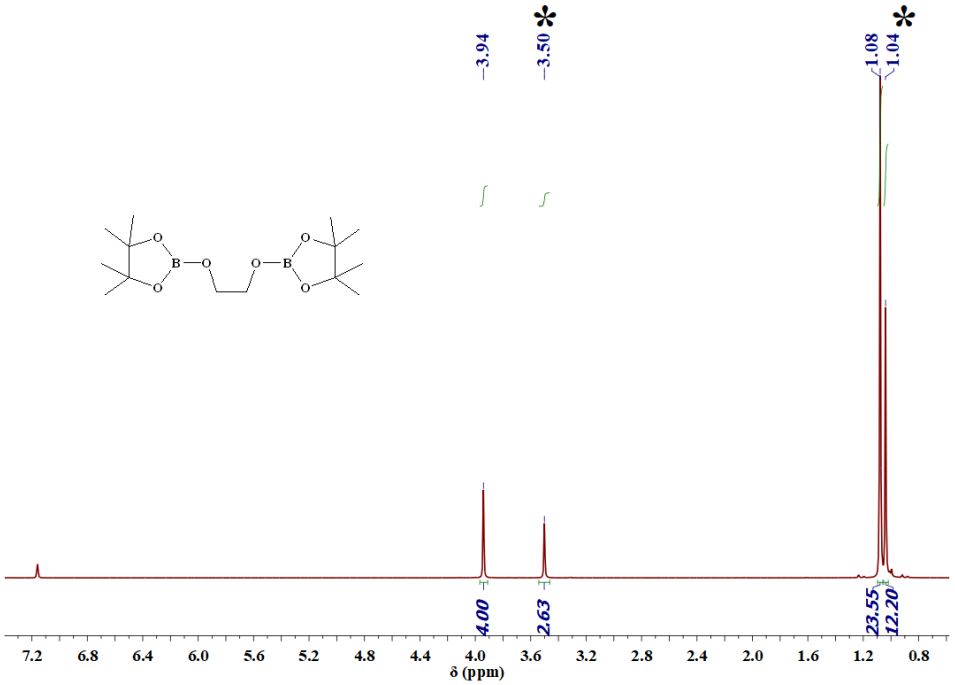


Figure S10. ^{1}H NMR spectrum of **2a** in reaction mixture.

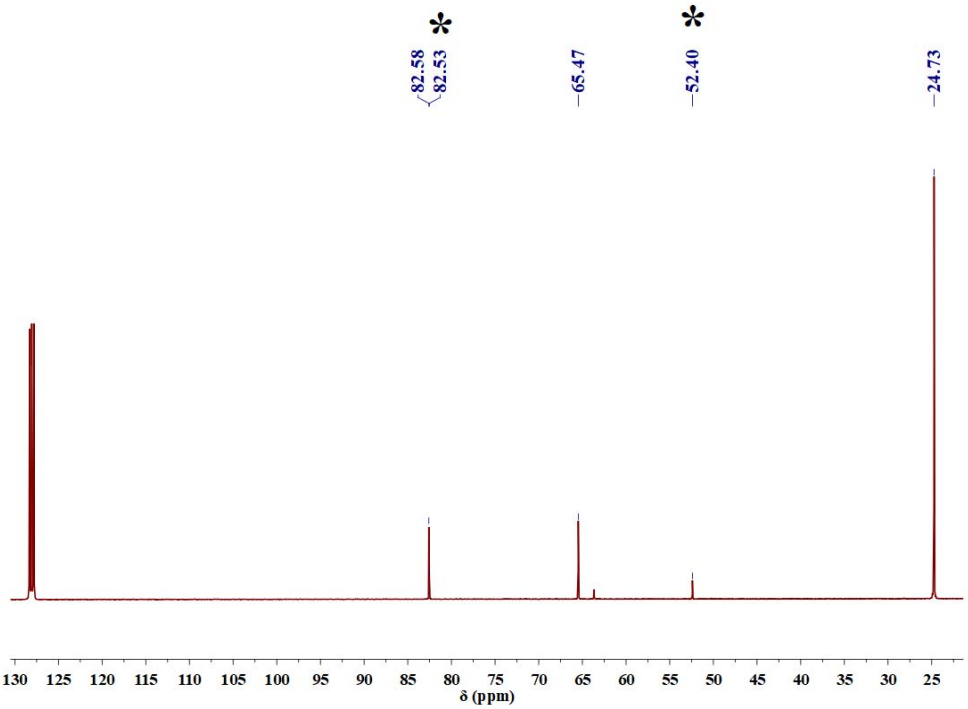


Figure S11. ^{13}C NMR spectrum of **2a** in reaction mixture.

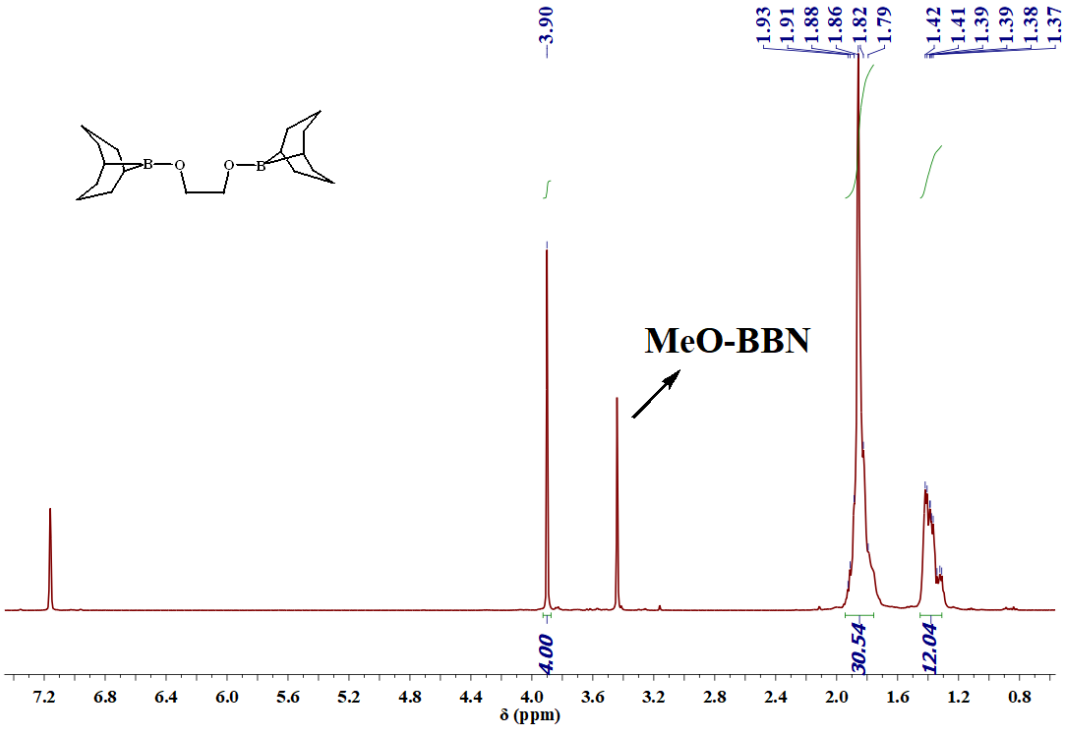


Figure S12. ^{1}H NMR spectrum of **3a** in reaction mixture.

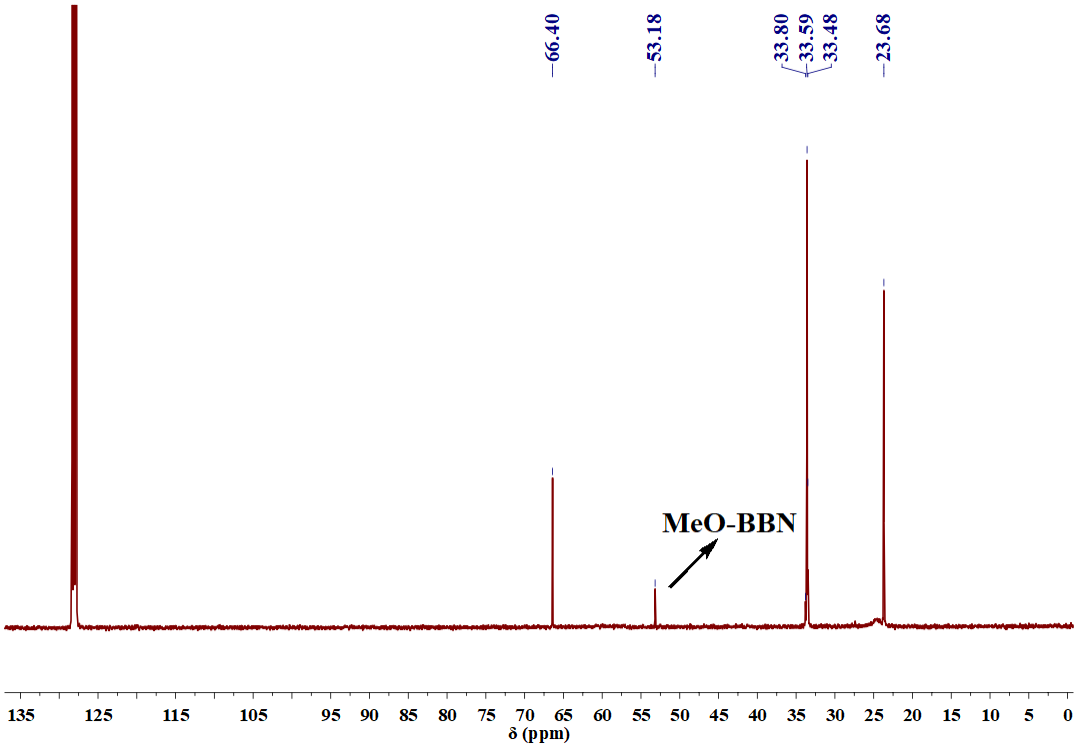


Figure S13. ^{13}C NMR spectrum of **3a** in reaction mixture.

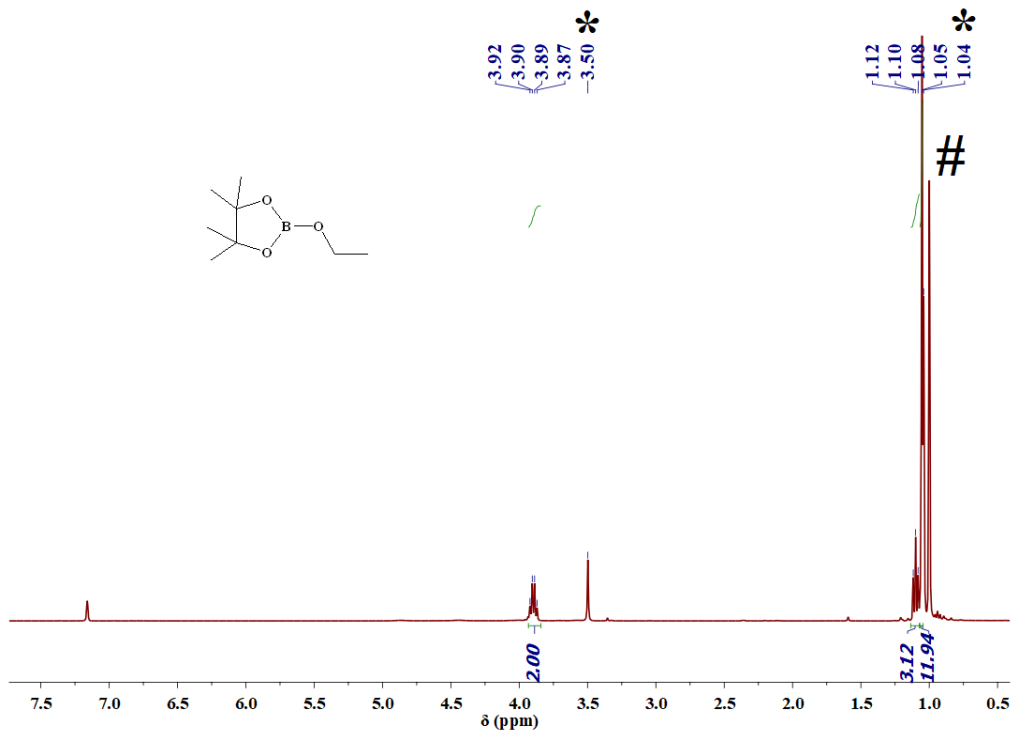


Figure S14. ^{1}H NMR spectrum of **2b** in reaction mixture.

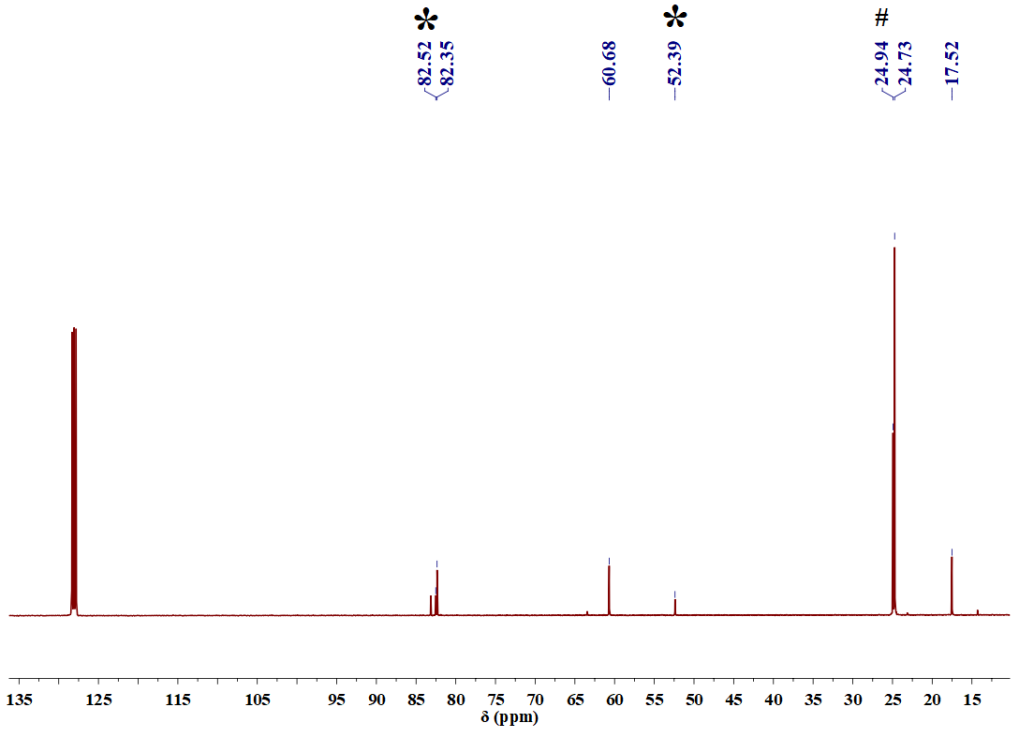


Figure S15. ^{13}C NMR spectrum of **2b** in reaction mixture.

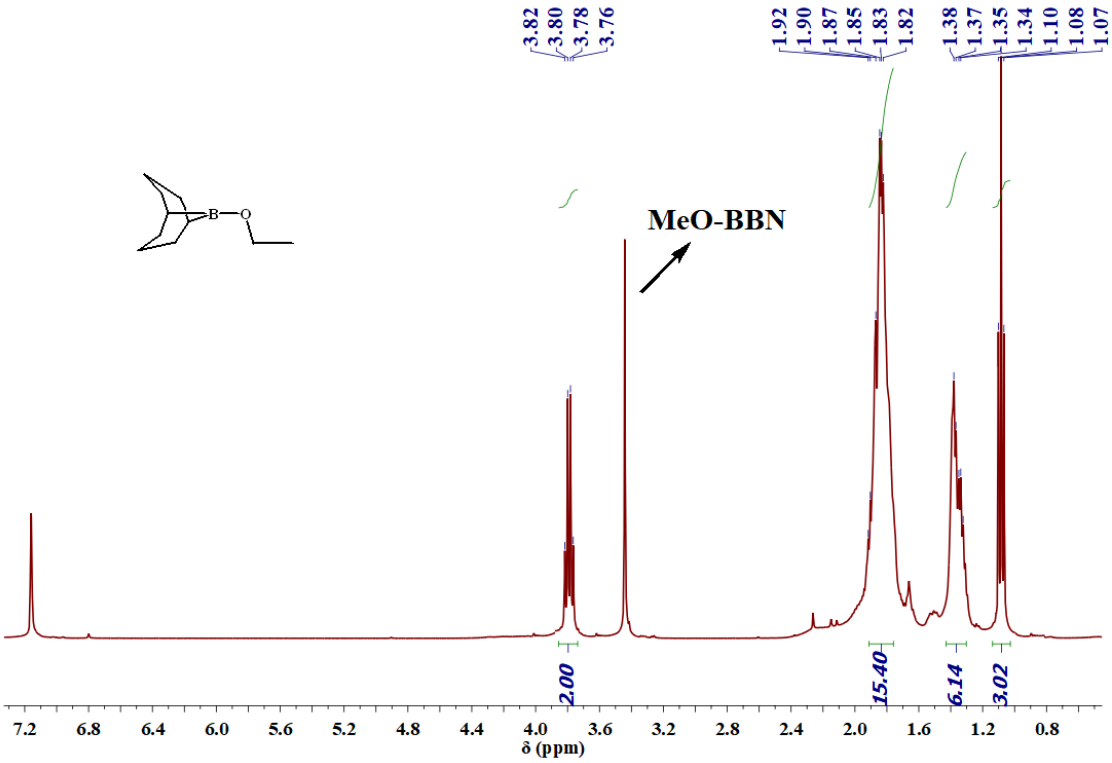


Figure S16. ^{1}H NMR spectrum of **3b** in reaction mixture.

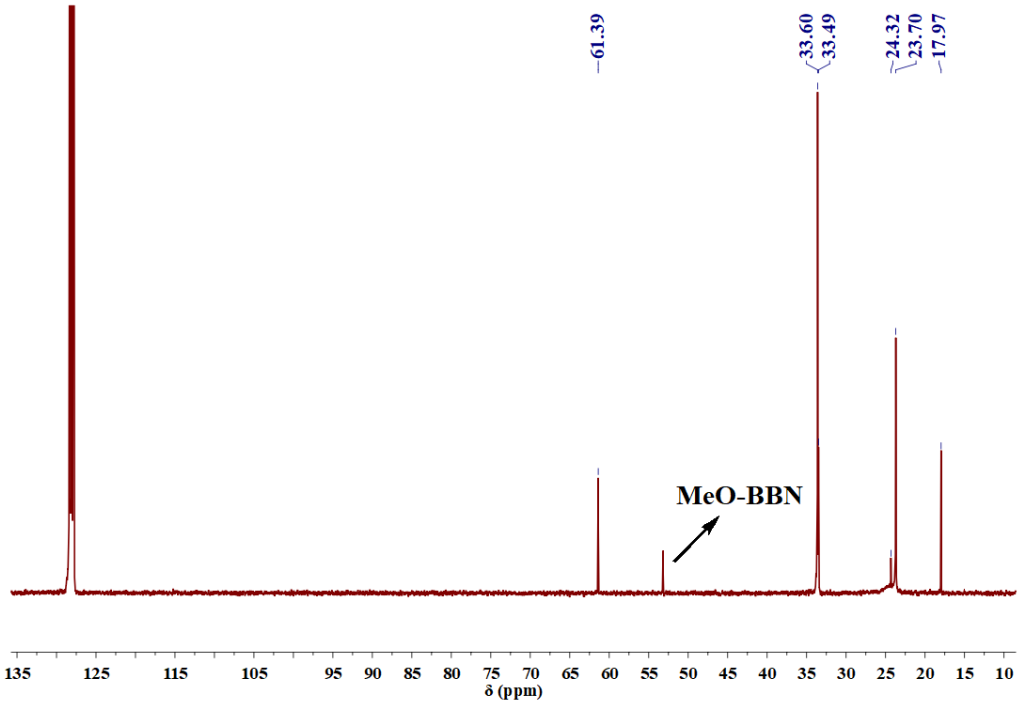


Figure S17. ^{13}C NMR spectrum of **3b** in reaction mixture.

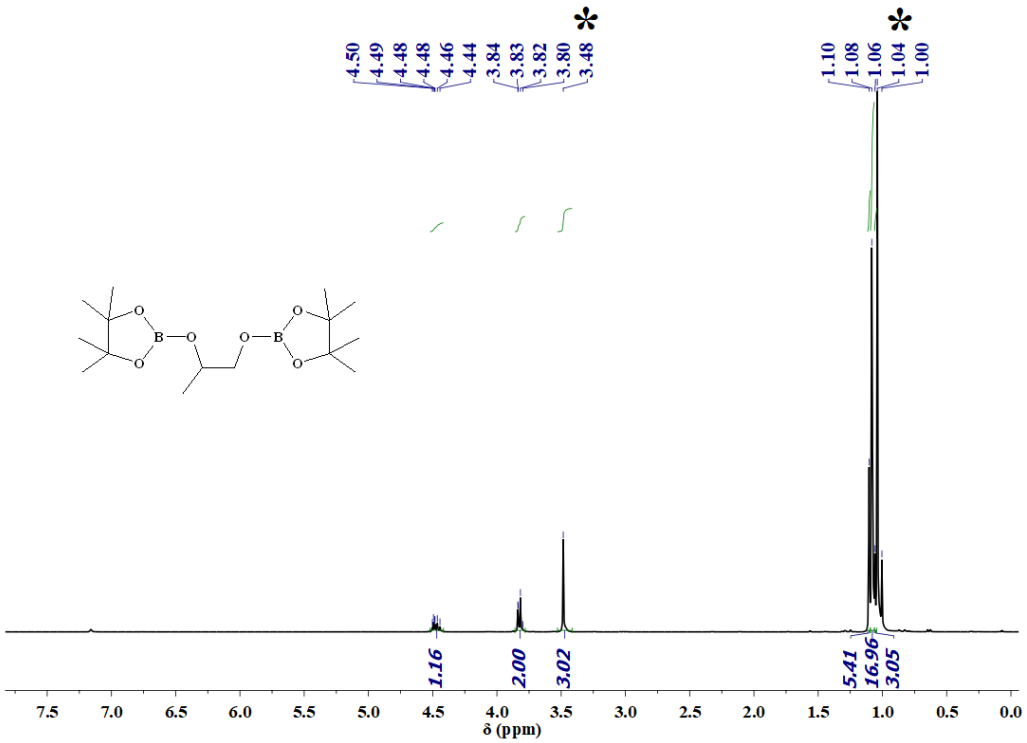


Figure S18. ^{1}H NMR spectrum of **2c** in reaction mixture.

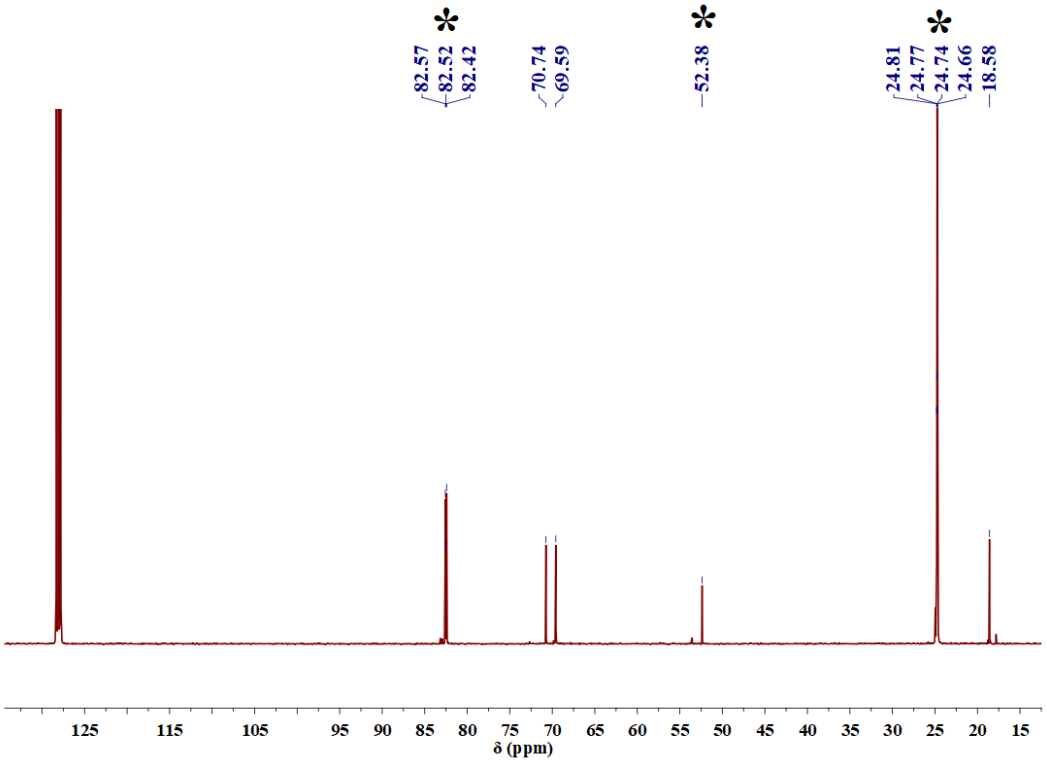


Figure S19. ^{13}C NMR spectrum of **2c** in reaction mixture.

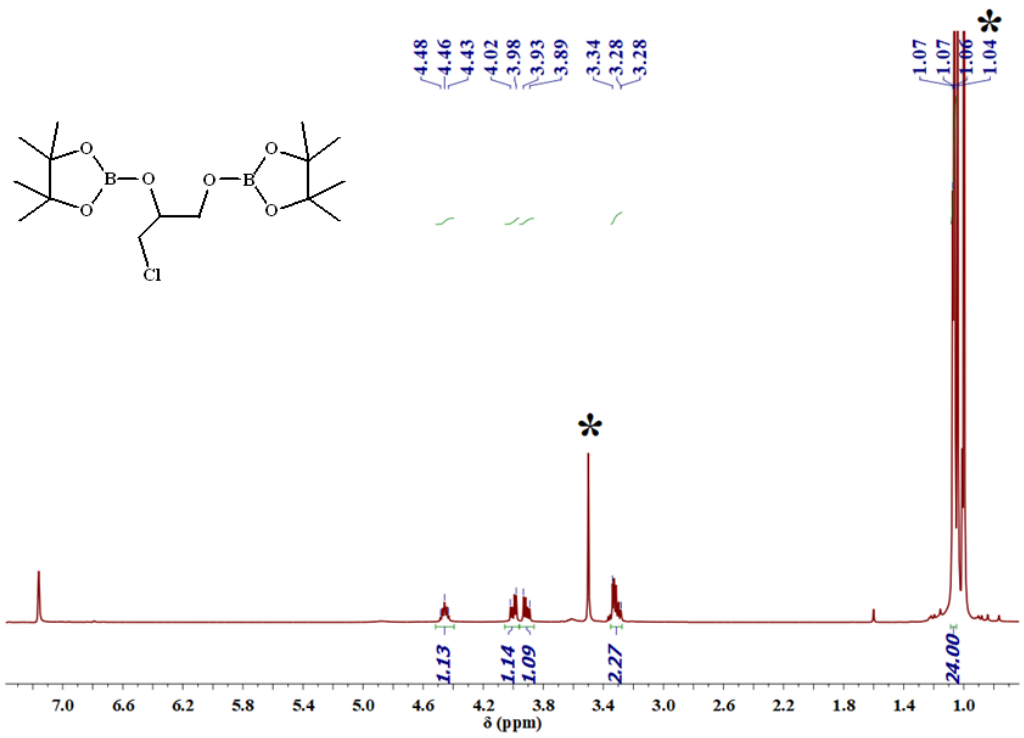


Figure S20. ^{1}H NMR spectrum of **2d** in reaction mixture.

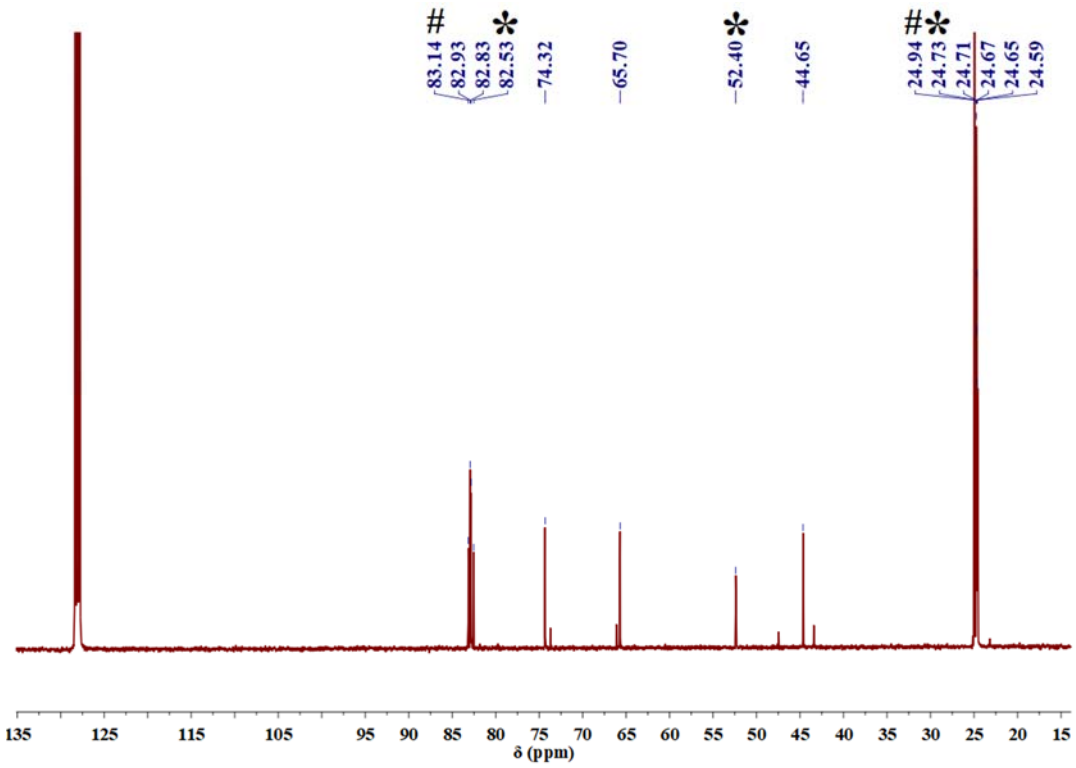


Figure S21. ^{13}C NMR spectrum of **2d** in reaction mixture.

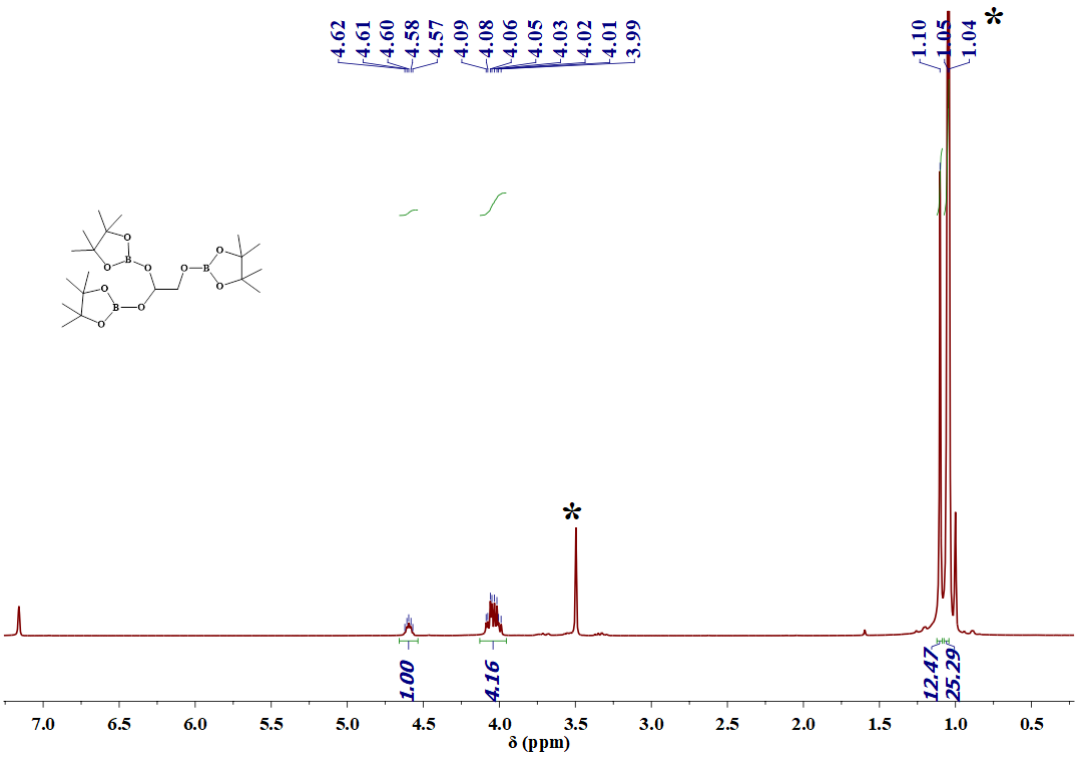


Figure S22. ^{1}H NMR spectrum of **2e** in reaction mixture.

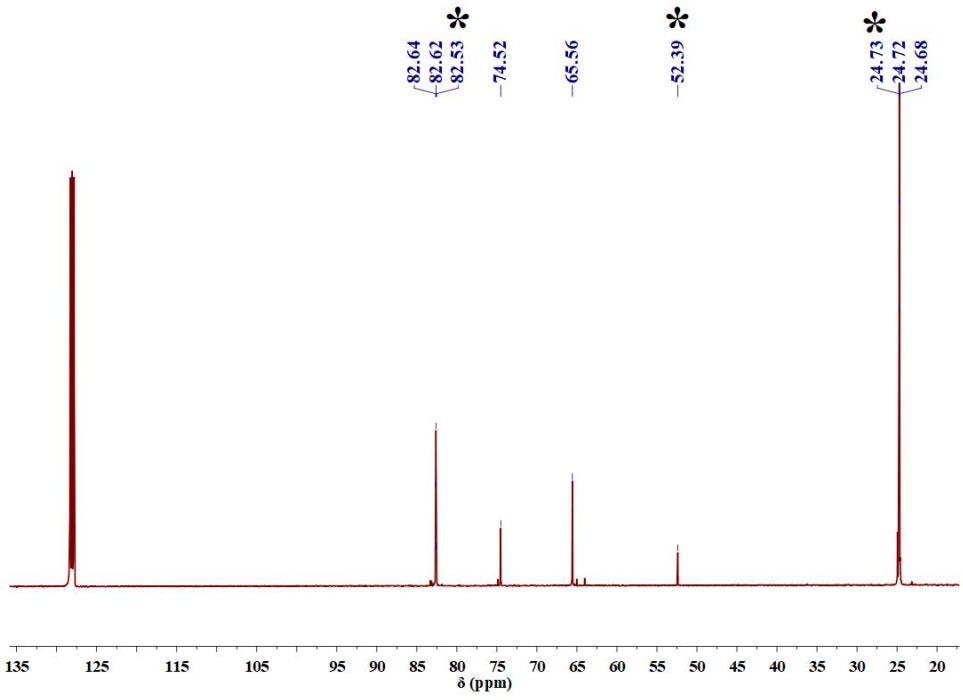


Figure S23. ^{13}C NMR spectrum of **2e** in reaction mixture.

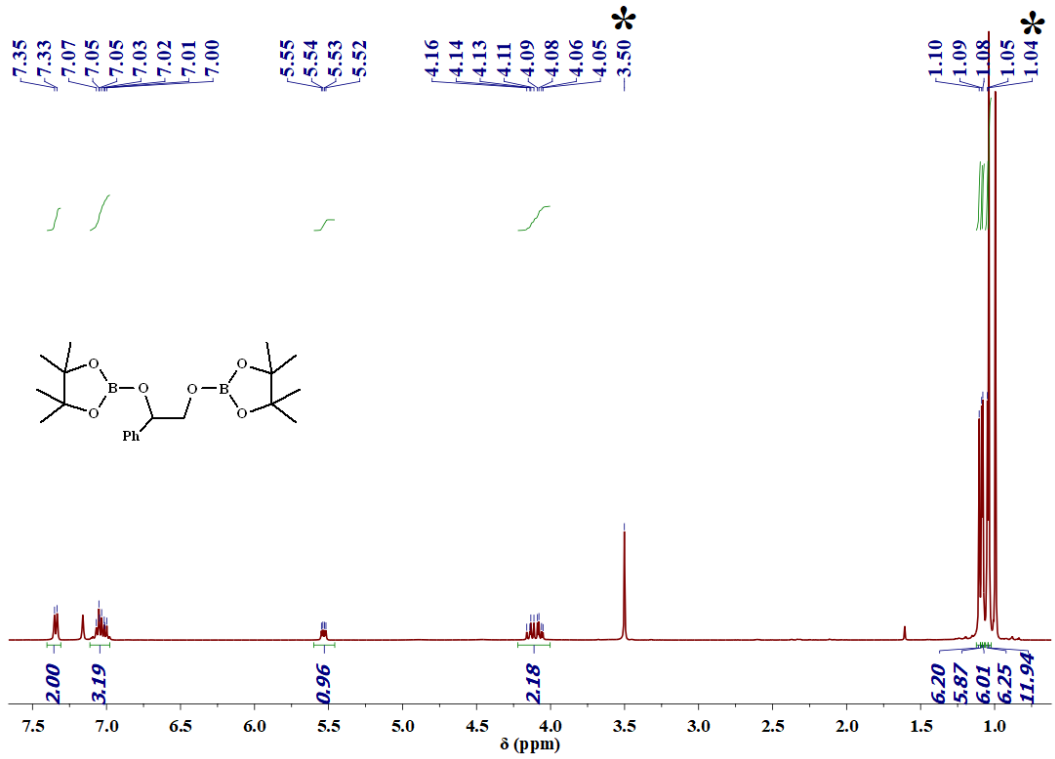


Figure S24. ^{1}H NMR spectrum of **2f** in reaction mixture.

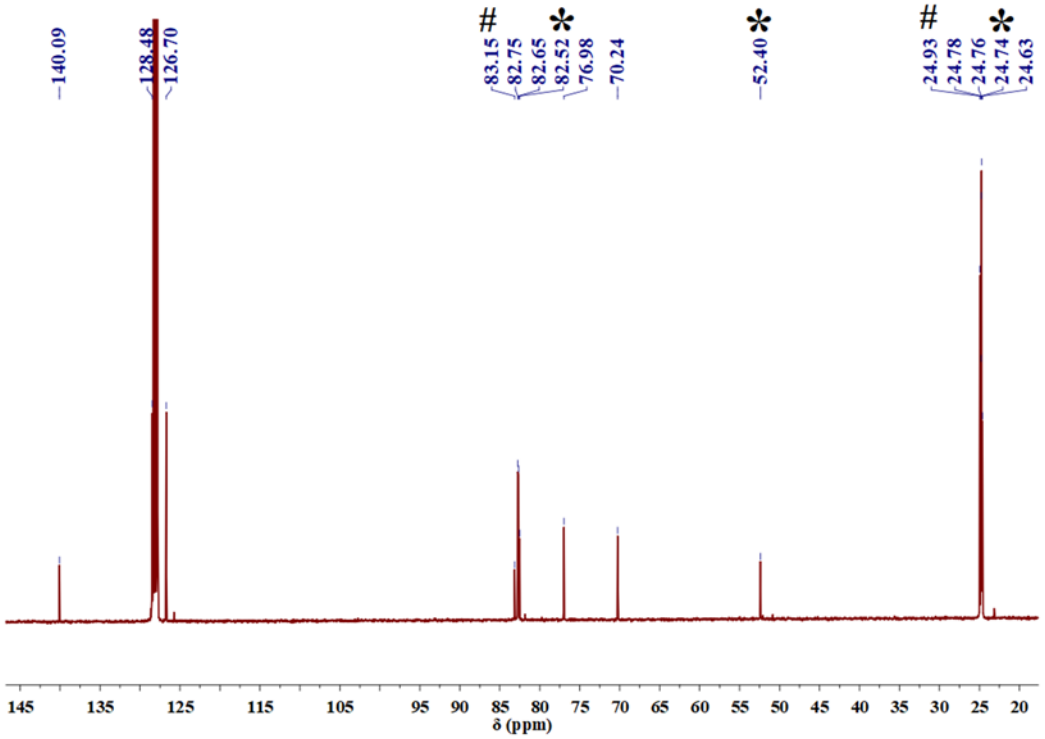


Figure S25. ^{13}C NMR spectrum of **2f** in reaction mixture.

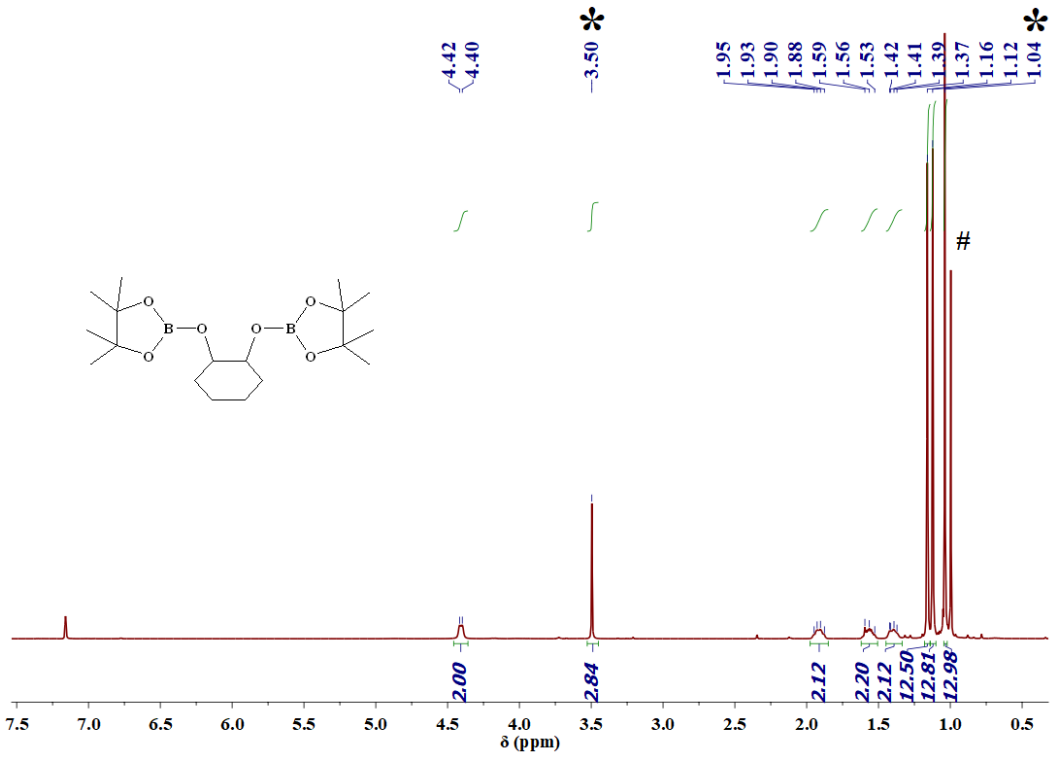


Figure S26. ^{1}H NMR spectrum of **2g** in reaction mixture.

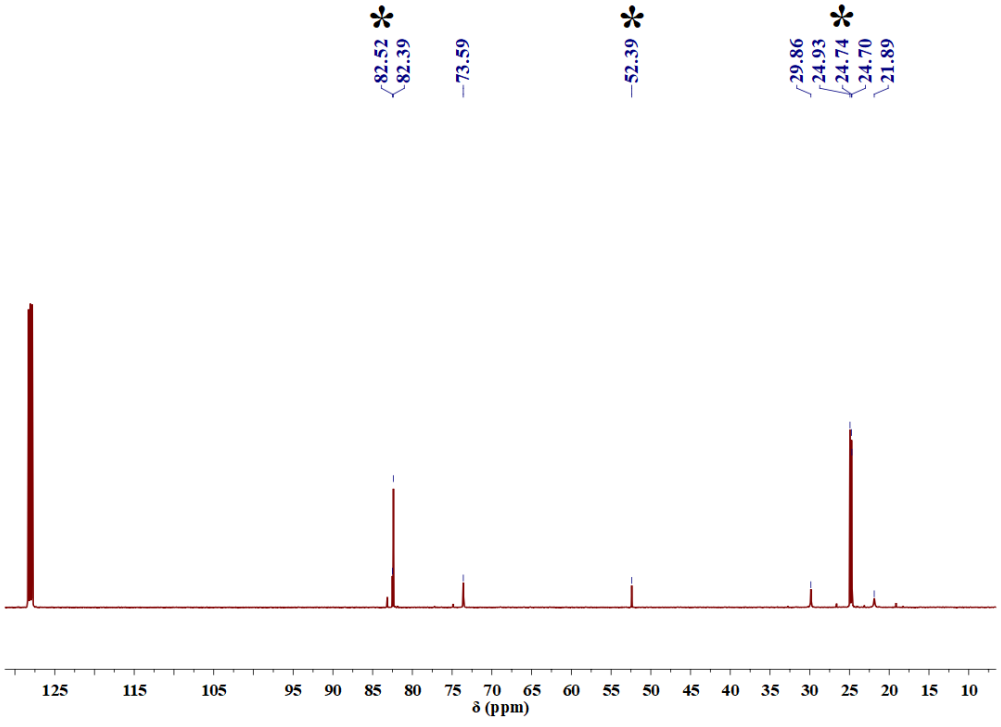


Figure S27. ^{13}C NMR spectrum of **2g** in reaction mixture (entry 5 in Table 2).

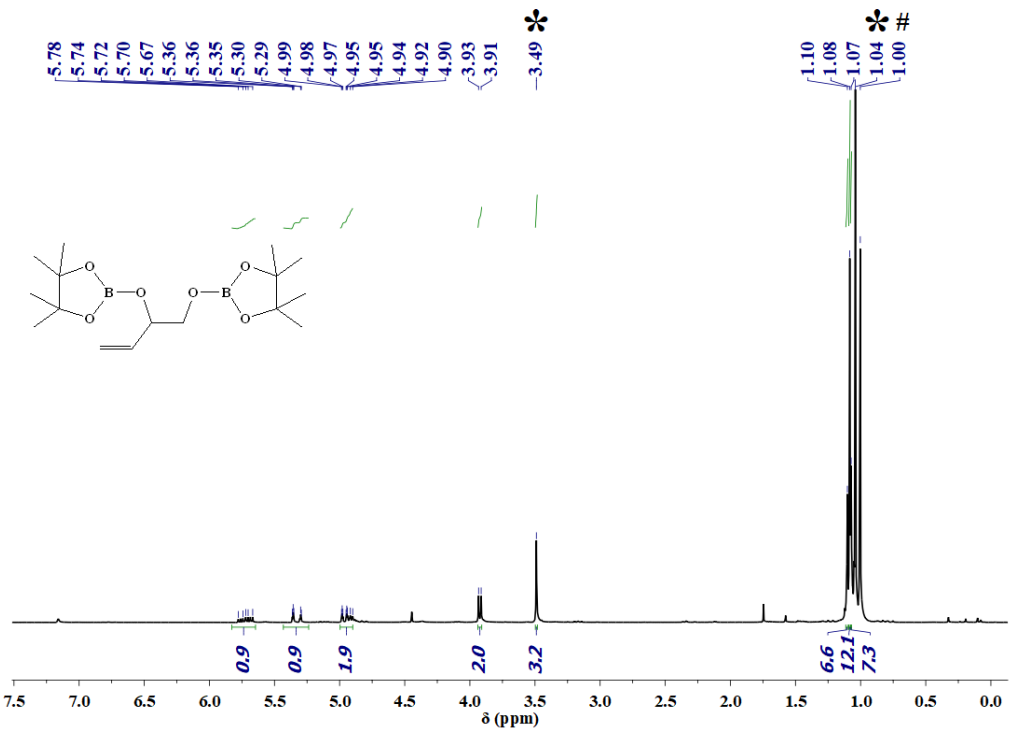


Figure S28. ^{1}H NMR spectrum of **2h** in reaction mixture.

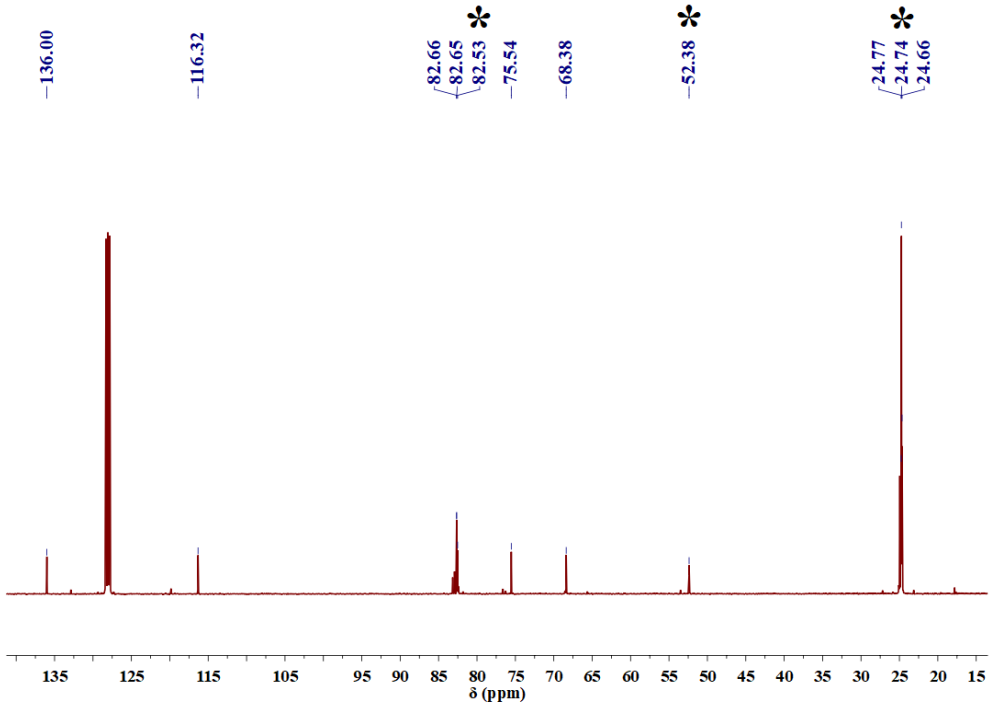


Figure S29. ^{13}C NMR spectrum of **2h** in reaction mixture.

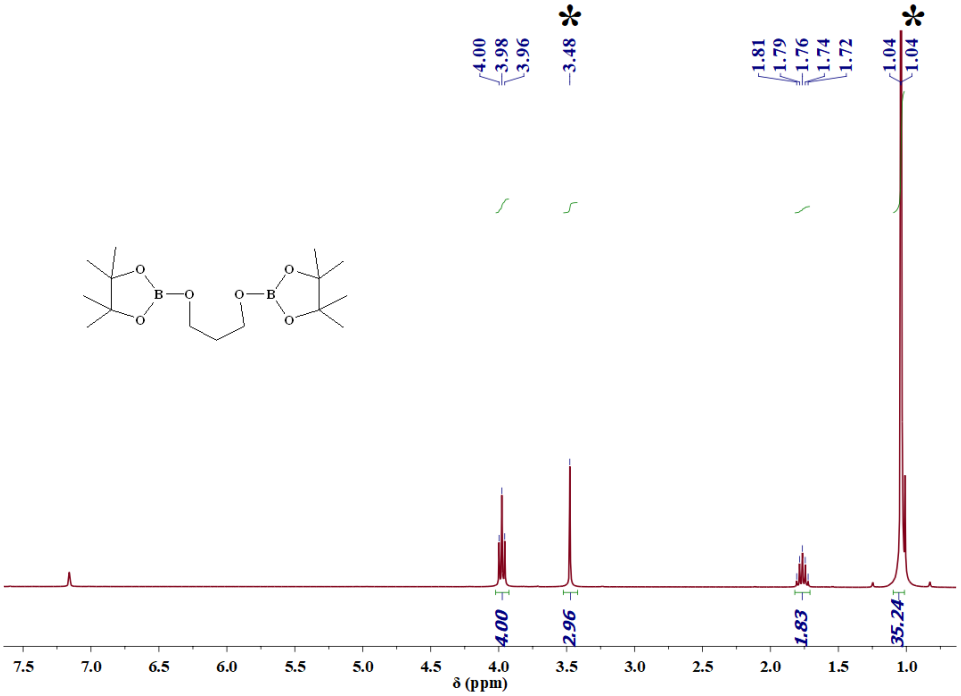


Figure S30. ^{1}H NMR spectrum of **2i** in reaction mixture.

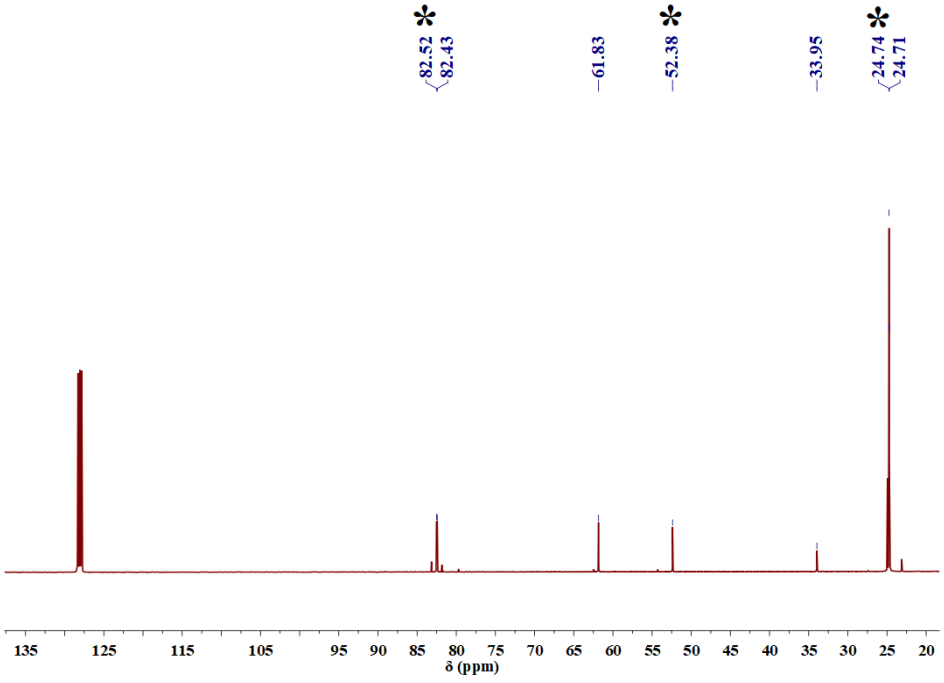


Figure S31. ^{13}C NMR spectrum of **2i** in reaction mixture.

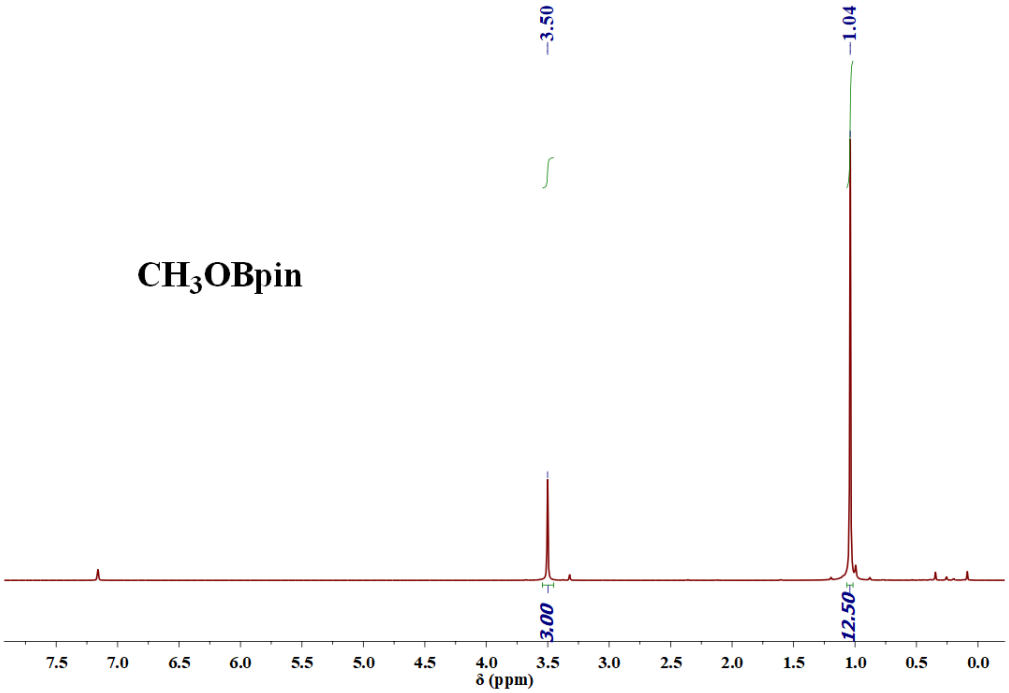


Figure S32. ^{1}H NMR spectrum of **3a** (Reaction of 1j and HBpin) in reaction mixture.

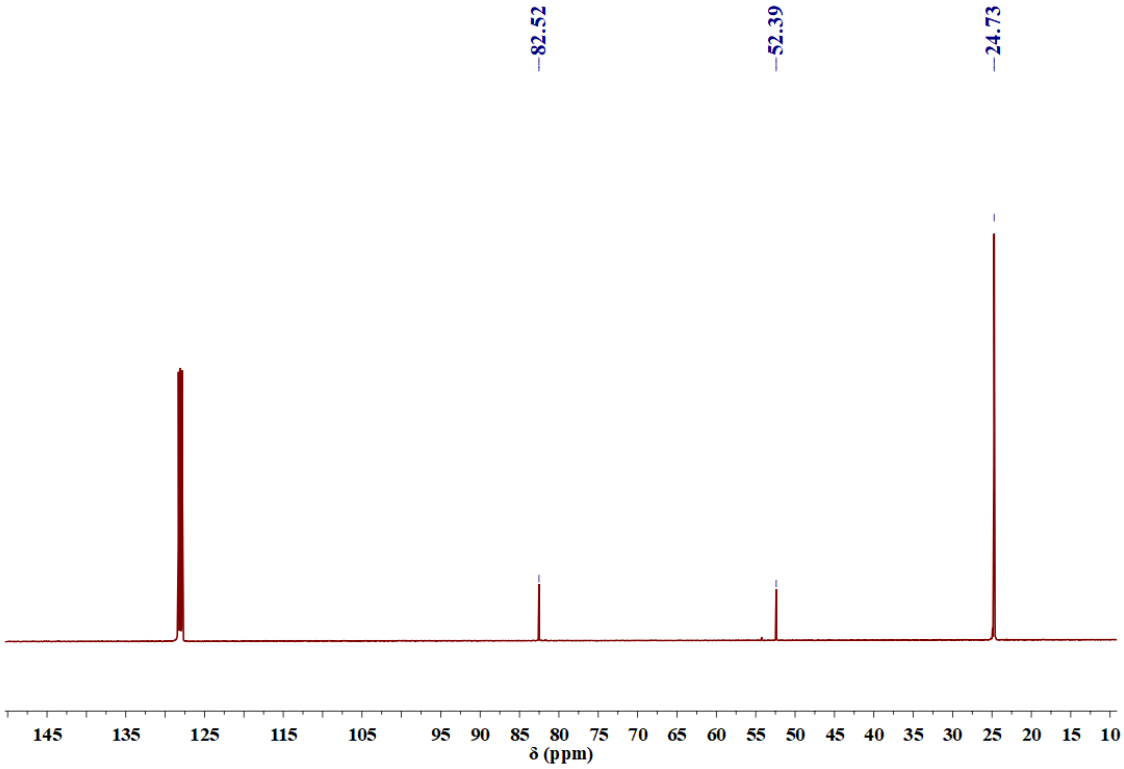


Figure S33. ^{13}C NMR spectrum of **3a** (Reaction of **1j** and HBpin) in reaction mixture.

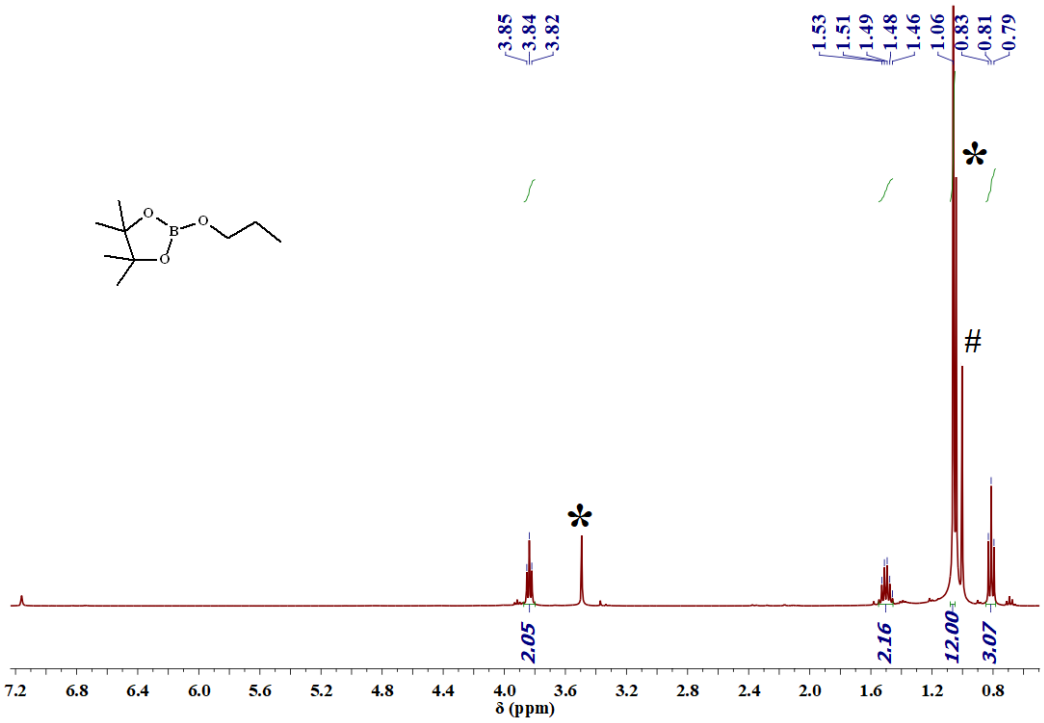


Figure S34. ^{1}H NMR spectrum of **2k** in reaction mixture.

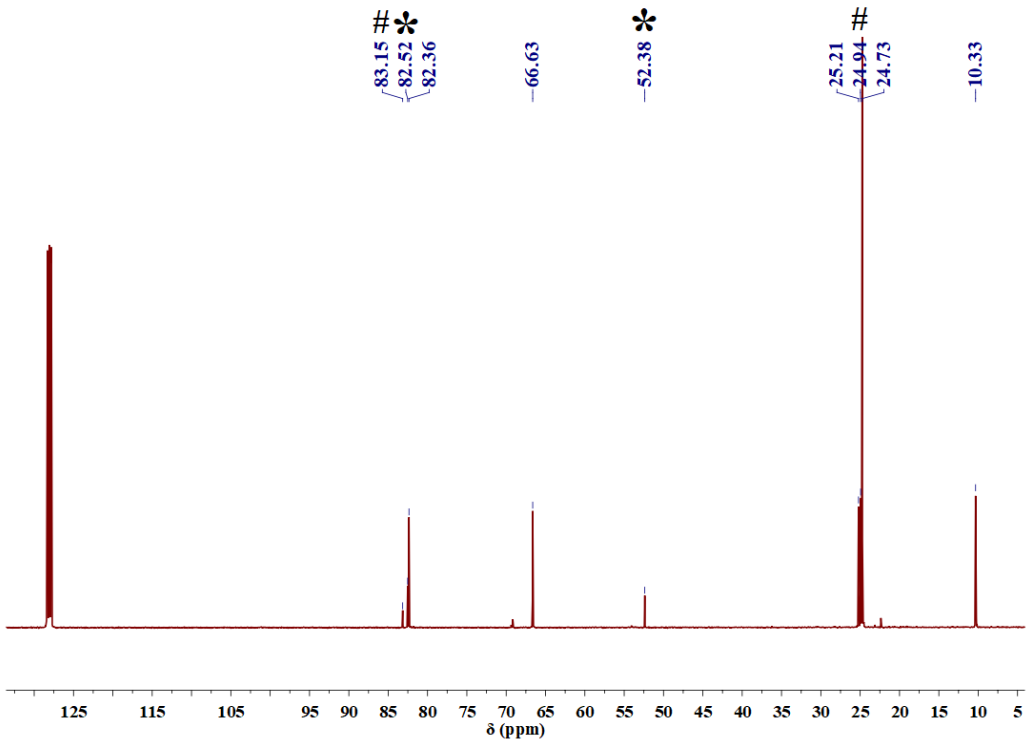


Figure S35. ^{13}C NMR spectrum of **2k** in reaction mixture.

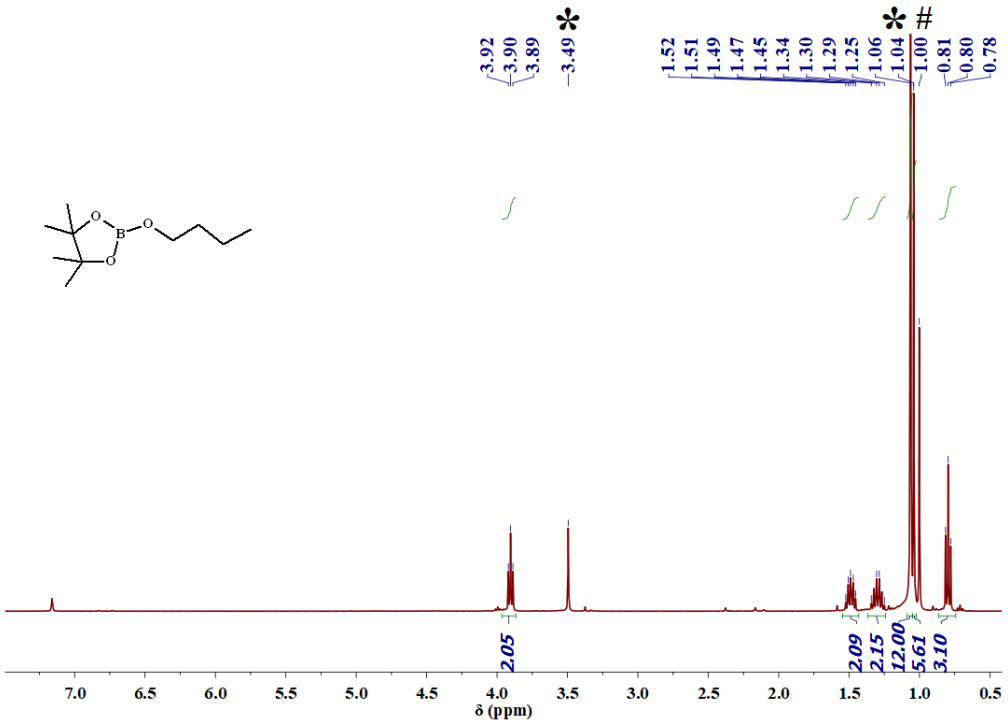


Figure S36. ^{1}H NMR spectrum of **2l** in reaction mixture.

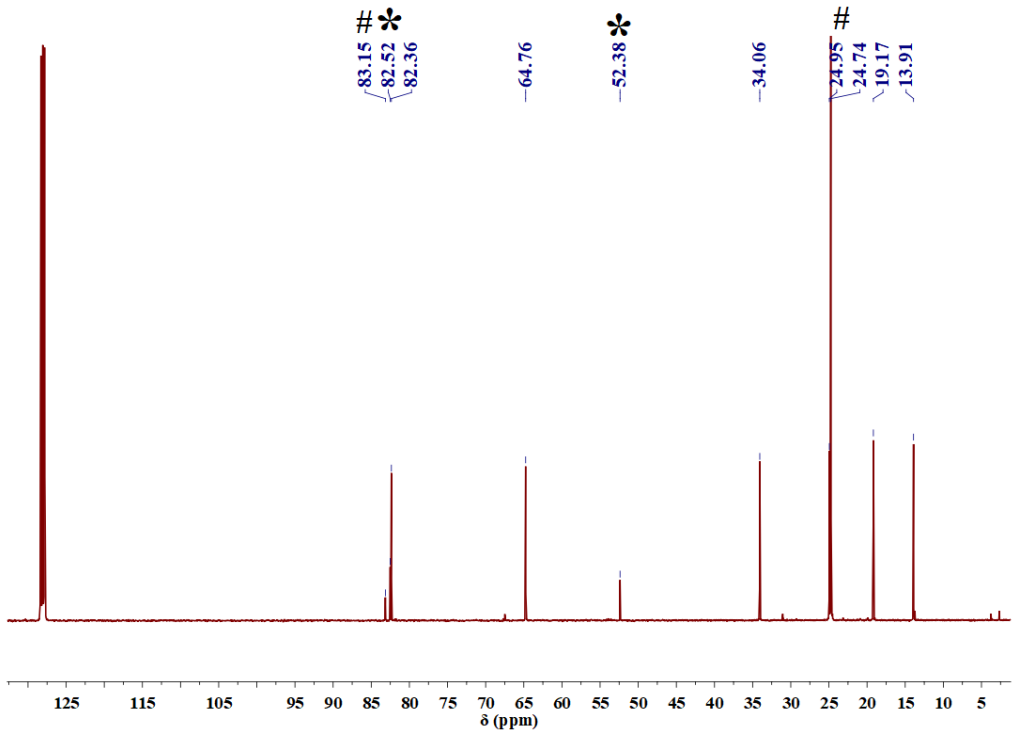


Figure S37. ^{13}C NMR spectrum of **2l** in reaction mixture.

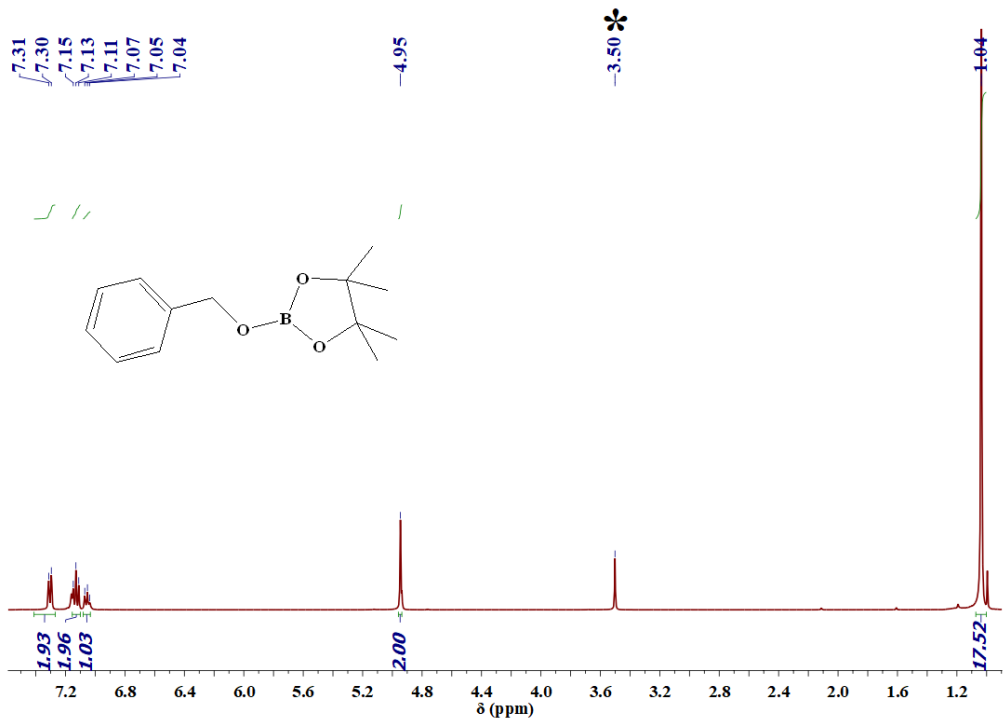


Figure S38. ^{1}H NMR spectrum of **2m** in reaction mixture.

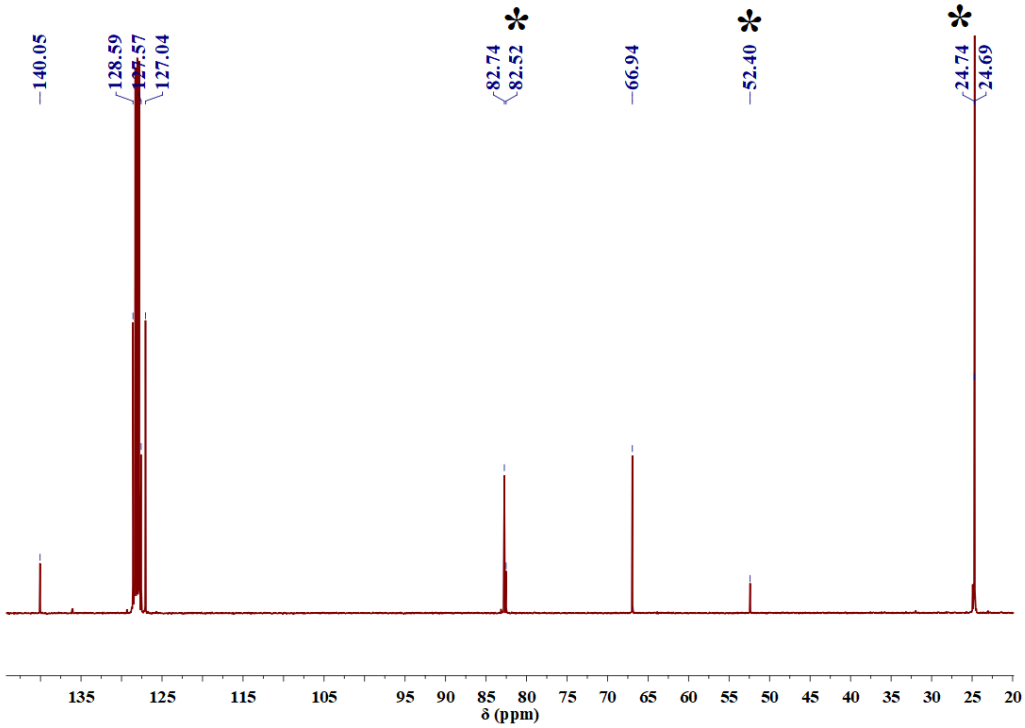


Figure S39. ^{13}C NMR spectrum of **2m** in reaction mixture.

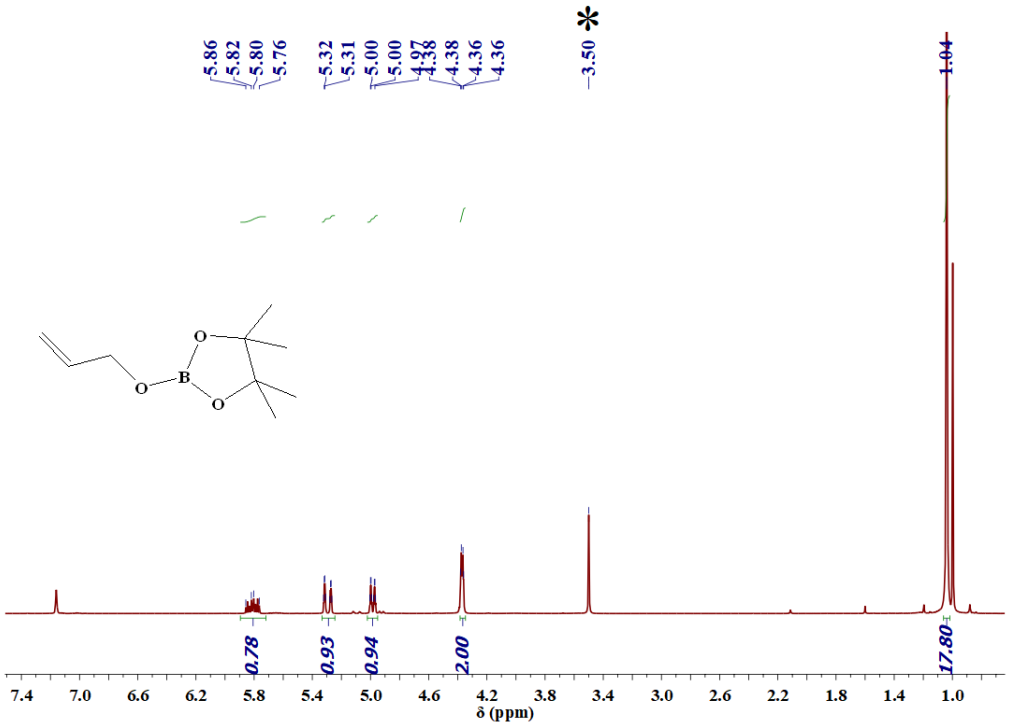


Figure S40. ^{1}H NMR spectrum of **2n** in reaction mixture.

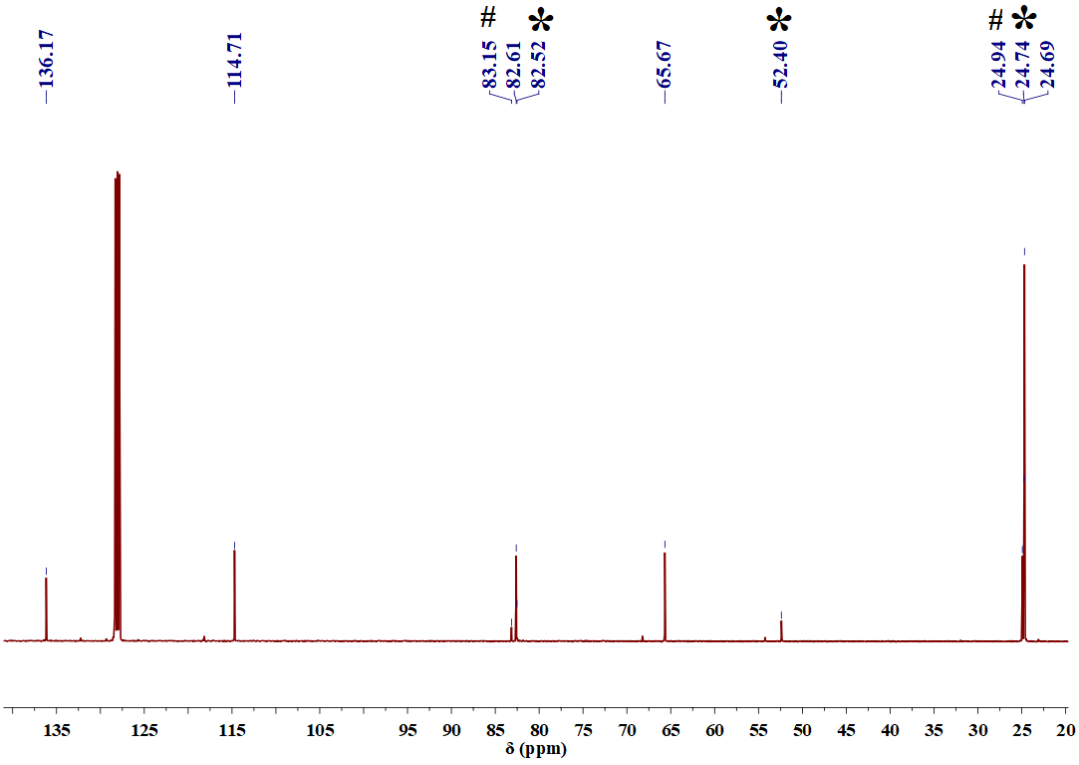


Figure S41. ^{13}C NMR spectrum of **2n** in reaction mixture.

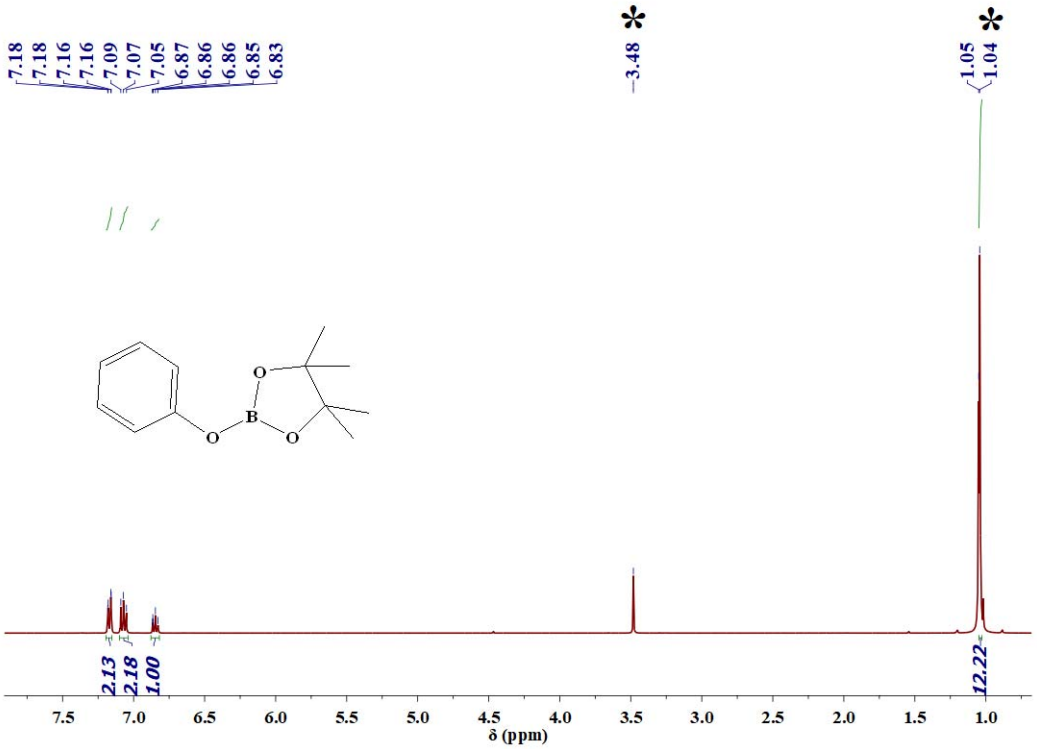


Figure S42. ^{1}H NMR spectrum of **2p** in reaction mixture.

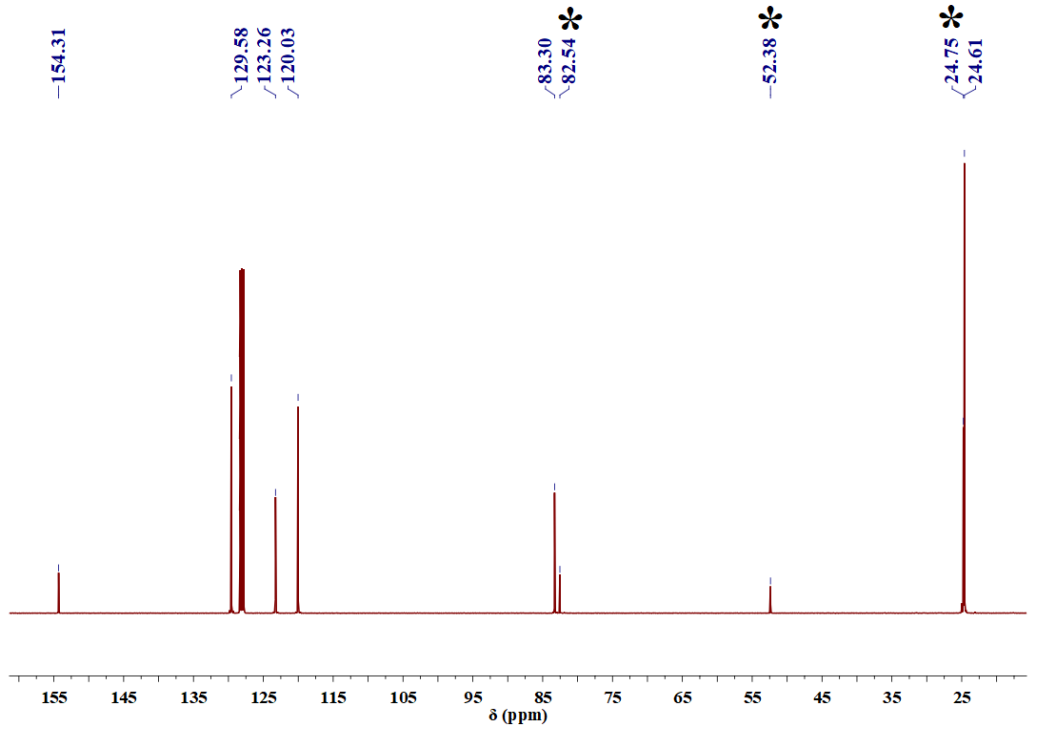


Figure S43. ^{13}C NMR spectrum of **2p** in reaction mixture.

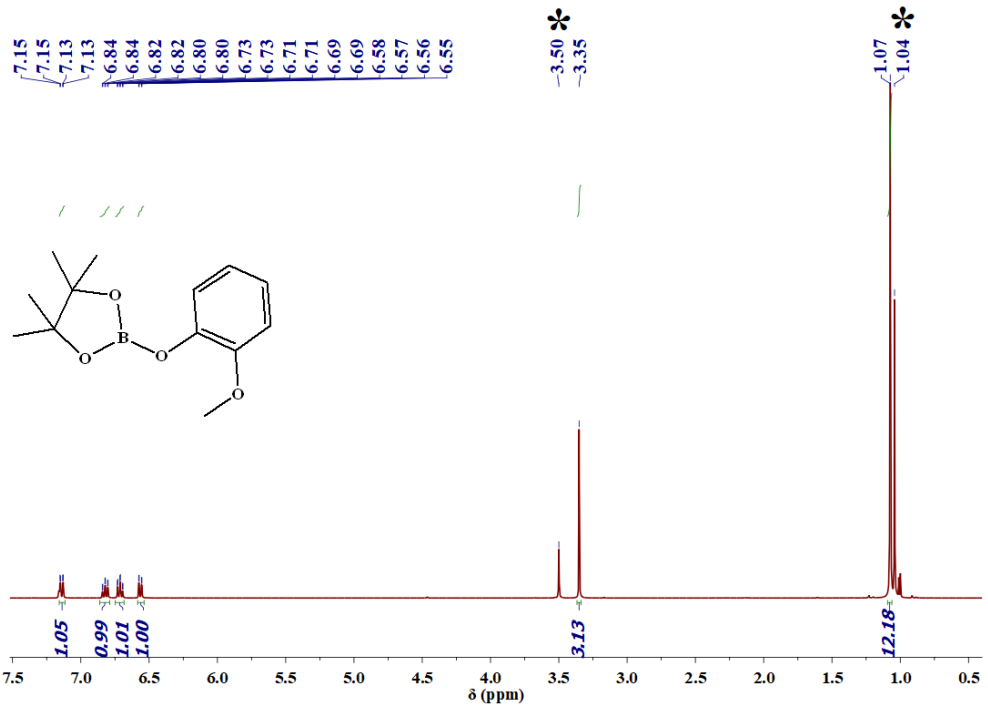


Figure S44. ^{1}H NMR spectrum of 2q in reaction mixture.

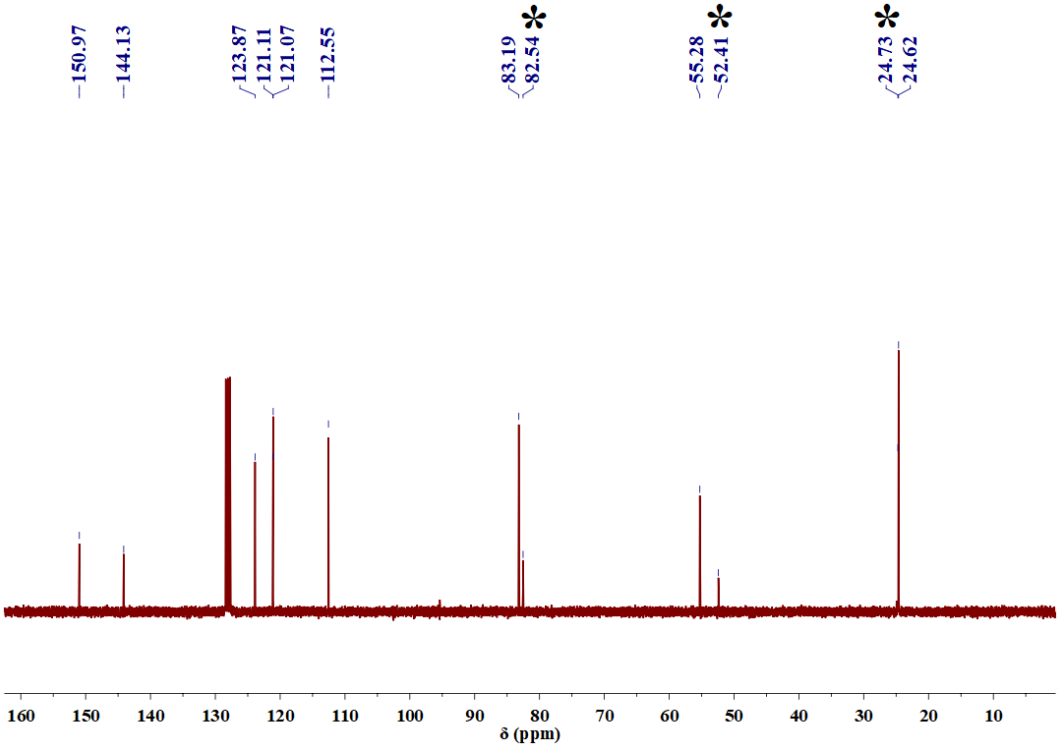


Figure S45. ^{13}C NMR spectrum of **2q** in reaction mixture.

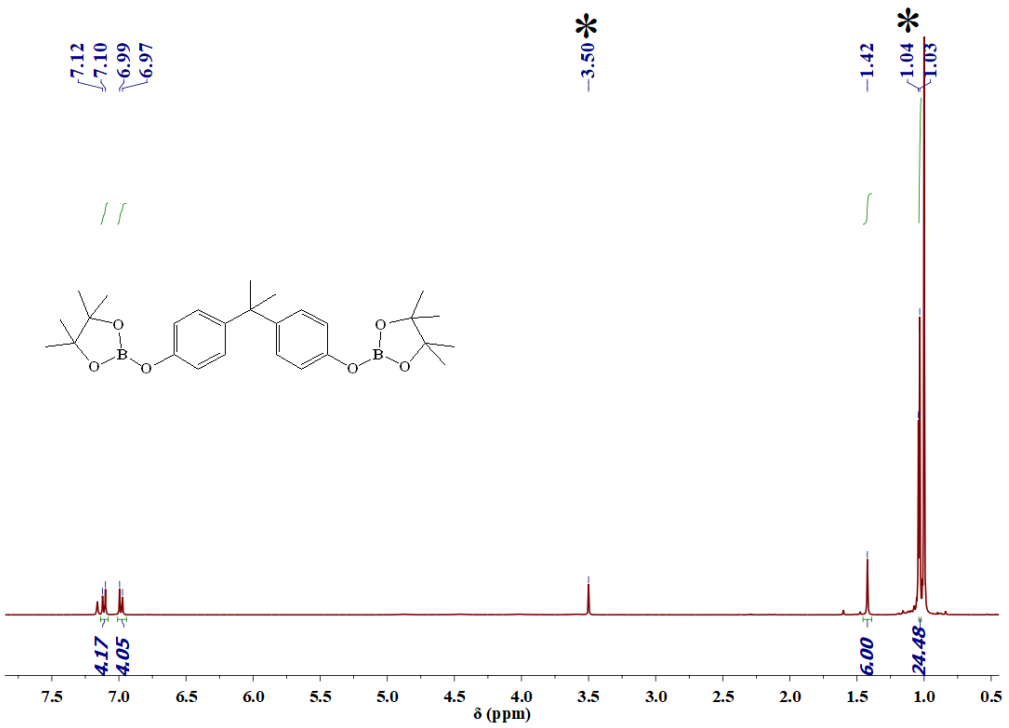


Figure S46. ^{1}H NMR spectrum of **2t** in reaction mixture.

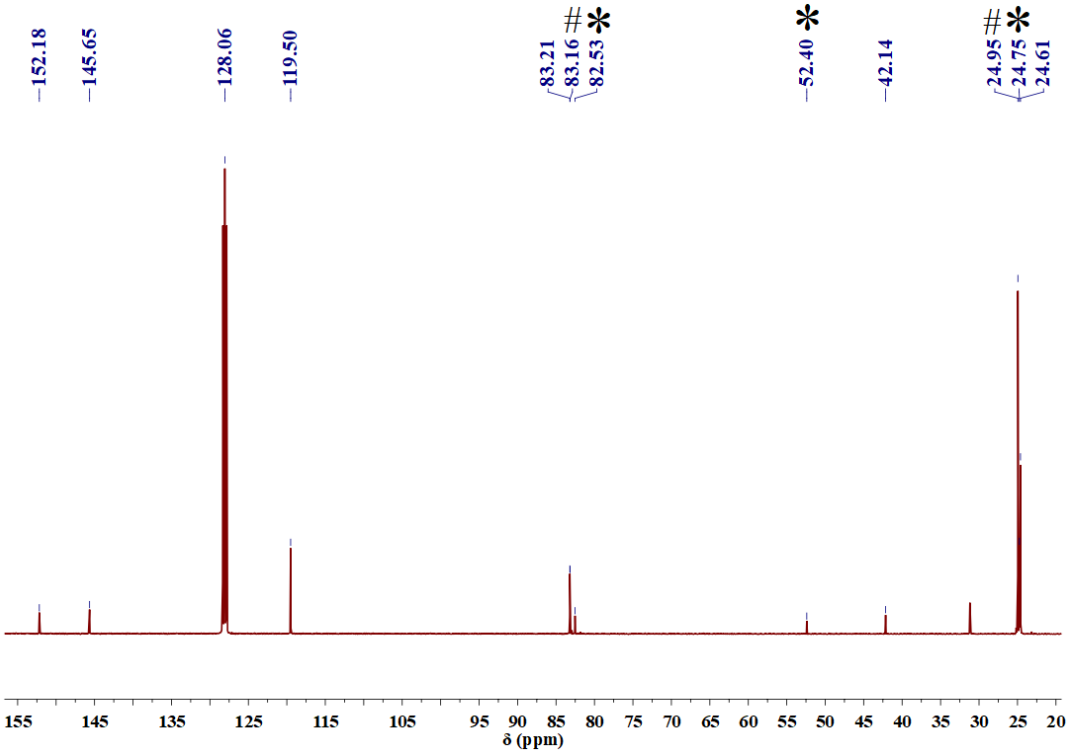


Figure S47. ^{13}C NMR spectrum of **2t** in reaction mixture.

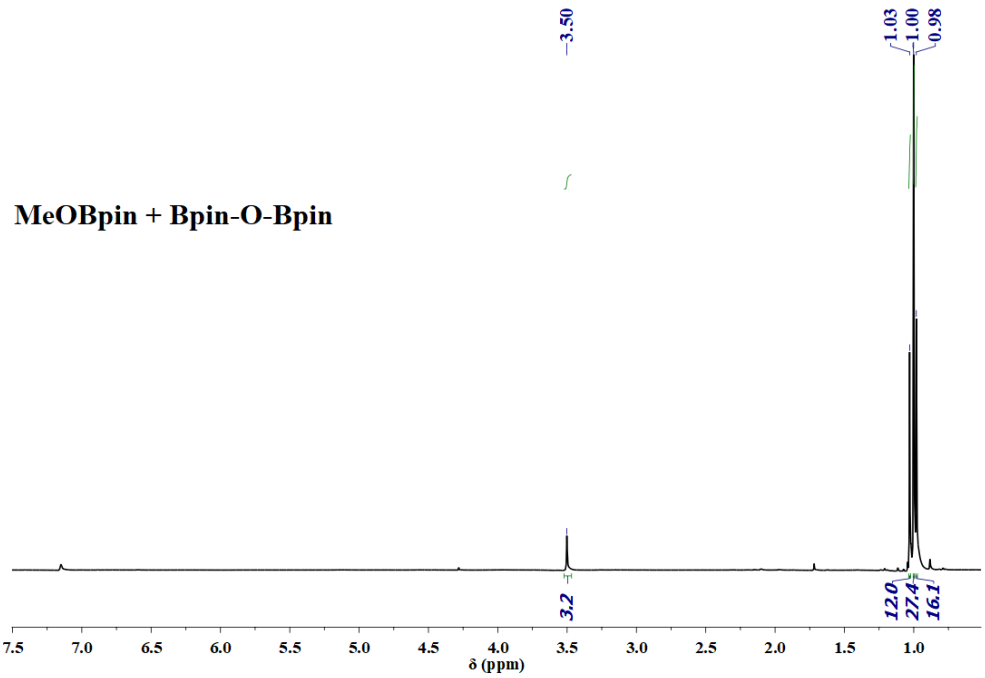


Figure S48. ^{1}H NMR spectrum of reduction of CO_2.

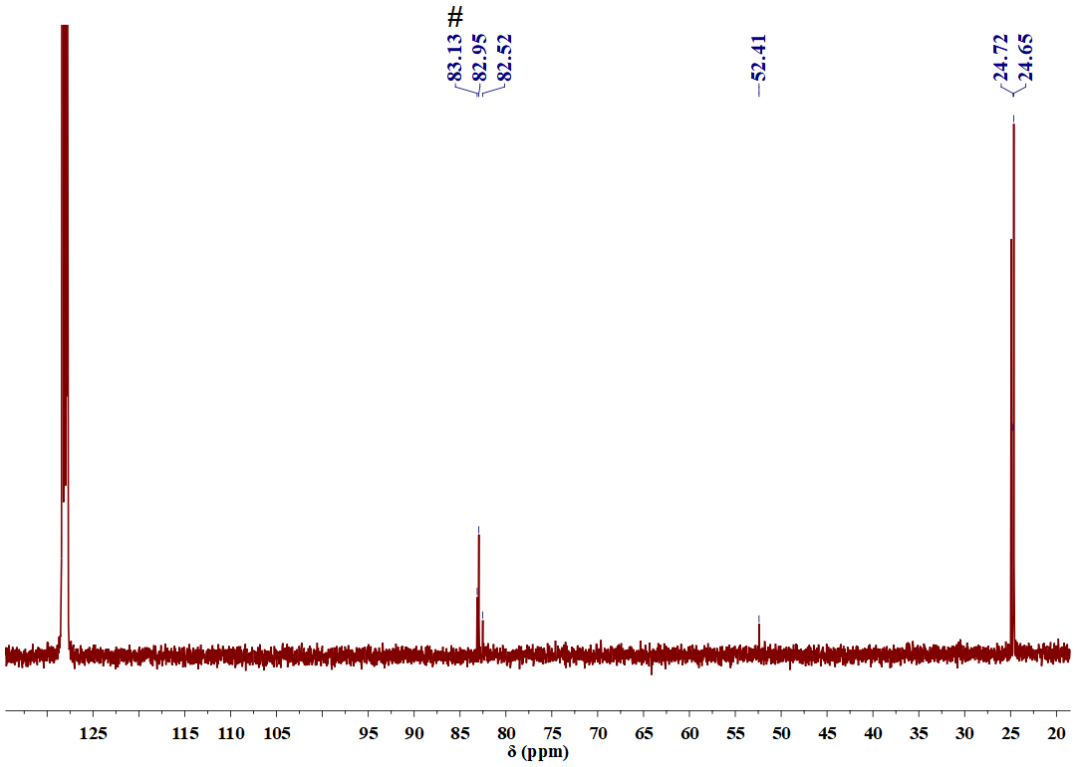


Figure S49. ^{13}C NMR spectrum of reduction of CO_2.

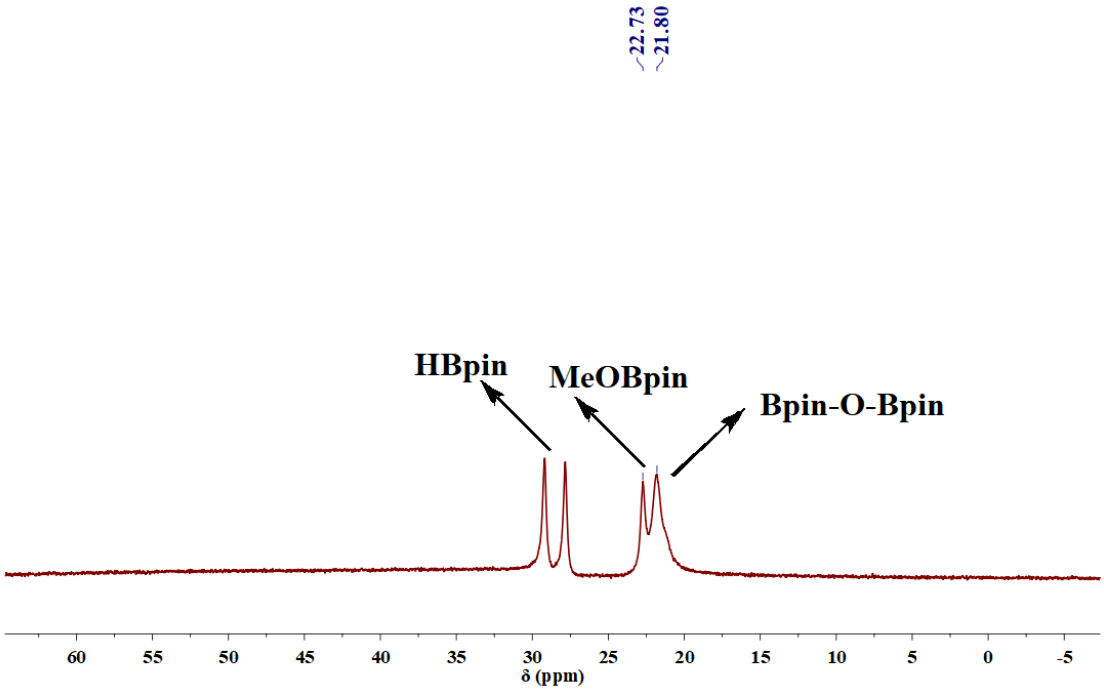


Figure S50. ^{11}B NMR spectrum of reduction of CO_2 (Entry 19, table 2).

5. Kinetic experiments

All the kinetic experiments were done in a similar method. In the glove box, to a J. Young NMR tube, typical amount of thorium catalyst (**Th-4**), ethylene carbonate and HBpin from a stock solution (**Th-4**, 10 mM, ethylene carbonate 100 mM and HBpin 300 mM) are transferred diluted to 0.6 ml by adding C_6D_6 and the NMR tube immediately loaded for measurement . All the experiments were done by changing either one substrate or the catalyst while keeping the other reagents constant and the data was collected early in the reaction (conversion less than 20%). The product concentrations were measured by the signal area ratio of the $–CH_2$- hydrogen of reagent and product. Reaction rates were determined by least-square fit of the initial product concentration versus time.

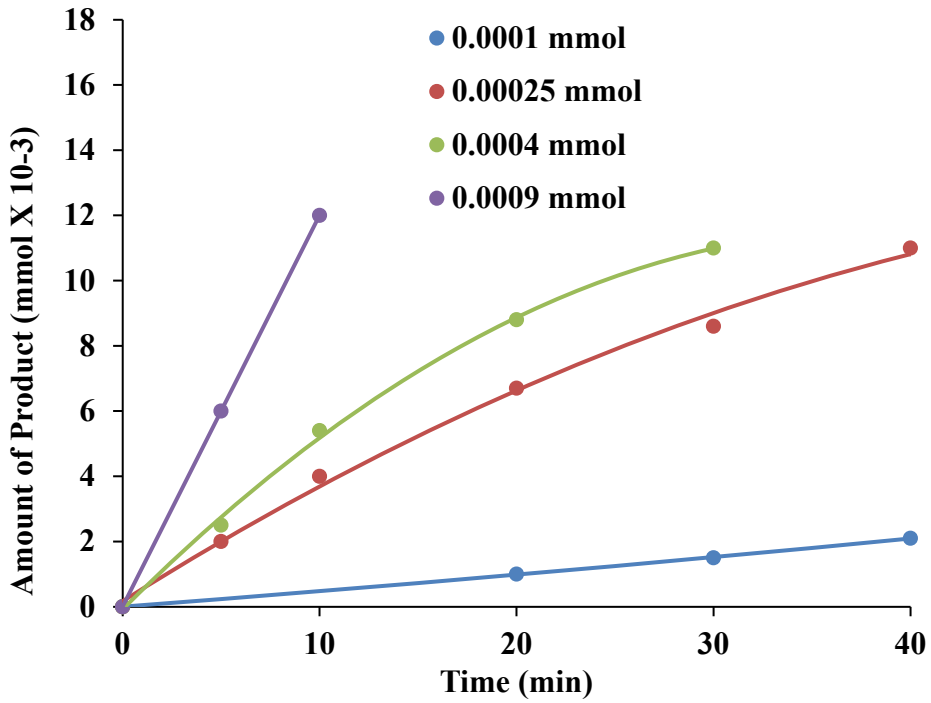


Figure S51. Plot of amount of product (X 10^{-3} mmol) vs. time (min) in the reaction of 0.1 mmol of ethylene carbonate and 0.3 mmol of HBpin catalyzed by different amount of **Th-4** at room temperature.

[**Th-4**] (mmol)×10^{-3}	Rate (mmol/min) ×10^{-3}	ln[**Th-4**]	ln(Rate)
0.10	0.060	-9.210	-9.721
0.25	0.315	-8.294	-8.026
0.40	0.440	-7.824	-7.728
0.90	0.920	-7.013	-6.991

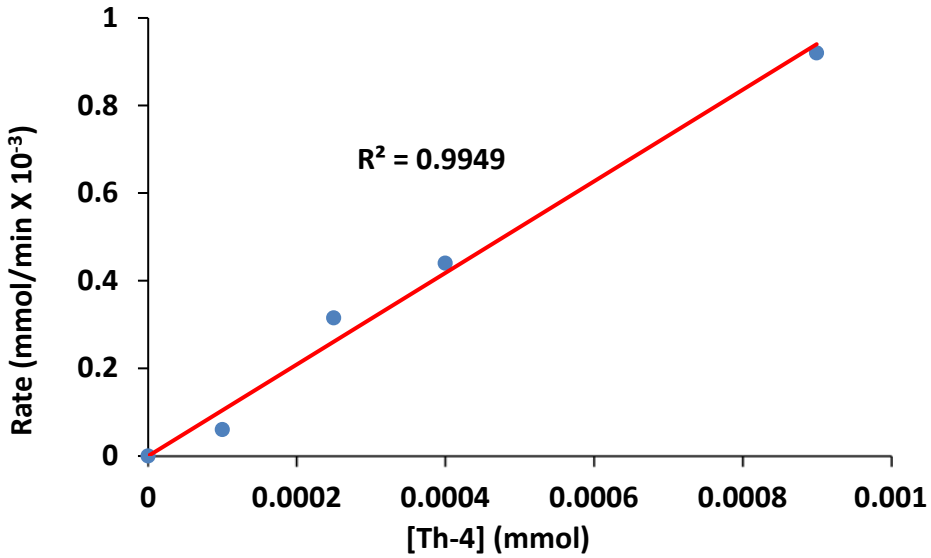


Figure S52. Plot of rate (X 10^{-3} mmol) vs. **Th-4** concentrations in the reaction of ethylene carbonate and HBpin at room temperature.

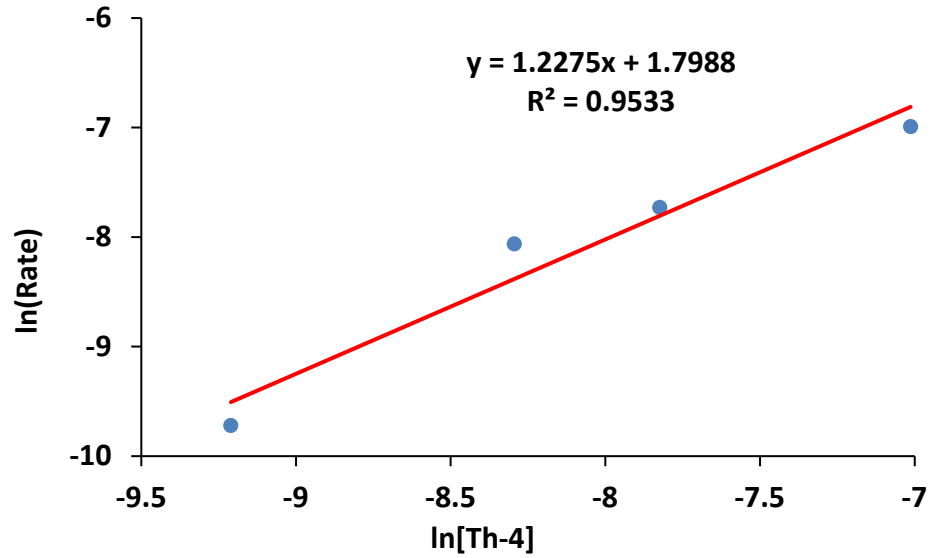


Figure S53. Plot of ln(rate) vs. ln[**Th-4**].

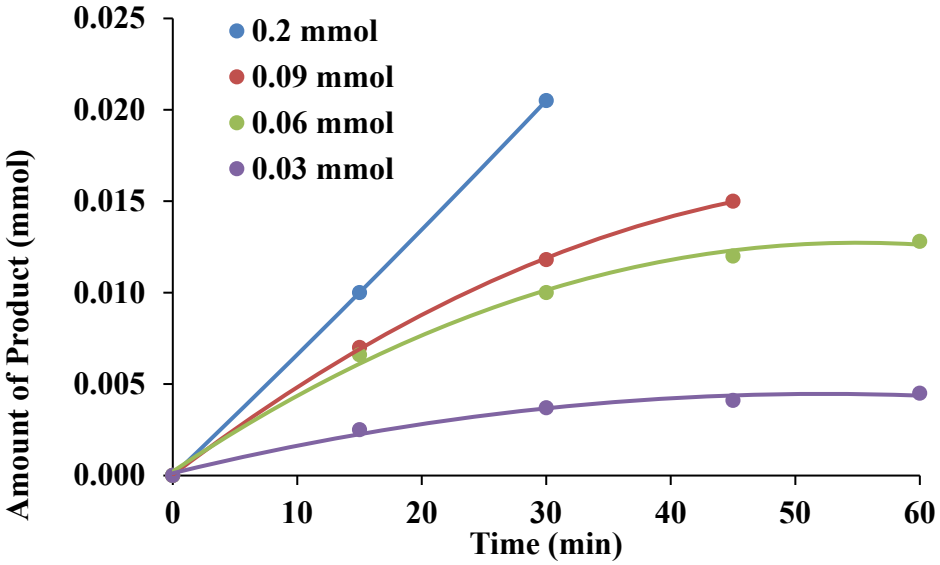


Figure S54. Plot of amount of product (X 10^{-3} mmol) vs. time in the reaction of 0.1 mmol of ethylene carbonate and different HBpin amount catalyzed by 0.001 mmol of **Th-4** at room temperature.

[HBpin] (mmol)	Rate (mmol/min) X 10^{-3}	ln[HBpin]	ln(rate)
0.03	0.122	-3.506	-9.003
0.06	0.313	-2.813	-8.069
0.09	0.395	-2.407	-7.836
0.20	0.684	-1.609	-7.287

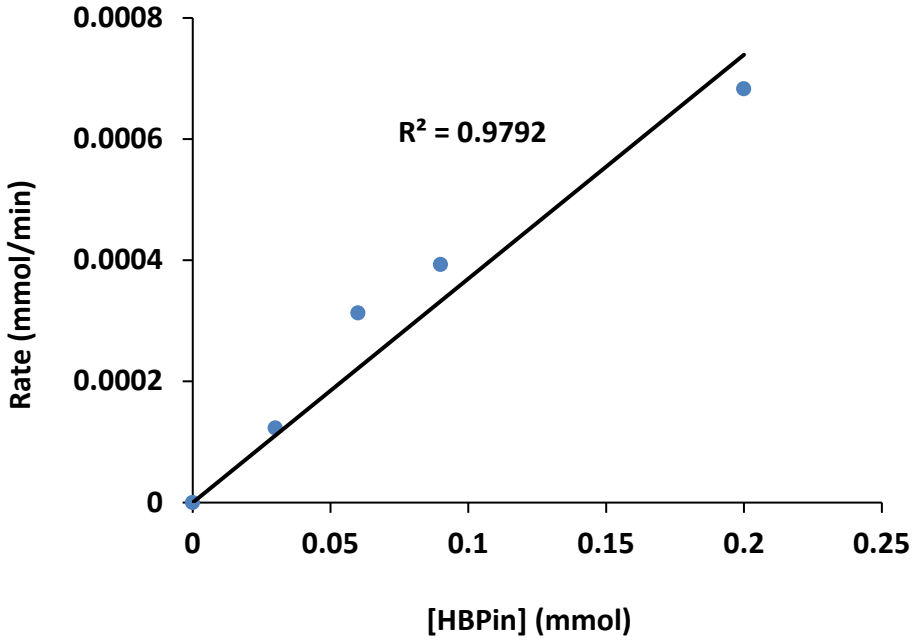


Figure S55. Plot of rate (X 10^{-3} mmol) vs. HBpin amount in the reaction of ethylene carbonate and HBpin at room temperature.

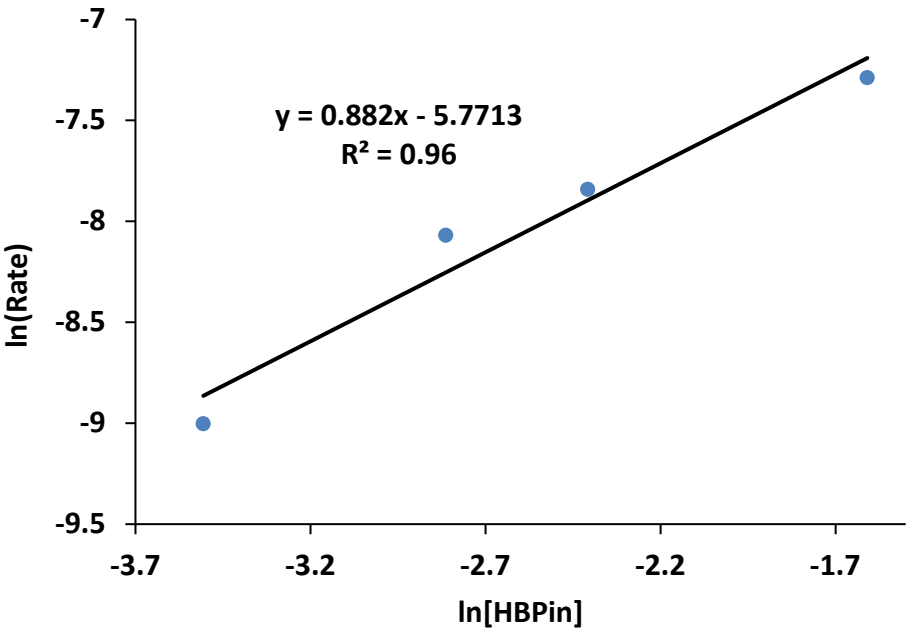


Figure S56. Plot of ln(rate) vs. ln[HBpin].

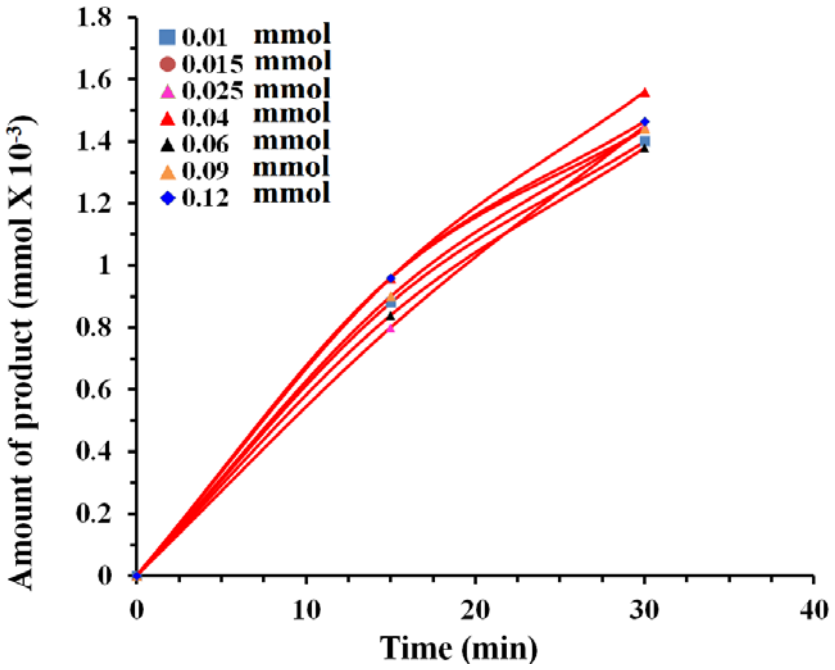


Figure S57. Plot of amount of product (X 10^{-3} mmol) vs. time in the reaction of different mmol of ethylene carbonate and 0.3 mmol of HBpin catalyzed by 0.0001 mmol of **Th-4** at room temperature.

[Ethylene Carbonate] (mmol)	Rate (mmol/min) X 10^{-3}	ln[Ethylene carbonate]	ln(rate)
0.01	0.0491	-4.605	-2.83532
0.015	0.0512	-4.199	-2.74887
0.025	0.0493	-3.688	-2.93182
0.040	0.0544	-3.218	-2.74887
0.060	0.048	-2.813	-2.8824
0.090	0.0504	-2.407	-2.81341
0.120	0.0518	-2.120	-2.74887

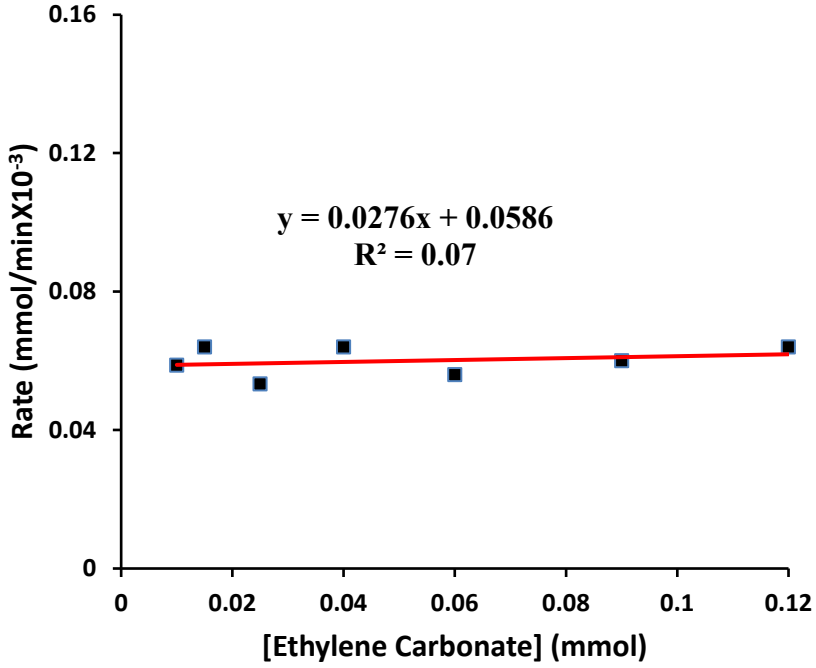


Figure S58. Plot of rate (X 10^{-3} mmol) vs. Ethylene carbonate amount in the reaction of ethylene carbonate and HBpin catalyzed by **Th-4** at room temperature.

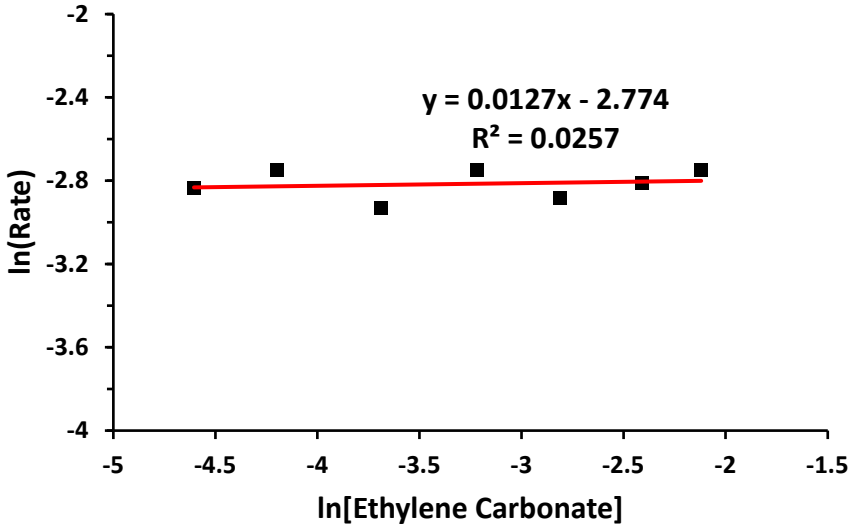


Figure S59. Plot of ln(rate) vs. ln[Ethylenecarbonate].

6. Activation parameters

Activation parameters including enthalpy ($\Delta H^{\ddagger}$), entropy ($\Delta S^{\ddagger}$) and activation energy (Ea) were calculated from kinetic data using Eyring and Arrhenius plots. Performed in a similar manner as the kinetic experiments. In a typical sample, the J. Young tube was loaded with desired amount

of thorium catalyst (**Th-4**) (0.001 mmol) from stock solution, ethylene carbonate (0.1 mmol), HBpin (0.3 mmol), from stock solution, diluted to final volume of 0.6 mL with C_6D_6, and sealed. Then the sample was inserted into Bruker Avance 300 spectrometer, which had been previously set to the desired temperature (40-70 °C). The data was collected at appropriate time intervals. Reaction rates at each temperature were determined by the least square fit of initial product concentration versus time. These data were then plotted as 1/T vs. ln(k/T) from which the enthalpy ($\Delta H^{\ddagger}$), and the entropy ($\Delta S^{\ddagger}$) of the transition state could be derived using the Eyring equation. And From a plot of 1/T vs. ln(k), the activation energy can be obtained using the Arrhenius equation. Enthalpy ($\Delta H^{\ddagger}$), entropy ($\Delta S^{\ddagger}$) and activation energy (Ea) were calculated from the slope and intercept of the least-square fit.

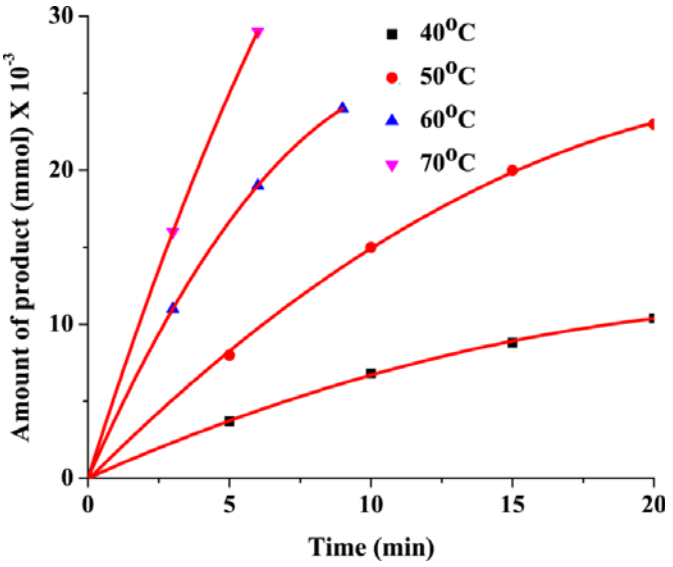


Figure S60. Plot of amount of product (X 10^{-3} mmol) vs. time (min) in the reaction of 0.1 mmol of ethylene carbonate and 0.3 mmol of HBpin catalyzed by 0.001 mmol **Th-4** at different temperature.

Temp (K)	Rate (mmol/min) X10^{-3}	1/T	k/T	Ln(k)	ln(k/T)
313	0.74	0.003195	2.36E-06	-7.20886	-12.9551
323	1.60	0.003096	4.95E-06	-6.43775	-12.2154
333	3.10	0.003003	9.31E-06	-5.77635	-11.5845
343	4.80	0.002915	1.4E-05	-5.33914	-11.1769

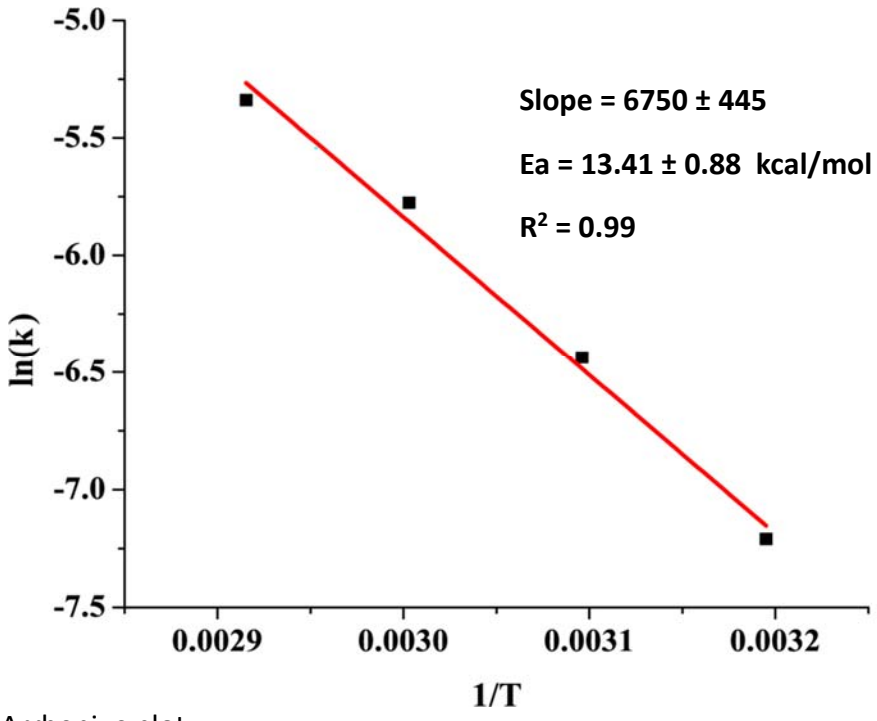


Figure S61. Arrhenius plot.

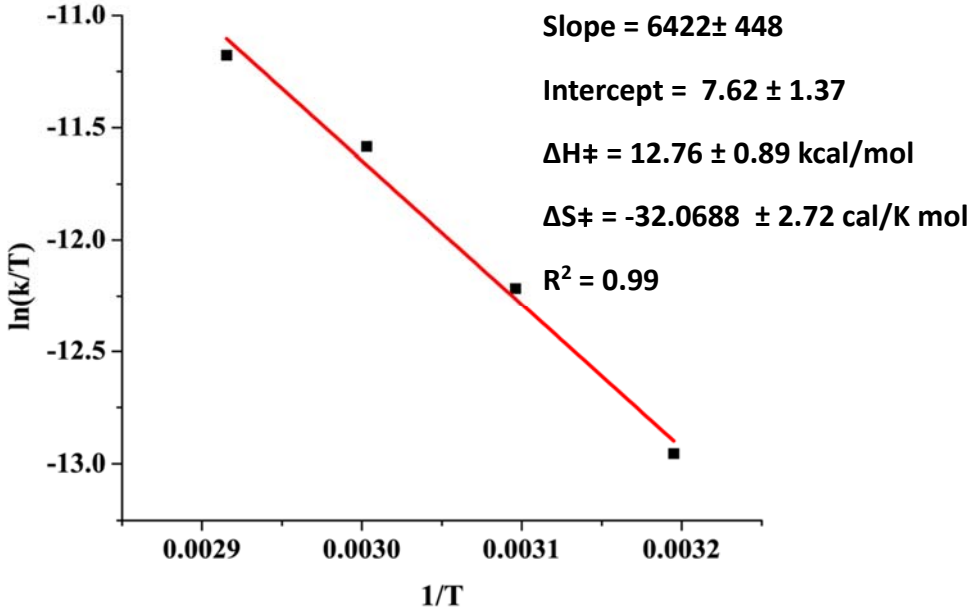


Figure S62. Eyring plot.

7. Kinetic Isotope Effect

In a typical sample, the J. Young tube was loaded with desired amount of thorium catalyst (**Th-4**) (0.0005 mmol, 0.5 mol %) from stock solution, ethylene carbonate (0.1 mmol), HBpin or DBpin (0.3 mmol), diluted to final volume of 0.6 mL with C_6D_6, and sealed. The data was collected early in the reaction (conversion less than 20%). The KIE value was calculated from the ratio (k_H/k_D) of the two slopes.

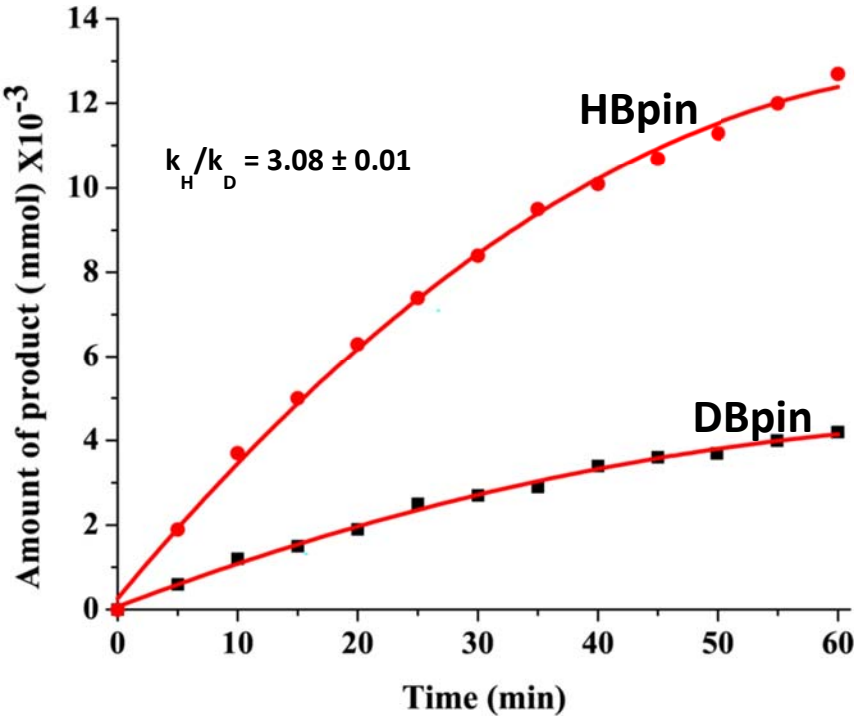


Figure S63. Plot of amount of product (X 10^{-3} mmol) vs. time (min) in the reaction of 0.1 mmol of ethylene carbonate and 0.3 mmol of HBpin (red dot) and 0.3 mmol of DBpin (black dot) catalyzed by 0.0005 mmol **Th-4** at room temperature.

8. Stoichiometric reactions and controlled experiments

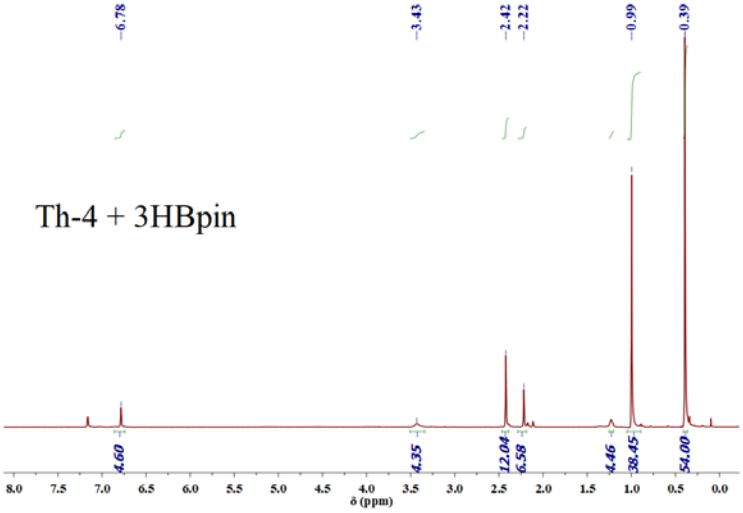


Figure S64. ^{1}H NMR spectrum **Th-4** + 3 equivalents of HBpin after 5 hours at room temperature in C_6D_6.

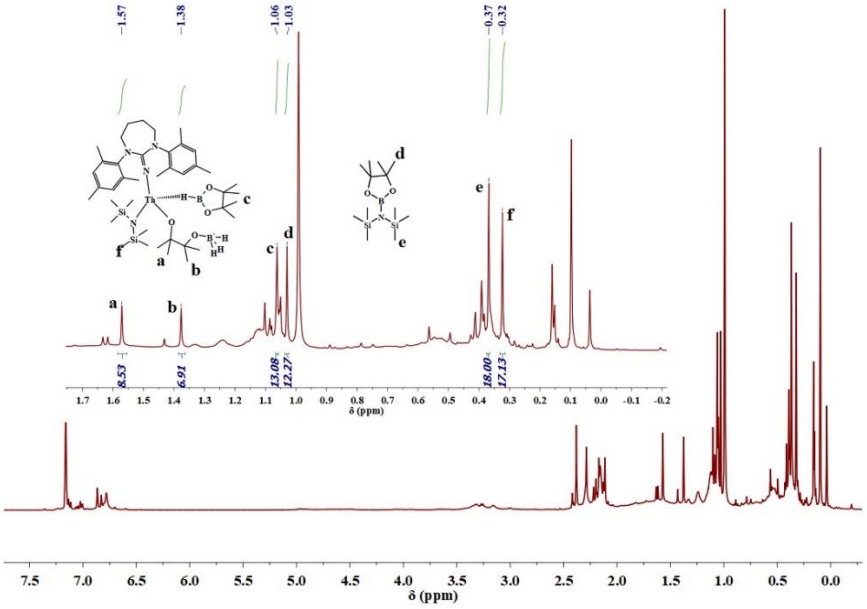


Figure S65. 1H NMR spectra of catalyst deactivation product obtained from 1:3 mixture of **Th-4** and HBpin in benzene-d6 after heating 80°C for 1 hour. Expanded portion with relevant peaks labeled are shown in inset.

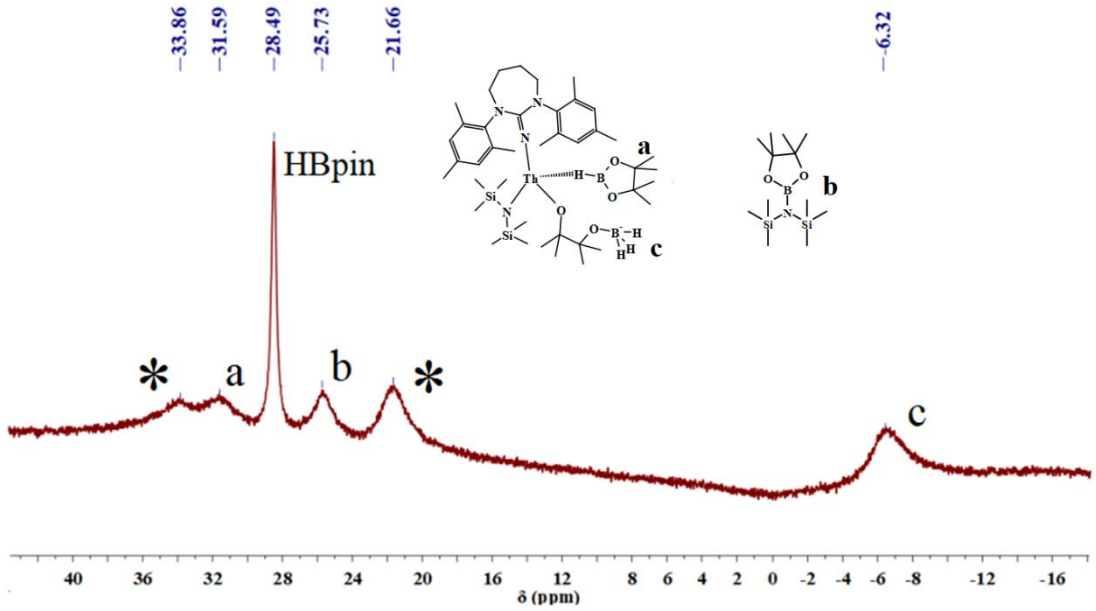


Figure S66. ^{11}B NMR spectra of catalyst deactivation product obtained from 1:3 mixture of **Th-4** and HBpin in benzene-d6 after heating 80°C for 1 hour. *indicates unidentified degradation products.

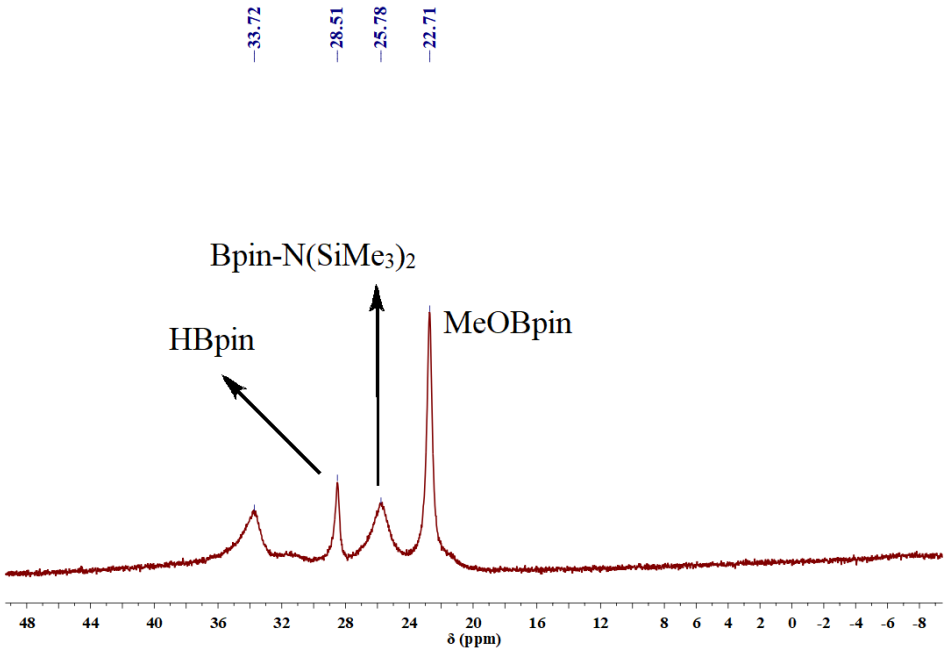


Figure S67. ^{11}B NMR spectra of catalyst deactivation product obtained from 1:3 mixture of **Th-4** and HBpin in benzene-d6 after heating 80°C for 1 hour and then adding 1 equivalent of dimethyl carbonate.

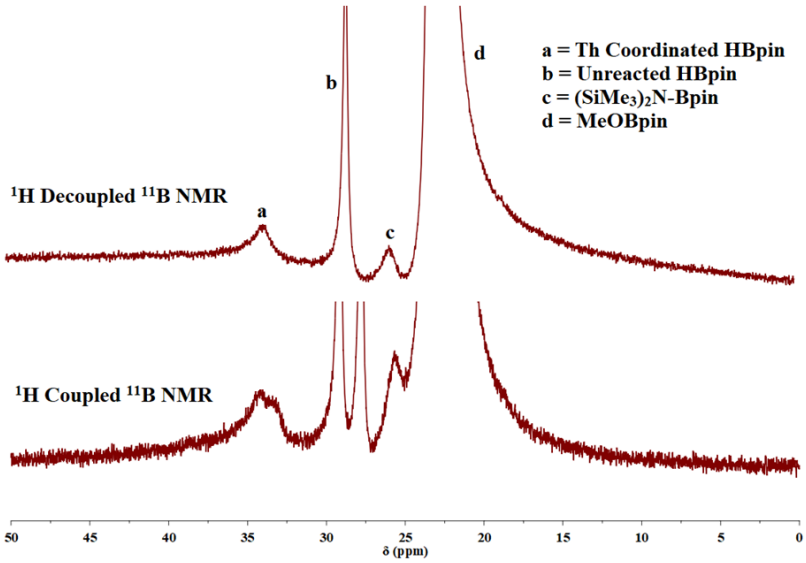


Figure S68. ^{11}B NMR spectra analysis of catalytic reaction of dimethyl carbonate with 3 equivalents of HBpin catalyzed by **Th-4** (1mol%) at 80°C after complete conversion of dimethyl carbonate to MeOBpin.

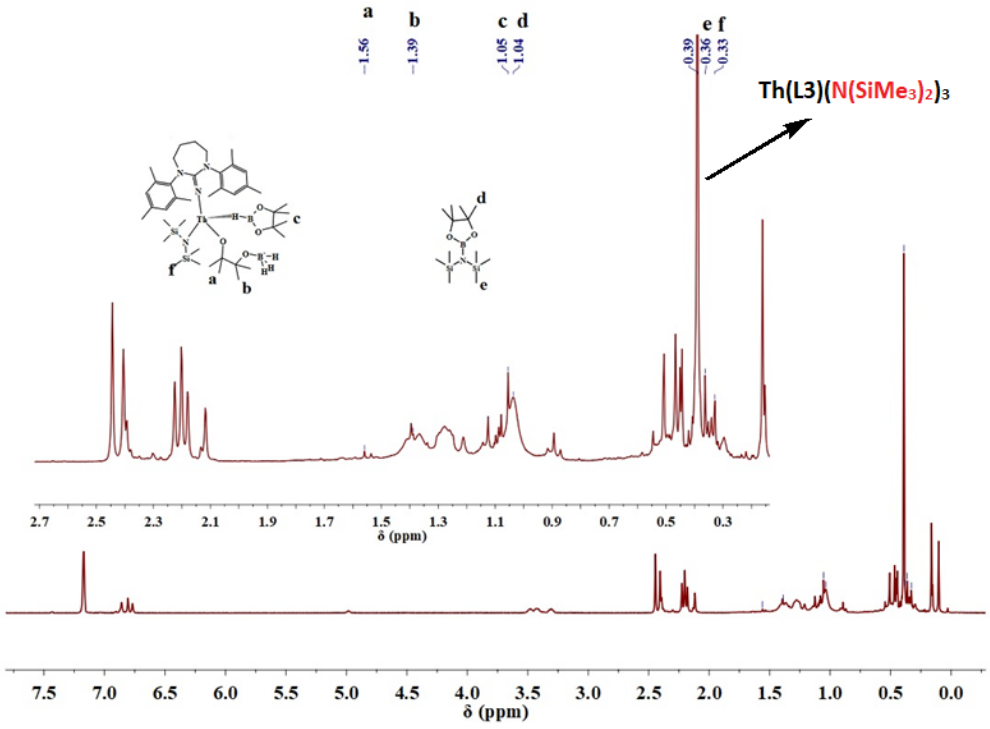


Figure S69. 1H NMR spectra of catalyst deactivation product obtained from reacton of **Th-4** and 1 equivalent HBpin in benzene-d6 after heating at 60°C for 1 hour. Expanded portion with relevant peaks labeled are shown in inset (Due to overlap of the peaks of several compounds, integration of the peaks are not taken).

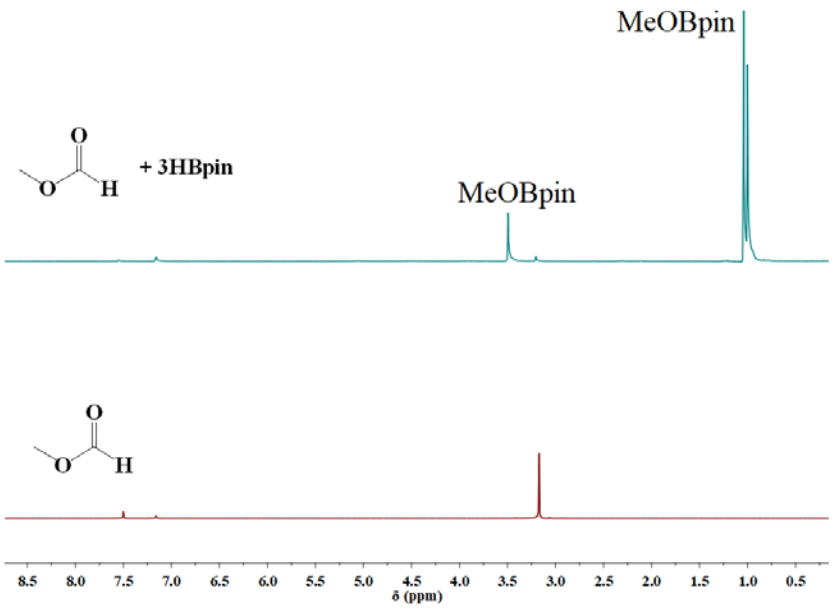


Figure S70. ^{1}H NMR spectrum of hydroboration of methyl formate catalyzed by **Th-4-H** at room temperature in 10 minutes.

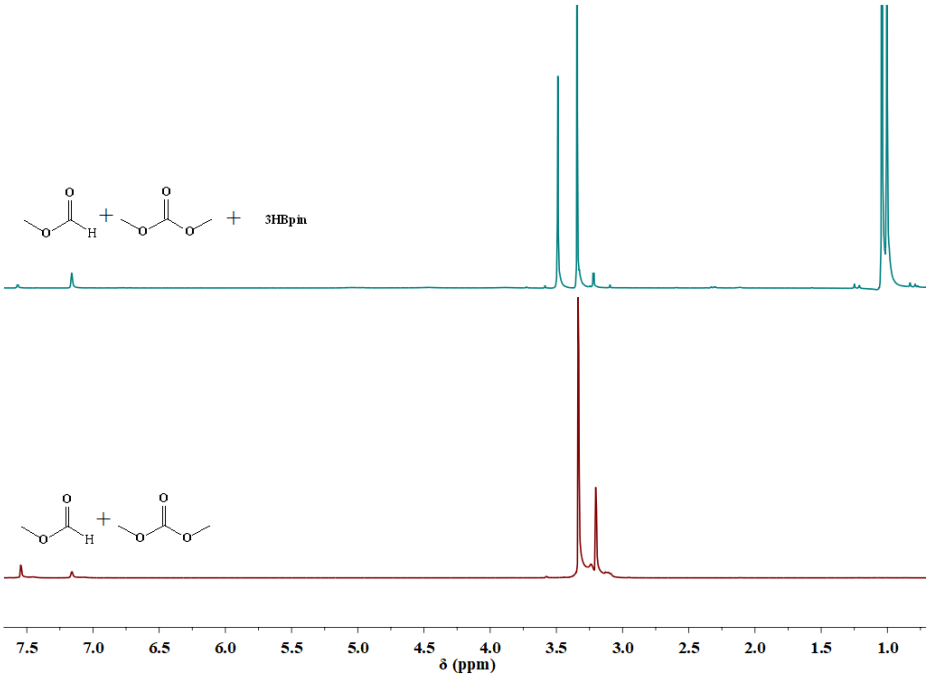


Figure S71. ^{1}H NMR spectrum of hydroboration of methyl formate in presence of dimethyl carbonate catalyzed by **Th-4-H** at room temperature in 10 minutes.

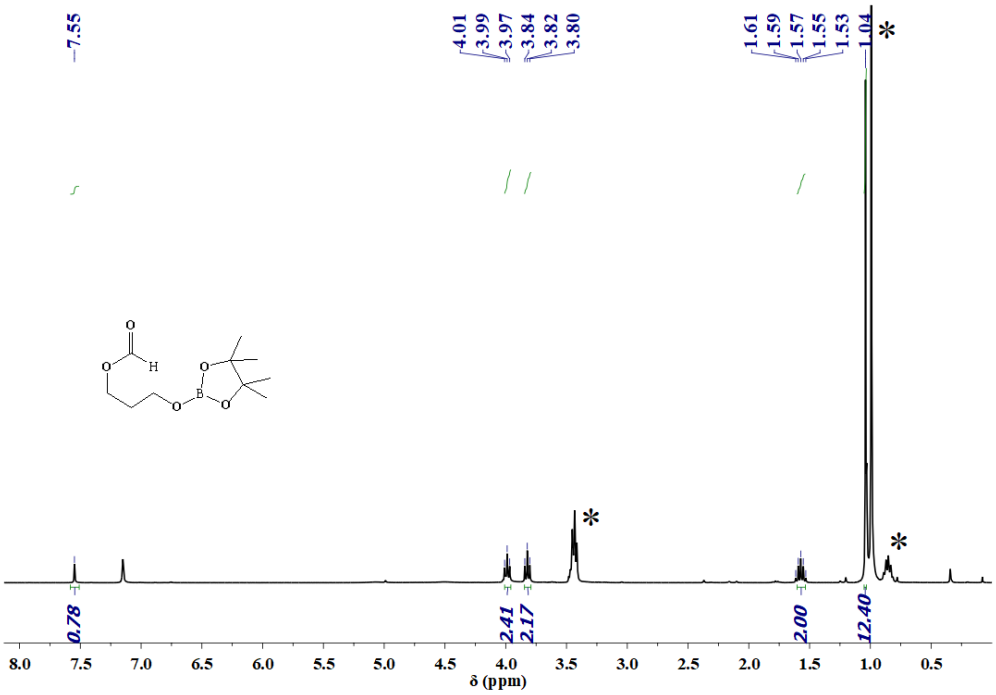
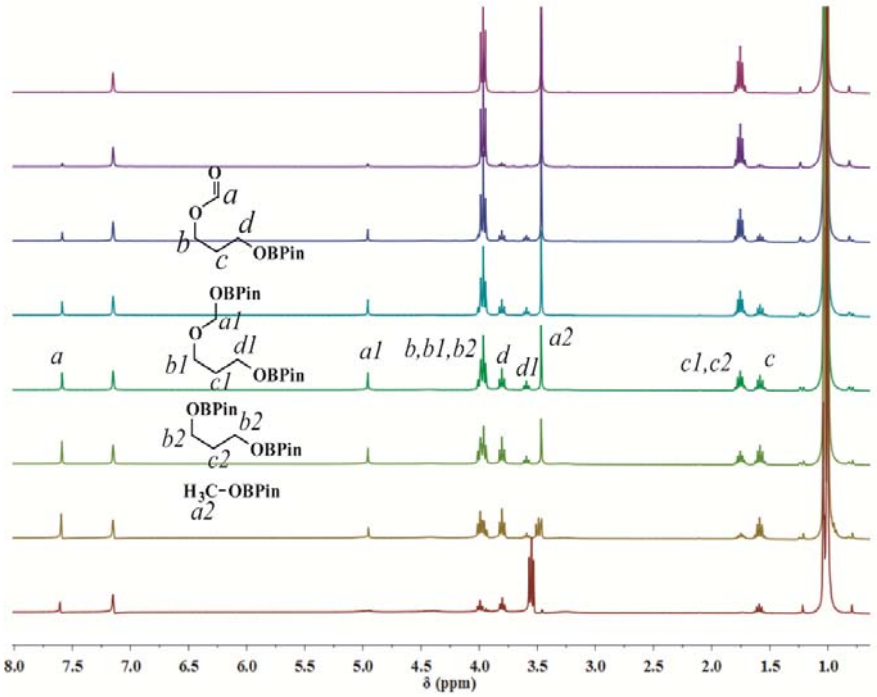
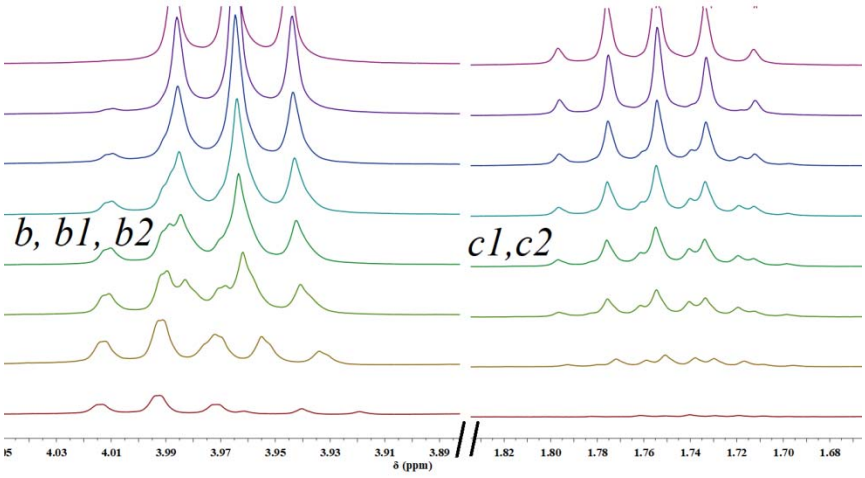


Figure S72. ^{1}H NMR spectrum of formate intermediate formed after 10 minutes of reaction of trimethylene carbonate and 1 equivalent of HBpin catalyzed by **Th-4** at room temperature. *Indicates the starting materials.



a)



b)

Figure S73. (a) ^{1}H NMR spectrum studies of reaction of trimethylene carbonate and 4.2 equivalent of HBpin catalyzed by **Th-4** at room temperature. Spectra were recorded after 30 minutes of interval. (b) Expansion of scale to visualize peaks for b, b1, b2 and c1, c2.

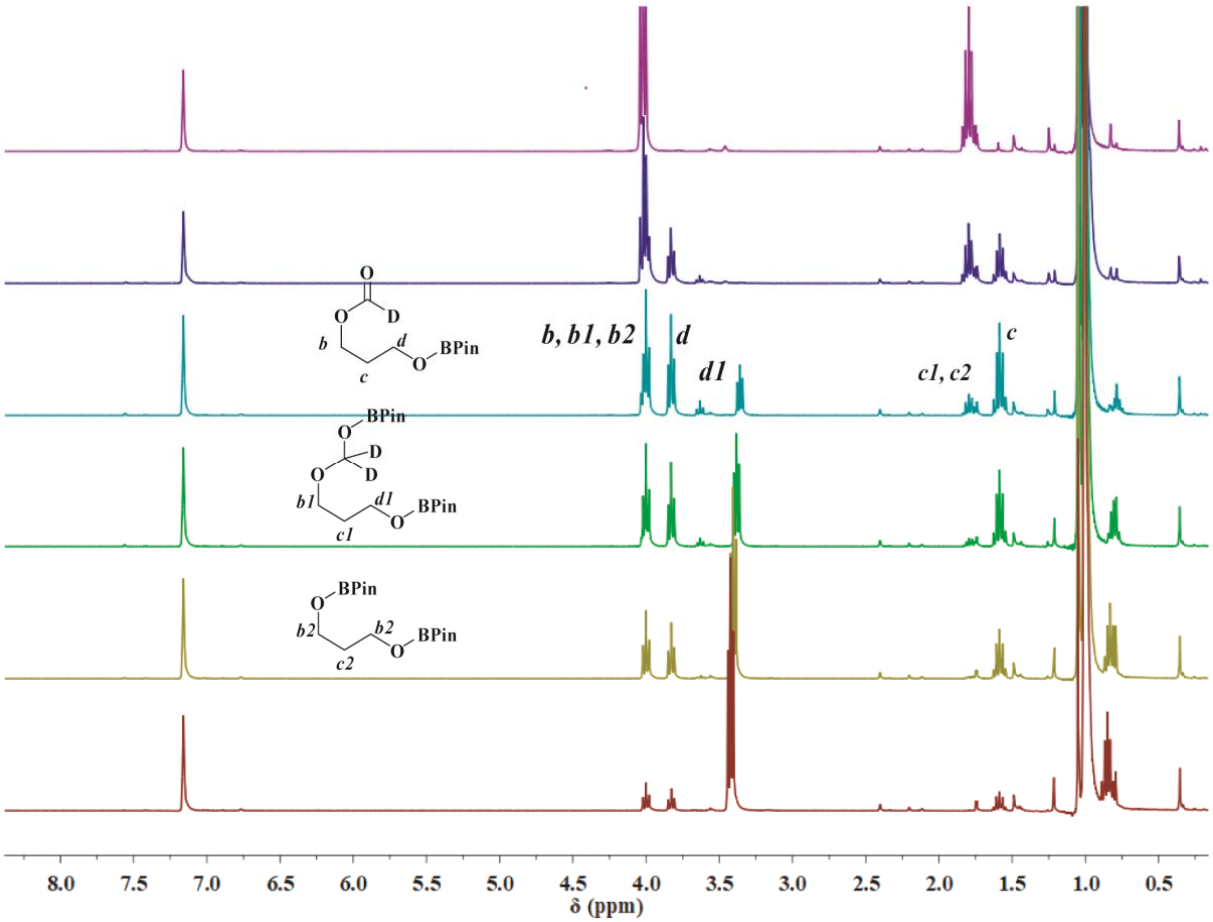


Figure S74. ^{1}H NMR spectrum studies of reaction of trimethylene carbonate and 4.2 equivalent of DBpin catalyzed by **Th-4** at room temperature. Spectra were recorded after 30 minutes of interval. Starting materials are at the bottom.

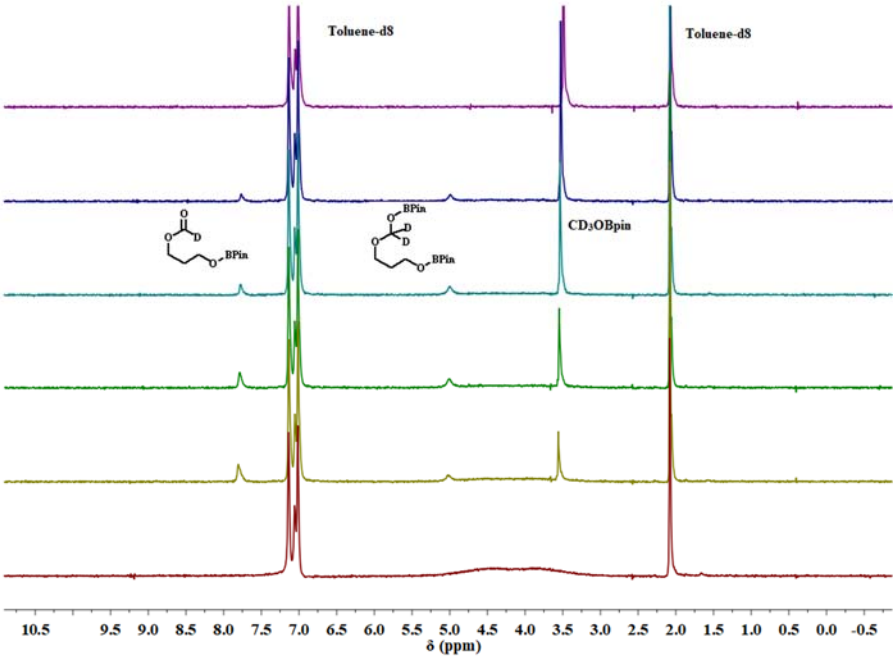


Figure S75. ^{2}H NMR spectrum studies of reaction of trimethylene carbonate and 4.2 equivalent of DBpin catalyzed by **Th-4** at room temperature. Spectra were recorded after 30 minutes of interval. Starting materials are at the bottom

Theoretical Study

9. Activation alternative mechanism

The activation step mechanism involving the carbonate (S74):

From **Th-4** complex (set as zero free energy) the carbonate coordinates to the metal forming an intermediate at 12.1 kcal/mol (Int-1'). The subsequent metathesis HBpin into Th-N* bond, from up (mechanism A) or from down (mechanism B), produces $(SiMe_3)_2N$-Bpin with a thorium alkoxide intermediate, Int-2-A, at 8.4 kcal/mol that evolves to the minimum Int-2-B at -43.8 kcal/mol from zero energy stabilized by the interaction of the carbonyl oxygen atom with the metal. However, the two suggested transitions state (TS1' and TS1'') involved in this metathesis step exceed 50 kcal/mol. For this reason, path A and B were ruled out.

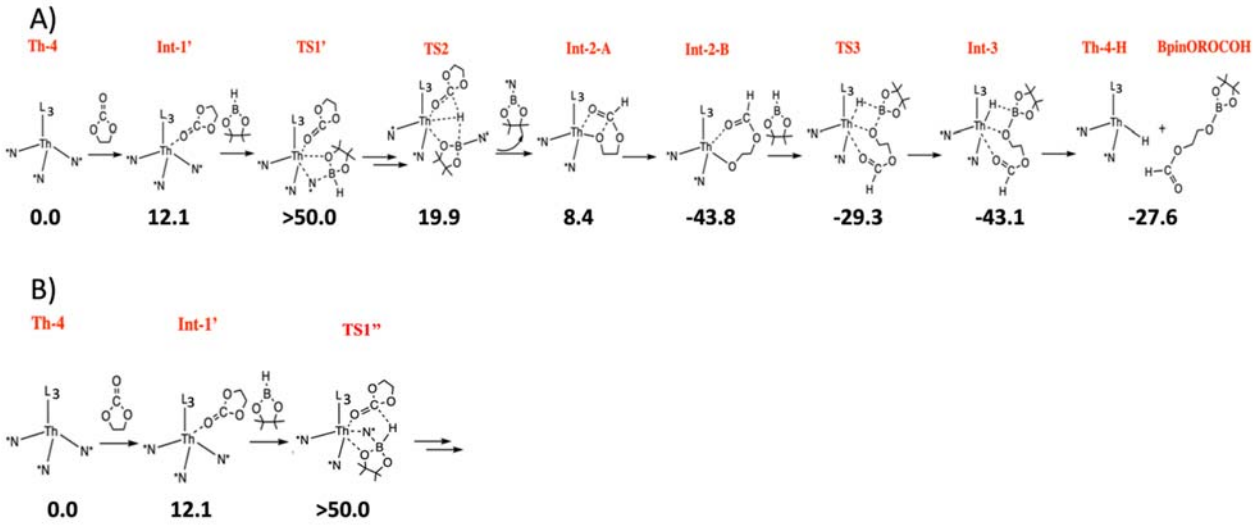


Figure S76. Proposed activation mechanisms of **Th-4** catalyst in presence of carbonate. The energy values are ΔG in kcal/mol in benzene solvent.

10. Deactivation mechanism

The deactivation of **Th-4-H** in presence of carbonate shows an energy barrier of 26 kcal/mol lower than the barrier observed for the deactivation reaction in absence of carbonate and the corresponding reaction product is about 30 kcal/mol more stable. These results, in agreement with the experimental observations, clearly indicate that the carbonate is essential in the reaction mixture to i) avoid the deactivation of the catalyst which otherwise occurs rapidly due to HBpin presence; ii) start the catalytic cycle.

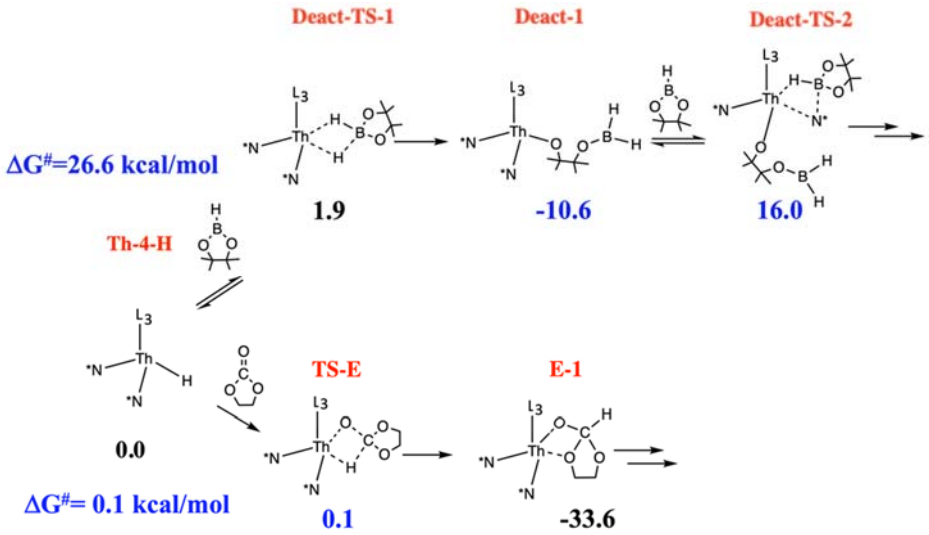


Figure S77. Proposed mechanism for the deactivation of the active species **Th-4-H** in absence and presence of carbonate. The energy values are ΔG in kcal/mol in benzene solvent.

11. Catalytic cycle

Starting from the intermediate **G**, lying at -66.9 kcal/mol, three catalytic cycles have been investigated.

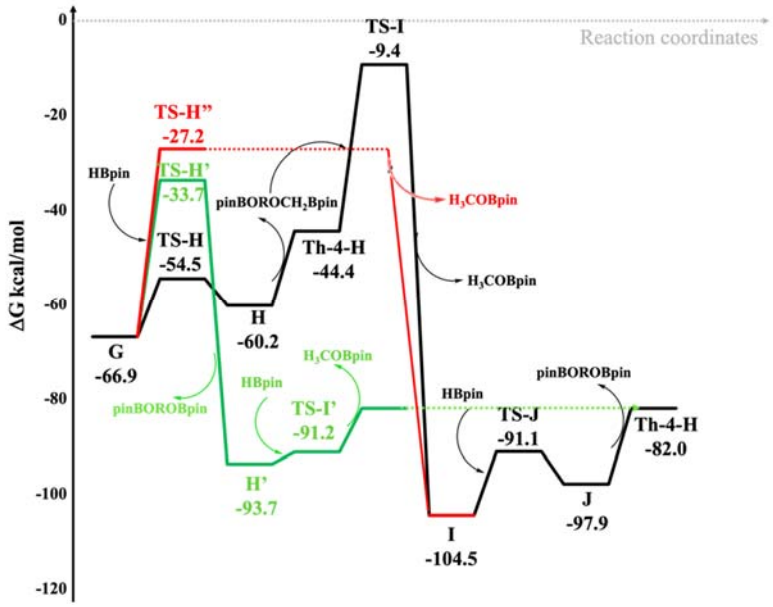
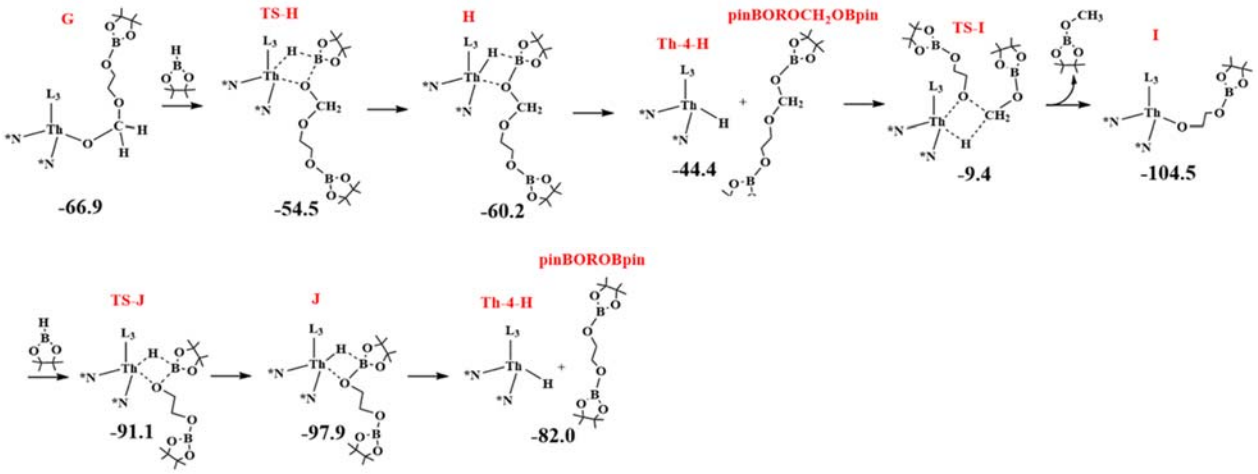
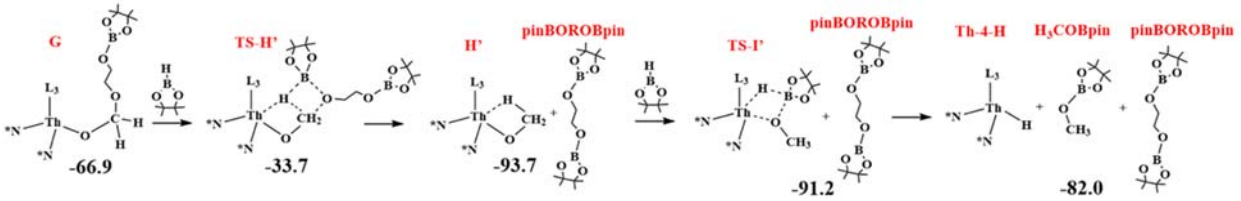


Figure S78. Competitive computed reaction pathways from intermediate **G** to **Th-4-H** passing from TS-H (black line), TS-H' (green line) and TS-H'' (red line). The Energy values are ΔG in kcal/mol in benzene solvent.

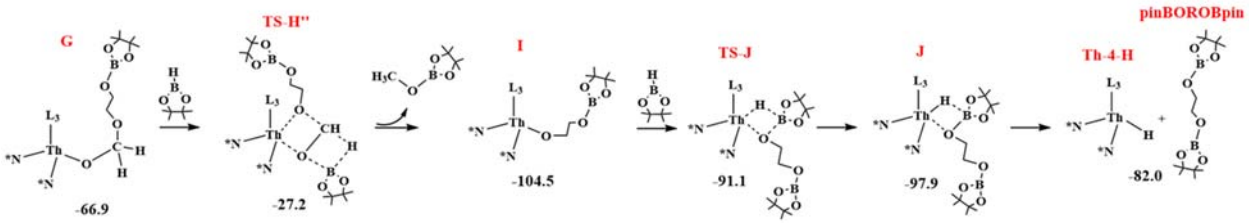
A)



B)



C)



Scheme S1. Proposed mechanism for the formation of the active thorium catalyst and the final product pinBOROBpin through A)TS-I, B)TS-H' and C) TS-H''. The energy values are ΔG in kcal/mol in benzene solvent.

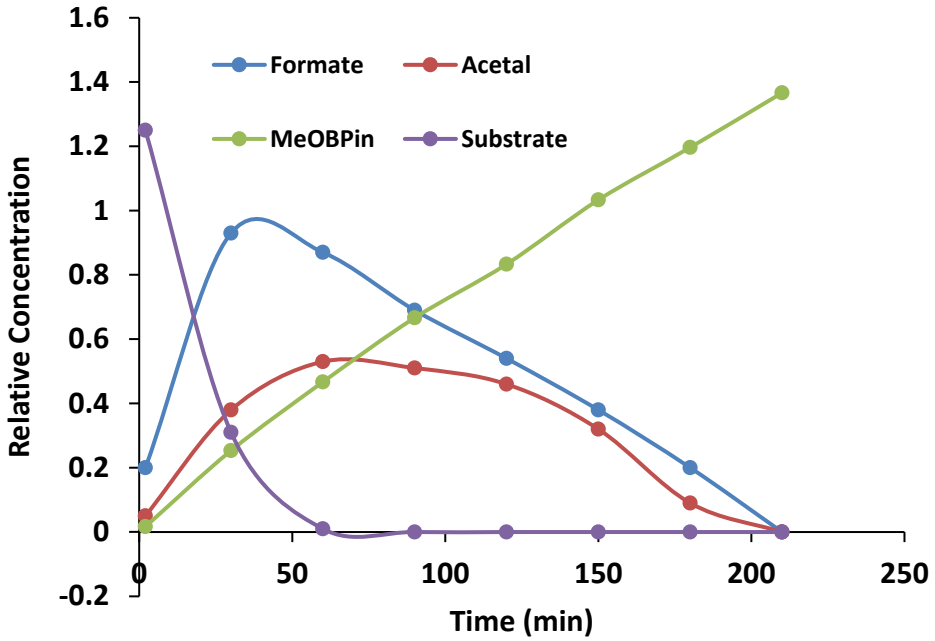


Figure 79: Changes of concentration of formate and acetal intermediate with respect to residual solvent peak as internal standard. Data were taken from NMR studies presented in Figure 2.

12. XYZ coordinates

Th-4

Th	-0.783659	-0.303288	0.027546
Si	-2.692901	1.868198	-1.911842
Si	-4.398717	0.931731	0.382389
Si	-0.658461	0.519365	3.406536
Si	-0.880649	-2.502703	3.078759
Si	-2.531450	-3.044811	-1.545393
Si	0.206837	-2.605436	-2.682449
N	1.280127	0.636330	-0.107696
N	3.634786	0.345812	0.361062
N	2.852104	2.453260	-0.271871
N	-2.817237	0.881150	-0.440449
N	-0.794374	-0.888657	2.323864
N	-1.009971	-2.114206	-1.467597
C	2.488971	1.108491	-0.021084
C	4.542800	0.873945	1.405894
H	4.929626	0.002173	1.969417
H	3.949848	1.481225	2.124900
C	5.736713	1.696147	0.902440
H	6.308174	1.085649	0.168731
H	6.424940	1.882055	1.756285
C	5.299834	3.017123	0.271226
H	4.943114	3.722333	1.053667
H	6.164306	3.512936	-0.222601
C	4.196231	2.828322	-0.780379
H	4.064378	3.784664	-1.321586
H	4.525660	2.077585	-1.525684
C	3.818111	-1.050410	0.031493
C	3.544971	-2.058370	0.998847
C	3.893872	-3.395336	0.719769
H	3.686699	-4.162944	1.484836
C	4.493391	-3.779372	-0.493963
C	4.733785	-2.770498	-1.443535

H	5.204068	-3.038923	-2.404869
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C	2.892440	-1.732553	2.317931
H	3.500010	-1.047020	2.943861
H	2.734273	-2.655108	2.907831
H	1.907540	-1.241917	2.170842
C	4.827023	-5.225333	-0.780821
H	5.110567	-5.771626	0.141872
H	5.659580	-5.318337	-1.507412
H	3.949918	-5.753433	-1.216552
C	4.785977	-0.400736	-2.266519
H	3.940665	0.271422	-2.515155
H	5.093683	-0.908997	-3.201519
H	5.635570	0.238641	-1.944321
C	1.883457	3.520278	-0.378764
C	1.465081	3.952804	-1.667782
C	0.684454	5.120031	-1.771960
H	0.369918	5.457357	-2.774268
C	0.290745	5.862730	-0.641794
C	0.707556	5.402750	0.621576
H	0.421687	5.971914	1.522453
C	1.511466	4.254648	0.777611
C	1.895849	3.224617	-2.921671
H	2.873826	3.600062	-3.296930
H	1.161854	3.371113	-3.737960
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H	1.494695	4.460399	2.936640
H	3.105737	4.104263	2.251258
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H	-4.315756	0.668338	-3.470252
H	-5.074848	2.141799	-2.777987
C	-1.141473	1.265838	-2.837557
H	-0.193953	1.358578	-2.258369
H	-0.991313	1.875646	-3.752896
H	-1.261469	0.210206	-3.158658
C	-2.497957	3.719932	-1.544431
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H	-2.247270	4.275931	-2.473334
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H	-3.509609	-0.516149	2.303001
H	-5.272028	-0.202779	2.442658
H	-4.094001	1.072096	2.869737
C	-5.756680	-0.051560	-0.527144
H	-5.964543	0.351066	-1.538437
H	-6.700806	0.013221	0.057248
H	-5.506613	-1.124790	-0.638912
C	-1.008414	2.084878	2.372966
H	-0.311071	2.219016	1.514173
H	-0.858487	2.976486	3.017386
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H	-2.917291	0.404020	4.587145
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H	-1.619196	-0.303261	5.601001
C	-2.635015	-2.950835	3.677389

H	-2.955513	-2.272143	4.495230
H	-2.634084	-3.984935	4.086661
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H	-0.577515	-4.823128	2.134256
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H	0.551495	-4.990626	-1.898691
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H	-2.973575	-3.596999	0.866692
H	-4.494160	-3.292092	-0.018148
H	-3.519511	-1.919489	0.548853
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H	-1.827829	-5.186702	-2.777490
H	-3.292234	-5.407051	-1.774244
H	-1.678473	-5.369443	-0.997868
C	-0.580807	7.089836	-0.782116
H	-0.508479	7.749009	0.106335
H	-0.308333	7.685873	-1.677420
H	-1.649584	6.802889	-0.896107
H	-6.014712	2.643463	1.215632
H	-5.405435	3.158060	-0.384158
H	-3.853184	2.291857	-4.072810

E(solv)= -4086.81214488 A.U
Thermal correction= 1.022026

Act-TS1

Th	-0.739747	0.114314	-0.595894
N	-1.524221	-2.229510	0.064689
N	-0.652312	0.860145	-2.861425
N	-2.630642	1.385814	0.030887
Si	-2.740019	2.323209	1.550936
Si	-1.065665	0.112800	-4.428870
Si	-0.349796	-3.361991	-0.698317
Si	-3.200624	-2.894785	0.232971
Si	-4.050708	1.618355	-1.036271
Si	0.084952	2.483404	-2.993499
C	-3.245647	-4.518772	1.230550
H	-3.009913	-4.343984	2.297744
H	-4.273321	-4.939878	1.178804
H	-2.551843	-5.292439	0.841106

C	-4.391826	-1.678536	1.065575
H	-4.375511	-1.804573	2.163953
H	-4.111850	-0.627612	0.856485
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C	-4.002225	-3.388831	-1.437210
H	-3.784458	-2.702923	-2.278597
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H	-5.105206	-3.392880	-1.297039
C	0.691116	-4.424859	0.473283
H	0.068410	-5.189374	0.980302
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H	1.207008	-3.825483	1.244910
C	-1.028358	-4.630811	-1.950158
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H	-1.616260	-4.192219	-2.778017
H	-0.138840	-5.130072	-2.394459
C	0.847004	-2.263281	-1.686971
C	-0.593885	3.628498	-4.360011
C	1.956209	2.393258	-3.317213
H	2.417577	3.403492	-3.282146
H	2.438245	1.755363	-2.550967
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C	0.403681	0.102598	-5.647469
H	1.302511	-0.368106	-5.197102
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H	0.686879	1.118893	-5.991984
C	-2.515616	0.950371	-5.343072
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H	-4.702159	-0.745569	-1.594590
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H	-3.044241	3.064918	-2.838997
H	-4.824018	3.248811	-2.772362
H	-3.793340	4.092228	-1.572473
C	-5.719908	1.783627	-0.121044
H	-5.798720	2.681468	0.524125
H	-6.516038	1.861984	-0.893544
H	-5.943476	0.892229	0.499242
C	-3.894898	1.543322	2.846342
O	0.164158	-2.183797	2.721116
C	-0.220363	-2.818949	3.980128
C	-1.611286	-2.113551	4.304860
O	-2.076205	-1.691198	2.991447
C	0.888585	-2.536691	5.002709
H	1.823970	-3.039027	4.683329
H	1.100040	-1.455707	5.099511
C	-0.335438	-4.336840	3.777700
H	-0.591373	-4.845266	4.729497
H	-1.101562	-4.597032	3.024226
H	0.635679	-4.739488	3.429204
C	-2.666132	-3.022699	4.943538
H	-3.605193	-2.452830	5.094417
H	-2.900676	-3.902078	4.315374
H	-2.324554	-3.383188	5.935910
B	-0.951877	-1.542705	2.170528
H	-0.725461	-0.432578	1.684635

H	-2.424785	-0.305906	5.190119
C	-1.454831	-0.840879	5.158818
H	-0.703995	-0.150369	4.726046
H	-1.156280	-1.077034	6.200311
H	0.615334	-2.935205	6.001845
H	1.652993	-2.900603	-2.105105
H	0.380876	-1.755150	-2.557259
H	1.390914	-1.500724	-1.082549
N	1.391621	0.605869	0.096444
C	2.667506	0.837517	0.202377
N	3.254148	1.742413	1.117119
N	3.654208	0.239991	-0.666024
C	4.729937	1.115360	-1.177029
C	6.051143	0.941596	-0.420236
C	5.750990	0.864804	1.080089
H	6.583143	0.025559	-0.754004
H	6.717707	1.801282	-0.655051
C	4.688099	1.870994	1.538467
H	5.458368	-0.166648	1.356315
H	6.664161	1.087851	1.673307
C	2.504421	2.758555	1.827553
C	3.845100	-1.170943	-0.833821
C	-1.050797	2.442429	2.387354
C	-3.271925	4.140615	1.293141
C	2.102264	2.516451	3.167774
C	1.604108	3.589286	3.930745
C	1.468347	4.887383	3.401848
C	1.866199	5.096682	2.068316
C	2.410477	4.063875	1.276575
C	2.200833	1.137506	3.773527
H	1.298760	3.398188	4.973650
C	0.882941	6.008846	4.230243
H	1.782446	6.107238	1.633398
C	2.947538	4.384006	-0.099396
H	-0.228188	6.008232	4.173214
H	1.152281	5.909807	5.301824
H	1.226555	7.002588	3.878164
H	2.664644	3.622474	-0.850205
H	2.577963	5.367390	-0.450952
H	4.059338	4.441644	-0.094233
H	1.791345	1.130758	4.802947
H	1.645480	0.392819	3.166704
H	3.251002	0.777453	3.834538
H	-0.074403	4.606192	-4.254569
H	-0.381146	3.254481	-5.382430
H	-1.682357	3.820499	-4.279912
H	-3.272785	4.650451	2.281362
H	-2.554557	4.681697	0.641112
H	-4.285872	4.260815	0.861277
H	-3.846134	2.143458	3.781457
H	-4.955527	1.494995	2.532052
H	-3.557810	0.512269	3.078494
H	-1.178479	3.003500	3.336808
H	-0.614758	1.458852	2.649204
H	-0.305362	2.993183	1.781801
C	4.157214	-1.693996	-2.130410
C	4.531709	-3.046416	-2.261576
C	4.574036	-3.933164	-1.172018
C	4.178007	-3.421646	0.076463
C	3.812560	-2.074921	0.277747
C	4.019817	-0.887838	-3.403964
H	4.774353	-3.422584	-3.270635
C	5.029400	-5.366351	-1.331843
H	4.158679	-4.094467	0.950457

C	3.343885	-1.685510	1.659033
H	4.863551	-5.736298	-2.364312
H	6.117205	-5.469552	-1.120228
H	4.499116	-6.046695	-0.634244
H	3.242381	-0.105791	-3.312383
H	4.965969	-0.386130	-3.707409
H	3.737435	-1.554356	-4.243943
H	3.735385	-2.396187	2.414307
H	3.649508	-0.668622	1.957187
H	2.235602	-1.704492	1.736768
C	-0.192965	3.432169	-1.367553
H	0.301685	4.422491	-1.452725
H	-1.270551	3.604149	-1.183495
H	0.242405	2.947509	-0.466364
H	4.371150	2.156329	-1.075534
H	4.869901	0.955893	-2.262464
H	5.028273	2.894359	1.250843
H	4.676711	1.873454	2.650361

E(solv)= -4498.64315818 A.U
Thermal correction= 1.199451

Act-1

Th	-0.715784	1.064034	0.119070
N	-1.161899	0.795935	2.402726
N	-2.832004	1.678981	-0.729140
N	0.692097	2.322711	-1.070214
C	1.448718	3.083834	-1.813813
N	1.934902	2.695198	-3.078179
C	3.312493	3.027114	-3.521108
C	3.492977	4.379855	-4.218250
C	3.310440	5.542931	-3.246930
C	1.980297	5.460184	-2.484821
N	1.865860	4.393304	-1.462226
C	1.820690	0.368252	-3.931682
C	2.928361	-0.094623	-3.016216
C	1.286392	-0.540306	-4.871501
C	0.227998	-0.197504	-5.730129
C	-0.304155	-1.172855	-6.756974
C	-0.316895	1.098887	-5.616248
C	0.192501	2.047826	-4.710570
C	-0.397708	3.437660	-4.668089
C	2.042922	4.805255	-0.092328
C	1.214361	5.815563	0.476996
C	0.066671	6.456080	-0.273730
C	1.484813	6.261371	1.787978
C	2.541566	5.747008	2.559019
C	2.789725	6.219570	3.973771
C	3.347241	4.751908	1.972196
C	3.125948	4.273099	0.667185
C	4.055897	3.227445	0.098617
H	3.997725	2.973299	-2.648904
H	3.616411	2.220219	-4.214440
H	4.508434	4.406559	-4.670582
H	2.771640	4.459341	-5.061568
H	4.147595	5.572819	-2.514216
H	3.336889	6.512312	-3.791387
H	1.827400	6.419699	-1.960093
H	1.144152	5.352707	-3.207971
H	-0.727000	6.777386	0.429352
H	-0.385512	5.772053	-1.016602
H	0.389249	7.369852	-0.820896
H	0.835460	7.041824	2.220312

H	3.874244	6.282927	4.199300
H	2.341101	7.216386	4.158200
H	2.345401	5.516977	4.712844
H	4.191052	4.334113	2.547391
H	4.627030	3.623329	-0.767957
H	4.790616	2.898798	0.859042
H	3.505441	2.329710	-0.252212
H	2.569477	-0.907176	-2.345445
H	3.300344	0.711361	-2.358359
H	3.788084	-0.498492	-3.592501
H	1.711572	-1.556749	-4.919185
H	0.039450	-2.207184	-6.556069
H	0.036990	-0.903066	-7.780749
H	-1.413936	-1.177193	-6.780118
H	-1.156596	1.390729	-6.269211
H	0.328561	4.201634	-5.018933
H	-1.294537	3.507285	-5.314068
H	-0.697714	3.723210	-3.638464
Si	0.311839	1.065434	3.359219
Si	-2.683910	0.467817	3.275399
C	1.621454	1.566939	2.067593
C	0.983247	-0.443381	4.277888
C	0.165013	2.506083	4.596791
C	-3.964191	-0.288922	2.102365
C	-2.486702	-0.741686	4.731118
C	-3.437675	2.051651	4.026796
H	1.962371	-0.183371	4.737174
H	0.313831	-0.781665	5.093046
H	1.140551	-1.283917	3.569290
H	1.833550	0.755736	1.333354
H	2.585569	1.745281	2.586336
H	1.404273	2.509307	1.518968
H	-0.516808	2.257669	5.437076
H	1.163291	2.718881	5.037577
H	-0.203503	3.437674	4.119486
H	-2.011242	-1.695864	4.425444
H	-1.898324	-0.314479	5.569470
H	-3.497139	-0.980964	5.128494
H	-3.628800	-1.276259	1.721589
H	-4.923676	-0.448542	2.638459
H	-4.157765	0.366369	1.230262
H	-4.406679	1.805603	4.513548
H	-2.779791	2.492425	4.803845
H	-3.637035	2.837193	3.270937
Si	-3.126882	3.356361	-0.216581
Si	-4.030768	0.987378	-1.867881
C	-4.734636	3.668815	0.754592
C	-3.078974	4.596564	-1.657452
C	-1.710606	3.824804	0.984234
C	-3.421253	1.137645	-3.660166
C	-4.462414	-0.822536	-1.477827
C	-5.738806	1.843015	-1.845862
H	-4.982699	2.833779	1.439903
H	-4.616039	4.586707	1.370303
H	-5.601703	3.829042	0.084394
H	-4.144089	0.665190	-4.359784
H	-2.430781	0.667132	-3.819086
H	-3.328381	2.207582	-3.942113
H	-2.124185	4.515812	-2.216616
H	-3.904204	4.421642	-2.378042
H	-3.177699	5.638464	-1.284072
H	-1.870063	4.880543	1.284670
H	-0.687845	3.805093	0.539511
H	-1.717804	3.228399	1.919853

H	-5.047325	-1.241074	-2.325155
H	-3.595105	-1.490724	-1.319794
H	-5.097285	-0.882915	-0.570490
H	-6.243317	1.761370	-0.861676
H	-6.374980	1.312612	-2.587952
H	-5.721460	2.912390	-2.140171
N	-0.187422	-3.149294	0.015192
Si	-0.645508	-3.098535	-1.691871
H	0.656847	-4.179710	3.170198
C	-2.291951	-3.961603	-2.102066
C	-0.854541	-1.244399	-2.141095
C	0.576598	-3.869474	-2.926251
C	-2.793917	-4.319392	1.154746
C	-0.415191	-3.993891	2.974458
C	-0.350624	-6.104459	0.749608
H	-3.168306	-3.591027	-1.536855
H	-2.225446	-5.059185	-1.946377
H	-2.495030	-3.800826	-3.183455
H	0.743233	-4.941812	-2.690808
H	0.162813	-3.810581	-3.956394
H	1.553837	-3.353174	-2.893840
H	-0.883072	-6.833016	1.399056
H	-0.577278	-6.369388	-0.305033
H	0.738702	-6.253362	0.905212
H	0.096108	-0.688867	-1.990681
H	-1.162652	-1.073103	-3.191533
H	-1.679830	-0.839244	-1.509071
H	-3.207177	-3.288654	1.157133
H	-3.151056	-4.821751	2.079766
H	-3.236757	-4.860634	0.295948
H	-1.024966	-4.659142	3.623927
H	-0.621759	-2.943188	3.261189
Si	-0.882498	-4.319889	1.167677
B	1.032309	-2.256769	0.334649
O	2.100450	-2.241933	-0.683093
C	3.246239	-2.925865	-0.140447
C	3.115696	-2.623108	1.412417
O	1.695518	-2.506437	1.599384
C	3.150539	-4.434604	-0.454353
C	4.526257	-2.375906	-0.787652
C	3.636188	-3.741255	2.329824
C	3.805134	-1.300966	1.804009
H	2.246481	-4.885492	-0.002880
H	3.086271	-4.576553	-1.551275
H	4.041389	-4.988319	-0.092017
H	3.082392	-4.686774	2.176616
H	3.509574	-3.443606	3.391277
H	4.716545	-3.933712	2.158838
H	5.428479	-2.815911	-0.312722
H	4.552209	-2.643690	-1.863894
H	4.591443	-1.274440	-0.710060
H	3.500403	-1.020061	2.831452
H	3.516456	-0.479613	1.120279
H	4.911033	-1.392310	1.785850
H	0.541383	-0.936160	0.330504
C	1.280537	1.678664	-3.872077

E(solv)= -4498.65367133 A.U
Thermal correction= 1.194220

HBpin

C	-0.795163	-0.190019	0.045653
C	0.795085	-0.190946	-0.045578

C	-1.379714	-1.071920	1.151114
C	-1.484055	-0.492946	-1.295235
C	1.482519	-0.493168	1.296009
C	1.378834	-1.074539	-1.150377
B	0.001563	1.954099	-0.000514
H	0.002524	3.163361	-0.000418
O	1.094736	1.206945	-0.362944
O	-1.093083	1.208750	0.361406
H	2.483991	-0.985049	-1.153939
H	1.122969	-2.141128	-0.982332
H	1.012735	-0.776621	-2.150908
H	2.564492	-0.270119	1.203749
H	1.075442	0.137360	2.111909
H	1.370406	-1.557663	1.585044
H	-2.484997	-0.983361	1.153831
H	-1.123004	-2.138364	0.984006
H	-1.014712	-0.772955	2.151657
H	-1.073419	0.132548	-2.113137
H	-1.377774	-1.558985	-1.580927
H	-2.564727	-0.263859	-1.203176

E(solv)= -411.853822590 A.U
Thermal correction= 0.15045

*N-Bpin

C	2.660092	-0.779854	0.083786
O	1.280182	-1.045571	0.458026
B	0.495639	0.009961	-0.011390
O	1.283499	1.064004	-0.475804
C	2.659166	0.800649	-0.084651
N	-0.941343	0.004146	-0.013616
C	3.587700	1.336086	-1.178336
C	2.915950	1.542924	1.238203
C	2.936773	-1.520116	-1.236302
C	3.575342	-1.313419	1.189434
H	4.646029	1.081436	-0.962360
H	3.322580	0.932181	-2.173687
H	3.507285	2.440975	-1.229807
H	3.968853	1.440628	1.570745
H	2.701362	2.621294	1.097412
H	2.255592	1.166440	2.045366
H	4.636409	-1.061093	0.984481
H	3.299517	-0.906523	2.180718
H	3.492491	-2.418070	1.242708
H	3.995085	-1.418581	-1.551857
H	2.719500	-2.598759	-1.102104
H	2.290654	-1.141536	-2.053964
Si	-1.829977	1.571244	-0.014323
Si	-1.790470	-1.585945	0.011326
C	-3.328677	1.469732	1.152714
C	-0.761254	2.981798	0.660307
C	-2.392013	2.013565	-1.770052
C	-3.396866	-1.489868	-1.001198
C	-0.753971	-2.938783	-0.815955
C	-2.176068	-2.097485	1.795535
H	-2.659997	-3.097273	1.826922
H	-1.238521	-2.153246	2.387414
H	-2.853466	-1.375968	2.297326
H	-3.887402	-2.486953	-0.980064
H	-4.134484	-0.753097	-0.626896
H	-3.181704	-1.249745	-2.063682
H	-1.369066	-3.860043	-0.906676
H	-0.440608	-2.640725	-1.838630

H	0.155704	-3.174235	-0.231648
H	-2.903671	2.999835	-1.785809
H	-1.515360	2.073890	-2.448809
H	-3.092636	1.261139	-2.186016
H	-1.394415	3.888787	0.769637
H	-0.346915	2.737323	1.660732
H	0.084950	3.216343	-0.012907
H	-3.843362	2.454806	1.158468
H	-4.083369	0.707153	0.875545
H	-3.000058	1.261768	2.192968

E(solv)= -1284.63804095 A.U
Thermal correction= 0.343173

Th-4-H

Th	2.916333	3.960747	6.958350
Si	-0.045104	2.205883	6.379626
Si	-0.456054	5.036955	7.623315
Si	3.842714	1.716028	9.429730
Si	5.647089	1.531129	6.926238
N	3.619641	5.048924	5.171657
N	5.002576	6.847540	4.448174
N	3.678209	5.697854	2.876542
N	0.579561	3.742207	6.989798
H	3.355517	5.465858	8.393543
N	4.253620	2.216243	7.779868
C	4.067913	5.814623	4.224264
C	4.856939	8.167581	3.794270
H	5.334424	8.904968	4.468102
H	3.778124	8.434817	3.739801
C	5.481269	8.291464	2.397432
H	6.553578	7.999987	2.452933
H	5.462559	9.363105	2.100379
C	4.756719	7.443031	1.351734
H	3.742736	7.855548	1.152544
H	5.304905	7.480066	0.384749
C	4.621702	5.971272	1.770200
H	4.262132	5.389040	0.900888
H	5.622955	5.568597	2.038955
C	5.824107	6.803389	5.636834
C	5.435277	7.500395	6.809588
C	6.303320	7.490514	7.921405
H	5.992410	8.023944	8.835297
C	7.534483	6.812785	7.906348
C	7.890846	6.122784	6.728842
H	8.855953	5.589729	6.687439
C	7.060613	6.102761	5.592118
C	4.133249	8.262065	6.890733
H	4.252378	9.319851	6.565457
H	3.755337	8.274027	7.931211
H	3.353287	7.801005	6.255537
C	8.437032	6.791476	9.120139
H	8.179673	7.597646	9.835965
H	9.504286	6.908240	8.838411
H	8.350631	5.825587	9.664676
C	7.503242	5.361155	4.351133
H	6.785682	4.562409	4.068656
H	8.490488	4.883564	4.507614
H	7.588977	6.039161	3.476077
C	2.444302	5.037285	2.526644
C	2.461857	3.741586	1.945067
C	1.248081	3.188375	1.482869
H	1.267973	2.186271	1.021218

C	0.021834	3.867068	1.592964
C	0.028489	5.130692	2.220471
H	-0.920771	5.681571	2.333904
C	1.212322	5.730990	2.687265
C	3.740830	2.948163	1.796548
H	4.251860	3.151985	0.829274
H	3.531962	1.859958	1.822771
H	4.460650	3.179817	2.604858
C	1.162550	7.099176	3.324857
H	1.600660	7.084326	4.344967
H	0.119188	7.461440	3.407411
H	1.735661	7.847538	2.737216
C	-0.864321	1.147515	7.732384
H	-0.180960	0.964605	8.587833
H	-1.772854	1.647272	8.130853
C	1.441184	1.237753	5.659600
H	1.862823	1.751975	4.766790
H	1.086235	0.244663	5.309250
H	2.268976	1.039252	6.376414
C	-1.277973	2.374796	4.944384
H	-2.256372	2.782816	5.267822
H	-1.462481	1.377859	4.488591
H	-0.865643	3.041579	4.159151
C	-2.085280	5.271911	6.665268
H	-1.913738	5.389420	5.575308
C	0.507921	6.672857	7.509542
H	1.496698	6.611794	8.018459
H	-0.064863	7.491136	7.995959
H	0.681540	6.968031	6.452947
C	-0.917791	4.760017	9.449203
H	-1.445627	3.794757	9.599579
H	-1.588939	5.570015	9.808844
H	-0.017088	4.755609	10.097700
C	5.818042	-0.355307	7.126066
H	6.054515	-0.649077	8.170294
H	6.647715	-0.724059	6.484476
H	4.892549	-0.887727	6.822524
C	7.284495	2.321728	7.480642
H	7.261393	3.423475	7.343346
H	8.138236	1.919508	6.892969
H	7.490137	2.122577	8.552799
C	5.422936	1.876074	5.067456
H	4.571975	1.299337	4.647930
H	6.335521	1.587058	4.503700
H	5.231749	2.952766	4.864179
C	3.152418	-0.054828	9.536050
H	2.301319	-0.199227	8.837876
H	2.782988	-0.261285	10.564060
H	3.917536	-0.820549	9.295526
C	2.461244	2.882296	10.038052
H	2.773707	3.951594	10.027427
H	2.201081	2.626794	11.087095
H	1.518768	2.790559	9.453721
C	5.301216	1.859184	10.639943
H	6.121368	1.154728	10.386425
H	4.969905	1.623401	11.674357
H	5.720658	2.886732	10.639042
C	-1.264540	3.266819	1.070645
H	-1.785720	3.964191	0.380808
H	-1.081165	2.320843	0.523085
H	-1.971782	3.043424	1.898447
H	-2.592243	6.190695	7.032595
H	-2.789094	4.426159	6.813470
H	-1.178435	0.160115	7.329994

E(solv)= -3214.014899 A.U
Thermal correction= 0.813312

Deact-TS-1

Th	-0.247411	-0.540151	0.399109
N	-0.402414	-2.678366	-0.521612
N	-0.042344	-0.410289	2.734309
N	1.276650	0.858232	-0.397784
C	2.043363	1.830517	-0.793888
N	1.565067	3.128898	-1.072823
C	2.037506	3.866079	-2.266696
C	3.290800	4.727595	-2.057949
C	4.542505	3.884070	-1.811292
C	4.349147	2.845104	-0.695977
N	3.433291	1.720276	-0.999823
C	-0.878557	3.557453	-1.201079
C	-0.975689	2.914042	-2.564871
C	-2.023599	4.151458	-0.632575
C	-2.004647	4.760410	0.636480
C	-3.259603	5.363231	1.227733
C	-0.789588	4.755702	1.349182
C	0.387324	4.190114	0.819441
C	1.672358	4.254705	1.613534
C	4.059949	0.425495	-1.129191
C	4.629251	-0.198425	0.011864
C	4.527457	0.435557	1.380428
C	5.325297	-1.412932	-0.155660
C	5.472347	-2.022686	-1.416032
C	6.193074	-3.343273	-1.568079
C	4.900513	-1.376046	-2.530026
C	4.201225	-0.158009	-2.416122
C	3.662118	0.521989	-3.654477
H	2.217543	3.143536	-3.093275
H	1.202023	4.517009	-2.588861
H	3.431704	5.368663	-2.955825
H	3.115680	5.419453	-1.204447
H	4.845239	3.361968	-2.745563
H	5.396428	4.538476	-1.529266
H	5.331639	2.390189	-0.462244
H	4.001385	3.358047	0.226598
H	4.706911	-0.309017	2.180085
H	3.527983	0.887973	1.539882
H	5.278481	1.244508	1.517412
H	5.766754	-1.896562	0.732348
H	6.752442	-3.397017	-2.524618
H	6.908222	-3.518705	-0.739246
H	5.470594	-4.189175	-1.564958
H	5.014064	-1.827260	-3.530463
H	4.194291	1.475751	-3.857535
H	3.783761	-0.125014	-4.545263
H	2.584632	0.766353	-3.559970
H	-1.981252	2.472158	-2.707437
H	-0.223232	2.111104	-2.686297
H	-0.813794	3.653201	-3.381330
H	-2.964676	4.120390	-1.206333
H	-3.030192	6.031936	2.081556
H	-3.944737	4.570749	1.602400
H	-3.826376	5.947860	0.473768
H	-0.748390	5.221516	2.348276
H	2.449010	4.847076	1.085065
H	1.503198	4.727906	2.600563
H	2.101964	3.246255	1.791074
Si	0.544671	-3.220272	-1.921264

Si	-1.634947	-3.697471	0.246230
C	0.934865	-1.685101	-2.966848
C	-0.336965	-4.466040	-3.057180
C	2.177549	-4.033477	-1.380982
C	-2.530835	-2.589535	1.523054
C	-2.997634	-4.336074	-0.905880
C	-0.879459	-5.192212	1.153196
H	0.309545	-4.653559	-3.942168
H	-0.510949	-5.444782	-2.562969
H	-1.311311	-4.083004	-3.422405
H	0.005509	-1.248166	-3.389549
H	1.609167	-1.940954	-3.810782
H	1.443235	-0.902139	-2.363862
H	1.991347	-4.907472	-0.721367
H	2.746394	-4.391900	-2.266186
H	2.823480	-3.319293	-0.829641
H	-3.437029	-3.489610	-1.472947
H	-2.643427	-5.106623	-1.618241
H	-3.801581	-4.795351	-0.289482
H	-3.049708	-1.744666	1.014640
H	-3.321266	-3.189252	2.021891
H	-1.886653	-2.182734	2.332599
H	-1.666572	-5.762505	1.692556
H	-0.399126	-5.890652	0.435077
H	-0.109195	-4.892500	1.893780
Si	1.173411	-1.464170	3.470865
Si	-1.055971	0.684602	3.688260
C	0.432081	-2.863438	4.528806
C	2.420045	-0.540138	4.572960
C	2.122176	-2.305834	2.046119
C	-0.070014	2.108263	4.474728
C	-2.348031	1.453523	2.523845
C	-2.000256	-0.192323	5.090514
H	-0.334697	-3.438777	3.969668
H	1.229434	-3.575147	4.835464
H	-0.044989	-2.479541	5.453803
H	-0.759017	2.832951	4.960181
H	0.514149	2.655191	3.706921
H	0.638419	1.747826	5.248277
H	2.840465	0.353677	4.068874
H	1.950208	-0.205643	5.521541
H	3.262400	-1.213348	4.843027
H	2.947532	-2.920443	2.464512
H	2.593483	-1.594673	1.332767
H	1.478104	-2.995935	1.460701
H	-2.982833	2.156537	3.104652
H	-1.905125	2.042880	1.691439
H	-3.024090	0.695088	2.076495
H	-2.578895	-1.063408	4.718675
H	-2.716765	0.514443	5.562959
H	-1.318393	-0.552725	5.889184
B	-3.166820	-0.166549	-2.214734
O	-3.832437	1.032498	-2.444438
C	-5.171446	0.916869	-1.881648
C	-5.390887	-0.659801	-1.845466
O	-4.029969	-1.174637	-1.793047
C	-5.146508	1.555345	-0.483918
C	-6.140796	1.679237	-2.791339
C	-6.162828	-1.170958	-0.624678
C	-6.023644	-1.214888	-3.134502
H	-4.405042	1.053394	0.168100
H	-4.839682	2.616282	-0.576904
H	-6.142522	1.524942	0.002322
H	-5.655123	-0.907941	0.322406

H	-6.246306	-2.275795	-0.670714
H	-7.190594	-0.752442	-0.602085
H	-7.188733	1.561477	-2.445021
H	-5.896894	2.760992	-2.771190
H	-6.074799	1.337875	-3.841694
H	-5.963969	-2.321859	-3.116236
H	-5.480207	-0.862120	-4.033877
H	-7.090592	-0.927548	-3.230805
H	-2.084423	-0.391402	-2.706430
C	0.340633	3.598240	-0.471885
H	-2.108995	0.222778	-0.405310

E(solv)= -3625.88895487 A.U
Thermal correction= 0.989444

Deact-1

Th	-0.232141	-0.823466	0.128670
N	0.065277	1.413182	-0.056359
C	0.165761	2.699608	-0.178876
N	-0.885556	3.549185	-0.620029
C	-0.623891	4.632218	-1.597612
C	-0.237099	5.993936	-1.004986
C	1.126864	5.960274	-0.318329
C	1.242603	4.811316	0.694701
N	1.332210	3.447736	0.121142
C	2.660200	2.888452	0.097386
C	3.377896	2.710203	1.312527
C	4.750639	2.387814	1.255460
C	5.432088	2.218105	0.038114
C	4.681846	2.336429	-1.150339
C	3.311929	2.663143	-1.148623
C	2.574905	2.795823	-2.460411
C	2.719572	2.869370	2.664814
C	6.914726	1.921636	-0.005251
C	-2.274153	3.187352	-0.469532
C	-2.986411	2.638649	-1.571532
C	-4.381889	2.475038	-1.467127
C	-5.088239	2.788910	-0.290211
C	-4.352858	3.293656	0.798730
C	-2.962800	3.520626	0.729155
C	-2.261962	4.173327	1.898613
C	-2.272599	2.258764	-2.849065
C	-6.580640	2.562837	-0.194551
H	0.164096	4.299497	-2.307452
H	-1.551476	4.757008	-2.188909
H	-0.241307	6.746825	-1.823788
H	-1.023374	6.311419	-0.284621
H	1.312238	6.917733	0.216360
H	1.941068	5.860792	-1.070346
H	2.160759	4.966149	1.291250
H	0.388257	4.848150	1.402010
H	1.631975	2.672864	2.616404
H	2.852904	3.893655	3.079224
H	3.164846	2.169307	3.399753
H	5.301239	2.259733	2.203150
H	7.490002	2.802064	-0.366977
H	7.308852	1.657039	0.996288
H	7.145921	1.084200	-0.696621
H	5.184926	2.191633	-2.121731
H	2.237970	3.839668	-2.635746
H	3.224184	2.506851	-3.309843
H	1.669744	2.153914	-2.486768
H	-1.365421	3.608532	2.220290
H	-1.928866	5.202000	1.642898

H	-2.940991	4.250524	2.770512
H	-4.882807	3.554632	1.730648
H	-7.032194	3.146197	0.632953
H	-7.097758	2.842705	-1.135598
H	-6.812165	1.491065	-0.007152
H	-4.933950	2.077139	-2.334318
H	-2.169601	3.119702	-3.545788
H	-1.254941	1.879464	-2.632118
H	-2.827817	1.469683	-3.392743
N	-0.526713	-1.615486	2.354716
Si	-0.338656	-0.605375	3.799595
Si	-0.845167	-3.350245	2.572770
C	-1.453024	-1.083818	5.271972
C	-0.810949	1.181774	3.362635
C	1.455473	-0.615615	4.439558
C	0.345487	-4.193294	3.798963
C	-0.638853	-4.223103	0.893590
C	-2.615246	-3.717337	3.176430
H	1.777723	-1.640167	4.719896
H	1.562642	0.030463	5.337823
H	2.161931	-0.242415	3.668536
H	-0.273094	1.546979	2.461933
H	-0.574885	1.865964	4.205328
H	-1.898706	1.260953	3.154880
H	-1.292145	-0.350514	6.092144
H	-2.529415	-1.054074	5.002452
H	-1.229717	-2.090162	5.682876
H	-2.798466	-3.327663	4.197656
H	-3.380653	-3.276051	2.505449
H	-2.786241	-4.815730	3.201896
H	0.230379	-3.809631	4.834310
H	1.406874	-4.058550	3.504370
H	0.142020	-5.285839	3.827901
H	-1.203757	-3.745218	0.063386
H	0.420243	-4.289125	0.577832
H	-1.025560	-5.261463	0.974990
N	-1.710217	-1.695465	-1.516359
Si	-3.397107	-1.709905	-0.996212
Si	-1.193157	-2.336805	-3.090621
C	-4.648903	-0.984872	-2.235833
C	-3.461818	-0.627867	0.580909
C	-4.074449	-3.442081	-0.580405
C	-0.083531	-1.045301	-3.945205
C	-2.605226	-2.703011	-4.318842
C	-0.228930	-3.954482	-2.877700
H	-2.809052	-0.981287	1.413241
H	-3.220079	0.435918	0.360692
H	-4.491607	-0.634366	0.996408
H	-4.247747	-0.099192	-2.765847
H	-5.570400	-0.672394	-1.698807
H	-4.944450	-1.735292	-2.996643
H	-5.131380	-3.368511	-0.243009
H	-3.499762	-3.959961	0.212758
H	-4.060523	-4.091661	-1.481599
H	-0.668747	-0.142493	-4.219209
H	0.370845	-1.452632	-4.873625
H	0.751145	-0.717904	-3.290189
H	-3.170217	-1.794371	-4.610402
H	-3.328708	-3.453099	-3.935871
H	-2.154160	-3.127191	-5.242506
H	-0.869381	-4.738189	-2.420343
H	0.127953	-4.338133	-3.857346
H	0.659004	-3.811248	-2.228718
B	3.561424	-3.912803	-3.367233

O	3.192468	-3.411381	-2.169823
C	3.812145	-2.259676	-1.501309
C	5.306523	-2.567173	-1.294965
C	3.642194	-1.024890	-2.389637
C	3.032605	-2.108531	-0.128348
C	2.999489	-3.455179	0.620701
C	3.690100	-1.044378	0.771314
O	1.690626	-1.686575	-0.379626
H	4.468706	-3.428986	-4.029578
H	4.162403	-1.173455	-3.357138
H	2.570831	-0.836591	-2.583861
H	4.065721	-0.127078	-1.900538
H	5.786953	-2.749368	-2.276965
H	5.459538	-3.466465	-0.666111
H	5.828050	-1.713271	-0.820703
H	2.522277	-4.238054	0.002246
H	4.017559	-3.799008	0.894177
H	2.424012	-3.330097	1.558952
H	3.721721	-0.054390	0.278765
H	4.716315	-1.322852	1.082869
H	3.080760	-0.943713	1.692682
H	2.942532	-4.886328	-3.757732

E(solv)= -3625.89996424 A.U
Thermal correction= 0.989202

Deact-TS-2

Th	-0.147953	-0.675219	-0.728534
N	-0.985354	-2.391609	1.035493
N	0.901120	-1.402520	-2.752464
O	-1.929602	0.112584	-1.642464
Si	0.169788	-2.815765	-3.534229
Si	0.540240	-3.215499	1.478887
Si	-2.493374	-3.392726	1.101141
Si	2.377317	-0.746397	-3.492047
C	-2.956468	-3.924406	2.871232
H	-3.261042	-3.066103	3.495694
H	-3.813780	-4.630043	2.819635
H	-2.124259	-4.456950	3.378706
C	-3.946534	-2.465494	0.327242
H	-4.149672	-1.525645	0.873850
H	-3.776392	-2.210941	-0.737663
H	-4.855103	-3.102816	0.378470
C	-2.434788	-5.108580	0.236441
H	-1.929854	-5.161524	-0.745061
H	-1.989874	-5.883398	0.892132
H	-3.496615	-5.396878	0.071292
C	0.997597	-3.176542	3.315347
H	0.277578	-3.764351	3.920993
H	2.004819	-3.623672	3.456877
H	1.004513	-2.139904	3.699305
C	0.712083	-5.037409	0.950168
H	0.096823	-5.723579	1.565943
H	0.459971	-5.215122	-0.114265
H	1.776016	-5.325130	1.099280
C	1.950585	-2.345231	0.511959
C	2.595127	-1.082303	-5.358528
C	3.935515	-1.475236	-2.677434
H	4.857041	-1.051367	-3.131562
H	3.977542	-1.293848	-1.584544
H	3.963446	-2.575080	-2.832266
C	1.305393	-4.347122	-3.484518
H	1.606116	-4.598780	-2.445480

H	0.787271	-5.233387	-3.911113
H	2.234022	-4.193659	-4.073740
C	-0.387078	-2.588240	-5.343777
H	0.443663	-2.704385	-6.067257
H	-1.148949	-3.361644	-5.583541
H	-0.852696	-1.596267	-5.517037
C	-1.399609	-3.230144	-2.553554
H	-2.176419	-2.447450	-2.658076
H	-1.838080	-4.180049	-2.924567
H	-1.212418	-3.384992	-1.470158
O	-0.686722	-0.262735	3.317341
C	-1.516301	-0.199315	4.518564
C	-2.978265	-0.014757	3.913296
O	-2.854249	-0.606240	2.589777
C	-1.028605	0.982562	5.367173
H	-0.001394	0.780748	5.732979
H	-1.004504	1.925302	4.790363
C	-1.347168	-1.495597	5.324163
H	-1.931318	-1.459795	6.266317
H	-1.664391	-2.383276	4.747065
H	-0.280690	-1.626338	5.594045
C	-4.095144	-0.715819	4.693370
H	-5.058409	-0.585984	4.159860
H	-3.918122	-1.800163	4.813745
H	-4.202561	-0.268337	5.703280
B	-1.506976	-0.508552	2.206628
H	-1.240196	0.156592	1.199631
H	-4.311772	1.502213	3.125325
C	-3.367819	1.461108	3.704590
H	-2.595047	2.002845	3.125891
H	-3.527931	1.989707	4.666199
H	-1.679688	1.127295	6.254506
H	2.910876	-2.777478	0.859268
H	1.923658	-2.538171	-0.586628
H	2.073178	-1.248296	0.687426
N	1.123715	1.045805	0.036843
C	1.848300	2.058205	0.408139
N	1.598478	3.409061	0.008998
N	3.010255	1.973853	1.222858
C	2.725677	4.287105	-0.379805
C	3.362182	5.103310	0.752879
H	3.500612	3.668048	-0.877679
H	2.349084	4.988270	-1.143775
C	4.176547	4.222220	1.695611
H	4.006480	5.890610	0.303365
H	2.558380	5.635245	1.309645
C	3.371833	3.022456	2.209494
H	5.096617	3.858944	1.186321
H	4.520244	4.805898	2.577919
H	3.972111	2.514348	2.987366
H	2.451585	3.389919	2.709551
C	0.280429	3.965154	-0.146898
C	3.761823	0.748399	1.390108
C	-0.590539	4.059422	0.982679
C	-1.804576	4.759652	0.863302
C	-2.200043	5.396092	-0.330117
C	-1.345569	5.266071	-1.435680
C	-0.128914	4.549415	-1.382335
C	-0.225550	3.476087	2.324775
H	-2.455776	4.829427	1.751275
C	-3.500479	6.163577	-0.409867
H	-1.638223	5.723323	-2.396579
C	0.668675	4.435821	-2.664451
H	-4.375954	5.491690	-0.275801

H	-3.566283	6.935845	0.386116
H	-3.615838	6.674155	-1.386832
H	1.327842	3.548433	-2.671425
H	-0.016785	4.357233	-3.532340
H	1.304306	5.331099	-2.848303
H	-1.033769	3.664240	3.057902
H	-0.046456	2.381676	2.281904
H	0.695014	3.945225	2.730208
H	3.527118	-0.567674	-5.680794
H	2.715056	-2.157124	-5.606100
H	1.762611	-0.676140	-5.968607
C	4.786255	0.422605	0.459058
C	5.601269	-0.699530	0.707902
C	5.460794	-1.489321	1.866116
C	4.458182	-1.127646	2.783929
C	3.599928	-0.027795	2.570919
C	5.060452	1.286271	-0.749458
H	6.393079	-0.945128	-0.019903
C	6.360188	-2.682115	2.104791
H	4.331475	-1.721826	3.704741
C	2.552435	0.309098	3.604815
H	7.429087	-2.421808	1.953978
H	6.247787	-3.080730	3.132782
H	6.130761	-3.509350	1.397936
H	4.157392	1.430069	-1.373615
H	5.411306	2.295811	-0.447487
H	5.845314	0.835264	-1.386688
H	2.467782	-0.504793	4.350790
H	2.800415	1.235907	4.165416
H	1.551013	0.454301	3.152718
C	2.356991	1.147805	-3.354263
H	3.317984	1.596530	-3.684128
H	1.556318	1.550559	-4.010034
H	2.142653	1.482062	-2.318955
C	-2.781186	0.809377	-2.554609
C	-4.086411	1.308166	-1.799656
C	-1.968101	1.994102	-3.111342
C	-3.155719	-0.134622	-3.712389
H	-3.809807	0.370598	-4.452047
H	-2.233316	-0.452628	-4.236007
H	-3.690414	-1.026337	-3.338129
H	-2.497573	2.530501	-3.923620
H	-1.709259	2.714201	-2.311787
H	-1.022271	1.594087	-3.530140
C	-4.853228	2.368070	-2.611808
O	-4.948953	0.126823	-1.685002
C	-3.760855	1.833562	-0.399015
H	-5.823065	2.576009	-2.116172
H	-4.290271	3.320128	-2.661604
H	-5.063172	2.026461	-3.645695
H	-4.674484	2.239516	0.079484
H	-3.356258	1.025122	0.236912
H	-3.010064	2.645684	-0.447408
B	-6.141166	0.076694	-1.056458
H	-6.628527	1.048140	-0.494671
H	-6.723516	-0.993067	-1.091123

E(solv)= -4037.74205188 A.U
Thermal correction= 1.171643

Deact-2

Th	-0.098956	0.927921	-2.021127
N	0.818110	-0.435108	-3.705641

O	-1.180545	2.490610	-3.097127
Si	0.252737	-2.083312	-3.996947
Si	1.999683	0.390200	-4.719108
C	1.543660	0.416534	-6.565272
C	3.762636	-0.306234	-4.552942
H	4.484431	0.311244	-5.130655
H	4.086660	-0.309321	-3.491394
H	3.833233	-1.347206	-4.929317
C	1.650336	-3.284278	-4.474811
H	2.458775	-3.286334	-3.714236
H	1.251715	-4.318815	-4.554176
H	2.104875	-3.030072	-5.455822
C	-1.065883	-2.147756	-5.368075
H	-0.663889	-1.786165	-6.337513
H	-1.439318	-3.183506	-5.520347
H	-1.937623	-1.509327	-5.111339
C	-0.535646	-2.731333	-2.389825
H	-1.428534	-2.158952	-2.055640
H	-0.877195	-3.778726	-2.535980
H	0.194734	-2.736227	-1.551389
N	1.280541	1.799537	-0.517757
C	2.066460	2.184379	0.437288
N	2.394460	3.531807	0.680432
N	2.670168	1.273969	1.328797
C	3.746730	3.938576	1.116536
C	4.021672	3.843279	2.624137
H	4.506966	3.340683	0.564716
H	3.873683	4.991085	0.799835
C	4.096649	2.399465	3.123110
H	4.978920	4.368500	2.836142
H	3.229741	4.400354	3.172742
C	2.849094	1.580407	2.764556
H	4.996265	1.894993	2.705204
H	4.213932	2.385105	4.228997
H	2.901039	0.604837	3.285120
H	1.944518	2.103235	3.148992
C	1.524197	4.561549	0.167018
C	2.686008	-0.120300	0.951237
C	0.309176	4.842769	0.849369
C	-0.501186	5.896466	0.383803
C	-0.147515	6.680503	-0.732349
C	1.047316	6.360715	-1.403619
C	1.889596	5.311774	-0.982812
C	-0.123510	4.031694	2.047475
H	-1.439577	6.115781	0.920901
C	-1.007925	7.841809	-1.179472
H	1.332207	6.936946	-2.300714
C	3.147692	5.011136	-1.767052
H	-2.064940	7.712748	-0.870519
H	-0.652373	8.798245	-0.735498
H	-0.984696	7.968320	-2.281257
H	3.420672	3.939985	-1.703449
H	3.012480	5.267789	-2.836417
H	4.020397	5.596634	-1.401188
H	-1.039196	4.453883	2.505784
H	-0.343298	2.979112	1.765290
H	0.666990	3.997981	2.825731
H	2.270105	1.030377	-7.140634
H	1.554026	-0.604420	-7.002505
H	0.531809	0.843928	-6.724283
C	3.724932	-0.591269	0.103810
C	3.768843	-1.961301	-0.217158
C	2.819206	-2.878547	0.278883
C	1.789527	-2.378624	1.097741

C	1.696272	-1.012991	1.442610
C	4.767040	0.353215	-0.448388
H	4.579905	-2.324575	-0.871014
C	2.922750	-4.353262	-0.042277
H	1.018930	-3.070683	1.477647
C	0.557098	-0.537384	2.316094
H	3.694276	-4.846912	0.589210
H	1.964224	-4.880086	0.137120
H	3.215127	-4.522859	-1.099058
H	4.306992	1.130844	-1.094995
H	5.304760	0.889107	0.361732
H	5.516579	-0.191920	-1.054926
H	-0.312100	-1.218634	2.236012
H	0.845137	-0.497098	3.389791
H	0.218021	0.476019	2.025201
C	2.061425	2.199585	-4.101730
H	2.861493	2.743808	-4.646941
H	1.114330	2.755863	-4.272792
H	2.324292	2.287708	-3.021244
C	-2.593016	2.650686	-3.229689
C	-3.224778	2.119680	-1.866933
C	-2.905523	4.136720	-3.483700
C	-3.061391	1.813199	-4.439060
H	-4.125633	1.996383	-4.691828
H	-2.446000	2.086340	-5.319590
H	-2.931322	0.727455	-4.252901
H	-3.998335	4.335683	-3.491376
H	-2.428657	4.780083	-2.719756
H	-2.498322	4.431034	-4.472465
C	-4.699196	1.710433	-1.967092
O	-2.425097	0.925744	-1.603848
C	-3.023968	3.122987	-0.720799
H	-5.069778	1.386362	-0.972963
H	-5.324015	2.564216	-2.302310
H	-4.841152	0.868734	-2.671257
H	-3.246041	2.631546	0.246310
H	-1.982160	3.503588	-0.691201
H	-3.703889	3.990613	-0.831831
B	-2.423868	0.019112	-0.375489
H	-1.195080	-0.367933	-0.347073
H	-2.628828	0.617669	0.681324
H	-3.107604	-0.992377	-0.534837

E(solv)= -2753.15644188 A.U.
Thermal correction= 0.794670

Deact-3

C	4.070785	-0.928722	1.076401
C	3.784445	-0.329232	-0.177848
C	4.008753	-1.050595	-1.384202
C	4.553743	-2.345152	-1.309983
C	4.892129	-2.947913	-0.080854
C	4.633223	-2.223585	1.096075
N	3.338314	1.038884	-0.252289
C	4.257016	2.068244	0.279335
C	4.892092	2.996944	-0.766789
C	3.881942	3.952807	-1.400911
C	2.654578	3.229058	-1.973700
N	1.746601	2.616496	-0.980362
C	0.429003	3.195983	-0.870294
C	0.065752	3.867095	0.325645
C	-1.182587	4.517505	0.386130
C	-2.077283	4.525312	-0.700027

C	-1.698688	3.833094	-1.867205
C	-0.467575	3.156213	-1.972462
C	0.993817	3.896379	1.517018
C	-3.418049	5.220180	-0.613142
C	-0.125976	2.402801	-3.238113
C	3.687591	-0.441825	-2.728691
C	5.493709	-4.335502	-0.041411
C	3.778701	-0.226464	2.383849
C	1.970574	1.316738	-0.474592
N	1.018922	0.472691	-0.237413
Th	-0.821928	-0.691282	0.286088
O	-1.231312	-1.397596	2.617792
C	-1.615817	-0.355962	3.562945
C	-0.264895	0.197641	4.051820
N	-1.915376	-1.269053	-1.706130
Si	-3.583912	-0.887861	-2.172852
C	-4.121498	0.738102	-1.353572
O	-1.915863	0.771556	1.441235
C	-2.453512	0.752537	2.761004
C	-3.962667	0.430198	2.698159
Si	-0.936337	-2.409850	-2.628126
C	0.567702	-2.868782	-1.530308
C	-0.248992	-1.693481	-4.251353
C	-1.819142	-4.044576	-3.036665
C	-4.799931	-2.246725	-1.629613
C	-3.777283	-0.660011	-4.057764
C	-2.290878	2.158978	3.373920
C	-2.382180	-0.971372	4.739735
H	-4.820723	-0.360022	-4.296790
H	-3.102072	0.132409	-4.443881
H	-3.566209	-1.591791	-4.624135
H	0.314161	-0.755325	-4.066514
H	0.437937	-2.415420	-4.743838
H	-1.062246	-1.459137	-4.968591
H	-2.675340	-3.890133	-3.726279
H	-1.116325	-4.748096	-3.533469
H	-2.204575	-4.535330	-2.118897
H	0.297747	-3.471717	-0.634576
H	1.242108	-3.517289	-2.128991
H	1.212090	-2.014025	-1.214267
H	2.986847	2.453858	-2.699849
H	2.048536	3.961376	-2.541399
H	4.363909	4.525073	-2.224091
H	3.541974	4.705452	-0.654966
H	5.380333	2.375226	-1.550116
H	5.705246	3.573773	-0.273415
H	5.064969	1.526767	0.807597
H	3.724965	2.678300	1.042856
H	-1.459005	5.044724	1.314691
H	-2.388512	3.810159	-2.728292
H	-3.615107	5.842685	-1.511189
H	-4.245889	4.480910	-0.545608
H	-3.483166	5.875802	0.278250
H	0.417959	1.465875	-3.004740
H	-1.043923	2.135819	-3.797333
H	0.514599	2.997509	-3.925852
H	0.559081	4.487888	2.346625
H	1.193667	2.871943	1.897824
H	1.978495	4.339892	1.259873
H	-5.842752	-1.977818	-1.905662
H	-4.565636	-3.222745	-2.102557
H	-4.762415	-2.390666	-0.529503
H	4.737828	-2.894604	-2.249134
H	4.863074	-2.681133	2.073277

H	4.748915	-5.107970	-0.332033
H	6.345306	-4.429874	-0.748063
H	5.864265	-4.592533	0.971197
H	2.606793	-0.200929	-2.817942
H	4.240294	0.507619	-2.888781
H	3.949904	-1.133732	-3.552985
H	3.517742	-0.963095	3.169636
H	4.652494	0.354144	2.754681
H	2.931786	0.479876	2.280043
H	-5.180455	0.959169	-1.607292
H	-4.039125	0.691450	-0.248415
H	-3.500639	1.594049	-1.691666
H	-4.445754	0.525736	3.692049
H	-4.449991	1.157239	2.017174
H	-4.153406	-0.588468	2.311532
H	-2.585609	2.179673	4.444608
H	-1.249531	2.520699	3.282157
H	-2.941165	2.870056	2.825450
H	-1.730025	-1.686055	5.281755
H	-2.695773	-0.182944	5.454931
H	-3.283115	-1.518436	4.404721
H	0.360390	-0.644915	4.407902
H	0.280595	0.701434	3.226075
H	-0.386616	0.923260	4.879667
O	1.054587	-4.432435	1.726097
B	1.436960	-3.211605	2.213706
O	1.841444	-3.221976	3.525483
C	1.506567	-4.541772	4.075528
C	1.314441	-5.434202	2.763013
H	1.446130	-2.210056	1.532613
C	0.214410	-4.367187	4.887060
C	2.651210	-4.984469	4.990367
C	0.120521	-6.391921	2.807498
C	2.584452	-6.187424	2.339089
B	-2.137548	-2.429198	1.962848
H	-2.935417	-1.852577	1.179010
H	-1.341944	-3.041104	1.201668
H	-2.714179	-3.206251	2.715631
H	-0.091060	-5.315497	5.373216
H	0.387320	-3.612962	5.681237
H	-0.619554	-4.008501	4.252125
H	2.466214	-6.002906	5.389806
H	3.625407	-4.984341	4.466041
H	2.728143	-4.290281	5.851520
H	0.052863	-6.944286	1.848484
H	0.237053	-7.136265	3.622262
H	-0.832496	-5.849729	2.952041
H	2.423829	-6.625434	1.333569
H	3.458741	-5.509561	2.277134
H	2.825485	-7.010934	3.041056

E(solv)= -3165.02313647 A.U
Thermal correction= 0.964027

Carbonate

C	0.992470	1.969940	-0.800495
C	-0.282273	1.125841	-0.619913
H	1.028864	2.868767	-0.154167
H	1.153918	2.276758	-1.857738
H	-0.755865	1.276640	0.375545
H	-1.041768	1.288941	-1.409530
C	1.563243	-0.225534	-0.470868
O	2.234116	-1.210138	-0.338532

O	0.210911	-0.218468	-0.708658
O	2.032900	1.063272	-0.408404

E(solv)= -342.375704 A.U
Thermal correction= 0.044062

E-Coor

Th	0.609874	-0.644144	0.129941
Si	-1.841004	-3.217450	-0.783056
Si	0.721526	-4.184054	0.568656
Si	4.208723	-0.423037	-0.724381
Si	2.201715	-0.773009	-3.000000
N	-0.513378	1.264877	-0.161915
N	-0.418204	3.515443	0.615606
N	-2.201745	2.857749	-0.772273
N	-0.243229	-2.867641	-0.111545
H	1.431631	-0.399106	2.072840
N	2.520531	-0.561295	-1.264614
C	-1.014881	2.455285	-0.113384
C	-1.232735	4.457896	1.414988
H	-0.585441	4.810849	2.240850
H	-2.079731	3.909819	1.883658
C	-1.772343	5.679727	0.658850
H	-0.921598	6.208570	0.173958
H	-2.201010	6.389775	1.400332
C	-2.824177	5.305753	-0.385339
H	-3.758490	4.958840	0.110010
H	-3.102076	6.200716	-0.984827
C	-2.337405	4.212776	-1.348567
H	-3.062055	4.134273	-2.179899
H	-1.365927	4.516828	-1.795053
C	0.980866	3.446933	0.962017
C	1.384512	3.009446	2.250482
C	2.748198	3.102297	2.602311
H	3.057864	2.762165	3.605010
C	3.718697	3.601889	1.716957
C	3.293807	3.993736	0.429938
H	4.036069	4.385278	-0.286291
C	1.946697	3.921586	0.031228
C	0.392679	2.474459	3.258520
H	0.011281	3.275989	3.930609
H	0.871938	1.702004	3.891400
H	-0.477028	2.009643	2.756465
C	5.177131	3.686482	2.107632
H	5.613359	4.673311	1.845080
H	5.776689	2.916945	1.574513
H	5.320081	3.525964	3.194896
C	1.544663	4.361685	-1.357248
H	0.810339	5.193833	-1.326131
H	1.067887	3.532857	-1.922698
H	2.425256	4.703959	-1.935709
C	-3.225531	1.906845	-1.120438
C	-3.483053	1.591470	-2.482433
C	-4.599364	0.787170	-2.797265
H	-4.797728	0.555299	-3.857779
C	-5.443055	0.252686	-1.809708
C	-5.132416	0.535546	-0.463485
H	-5.770331	0.120271	0.335556
C	-4.050254	1.356097	-0.096683
C	-2.594398	2.080898	-3.604865
H	-2.973800	3.020044	-4.066295
H	-2.542816	1.325363	-4.414203

H	-1.563114	2.273939	-3.253256
C	-3.800819	1.658137	1.361091
H	-2.796041	1.310300	1.678188
H	-4.549051	1.153120	2.002732
H	-3.856530	2.748568	1.564750
C	-1.950468	-4.858983	-1.749094
H	-1.207680	-4.904672	-2.572582
H	-1.800371	-5.749927	-1.103886
C	-2.312889	-1.841047	-1.998799
H	-2.243159	-0.823161	-1.554922
H	-3.365201	-1.963819	-2.329552
H	-1.672261	-1.868066	-2.904833
C	-3.199760	-3.289359	0.557157
H	-2.967341	-4.042958	1.338905
H	-4.178247	-3.564813	0.107097
H	-3.323547	-2.303353	1.050627
C	-0.222607	-5.192382	1.889786
H	-0.588398	-4.531431	2.702772
C	2.261714	-3.438714	1.400720
H	2.034915	-2.648355	2.149863
H	2.949185	-3.005924	0.642633
H	2.828151	-4.239740	1.921564
C	1.383825	-5.435079	-0.705274
H	0.581299	-6.031416	-1.183988
H	2.076214	-6.145405	-0.202487
H	1.950672	-4.922226	-1.509121
C	1.956593	-2.603750	-3.459358
H	2.880069	-3.187222	-3.257845
H	1.711157	-2.719332	-4.537210
H	1.137373	-3.061488	-2.867075
C	3.522104	-0.099637	-4.199977
H	3.677006	0.992944	-4.087876
H	3.162174	-0.283865	-5.235953
H	4.506228	-0.602070	-4.100032
C	0.617423	0.185044	-3.453634
H	-0.253710	0.003083	-2.789572
H	0.295971	-0.066800	-4.487120
H	0.823002	1.275578	-3.414139
C	5.243263	-1.941117	-1.247631
H	4.822881	-2.883684	-0.837763
H	6.285361	-1.846481	-0.871820
H	5.298590	-2.052819	-2.350996
C	4.349109	-0.274967	1.166527
H	3.809019	0.612996	1.555519
H	5.426389	-0.158370	1.417736
H	3.968285	-1.157726	1.716382
C	5.092733	1.127616	-1.396584
H	5.292106	1.086712	-2.485277
H	6.071419	1.246311	-0.882007
H	4.488320	2.034916	-1.188775
C	-6.626558	-0.620088	-2.165161
H	-7.554572	-0.271560	-1.663929
H	-6.814011	-0.631060	-3.257563
H	-6.465125	-1.672110	-1.843065
H	0.445382	-5.956615	2.343462
H	-1.096491	-5.728190	1.462490
H	-2.961813	-4.947001	-2.202833
O	-1.307668	-0.751138	2.022401
C	-1.498654	-1.210104	3.129522
O	-0.645127	-2.016210	3.795239
O	-2.618226	-0.964942	3.854521
C	-1.273204	-2.488407	5.005448
H	-1.584547	-3.542859	4.850060
H	-0.535251	-2.440465	5.828614

C	-2.463927	-1.524365	5.175133
H	-2.256120	-0.698242	5.887863
H	-3.407806	-2.026471	5.461772

E(solv)= -3556.40457919 A.U
Thermal correction= 0.878703

TS-E

Th	-0.206605	1.432119	0.260234
N	-0.182281	0.963449	2.567817
N	-2.397637	1.785638	-0.487513
N	1.053802	2.799080	-0.980006
C	1.763706	3.507680	-1.802452
N	2.406600	2.964403	-2.939547
C	3.770026	3.388428	-3.326489
C	3.849274	4.615967	-4.245282
C	3.414323	5.903446	-3.545613
C	2.039159	5.776565	-2.872794
N	1.978390	4.899396	-1.682154
C	2.601923	0.501769	-3.187865
C	3.758513	0.451042	-2.216868
C	2.165541	-0.681248	-3.822218
C	1.088209	-0.696364	-4.724962
C	0.624552	-1.977108	-5.384126
C	0.435371	0.525383	-4.992097
C	0.843658	1.734557	-4.399971
C	0.142855	3.025462	-4.755523
C	1.790987	5.565925	-0.416982
C	0.588051	6.273265	-0.156071
C	-0.554931	6.270029	-1.144978
C	0.473468	6.999170	1.048484
C	1.509484	7.040626	1.998987
C	1.362657	7.807073	3.294962
C	2.690151	6.324249	1.714570
C	2.855744	5.589992	0.524875
C	4.150880	4.858295	0.260355
H	4.373728	3.569499	-2.409971
H	4.232081	2.528238	-3.847312
H	4.895442	4.713007	-4.610578
H	3.219996	4.433471	-5.144604
H	4.164844	6.200100	-2.779567
H	3.367674	6.740104	-4.277095
H	1.718203	6.781698	-2.537774
H	1.292827	5.430486	-3.620465
H	-1.514216	6.502692	-0.643206
H	-0.649397	5.284744	-1.644212
H	-0.416795	7.030804	-1.944784
H	-0.463655	7.546267	1.248411
H	1.187025	7.119417	4.151150
H	2.280611	8.384855	3.532235
H	0.511772	8.516102	3.258185
H	3.520047	6.343808	2.441579
H	4.643173	5.225377	-0.664506
H	4.861255	4.991862	1.099713
H	3.983644	3.768755	0.129204
H	3.835229	-0.551393	-1.757410
H	3.627992	1.187875	-1.400652
H	4.729768	0.669029	-2.714145
H	2.686374	-1.624154	-3.586161
H	0.564128	-1.868907	-6.488095
H	-0.391039	-2.264903	-5.034907
H	1.308245	-2.821619	-5.164388
H	-0.411672	0.542077	-5.698948

H	0.841277	3.753405	-5.219904
H	-0.681897	2.845273	-5.472420
H	-0.288490	3.520173	-3.859940
Si	1.125046	1.682870	3.521006
Si	-1.346932	-0.167532	3.276885
C	2.235258	2.615761	2.290022
C	2.248305	0.442520	4.421208
C	0.498297	2.938441	4.810379
C	-2.354679	-0.970108	1.869955
C	-0.554734	-1.597543	4.250284
C	-2.562698	0.688097	4.472435
H	3.137474	0.977324	4.821307
H	1.749222	-0.058065	5.275606
H	2.602217	-0.334182	3.713486
H	2.735804	1.916691	1.586677
H	3.039351	3.139255	2.849117
H	1.715218	3.402389	1.700927
H	-0.127381	2.451655	5.587717
H	1.357292	3.419330	5.327408
H	-0.108584	3.741165	4.342172
H	0.255341	-2.076778	3.665046
H	-0.132529	-1.261845	5.219436
H	-1.327294	-2.365169	4.475456
H	-1.691715	-1.533785	1.178454
H	-3.080187	-1.691651	2.302446
H	-2.931699	-0.240967	1.263239
H	-3.367071	-0.015738	4.778660
H	-2.046786	1.023302	5.397019
H	-3.045860	1.578705	4.020569
Si	-3.208488	3.108404	0.370544
Si	-3.247672	0.933322	-1.798955
C	-4.628560	2.550721	1.508357
C	-3.924573	4.446999	-0.776110
C	-1.896168	3.915183	1.503326
C	-3.358017	1.983997	-3.382800
C	-2.363767	-0.680312	-2.272496
C	-5.033477	0.450614	-1.331616
H	-4.314098	1.732837	2.188092
H	-4.969191	3.401520	2.138076
H	-5.504466	2.190361	0.931926
H	-3.828404	1.396494	-4.201169
H	-2.346761	2.286429	-3.721162
H	-3.957554	2.906437	-3.243418
H	-3.180103	4.798268	-1.518162
H	-4.809061	4.070919	-1.331562
H	-4.259129	5.322179	-0.177781
H	-2.349029	4.783868	2.027172
H	-1.003816	4.310755	0.967782
H	-1.551396	3.217012	2.297985
H	-2.929177	-1.159302	-3.101645
H	-1.320650	-0.516230	-2.613875
H	-2.326701	-1.392068	-1.422428
H	-5.075229	-0.143445	-0.394687
H	-5.466926	-0.171854	-2.144644
H	-5.696308	1.332435	-1.206780
C	2.109106	-1.609716	0.597322
O	2.426760	-2.200233	-0.588335
C	1.497117	-3.270149	-0.836326
C	0.993899	-3.612966	0.576886
O	1.272875	-2.410980	1.316882
H	0.687532	-2.880986	-1.488558
H	2.032445	-4.100163	-1.336320
H	-0.093791	-3.815606	0.619226
H	1.545515	-4.456884	1.045477

O	2.564899	-0.561451	0.991938
C	1.937671	1.717413	-3.491587
H	0.136617	-0.515499	-0.556661

E(solv)= -3556.407302 A.U
Thermal correction= 0.880939

E-1

C	1.176591	2.455813	-0.136164
O	-0.043929	2.021948	-0.724669
C	-0.836276	3.197433	-0.964688
O	0.113874	4.219770	-1.265606
C	1.176639	4.001271	-0.351149
O	-1.708917	2.999948	-1.964115
Th	-3.407909	2.856740	-3.340642
N	-2.611177	1.683754	-5.070523
C	-1.994547	0.964330	-5.957178
N	-0.707142	1.263029	-6.440426
C	0.122345	2.212532	-5.738767
C	0.337553	3.507274	-6.284663
C	1.240038	4.373852	-5.634773
C	1.927442	4.000925	-4.466411
C	1.685884	2.715358	-3.945874
C	0.795128	1.811492	-4.553084
C	-0.347962	3.976455	-7.549250
C	2.854831	4.968186	-3.767349
C	0.575038	0.445988	-3.948560
N	-3.947018	5.132528	-3.702227
Si	-4.354178	6.084815	-2.260842
C	-6.111859	6.818774	-2.302255
N	-4.974418	1.658674	-2.019952
Si	-4.814774	0.734235	-0.510207
C	-3.287664	1.242662	0.493031
N	-2.542283	-0.210295	-6.535715
C	-3.970856	-0.360911	-6.645430
C	-4.678224	-1.230419	-5.769452
C	-6.046139	-1.470341	-6.009047
C	-6.750175	-0.839993	-7.053159
C	-6.039248	0.062535	-7.866373
C	-4.661550	0.306698	-7.694165
C	-4.004317	-1.883786	-4.583591
C	-8.216587	-1.129616	-7.286215
C	-3.946064	1.243118	-8.638713
C	-1.732327	-1.443948	-6.644940
C	-0.881179	-1.577801	-7.914391
C	0.249666	-0.553244	-7.970849
C	-0.254926	0.885963	-7.797967
Si	-3.719501	5.952289	-5.259006
C	-1.981328	6.714444	-5.392064
C	-4.972395	7.344660	-5.612016
C	-3.941216	4.677759	-6.656546
C	-3.135550	7.510423	-1.937603
C	-4.269188	4.943181	-0.735705
Si	-6.552718	1.760469	-2.809229
C	-7.755493	2.989813	-1.995925
C	-7.475251	0.108202	-2.973098
C	-6.202727	2.423789	-4.575287
C	-4.651917	-1.136265	-0.837566
C	-6.310685	0.970545	0.652323
H	-1.079164	-1.535923	-5.748081
H	-2.440671	-2.292613	-6.610401
H	-0.469218	-2.610423	-7.950582
H	-1.541394	-1.471090	-8.804184

H	0.776032	-0.619058	-8.948353
H	1.012135	-0.768786	-7.189562
H	0.569717	1.577349	-8.051344
H	-1.074313	1.077544	-8.524451
H	-1.327971	3.484052	-7.697222
H	0.264318	3.769626	-8.455021
H	-0.516099	5.070952	-7.519086
H	1.405154	5.378189	-6.060660
H	3.672626	4.441263	-3.233783
H	3.315090	5.685434	-4.477140
H	2.295929	5.564962	-3.013320
H	2.216683	2.393417	-3.035288
H	0.744071	-0.363616	-4.689234
H	1.249334	0.279157	-3.087283
H	-0.465886	0.338318	-3.576932
H	-3.479139	2.094374	-8.101074
H	-3.135465	0.720873	-9.189752
H	-4.647058	1.664083	-9.386038
H	-6.567811	0.581127	-8.684285
H	-8.656881	-0.440011	-8.033911
H	-8.369174	-2.166566	-7.657516
H	-8.803364	-1.036768	-6.347966
H	-6.583472	-2.165045	-5.341034
H	-3.565405	-2.874819	-4.833316
H	-3.188735	-1.246673	-4.188808
H	-4.730793	-2.052849	-3.765422
H	-1.836772	7.514352	-4.636487
H	-1.816934	7.165414	-6.394970
H	-1.193055	5.952116	-5.219268
H	-3.348249	3.753543	-6.482752
H	-3.613858	5.108782	-7.626551
H	-5.005110	4.379454	-6.763642
H	-4.819454	7.714183	-6.649536
H	-6.021292	6.990464	-5.531343
H	-4.850214	8.214142	-4.932955
H	-6.217192	7.612058	-3.069206
H	-6.878321	6.044366	-2.514259
H	-6.354836	7.271658	-1.316472
H	-3.177047	8.294003	-2.723180
H	-2.092998	7.132779	-1.882988
H	-3.373148	8.001576	-0.968996
H	-4.875347	4.016317	-0.835100
H	-3.226620	4.647779	-0.496793
H	-4.663416	5.492497	0.145530
H	-5.888654	3.494145	-4.593037
H	-5.465960	1.807981	-5.143398
H	-7.141662	2.388760	-5.165916
H	-6.868412	-0.646181	-3.511354
H	-8.418035	0.258501	-3.542217
H	-7.748924	-0.307173	-1.980894
H	-8.669605	3.107817	-2.617556
H	-7.294395	3.991993	-1.879384
H	-8.074816	2.648341	-0.990251
H	-5.528249	-1.543405	-1.383195
H	-4.565559	-1.689796	0.122692
H	-3.743410	-1.360070	-1.435060
H	-7.263565	0.599603	0.219921
H	-6.453408	2.037157	0.925827
H	-6.136869	0.404735	1.593364
H	-3.324930	2.314022	0.781385
H	-3.266474	0.647520	1.431744
H	-2.330175	1.061567	-0.036196
H	1.227272	2.193090	0.946391
H	2.022994	1.949728	-0.650473

H	1.000018	4.536958	0.613758
H	2.115174	4.387917	-0.796518
H	-1.369005	3.470707	-0.009375

E(solv)= -3556.467894 A.U
Thermal correction= 0.887923

E-2

Th	2.687692	4.058587	6.994224
Si	-0.264081	2.556472	6.216681
Si	-0.705159	5.281711	7.697497
Si	3.359704	1.515493	9.367148
Si	5.490545	1.723668	7.173855
N	3.462567	5.086639	5.164989
N	4.757288	6.916696	4.348889
N	3.732829	5.443396	2.817040
N	0.321844	4.021134	6.999305
O	3.096157	5.423456	8.623075
N	3.935853	2.231320	7.853885
C	3.948065	5.771542	4.177693
C	4.677764	8.082721	3.440121
H	5.022743	8.955595	4.026432
H	3.614552	8.273160	3.175027
C	5.511823	7.998859	2.154468
H	6.568124	7.770389	2.419508
H	5.518224	9.004980	1.680540
C	4.974232	6.957565	1.174791
H	3.990796	7.280638	0.766047
H	5.659388	6.861142	0.303988
C	4.815658	5.572732	1.818301
H	4.601715	4.838978	1.019582
H	5.778068	5.267792	2.285434
C	5.387826	7.160729	5.626030
C	4.815227	8.086603	6.540182
C	5.516852	8.393686	7.722496
H	5.074666	9.116486	8.429204
C	6.751189	7.793685	8.042108
C	7.278921	6.858323	7.130521
H	8.243218	6.372426	7.356443
C	6.628461	6.537116	5.920600
C	3.483487	8.747452	6.264184
H	3.586290	9.647061	5.618397
H	3.005668	9.083142	7.205402
H	2.787317	8.054014	5.752717
C	7.477033	8.156006	9.318994
H	6.776759	8.215440	10.178015
H	7.966556	9.151040	9.232964
H	8.267009	7.418566	9.564831
C	7.267019	5.567059	4.954124
H	6.616966	4.688830	4.761397
H	8.232227	5.192084	5.346980
H	7.461207	6.044667	3.970685
C	2.553147	4.720991	2.413200
C	2.640407	3.381168	1.943836
C	1.481740	2.762727	1.424200
H	1.561777	1.725737	1.055185
C	0.239932	3.415645	1.364774
C	0.170608	4.727533	1.879239
H	-0.792548	5.265657	1.856726
C	1.295150	5.392227	2.401007
C	3.930773	2.591975	1.967660
H	4.489457	2.672833	1.008513
H	3.722617	1.514078	2.121761

H	4.606878	2.927612	2.775771
C	1.151438	6.805670	2.911866
H	1.433903	6.881464	3.983396
H	0.106841	7.158980	2.809402
H	1.804620	7.509829	2.354388
C	-1.080182	1.326846	7.417308
H	-0.402647	1.042772	8.248905
H	-1.993723	1.770053	7.868235
C	1.294951	1.728906	5.455923
H	1.765812	2.373302	4.675846
H	0.985211	0.802159	4.928852
H	2.076598	1.404661	6.183269
C	-1.461841	2.828997	4.770551
H	-2.444052	3.215494	5.108544
H	-1.641902	1.864292	4.248514
H	-1.036120	3.542437	4.035205
C	-2.480430	5.316285	7.007690
H	-2.498233	5.482314	5.910720
C	0.069115	6.980826	7.327023
C	-0.853096	5.101399	9.587188
H	-1.313388	4.129935	9.866193
H	-1.483599	5.909946	10.016291
H	0.143063	5.148485	10.074070
C	5.898139	-0.121687	7.415352
H	6.006405	-0.406902	8.482269
H	6.864096	-0.350296	6.914503
H	5.123205	-0.775299	6.963075
C	6.930681	2.735241	7.899112
H	6.784602	3.824090	7.733495
H	7.898860	2.447102	7.435079
H	7.021288	2.576024	8.994048
C	5.433699	2.012453	5.294458
H	4.740752	1.291634	4.811732
H	6.436704	1.876147	4.836901
H	5.080541	3.035308	5.036380
C	2.700922	-0.257114	9.137327
H	1.915585	-0.297014	8.353166
H	2.251904	-0.631591	10.082830
H	3.502666	-0.965062	8.844099
C	1.911546	2.568091	10.025338
H	2.265534	3.526389	10.457632
H	1.394415	2.010182	10.834772
H	1.131761	2.811435	9.269065
C	4.674036	1.487848	10.744195
H	5.540027	0.840967	10.492294
H	4.233128	1.098241	11.687310
H	5.061989	2.507933	10.948493
C	-0.985004	2.745643	0.784401
H	-1.796441	2.664867	1.539237
H	-1.397156	3.326199	-0.068758
H	-0.759033	1.723817	0.419776
H	-3.037531	6.152156	7.484132
H	-3.041542	4.382939	7.225173
H	-1.386128	0.396460	6.891776
C	3.786734	5.973312	9.707398
C	3.058902	7.207476	10.256076
H	3.897695	5.224767	10.531936
H	4.813997	6.282583	9.406811
O	3.887639	7.875054	11.227291
H	2.869420	7.931194	9.437808
H	2.078863	6.929120	10.706862
H	-0.487330	7.793082	7.841761
H	1.123780	7.026622	7.672015
H	0.054255	7.198664	6.238073

C	3.562886	7.757876	12.540977
O	4.224329	8.240887	13.424717
H	2.608982	7.172211	12.693503

E(solv)= -3556.474772 A.U
Thermal correction= 0.881462
TS-F

Th	0.687409	-1.005412	0.404026
N	-1.113752	-2.098613	-0.402340
C	-2.095359	-2.720999	-0.966969
N	-2.611592	-2.354657	-2.239414
C	-4.041290	-2.498567	-2.594419
C	-4.484648	-3.881906	-3.087020
C	-4.495746	-4.917815	-1.967606
C	-3.146766	-5.004716	-1.242355
N	-2.773057	-3.843242	-0.407924
C	-2.902900	-3.995271	1.019033
C	-3.742091	-3.093154	1.738352
C	-3.938330	-3.289126	3.117366
C	-3.349148	-4.358257	3.819926
C	-2.532151	-5.237219	3.090177
C	-2.288134	-5.080218	1.708643
C	-1.388237	-6.089412	1.028041
C	-4.464318	-1.965319	1.044311
C	-3.567001	-4.528883	5.306126
H	-5.093924	-2.347021	0.213310
H	-5.127510	-1.432422	1.752364
H	-3.766312	-1.215554	0.617701
H	-0.838057	-5.653464	0.172964
H	-0.644265	-6.490058	1.744859
H	-1.955987	-6.966530	0.644303
H	-2.049790	-6.080569	3.613578
H	-4.596993	-2.587831	3.657565
H	-3.303853	-5.550949	5.645546
H	-4.622165	-4.333697	5.590427
H	-2.939183	-3.815153	5.883654
C	-1.832212	-1.564813	-3.156892
C	-0.750807	-2.163348	-3.861973
C	-0.122486	-1.435786	-4.892509
C	-0.526007	-0.134585	-5.250660
C	-1.557133	0.458341	-4.495975
C	-2.212897	-0.222646	-3.449106
C	-3.299772	0.491570	-2.673592
H	-3.181438	1.589929	-2.761591
H	-3.283152	0.225471	-1.597601
H	-4.318228	0.255329	-3.052804
H	-1.865259	1.493113	-4.724946
C	0.107666	0.592448	-6.417391
H	0.125913	1.690621	-6.258708
H	1.147103	0.251697	-6.601825
H	-0.461894	0.413010	-7.356347
H	0.696992	-1.919646	-5.450891
C	-0.272936	-3.552626	-3.528159
H	0.459068	-3.916664	-4.275032
H	0.219891	-3.563466	-2.532330
H	-1.113847	-4.274814	-3.483045
N	1.545257	-0.481353	2.588168
Si	2.793345	0.763372	2.480417
Si	1.120734	-1.033144	4.225537
C	2.249790	2.505264	3.023048
C	4.404592	0.331407	3.402096
C	3.302321	0.977502	0.645860
C	2.370961	-2.315656	4.902232

C	1.066068	0.365869	5.521029
C	-0.602807	-1.833203	4.306777
H	-1.386435	-1.056670	4.204504
H	-0.794282	-2.617711	3.547432
H	-0.719240	-2.307038	5.305809
H	0.720321	-0.052416	6.491414
H	2.051444	0.843985	5.701251
H	0.343715	1.145753	5.204762
H	2.443853	-3.226455	4.272508
H	3.391844	-1.889918	4.987094
H	2.058103	-2.639633	5.919255
H	2.069942	2.577137	4.113840
H	3.028652	3.252915	2.756547
H	1.306681	2.778934	2.507485
H	4.264353	0.294291	4.502477
H	4.802978	-0.652135	3.076551
H	5.179638	1.101055	3.194486
H	4.217285	1.606312	0.618656
H	3.563738	0.024213	0.143451
H	2.544122	1.505053	0.034866
N	2.507742	-2.392238	-0.482198
Si	2.416594	-3.951198	0.353794
Si	3.921578	-2.212776	-1.542950
C	3.790057	-0.824013	-2.841114
C	4.293638	-3.768807	-2.592291
C	5.544625	-1.856455	-0.593865
C	3.987713	-4.456610	1.307125
C	1.932244	-5.444202	-0.733278
C	1.051271	-3.794534	1.674188
H	4.604167	-4.639571	-1.978827
H	5.132949	-3.541889	-3.285188
H	3.422423	-4.077778	-3.206947
H	4.710033	-0.858981	-3.463619
H	3.731892	0.187901	-2.393554
H	2.918990	-0.975810	-3.510664
H	5.812870	-2.677732	0.100572
H	6.379761	-1.745431	-1.319920
H	5.498240	-0.921823	0.001693
H	4.829560	-4.721864	0.634170
H	3.773699	-5.350120	1.933228
H	4.327826	-3.642813	1.980421
H	2.722797	-5.724916	-1.456826
H	1.744928	-6.327287	-0.084295
H	1.005824	-5.244864	-1.310307
H	0.971353	-4.748922	2.232344
H	0.032935	-3.596163	1.267470
H	1.312840	-3.026322	2.429219
H	-4.235019	-1.772686	-3.404306
H	-4.670709	-2.192851	-1.731574
H	-3.812103	-4.207440	-3.912075
H	-5.499862	-3.781106	-3.530469
H	-4.738308	-5.924666	-2.373746
H	-5.289988	-4.678066	-1.225631
H	-2.339152	-5.198517	-1.982957
H	-3.176174	-5.883510	-0.574917
O	-0.270749	1.090786	0.389962
C	-0.695930	2.097813	-0.473565
B	-1.828954	0.694716	1.943082
H	-1.525734	-0.478364	1.810395
O	-2.947141	1.241201	1.309530
C	-3.553985	2.208616	2.212922
C	-2.379619	2.522812	3.252963
O	-1.517311	1.360593	3.120692
C	-4.767114	1.517280	2.860504

C	-1.561747	3.777793	2.907093
C	-4.032465	3.416815	1.399778
C	-2.831411	2.611147	4.717280
H	-5.322226	2.199438	3.535672
H	-5.459418	1.184100	2.061234
H	-4.459331	0.623637	3.438525
H	-1.195275	3.754992	1.862729
H	-0.675518	3.825437	3.570366
H	-2.153343	4.704715	3.051369
H	-3.210213	3.886672	0.827560
H	-4.481881	4.187526	2.059726
H	-1.950650	2.795902	5.364982
H	-3.544570	3.448198	4.866873
H	-3.308483	1.673880	5.059814
H	-4.808652	3.094709	0.675948
H	-1.259709	2.874146	0.098832
C	0.414491	2.867537	-1.195364
H	-1.417096	1.726624	-1.240172
H	0.064577	3.883778	-1.461437
H	1.315891	2.961234	-0.555150
O	0.835457	2.337071	-2.499333
C	1.128648	1.059434	-2.660238
O	1.102724	0.178201	-1.805854
H	1.432398	0.861563	-3.711128

E(solv)= -3968.331428 A.U
Thermal correction= 1.064743

F

Th	0.776173	-1.066093	0.579764
N	-0.997412	-2.162211	-0.255651
C	-2.076542	-2.634979	-0.791590
N	-2.713414	-2.052196	-1.932752
C	-4.180627	-1.858525	-1.911617
C	-5.015391	-3.024264	-2.460672
C	-4.980943	-4.243899	-1.543474
C	-3.546994	-4.669663	-1.205271
N	-2.780082	-3.765561	-0.316638
C	-2.589767	-4.274484	1.022262
C	-3.289686	-3.679120	2.105810
C	-3.218647	-4.287854	3.373424
C	-2.474847	-5.461768	3.605828
C	-1.780373	-6.021008	2.517835
C	-1.821463	-5.451966	1.228320
C	-1.070863	-6.117353	0.097219
C	-4.107859	-2.425470	1.914078
C	-2.399082	-6.073597	4.987076
H	-4.953390	-2.590812	1.213089
H	-4.532374	-2.079194	2.876276
H	-3.494451	-1.600409	1.496083
H	-0.757577	-5.382219	-0.668969
H	-0.167442	-6.636298	0.473456
H	-1.690852	-6.884082	-0.418310
H	-1.182045	-6.935573	2.671391
H	-3.769591	-3.824410	4.209122
H	-2.117759	-7.145276	4.946832
H	-3.366821	-5.991284	5.523587
H	-1.637959	-5.556640	5.612333
C	-1.993750	-1.500576	-3.043265
C	-1.093554	-2.322403	-3.794584
C	-0.555076	-1.833559	-5.001431
C	-0.885113	-0.566279	-5.524877
C	-1.714092	0.250638	-4.736761

C	-2.238639	-0.162864	-3.490600
C	-2.998877	0.865952	-2.679656
H	-2.586206	1.874433	-2.884813
H	-2.924972	0.702663	-1.586091
H	-4.077884	0.916145	-2.949832
H	-1.939265	1.275546	-5.078941
C	-0.372489	-0.116222	-6.874940
H	-0.388759	0.988198	-6.973400
H	0.665278	-0.463851	-7.058146
H	-0.998964	-0.526899	-7.697686
H	0.123196	-2.491659	-5.570442
C	-0.726452	-3.719510	-3.359472
H	-0.006788	-4.174228	-4.066726
H	-0.268089	-3.728561	-2.348857
H	-1.619746	-4.377699	-3.321014
N	1.432030	-0.451856	2.780148
Si	2.777858	0.695378	2.899075
Si	0.588025	-0.815935	4.305043
C	2.228506	2.495738	3.204152
C	4.072661	0.247024	4.223579
C	3.740700	0.670172	1.254083
C	1.515319	-2.112592	5.359940
C	0.319855	0.704759	5.416156
C	-1.143403	-1.507318	3.951459
H	-1.814179	-0.692858	3.611397
H	-1.166123	-2.310916	3.186893
H	-1.568130	-1.940876	4.881729
H	-0.339286	0.420907	6.265430
H	1.257723	1.111806	5.847239
H	-0.183008	1.503465	4.833748
H	1.615955	-3.092310	4.848671
H	2.534577	-1.772815	5.635998
H	0.953752	-2.286994	6.304052
H	2.180143	2.734130	4.286391
H	2.943298	3.209247	2.739178
H	1.213497	2.665611	2.787508
H	3.665303	0.315503	5.253537
H	4.468593	-0.780013	4.079793
H	4.927682	0.954988	4.160082
H	4.556234	1.422961	1.301015
H	4.192067	-0.323766	1.066725
H	3.143717	0.927954	0.352627
N	2.678293	-2.294139	-0.207552
Si	2.789060	-3.780145	0.745474
Si	3.780008	-2.149996	-1.595387
C	4.431017	-0.391291	-1.963153
C	2.955805	-2.801512	-3.184060
C	5.413722	-3.125230	-1.386576
C	4.296395	-3.889868	1.900971
C	2.702646	-5.379056	-0.290302
C	1.261754	-3.799842	1.892795
H	2.690990	-3.874350	-3.078332
H	3.631659	-2.702981	-4.061010
H	2.020678	-2.245828	-3.400728
H	5.009796	-0.438241	-2.911484
H	5.124116	-0.042999	-1.170531
H	3.648517	0.380171	-2.091498
H	5.280149	-4.214712	-1.231007
H	6.017101	-2.998495	-2.311926
H	6.019453	-2.732166	-0.543003
H	5.253608	-3.971225	1.348300
H	4.210383	-4.783126	2.557324
H	4.353710	-2.995123	2.555543
H	3.572920	-5.499305	-0.967315

H	2.679429	-6.266654	0.378798
H	1.785950	-5.398076	-0.914732
H	1.220055	-4.769795	2.429899
H	0.282086	-3.716835	1.366403
H	1.333187	-3.021965	2.681639
H	-4.407659	-0.959698	-2.508214
H	-4.489120	-1.626738	-0.870735
H	-4.637553	-3.291036	-3.473305
H	-6.061613	-2.672545	-2.598538
H	-5.493235	-5.106050	-2.024432
H	-5.534311	-4.037804	-0.600630
H	-2.981943	-4.823561	-2.149448
H	-3.581150	-5.649541	-0.692973
O	0.005755	1.321202	0.312800
C	0.310113	2.594144	-0.234105
B	-1.245740	1.253742	1.203552
H	-1.235575	0.007257	1.481059
O	-2.424608	1.682723	0.467073
C	-3.293192	2.385383	1.368571
C	-2.277149	3.003782	2.432623
O	-1.172638	2.084691	2.394123
C	-4.266816	1.373303	2.007172
C	-1.778278	4.411646	2.041924
C	-4.098279	3.423787	0.574454
C	-2.823479	3.065648	3.868404
H	-5.018182	1.865141	2.658521
H	-4.806731	0.838395	1.199372
H	-3.722397	0.620497	2.610609
H	-1.436966	4.455453	0.989480
H	-0.919240	4.679277	2.690809
H	-2.563818	5.183921	2.177546
H	-3.438305	4.083136	-0.020885
H	-4.713538	4.056779	1.247481
H	-2.062748	3.515571	4.539068
H	-3.738739	3.691907	3.927685
H	-3.058481	2.058055	4.260054
H	-4.785722	2.909745	-0.128820
H	0.713282	3.265480	0.559681
C	1.344242	2.553254	-1.342544
H	-0.629043	3.048926	-0.620353
H	1.592853	3.586657	-1.651053
H	2.275779	2.038602	-1.030215
O	0.854026	1.924811	-2.569477
C	0.868849	0.603258	-2.635090
O	1.243766	-0.146889	-1.733212
H	0.521963	0.239889	-3.627342

E(solv)= -3968.354444 A.U
Thermal correction= 1.065730

BpinOROCOH

C	-0.129159	0.005823	-0.010344
C	-0.052400	-0.063648	1.579310
C	1.223067	-0.011729	-0.725476
C	-0.987992	1.175359	-0.518754
C	1.161836	-0.859779	2.086641
C	-0.131540	1.290139	2.288653
B	-1.558875	-1.578122	0.797625
O	-2.493843	-2.574868	0.836450
O	-1.241935	-0.836860	1.916907
O	-0.848011	-1.222873	-0.337493
H	-0.085297	1.138759	3.386106
H	0.719016	1.941000	1.998052

H	-1.076641	1.819229	2.062387
H	1.033837	-1.056484	3.169940
H	1.247399	-1.838603	1.572501
H	2.110294	-0.303752	1.943172
H	1.067618	0.024044	-1.822964
H	1.833358	0.869682	-0.439156
H	1.797145	-0.929304	-0.496074
H	-1.966013	1.212256	0.002644
H	-0.481198	2.151508	-0.379588
H	-1.181420	1.036752	-1.601617
C	-2.845017	-3.275273	-0.353300
C	-4.049364	-2.597222	-1.016858
H	-1.995934	-3.313983	-1.069705
H	-3.116779	-4.312173	-0.064709
O	-4.394553	-3.272809	-2.249315
H	-4.918480	-2.595421	-0.328343
H	-3.791879	-1.559730	-1.308285
C	-5.310424	-4.267398	-2.165212
H	-5.473231	-4.679307	-3.194469
O	-5.867447	-4.648158	-1.159948

E(solv)= -754.281981 A.U
Thermal correction= 0.212861

TS-G

Th	-0.147934	-0.116446	0.231221
Si	0.171077	1.456651	3.389640
Si	2.825996	0.365690	2.242809
Si	1.065716	-2.335562	-2.357912
Si	0.714605	-3.471960	0.516571
N	-2.322225	0.084680	-0.204249
N	-4.082496	1.131579	-1.436579
N	-4.615940	-0.518760	0.141654
N	1.074264	0.605514	2.124004
H	0.831571	0.988213	-1.317270
N	0.595537	-2.145577	-0.647938
C	-3.583495	0.224247	-0.479262
C	-5.342429	1.873964	-1.208327
H	-5.250080	2.825946	-1.765966
H	-5.422226	2.139133	-0.131239
C	-6.627207	1.159692	-1.652919
H	-6.519621	0.849964	-2.715972
H	-7.463823	1.891972	-1.623309
C	-6.956489	-0.049161	-0.777410
H	-7.273125	0.284266	0.235679
H	-7.816541	-0.610194	-1.204907
C	-5.773000	-1.018091	-0.635564
H	-6.127085	-1.932490	-0.120486
H	-5.427893	-1.327874	-1.646448
C	-3.211589	1.659092	-2.460145
C	-2.607518	2.933510	-2.298504
C	-1.839724	3.456070	-3.360125
H	-1.358420	4.438549	-3.224871
C	-1.653838	2.755398	-4.565875
C	-2.253578	1.486068	-4.689356
H	-2.115596	0.911446	-5.621059
C	-3.035339	0.924302	-3.662361
C	-2.779747	3.745634	-1.035232
H	-3.566291	4.524238	-1.153500
H	-1.833590	4.254645	-0.768341
H	-3.063887	3.108295	-0.176493
C	-0.863653	3.354955	-5.709018
H	-0.058668	4.030312	-5.353875

H	-1.520111	3.958582	-6.375056
H	-0.399551	2.568892	-6.339330
C	-3.687323	-0.424694	-3.865011
H	-4.795729	-0.347831	-3.862558
H	-3.412050	-1.141679	-3.063663
H	-3.382485	-0.867685	-4.833290
C	-4.383934	-1.151544	1.416595
C	-4.000159	-2.517049	1.477818
C	-3.860450	-3.128123	2.741808
H	-3.563372	-4.189808	2.784984
C	-4.079379	-2.425920	3.941766
C	-4.463059	-1.072848	3.849412
H	-4.655148	-0.503250	4.774719
C	-4.630024	-0.421608	2.611568
C	-3.760483	-3.319542	0.219937
H	-4.712373	-3.645691	-0.252967
H	-3.181460	-4.236502	0.441377
H	-3.205377	-2.726736	-0.535087
C	-5.100560	1.014716	2.574728
H	-4.410754	1.662701	1.996727
H	-5.177028	1.431328	3.598354
H	-6.100944	1.100260	2.100079
C	0.124424	0.493201	5.033112
H	-0.237642	-0.545647	4.884627
H	1.125287	0.437165	5.510761
C	-1.618690	1.616659	2.764965
H	-1.675946	2.242783	1.848759
H	-2.226359	2.127368	3.541522
H	-2.121308	0.646011	2.562543
C	0.763363	3.222714	3.761483
H	1.747386	3.255538	4.270542
H	0.026301	3.723789	4.426336
H	0.829167	3.806096	2.820825
C	3.800860	1.937461	2.701708
H	3.515290	2.808857	2.076767
C	3.467738	-0.194088	0.544254
H	3.361491	0.606286	-0.217948
H	2.933737	-1.086339	0.155198
H	4.545024	-0.457275	0.607496
C	3.307716	-0.956108	3.529159
H	3.038525	-0.638870	4.558276
H	4.405389	-1.131543	3.511350
H	2.808269	-1.928655	3.339896
C	2.505210	-4.026683	0.849806
H	2.976731	-4.423355	-0.074655
H	2.529150	-4.839236	1.608195
H	3.141948	-3.197098	1.219088
C	-0.260566	-5.041995	0.053870
H	-1.250338	-4.798721	-0.382156
H	-0.428863	-5.658213	0.963975
H	0.286030	-5.670953	-0.677192
C	-0.036375	-2.829301	2.155038
H	0.438248	-1.896144	2.535814
H	0.117089	-3.592658	2.947996
H	-1.135396	-2.665784	2.089611
C	2.808868	-1.662676	-2.709796
H	2.862210	-0.576990	-2.488379
H	3.064492	-1.807159	-3.782074
H	3.587228	-2.173723	-2.105093
C	-0.162129	-1.399980	-3.459062
H	-1.170543	-1.859140	-3.403260
H	0.167441	-1.433657	-4.519756
H	-0.251738	-0.330097	-3.174134
C	1.059696	-4.146184	-2.958579

H	1.780234	-4.789437	-2.411179
H	1.360950	-4.156116	-4.028925
H	0.056560	-4.614629	-2.888883
C	-3.891219	-3.088174	5.288829
H	-4.710917	-2.826690	5.990148
H	-3.853467	-4.192499	5.201711
H	-2.942337	-2.760132	5.767098
H	4.886203	1.750083	2.549511
H	3.660654	2.224804	3.764047
H	-0.558168	0.992511	5.754826
O	0.217949	3.476956	0.307590
C	1.150867	3.419278	-0.469073
O	1.135531	4.064224	-1.655326
H	2.116280	2.888102	-0.264439
C	2.245883	3.864597	-2.546424
C	2.861469	5.223621	-2.889618
H	3.006096	3.197748	-2.082523
H	1.859116	3.362429	-3.457340
O	3.976197	5.037729	-3.754736
H	2.093122	5.881787	-3.349975
H	3.225078	5.711287	-1.959243
B	3.859171	5.245409	-5.101257
O	2.676951	5.584052	-5.741918
C	3.042637	5.963659	-7.106418
C	4.428132	5.203080	-7.304319
O	4.945874	5.135398	-5.942645
C	3.188793	7.494315	-7.119812
C	1.927484	5.527728	-8.058167
C	5.446857	5.939820	-8.176951
C	4.253379	3.755488	-7.794039
H	3.391310	7.880671	-8.139136
H	2.244583	7.949086	-6.758116
H	4.007608	7.828476	-6.450736
H	2.212269	5.724217	-9.112508
H	1.692800	4.451961	-7.951056
H	1.002747	6.100768	-7.843514
H	6.380823	5.345791	-8.242180
H	5.059132	6.080668	-9.207083
H	5.706101	6.929871	-7.756671
H	5.221617	3.225012	-7.695545
H	3.504357	3.209923	-7.185041
H	3.939319	3.713374	-8.856581

E(solv)= -3968.306619 A.U
Thermal correction= 1.048687

G

Th	2.032524	4.217885	6.620002
Si	0.574695	1.146670	6.235947
Si	-1.503284	3.459983	5.962710
Si	2.577235	3.442091	10.056330
Si	5.161246	3.660039	8.423678
N	3.060463	4.765609	4.709624
N	4.128739	6.536914	3.505104
N	3.716991	4.494028	2.428508
N	0.137187	2.852668	6.241085
N	3.390724	3.699470	8.502311
C	3.594292	5.232268	3.624206
C	3.864799	7.359674	2.302823
H	3.882375	8.416173	2.634500
H	2.833561	7.156657	1.938816
C	4.859271	7.185067	1.146465
H	5.888774	7.372829	1.524590

H	4.656866	7.972408	0.387209
C	4.777669	5.799728	0.503829
H	3.825709	5.689372	-0.061536
H	5.596452	5.675270	-0.238770
C	4.882106	4.661876	1.530789
H	4.999937	3.704941	0.987035
H	5.796928	4.800679	2.146421
C	4.556662	7.257128	4.681586
C	3.674205	8.158654	5.332071
C	4.161894	8.924065	6.412754
H	3.468787	9.615883	6.919094
C	5.491514	8.826099	6.861844
C	6.339375	7.910327	6.206139
H	7.384580	7.807799	6.544186
C	5.901657	7.123515	5.123558
C	2.241986	8.334186	4.882740
H	2.156276	9.084831	4.065728
H	1.621263	8.682529	5.729973
H	1.820234	7.381286	4.507254
C	6.009831	9.687844	7.991837
H	6.557162	10.572754	7.597189
H	6.722675	9.128412	8.632461
H	5.193030	10.069028	8.637047
C	6.872124	6.185589	4.441640
H	6.482498	5.148349	4.391652
H	7.837838	6.156568	4.983842
H	7.082612	6.502676	3.397933
C	2.879584	3.349829	2.165992
C	3.406154	2.036223	2.299293
C	2.631007	0.945815	1.854777
H	3.050492	-0.071042	1.944173
C	1.345031	1.113101	1.305657
C	0.825608	2.421553	1.243504
H	-0.185243	2.580147	0.830719
C	1.566840	3.545512	1.658972
C	4.778068	1.791953	2.888124
H	5.580712	1.836923	2.118813
H	4.834960	0.785731	3.349359
H	5.024419	2.544405	3.662871
C	0.976390	4.929832	1.526103
H	0.951217	5.458229	2.502043
H	-0.059788	4.884319	1.137411
H	1.570136	5.561890	0.832415
C	-0.064449	0.199020	7.756667
H	0.264097	0.667965	8.707058
H	-1.175325	0.176450	7.763872
C	2.492294	1.127608	6.244486
H	2.902179	1.641585	5.343175
H	2.858610	0.080958	6.192637
H	2.959135	1.564885	7.157376
C	0.055704	0.171870	4.692463
H	-1.031523	-0.042830	4.676258
H	0.591690	-0.801817	4.667956
H	0.318284	0.731989	3.772242
C	-1.426358	4.931829	4.757134
H	-0.729428	5.723308	5.104837
C	-2.329342	4.017699	7.583314
H	-1.734332	4.795805	8.103505
H	-2.442412	3.163241	8.284096
H	-3.342463	4.432684	7.391759
C	-2.693517	2.193591	5.179078
H	-2.367842	1.874028	4.167864
H	-3.695189	2.665271	5.076165
H	-2.823174	1.284954	5.804279

C	5.973735	2.335660	9.529341
H	5.819347	2.522290	10.612559
H	7.071076	2.340098	9.349557
H	5.600548	1.315430	9.300925
C	5.919816	5.336762	8.898586
H	5.580794	6.138115	8.209265
H	7.030158	5.300415	8.855493
H	5.629673	5.629754	9.928863
C	5.686779	3.241567	6.640495
H	5.464155	2.181031	6.399789
H	6.780670	3.391822	6.518939
H	5.176809	3.875527	5.882430
C	2.674603	1.638838	10.665791
H	2.306472	0.927769	9.896766
H	2.044649	1.508415	11.572588
H	3.708459	1.339440	10.931467
C	0.728198	3.839908	9.834460
H	0.553269	4.920539	9.656443
H	0.177112	3.561000	10.757535
H	0.252168	3.276454	9.001524
C	3.237110	4.557689	11.449393
H	4.294542	4.332509	11.702560
H	2.638395	4.410050	12.374268
H	3.174476	5.631754	11.176250
C	0.535880	-0.074248	0.832675
H	-0.216570	0.220571	0.073510
H	1.182302	-0.859373	0.389762
H	-0.015117	-0.544222	1.677202
H	-2.425666	5.398308	4.622971
H	-1.075581	4.585872	3.762379
H	0.289205	-0.854786	7.754268
O	0.936547	5.994088	7.212734
C	0.114471	7.054807	7.569913
O	0.813152	8.201598	8.007071
H	-0.484962	7.398706	6.695300
H	-0.586497	6.724082	8.382776
C	1.437064	8.068259	9.277680
C	1.676440	9.471828	9.831145
H	0.776199	7.508811	9.984065
H	2.398908	7.509298	9.204192
O	2.169169	9.356935	11.164485
H	2.383704	10.035621	9.185113
H	0.710571	10.025459	9.836690
B	3.119996	10.203793	11.652266
O	3.805347	11.144504	10.895243
C	4.536760	11.985081	11.840269
C	4.662537	11.030567	13.110471
O	3.484441	10.184401	12.983872
C	3.663807	13.223736	12.102447
C	5.868421	12.398071	11.210637
C	4.604701	11.747223	14.461919
C	5.891829	10.108164	13.048118
H	6.481294	12.977852	11.931554
H	6.454649	11.521689	10.875628
H	5.683580	13.042265	10.327054
H	5.794531	9.329941	13.831445
H	5.962126	9.595171	12.067688
H	6.836096	10.662564	13.223060
H	4.675549	11.003144	15.280998
H	5.449464	12.458347	14.572361
H	3.655375	12.300714	14.591557
H	4.175818	13.961373	12.752961
H	3.435702	13.714091	11.134550
H	2.701876	12.945290	12.578698

E(solv)= -3968.389071 A.U
Thermal correction= 1.059339

TS-H

Th	0.548314	-0.984428	0.229009
N	-1.066000	-2.488181	-0.101858
C	-2.036483	-3.258216	-0.483640
N	-2.583789	-3.239934	-1.793714
C	-4.046470	-3.326224	-1.999163
C	-4.624050	-4.743574	-2.115825
C	-4.565881	-5.508563	-0.795169
C	-3.159165	-5.507317	-0.181668
N	-2.675850	-4.208958	0.343833
C	-2.627218	-4.123612	1.783558
C	-3.549392	-3.285584	2.469389
C	-3.615000	-3.361558	3.873363
C	-2.790555	-4.224120	4.622846
C	-1.863494	-5.014941	3.921137
C	-1.763891	-4.984394	2.514311
C	-0.773625	-5.894352	1.820852
C	-4.456235	-2.334520	1.725072
C	-2.873332	-4.259640	6.132590
H	-5.065297	-2.862541	0.962062
H	-5.152963	-1.829202	2.422743
H	-3.883472	-1.546975	1.189295
H	-0.438845	-5.473385	0.853034
H	0.119013	-6.061518	2.455329
H	-1.209344	-6.896508	1.610330
H	-1.192543	-5.687276	4.483048
H	-4.342801	-2.720702	4.399787
H	-3.922482	-4.183374	6.486178
H	-2.317978	-3.407611	6.584267
H	-2.437439	-5.191047	6.546705
C	-1.803008	-2.862012	-2.944139
C	-0.847764	-3.776564	-3.473544
C	-0.225796	-3.483871	-4.702870
C	-0.510401	-2.312883	-5.431126
C	-1.423850	-1.404943	-4.866339
C	-2.068168	-1.644369	-3.634377
C	-3.027182	-0.605226	-3.101335
H	-2.736975	0.400743	-3.463676
H	-3.051416	-0.573733	-1.995089
H	-4.069073	-0.776246	-3.454758
H	-1.645652	-0.463560	-5.398158
C	0.175711	-2.018577	-6.746101
H	-0.496057	-1.483182	-7.448133
H	1.068754	-1.372224	-6.595635
H	0.524096	-2.946621	-7.242922
H	0.495634	-4.210623	-5.112456
C	-0.515901	-5.066883	-2.763661
H	0.256844	-5.636901	-3.315645
H	-0.134064	-4.878726	-1.738067
H	-1.409287	-5.718928	-2.665571
N	1.189626	0.086908	2.244030
Si	2.375924	1.392664	2.015513
Si	0.503765	-0.114897	3.869302
C	1.601128	3.129169	1.992438
C	3.779901	1.396181	3.306480
C	3.226409	1.133024	0.333301
C	1.702721	-0.957064	5.093802
C	-0.033569	1.529832	4.667336
C	-1.037591	-1.214271	3.792481

H	-1.881723	-0.717235	3.274045
H	-0.863710	-2.189501	3.291336
H	-1.374505	-1.443158	4.825417
H	-0.583488	1.326460	5.611937
H	0.828013	2.182419	4.919679
H	-0.705330	2.096345	3.989673
H	1.981245	-1.980676	4.767716
H	2.639782	-0.381996	5.234297
H	1.212680	-1.047808	6.088048
H	1.324194	3.477354	3.008282
H	2.320869	3.862681	1.568382
H	0.681543	3.136650	1.372336
H	3.425717	1.647046	4.328217
H	4.298883	0.416000	3.354369
H	4.531546	2.164810	3.022543
H	3.973438	1.944723	0.198936
H	3.764656	0.166734	0.277652
H	2.539555	1.226840	-0.536473
N	2.397803	-2.149189	-0.651276
Si	3.016168	-3.368352	0.467052
Si	3.096131	-1.884659	-2.256937
C	1.951792	-0.696976	-3.198420
C	3.273160	-3.482617	-3.279003
C	4.833846	-1.102884	-2.221518
C	4.774175	-3.013288	1.102379
C	3.001206	-5.148116	-0.208289
C	1.853245	-3.339062	1.980246
H	4.105900	-4.118484	-2.912468
H	3.496178	-3.225401	-4.337269
H	2.344605	-4.087171	-3.262154
H	2.361862	-0.510610	-4.214101
H	1.865581	0.293307	-2.701866
H	0.931383	-1.114668	-3.334497
H	5.564334	-1.739589	-1.679950
H	5.210324	-0.976950	-3.260368
H	4.832358	-0.104327	-1.739519
H	5.532002	-3.099534	0.295624
H	5.053277	-3.737057	1.898679
H	4.849373	-1.991677	1.529953
H	3.757750	-5.301711	-1.004339
H	3.230479	-5.861763	0.612733
H	2.010238	-5.417765	-0.628513
H	2.126997	-4.160055	2.675539
H	0.783337	-3.505944	1.716713
H	1.940288	-2.394500	2.556986
H	-4.271087	-2.784002	-2.935631
H	-4.558446	-2.774836	-1.181448
H	-4.067478	-5.294481	-2.906842
H	-5.675567	-4.665305	-2.470392
H	-4.877319	-6.565529	-0.947377
H	-5.281935	-5.074946	-0.061988
H	-2.430305	-5.894858	-0.924930
H	-3.149238	-6.210932	0.672032
O	-0.427398	0.812254	-0.828629
C	-0.333127	1.827621	-1.749382
B	-1.987483	1.035528	0.577480
H	-1.495773	0.092600	1.182346
O	-3.243796	0.830664	0.004350
C	-3.959406	2.099784	-0.040657
C	-3.100974	3.023503	0.945379
O	-1.810263	2.354933	0.989056
C	-5.398594	1.840026	0.425617
C	-2.894095	4.462034	0.458981
C	-3.992011	2.602429	-1.493172

C	-3.642224	3.042912	2.386804
H	-5.977912	2.784885	0.479425
H	-5.907559	1.170915	-0.297613
H	-5.428751	1.350962	1.417117
H	-2.393514	4.498932	-0.527336
H	-2.256585	5.009631	1.182076
H	-3.861183	5.000332	0.380696
H	-2.976509	2.785157	-1.892518
H	-4.575467	3.541072	-1.583010
H	-2.907272	3.557179	3.038005
H	-4.607807	3.582950	2.461280
H	-3.781057	2.016887	2.781697
H	-4.476181	1.837853	-2.132618
H	-0.629507	1.478561	-2.774841
H	-0.997396	2.675161	-1.445237
O	1.023067	2.290598	-1.811080
C	1.275326	3.244690	-2.833669
H	2.352308	3.161155	-3.094119
H	0.688288	3.015040	-3.756234
C	0.975860	4.686038	-2.389552
O	1.153523	5.573500	-3.494162
H	-0.080567	4.776725	-2.057627
H	1.629855	4.962028	-1.535110
B	2.310054	6.285521	-3.636876
O	3.340668	6.299780	-2.710612
C	4.457775	6.998202	-3.338637
C	3.725215	7.870393	-4.453595
O	2.540048	7.074822	-4.746777
C	5.383573	5.921386	-3.929454
C	5.195687	7.806140	-2.268980
C	4.520327	8.058882	-5.747902
C	3.236183	9.230127	-3.925835
H	6.306814	6.358422	-4.360889
H	5.676777	5.218278	-3.123929
H	4.870080	5.338622	-4.720962
H	6.006034	8.413697	-2.722335
H	4.511179	8.480735	-1.720972
H	5.656891	7.118679	-1.531105
H	2.553124	9.679675	-4.674301
H	2.672407	9.115230	-2.977867
H	4.074942	9.934214	-3.752266
H	3.929050	8.664172	-6.464594
H	5.473528	8.593004	-5.554132
H	4.748519	7.090898	-6.232768

E(solv)= -4380.240576 A.U
Thermal correction= 1.234045

H

Th	-0.786201	-0.209719	-0.838943
N	-2.470315	0.722936	0.254227
C	-3.321290	1.337927	1.019706
N	-2.979740	2.442533	1.838216
C	-3.537117	2.569915	3.203497
C	-4.892242	3.281588	3.314781
C	-6.035886	2.452620	2.735592
C	-5.750206	1.995988	1.299263
N	-4.682061	0.982353	1.133111
C	-5.152981	-0.338293	0.790017
C	-5.046376	-1.389450	1.742272
C	-5.686352	-2.612920	1.468931
C	-6.409228	-2.839183	0.280442
C	-6.462416	-1.796030	-0.660819

C	-5.849249	-0.546270	-0.431237
C	-5.982770	0.546841	-1.469253
C	-4.275313	-1.215020	3.028925
C	-7.063979	-4.176149	0.013817
H	-4.663900	-0.364458	3.627224
H	-4.347847	-2.126157	3.654660
H	-3.197133	-1.014470	2.845506
H	-5.128567	1.250681	-1.435627
H	-6.039888	0.116677	-2.488661
H	-6.908597	1.146772	-1.323242
H	-7.005103	-1.951445	-1.609141
H	-5.615712	-3.419750	2.218299
H	-7.551167	-4.581060	0.925113
H	-6.314756	-4.931044	-0.313133
H	-7.830511	-4.107095	-0.783980
C	-1.913272	3.350764	1.498159
C	-2.096940	4.270148	0.423536
C	-1.133714	5.273045	0.204188
C	0.015183	5.403067	1.008283
C	0.191519	4.464082	2.038954
C	-0.738352	3.433956	2.301231
C	-0.448638	2.476875	3.435048
H	0.643455	2.423215	3.617169
H	-0.807067	1.446546	3.239855
H	-0.901739	2.814553	4.394122
H	1.092187	4.526239	2.673888
C	1.036620	6.486052	0.742902
H	1.634450	6.716966	1.647673
H	1.750968	6.177612	-0.052415
H	0.556646	7.425162	0.398308
H	-1.300856	5.989766	-0.617223
C	-3.318861	4.213604	-0.460825
H	-3.297925	5.020363	-1.219323
H	-3.387777	3.242494	-0.995305
H	-4.252735	4.329642	0.128073
N	-0.399211	-2.417639	-1.555183
Si	1.254033	-2.703768	-2.150817
Si	-1.463524	-3.831309	-1.381480
C	2.385587	-3.563287	-0.891258
C	1.306506	-3.685619	-3.783275
C	2.037587	-1.009381	-2.527342
C	-2.226504	-4.397932	-3.037782
C	-0.592316	-5.360494	-0.654878
C	-2.893885	-3.386942	-0.224187
H	-2.532280	-3.132634	0.792984
H	-3.501116	-2.532216	-0.589931
H	-3.585386	-4.249922	-0.126989
H	-1.344834	-6.157054	-0.467146
H	0.169055	-5.783213	-1.343364
H	-0.092986	-5.126306	0.307220
H	-2.868430	-3.619314	-3.498889
H	-1.452286	-4.679094	-3.780630
H	-2.864533	-5.292174	-2.864274
H	2.176606	-4.648825	-0.805958
H	3.447595	-3.449232	-1.200090
H	2.259281	-3.112819	0.115811
H	0.946710	-4.728791	-3.661757
H	0.695298	-3.202954	-4.574365
H	2.355036	-3.740523	-4.148747
H	3.056632	-1.189856	-2.932166
H	1.471057	-0.439099	-3.289404
H	2.196408	-0.375492	-1.626609
N	-0.682826	1.222754	-2.708693
Si	-1.907877	0.808659	-3.910098

Si	0.432490	2.582191	-2.899252
C	1.361929	2.785881	-1.254145
C	-0.438768	4.224731	-3.310814
C	1.728607	2.334854	-4.274162
C	-1.193292	0.161920	-5.549383
C	-3.127774	2.209477	-4.321741
C	-2.924381	-0.608900	-3.133323
H	-0.786649	4.252074	-4.364573
H	0.270303	5.070133	-3.176075
H	-1.313696	4.403017	-2.655043
H	2.062342	3.645640	-1.318820
H	1.978014	1.896236	-1.000974
H	0.673383	2.998746	-0.408015
H	1.252920	2.183756	-5.265831
H	2.371909	3.238815	-4.350103
H	2.390483	1.466622	-4.080553
H	-0.657186	0.956754	-6.109408
H	-2.004380	-0.218789	-6.207264
H	-0.479046	-0.669146	-5.373232
H	-2.648352	3.027812	-4.896498
H	-3.961327	1.810960	-4.940024
H	-3.564910	2.652961	-3.403387
H	-3.791351	-0.850361	-3.782748
H	-3.355880	-0.349124	-2.138207
H	-2.332035	-1.543774	-3.043657
H	-2.800485	3.139874	3.796441
H	-3.599824	1.559488	3.660383
H	-4.826646	4.265600	2.798606
H	-5.082012	3.503627	4.388034
H	-6.978539	3.043032	2.730581
H	-6.229723	1.559433	3.370316
H	-5.514631	2.881387	0.670529
H	-6.671142	1.545730	0.883832
O	0.755081	-0.104892	1.057543
C	1.968265	0.466464	1.456871
B	0.119260	-1.237389	1.932958
H	-0.840511	-1.566234	1.159417
O	-0.410441	-0.805449	3.212012
C	0.182574	-1.576854	4.274748
C	0.846418	-2.804963	3.497545
O	1.103155	-2.255732	2.194949
C	-0.921144	-1.978003	5.266314
C	2.171867	-3.296976	4.093439
C	1.210897	-0.701392	5.020558
C	-0.116700	-3.999834	3.341234
H	-0.524719	-2.634176	6.069484
H	-1.338905	-1.069475	5.747311
H	-1.752562	-2.502518	4.759442
H	2.938576	-2.498600	4.097611
H	2.565320	-4.137735	3.486275
H	2.035500	-3.660961	5.133182
H	2.055485	-0.403496	4.367670
H	1.631650	-1.217643	5.907958
H	0.337486	-4.731940	2.643442
H	-0.312207	-4.515742	4.303582
H	-1.087025	-3.680808	2.910845
H	0.711128	0.225312	5.369112
H	1.840513	1.568153	1.597703
H	2.290896	-0.005587	2.411623
O	2.925288	0.233838	0.431870
C	4.226209	0.730517	0.733978
H	4.703951	0.996506	-0.232856
H	4.173890	1.660820	1.348703
C	5.090416	-0.310922	1.462600

O	6.319616	0.288692	1.872654
H	4.571230	-0.668122	2.377016
H	5.263772	-1.187216	0.802654
B	7.439122	0.179118	1.097801
O	7.516745	-0.574218	-0.062626
C	8.796542	-0.251337	-0.686131
C	9.644974	0.293661	0.548474
O	8.612905	0.826942	1.428449
C	8.517589	0.826748	-1.747058
C	9.354585	-1.514709	-1.344777
C	10.626153	1.418141	0.208178
C	10.363790	-0.824486	1.322748
H	9.425503	1.079737	-2.331141
H	7.748223	0.448494	-2.450103
H	8.129884	1.756796	-1.283919
H	10.365080	-1.328022	-1.763488
H	9.417472	-2.355488	-0.628581
H	8.692623	-1.827582	-2.177657
H	10.742884	-0.410803	2.278772
H	9.672081	-1.656900	1.564199
H	11.223379	-1.235610	0.755782
H	11.158053	1.739879	1.126409
H	11.385703	1.074394	-0.524156
H	10.107362	2.302528	-0.207615

E(solv)= -4380.251466 A.U
Thermal correction= 1.23584

BpinOROCH$_2$OBpin

C	0.912095	-1.013221	-0.930311
O	1.209102	-1.833002	-2.096851
B	0.238674	-1.547227	-3.037874
O	-0.558046	-0.460832	-2.713949
C	0.060567	0.179173	-1.557570
O	0.107300	-2.290485	-4.174132
C	0.935083	1.325499	-2.092248
C	-1.043949	0.729083	-0.653017
C	2.231948	-0.590852	-0.280679
C	0.096374	-1.885134	0.039668
H	1.387809	1.918587	-1.272035
H	1.750990	0.941706	-2.737686
H	0.305416	2.003092	-2.703529
H	-0.617313	1.157820	0.277301
H	-1.593363	1.535806	-1.179655
H	-1.775333	-0.054502	-0.379194
H	-0.106879	-1.362653	0.996324
H	-0.872327	-2.187483	-0.407348
H	0.670341	-2.807283	0.261063
H	2.053518	0.096678	0.571971
H	2.759544	-1.485804	0.107053
H	2.903410	-0.091938	-1.004696
C	-0.870398	-1.962809	-5.158785
C	-0.329247	-2.372666	-6.524968
H	-1.814513	-2.517603	-4.958072
H	-1.111403	-0.877614	-5.147104
O	-1.336970	-2.082372	-7.490699
H	0.608566	-1.806558	-6.750281
H	-0.072621	-3.456129	-6.519568
C	-0.987183	-2.406166	-8.802643
O	-0.920589	-3.813904	-9.011008
H	0.024257	-2.007188	-9.057133
H	-1.762677	-1.950355	-9.452791
B	-2.010239	-4.488473	-9.495427

O	-3.177696	-3.882685	-9.927498
C	-3.959731	-4.917385	-10.597571
C	-3.378850	-6.249360	-9.947106
O	-2.012805	-5.863189	-9.613501
C	-3.660660	-4.804313	-12.101702
C	-5.443622	-4.659110	-10.328473
C	-3.329089	-7.456916	-10.886060
C	-4.074839	-6.625914	-8.627954
H	-2.901276	-8.328472	-10.350408
H	-4.346686	-7.733770	-11.231201
H	-2.694837	-7.261775	-11.771438
H	-3.480685	-7.413102	-8.121967
H	-4.138474	-5.755764	-7.943668
H	-5.098960	-7.016341	-8.796188
H	-4.276354	-5.506006	-12.700052
H	-3.887178	-3.771997	-12.436688
H	-2.591824	-5.006608	-12.316185
H	-6.070421	-5.470218	-10.753292
H	-5.653795	-4.578596	-9.245341
H	-5.750628	-3.705939	-10.804858

E(solv)= -1166.18432 A.U
Thermal correction= 0.388798

TS-I

Th	0.300206	0.004855	-0.200072
Si	0.597697	0.845642	3.397024
Si	3.186498	0.221978	1.928602
Si	2.309685	-2.788857	-1.835364
Si	0.209708	-3.403906	0.261471
N	-1.889392	0.133094	-0.738401
N	-3.389453	-0.056405	-2.597496
N	-4.213433	0.707606	-0.538556
N	1.429627	0.419693	1.896715
N	1.080803	-2.193377	-0.696423
C	-3.073191	0.250645	-1.246770
C	-4.226730	0.859128	-3.403155
H	-3.888866	0.760441	-4.452659
H	-4.020260	1.908574	-3.098978
C	-5.738404	0.600525	-3.346237
H	-5.934027	-0.458848	-3.625208
H	-6.233382	1.224959	-4.122726
C	-6.326901	0.903208	-1.968486
H	-6.321048	1.999480	-1.776099
H	-7.392204	0.585301	-1.927449
C	-5.570627	0.195442	-0.833382
H	-6.159783	0.307272	0.095752
H	-5.511298	-0.892288	-1.048671
C	-2.613641	-1.014805	-3.346789
C	-1.610448	-0.577155	-4.251780
C	-0.983961	-1.528321	-5.083618
H	-0.208258	-1.181385	-5.787636
C	-1.315023	-2.895196	-5.043974
C	-2.284730	-3.306611	-4.107663
H	-2.552661	-4.374827	-4.043121
C	-2.941004	-2.395163	-3.257547
C	-1.225642	0.878088	-4.361607
H	-1.842984	1.418947	-5.112980
H	-0.170096	0.985756	-4.671696
H	-1.343202	1.400285	-3.392408
C	-0.679703	-3.883503	-5.997304
H	0.337187	-3.562626	-6.301372
H	-1.282579	-3.984540	-6.927393

H	-0.600441	-4.895289	-5.550148
C	-3.992746	-2.894490	-2.293338
H	-4.993841	-2.476524	-2.531050
H	-3.761022	-2.605815	-1.246616
H	-4.071140	-3.998779	-2.328964
C	-4.094819	1.509890	0.650340
C	-4.451100	0.966644	1.914107
C	-4.504202	1.823162	3.033834
H	-4.792877	1.396741	4.009864
C	-4.160677	3.182921	2.955505
C	-3.749075	3.682104	1.701948
H	-3.455301	4.741197	1.610890
C	-3.724974	2.880640	0.544719
C	-4.747012	-0.505939	2.095236
H	-5.829565	-0.741411	1.990770
H	-4.442967	-0.840947	3.107176
H	-4.203354	-1.119271	1.350000
C	-3.350652	3.496318	-0.783506
H	-2.526253	2.940539	-1.277288
H	-3.026063	4.547031	-0.651186
H	-4.211786	3.490908	-1.486007
C	0.977880	-0.358686	4.829601
H	0.768319	-1.412602	4.549376
H	2.039099	-0.303046	5.152352
C	-1.279541	0.801589	3.114996
H	-1.612938	1.399038	2.239233
H	-1.784993	1.239509	4.000772
H	-1.678915	-0.224072	2.986032
C	0.965480	2.599272	4.056348
H	2.023416	2.737568	4.356394
H	0.339018	2.781550	4.957196
H	0.721743	3.391081	3.317618
C	4.127987	1.503165	2.984532
H	3.886546	2.546592	2.693345
C	3.877924	0.468663	0.163478
H	3.828131	1.537520	-0.129533
H	3.371584	-0.135442	-0.619827
H	4.946836	0.166823	0.140740
C	3.738019	-1.492579	2.537169
H	3.405633	-1.682346	3.578831
H	4.845210	-1.586816	2.511758
H	3.314306	-2.289587	1.893965
C	1.304078	-4.552094	1.317027
H	1.929500	-5.218960	0.687540
H	0.656160	-5.203191	1.943820
H	1.977924	-3.988335	1.993897
C	-0.949924	-4.542721	-0.731170
H	-1.483118	-3.980436	-1.523028
H	-1.704399	-4.996196	-0.051874
H	-0.402323	-5.372737	-1.221359
C	-0.902935	-2.456641	1.493713
H	-0.304101	-1.893064	2.239437
H	-1.513336	-3.190193	2.061720
H	-1.630964	-1.761708	1.012493
C	3.944622	-3.256628	-0.967878
H	4.416200	-2.383060	-0.473503
H	4.668646	-3.651986	-1.713673
H	3.799396	-4.038690	-0.194699
C	2.775340	-1.538543	-3.194930
H	1.882068	-1.189112	-3.750326
H	3.466599	-2.038654	-3.908255
H	3.305588	-0.646832	-2.800584
C	1.750156	-4.347978	-2.784033
H	1.667217	-5.244159	-2.134672

H	2.498855	-4.582026	-3.571842
H	0.769967	-4.187194	-3.278413
C	-4.194878	4.079103	4.173911
H	-4.781384	5.003270	3.984449
H	-4.645456	3.565557	5.046708
H	-3.172104	4.401487	4.467191
H	5.220346	1.355155	2.836571
H	3.927561	1.395846	4.070858
H	0.351418	-0.112997	5.714778
O	0.886799	2.297091	-0.648369
C	2.084642	2.209045	-2.334359
O	1.399614	2.560175	-3.430808
H	2.522651	3.054786	-1.770205
H	2.754062	1.355247	-2.489653
C	1.230225	3.384006	0.177166
B	0.996177	3.868694	-3.682671
O	1.379655	4.957531	-2.938786
C	1.016475	6.138484	-3.735503
C	-0.137372	5.567371	-4.672766
O	0.214419	4.147085	-4.772480
C	2.278215	6.546198	-4.512570
C	0.587264	7.258051	-2.788021
C	-0.171140	6.157041	-6.083704
C	-1.528775	5.637332	-4.026088
H	0.235495	8.139186	-3.363688
H	-0.215554	6.943546	-2.094555
H	1.455023	7.578118	-2.176191
H	2.119263	7.479801	-5.088834
H	3.104547	6.718932	-3.794355
H	2.597585	5.751534	-5.217162
H	-0.990923	5.688143	-6.664312
H	-0.359492	7.249807	-6.049138
H	0.774663	5.977580	-6.628778
H	-2.237241	5.037450	-4.631477
H	-1.520815	5.222281	-2.998376
H	-1.906020	6.678526	-3.979944
H	2.070088	3.970561	-0.282476
C	0.045651	4.339768	0.355682
H	1.588908	3.034667	1.171556
O	0.458009	5.413443	1.207768
H	-0.280180	4.718716	-0.636761
H	-0.811341	3.801080	0.818214
B	-0.212441	6.595833	1.259584
O	-1.288625	6.942851	0.446245
C	-1.823650	8.198881	0.969718
C	-0.581153	8.787638	1.777641
O	0.147939	7.587405	2.152312
C	-3.012200	7.842975	1.876952
C	-2.295854	9.062706	-0.201743
C	-0.946080	9.552825	3.052872
C	0.359174	9.634484	0.902285
H	-2.643316	10.054246	0.155270
H	-1.493884	9.220445	-0.947342
H	-3.147295	8.569843	-0.713856
H	-3.512353	8.748920	2.274592
H	-3.757878	7.268568	1.291087
H	-2.690454	7.216059	2.732682
H	-0.020117	9.901817	3.552977
H	-1.566133	10.443952	2.822651
H	-1.494498	8.914053	3.770808
H	1.296003	9.823019	1.463922
H	0.627555	9.101974	-0.032679
H	-0.089215	10.612497	0.633995
H	1.145219	0.492487	-2.133234

E(solv)= -4380.157208 A.U
Thermal correction= 1.229590

I

Th	2.221012	4.873770	6.500793
Si	-0.579197	3.604162	5.036567
Si	-0.624246	6.732193	5.100552
Si	1.108147	3.557177	9.635202
Si	3.862647	2.543150	8.757919
N	3.892160	4.836514	5.007469
N	5.946868	5.856859	4.349615
N	5.079286	4.071485	3.079681
N	0.131175	5.164779	5.429739
N	2.402193	3.485299	8.429202
C	4.900419	4.919158	4.199297
C	6.569542	6.525166	3.184233
H	6.956275	7.495166	3.551819
H	5.787299	6.756669	2.428024
C	7.717715	5.764193	2.507374
H	8.482163	5.505299	3.273275
H	8.214467	6.451887	1.788079
C	7.242078	4.502035	1.788533
H	6.629108	4.768664	0.898656
H	8.114946	3.928086	1.406485
C	6.421013	3.578319	2.700101
H	6.270223	2.615816	2.177107
H	7.001252	3.356339	3.622882
C	6.138454	6.512146	5.623057
C	5.593300	7.805253	5.849954
C	5.907355	8.471957	7.050242
H	5.490194	9.478823	7.222224
C	6.722717	7.890954	8.042480
C	7.223272	6.596756	7.801801
H	7.862207	6.117727	8.562811
C	6.956738	5.896965	6.606153
C	4.703596	8.478696	4.829304
H	5.290032	9.055791	4.080529
H	4.014815	9.195144	5.319105
H	4.092863	7.740960	4.273239
C	7.037472	8.640256	9.318472
H	6.107351	8.943885	9.844594
H	7.605874	9.571758	9.106914
H	7.644464	8.026802	10.013927
C	7.568538	4.533088	6.380498
H	6.799169	3.763456	6.165634
H	8.136313	4.202324	7.272260
H	8.267417	4.538763	5.517120
C	3.948539	3.436395	2.452304
C	3.745592	2.033303	2.562681
C	2.709712	1.432910	1.813423
H	2.565906	0.341917	1.897643
C	1.859782	2.172193	0.974413
C	2.052760	3.568681	0.920526
H	1.395069	4.179550	0.278726
C	3.074982	4.215381	1.638519
C	4.605345	1.154023	3.444139
H	5.454323	0.702073	2.884112
H	4.009373	0.311465	3.849140
H	5.030798	1.712768	4.298488
C	3.242632	5.710622	1.513013
H	3.133129	6.215577	2.496080
H	2.487021	6.138148	0.825317

H	4.247663	5.977090	1.123114
C	-2.114263	3.182469	6.078646
H	-1.903811	3.226836	7.167131
H	-2.936751	3.899403	5.869381
C	0.794135	2.313873	5.417532
H	1.691788	2.464031	4.771742
H	0.415692	1.299506	5.171863
H	1.117013	2.256323	6.484261
C	-1.038605	3.345744	3.212722
H	-1.913098	3.955959	2.910519
H	-1.297746	2.278182	3.042746
H	-0.184873	3.602356	2.552381
C	0.703466	7.965602	4.520417
H	1.517642	8.058895	5.268721
C	-1.463424	7.453738	6.649100
H	-0.735011	7.596993	7.473803
H	-2.266064	6.784443	7.024886
H	-1.922976	8.440844	6.425176
C	-1.953407	6.677803	3.734741
H	-1.540755	6.333719	2.763897
H	-2.357207	7.702652	3.583840
H	-2.811720	6.022996	3.995478
C	3.581526	0.937270	9.746268
H	3.171982	1.114594	10.762154
H	4.553494	0.411698	9.870171
H	2.892845	0.246274	9.216206
C	5.154956	3.584106	9.690307
H	5.383622	4.520689	9.137773
H	6.106935	3.026900	9.827775
H	4.785218	3.874705	10.696097
C	4.603797	2.001103	7.091101
H	3.960423	1.230289	6.616881
H	5.614135	1.559924	7.227861
H	4.697815	2.844047	6.370937
C	0.077658	1.954358	9.676697
H	-0.353888	1.726400	8.679310
H	-0.766056	2.045654	10.394837
H	0.687443	1.080228	9.984157
C	-0.079492	4.982142	9.196780
H	0.353172	5.972464	9.447938
H	-1.014813	4.871365	9.786304
H	-0.387376	5.008168	8.127688
C	1.730332	3.897895	11.403544
H	2.390139	3.092848	11.788788
H	0.868249	3.982741	12.100261
H	2.295406	4.852427	11.449707
C	0.765926	1.509486	0.167657
H	0.853812	1.754562	-0.912377
H	0.794242	0.406131	0.268174
H	-0.239288	1.853235	0.494428
H	0.266771	8.975932	4.369139
H	1.155185	7.644429	3.557887
H	-2.492757	2.164157	5.843377
O	2.315598	6.795913	7.451802
C	2.460210	7.959892	8.215205
C	3.257834	7.671807	9.494832
H	2.994268	8.749272	7.634363
H	1.459193	8.372475	8.490442
O	3.521059	8.881493	10.215293
H	2.706668	6.944503	10.128943
H	4.235985	7.226772	9.216963
B	2.679246	9.287526	11.210554
O	1.527593	8.613492	11.588008
C	1.069384	9.233265	12.827596

C	1.730029	10.679659	12.743151
O	2.924083	10.432578	11.944935
C	1.624207	8.386490	13.985308
C	-0.460830	9.219685	12.845240
C	2.155712	11.273323	14.088520
C	0.868442	11.689240	11.965099
H	-0.851443	9.752459	13.736857
H	-0.885559	9.689155	11.937877
H	-0.824829	8.173128	12.887231
H	1.259026	8.742042	14.970063
H	1.295897	7.336162	13.851463
H	2.732954	8.397642	13.998306
H	2.615909	12.269287	13.927595
H	1.281245	11.405168	14.758861
H	2.901767	10.636152	14.599996
H	1.478669	12.589938	11.752090
H	0.532619	11.270368	10.994901
H	-0.026105	12.003164	12.540323

E(solv)= -3853.871102 A.U
Thermal correction= 1.029023

TS-J

Th	0.583973	-0.246986	0.816515
N	1.988650	0.896048	-0.498643
C	2.624186	1.678074	-1.315344
N	4.030828	1.694551	-1.473407
C	4.776044	2.954924	-1.694862
C	4.895425	3.423895	-3.150571
C	3.559590	3.905970	-3.711567
C	2.443581	2.865946	-3.540194
N	1.982885	2.626591	-2.154616
C	4.849219	0.548414	-1.163425
C	5.671892	0.551552	-0.003485
C	6.595682	-0.498122	0.179646
C	6.727620	-1.551200	-0.743401
C	5.874352	-1.547141	-1.864032
C	4.932602	-0.526098	-2.091357
C	4.042843	-0.584368	-3.310509
C	7.711465	-2.676921	-0.514502
C	5.601241	1.659715	1.023741
H	4.203769	0.288388	-3.978054
H	2.967032	-0.584655	-3.033170
H	4.241937	-1.500396	-3.900709
H	5.942828	-2.369882	-2.596141
H	8.588104	-2.342576	0.076714
H	8.081945	-3.098019	-1.471519
H	7.239042	-3.513221	0.047494
H	7.233665	-0.486545	1.080159
H	6.322974	2.478589	0.806829
H	5.849884	1.275426	2.032600
H	4.592619	2.113864	1.065301
H	4.320058	3.761688	-1.082416
H	5.794484	2.790542	-1.296548
H	5.649391	4.240593	-3.193159
H	5.299558	2.591825	-3.769129
H	3.656214	4.138510	-4.795063
H	3.251434	4.852649	-3.213995
H	2.759744	1.900377	-3.990442
H	1.562344	3.207408	-4.112615
C	0.708902	3.203307	-1.805367
C	-0.465196	2.876987	-2.540090
H	-2.558359	3.334386	-2.852446

C	-1.655273	3.589798	-2.272151
C	-1.728485	4.602231	-1.300451
C	-0.557979	4.886449	-0.568019
C	0.655291	4.212617	-0.800217
C	-0.483356	1.814904	-3.614705
C	-3.016789	5.344974	-1.025354
C	1.883406	4.601271	-0.013056
H	1.644082	5.378504	0.738565
H	2.677712	5.007888	-0.674144
H	2.316779	3.730680	0.521642
H	-0.188774	2.223409	-4.607273
H	0.188659	0.966509	-3.385774
H	-1.504595	1.404566	-3.733657
H	-0.582181	5.675239	0.202754
H	-3.766034	5.175145	-1.824249
H	-2.846422	6.438825	-0.940704
H	-3.472676	5.015457	-0.065993
N	0.403944	1.241557	2.663503
Si	-0.969023	2.292971	3.042903
Si	1.854898	1.256805	3.676427
C	-1.929193	1.775614	4.607878
C	-0.489352	4.116812	3.308899
C	-2.184346	2.211614	1.586813
C	1.533346	0.841787	5.505961
C	2.816468	2.901737	3.661250
C	3.035306	-0.069129	2.979463
H	3.303962	0.107020	1.911855
H	2.630784	-1.097391	3.079160
H	3.993036	-0.035289	3.540085
H	0.950144	-0.094463	5.626297
H	2.498103	0.714337	6.043196
H	0.976688	1.655259	6.016935
H	3.793037	2.765340	4.174723
H	2.274894	3.714697	4.186016
H	3.021135	3.246080	2.626928
H	-3.076671	2.840277	1.791277
H	-1.730925	2.578398	0.641706
H	-2.553260	1.177716	1.424871
H	-2.303960	0.733351	4.549904
H	-1.309101	1.859303	5.523946
H	-2.809991	2.441455	4.741010
H	0.160328	4.492949	2.493477
H	-1.406136	4.744959	3.335999
H	0.043153	4.270044	4.270821
N	0.868443	-2.442721	1.665250
Si	-0.421219	-2.979301	2.752776
Si	2.145177	-3.593023	1.214851
C	-1.781138	-1.643887	2.738193
C	-1.264379	-4.609010	2.248591
C	0.138971	-3.154880	4.564990
C	1.511722	-5.087985	0.222733
C	3.417444	-2.719682	0.116169
C	3.094356	-4.280340	2.722126
H	-2.265926	-1.548283	1.745755
H	-2.574606	-1.919714	3.464185
H	-1.400475	-0.649832	3.058311
H	-2.195948	-4.741679	2.840777
H	-1.531768	-4.605399	1.171928
H	-0.622416	-5.493508	2.440441
H	0.894905	-3.955802	4.696139
H	-0.728600	-3.401971	5.214888
H	0.584072	-2.209560	4.939949
H	0.976811	-5.824079	0.856056
H	0.816325	-4.753992	-0.574602

H	2.368780	-5.615622	-0.250257
H	2.460393	-4.933075	3.358573
H	3.503712	-3.473460	3.365643
H	3.950720	-4.897562	2.372129
H	4.200276	-3.449799	-0.178126
H	3.934330	-1.875937	0.616524
H	2.973328	-2.333126	-0.823751
O	-1.193670	-0.554903	-0.558323
C	-2.385885	-0.090544	-1.158415
H	-2.391396	-0.374332	-2.235212
H	-2.435614	1.021417	-1.122119
C	-3.635422	-0.685060	-0.497221
H	-3.504588	-1.783845	-0.385831
H	-3.806958	-0.261221	0.516012
O	-4.756888	-0.419024	-1.346849
B	-5.996889	-0.195166	-0.823161
O	-7.082029	0.094338	-1.629385
C	-8.262383	0.029656	-0.778195
C	-7.653629	0.281734	0.672608
O	-6.296028	-0.232461	0.529737
C	-8.347913	-0.477818	1.805499
C	-7.536823	1.774608	1.024216
H	-8.527286	2.230238	1.226602
H	-7.049927	2.343903	0.206672
H	-6.912537	1.882022	1.933979
C	-9.263415	1.088159	-1.247900
C	-8.861062	-1.378411	-0.940157
H	-9.814983	-1.489498	-0.385927
H	-9.058784	-1.561763	-2.015427
H	-8.157075	-2.158741	-0.586370
H	-9.623194	0.836674	-2.266215
H	-10.144427	1.128557	-0.574278
H	-8.804436	2.093977	-1.291552
H	-9.410603	-0.171116	1.895043
H	-8.307444	-1.572400	1.649176
H	-7.846341	-0.254861	2.769125
H	0.833245	-1.716055	-1.169735
B	-0.190162	-1.957763	-1.802234
O	-0.776808	-3.213025	-1.672345
C	-1.427702	-3.569829	-2.926542
C	-0.824889	-2.502739	-3.954086
O	-0.349465	-1.434644	-3.086237
C	-2.950388	-3.465522	-2.744944
C	-1.065526	-5.028232	-3.241065
C	-1.841464	-1.924254	-4.944822
C	0.403072	-3.024150	-4.723724
H	0.860445	-2.181789	-5.281045
H	1.170936	-3.430523	-4.035703
H	0.131668	-3.813874	-5.453216
H	-1.345374	-1.171342	-5.590371
H	-2.248995	-2.719080	-5.603224
H	-2.688368	-1.429624	-4.432788
H	-1.474593	-5.336539	-4.225507
H	0.028152	-5.192669	-3.244411
H	-1.502866	-5.692701	-2.468672
H	-3.488009	-3.849933	-3.635753
H	-3.249957	-4.082245	-1.873486
H	-3.291399	-2.429376	-2.565835

E(solv)= -4265.725301 A.U
Thermal correction= 1.207983

J

Th	0.553854	-0.255675	0.738413
N	1.943016	0.901647	-0.548493
C	2.592171	1.690180	-1.353681
N	3.999577	1.719441	-1.472197
C	4.739645	2.985754	-1.678778
C	4.887851	3.456589	-3.130893
C	3.560911	3.927442	-3.720739
C	2.451812	2.876114	-3.580319
N	1.957597	2.624486	-2.207854
C	4.818474	0.576764	-1.147763
C	5.618040	0.581670	0.027376
C	6.536751	-0.469741	0.229981
C	6.685737	-1.523386	-0.689065
C	5.857204	-1.517829	-1.828781
C	4.921999	-0.496212	-2.076124
C	4.060797	-0.549839	-3.315479
C	7.664636	-2.650137	-0.444651
C	5.531193	1.691766	1.051299
H	4.244536	0.321236	-3.979382
H	2.978709	-0.544192	-3.063885
H	4.267599	-1.467354	-3.900347
H	5.941101	-2.339690	-2.560243
H	8.450449	-2.361310	0.281983
H	8.163733	-2.968641	-1.383276
H	7.149180	-3.546304	-0.033472
H	7.156890	-0.458617	1.142761
H	6.260265	2.507356	0.846944
H	5.759483	1.308757	2.065436
H	4.523998	2.150432	1.073347
H	4.263127	3.788151	-1.076338
H	5.749863	2.828571	-1.257644
H	5.635122	4.280072	-3.154754
H	5.314097	2.629484	-3.741097
H	3.679853	4.164343	-4.800917
H	3.231745	4.869471	-3.227874
H	2.786092	1.915372	-4.026935
H	1.581362	3.212383	-4.171276
C	0.666962	3.184444	-1.889001
C	-0.484734	2.852209	-2.657051
H	-2.576257	3.286297	-3.008336
C	-1.689760	3.546600	-2.405321
C	-1.798512	4.547816	-1.425322
C	-0.646903	4.844091	-0.668230
C	0.579922	4.188474	-0.880651
C	-0.468016	1.810498	-3.751791
C	-3.102448	5.271009	-1.172661
C	1.788105	4.595551	-0.071790
H	1.521857	5.362892	0.680935
H	2.583156	5.023767	-0.718337
H	2.232674	3.731799	0.464541
H	-0.101969	2.228572	-4.715981
H	0.157575	0.931707	-3.503302
H	-1.492473	1.437437	-3.942801
H	-0.696790	5.628796	0.105404
H	-3.840390	5.077472	-1.976473
H	-2.951753	6.368742	-1.100883
H	-3.562442	4.946711	-0.213589
N	0.308607	1.227165	2.577176
Si	-1.095380	2.246611	2.925943
Si	1.744173	1.282967	3.611648
C	-2.069326	1.721847	4.478885
C	-0.671755	4.085653	3.179574
C	-2.276363	2.118535	1.442405
C	1.403833	0.904760	5.444972

C	2.675113	2.943891	3.576104
C	2.952558	-0.039978	2.956105
H	3.233954	0.117157	1.888469
H	2.564394	-1.072557	3.072979
H	3.903800	0.023279	3.525320
H	0.833811	-0.037078	5.581246
H	2.363800	0.804831	5.996391
H	0.829433	1.721973	5.929687
H	3.642957	2.841158	4.113160
H	2.103942	3.755477	4.070577
H	2.893823	3.270067	2.538983
H	-3.194213	2.716250	1.625410
H	-1.815153	2.507308	0.509587
H	-2.614141	1.074981	1.269344
H	-2.419777	0.671017	4.429819
H	-1.463993	1.830865	5.402113
H	-2.966097	2.369852	4.591418
H	-0.018179	4.471486	2.371962
H	-1.605976	4.688100	3.183987
H	-0.161494	4.263675	4.149449
N	0.786550	-2.396630	1.650066
Si	-0.509153	-2.942908	2.727468
Si	2.022826	-3.562881	1.126815
C	-1.922177	-1.671302	2.601380
C	-1.269698	-4.618586	2.254904
C	0.029524	-3.030960	4.550033
C	1.324480	-4.941940	0.021066
C	3.316861	-2.642652	0.094009
C	2.930635	-4.370442	2.596981
H	-2.377570	-1.670082	1.589832
H	-2.729050	-1.932741	3.317957
H	-1.597526	-0.642135	2.865741
H	-2.172093	-4.800667	2.878175
H	-1.575097	-4.622872	1.188397
H	-0.574904	-5.467681	2.421121
H	0.826516	-3.786817	4.706715
H	-0.829149	-3.307861	5.199391
H	0.420628	-2.053937	4.902163
H	0.833099	-5.750100	0.598919
H	0.571847	-4.515131	-0.674794
H	2.141367	-5.404397	-0.574512
H	2.261153	-5.018616	3.201262
H	3.375819	-3.613225	3.276296
H	3.756036	-5.013480	2.220624
H	4.068822	-3.370853	-0.275423
H	3.870184	-1.862259	0.654575
H	2.872520	-2.166078	-0.804839
O	-1.245254	-0.648687	-0.851932
C	-2.467559	-0.099487	-1.369917
H	-2.475791	-0.255571	-2.468021
H	-2.478837	0.993836	-1.184041
C	-3.698606	-0.766114	-0.752443
H	-3.604139	-1.868714	-0.846671
H	-3.797532	-0.522073	0.328092
O	-4.841699	-0.301373	-1.475854
B	-6.067830	-0.244163	-0.879798
O	-7.175911	0.244558	-1.545742
C	-8.330925	-0.060027	-0.711761
C	-7.680395	-0.209231	0.734797
O	-6.326692	-0.652630	0.419088
C	-8.340365	-1.255052	1.636247
C	-7.551243	1.130616	1.478904
H	-8.533593	1.508428	1.827768
H	-7.085902	1.905065	0.836131

H	-6.900973	0.986966	2.365235
C	-9.345270	1.078578	-0.846583
C	-8.934227	-1.374383	-1.237324
H	-9.872697	-1.640409	-0.709953
H	-9.161997	-1.256721	-2.315835
H	-8.221334	-2.217231	-1.131796
H	-9.732469	1.112413	-1.885108
H	-10.207598	0.925085	-0.165256
H	-8.889041	2.062040	-0.625380
H	-9.400002	-0.993673	1.836882
H	-8.303862	-2.264832	1.185821
H	-7.810185	-1.299138	2.609284
H	0.575212	-1.801429	-1.090366
B	-0.552915	-1.756887	-1.698081
O	-1.226348	-3.038447	-1.666000
C	-1.502536	-3.475922	-3.013092
C	-0.544256	-2.550151	-3.888110
O	-0.429367	-1.363772	-3.083375
C	-2.997785	-3.251786	-3.319313
C	-1.204993	-4.979266	-3.123666
C	-1.107488	-2.163576	-5.261668
C	0.863815	-3.157063	-4.065223
H	1.528743	-2.387784	-4.507897
H	1.296957	-3.461435	-3.091370
H	0.861966	-4.039225	-4.737867
H	-0.381045	-1.518259	-5.797540
H	-1.288398	-3.061936	-5.888084
H	-2.056305	-1.601194	-5.170273
H	-1.348113	-5.339476	-4.164378
H	-0.174400	-5.222686	-2.804562
H	-1.900545	-5.545835	-2.470866
H	-3.285293	-3.668528	-4.306901
H	-3.602594	-3.768619	-2.546096
H	-3.274724	-2.179504	-3.307350

E(solv)= -4265.737884 A.U
Thermal correction= 1.209721

BpinOROBpin

C	0.287289	-1.080645	-0.041054
O	1.314381	-1.020706	-1.073539
B	0.716681	-0.473668	-2.192498
O	-0.544598	0.050932	-1.957078
C	-0.735768	0.045658	-0.510871
O	1.335721	-0.475709	-3.409023
C	-0.359499	1.447792	-0.003075
C	-2.207047	-0.250335	-0.212412
C	0.945067	-0.829288	1.317772
C	-0.316275	-2.494906	-0.087820
H	-0.551035	1.560318	1.083217
H	0.709602	1.671863	-0.194014
H	-0.968446	2.200884	-0.542646
H	-2.379778	-0.338805	0.880110
H	-2.840034	0.577313	-0.592005
H	-2.543753	-1.184131	-0.701020
H	-1.051724	-2.660165	0.725432
H	-0.817115	-2.686890	-1.058357
H	0.500337	-3.235991	0.024902
H	0.186069	-0.794705	2.126568
H	1.651255	-1.652751	1.547596
H	1.517628	0.117390	1.327475
C	0.729024	0.164339	-4.530406
C	1.271641	1.589705	-4.687392

H	0.987610	-0.428594	-5.434003
H	-0.377912	0.194411	-4.433992
O	0.664790	2.229539	-5.808843
H	1.013080	2.182701	-3.783826
H	2.378559	1.559677	-4.783938
B	1.284754	2.229272	-7.024896
O	0.687129	2.776274	-8.143888
C	1.714704	2.837892	-9.175783
C	2.738896	1.712666	-8.705868
O	2.546844	1.706416	-7.259819
C	2.316401	4.252923	-9.128160
C	1.057987	2.586205	-10.535064
C	4.209964	2.010712	-9.003317
C	2.364781	0.310291	-9.214603
H	4.843800	1.183601	-8.623973
H	4.383162	2.100157	-10.095686
H	4.545220	2.944597	-8.513887
H	2.974201	-0.442266	-8.674814
H	1.295801	0.084762	-9.024705
H	2.557423	0.198430	-10.300775
H	1.817491	2.552617	-11.343429
H	0.486463	1.638905	-10.545334
H	0.351062	3.408972	-10.765096
H	3.051970	4.419504	-9.941039
H	1.498847	4.992959	-9.240959
H	2.816557	4.445209	-8.157333

E(solv)= -1051.667738 A.U
Thermal correction= 0.359779

TS-H'

Th	2.208345	4.364397	6.570466
Si	0.832946	1.270997	6.629548
Si	-1.342319	3.479166	6.219909
Si	3.088268	3.845873	9.950987
Si	5.503809	4.255267	8.096596
N	2.972774	4.879467	4.570005
N	3.761633	6.621209	3.143262
N	3.282030	4.520739	2.228348
N	0.339434	2.957661	6.465031
N	3.741093	4.117055	8.311978
C	3.320510	5.310866	3.389342
C	3.305511	7.366634	1.947507
H	3.312321	8.438555	2.225054
H	2.247355	7.096828	1.739219
C	4.146182	7.170208	0.678568
H	5.208587	7.404900	0.909315
H	3.819612	7.917016	-0.077852
C	4.027744	5.755867	0.108905
H	3.016695	5.595895	-0.326625
H	4.750247	5.618441	-0.725198
C	4.298737	4.667087	1.158486
H	4.349457	3.686852	0.646051
H	5.292498	4.841887	1.624307
C	4.382136	7.404910	4.186623
C	3.605867	8.324965	4.939446
C	4.262391	9.172106	5.856263
H	3.651399	9.884394	6.432762
C	5.658264	9.136136	6.043532
C	6.396435	8.194328	5.300176
H	7.489713	8.138298	5.437076
C	5.789047	7.327551	4.369707
C	2.110287	8.445683	4.759226

H	1.857681	9.185719	3.967669
H	1.646816	8.808002	5.697117
H	1.652911	7.479916	4.467877
C	6.341885	10.093282	6.994812
H	6.392848	11.115697	6.560628
H	7.379714	9.774633	7.218587
H	5.795737	10.185101	7.956671
C	6.651557	6.380598	3.564860
H	6.284387	5.335040	3.612299
H	7.694125	6.386416	3.939448
H	6.682942	6.665799	2.491448
C	2.474167	3.325597	2.153560
C	3.073986	2.053536	2.360334
C	2.317190	0.896290	2.090173
H	2.790508	-0.090225	2.233763
C	0.984089	0.960593	1.636478
C	0.401768	2.234374	1.492627
H	-0.643598	2.311479	1.148828
C	1.120701	3.422750	1.737036
C	4.507104	1.928169	2.827541
H	5.227823	1.987373	1.982163
H	4.678119	0.952201	3.324101
H	4.772187	2.735396	3.539058
C	0.459885	4.762004	1.503057
H	0.577279	5.438954	2.373636
H	-0.624392	4.640821	1.311756
H	0.896359	5.284301	0.625170
C	0.320664	0.488411	8.282818
H	0.680195	1.069228	9.156398
H	-0.786512	0.430924	8.354670
C	2.751228	1.318305	6.504577
H	3.084364	1.718575	5.517506
H	3.141937	0.279992	6.548241
H	3.282256	1.864061	7.319464
C	0.275659	0.108836	5.240270
H	-0.804404	-0.131287	5.298432
H	0.837055	-0.848083	5.312051
H	0.485147	0.558194	4.248756
C	-1.381904	4.885111	4.938810
H	-0.667790	5.704766	5.162524
C	-2.119063	4.076492	7.849754
H	-1.543747	4.900502	8.318892
H	-2.172181	3.249178	8.589147
H	-3.154593	4.442605	7.680842
C	-2.490215	2.116505	5.548956
H	-2.158596	1.735378	4.561437
H	-3.507499	2.546441	5.420562
H	-2.585702	1.253308	6.240752
C	6.505593	3.038217	9.165195
H	6.386421	3.216572	10.253718
H	7.585803	3.155095	8.929470
H	6.229498	1.983379	8.956811
C	6.098017	6.016782	8.465438
H	5.638134	6.744211	7.764137
H	7.201386	6.097916	8.359293
H	5.828164	6.326076	9.495944
C	5.912128	3.821740	6.288529
H	5.724420	2.746836	6.081028
H	6.985793	4.019663	6.084540
H	5.321888	4.420976	5.562312
C	3.334939	2.047774	10.532886
H	2.916204	1.311622	9.815903
H	2.824515	1.893134	11.508255
H	4.406838	1.802941	10.677208

C	1.207385	4.163360	9.892436
H	0.978352	5.246237	9.826405
H	0.754375	3.792544	10.836622
H	0.666746	3.642347	9.070179
C	3.817946	4.987248	11.274342
H	4.899877	4.802850	11.440290
H	3.304608	4.797997	12.242240
H	3.690017	6.062814	11.032636
C	0.206887	-0.300856	1.331511
H	-0.736537	-0.080604	0.793480
H	0.800747	-1.002363	0.709040
H	-0.059784	-0.844268	2.264296
H	-2.394920	5.337059	4.879774
H	-1.130104	4.485096	3.934956
H	0.712491	-0.547651	8.373285
O	0.952603	6.210705	7.190483
C	0.172495	7.170298	7.527903
O	1.238545	8.778177	8.138616
H	-0.351364	7.744690	6.733072
H	-0.348669	7.119875	8.511078
C	1.868906	8.320047	9.336155
C	3.092650	9.176419	9.661056
H	1.168069	8.342309	10.201992
H	2.223702	7.277845	9.179761
O	3.744923	8.605865	10.804335
H	3.784444	9.175438	8.790251
H	2.769007	10.216281	9.864958
B	4.645712	9.349122	11.509613
O	5.062530	10.621750	11.148326
C	5.838664	11.142010	12.269612
C	6.300091	9.806765	13.009046
O	5.238922	8.872044	12.663809
C	4.885158	12.000090	13.117545
C	6.978202	12.002652	11.718733
C	6.380546	9.909724	14.534514
C	7.611128	9.231121	12.446381
H	7.632664	12.364818	12.538464
H	7.598922	11.446393	10.991061
H	6.559517	12.888838	11.199886
H	7.758128	8.210668	12.853900
H	7.574148	9.152649	11.340962
H	8.489274	9.847840	12.725771
H	6.665098	8.925404	14.958602
H	7.147396	10.649907	14.843709
H	5.409109	10.198965	14.977979
H	5.412074	12.496055	13.957672
H	4.438966	12.785112	12.474731
H	4.057256	11.390687	13.533014
C	0.255977	12.071734	9.163971
C	0.592682	12.090182	7.606291
C	-0.143295	13.175786	6.804776
H	0.126478	14.195295	7.153736
H	0.133240	13.098354	5.732500
H	-1.240886	13.053370	6.875081
C	2.107619	12.204737	7.325341
H	2.284750	11.985990	6.252208
H	2.506713	13.218255	7.540783
H	2.683479	11.469541	7.921159
C	1.226290	12.878789	10.039701
H	1.224051	13.953432	9.759006
H	0.919335	12.805278	11.103790
H	2.264312	12.500479	9.963259
C	-1.191526	12.525708	9.456708
H	-1.421171	12.314071	10.521174

H	-1.342327	13.610268	9.275275
H	-1.913649	11.958433	8.835524
B	0.063241	9.910148	8.303637
H	-0.979242	9.231713	8.319433
O	0.125813	10.809439	7.170595
O	0.364525	10.682704	9.497329

E(solv)= -4380.201213A.U
Thermal correction= 1.227949

H’

Th	-0.501406	-1.509880	-0.297661
Si	-1.937046	-4.589241	-0.210496
Si	-4.071329	-2.348677	-0.566280
Si	0.406294	-1.987595	3.050081
Si	2.831089	-1.820024	1.180272
N	0.273664	-1.140407	-2.347260
N	1.165826	0.536521	-3.794402
N	0.570321	-1.557455	-4.672801
N	-2.403279	-2.904875	-0.376943
N	1.080163	-1.808629	1.422762
C	0.640986	-0.748069	-3.522481
C	0.725349	1.292611	-4.985673
H	0.804219	2.366788	-4.726838
H	-0.352168	1.087464	-5.171393
C	1.526391	1.031529	-6.269602
H	2.603063	1.225352	-6.067758
H	1.214075	1.774872	-7.035951
C	1.338468	-0.388290	-6.807900
H	0.311806	-0.514526	-7.217443
H	2.035971	-0.568614	-7.655267
C	1.585720	-1.467726	-5.743083
H	1.606420	-2.456970	-6.240488
H	2.586709	-1.314008	-5.285450
C	1.796559	1.300677	-2.744163
C	1.048055	2.241696	-1.987219
C	1.722072	3.034129	-1.034912
H	1.127699	3.745246	-0.439839
C	3.110319	2.934208	-0.823250
C	3.826230	1.994623	-1.589819
H	4.915973	1.899861	-1.446337
C	3.197923	1.171421	-2.544882
C	-0.432027	2.442184	-2.212890
H	-0.622145	3.112770	-3.080506
H	-0.903532	2.901255	-1.324996
H	-0.940602	1.480360	-2.419428
C	3.805230	3.782978	0.218260
H	3.706866	3.331923	1.230446
H	3.373031	4.803415	0.271306
H	4.890271	3.879410	0.010663
C	4.032858	0.206576	-3.356876
H	3.648112	-0.831832	-3.292782
H	5.081813	0.198337	-3.000347
H	4.045724	0.480958	-4.433013
C	-0.292283	-2.712793	-4.723626
C	0.250053	-4.012630	-4.528287
C	-0.566567	-5.132423	-4.781054
H	-0.138634	-6.140363	-4.643130
C	-1.906005	-5.005002	-5.200726
C	-2.431315	-3.705119	-5.328451
H	-3.481593	-3.577815	-5.641321
C	-1.650666	-2.552750	-5.102917
C	1.682170	-4.207039	-4.082108

H	2.394025	-4.187558	-4.936973
H	1.810030	-5.187625	-3.581689
H	1.995212	-3.410783	-3.377678
C	-2.253869	-1.182831	-5.313156
H	-2.128438	-0.536281	-4.420495
H	-3.338014	-1.256788	-5.528099
H	-1.777954	-0.654110	-6.166333
C	-2.467195	-5.349766	1.450754
H	-2.125851	-4.745714	2.316011
H	-3.575515	-5.408710	1.505310
C	-0.020973	-4.594050	-0.344434
H	0.308543	-4.215514	-1.340192
H	0.351686	-5.637761	-0.277775
H	0.520728	-4.033561	0.452464
C	-2.531859	-5.750620	-1.587204
H	-3.618716	-5.956564	-1.523492
H	-1.999317	-6.723820	-1.511912
H	-2.314128	-5.314752	-2.583062
C	-4.151931	-0.986354	-1.892799
H	-3.409414	-0.180068	-1.720084
C	-4.786663	-1.707065	1.077808
H	-4.166438	-0.906899	1.526898
H	-4.849779	-2.531180	1.820584
H	-5.813355	-1.305574	0.933796
C	-5.279709	-3.705552	-1.147388
H	-5.006134	-4.113748	-2.142080
H	-6.296480	-3.263495	-1.233498
H	-5.351575	-4.553576	-0.433730
C	3.736238	-3.110378	2.251910
H	3.647609	-2.903409	3.338787
H	4.820007	-3.105667	2.003380
H	3.353925	-4.136057	2.066116
C	3.589206	-0.115475	1.536381
H	3.221290	0.633052	0.803816
H	4.697985	-0.142789	1.461293
H	3.322255	0.242429	2.552027
C	3.200594	-2.284720	-0.628983
H	2.934358	-3.343471	-0.833170
H	4.284371	-2.163086	-0.840398
H	2.643800	-1.647474	-1.348913
C	0.508745	-3.783326	3.683319
H	0.074630	-4.504604	2.960426
H	-0.050399	-3.889073	4.638473
H	1.556255	-4.092875	3.875621
C	-1.443780	-1.528082	2.984917
H	-1.599272	-0.444732	2.809228
H	-1.910545	-1.783783	3.960097
H	-2.025638	-2.079898	2.212378
C	1.228085	-0.879214	4.351834
H	2.291812	-1.150931	4.517736
H	0.707273	-0.998243	5.327015
H	1.197344	0.196490	4.083287
C	-2.750606	-6.228664	-5.478992
H	-2.218060	-6.949046	-6.134862
H	-2.996171	-6.768470	-4.538372
H	-3.707963	-5.962469	-5.969813
H	-5.159005	-0.518482	-1.926151
H	-3.949364	-1.428896	-2.890196
H	-2.073612	-6.381872	1.574215
O	-1.639529	0.317812	0.237690
C	-2.660802	1.249424	0.516083
H	-2.731155	2.034477	-0.263146
H	-3.653554	0.754962	0.592954
H	-2.496561	1.756985	1.495012

E(solv)= -3328.620776 A.U
Thermal correction= 0.852924

TS-I’

Th	0.464524	-1.004249	0.276107
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C	-2.082599	-3.320294	-0.464791
N	-2.622686	-3.310066	-1.777570
C	-4.083691	-3.397482	-1.991136
C	-4.659277	-4.816536	-2.098436
C	-4.607747	-5.571378	-0.771385
C	-3.204000	-5.569345	-0.150745
N	-2.720853	-4.268087	0.366564
C	-2.651060	-4.177253	1.804976
C	-3.566873	-3.340727	2.500472
C	-3.606274	-3.405519	3.906011
C	-2.762922	-4.257511	4.646690
C	-1.842772	-5.047229	3.934409
C	-1.767580	-5.025355	2.525924
C	-0.780241	-5.928358	1.819407
C	-4.494481	-2.404461	1.762740
C	-2.819164	-4.283687	6.157895
H	-5.113546	-2.945497	1.017053
H	-5.181455	-1.895128	2.467162
H	-3.936702	-1.620412	1.206668
H	-0.462011	-5.504007	0.847381
H	0.122132	-6.089644	2.441684
H	-1.211634	-6.933310	1.613438
H	-1.157311	-5.710652	4.489382
H	-4.328869	-2.765851	4.440957
H	-3.862363	-4.211004	6.529313
H	-2.260978	-3.425740	6.594696
H	-2.370765	-5.209976	6.570146
C	-1.831824	-2.922372	-2.917677
C	-0.863944	-3.831419	-3.437799
C	-0.223675	-3.529372	-4.653310
C	-0.496924	-2.350530	-5.376513
C	-1.418253	-1.448750	-4.819099
C	-2.087179	-1.700956	-3.600877
C	-3.056556	-0.667077	-3.077450
H	-2.759603	0.342327	-3.424604
H	-3.101892	-0.643983	-1.971913
H	-4.091391	-0.836139	-3.452280
H	-1.628009	-0.501700	-5.345242
C	0.194910	-2.069167	-6.691530
H	-0.146689	-1.113703	-7.137309
H	1.297241	-2.007952	-6.564688
H	0.003154	-2.875949	-7.431335
H	0.505009	-4.252520	-5.056709
C	-0.533138	-5.119371	-2.723309
H	0.242948	-5.689916	-3.270106
H	-0.155233	-4.924926	-1.697156
H	-1.425860	-5.771961	-2.623860
N	1.127486	0.137905	2.255986
Si	2.233985	1.496934	1.981203
Si	0.499711	-0.104799	3.896834
C	1.406574	3.207573	2.067988
C	3.730760	1.509251	3.161022
C	2.962027	1.335007	0.224881
C	1.767645	-0.918506	5.069368
C	-0.072507	1.504810	4.741500
C	-1.013378	-1.246979	3.841469

H	-1.884602	-0.753822	3.365004
H	-0.841059	-2.206584	3.309658
H	-1.311830	-1.510594	4.877954
H	-0.594115	1.261334	5.692680
H	0.771836	2.180625	4.990974
H	-0.778524	2.062386	4.091890
H	2.068515	-1.929707	4.725091
H	2.689868	-0.311806	5.173069
H	1.323573	-1.030739	6.082697
H	1.218000	3.528822	3.112423
H	2.060070	3.972815	1.595162
H	0.430057	3.196106	1.541226
H	3.434456	1.709626	4.211999
H	4.280849	0.545312	3.139549
H	4.438849	2.312380	2.861410
H	3.713862	2.139130	0.077042
H	3.473879	0.364105	0.070648
H	2.213572	1.468036	-0.585451
N	2.380964	-2.051327	-0.648120
Si	3.030218	-3.267177	0.455359
Si	3.082934	-1.757679	-2.245139
C	1.964220	-0.534187	-3.176725
C	3.239249	-3.333454	-3.303701
C	4.833508	-1.002590	-2.198153
C	4.759271	-2.853903	1.132025
C	3.090311	-5.036619	-0.243706
C	1.840733	-3.308728	1.950247
H	4.057138	-3.993399	-2.947035
H	3.472852	-3.058207	-4.355226
H	2.298770	-3.919213	-3.304163
H	2.352156	-0.378916	-4.205911
H	1.944872	0.463940	-2.691830
H	0.918970	-0.897644	-3.275829
H	5.562456	-1.678435	-1.703930
H	5.193635	-0.831765	-3.236379
H	4.863539	-0.028285	-1.669419
H	5.533409	-2.879872	0.336847
H	5.058787	-3.587154	1.911954
H	4.777968	-1.842888	1.589828
H	3.863971	-5.153328	-1.029598
H	3.332616	-5.752753	0.571323
H	2.115330	-5.334204	-0.682039
H	2.139278	-4.125291	2.640285
H	0.782631	-3.520529	1.669436
H	1.883117	-2.370077	2.542454
H	-4.302151	-2.863099	-2.933772
H	-4.601622	-2.839595	-1.181193
H	-4.097889	-5.373506	-2.881753
H	-5.709158	-4.742748	-2.458797
H	-4.921176	-6.628672	-0.917221
H	-5.326091	-5.130352	-0.044882
H	-2.473025	-5.965333	-0.887968
H	-3.199819	-6.265768	0.709140
O	-0.431200	0.787941	-0.754850
C	-0.319967	1.903821	-1.602673
B	-2.069617	0.961658	0.617079
H	-1.615049	-0.013111	1.201704
O	-3.300269	0.797764	-0.016582
C	-3.990439	2.081469	-0.051872
C	-3.170623	2.951355	1.011021
O	-1.893485	2.258687	1.093789
C	-5.457052	1.832853	0.326317
C	-2.919426	4.404545	0.593677
C	-3.931524	2.636623	-1.484202

C	-3.782989	2.922684	2.423483
H	-6.021460	2.786450	0.384796
H	-5.937370	1.201696	-0.448734
H	-5.550648	1.307533	1.295117
H	-2.367878	4.474365	-0.363000
H	-2.315094	4.914356	1.370974
H	-3.874865	4.958873	0.487574
H	-2.891994	2.810230	-1.818768
H	-4.492082	3.589493	-1.571247
H	-3.075852	3.401618	3.130149
H	-4.744534	3.472956	2.470931
H	-3.953790	1.884258	2.770712
H	-4.395029	1.905835	-2.176589
H	-0.884603	1.750531	-2.551013
H	-0.708051	2.815552	-1.094512
H	0.740573	2.107514	-1.878021

E(solv)= -3740.481766 A.U
Thermal correction= 1.021476

CH_3OBpin

C	-1.718713	0.124679	1.587056
O	-0.322103	0.446609	1.332082
B	-0.086047	0.161372	-0.000016
O	-1.236094	-0.116222	-0.725322
C	-2.363386	0.225901	0.134081
O	1.173233	0.164678	-0.518409
C	-2.792958	1.656324	-0.232554
C	-3.503133	-0.758090	-0.139565
C	-2.270976	1.121503	2.609141
C	-1.759388	-1.302911	2.158892
H	-3.699420	1.971593	0.322767
H	-1.983139	2.384469	-0.023979
H	-3.018715	1.697465	-1.317285
H	-4.354667	-0.580996	0.549501
H	-3.871529	-0.625594	-1.177258
H	-3.171841	-1.808059	-0.030143
H	-2.785220	-1.600994	2.456348
H	-1.378868	-2.041552	1.424439
H	-1.108395	-1.349389	3.054891
H	-3.355054	0.957352	2.780427
H	-1.748279	0.988825	3.578075
H	-2.116993	2.168034	2.284532
C	1.395573	-0.086033	-1.900305
H	2.123515	0.657220	-2.288482
H	1.831804	-1.099585	-2.038321
H	0.458482	-0.019829	-2.492585

E(solv)= -526.4297122 A.U
Thermal correction= 0.178899

13. References

1. Szewczyk, M.; Magre, M.; Zubar, V.; Rueping, M. Reduction of Cyclic and Linear Organic Carbonates Using a Readily Available Magnesium Catalyst. *ACS Catal.* **2019**, *9*, 11634–11639.

2. (a) Yang, Y.; Xu, M.; Song, D. Organocatalysts with Carbon-Centered Activity for CO_2 Reduction with Boranes. *Chem. Commun.* **2015**, *5*, 11293–11296. (b) Hojoh, K.; Shido, Y.; Ohmiya, H.; Sawamura, M. Construction of Quaternary Stereogenic Carbon Centers through Copper-Catalyzed Enantioselective Allylic Cross-Coupling with Alkylboranes. *Angew. Chem. Int. Ed.* **2014**, *53*, 4954–4958.