

SUPPORTING INFORMATION FOR

**Moisture-Tolerant Frustrated Lewis Pair Catalyst for
Hydrogenation of Aldehydes and Ketones**

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Materials and methods

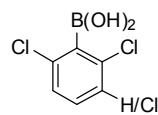
When experiments were performed on double-manifold N₂(H₂)/vacuum lines or in a nitrogen glovebox, the glasswares were heated to 120°C overnight and either attached to the vacuum lines or placed into the glovebox while hot.

NMR experiments were performed on a 250 MHz Bruker spectrometer (¹H, ¹³C, ¹⁹F) 400 MHz Bruker NMR System spectrometers (¹H, ¹³C, ¹⁹F, ¹⁰B). 600 MHz Varian NMR (molecular dynamic investigations). ¹H, ¹³C NMR spectra are referenced to residual solvent peaks. ¹⁰B, ¹⁹F NMR spectra were referenced externally to BF₃·Et₂O at 0 ppm and CFCl₃ at 0 ppm, respectively. Mass spectra were recorded on Thermo LTQ FT Ultra mass spectrometer operated in electrospray ionization (ESI) mode. The IR spectra were recorded with Mettler Toledo ReactIR 15 infrared spectrometer equipped with MCT detector and diamond head. Melting points are uncorrected. Diethyl ether, tetrahydrofuran, toluene and hexanes were distilled from sodium/benzophenone prior to use. Trimethylborate was freshly distilled from sodium before quenching the aryllithiums. Hydrogen gas (99.96 %) was purchased from Linde. Benzene-d₆, toluene-d₈ and THF-d₈ were purchased from Euriso-top and used in glovebox over 4 Å molecular sieves.

Commercially available liquid aldehydes and ketones were distilled under high vacuum (using vacuum pump) and kept in glovebox over 4 Å molecular sieves. The solids were used without further purification. Puriss. grade THF was purchased from Molar Chemicals. It contained 0.0078% water determined by Karl-Fischer method. Reactor bodies were purchased from Parr Instrument Company (*V* = 22 cm³), the valves were purchased from Swagelok.

General procedure for the synthesis of the new catalysts

General procedure of boronic acid synthesis



At $-75\text{ }^{\circ}\text{C}$, chlorobenzene (50.0 mmol) was added to a solution of n-butyllithium (22 mL in hexanes, 2.5 M) (55.0 mmol) in tetrahydrofuran (70 mL). After a few minutes the 2-lithio-1,3-dichlorobenzene precipitated as a white solid from the solution. After 2 h stirring at this temperature, the reaction mixture was treated with 12.0 mL of trimethylborate. The mixture was slowly allowed to warm to rt. and stirred overnight. Next day, 70 mL of 1M HCl was added to the slurry at $0\text{ }^{\circ}\text{C}$ and the mixture was stirred at rt. for two hours. After that the phases were separated and the aqueous phase was washed with ether. The combined organic layer was washed with brine three times, dried over anhydrous Na_2SO_4 , filtered off and evaporated to dryness. The resulted amorphous solid was washed with hexane and dried. The product was obtained as a white powder.

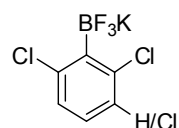
(2,6-dichlorophenyl)boronic acid

white solid, mp.: $137\text{--}138\text{ }^{\circ}\text{C}$, yield: 78%, IR: $\nu_{\text{max}} = 1696, 1588, 1555, 1403, 1329, 1307, 1148, 1077, 781, 733\text{ cm}^{-1}$. $^1\text{H-NMR}$ (600 MHz, dimethyl sulfoxide- d_6) $\delta = 7.31\text{--}7.36$ (ABC multiplet, $J=8.1\text{ Hz}$, $J=2.3\text{ Hz}$, 3H); 8.58 (s, 2H) ppm; $^{13}\text{C-NMR}$ (125 MHz, dimethyl sulfoxide- d_6) $\delta = 126.7; 130.6; 135.8; 138.7$ ppm; $^{10}\text{B-NMR}$ (64 MHz, dimethyl sulfoxide- d_6) $\delta = 27.6$ ppm. HR-MS ESI Exact mass calculated for $\text{C}_6\text{H}_4\text{O}_2^{10}\text{BCl}_2$ [M] 188.9687; Found: 188.9684.

(2,3,6-trichlorophenyl)boronic acid.

white solid, mp.: $149\text{--}150\text{ }^{\circ}\text{C}$, yield: 63%, IR: $\nu_{\text{max}} = 1701, 1570, 1401, 1311, 1232, 1175, 1086, 1033, 823, 771\text{ cm}^{-1}$. $^1\text{H-NMR}$ (600 MHz, dimethyl sulfoxide- d_6) $\delta = 7.40$ (d, $J=8.6\text{ Hz}$, 1H); 7.58 (d, $J=8.6\text{ Hz}$, 1H); 8.70 (s, 2H) ppm; $^{13}\text{C-NMR}$ (125 MHz, dimethyl sulfoxide- d_6) $\delta = 128.4; 129.6; 130.7; 133.3; 134.0; 414.0$ ppm; $^{10}\text{B-NMR}$ (64 MHz, dimethyl sulfoxide- d_6) $\delta = 27.3$ ppm. HR-MS ESI Exact mass calculated for $\text{C}_6\text{H}_3\text{O}_2^{10}\text{BCl}_3$ [M] 222.9297; Found: 222.9293.

General procedure of potassium aryltrifluoroborate salts



60 mL methanol was added to 39.0 mmol boronic acid in a PE-flask. The solution was treated with 156.0 mmol (4 equiv.) KHF_2 dissolved in 43 mL of distilled water. The resulting suspension was stirred overnight. Next day, acetone was added to the suspension, decanted from the solid residue and evaporated to dryness. The resulted white solid was dried on rotary evaporator on $60\text{ }^{\circ}\text{C}$ for two hours. The formed white solid was dissolved in acetone, filtered off and evaporated to dryness. It was scoured with hexane, filtered, washed three times with hexane and dried in vacuum exicator pistol over phosphorus(V)-oxide at $70\text{ }^{\circ}\text{C}$ overnight. The products were obtained as white powders.

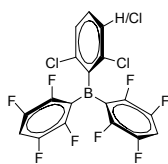
Potassium (2,6-dichlorophenyl)trifluoroborate (2a)

white solid, mp (decomp.): $268\text{--}272\text{ }^{\circ}\text{C}$, yield: 93%, IR: $\nu_{\text{max}} = 1704, 1582, 1554, 1409, 1240, 1156, 1081, 1020, 940, 766, 733\text{ cm}^{-1}$. $^1\text{H-NMR}$ (600 MHz, dimethyl sulfoxide- d_6) $\delta = 7.00$ (dd, $J=8.5\text{ Hz}$, $J=7.3\text{ Hz}$, 1H); 7.09 (d, $J=7.8\text{ Hz}$, 2H); $^{19}\text{F-NMR}$ (564 MHz, dimethyl sulfoxide- d_6) $\delta = -133.4$ (dd, $J=44.2\text{ Hz}$, $J=93.4\text{ Hz}$, 3F); $^{13}\text{C-NMR}$ (125 MHz, dimethyl sulfoxide- d_6) $\delta = 127.5; 127.8; 139.2; 144.1$ ppm; $^{10}\text{B-NMR}$ (64 MHz, dimethyl sulfoxide- d_6) $\delta = 2.0$ ppm. HR-MS ESI Exact mass calculated for $\text{C}_6\text{H}_3^{10}\text{BCl}_2\text{F}_3$ [M] 212.9662; Found: 212.9659.

Potassium (2,3,6-trichlorophenyl)trifluoroborate (2b)

white solid, mp (decomp.): $280\text{--}284\text{ }^{\circ}\text{C}$, yield: 96%, IR: $\nu_{\text{max}} = 1704, 1561, 1411, 1339, 1237, 1169, 1086, 1026, 951, 800, 744\text{ cm}^{-1}$. $^1\text{H-NMR}$ (600 MHz, dimethyl sulfoxide- d_6) $\delta = 7.13$ (d, $J=8.5\text{ Hz}$, 1H); 7.28 (d, $J=8.5\text{ Hz}$, 1H); $^{19}\text{F-NMR}$ (564 MHz, dimethyl sulfoxide- d_6) $\delta = -133.8$ (dd, $J=43.2\text{ Hz}$, $J=90.3\text{ Hz}$, 3F); $^{13}\text{C-NMR}$ (125 MHz, dimethyl sulfoxide- d_6) $\delta = 128.1; 129.0; 130.2; 136.6; 137.3; 144.8$ ppm; $^{10}\text{B-NMR}$ (64 MHz, dimethyl sulfoxide- d_6) $\delta = 1.9$ ppm. HR-MS ESI Exact mass calculated for $\text{C}_6\text{H}_2^{10}\text{BCl}_3\text{F}_3$ [M] 246.9273; Found: 246.9268.

General procedure of arylbis(2,3,5,6-tetrafluorophenyl)boranes



The Grignard reagent, (*p*-C₆F₄H)MgCl was prepared from slow addition of ⁱPrMgCl (prepared from 45.0 mmol activated magnesium turnings, 45.0 mmol 2-chloropropane, 24 mL of diethylether), to a solution of *p*-C₆F₄HBr (10.304 g, 45.0 mmol) in Et₂O (132 mL). The cloudy solution was stirred for 1 hour at ambient temperature^{1a}. After that the Grignard reagent was added to the suspension of trifluoroborate salt **2a/2b** (20.0 mmol in 16 mL of ether) at 0°C and then it was allowed to warm to rt. and stirred overnight. Next day, the solvent was evaporated, and the solid residue was extracted with 100 ml hot toluene. The combined solution was evaporated to dryness. The solid was washed with hexane three times and dried under vacuum. The products were obtained as white microcrystalline solids.

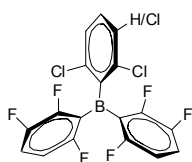
(2,6-dichlorophenyl)bis(2,3,5,6-tetrafluorophenyl)borane (4a)

white solid, mp.: 163-165°C, yield: 68%, IR: ν_{\max} = 1646, 1475, 1363, 1288, 1176, 921, 862, 778, 662 cm⁻¹. ¹H-NMR (400 MHz, benzene-*d*₆) δ = 6.84 (d, *J* = 8.1 Hz, 2H); 6.57 (t, *J* = 8.1 Hz, 1H); 6.27 (pm, *J* = 8.5 Hz, 2H) ppm; ¹⁹F-NMR (376 MHz, benzene-*d*₆) δ = -129.1 (m, 4F); -138.0 (m, 4F) ppm; ¹³C-NMR (100 MHz, benzene-*d*₆) δ = 148.2 (dm, *J* = 255 Hz); 145.6 (dm, *J* = 256 Hz); 140.7 (br m); 134.4 (C-Cl); 131.4; 126.8; 118.7 (br m); 111.4 (t, *J* = 22.6 Hz) ppm; ¹¹B-NMR (128 MHz, benzene-*d*₆) δ = 63.4 ppm, HR-MS ESI Exact mass calculated for C₁₈H₆O¹⁰BCl₂F₈ [M+OH⁻] 470.9767; Found: 470.9767.

(2,3,6-trichlorophenyl)bis(2,3,5,6-tetrafluorophenyl)borane (4b)

white solid, mp.: 140-142°C, yield: 44%, IR: ν_{\max} = 1643, 1603, 1476, 1368, 1286, 1178, 921, 865 cm⁻¹. ¹H-NMR (400 MHz, benzene-*d*₆) δ = 6.73 (d, *J* = 8.6 Hz, 1H); 6.57 (d, *J* = 8.6 Hz, 1H); 6.23 (pm, *J* = 8.4 Hz, 2H) ppm; ¹⁹F-NMR (376 MHz, benzene-*d*₆) δ = -128.8 (m, 4F); -137.8 (m, 4F) ppm; ¹³C-NMR (100 MHz, benzene-*d*₆) δ = 148.2 (dm, *J* = 270 Hz); 145.6 (dm, *J* = 250 Hz); 142.4 (br m); 132.2; 132.0; 131.6; 131.2; 128.2; 118.1 (br m); 111.7 (t, *J* = 22.6 Hz) ppm; ¹¹B-NMR (128 MHz, benzene-*d*₆) δ = 62.5 ppm, HR-MS ESI Exact mass calculated for C₁₈H₅O¹⁰BCl₃F₈ [M+OH⁻] 504.9377; Found: 504.9379.

General procedure of arylbis(2,3,6-trifluorophenyl)boranes



The Grignard reagent, (*m,p*-C₆F₃H₂)MgCl was prepared from slow addition of ⁱPrMgCl (prepared from 46.0 mmol activated magnesium, 5 mL 2-chloropropane, 20 ml THF, stirred at 50°C for 1.5 hours), to a solution of *m,p*-C₆F₃H₂Br (10.368 g, 46.0 mmol) in THF (132 mL) at -20°C. The clear solution was allowed to warm to 0°C slowly, then the cooling bath was removed and the mixture was stirred for 1 hour at ambient temperature. After that the Grignard reagent was added to a suspension of trifluoroborate salt **2a/2b** (20.0 mmol in 14 ml THF) at 0°C and then it was allowed to warm to rt. and stirred overnight. Next day, the solvent was evaporated, the solid residue was dried under vacuum at 80°C for 2 hours and then extracted with 100 ml toluene. The resulted yellow solution was evaporated to dryness. The crude product was suspended in 10 ml hexane and filtered off. The filtered solid was washed with hexane three times and dried on vacuum pump. The products were obtained as white microcrystalline solids.

(2,3,6-trichlorophenyl)bis(2,3,6-trifluorophenyl)borane (4d)

white solid, mp.: 141-144°C, yield: 45%, IR: ν_{\max} = 1633, 1476, 1424, 1230, 1223, 1174, 977, 950, 816 cm⁻¹. ¹H-NMR (400 MHz, benzene-*d*₆) δ = 6.75 (d, *J* = 8.6 Hz, 1H); 6.62 (d, *J* = 8.6 Hz, 1H); 6.47 (o, *J* = 4.7 Hz, 2H); 6.12 (tm, *J* = 8.9 Hz, 2H) ppm; ¹⁹F-NMR (376 MHz, benzene-*d*₆) δ = -103.1 (p, *J* = 7.0 Hz, 2F); -122.7 (dd, *J* = 8.9 Hz, 21.8 Hz, 2F); -142.2 (m, 2F) ppm; ¹³C-NMR (100 MHz, benzene-*d*₆) δ = 160.7 (dd, *J* = 8.6 Hz, 251 Hz); 152.1 (dt, *J* = 12.3, 255 Hz); 146.9 (dd, *J* = 14.7 Hz, 246 Hz); 143.7 (br m); 132.4; 132.2; 131.1; 131.0; 128.1; 122.6 (dd, *J* = 11.4 Hz, 19.5 Hz); 118.0 (br m); 111.2 (dt, *J* = 4.8 Hz, 27.7 Hz) ppm; ¹¹B-NMR (128 MHz, benzene-*d*₆) δ = 62.2 ppm, HR-MS ESI Exact mass calculated for C₁₈H₇O¹⁰BCl₃F₆ [M+OH⁻] 468.9566; Found: 468.9566.

(2,6-dichlorophenyl)bis(2,3,6-trifluorophenyl)borane (4c)

white solid, mp 122-124°C, yield: 43% IR: ν_{\max} = 2934, 1633, 1590, 1480, 1426, 1254, 1226, 980, 820, 781 cm⁻¹. ¹H-NMR (400 MHz, benzene-*d*₆) δ = 6.86 (d, *J* = 8.1 Hz, 2H); 6.56 (t, *J* = 8.1 Hz, 1H); 6.47 (o, *J* = 4.7 Hz,

2H); 6.14 (tm, $J = 8.9$ Hz, 2H) ppm; ^{19}F -NMR (376 MHz, benzene- d_6) $\delta = -103.3$ (p, $J = 7.3$ Hz, 2F); -122.9 (dd, $J = 8.9$ Hz, 21.7 Hz, 2F); -142.5 (m, 2F) ppm; ^{13}C -NMR (100 MHz, benzene- d_6) $\delta = 160.6$ (dd, $J = 8.5$ Hz, 251 Hz); 152.8 (dt, $J = 12.4$, 255 Hz); 146.9 (dd, $J = 14.7$ Hz, 246 Hz); 142.0 (br m); 134.6; 130.9; 126.8; 122.6 (dd, $J = 11.4$ Hz, 19.5 Hz); 118.7 (br m); 111.2 (dt, $J = 4.8$ Hz, 27.7 Hz) ppm; ^{11}B -NMR (128 MHz, benzene- d_6) $\delta = 63.8$ ppm, HR-MS ESI Exact mass calculated for $\text{C}_{18}\text{H}_8\text{O}^{10}\text{BCl}_2\text{F}_6$ [M+OH] 434.9955; Found: 434.9953.

General procedure for the hydrogenations:

Reactions for catalyst screening were carried out in glove box in the following manner: 1 mmol substrate and 0.1 mmol catalyst was dissolved in 1.25 ml abs. THF (dioxane was used when **1a** was applied as catalyst) in the glove box, in a glass vial, and the vial was placed in a high pressure reactor. The reactions took place under 100 bar H_2 pressure at 50°C . After then the solvent was removed and the residue was taken up in CDCl_3 and measured with ^1H -NMR (except **Table 2, entry 8**, when THF- d_8 was used as solvent). Conversion was calculated according to NMR spectra and GC-MS. The identification of the products was aided by GC-MS.

General procedure for the bench manipulations :

Procedure A

1.0 mmol benzaldehyde and 0.1 mmol catalyst (**4a**, stored at air in an opened vial for several months) was dissolved in 1.25 ml puriss. grade THF in a glass vial, and the vial was placed in a high pressure reactor (the vial and the reactor was not dried). The reactions were carried out under 20 bar H_2 pressure at 55°C for 42 hours. Then, the solvent was removed and the residue was dissolved in CDCl_3 and measured with ^1H -NMR/GC-MS.

Procedure B:

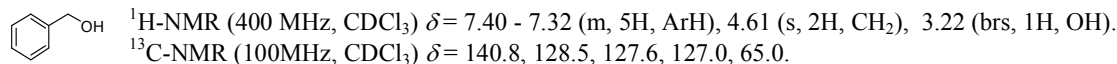
1.0 mmol aldehyde and 0.1 mmol catalyst (**4a**, **4b** stored at air in an opened vial for several months) was dissolved in 1.25 ml puriss. grade THF in a glass vial, and the vial was placed in a high pressure reactor (the vial and the reactor was not dried). The reactions were carried out under 100 bar H_2 pressure at 55°C for 137 hours. Then, the solvent was removed, the residue was dissolved in CDCl_3 and measured with ^1H -NMR/ GC-MS.

Procedure C:

1.0 mmol aldehyde and 0.1 mmol catalyst (**4a**, stored at air in an opened vial for several months) was dissolved in 1.25 ml puriss. grade diethyl-ether in a glass vial, and the vial was placed in a high pressure reactor (the vial and the reactor was not dried). The reactions were carried out under 20 bar H_2 pressure at 55°C for 87 hours. Then, the solvent was removed, the residue was dissolved in CDCl_3 and measured with ^1H -NMR/ GC-MS.

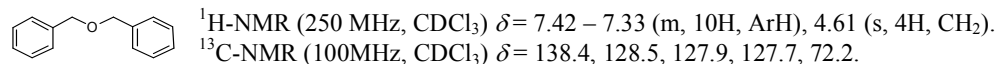
Product characterization

Benzyl alcohol¹ (Table 1. Entry 1-4, 16-19) Procedure A

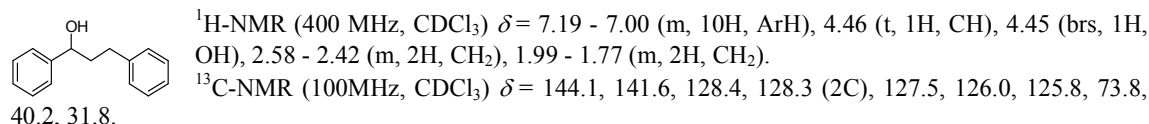


Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 75%)

Dibenzylether² (Table 1. Entry 1-4, 16-19) Procedure A

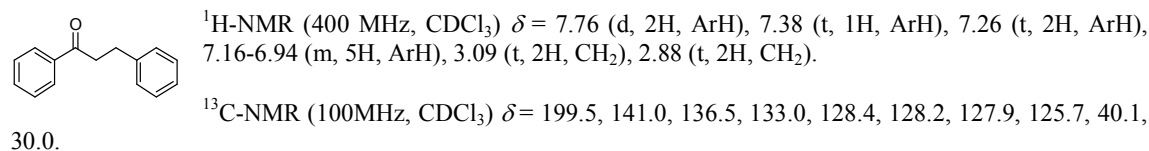


1,3-Diphenylpropanol³ (Table 1. Entry 5-11) Procedure B (cat. 4b)



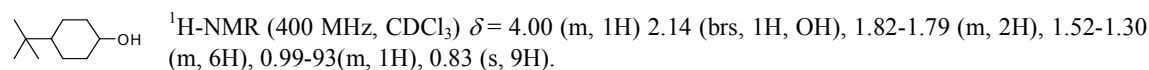
Purified by column chromatography with hexane : ethyl acetate 3:1 (Yield: 45%)

Dihydrochalcone⁴ (Table 1. Entry 5-11) Procedure B (cat.4b)



Purified by column chromatography with hexane : ethyl acetate 3:1 (Yield: 21%)

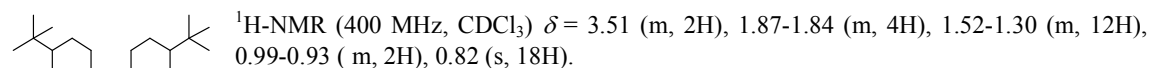
4-tertbutylcyclohexanol⁵ (Table 1. Entry 12-15) Procedure C



¹³C-NMR (100MHz, CDCl₃) δ = 69.6, 48.0, 33.3, 32.5, 27.6, 20.8.

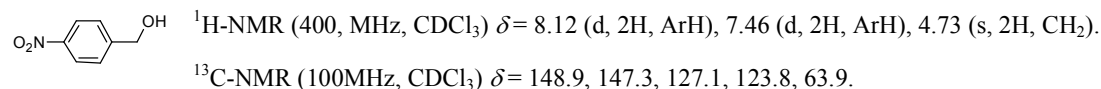
Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 65%)

4,4'-oxybis(tert-butylcyclohexane)^{5,6} (Table 1. Entry 12-15) Procedure C



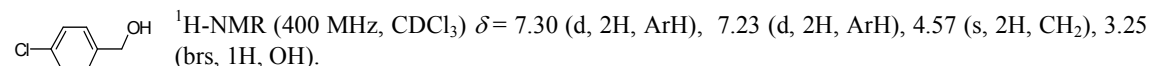
¹³C-NMR (100MHz, CDCl₃) δ = 69.4, 47.6, 32.9, 31.4, 27.4, 21.1.

4-Nitrobenzylalcohol⁷ (Table 2. Entry 1.) Procedure A



Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 95%)

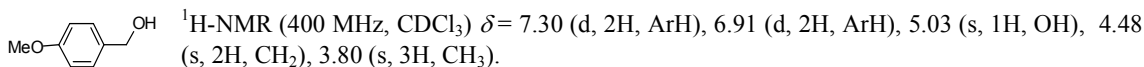
4-Chlorobenzylalcohol¹ (Table 2. Entry 2) Procedure A



¹³C-NMR (100MHz, CDCl₃) δ = 139.5, 133.4, 128.7, 128.3, 64.5.

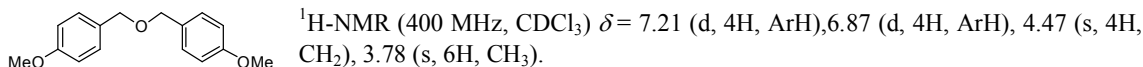
Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 93%)

4-Methoxybenzylalcohol⁸ (Table 2. Entry 3) Procedure A



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 159.2, 132.6, 128.7 (2C), 113.8 (2C), 64.7, 55.2.

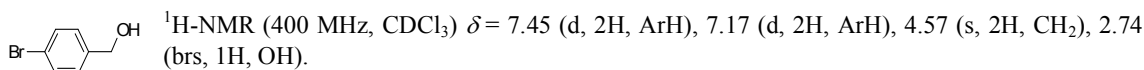
Di-(4-methoxybenzyl)ether⁸ (Table 2. Entry 3) Procedure A (80°C)



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 159.2, 130.3, 129.3 (2C), 113.8 (2C), 71.4, 55.2.

Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 73%)

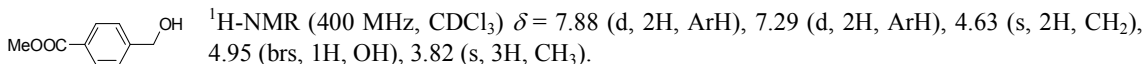
4-Bromobenzylalcohol¹ (Table 2. Entry 4) Procedure A



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 139.8, 131.7, 128.7, 121.5, 64.5.

Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 75%)

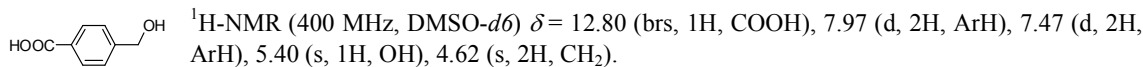
Methyl 4-(hydroxymethyl)benzoate⁹ (Table 2. Entry 5) Procedure A



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 167.3, 146.2, 129.8, 129.0, 126.5, 64.5, 52.2.

Purified by flash chromatography with hexane : ethyl acetate 50:1 – 10:1 (Yield: 76%)

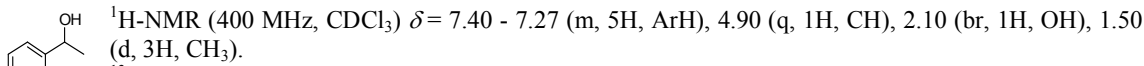
4-Hydroxymethylbenzoic acid¹⁰ (Table 2. Entry 6) Procedure B (cat. 4b)



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 167.5, 147.9, 129.4, 129.3, 126.3, 62.7.

Purified by digestion with diethyl ether:hexane 1:1. (Yield: 76%)

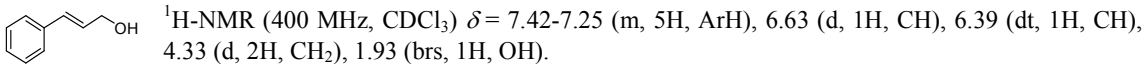
1-Phenylethanol¹¹ (Table 2. Entry 7) Procedure B (cat. 4a)



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 145.9, 128.6, 127.6, 125.5, 70.5, 25.2.

Purified by column chromatography with hexane : ethyl acetate 3:1 (Yield: 60%)

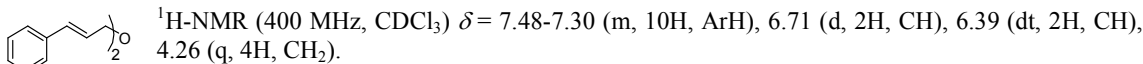
(E)-3-phenylprop-2-en-1-ol¹² (Table 2. Entry 9) Procedure A



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 136.8, 131.2, 128.7, 128.6, 127.8, 126.6, 63.8.

Purified by column chromatography with hexane : ethyl acetate 3:1 (Yield: 60%).

((1E,1'E)-oxybis(prop-1-ene-3,1-diyl)dibenzene¹³ (Table 2. Entry 9) Procedure A



$^{13}\text{C-NMR}$ (100MHz, CDCl_3) δ = 136.8, 132.6, 128.6, 127.8, 126.6, 126.1, 70.8.

Purified by column chromatography with hexane : ethyl acetate 3:1 (Yield: 21%).

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NMR spectra

NMR spectra of the arylboronic acids

(2,6-dichlorophenyl)boronic acid

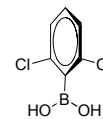
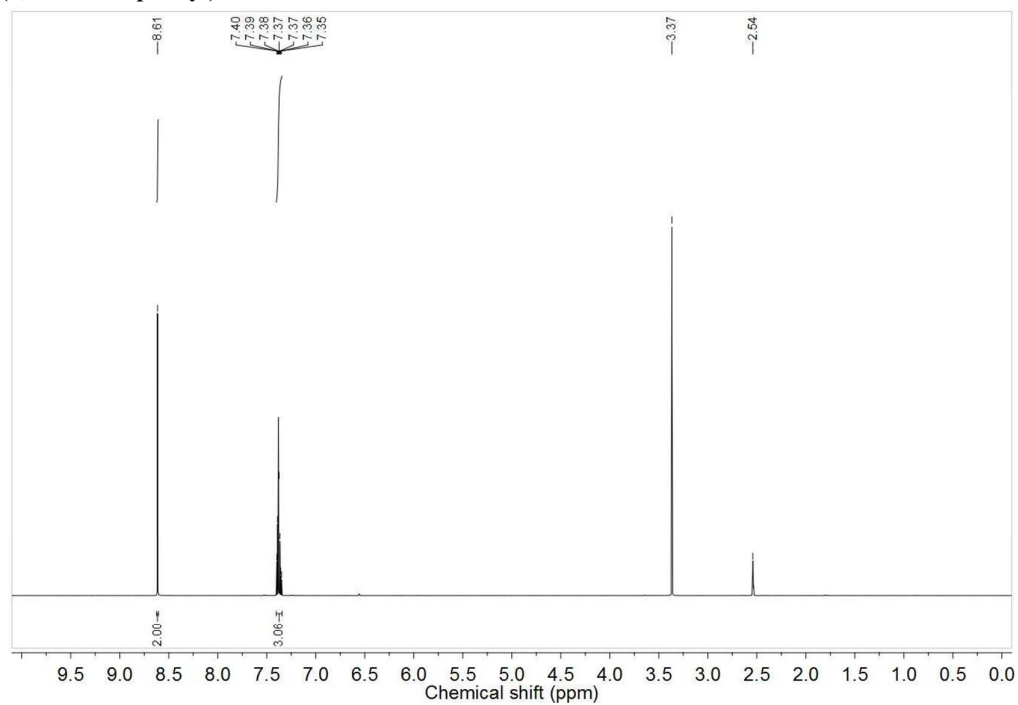


Figure S1 ¹H-NMR, 600 MHz, DMSO-*d*₆

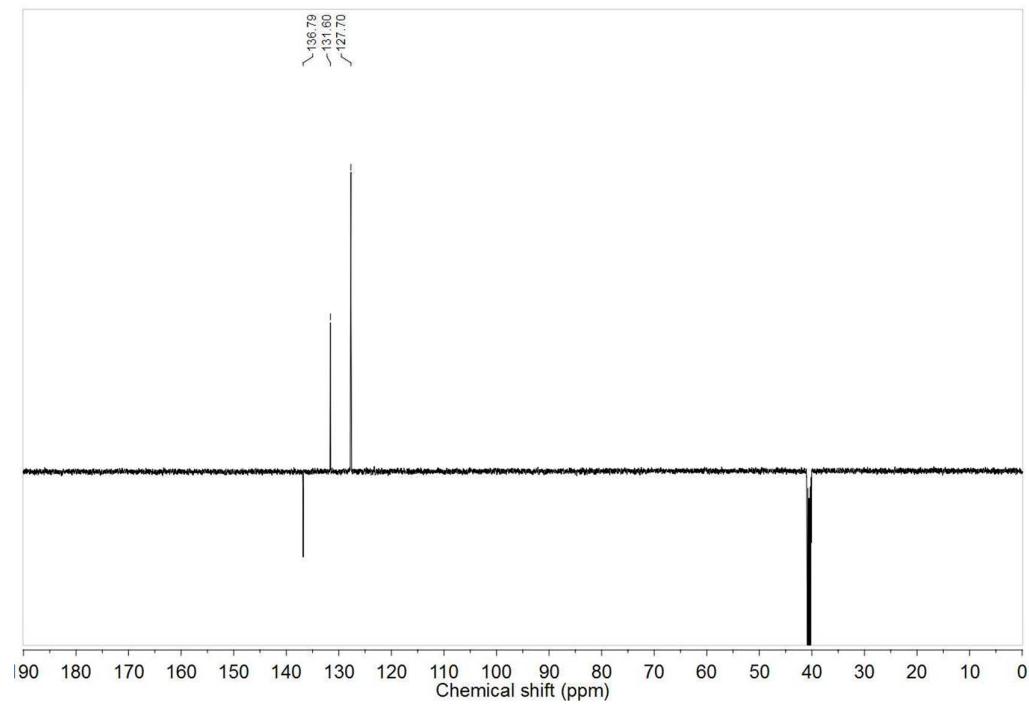


Figure S2 DEPT-Q-NMR, 125 MHz, DMSO-*d*₆

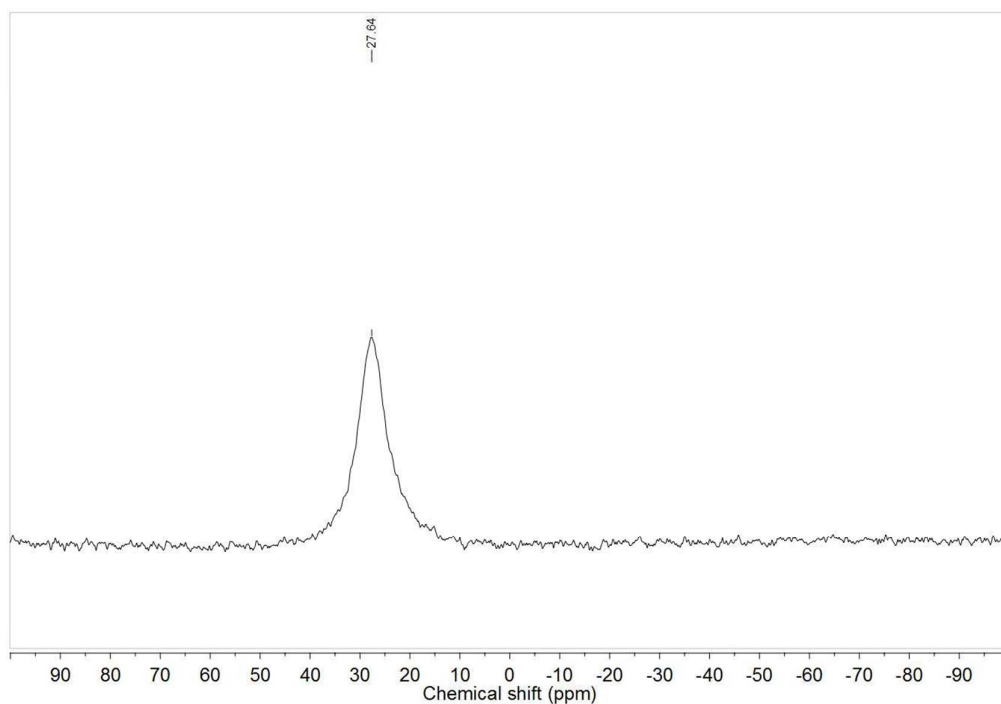


Figure S3 ^{10}B -NMR, 64 MHz, $\text{DMSO-}d_6$

(2,3,6-trichlorophenyl)boronic acid

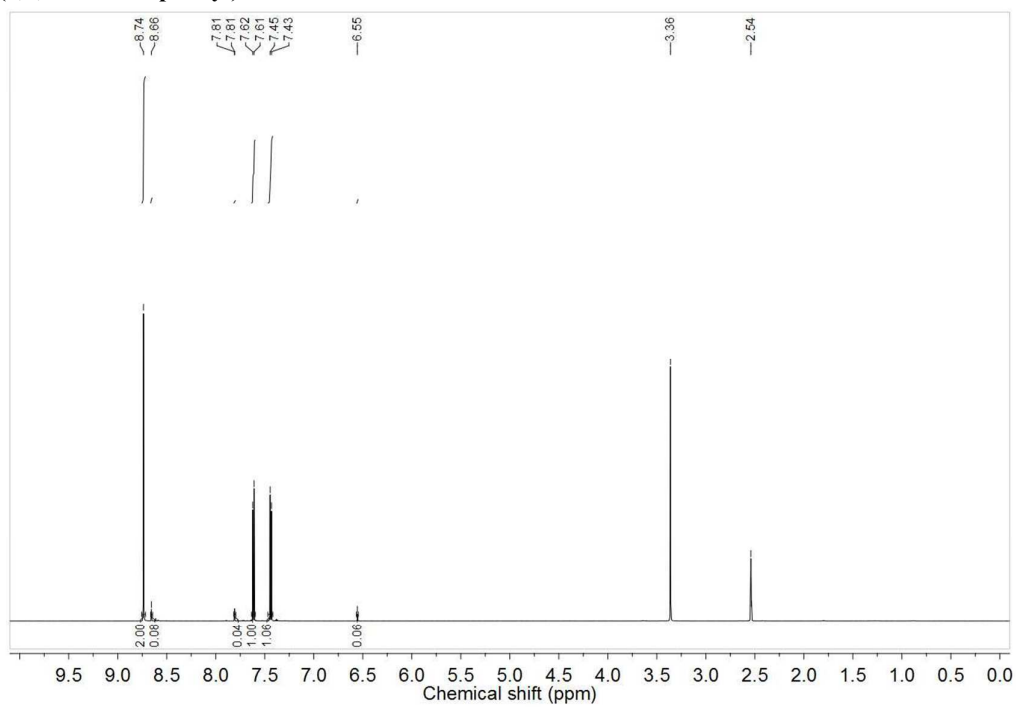
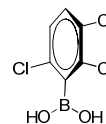


Figure S4 ^1H -NMR, 600 MHz, $\text{DMSO-}d_6$



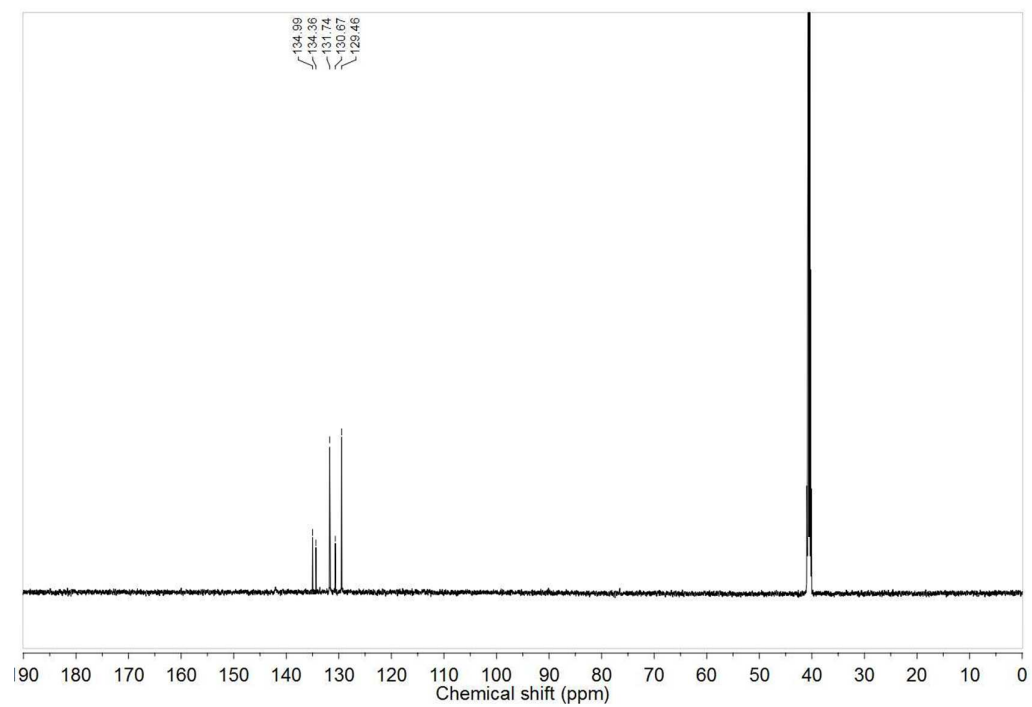


Figure S5 ^{13}C -NMR, 125 MHz, DMSO- d_6

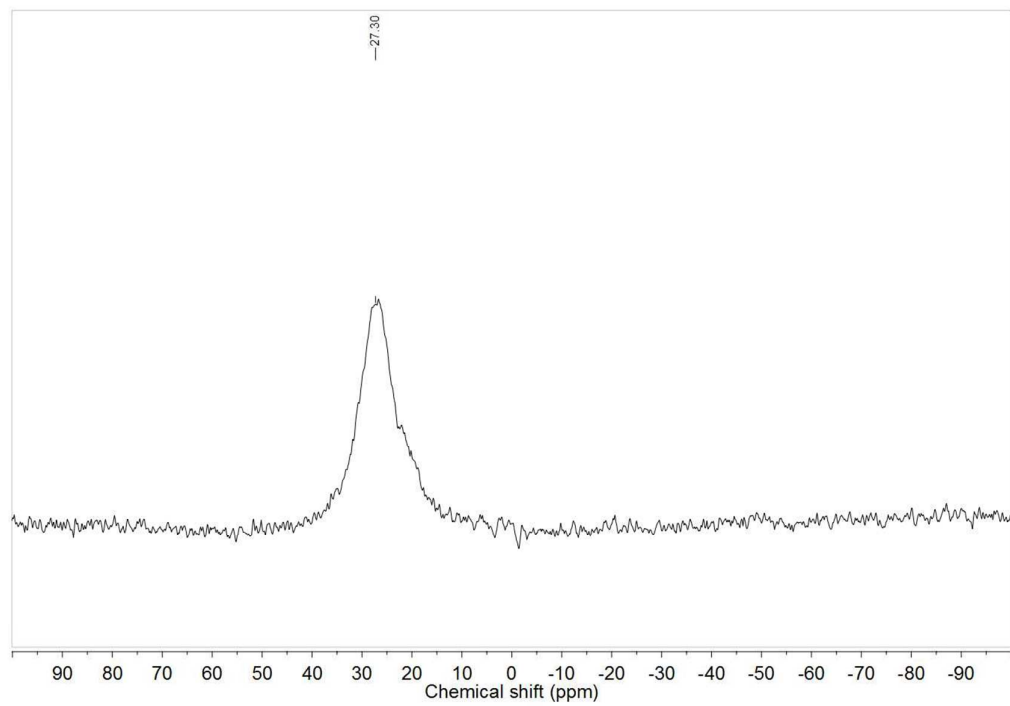


Figure S6 ^{10}B -NMR, 64 MHz, DMSO- d_6

NMR spectra of the potassium aryltrifluoroborates

Potassium (2,6-dichlorophenyl)trifluoroborate (2a)

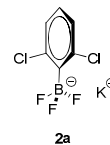
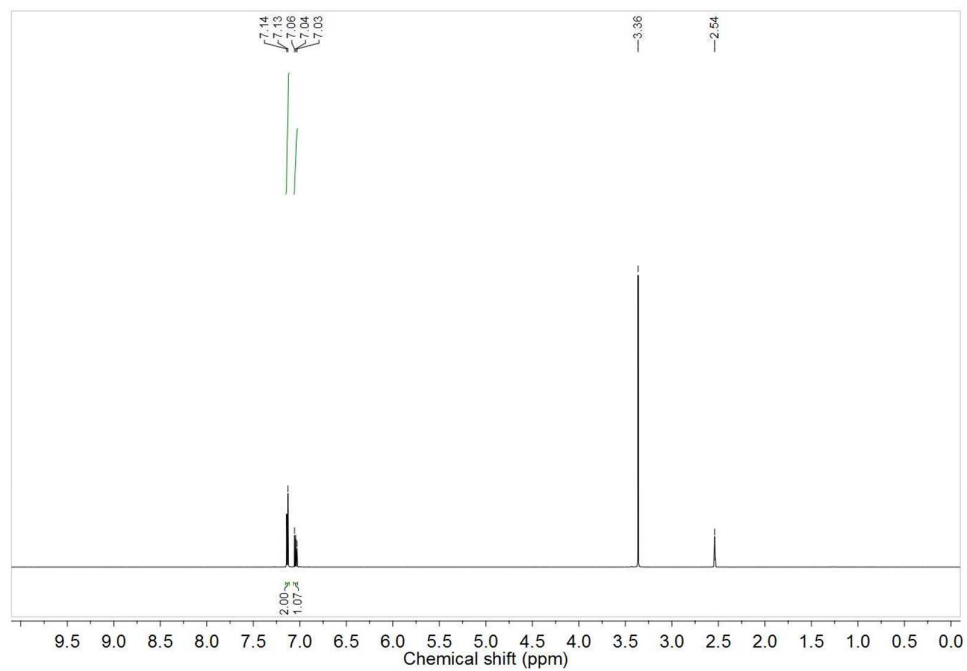


Figure S7 $^1\text{H-NMR}$, 600 MHz, $\text{DMSO-}d_6$

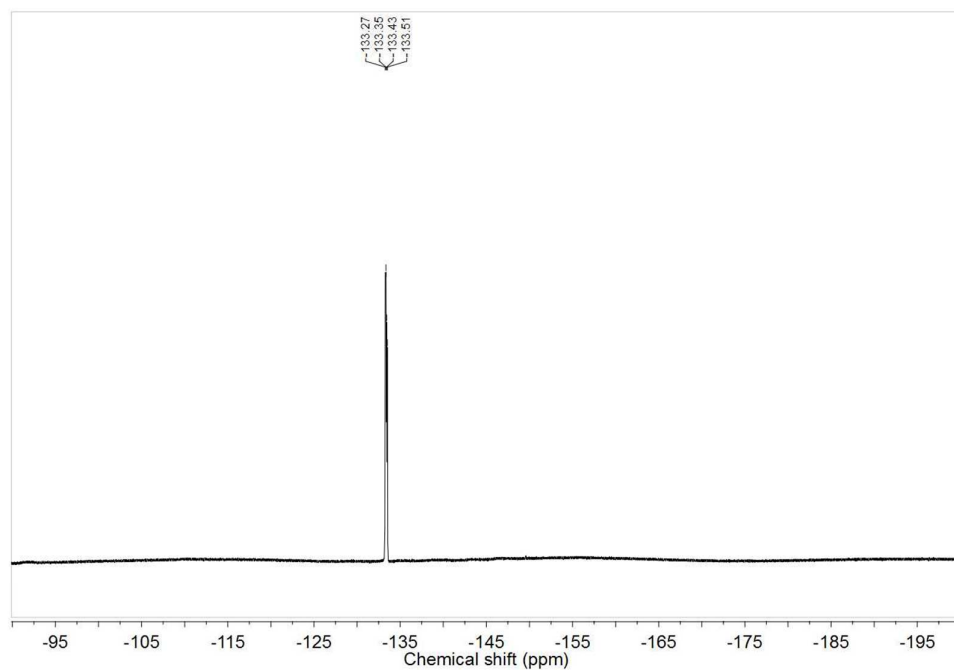


Figure S8 $^{19}\text{F-NMR}$, 564 MHz, $\text{DMSO-}d_6$

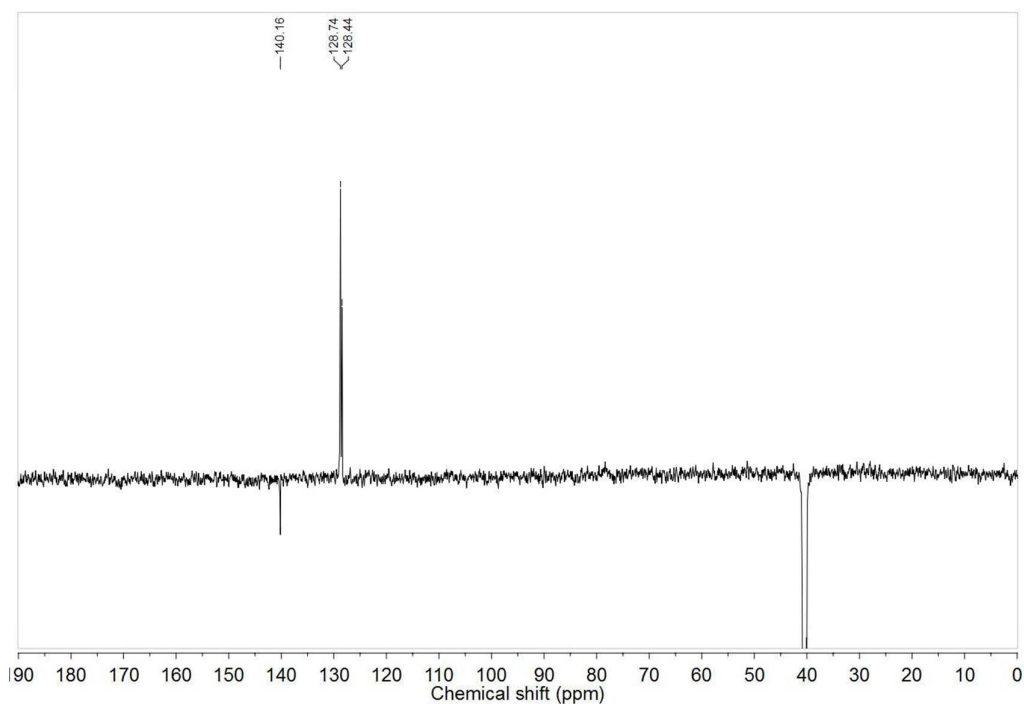


Figure S9 DEPT-Q-NMR, 125 MHz, DMSO-*d*₆

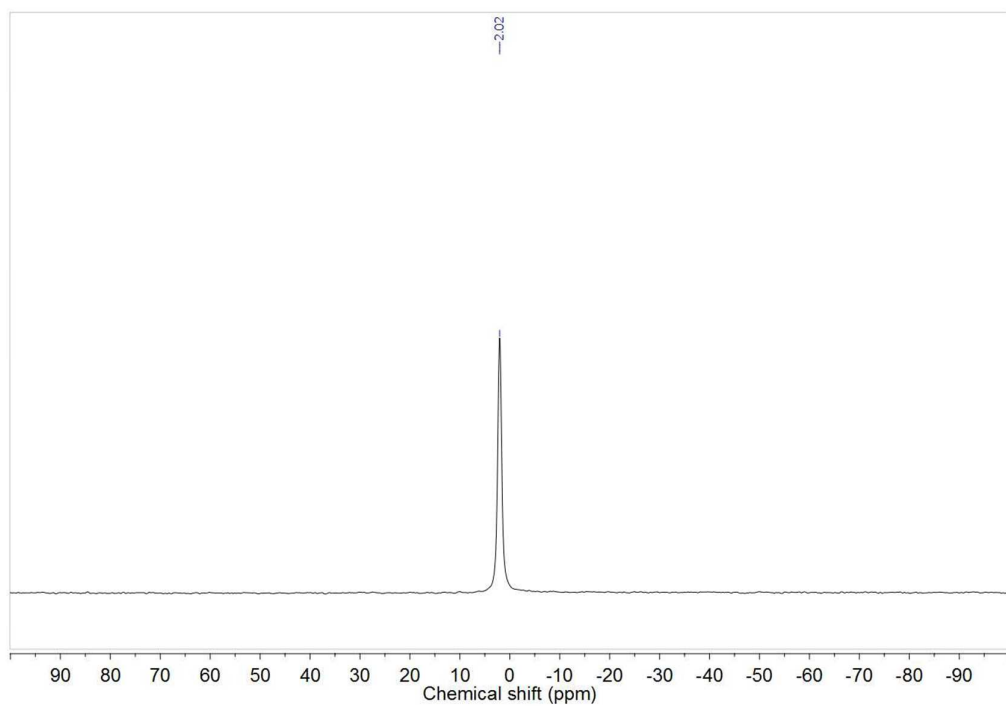
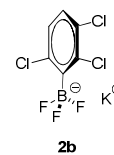


Figure S10 ¹⁰B-NMR, 64 MHz, DMSO-*d*₆

Potassium (2,3,6-trichlorophenyl)trifluoroborate (2b)



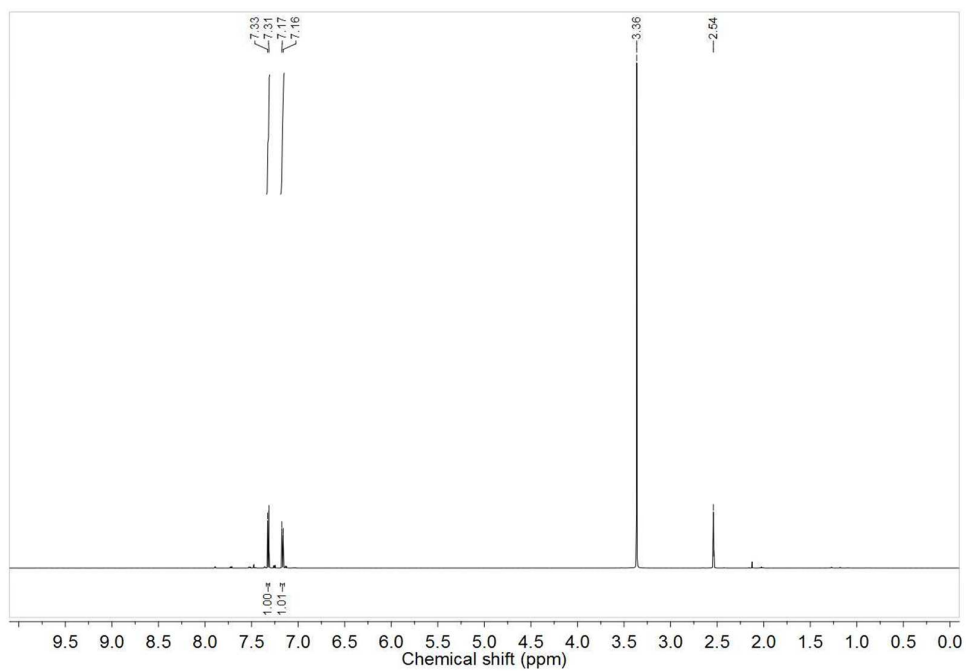


Figure S11 $^1\text{H-NMR}$, 600 MHz, $\text{DMSO-}d_6$

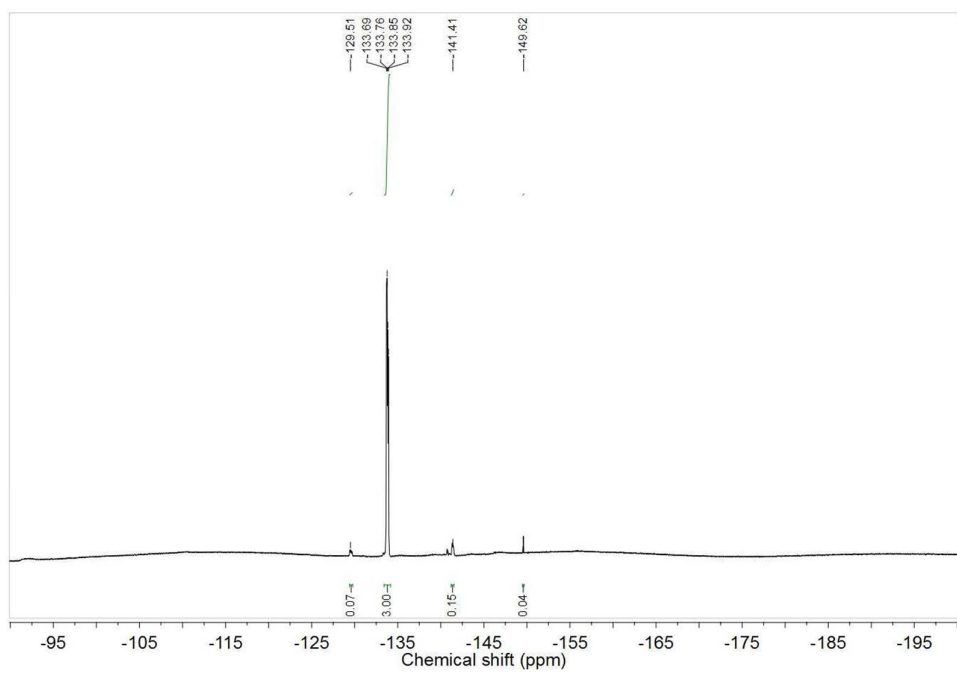


Figure S12 $^{19}\text{F-NMR}$, 564 MHz, $\text{DMSO-}d_6$

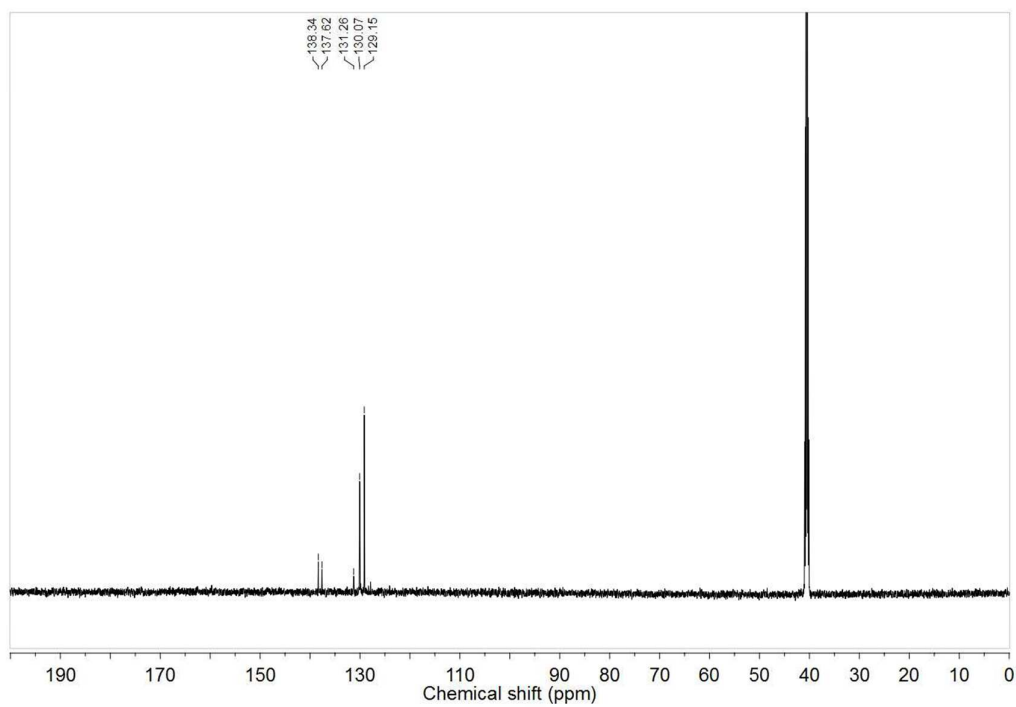


Figure S13 ^{13}C -NMR, 125 MHz, $\text{DMSO-}d_6$

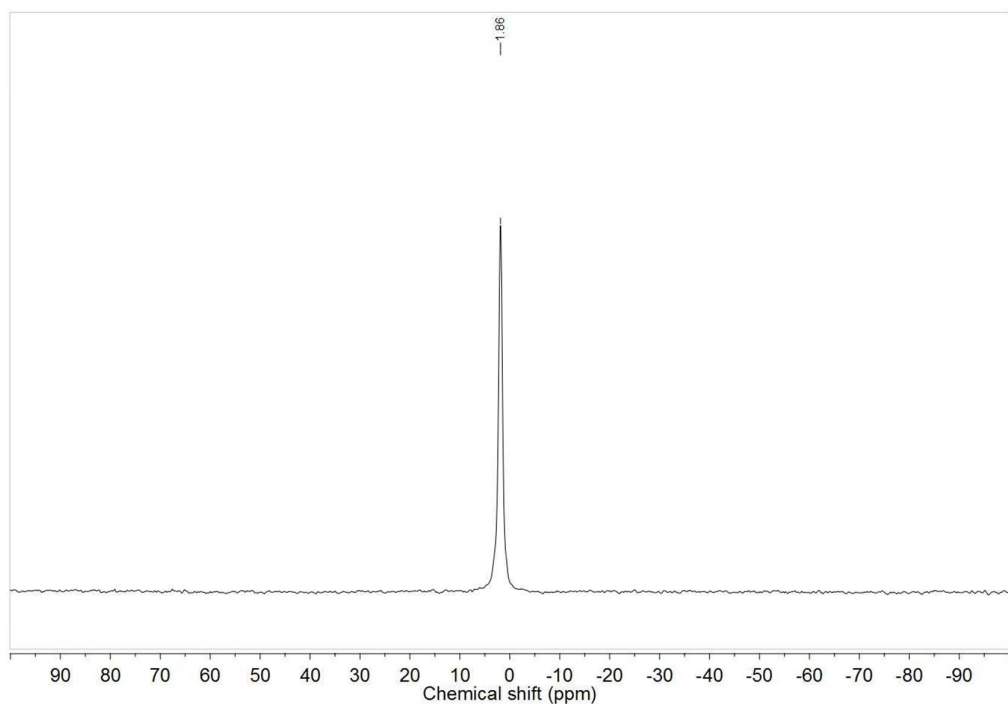


Figure S14 ^{10}B -NMR, 64 MHz, $\text{DMSO-}d_6$

NMR spectra of the boranes

(2,6-dichlorophenyl)bis(2,3,5,6-tetrafluorophenyl)borane (4a)

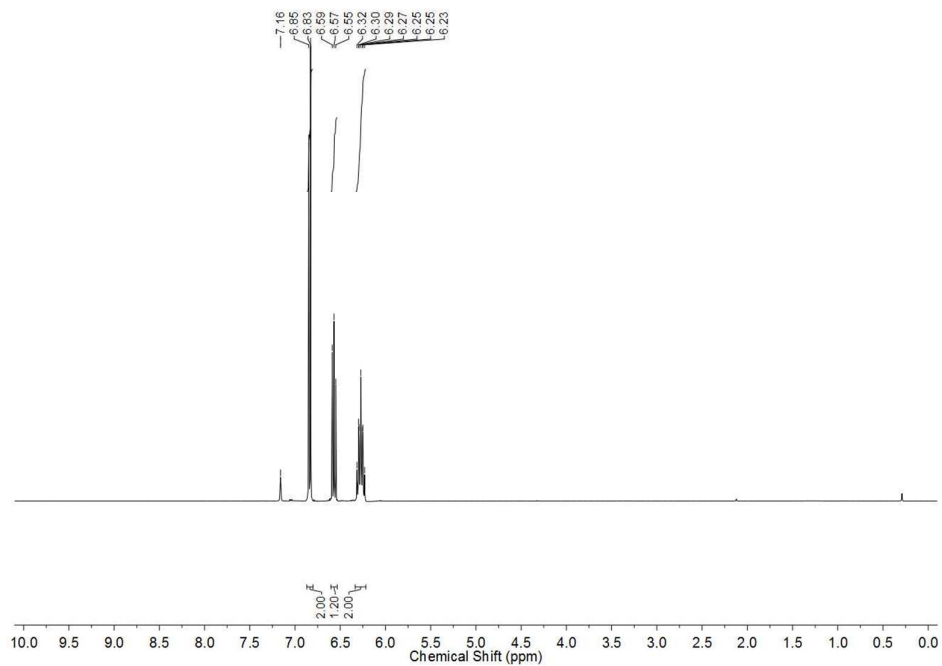
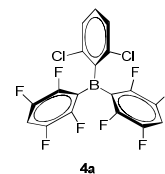


Figure S15 $^1\text{H-NMR}$, 400 MHz, C_6D_6

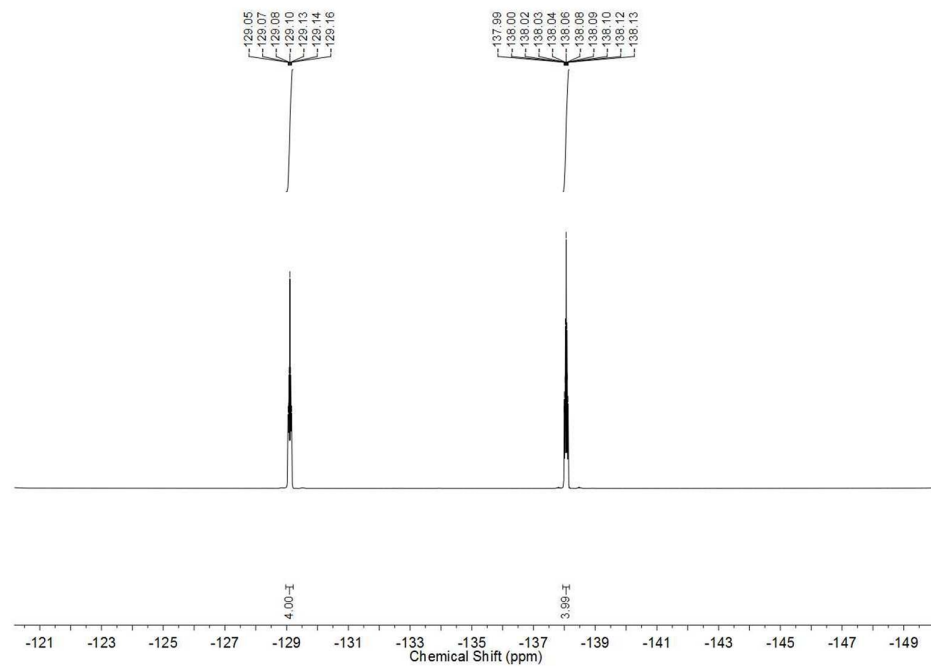


Figure S16 $^{19}\text{F-NMR}$, 376 MHz, C_6D_6

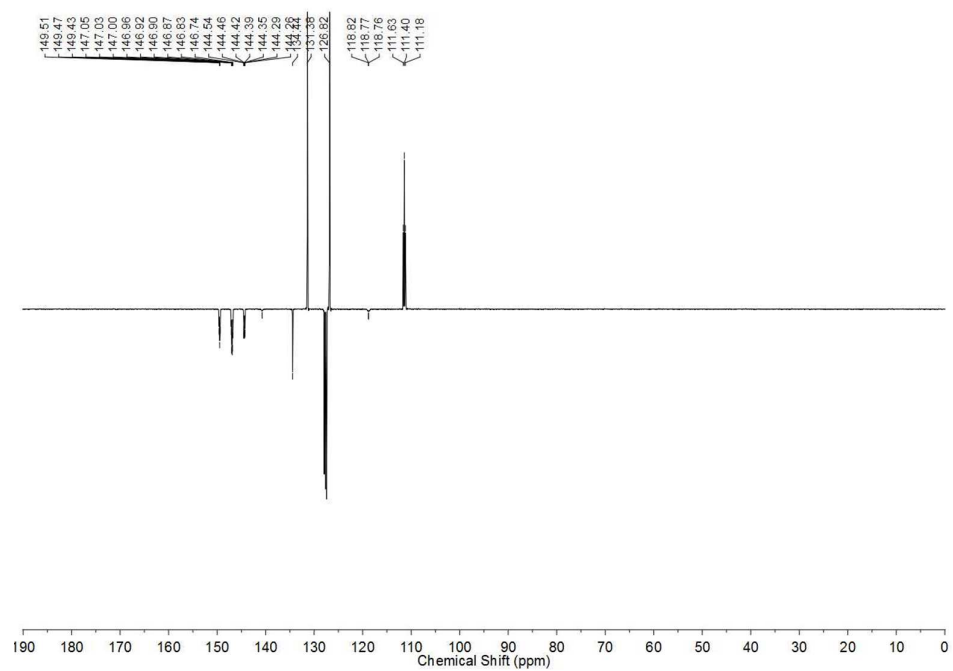


Figure S17 DEPT-Q-NMR, 100 MHz, C₆D₆

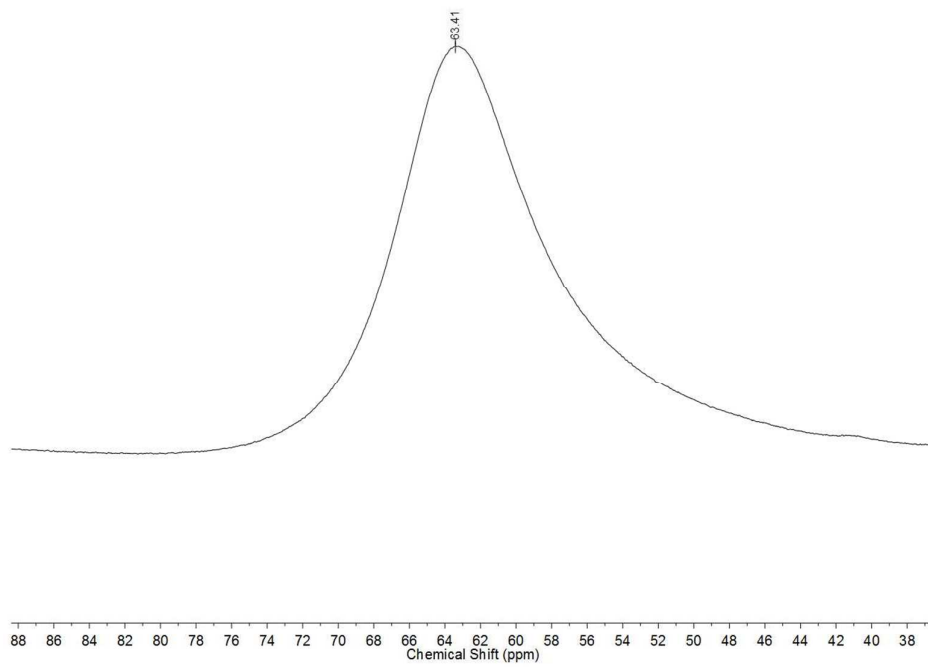


Figure S18 ¹¹B-NMR, 128 MHz, C₆D₆

(2,3,6-trichlorophenyl)bis(2,3,5,6-tetrafluorophenyl)borane (4b)

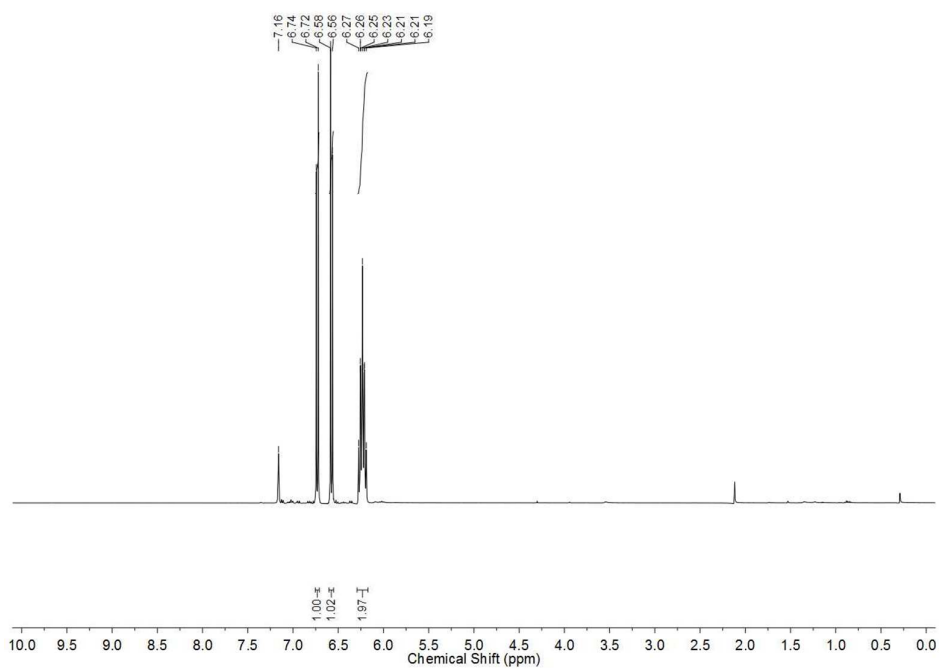
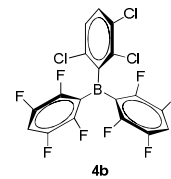


Figure S19 $^1\text{H-NMR}$, 400 MHz, C_6D_6

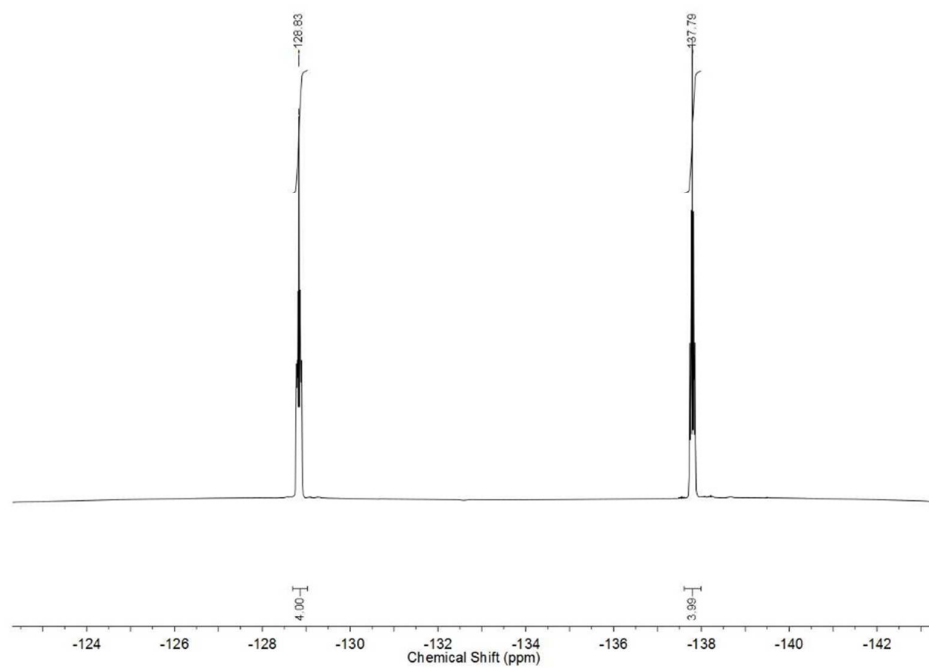


Figure S20 $^{19}\text{F-NMR}$, 376 MHz, C_6D_6

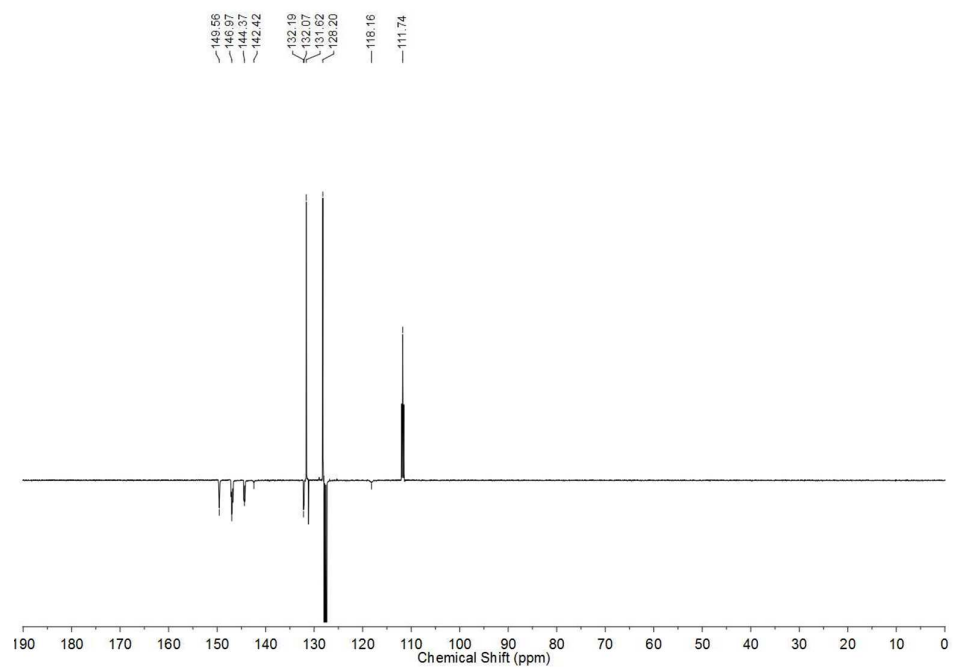


Figure S21 DEPT-Q-NMR, 100 MHz, C₆D₆

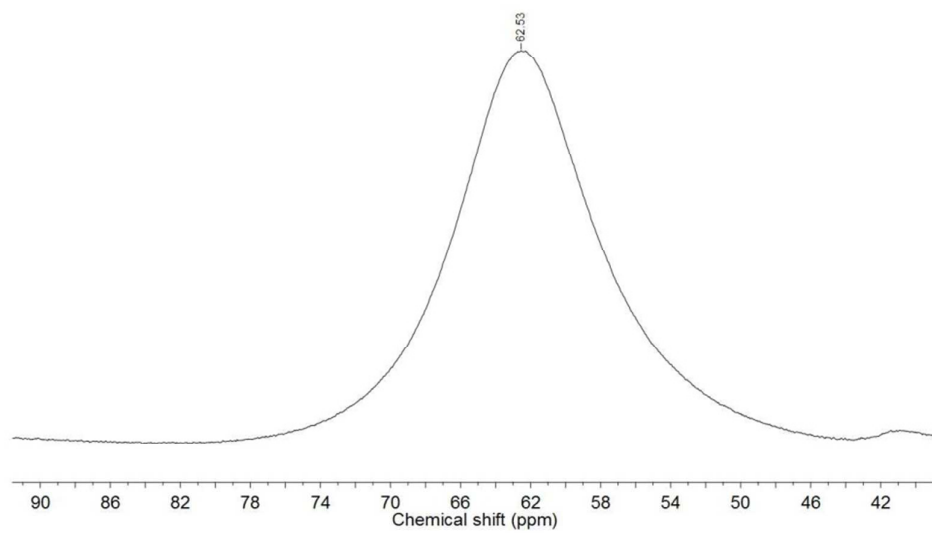


Figure S22 ¹¹B-NMR, 128 MHz, C₆D₆

(2,3,6-trichlorophenyl)bis(2,3,6-trifluorophenyl)borane (4d)

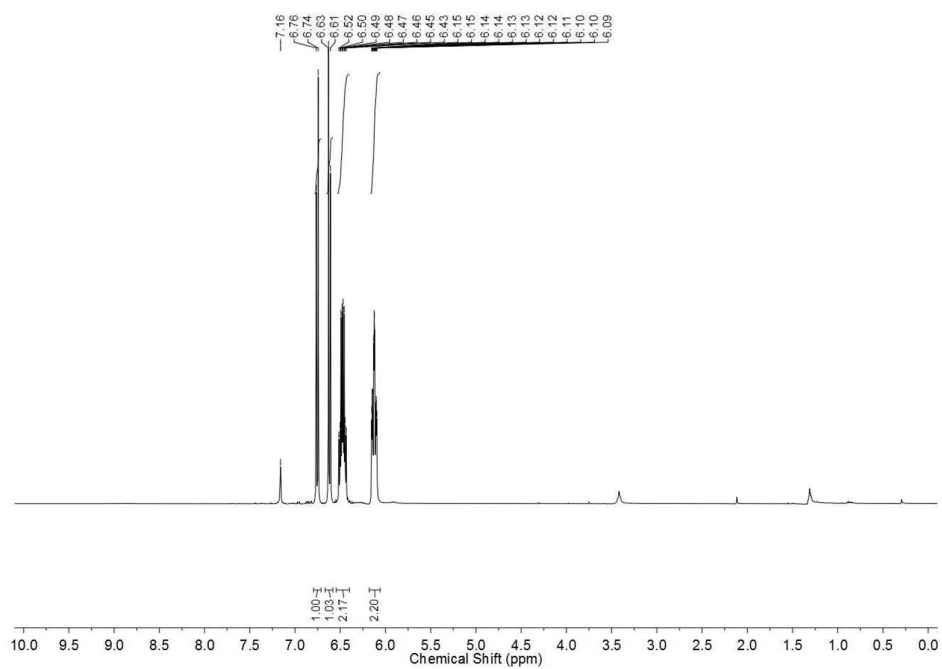
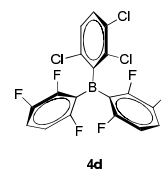


Figure S23 $^1\text{H-NMR}$, 400 MHz, C_6D_6

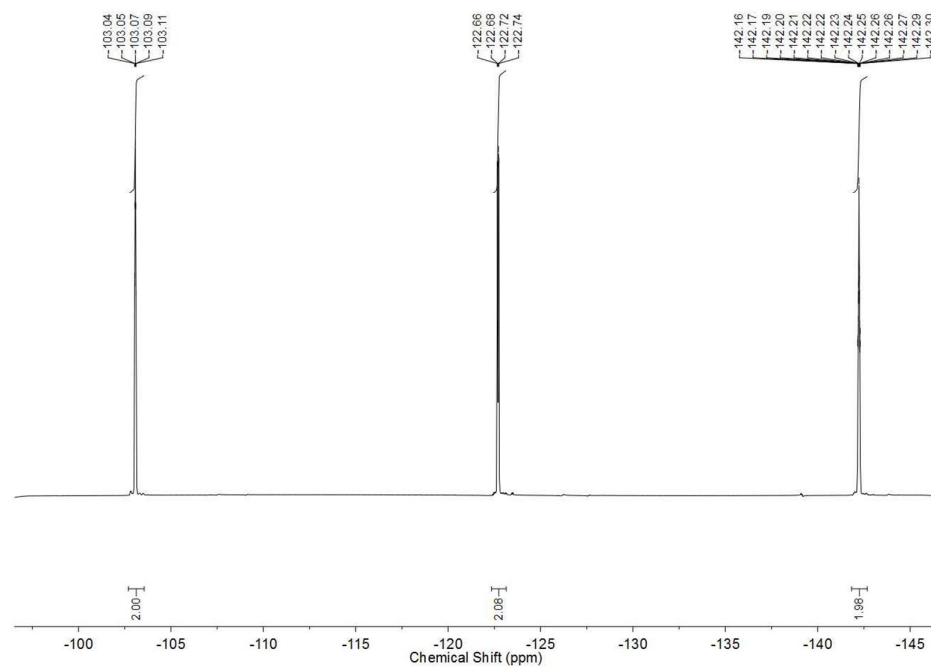


Figure S24 $^{19}\text{F-NMR}$, 376 MHz, C_6D_6

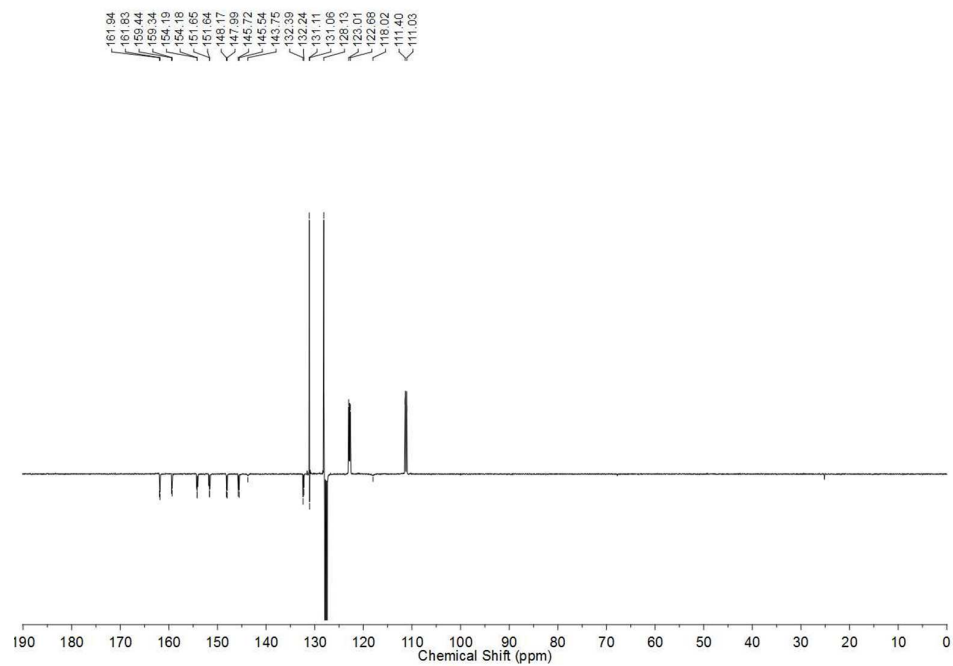


Figure S25 DEPT-Q-NMR, 100 MHz, C₆D₆

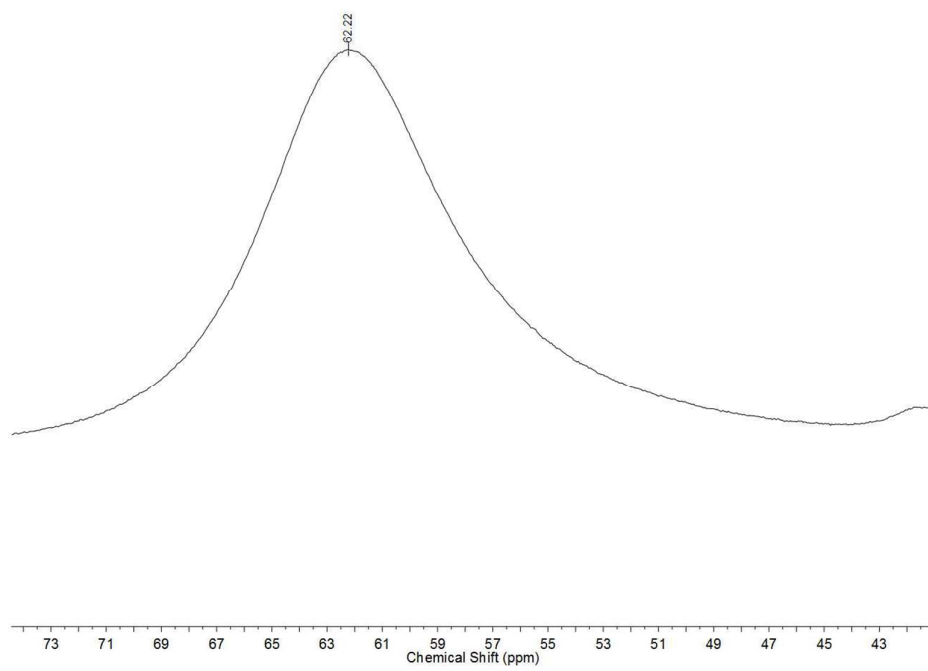


Figure S26 ¹¹B-NMR, 128 MHz, C₆D₆

(2,6-dichlorophenyl)bis(2,3,6-trifluorophenyl)borane (4c)

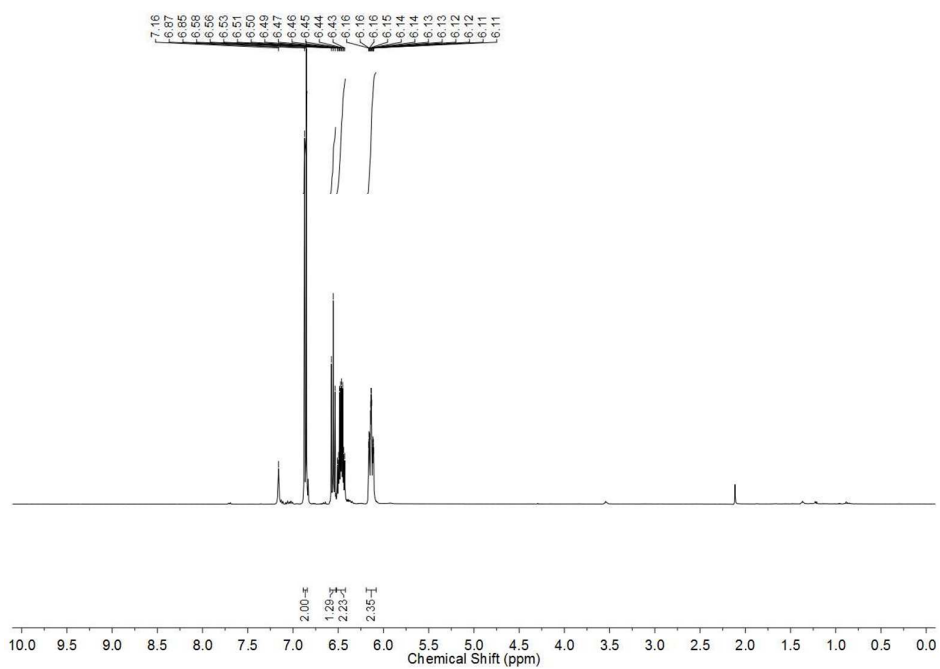
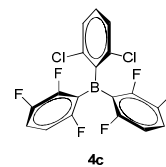


Figure S27 ¹H-NMR, 400 MHz, C₆D₆

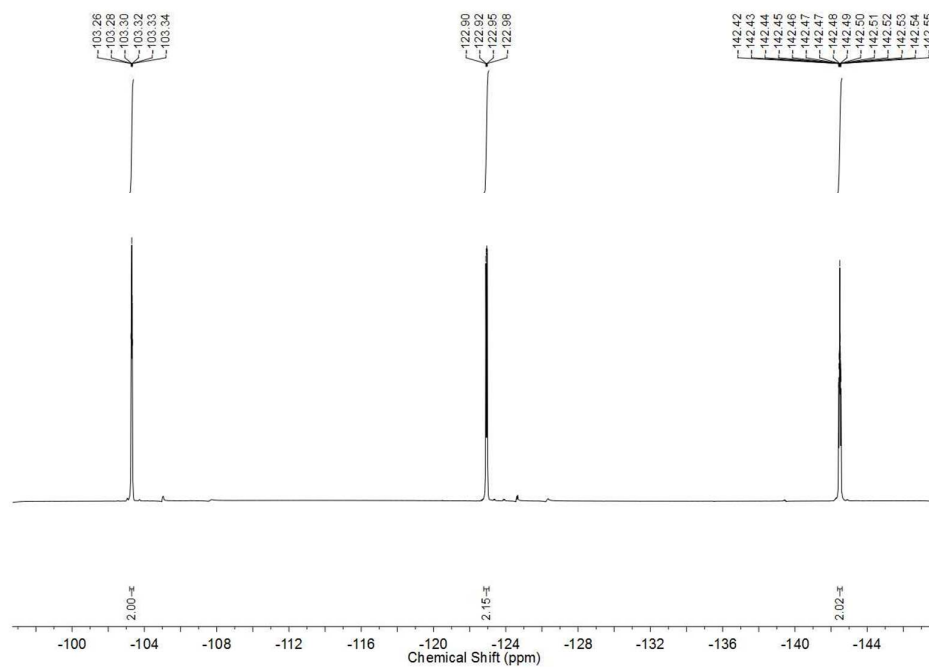


Figure S28 ¹⁹F-NMR, 376 MHz, C₆D₆

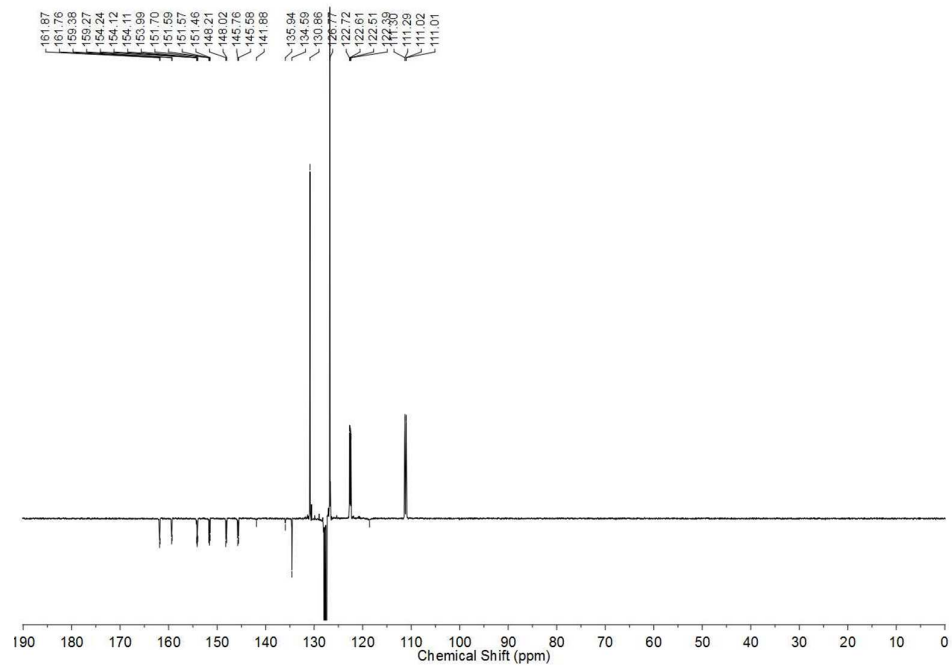


Figure S29 DEPT-Q-NMR, 100 MHz, C₆D₆

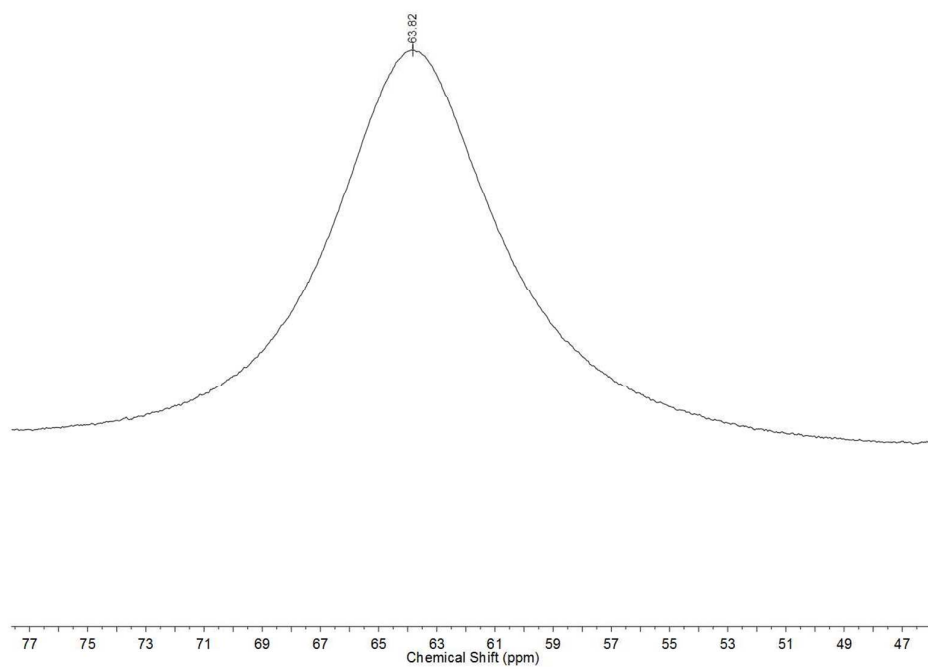
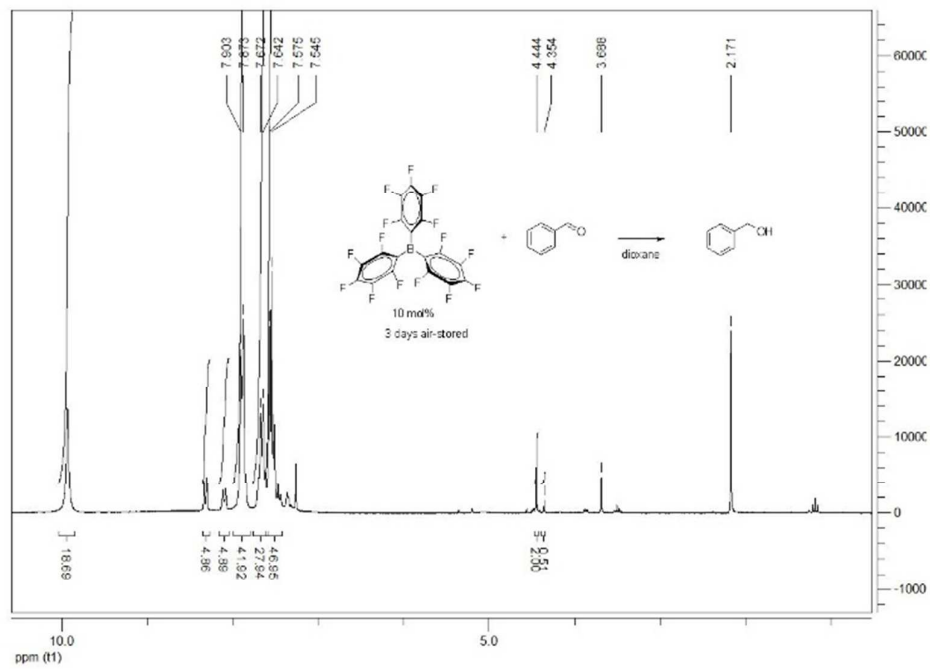
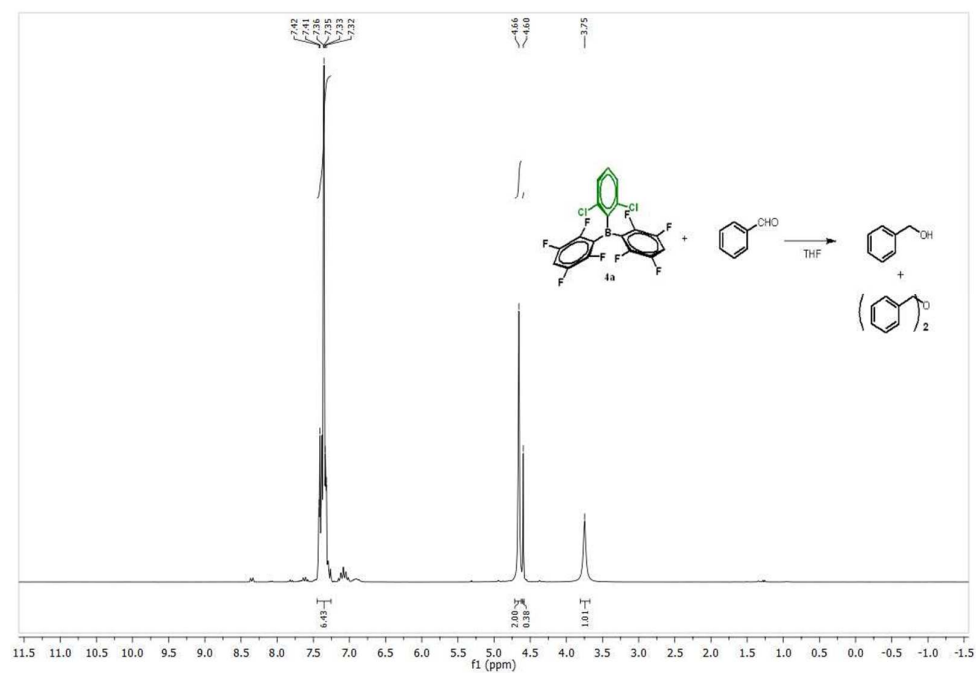
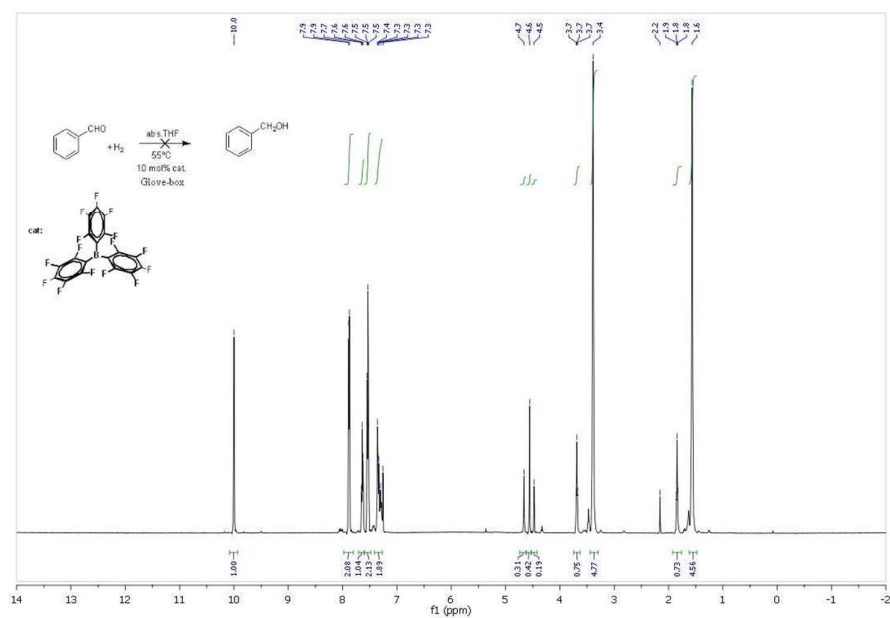
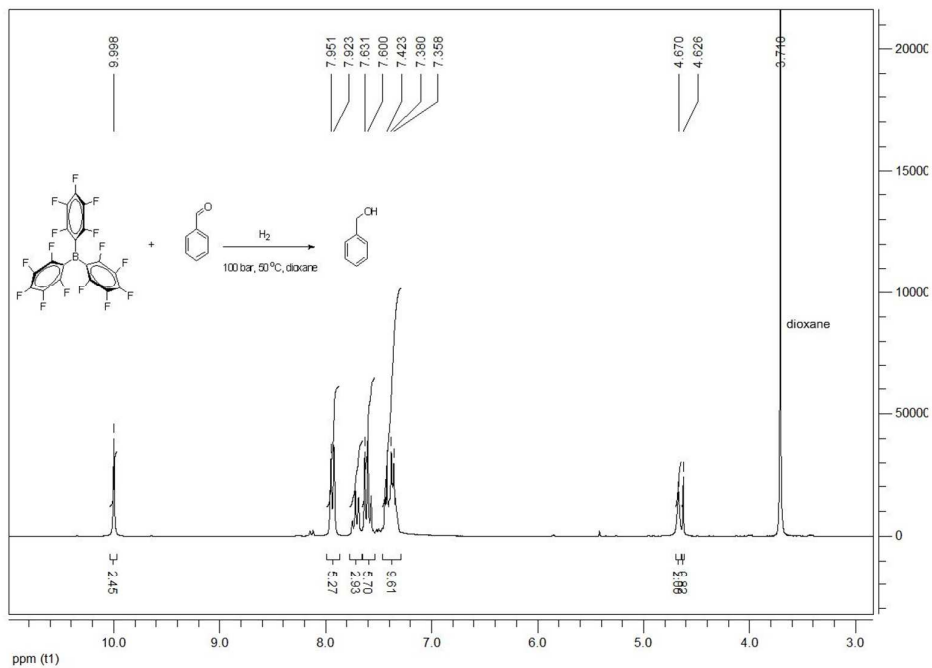
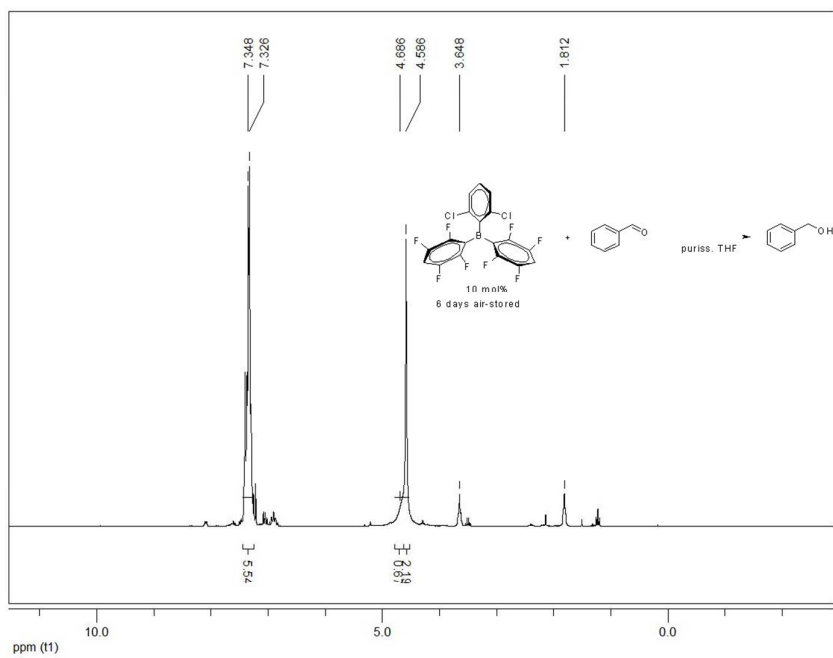
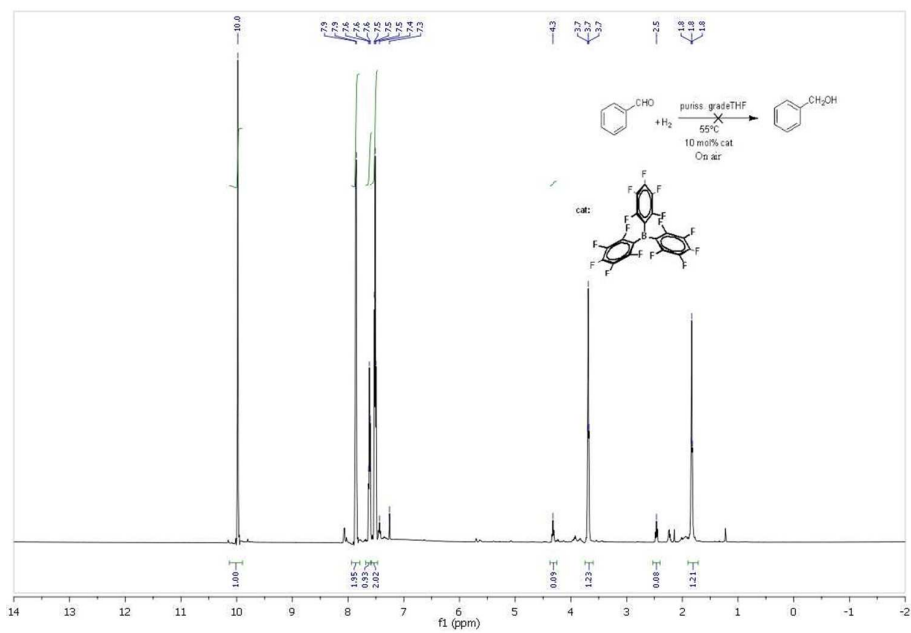


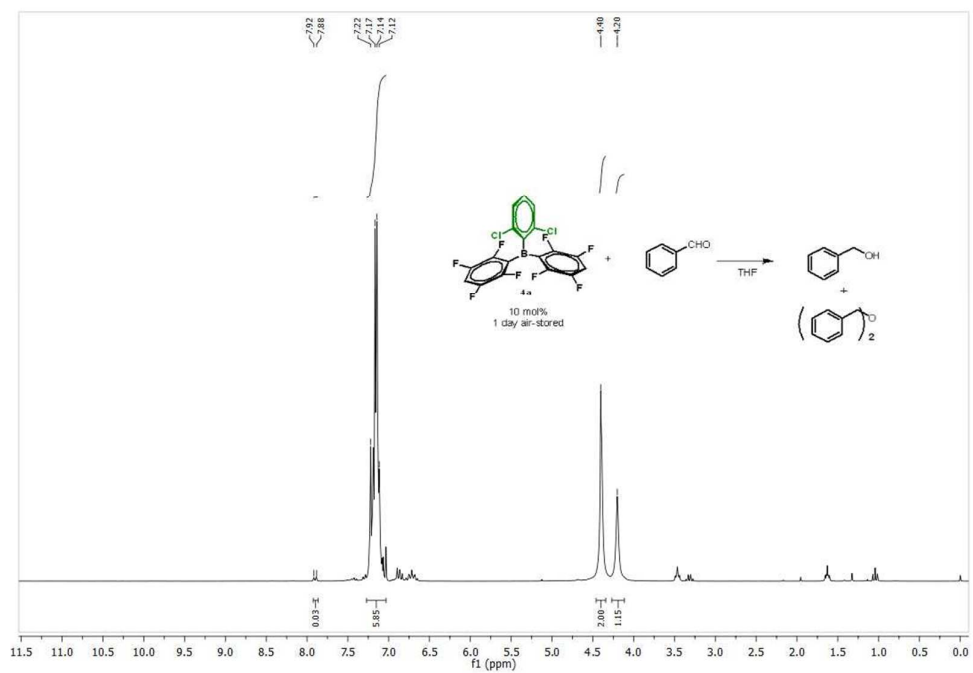
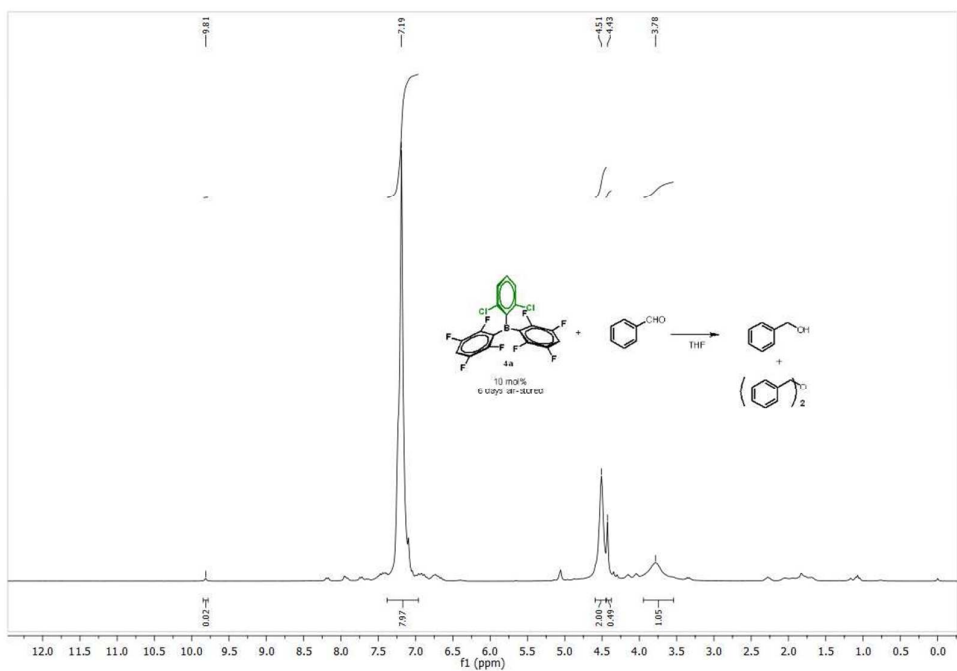
Figure S30 ¹¹B-NMR, 128 MHz, C₆D₆

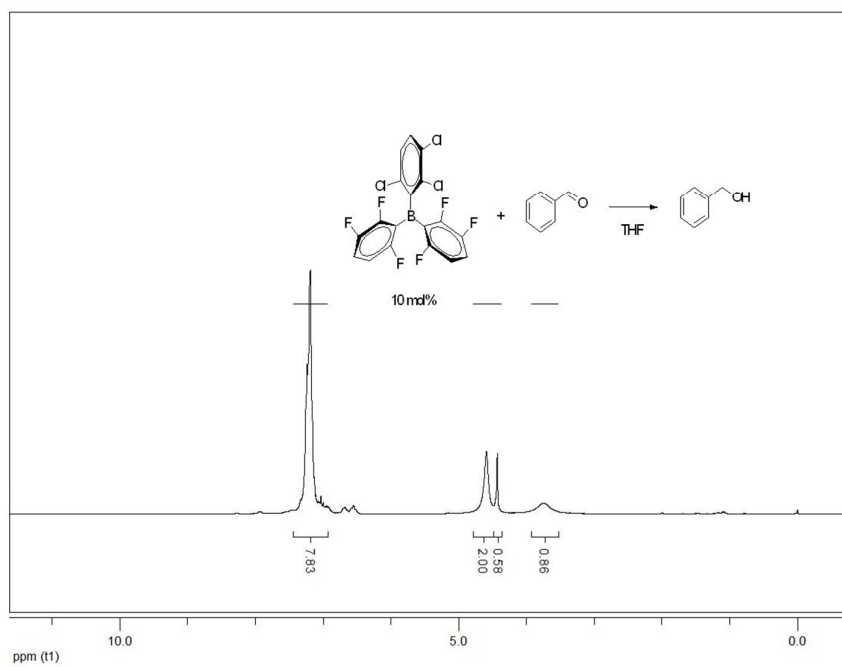
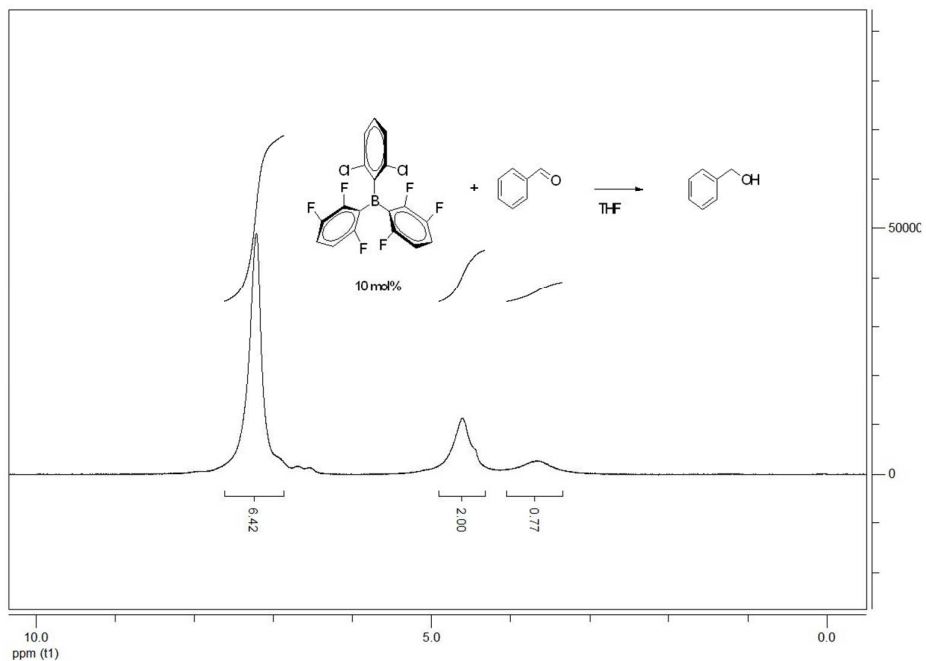
NMR spectra of the crude products - Catalyst and solvent screen

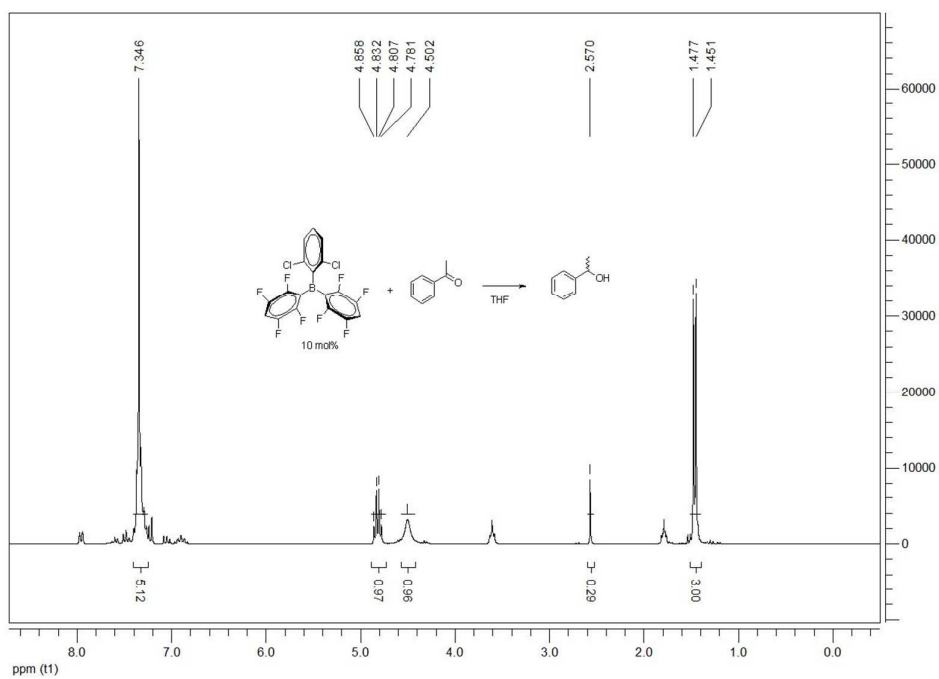
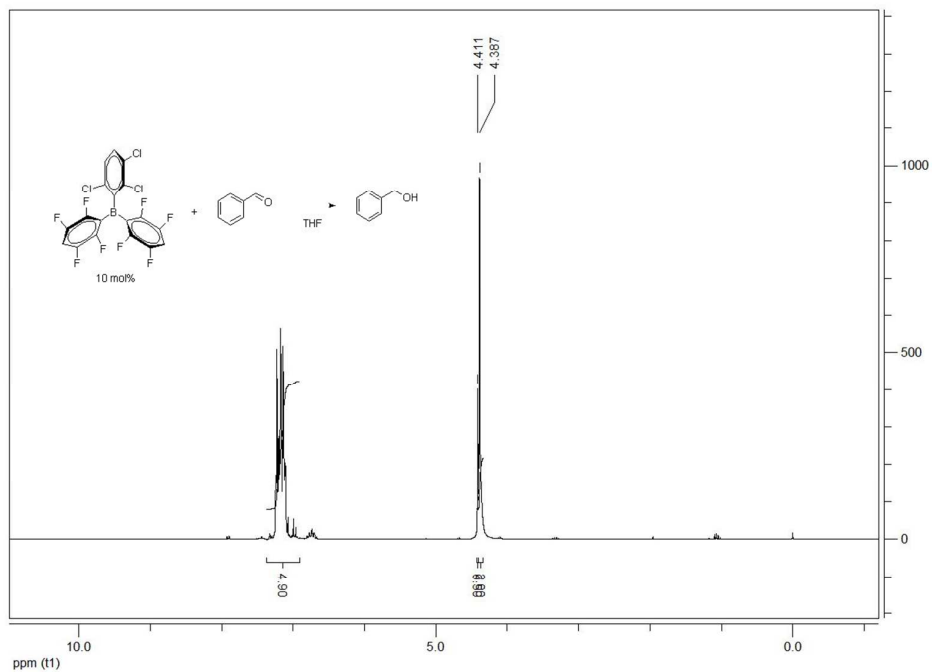


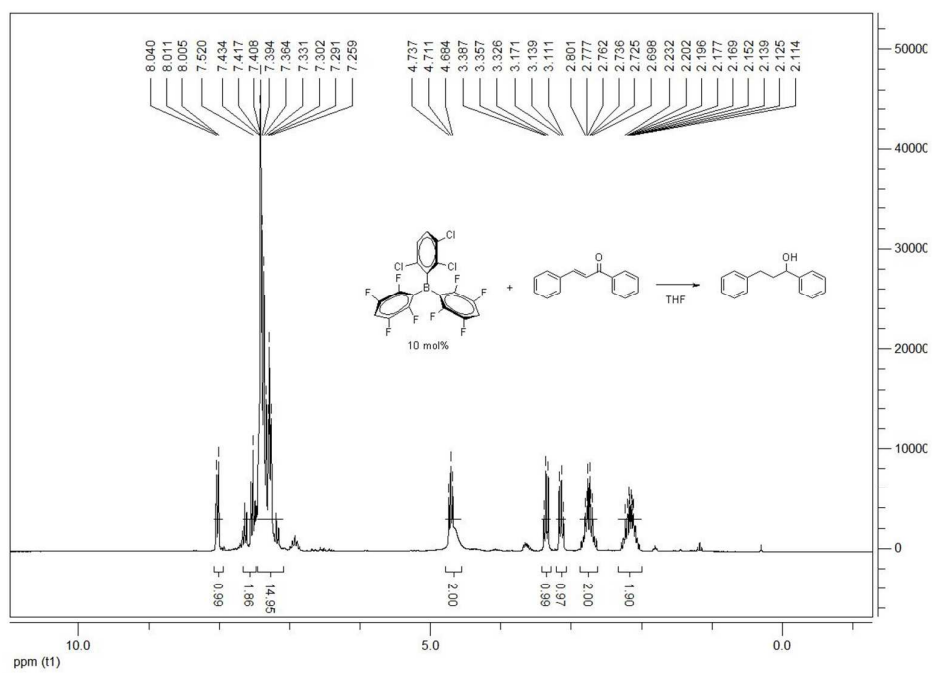
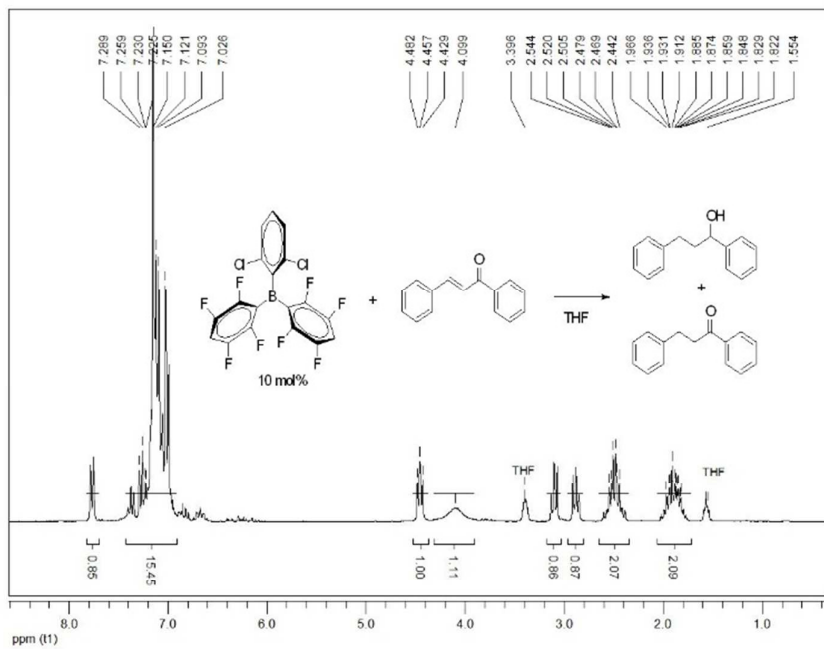


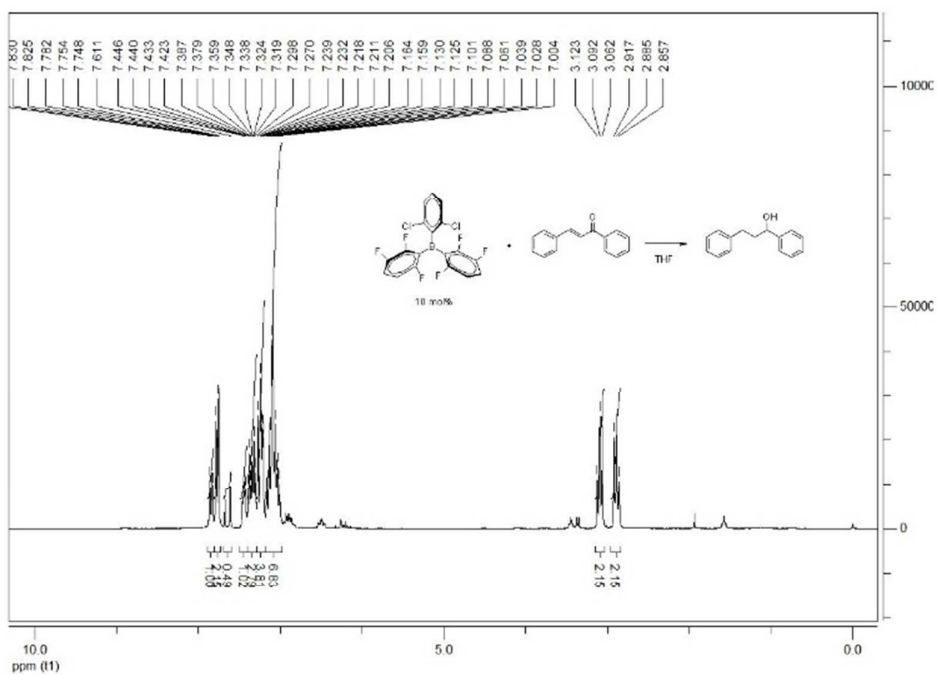
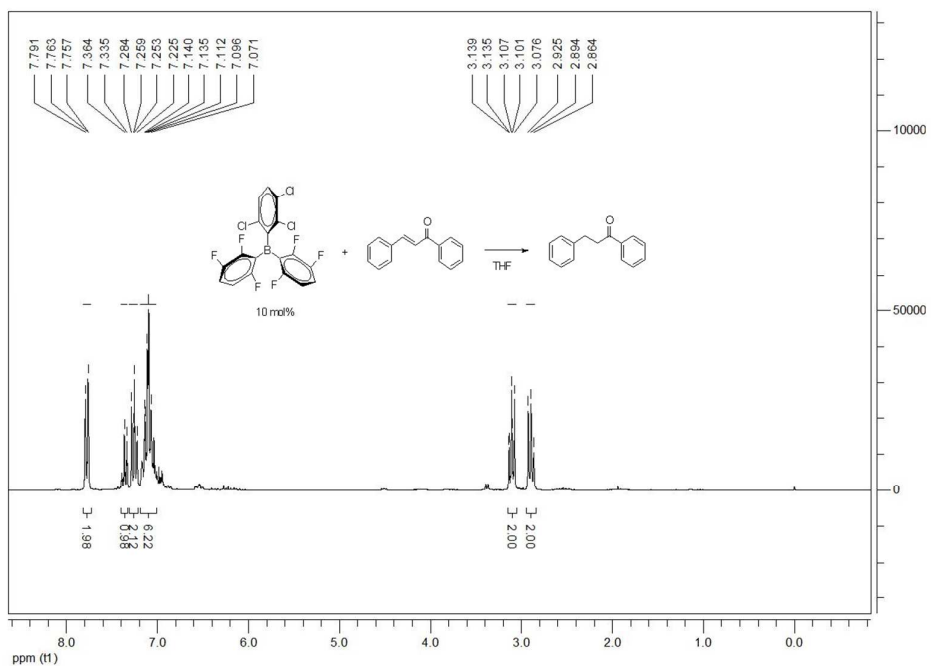


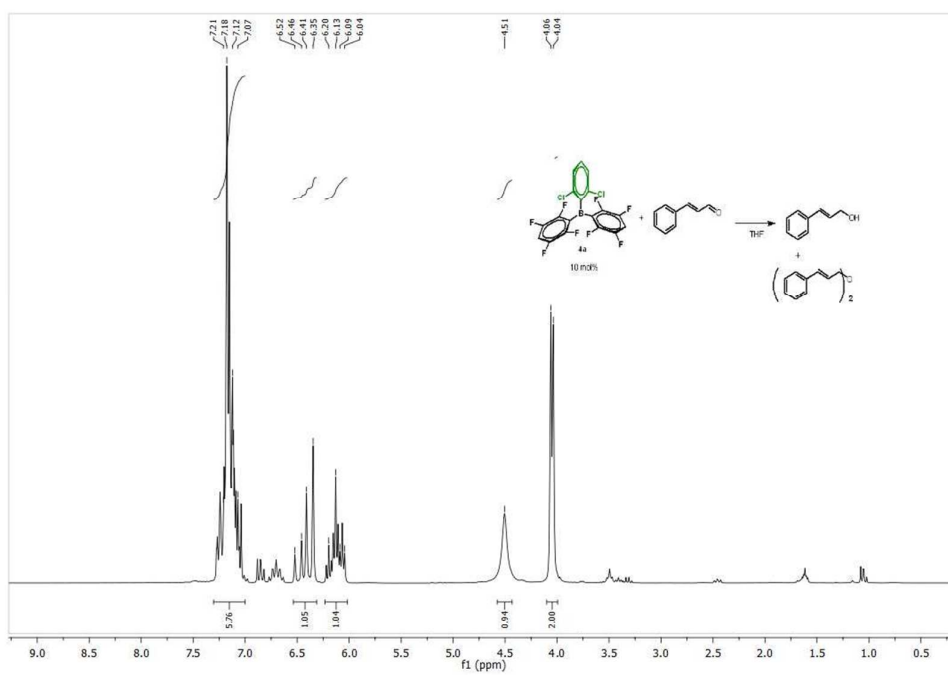
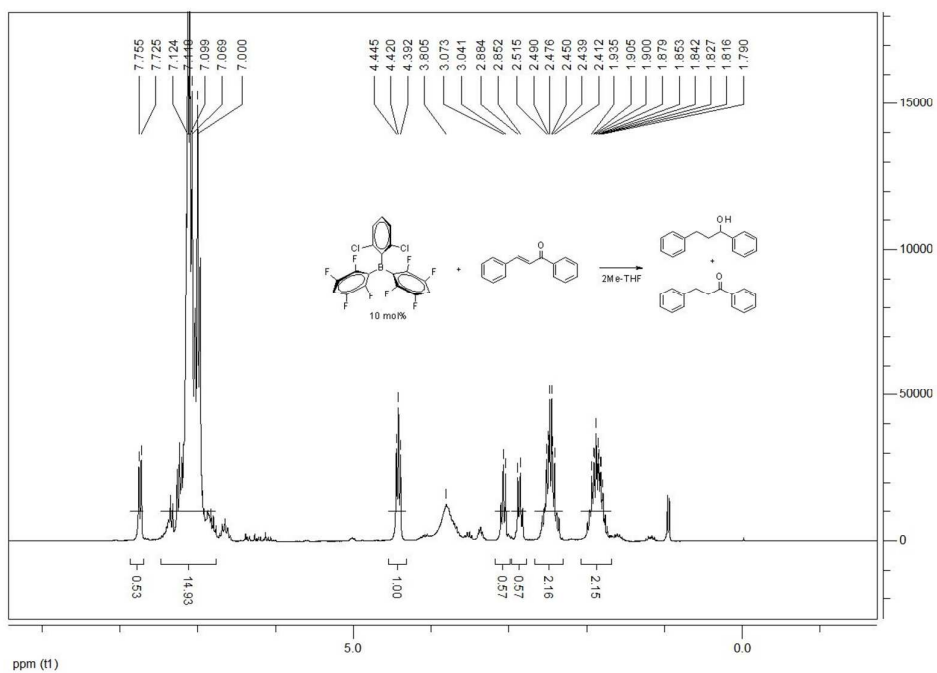


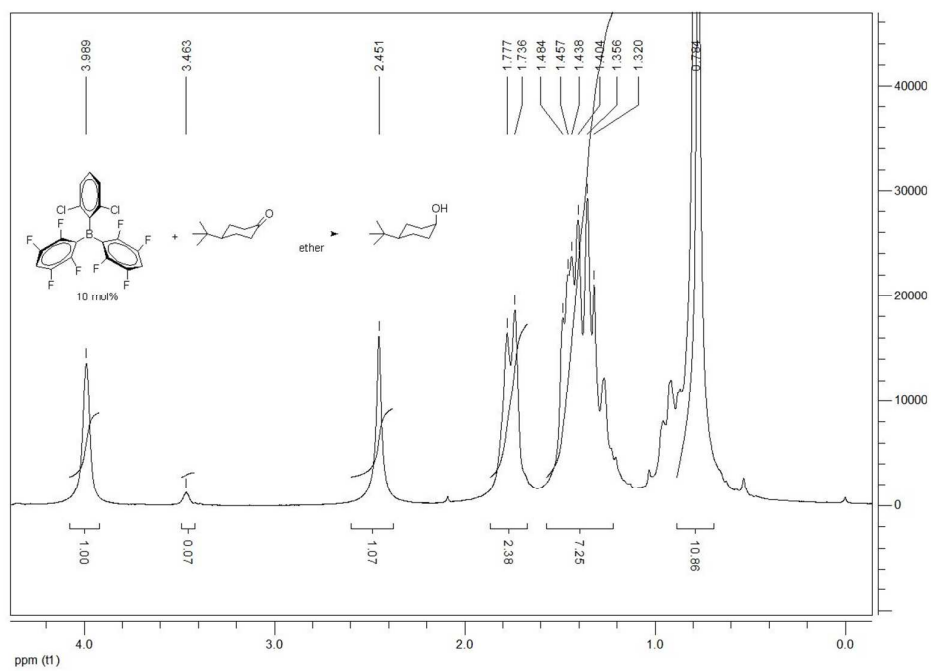
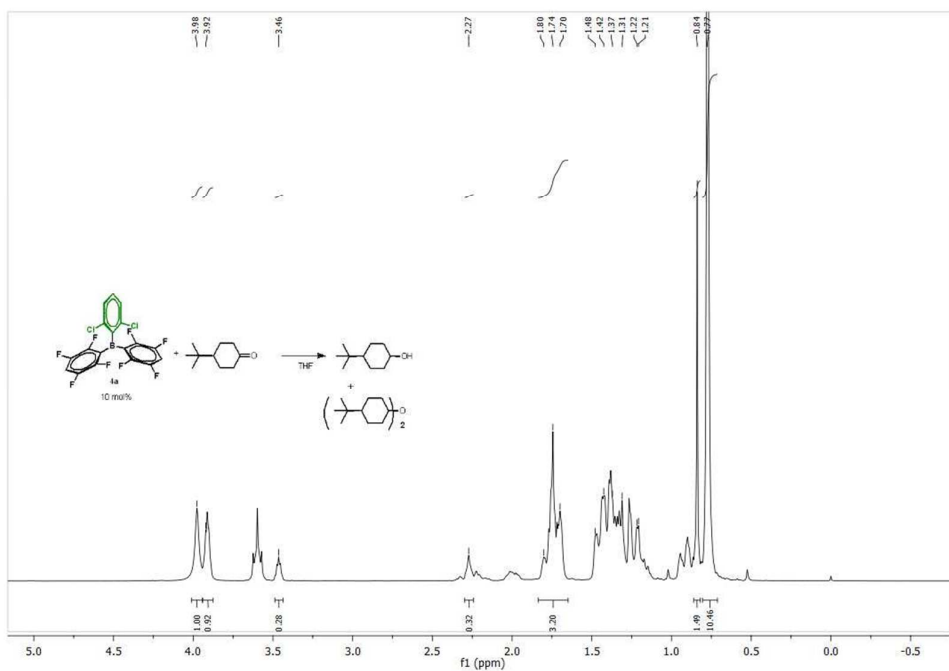




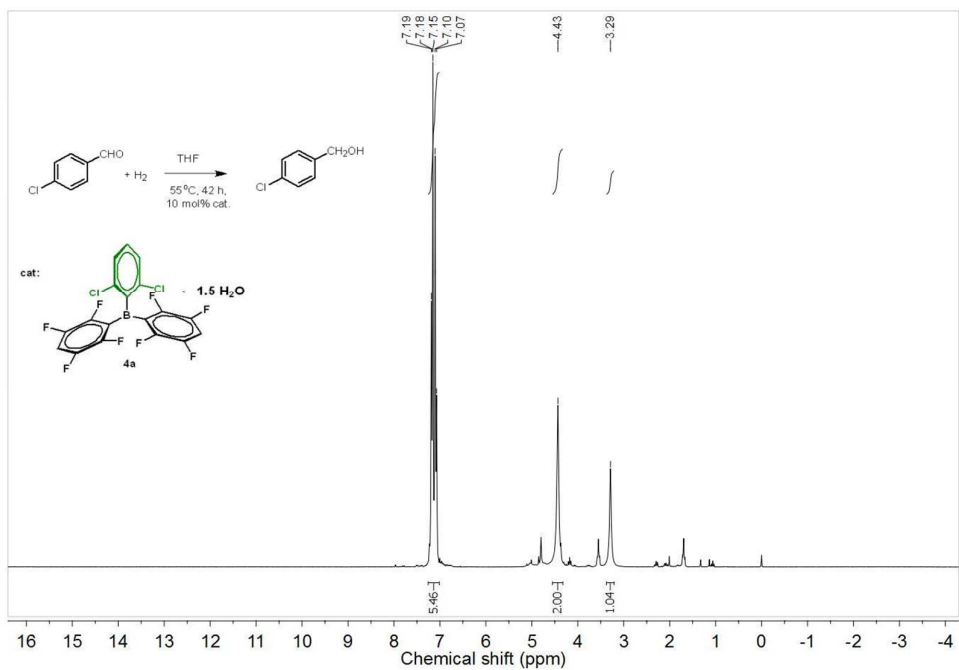
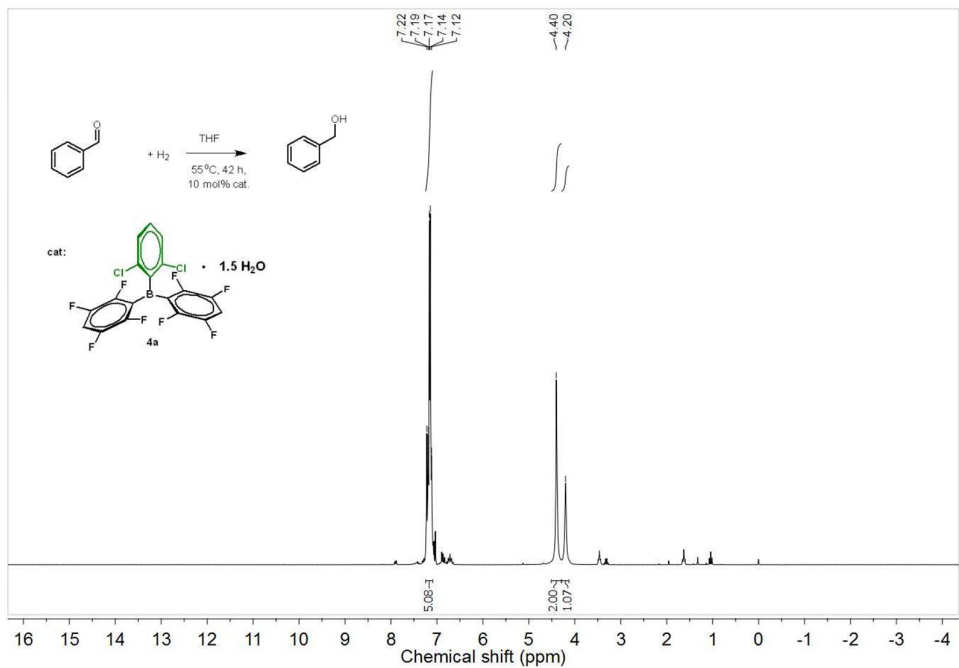


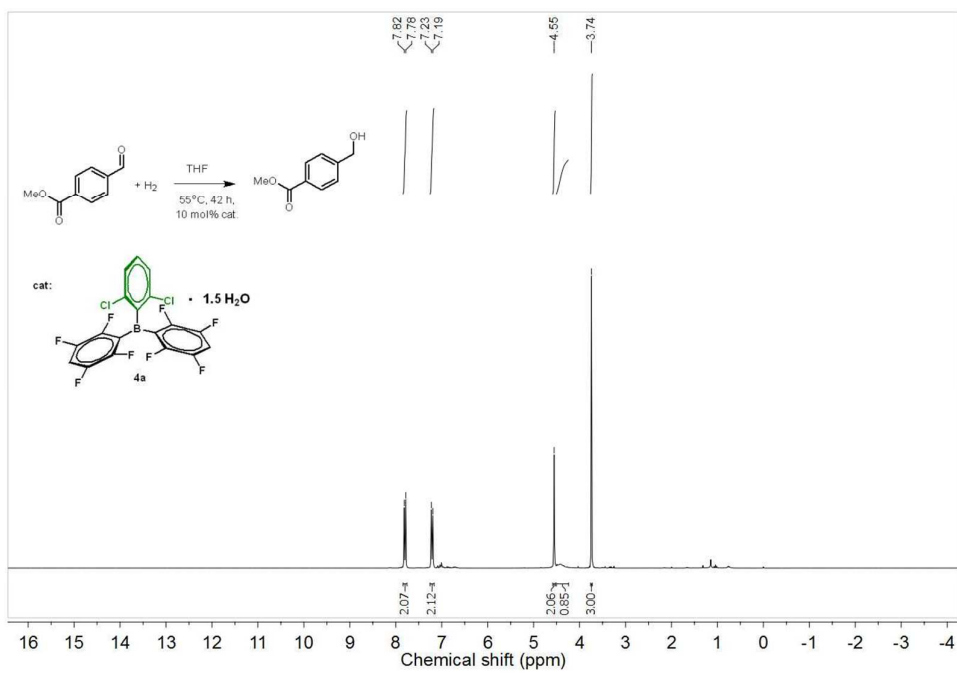
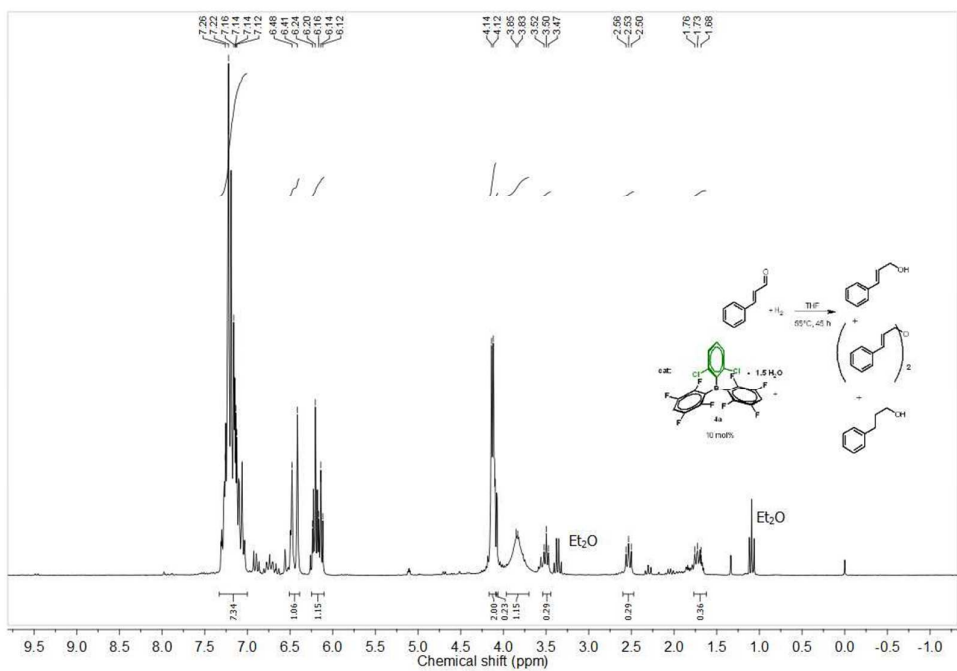


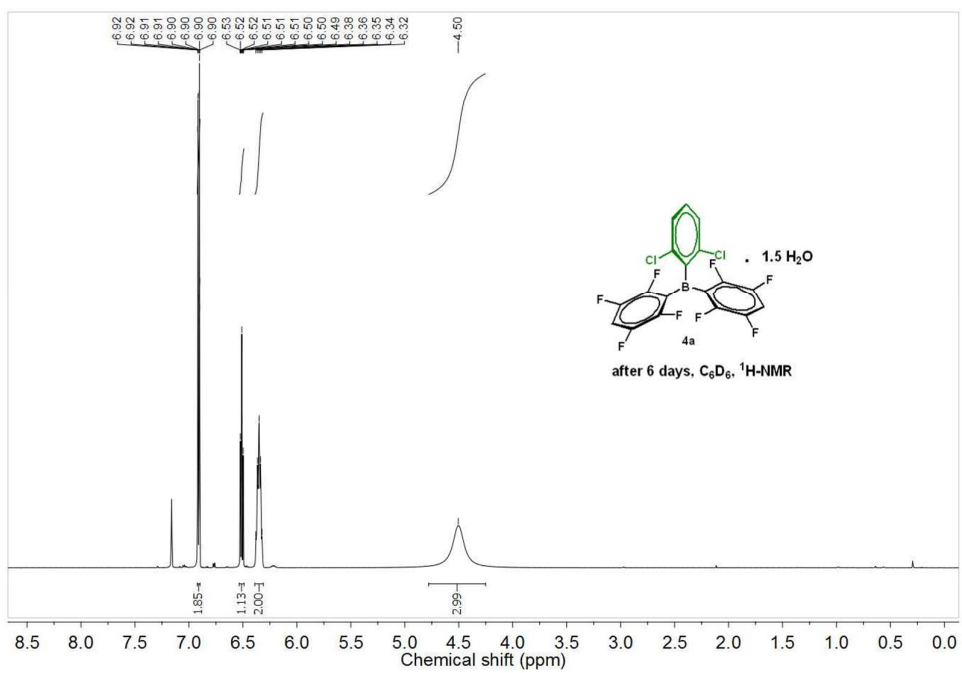
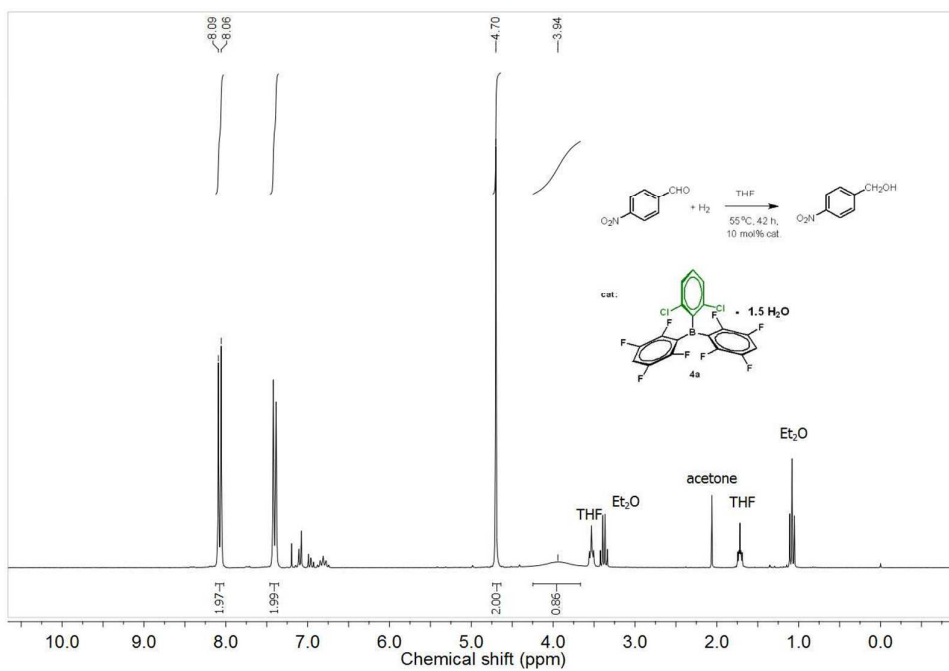


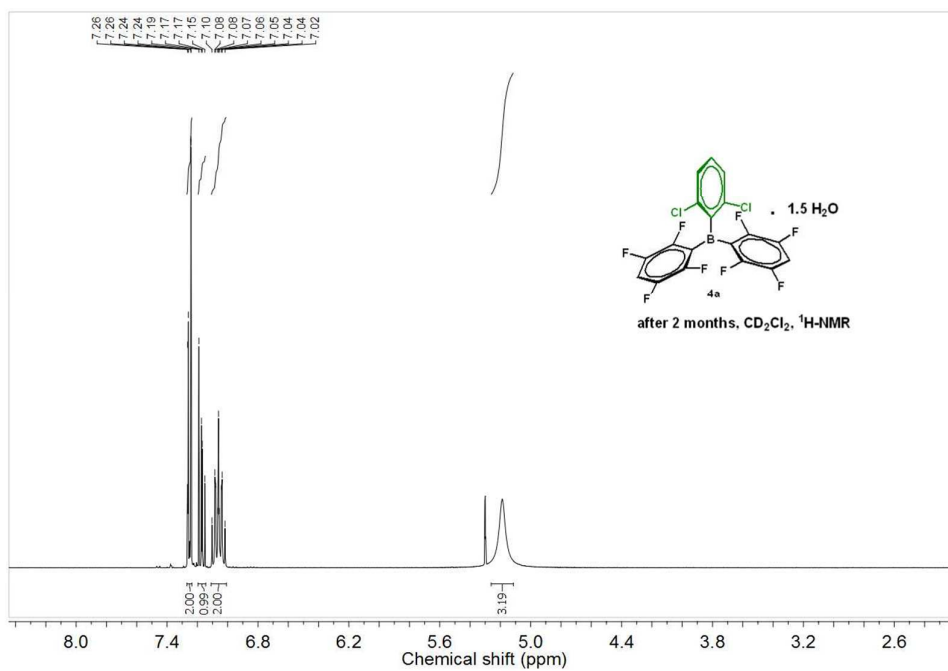


NMR spectra of the crude products – tests with 4a · 1.5H₂O at 100 bar

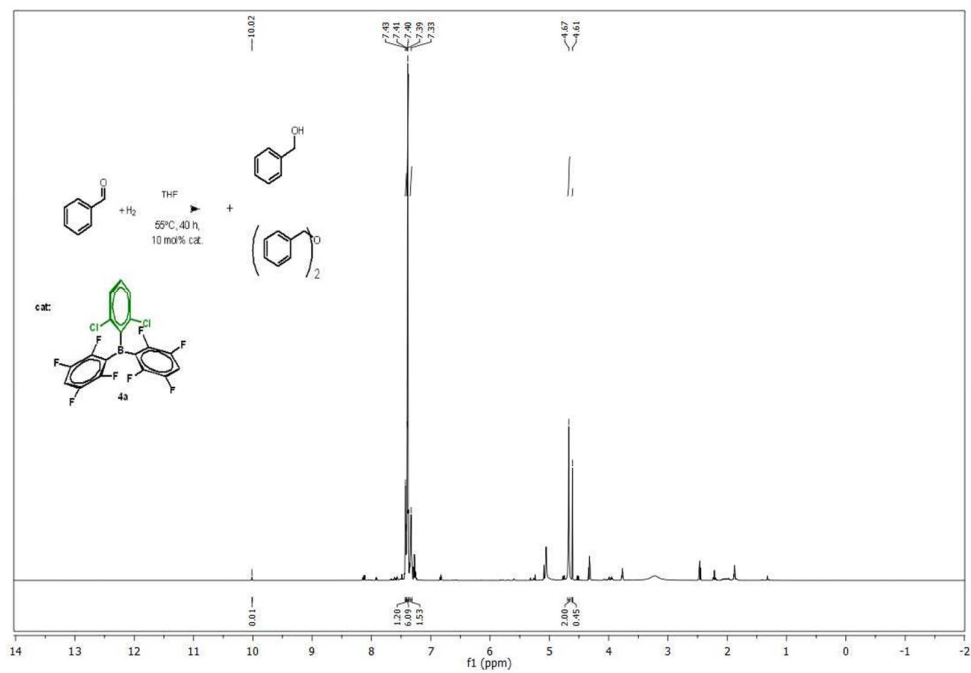


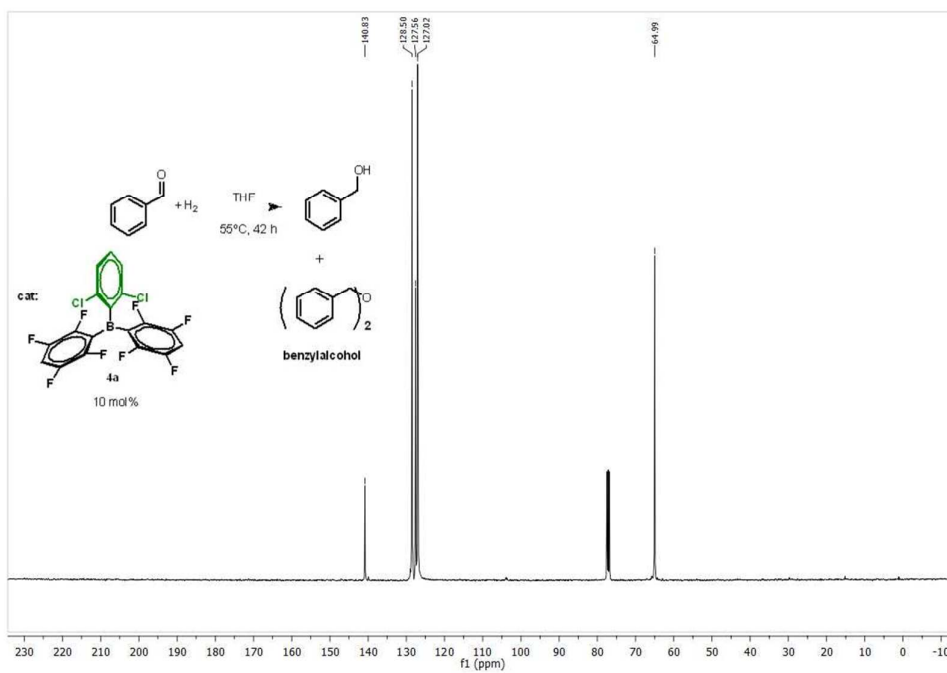
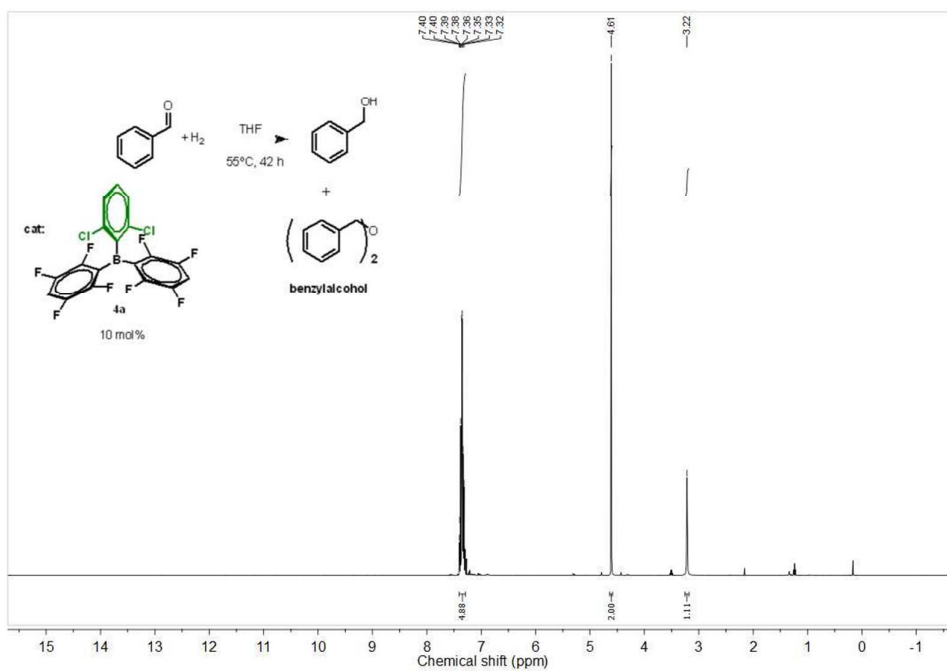


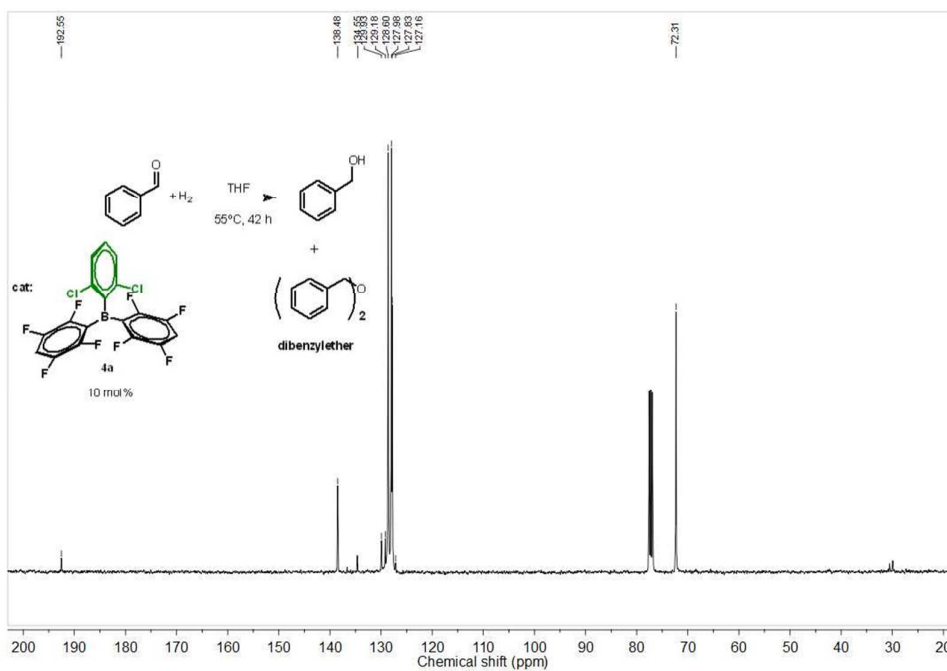
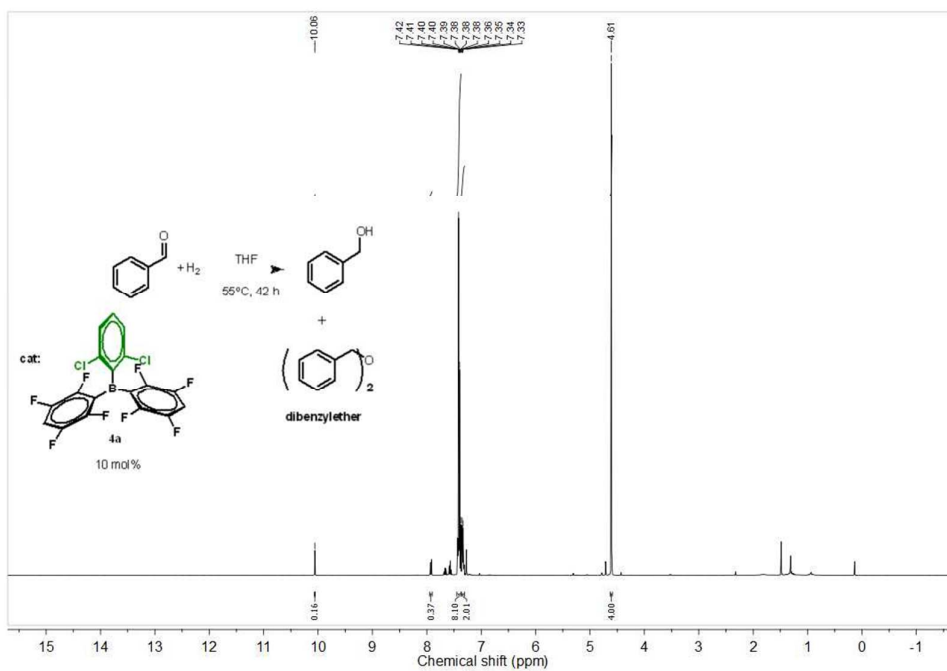


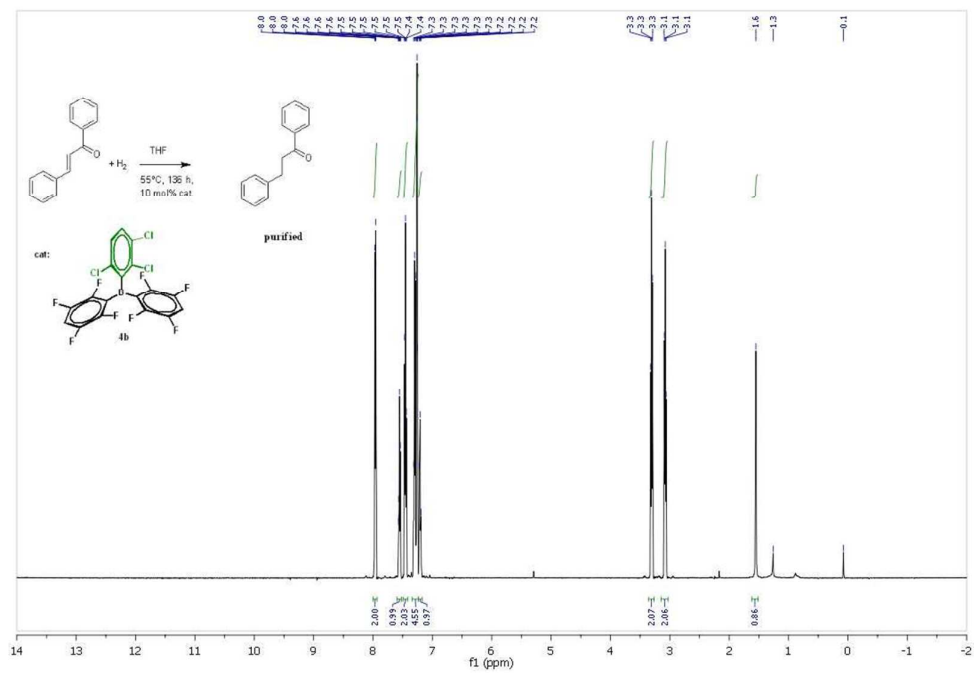
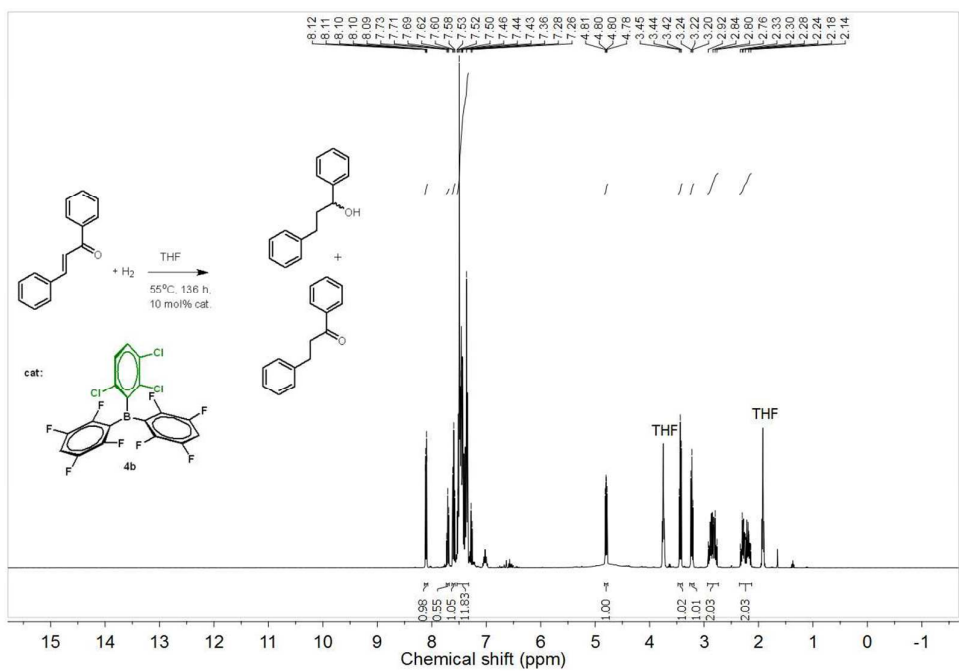


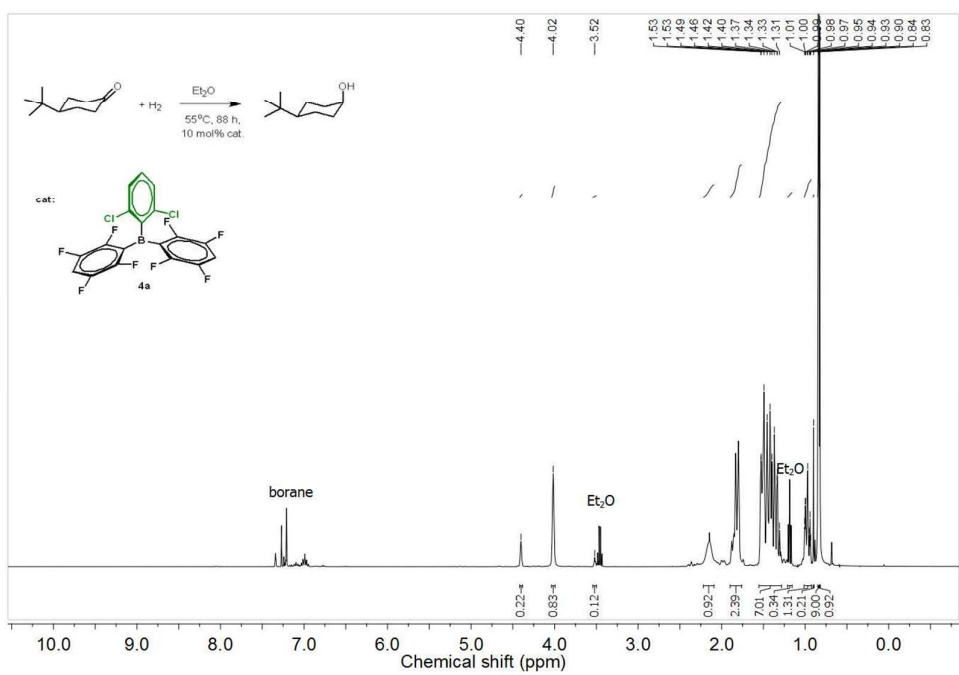
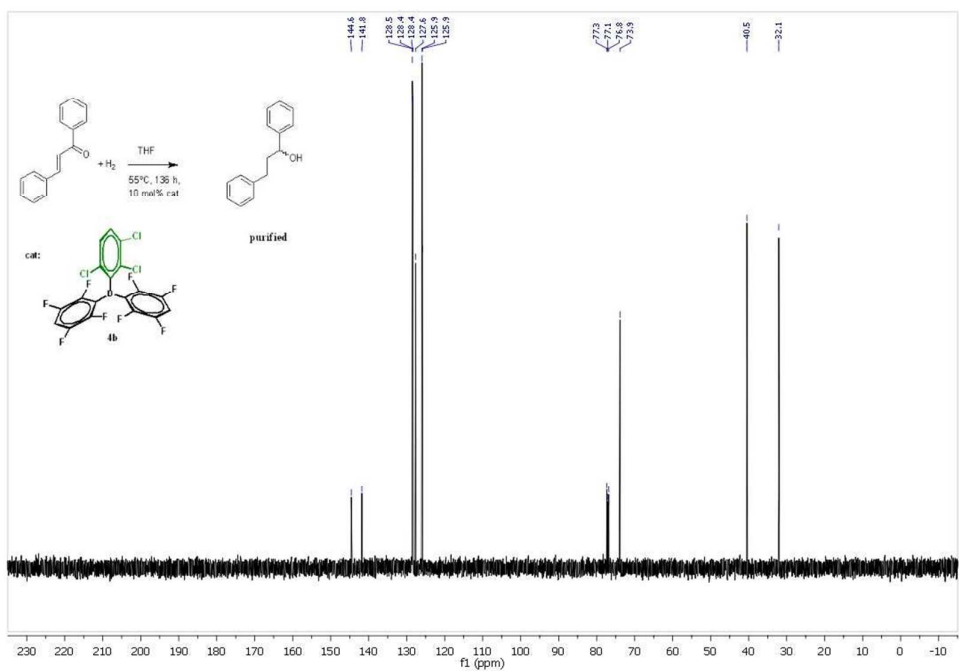
NMR spectra of the crude and isolated products – Substrate scope

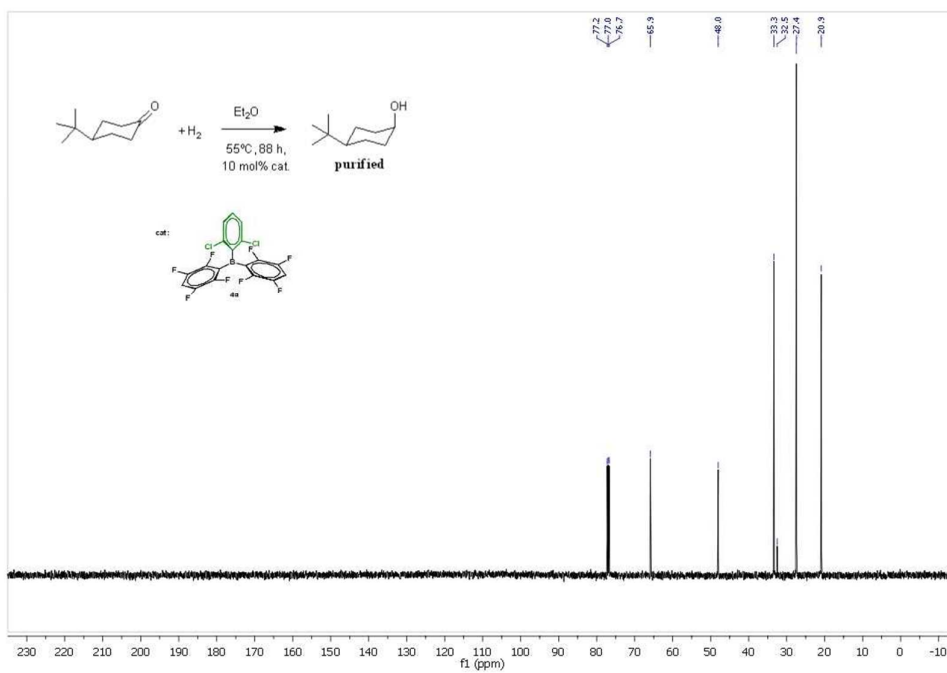
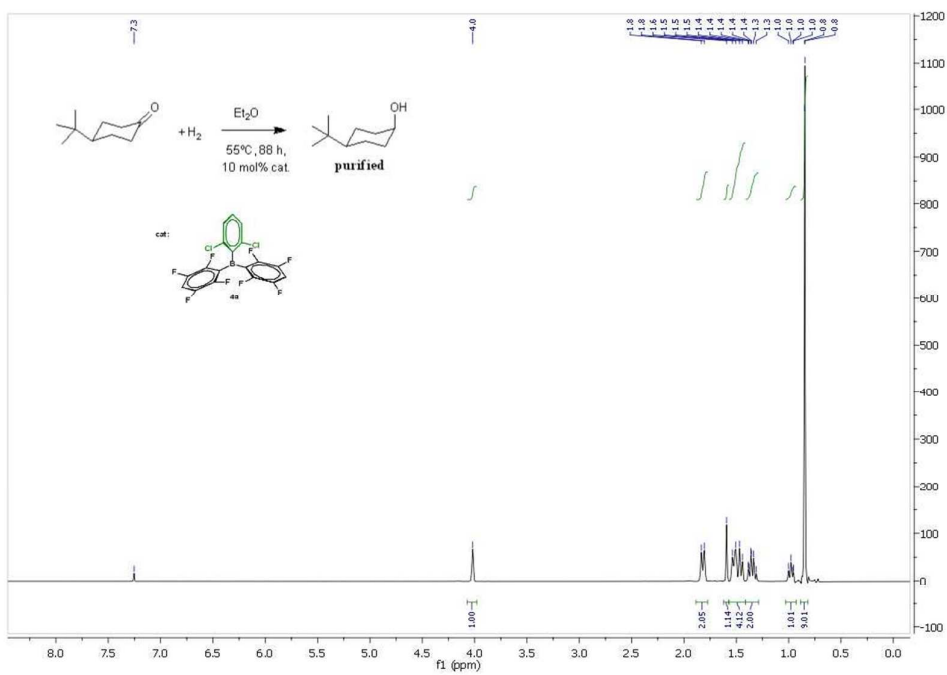


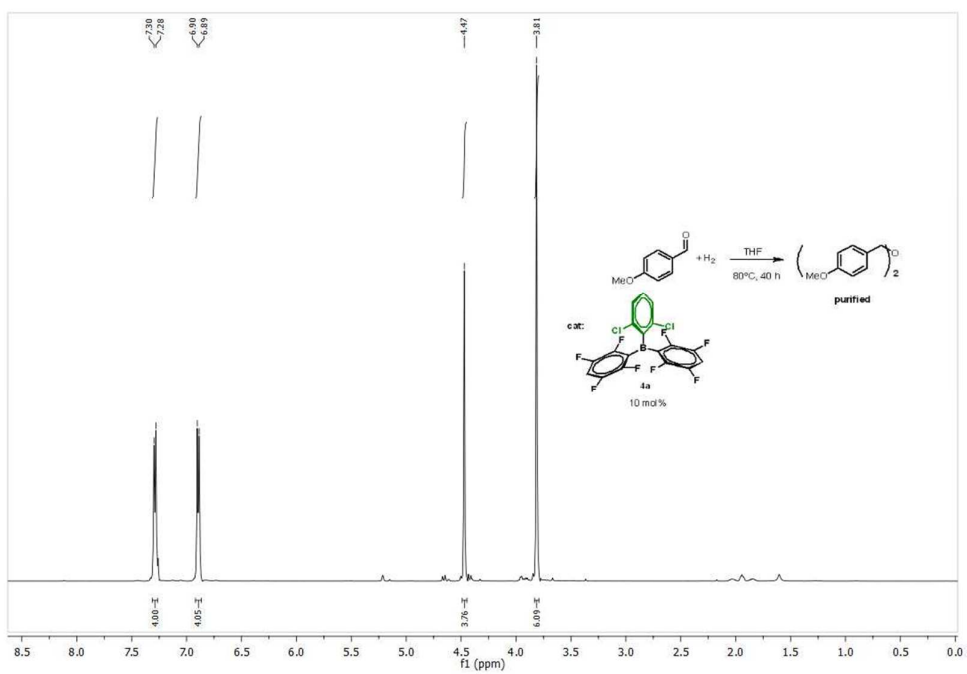
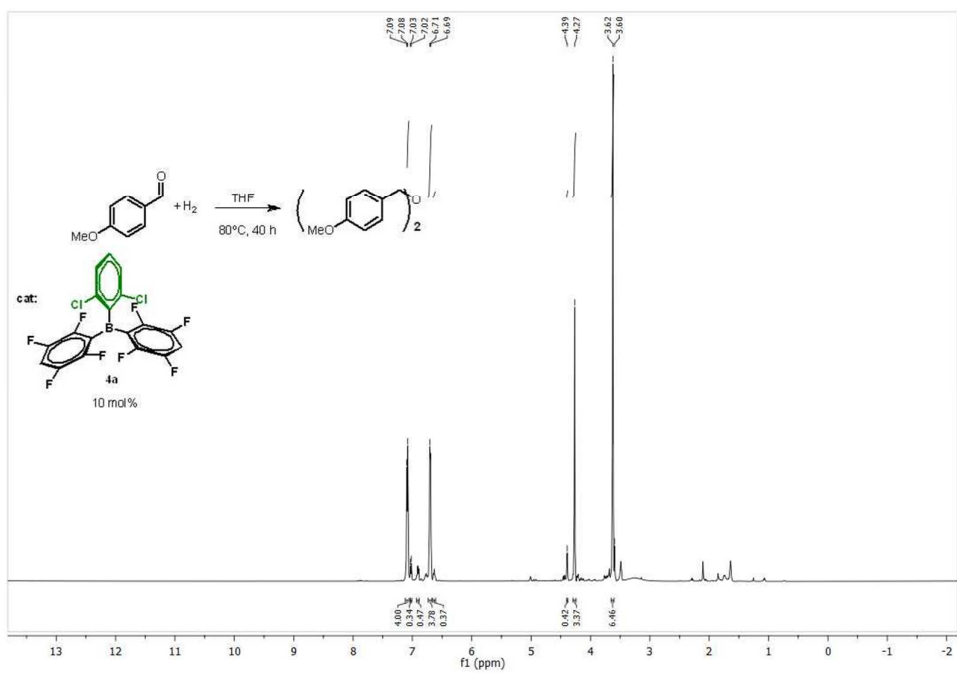


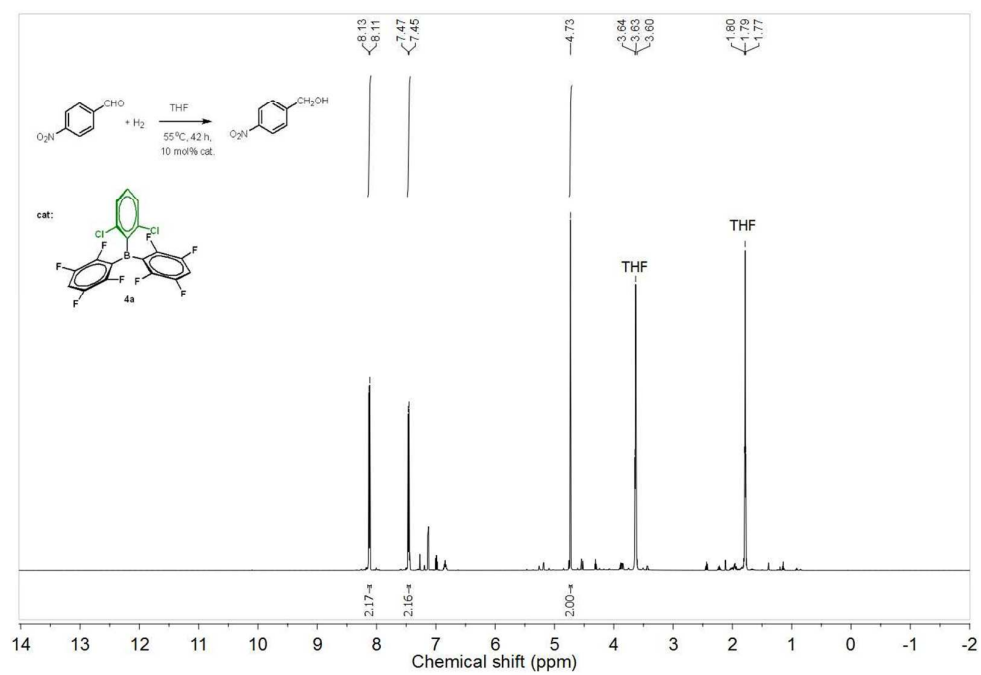
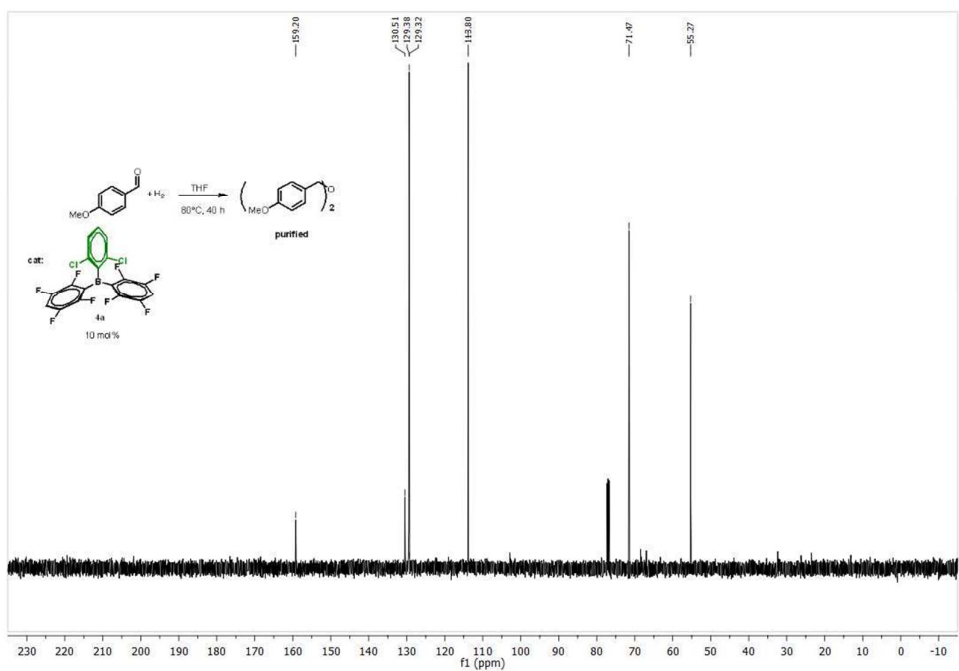


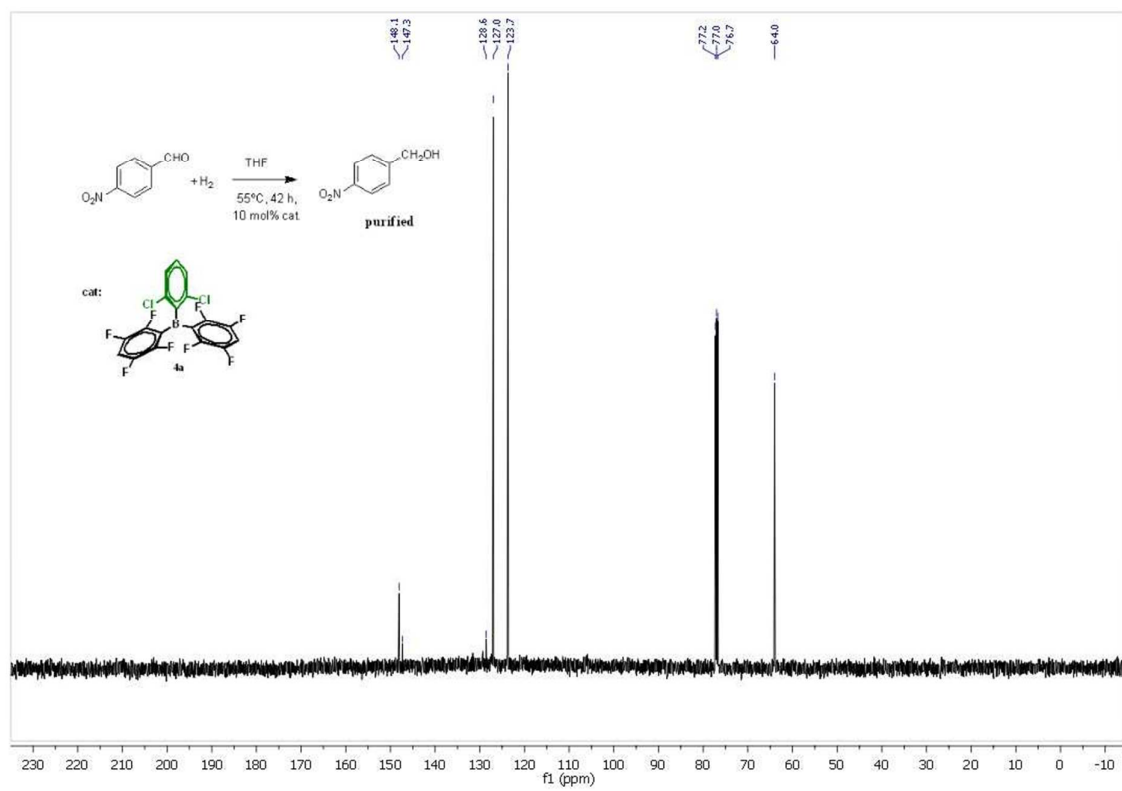
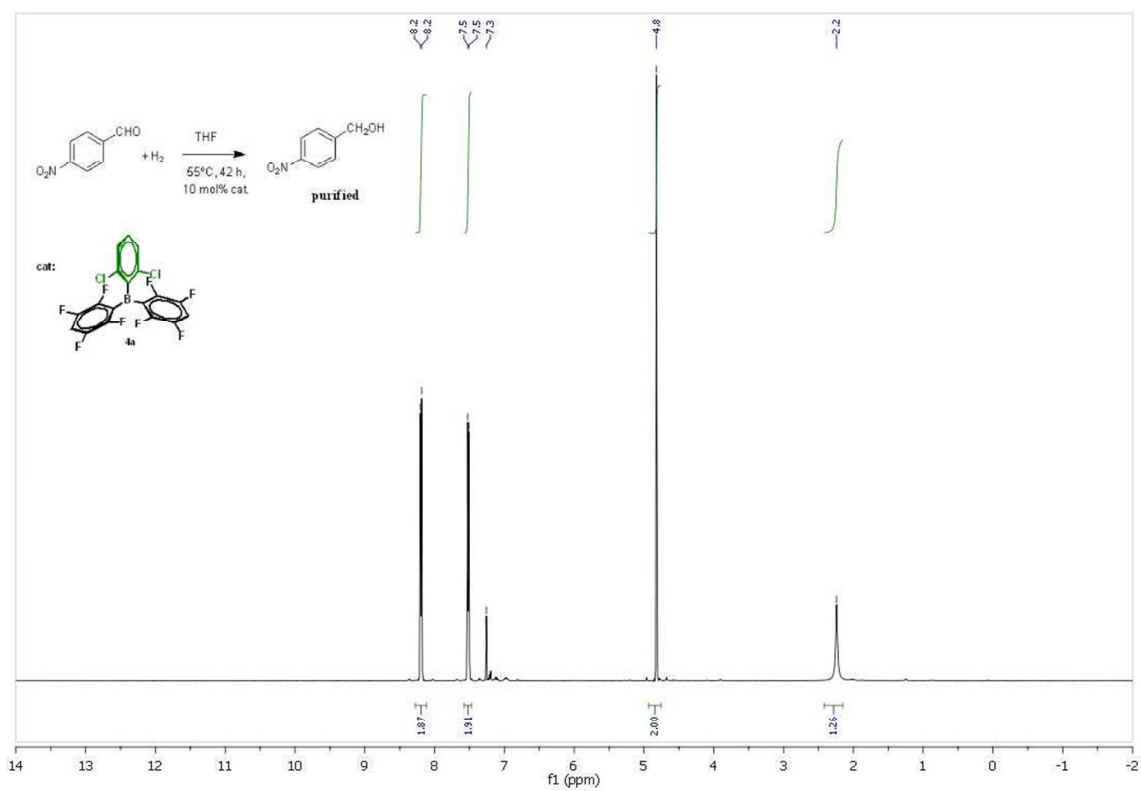


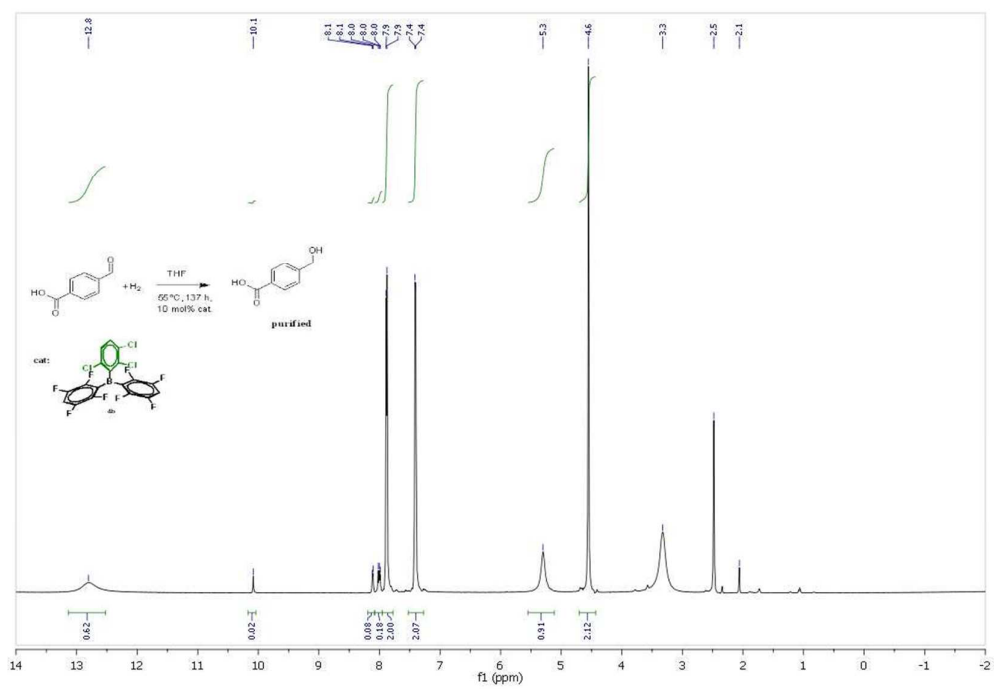
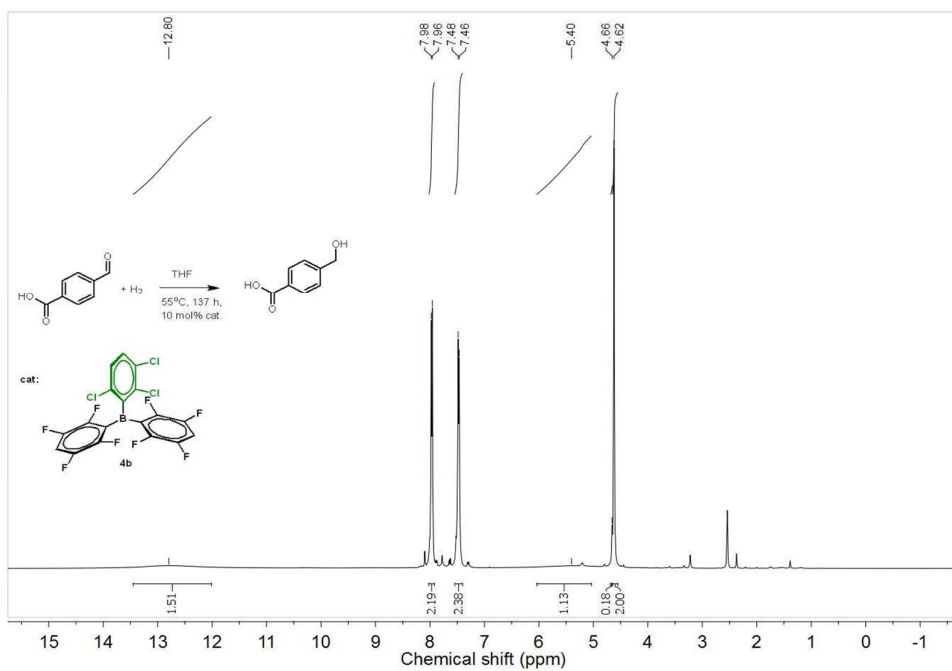


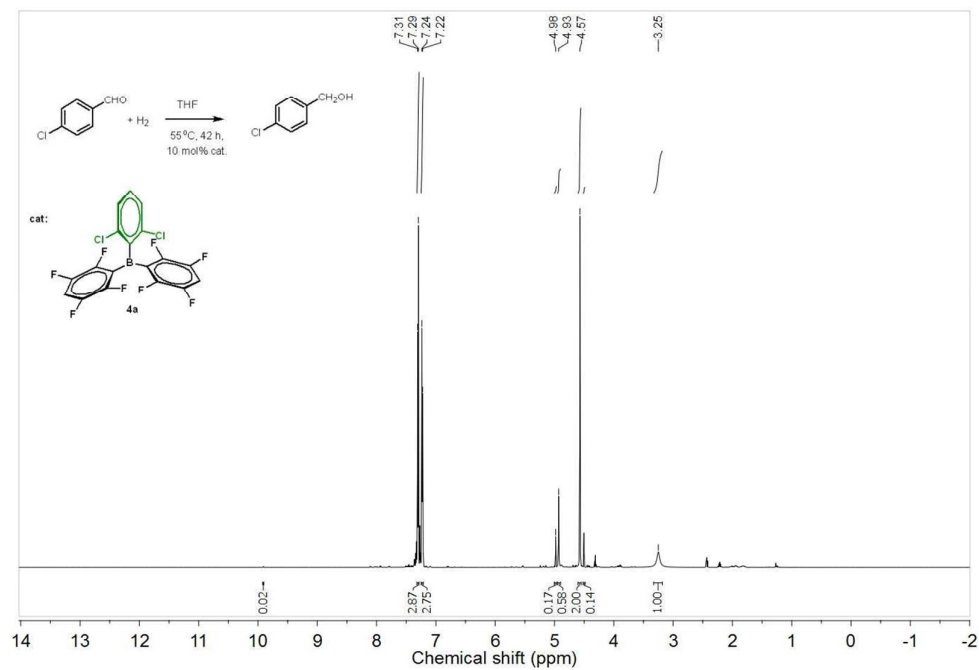
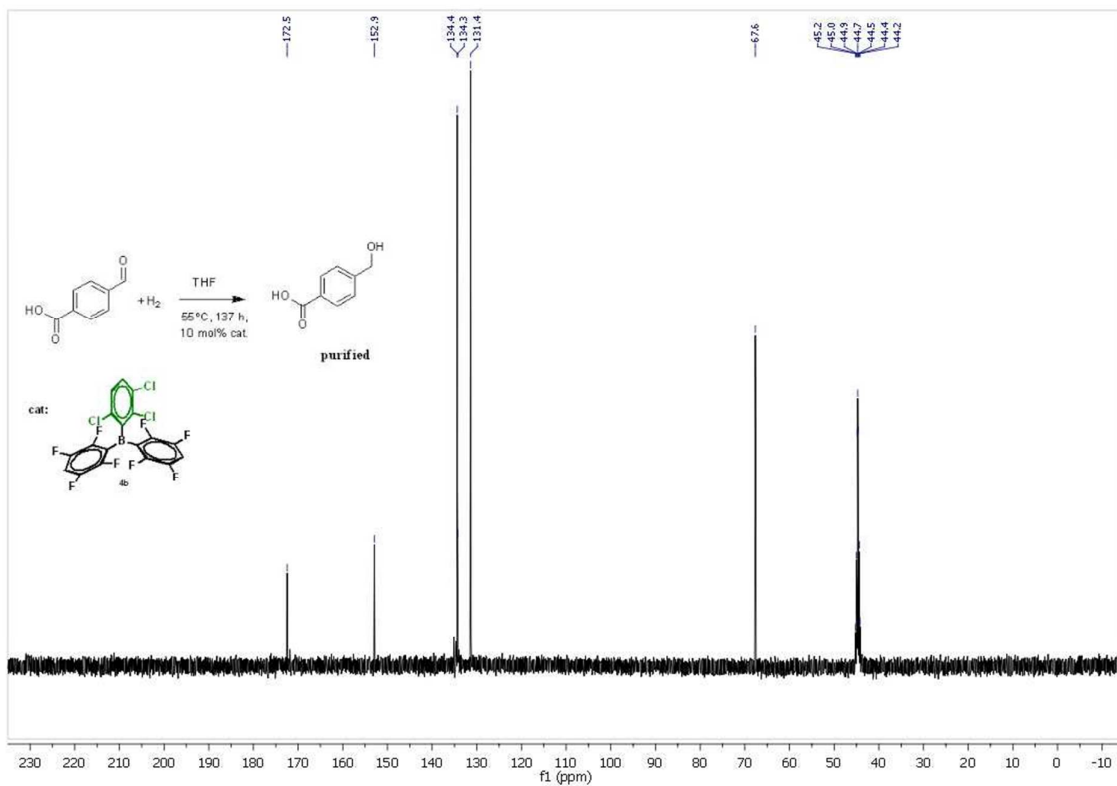


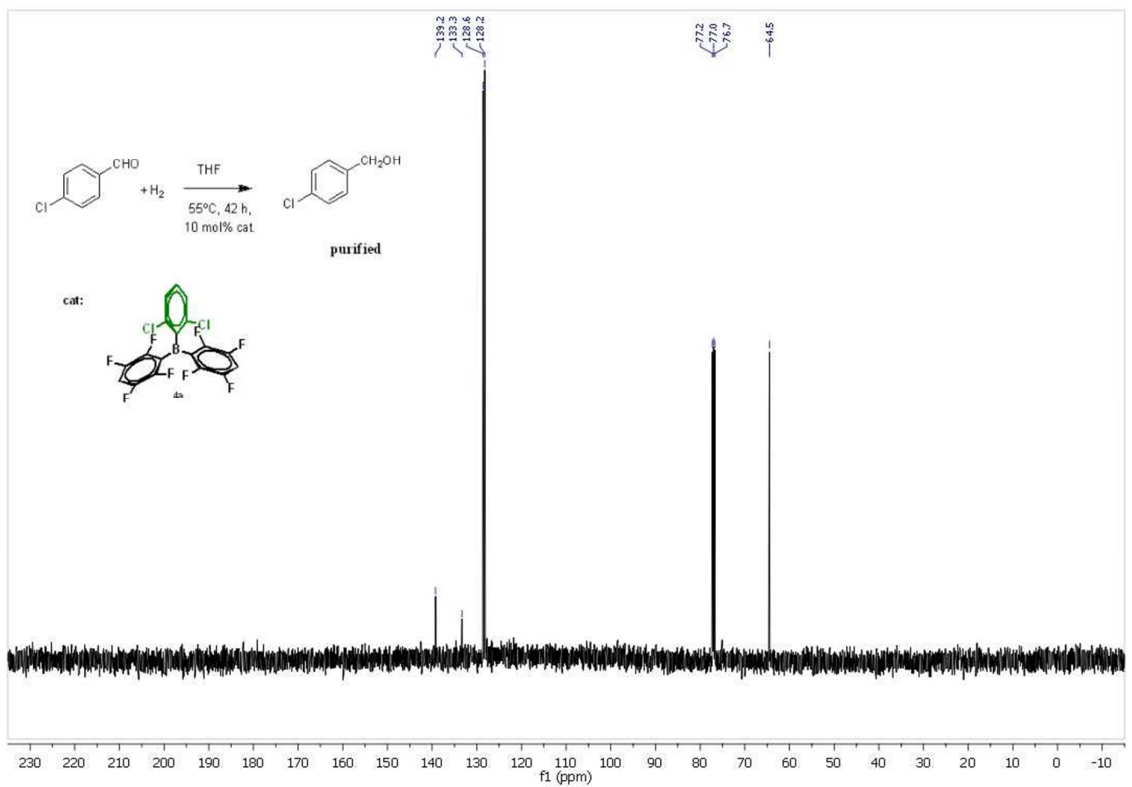
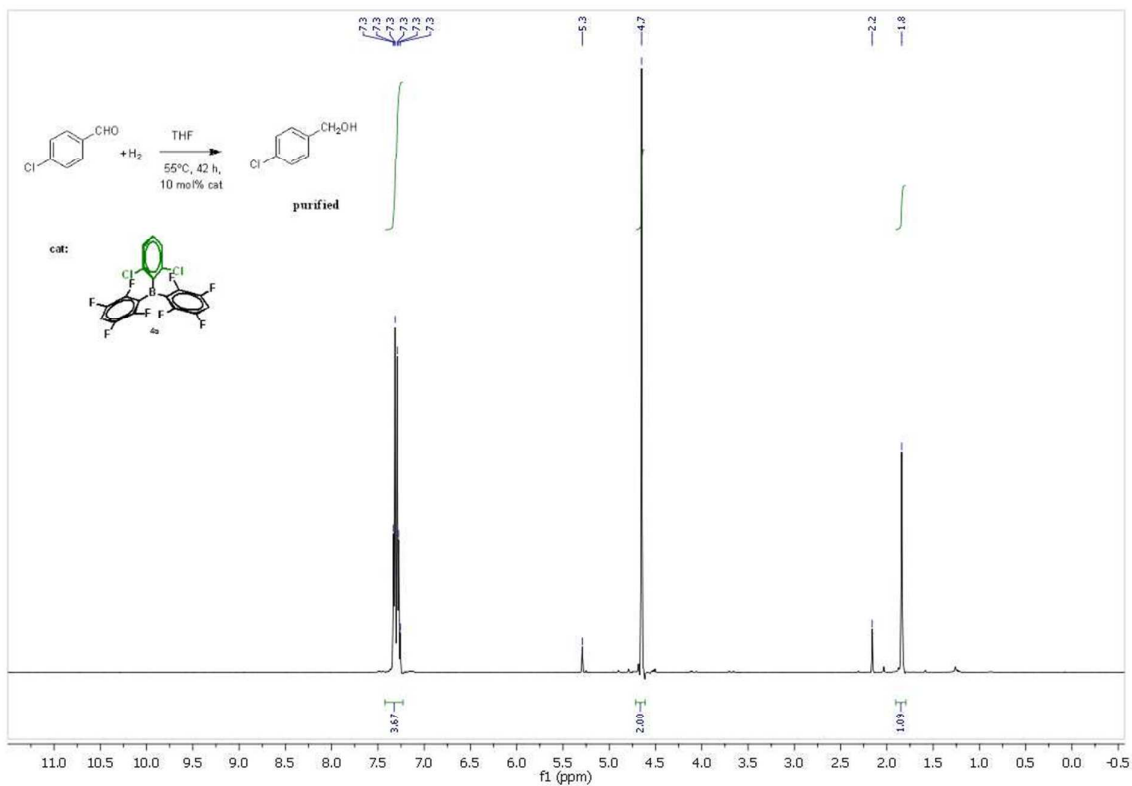


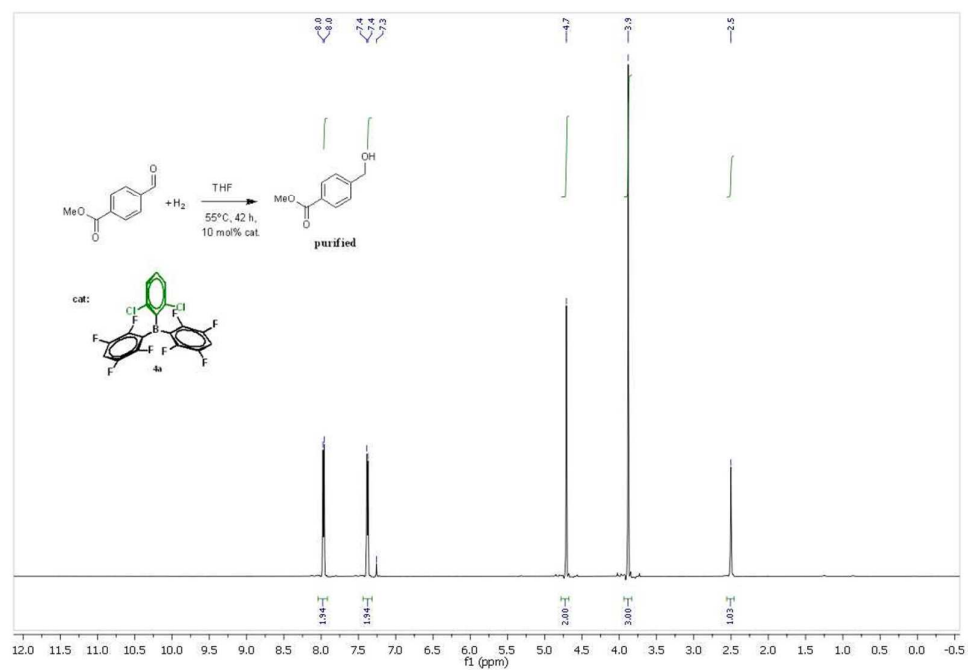
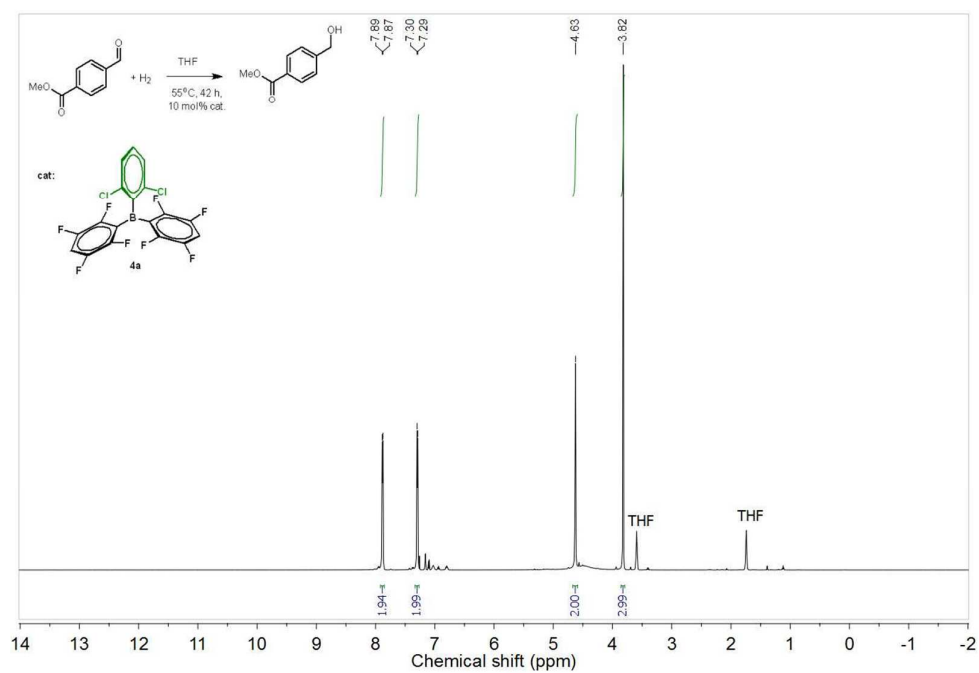


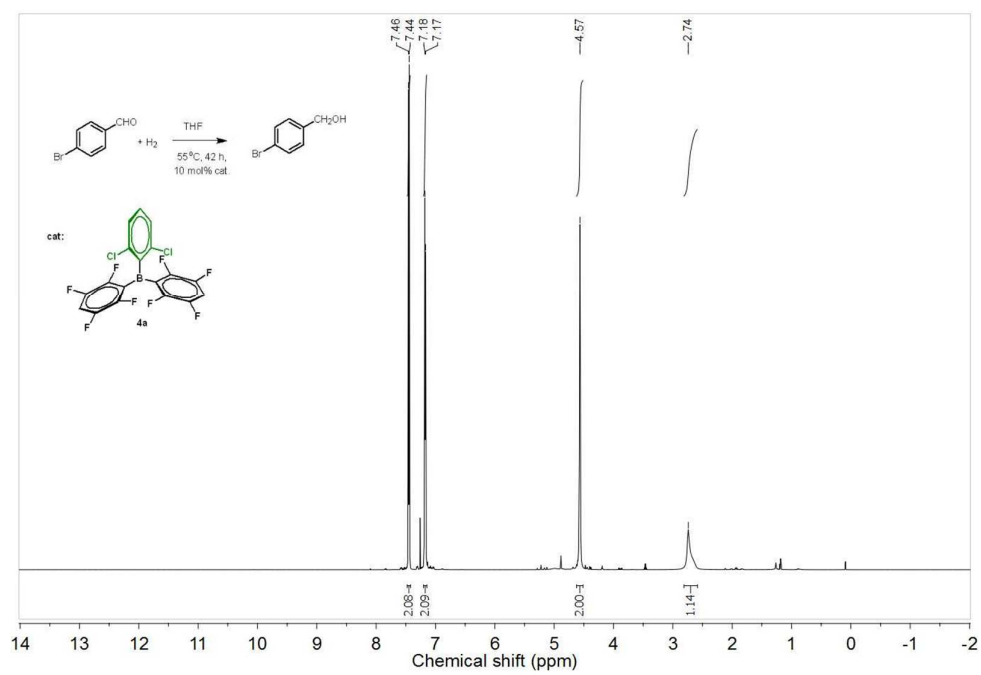
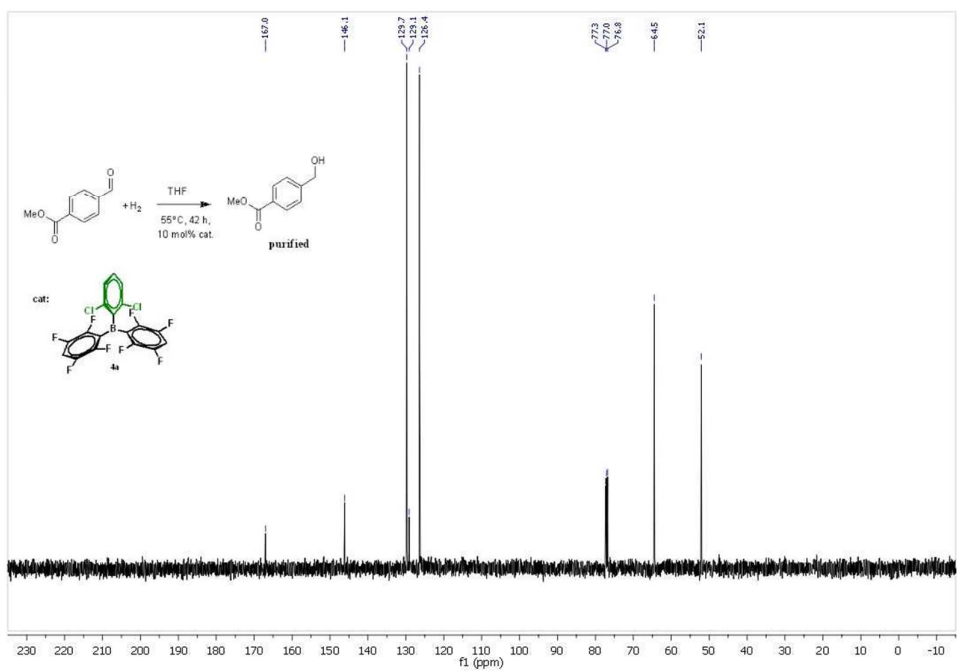


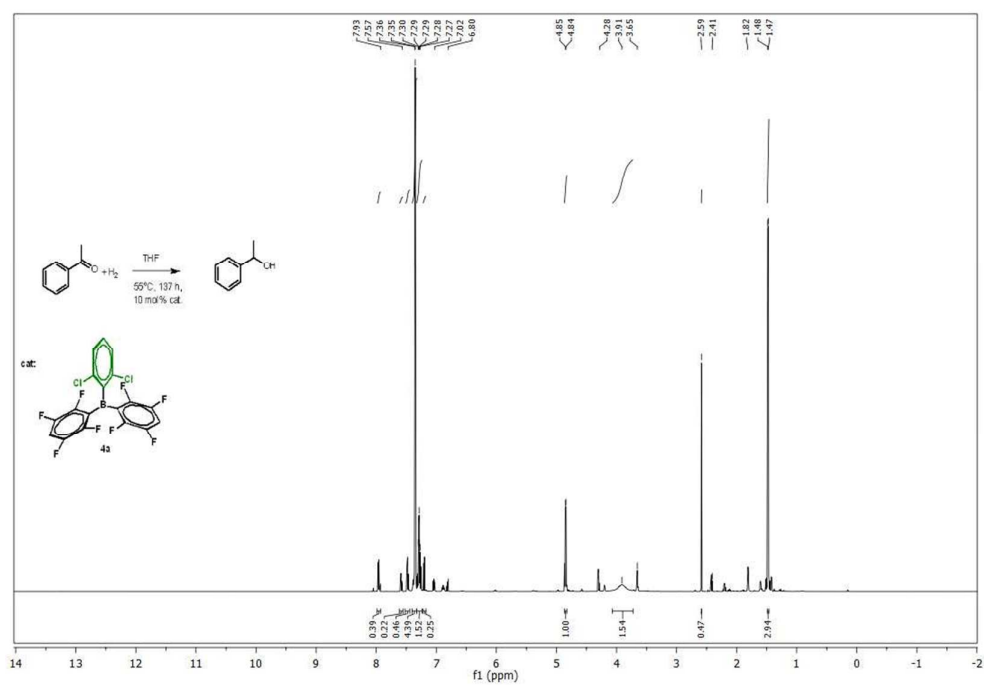
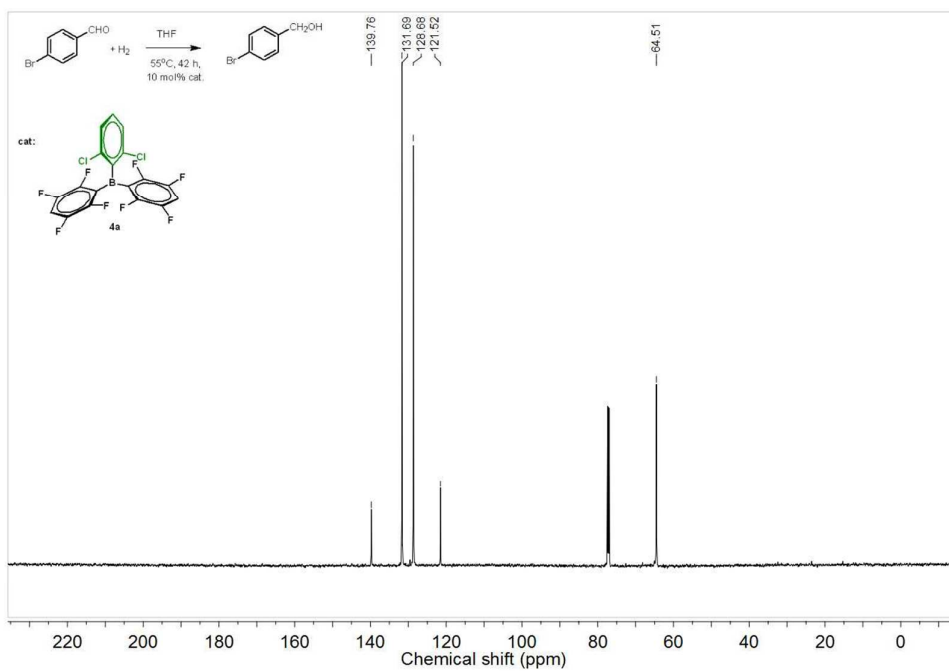


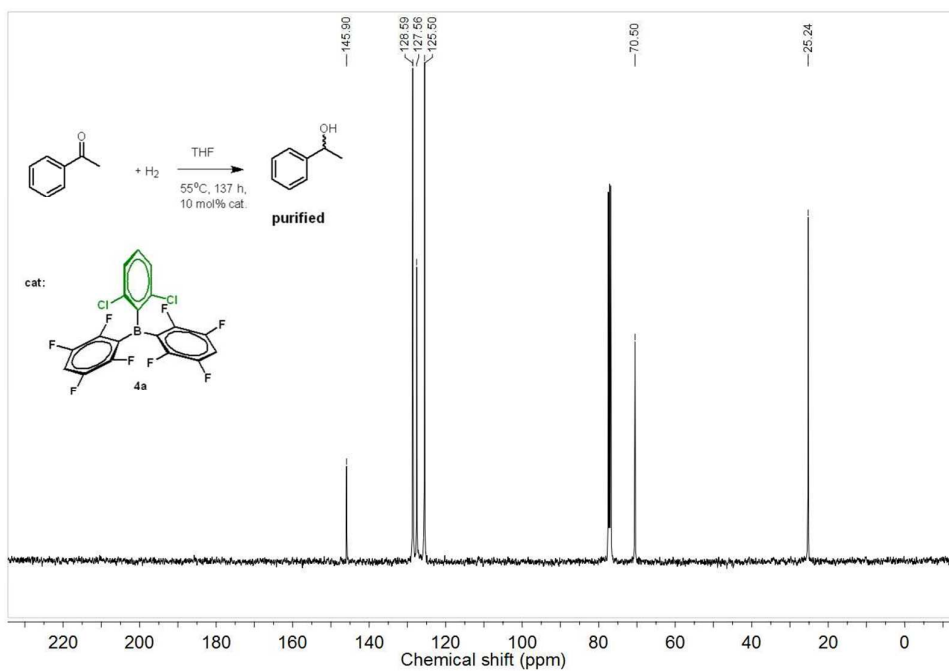
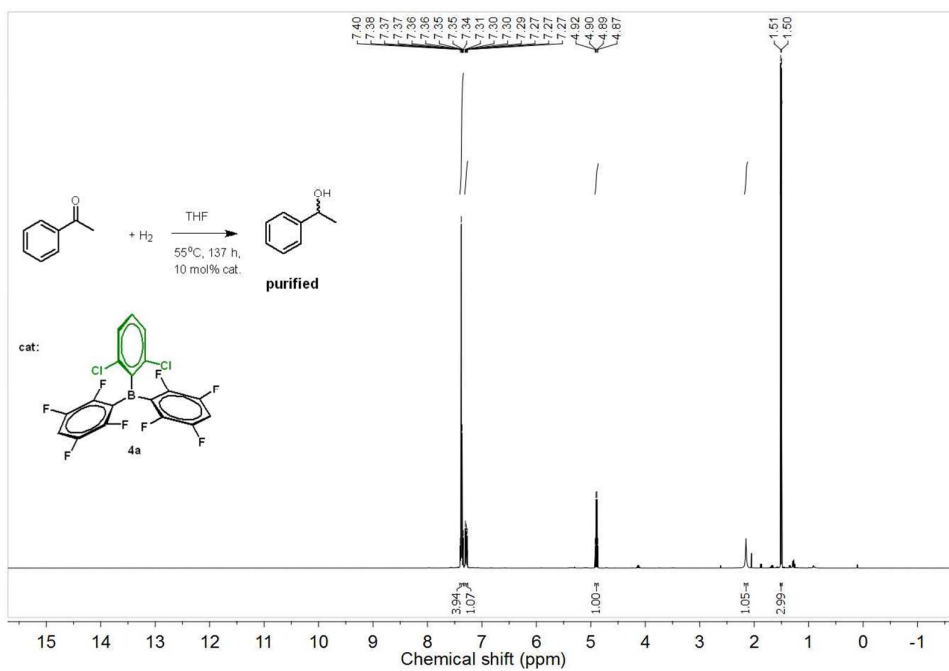


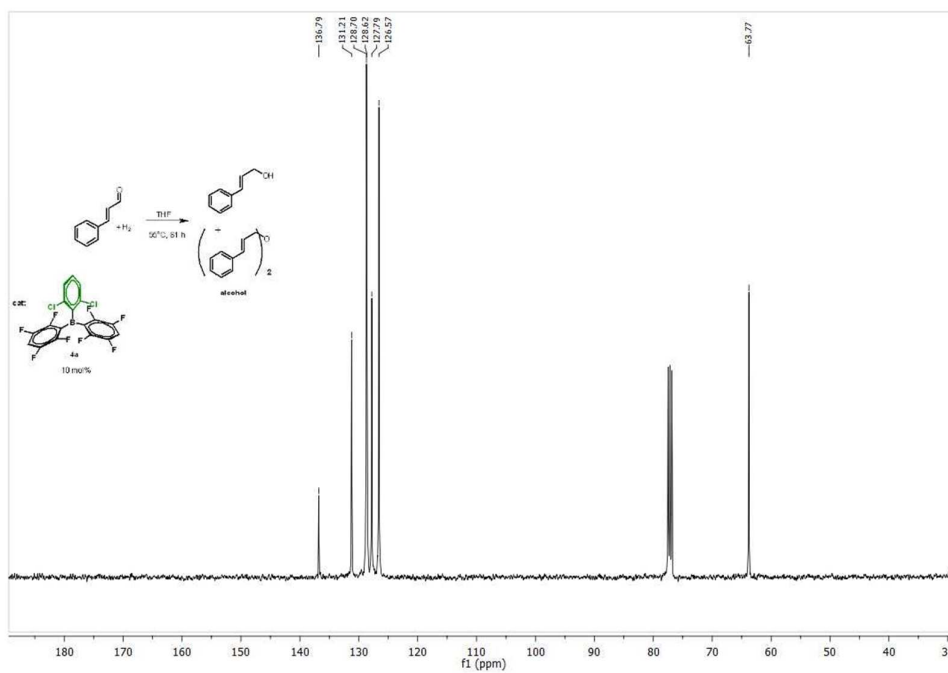
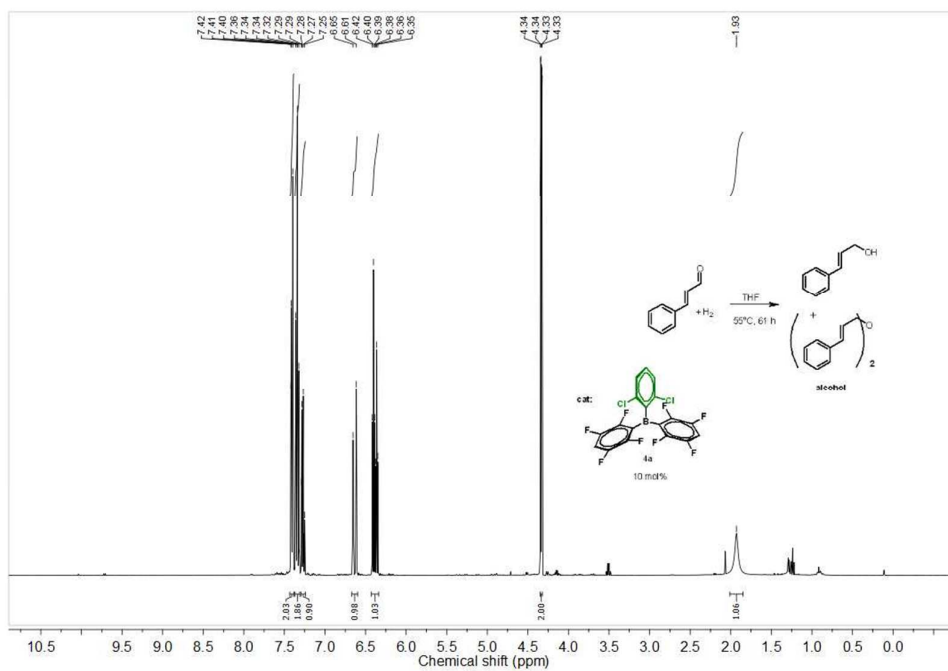


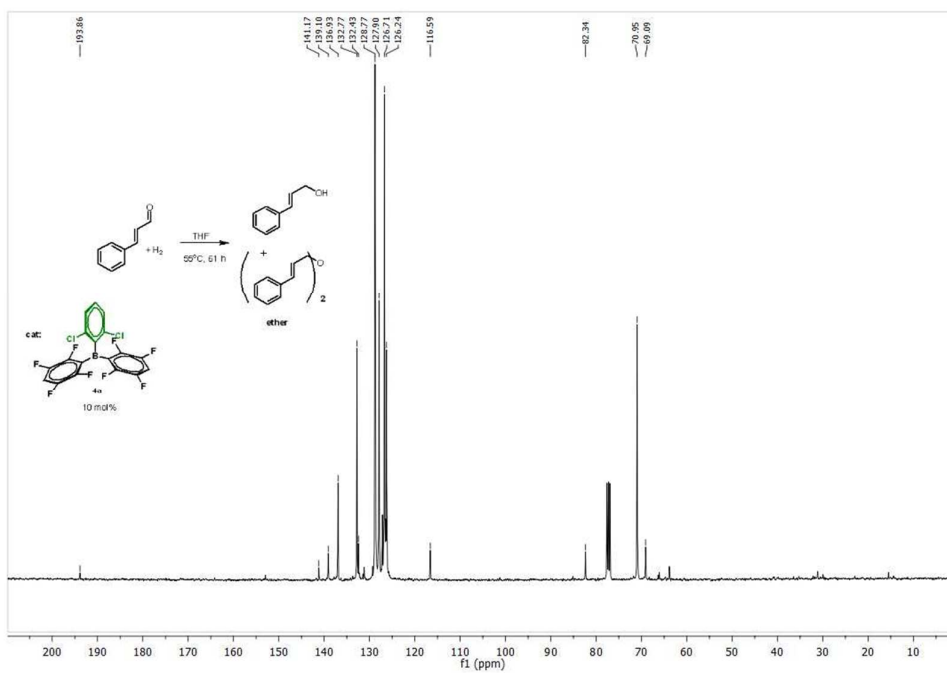
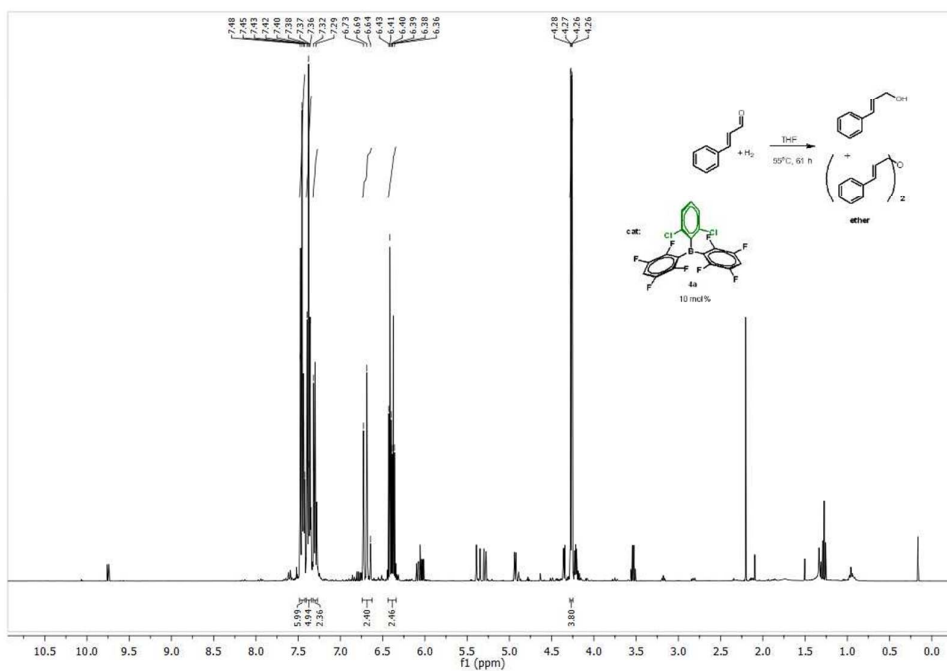




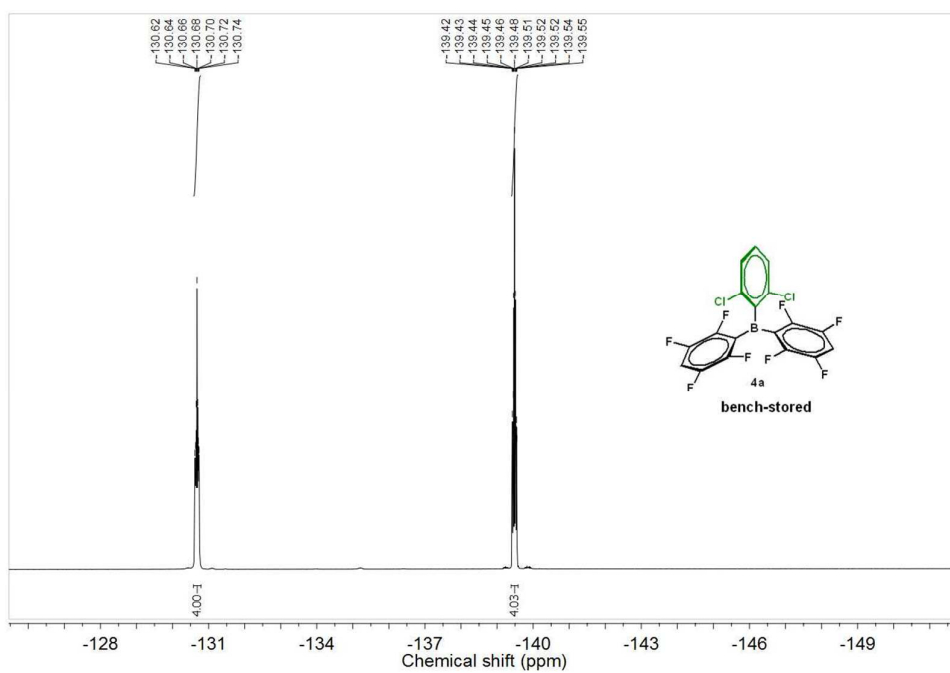
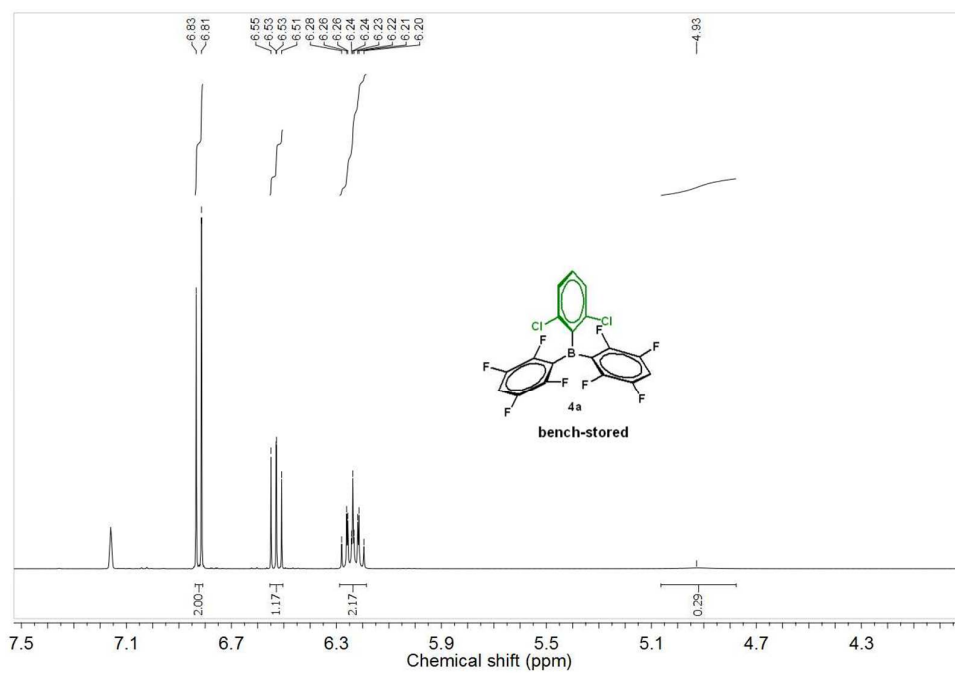


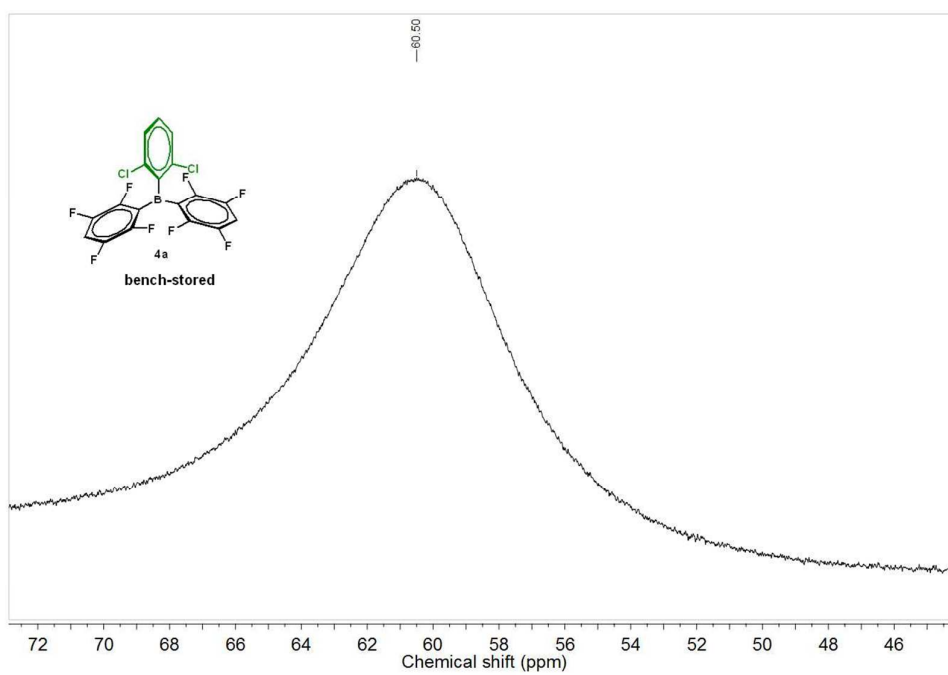
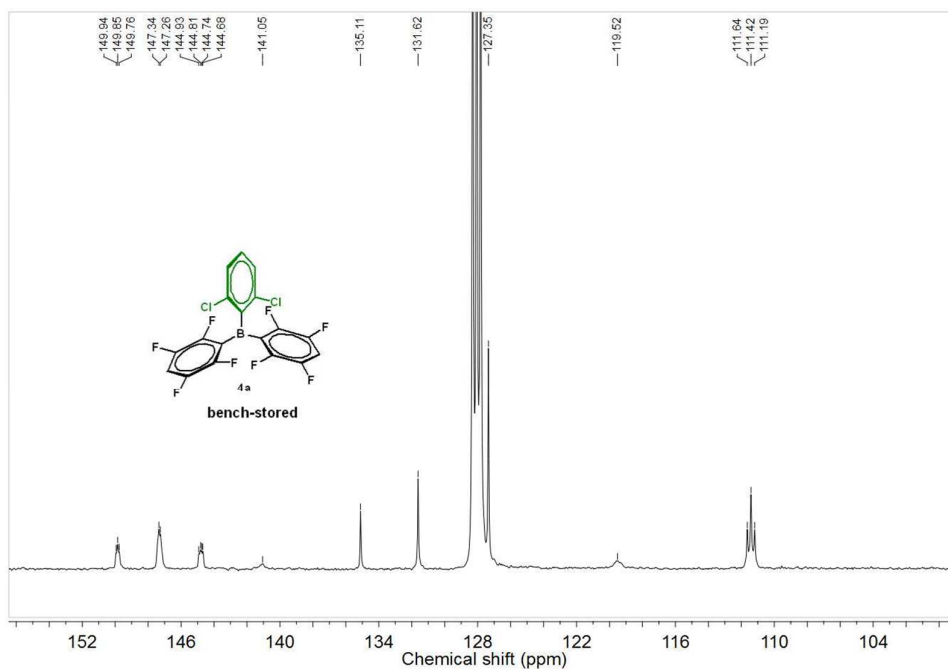


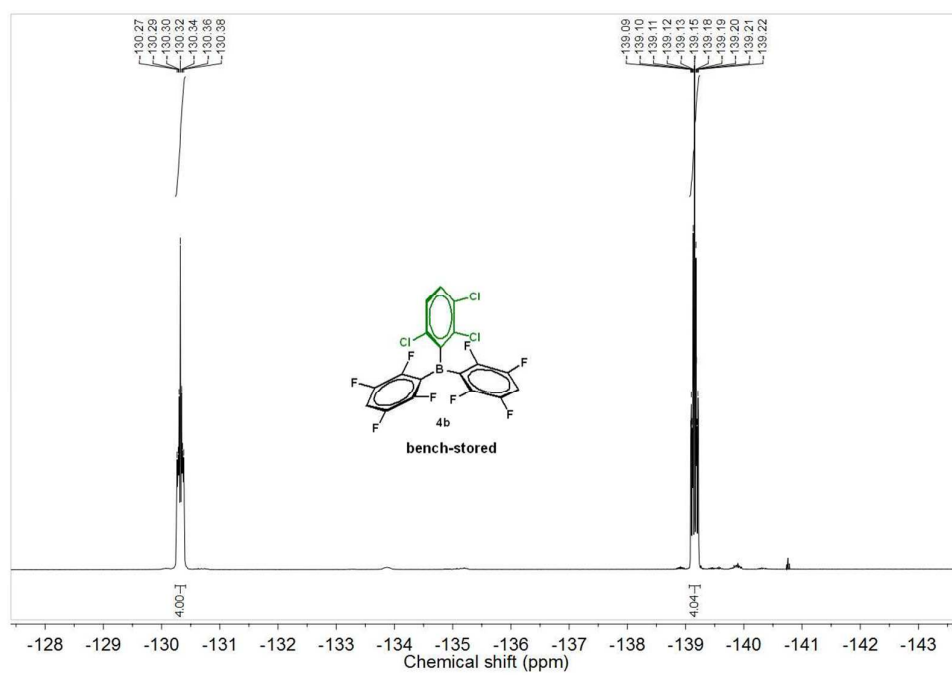
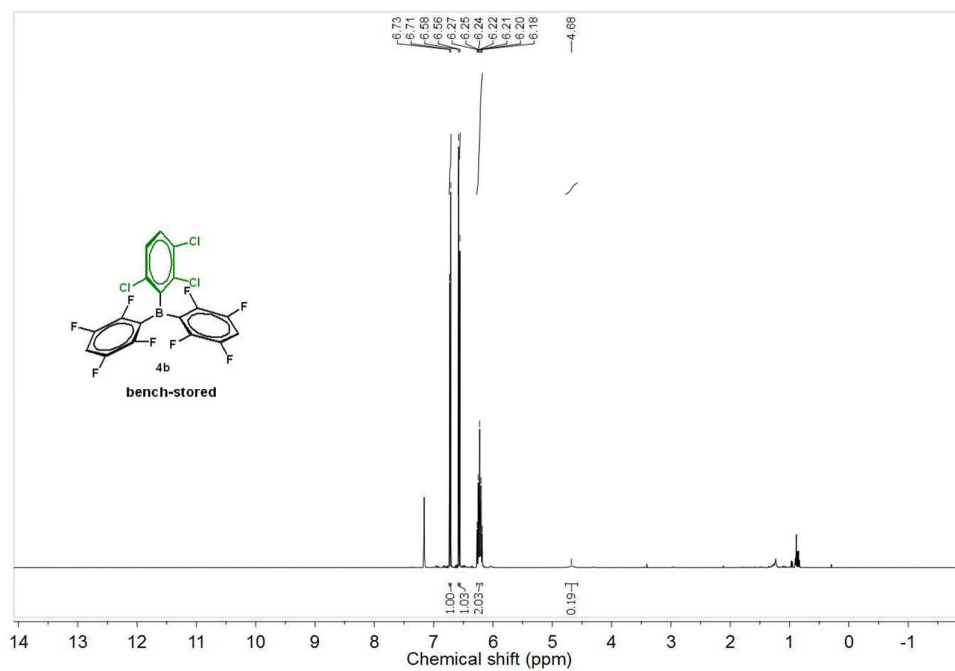


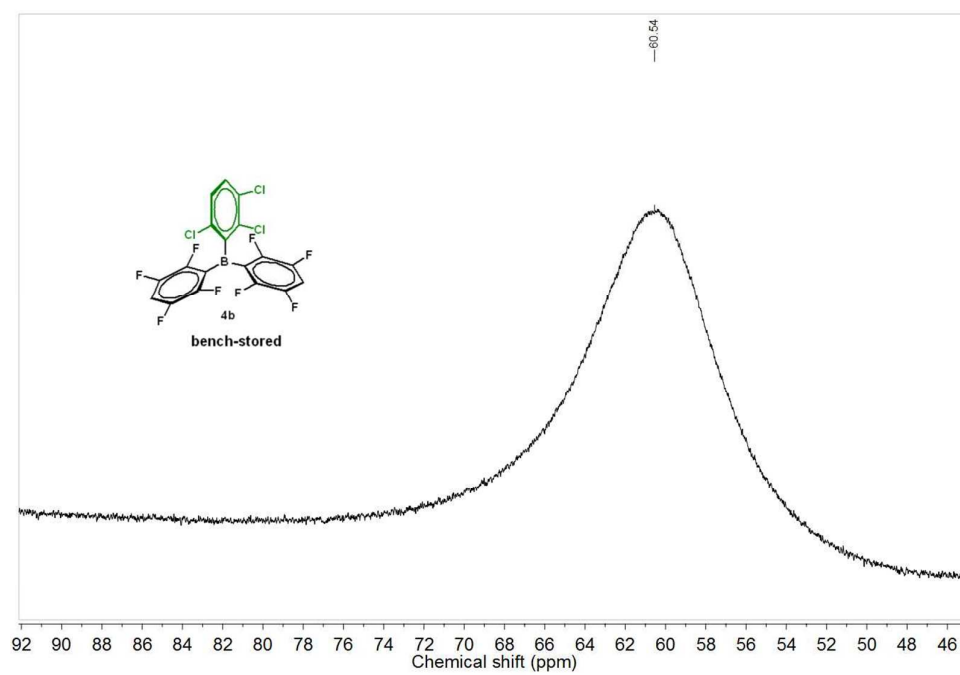
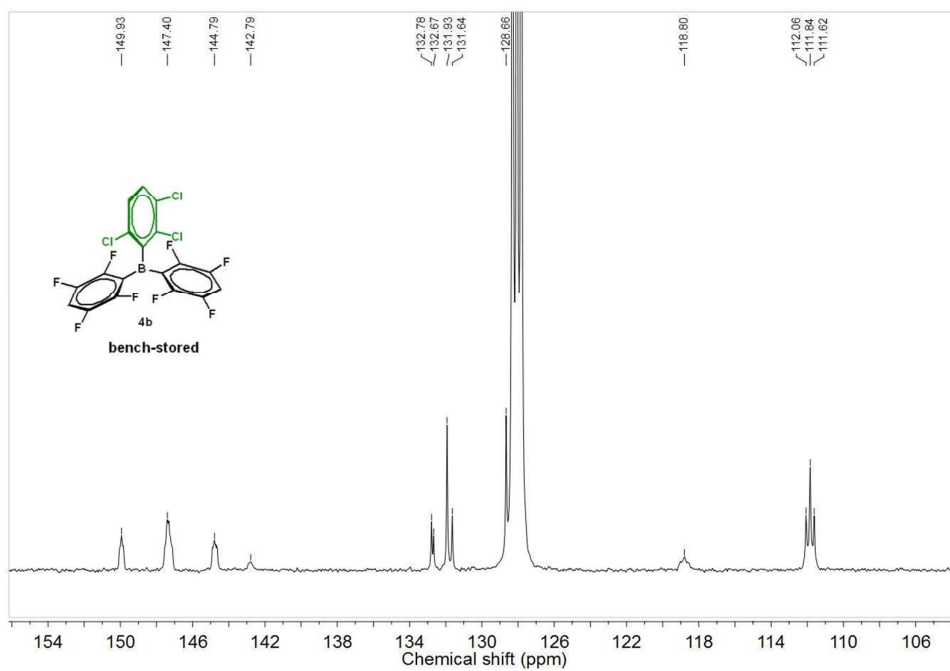


NMR spectra of the bench-stored boranes in C₆D₆ (4a and 4b)









NMR Complexation Studies

Boron has two naturally occurring NMR active isotopes both with spins larger than 1/2. Measuring the ^{11}B isotope is much more favored against the ^{10}B isotope, because it has a larger abundance (80%) and lower quadrupole moment, which results better resolution. In FLP chemistry this background problem can make the characterization of the products difficult. In general the chemical shifts of Ar_3B type compounds are in the range of 50 – 100 ppm and the signals of their Ar_3BL complexes are shifted upfield. Compound **4a** has a relatively broad signal at 63.4 ppm, so the chemical shift of its complexes should be found in the region of the ^{11}B background as the Figure S31 shows. Signals with smaller intensities cannot be reliably detected below 30 ppm.

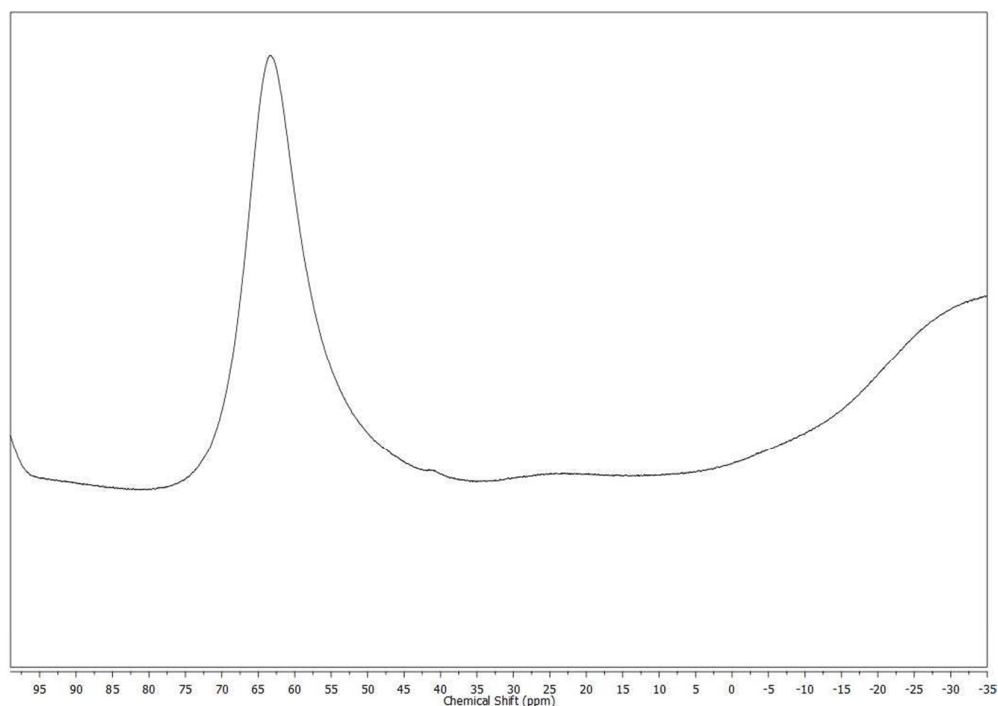


Figure S31 ^{11}B solution NMR spectra of borane **4a** in benzene at 25 °C.

To overcome this problem, measuring of ^{10}B is an appealing alternative. As it was previously demonstrated, the ^{10}B spectrum has a flat baseline.¹ The signal is slightly broader, but the region where the complexes of borane **4a** should be found is completely flat, as the Figure S32 shows.

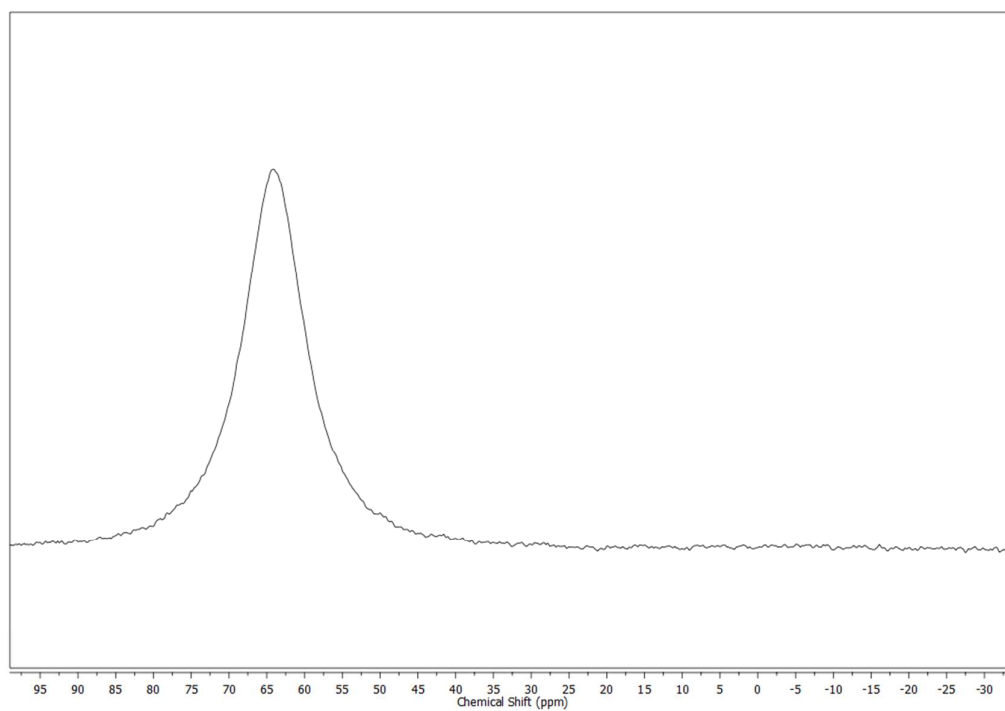


Figure S32 ^{10}B solution NMR spectra of borane **4a** in benzene at 25 °C.

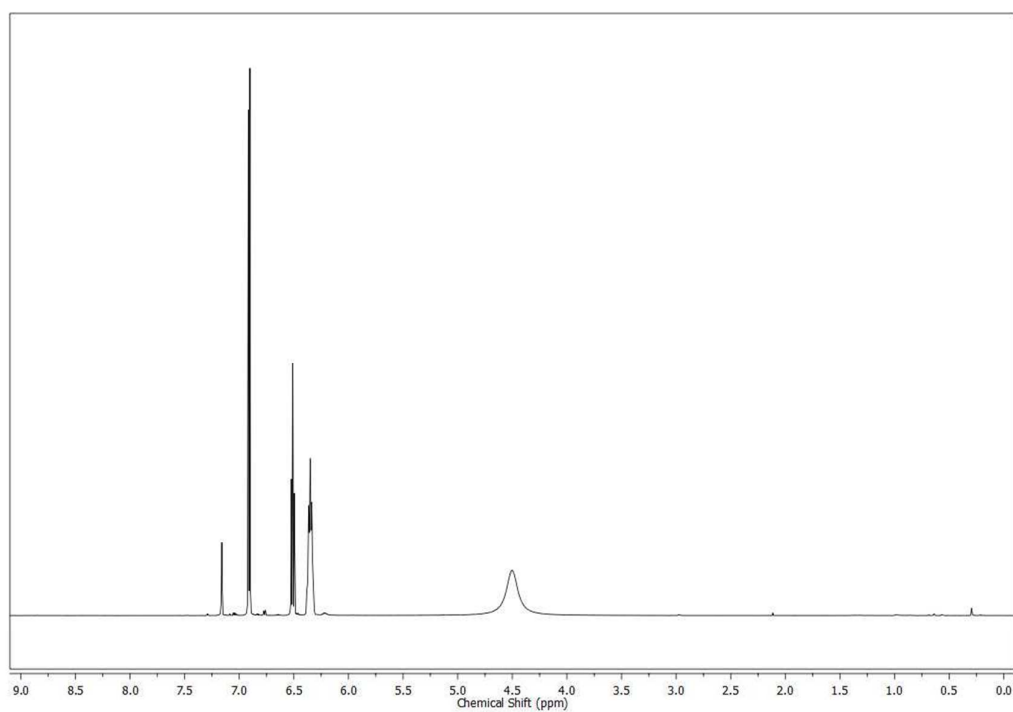


Figure S33 ^1H solution NMR spectra of borane **4a** stored in an open vial for 6 days in benzene at 20 °C

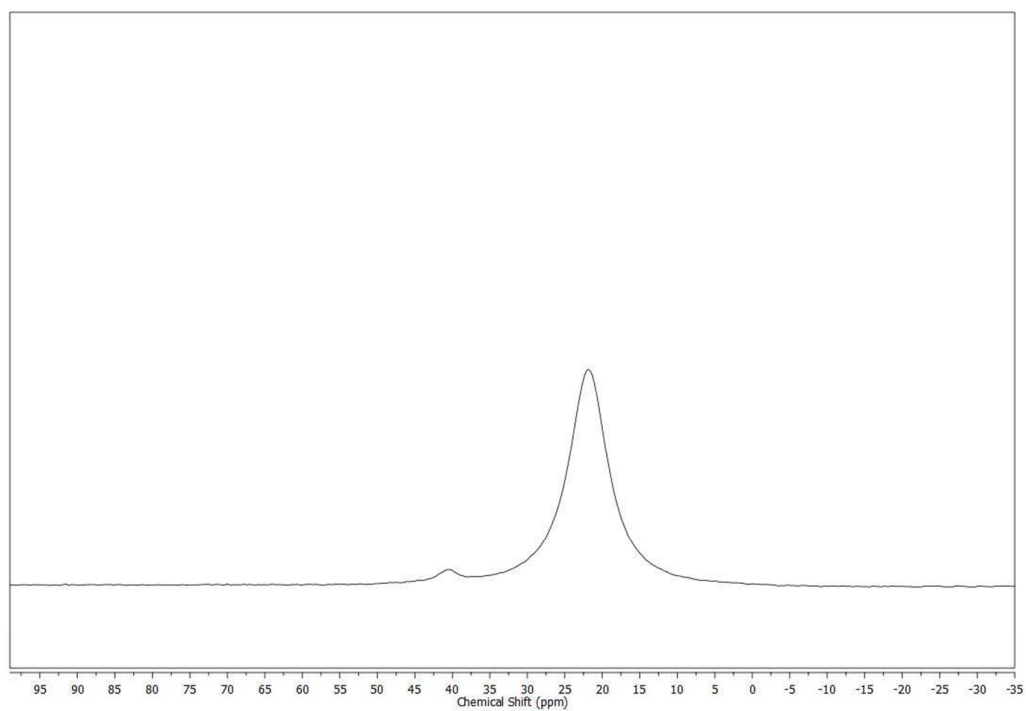


Figure S34 ^{10}B solution NMR spectra of borane **4a** stored in an open vial for 6 days in benzene at 20 °C. The signal around 40 ppm belongs to decomposition products.

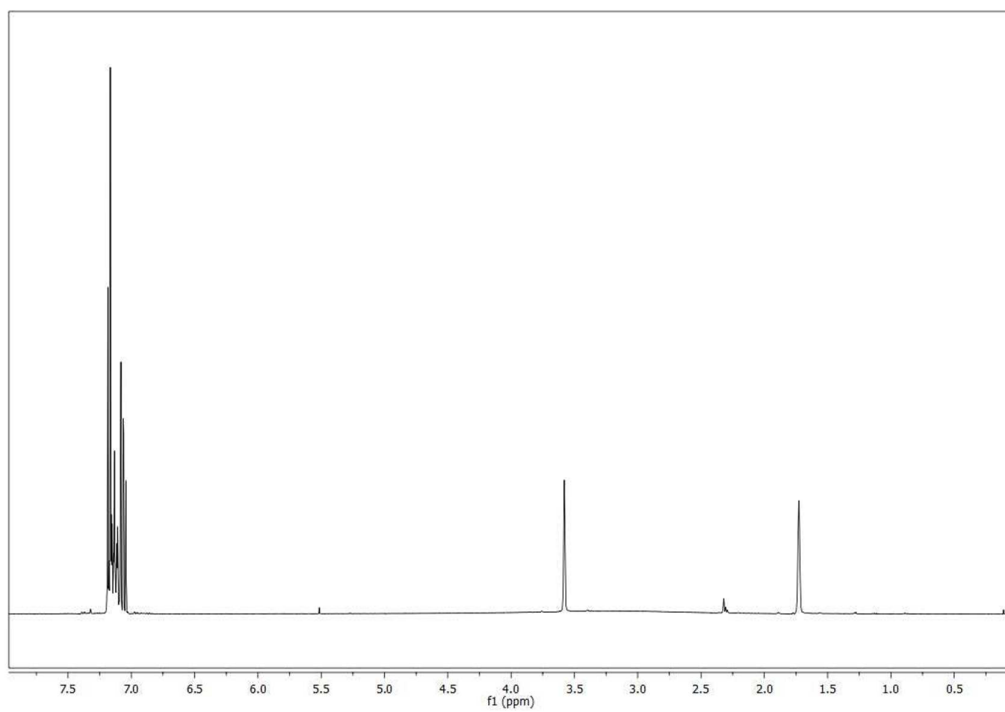


Figure S35 ^1H solution NMR of borane **4a** with 3 equiv. water at 20°C

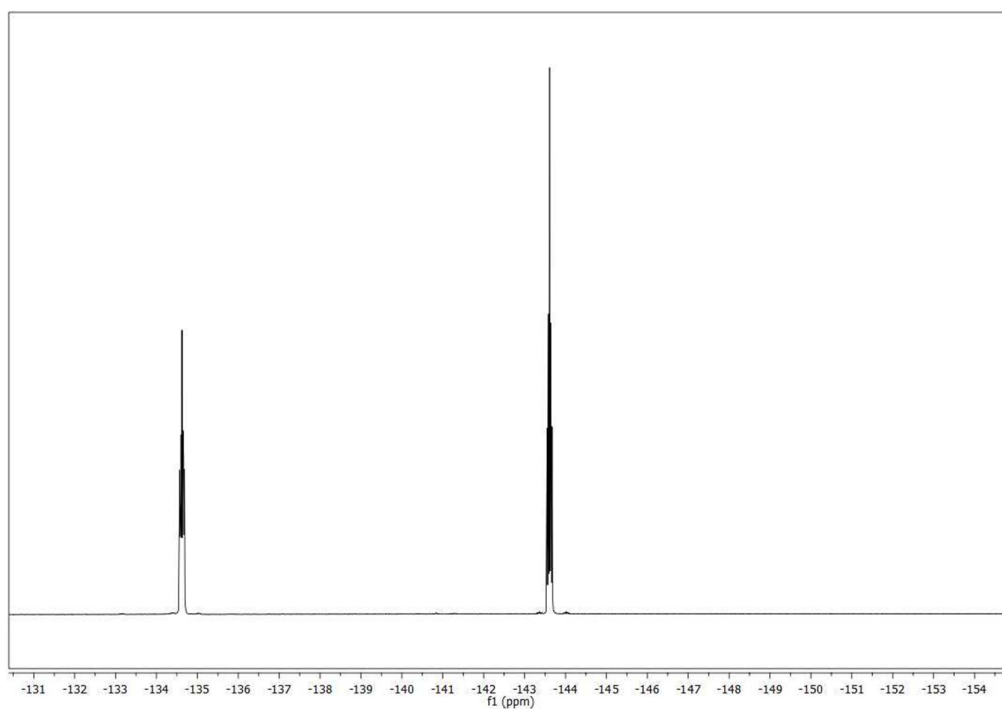


Figure S36 ^{19}F solution NMR of borane **4a** with 3 equiv. water at 20°C

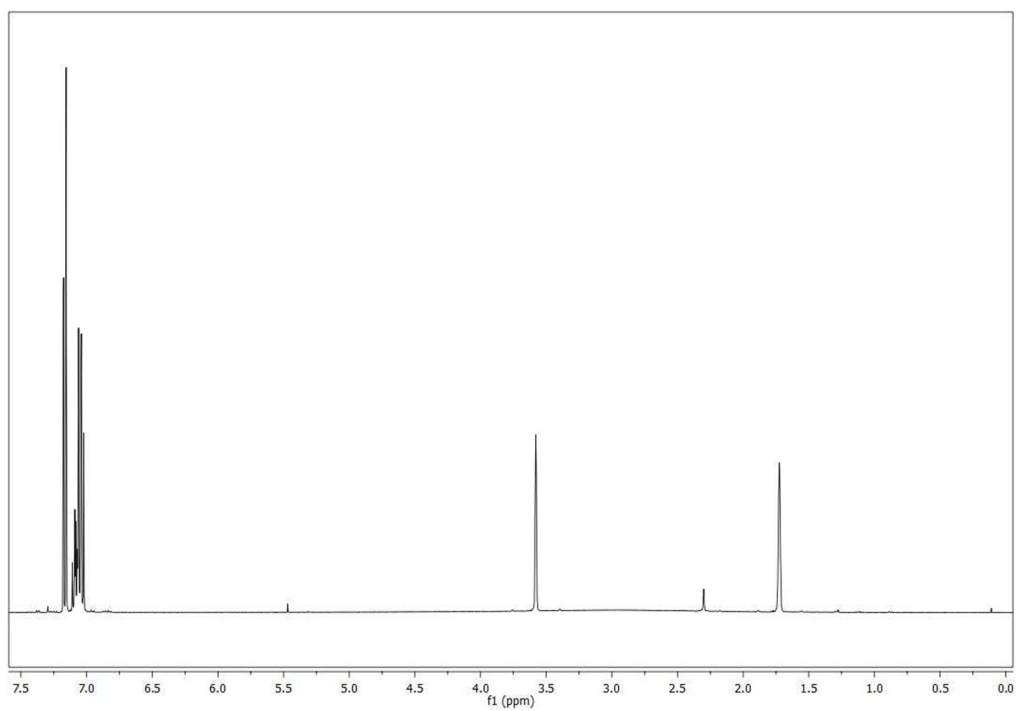


Figure S37 ^1H solution NMR of borane **4a** with 3 equiv. water at 49°C

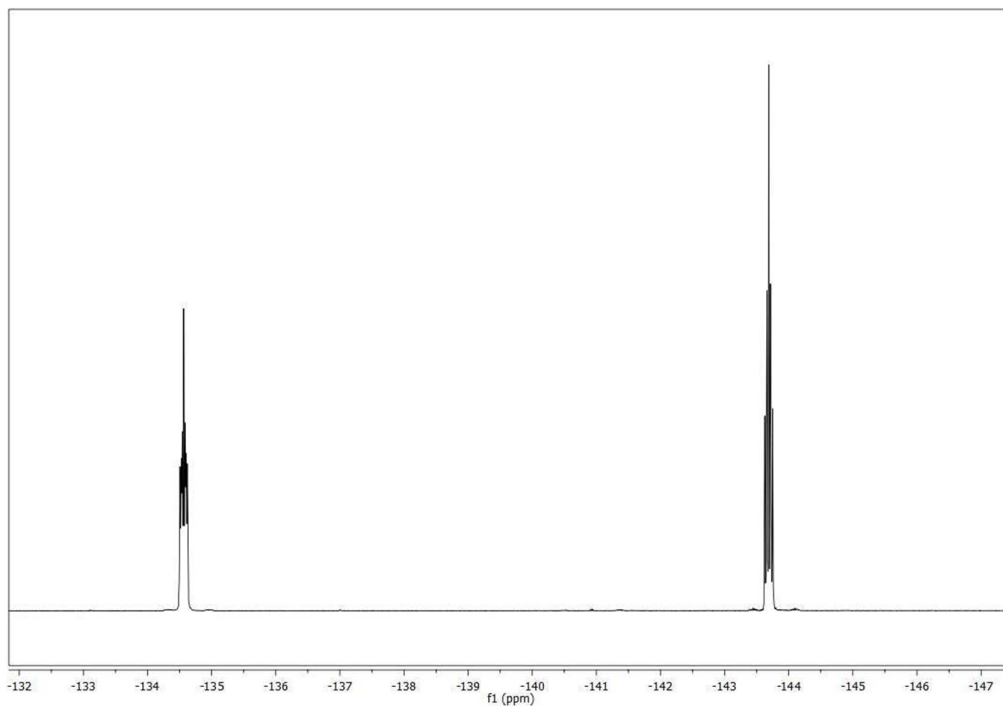


Figure S38 ^{19}F solution NMR of borane **4a** with 3 equiv. water at 49°C

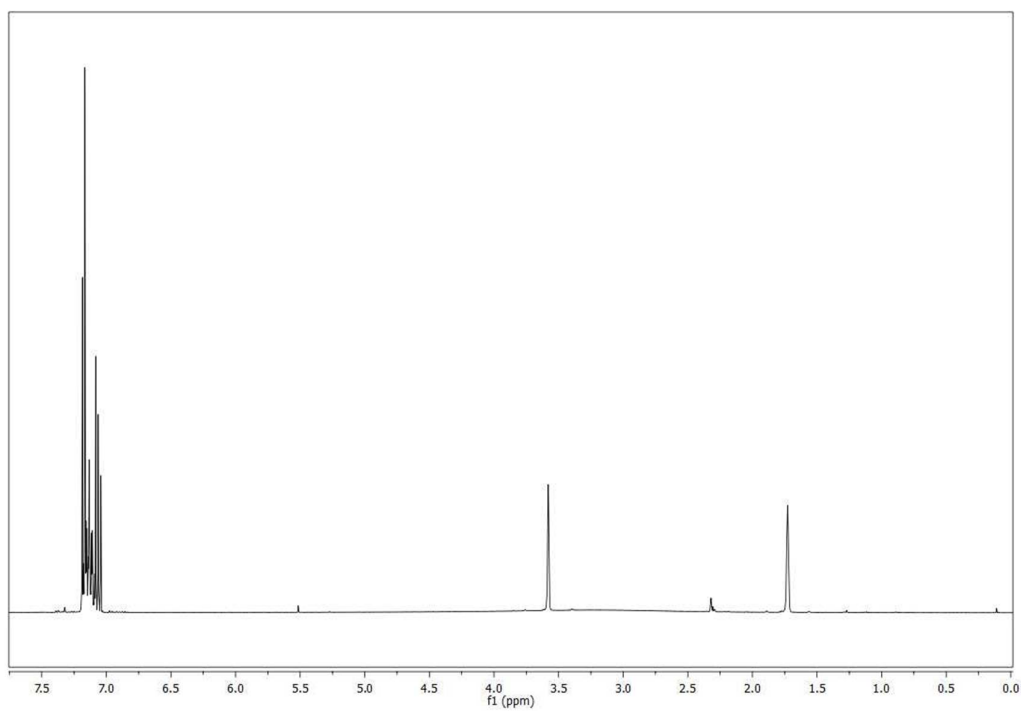


Figure S39 ^1H solution NMR of borane **4a** with 3 equiv. water, after cooled back from 50°C to 20°C

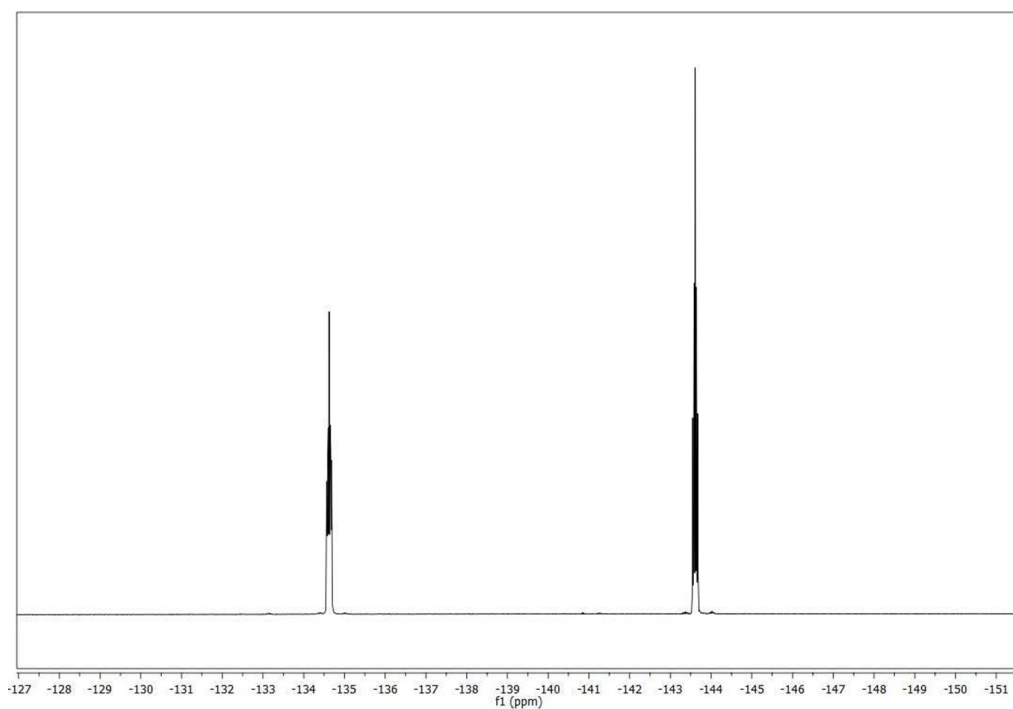


Figure S40 ^{19}F solution NMR of borane **4a** with 3 equiv. water, after cooled back from 50°C to 20°C

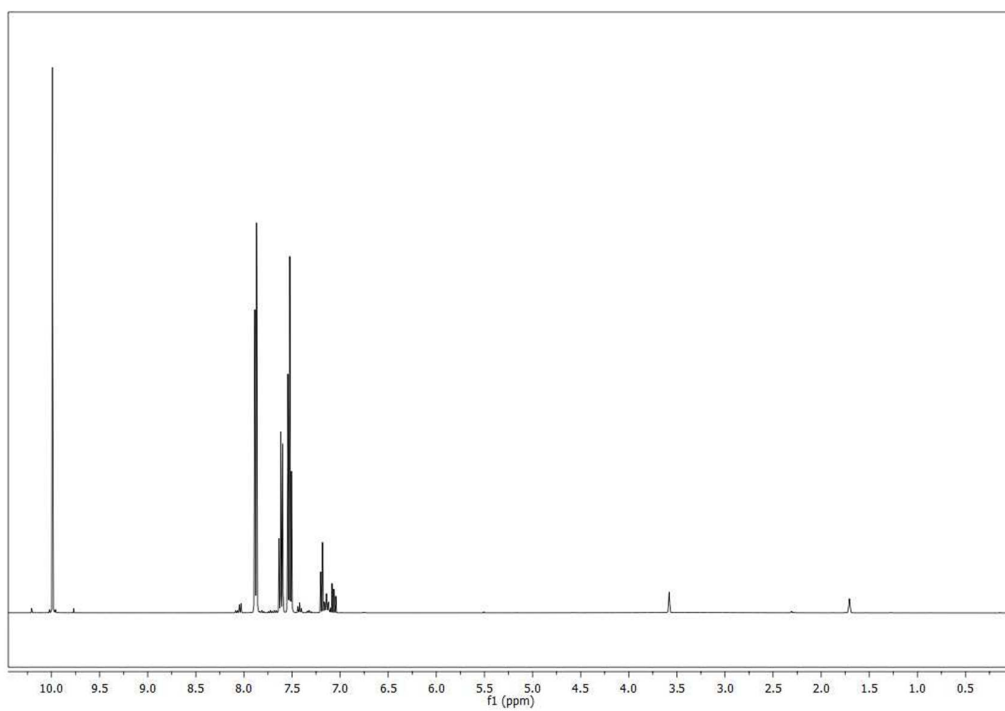


Figure S41 ^1H solution NMR of borane **4a** with 3 equiv. water and 10 equiv. benzaldehyde at 20°C

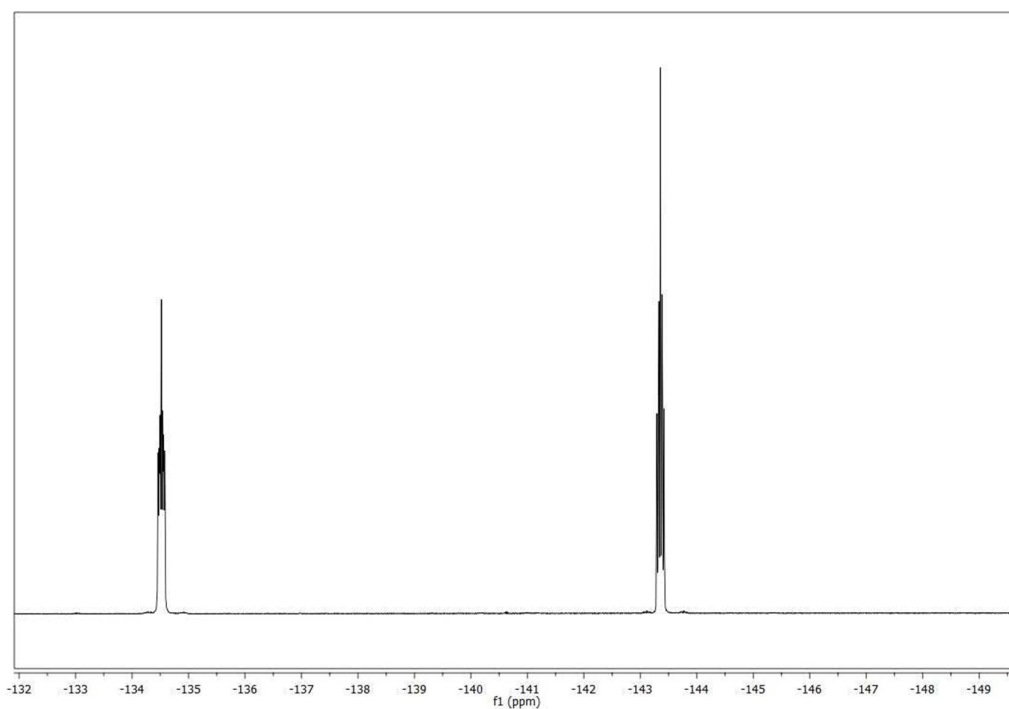


Figure S42 ^{19}F solution NMR of borane **4a** with 3 equiv. water and 10 equiv. benzaldehyde at 20°C

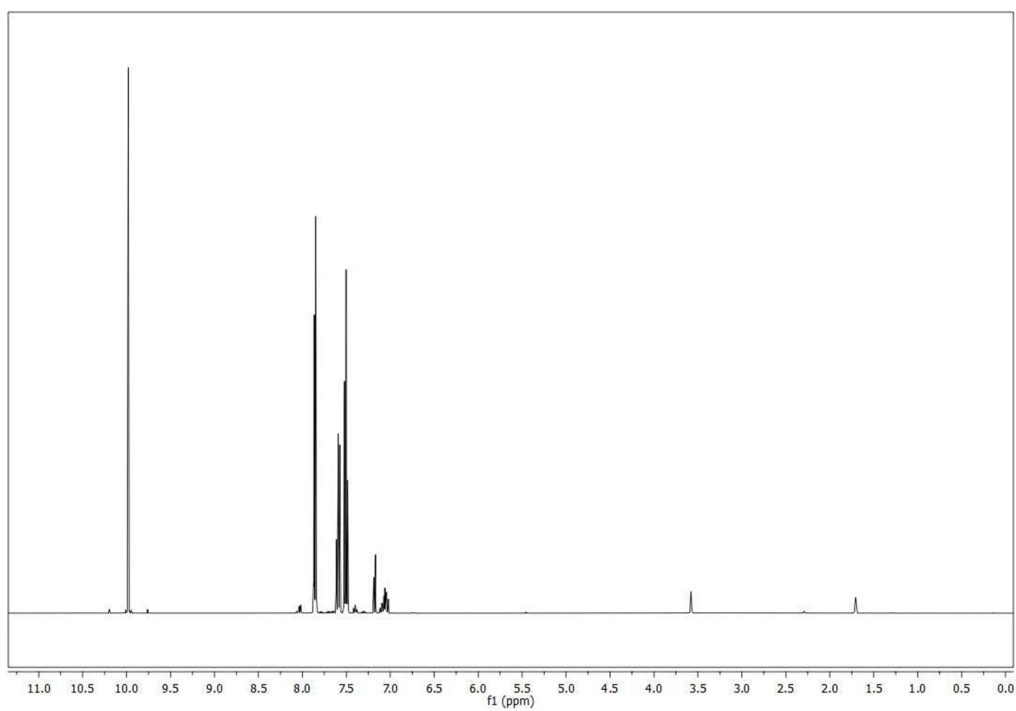


Figure S43 ^1H solution NMR of borane **4a** with 3 equiv. water and 10 equiv. benzaldehyde at 49°C

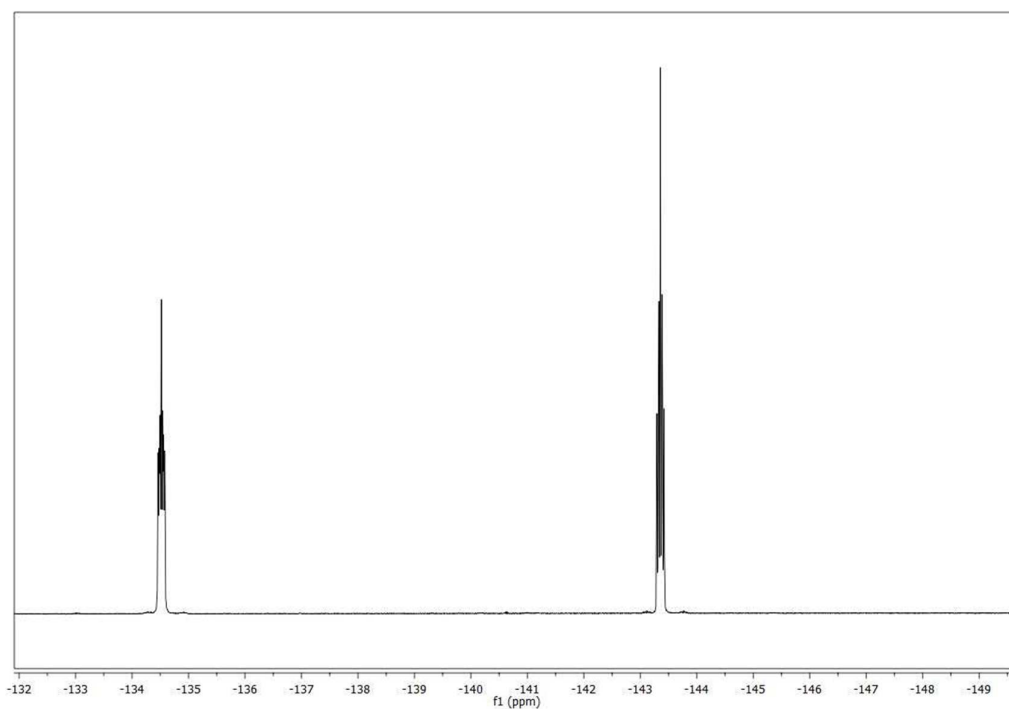


Figure S44 ^{19}F solution NMR of borane **4a** with 3 equiv. water and 10 equiv. benzaldehyde at 49°C

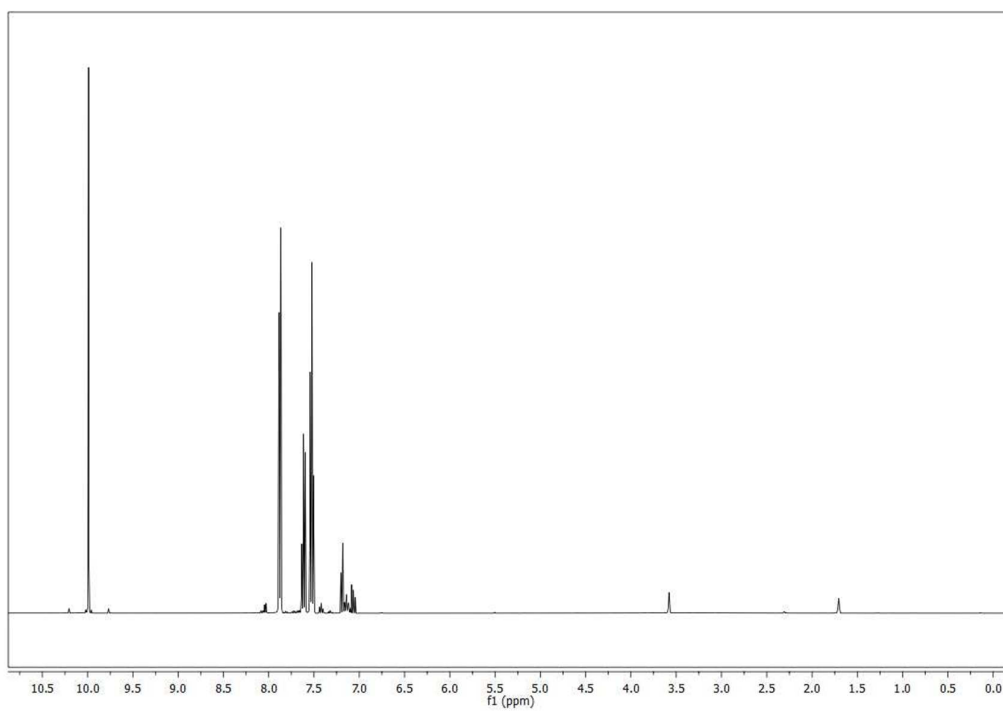


Figure S45 ^1H solution NMR of borane **4a** with 3 equiv. water and 10 equiv. benzaldehyde, after cooled back from 50°C to 20°C

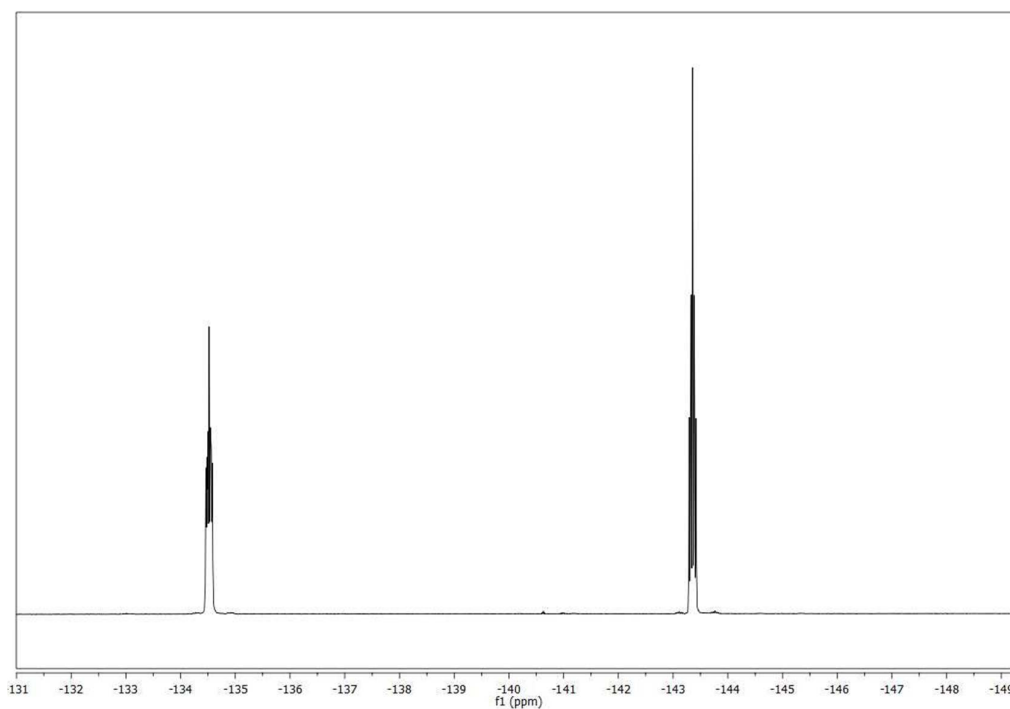


Figure S46 ^{19}F solution NMR of borane **4a** with 3 equiv. water and 10 equiv. benzaldehyde, after cooled back from 50°C to 20°C

Experimental

Solution state boron NMR spectra were performed on a 14.1T (^1H frequency of 600 MHz and 64.4 MHz for ^{10}B) Varian NMR System spectrometer. Direct detection tunable dual-broadband $\{^1\text{H}-^{19}\text{F}\}/\{^31\text{P}-^{15}\text{N}\}$ Chemagnetics probe equipped with Z-gradients was used. Spectra were referenced to $\text{BF}_3\text{-Et}_2\text{O}$ (0ppm) dissolved in CDCl_3 . 5-10 thousand transients were recorded by using 20.25 μs of $\pi/2$ pulse, 2s of relaxation delay and 50 kHz spectral width.

References:

¹ Király, P. *Magnetic Resonance in Chemistry* **2012**, *50*, 620–626.

Computational methodology

The conformational space of the examined species was extensively explored via Monte Carlo sampling using a slightly modified version of the OPLS_2005 force field. The modification concerns the partial atomic charges used to estimate the energy contribution of Coulomb interactions. These parameters were obtained from DFT calculations as electrostatic potential (ESP) derived atomic charges. The conformational analysis was carried out using the *MacroModel* software.¹

The energetically most favored structures were subject to quantum chemical calculations. Density functional theory was used in electronic structure calculations, which were carried out with the dispersion-corrected, range-separated hybrid exchange-correlation functional ω B97X-D² For geometry optimizations, the 6-311G(d,p) basis set was employed, but additional single-point energy calculations were performed for each optimized structure with the larger 6-311++G(3df,3pd) basis set.³ In all DFT calculations the numerical integrations were performed using the ultrafine grid.

Normal coordinate analysis was carried out at the ω B97X-D/6-311G(d,p) level of theory to verify the nature of the stationary points (i.e. minima or first-order saddle points) and to estimate the zero point energies as well as the thermal and entropic contributions to the gas-phase Gibbs free energies. The thermochemical data were computed in terms of the ideal gas – rigid rotor – harmonic oscillator model either for room temperature ($T = 298.15$ K), or for temperature used experimentally in catalytic hydrogenation reactions ($T = 323.15$ K). The free energies were computed for a hypothetical ideal gas with $p = 1$ atm, however, concentration corrections were applied using $c = 1$ mol/dm³ for all reaction components, except for THF, for which the molar concentration of liquid state THF was used (12.2 mol/dm³ at $T = 298.15$ K and 11.9 mol/dm³ at $T = 323.15$ K).

The solvent effects were estimated by means of solvation free energies (solvent = THF) calculated at the ω B97X-D/6-311G(d,p) level for gas-phase optimized geometries. In these calculations, the integral equation formalism polarizable continuum model (IEFPCM) was applied.⁴ The atomic radii and non-electrostatic terms in the IEFPCM calculations were those of the SMD solvation model.⁵

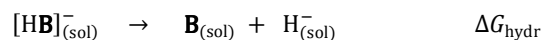
The energetics reported in the paper correspond to solution phase Gibbs free energies, which are obtained from ω B97X-D/6-311++G(3df,3pd) electronic energies and all other contributions computed at the ω B97X-D/6-311G(d,p) level. All DFT calculations were carried out with the *Gaussian 09* software.⁶

Computational Results

In the present computational study, we estimated the hydride affinity of the newly prepared boranes, examined the association (dative bond formation) of borane $B(C_6Cl_2H_3)(C_6F_4H)_2$ with various Lewis bases relevant to this work, and explored the mechanism of catalytic hydrogenation of benzaldehyde (as a representative of carbonyl substrates). Herein, we provide the details of our computational results.

Acidic properties of new boranes

In order to evaluate the Lewis-acidity of the newly synthesized borane species and make comparison with previously used boranes, hydride affinity values were calculated as the Gibbs free energy of hydride detachment defined by the following reaction:



Here, $B_{(sol)}$ denotes the solvated borane species, $[HB]_{(sol)}^-$ the solvated borohydride and $H_{(sol)}^-$ the solvated hydride anion. Standard conditions ($T = 298.15$ K and $c = 1$ mol/dm³) and tetrahydrofuran as a solvent were used for free energy calculations. The results are summarized in Figure S47.

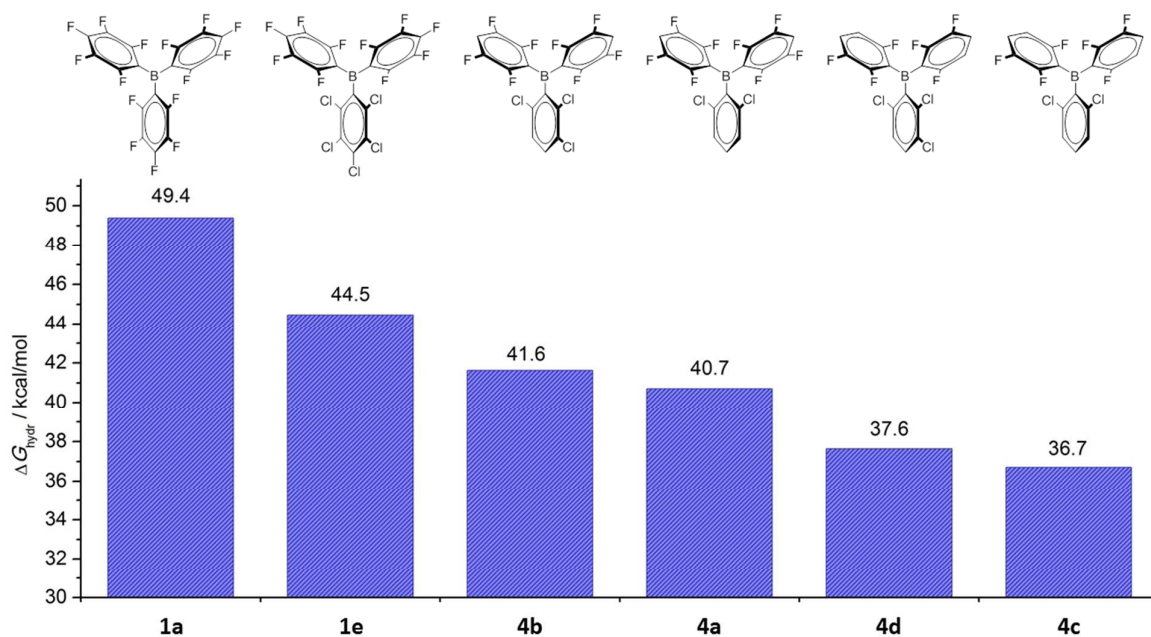


Figure S47 Computed hydride affinities of a series of boranes relevant to this work.

The results reveal a significant reduction of acidity along the $\text{B}(\text{C}_6\text{F}_5)_3 \rightarrow \text{B}(\text{C}_6\text{Cl}_2\text{H}_3)(\text{C}_6\text{F}_3\text{H}_2)_2$ series. As pointed out by Ashley and coworkers, despite the powerful electron-withdrawing property of the C_6Cl_5 group, borane $\text{B}(\text{C}_6\text{Cl}_5)(\text{C}_6\text{F}_5)_2$ (**1e**) is a weaker Lewis acid than the parent compound $\text{B}(\text{C}_6\text{F}_5)_3$ (**1a**), which is due to the increased steric hindrance introduced by *ortho*-Cl substituents.⁷ The effect is notable: the hydride affinity of (**1e**) is found to be about 5 kcal/mol lower than that of (**1a**). Steric effects remain unchanged in the new boranes, therefore one expects a correlation between the Lewis acidity and the number of halogen atoms (i.e. solely electronic effects). This is indeed supported by our results, which show gradual decrease of hydride affinity along the investigated series. The acidity of borane $\text{B}(\text{C}_6\text{Cl}_2\text{H}_3)(\text{C}_6\text{F}_4\text{H})_2$ (**4a**) used for catalytic hydrogenation in our present work is about 3 kcal/mol reduced relative to (**1e**), and further weakening by 4 kcal/mol is found for the last member of the series ($\text{B}(\text{C}_6\text{Cl}_2\text{H}_3)(\text{C}_6\text{F}_3\text{H}_2)_2$).

We note that the optimized structures of (**1e**) and new boranes (and the corresponding borohydrides) are very similar underlying again the invariance of steric properties in this series of boranes. The most stable forms of borane (**4a**) and its hydride are depicted in Figure S48. We mention that the borohydride species have several energetically close lying isomers differing in the orientation of the aryl groups.

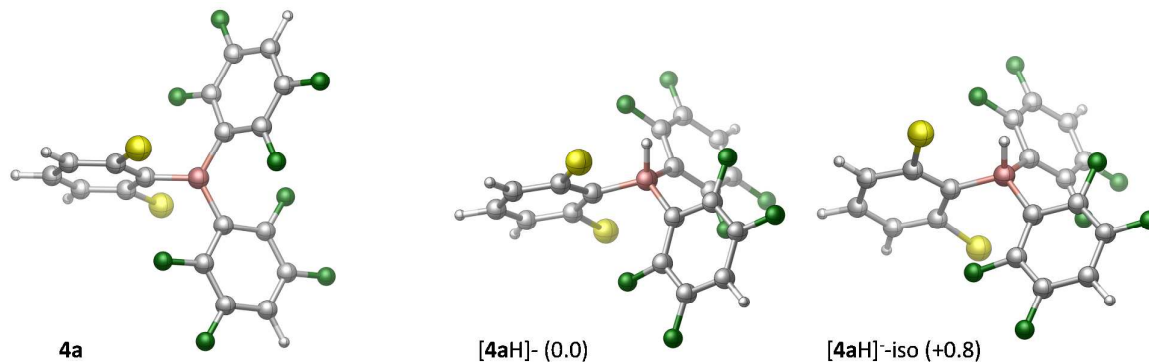


Figure S48 The structure of borane **4a**, and the two most stable forms of the corresponding borohydride (relative stabilities are given in kcal/mol).

Datively bound borane-base complexes

Datively bound 1:1 complexes of borane **4a** with various bases were examined computationally. The bases include the prototype carbonyl substrate benzaldehyde (denoted as **5**), the corresponding alcohol product (**8a**), the solvent molecule (THF), and water. Association of these molecules with more acidic boranes **1e** and **1a** was also considered for comparison. The most stable forms of **4a**-base complexes are shown in Figure S49.⁸ The relative stabilities of these forms along with those of analogous structures for complexes with boranes **1a** and **1e** are reported in Figure S50.

We note first that there are a few indications that the present computational approach underestimates the stability of datively bound species. For instance, the **1e**-THF adduct can be clearly detected by NMR at room temperature,⁹ whereas the calculations predict $\Delta G = +3.1$ kcal/mol for adduct formation in this case (plus sign corresponds to endergonic association). Nevertheless, it is quite likely that the trends obtained for the relative stabilities can be considered as reasonable predictions.

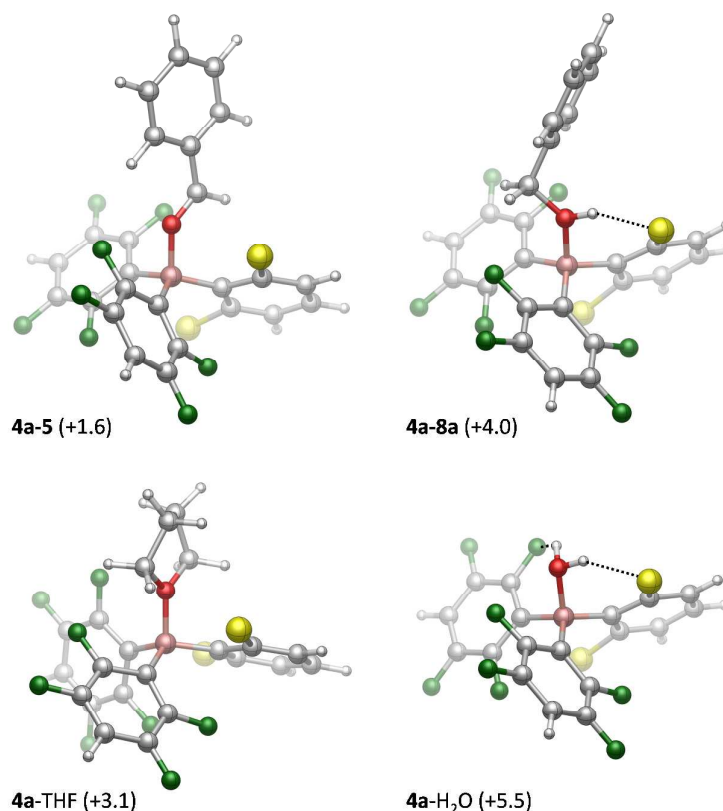


Figure S49 Gibbs free energy of association for various borane/base pairs ($T = 25$ °C, $c = 1$ mol/dm³, solvent = THF).

Figure S50 reveals that sterically hindered boranes **1e** and **4a** form much weaker adducts than the perfluoro compound **1a**, which is in line with previous observations regarding the coordination properties of the $B(C_6Cl_5)_n(C_6F_5)_{3-n}$ ($n = 1-3$) series of boranes.⁷ Among the investigated bases, the aldehyde is found to form the strongest complex with boranes **4a** and **1e**. THF complexes are slightly destabilized, and 1:1 adduct formation with **5** and H₂O is predicted to be even less favored thermodynamically. Interestingly, the relative stabilities **4a-8a/1e-8a** and **4a-H₂O/1e-H₂O** complexes do not reflect the acidic strengths of the two boranes (the more electrophilic borane **1e** would be expected to form stronger dative bonds). This can be associated with the presence of intramolecular OH \cdots Cl and OH \cdots F hydrogen bonds in these complexes (see Figure S49), which become stronger when going from **1e** to **4a**, i.e. by reducing the number of halogen substituents on the phenyl rings.¹⁰

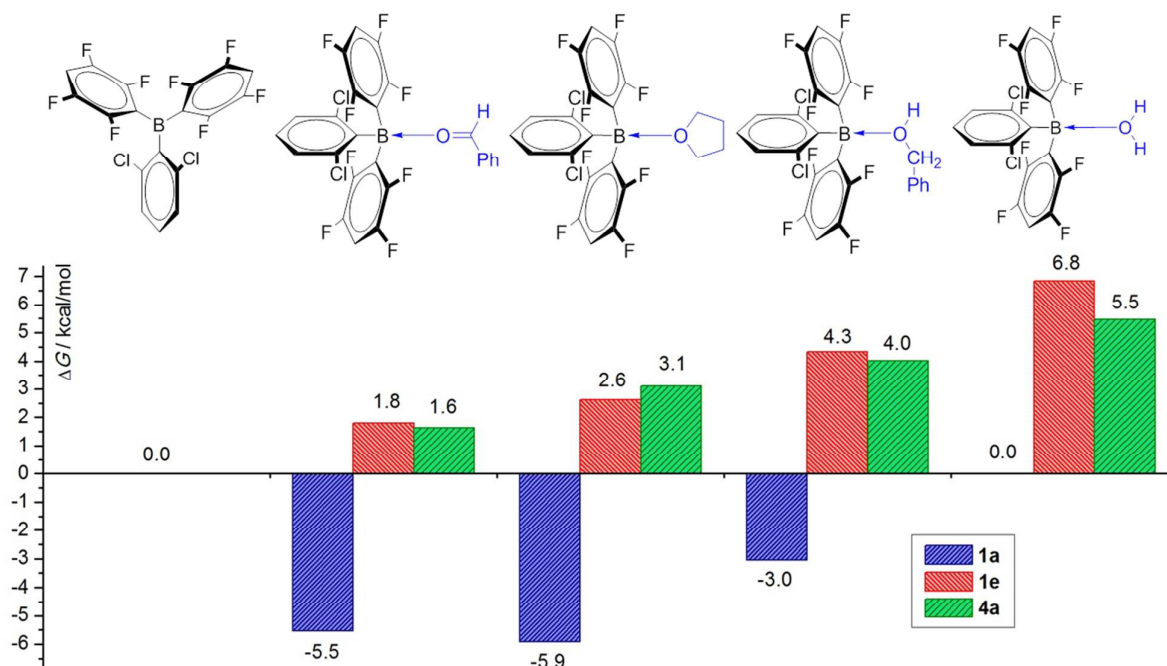


Figure S50 Gibbs free energy of association for various borane/base pairs ($T = 25\text{ }^{\circ}\text{C}$, $c = 1\text{ mol/dm}^3$, solvent = THF).

In light of our experimental findings regarding the existence of datively bound alcohol and water adducts of borane **4a** in THF solutions, the endergonicities predicted for the **4a-8a** and **4a-H₂O** complexes seem surprising. However, considering the enhanced Brønsted acidity of coordinated alcohol and water molecules,¹¹ we anticipate that the explicit treatment of additional solvent (THF) species might be required to characterize properly the stability of these adducts. We have, therefore, carried out calculations for the borane-**8a**(THF), borane-H₂O(THF) and borane-H₂O(THF)₂ complexes, wherein the THF molecules are attached to the original 1:1 complexes via OH...O hydrogen bonds. The optimized structures of these complexes for borane = **4a** are depicted in Figure S51, and the stability data are given in Figures S52 and S53.

The short H...O bond distances found in these adducts are clear indications of strong H-bonding interactions between the OH groups of coordinated base species and the THF molecule. THF association provides extra stabilization for these systems as revealed by the computed Gibbs free energies (see Figure S51). For instance, the **4a-8a**(THF) adduct is stabilized by about 4 kcal/mol (with respect to **4a-8a** + THF), and this effect is further enhanced in **4a-H₂O**(THF) ($\Delta G = -8.4\text{ kcal/mol}$). The association of the second THF molecule to the water adduct is still exergonic (by 2.4 kcal/mol), so the overall stabilization amounts to 10.8 kcal/mol. These results are consistent with previous and our present experimental observations that alcohol and water adducts are remarkably stable in THF (or in other etheric solutions).

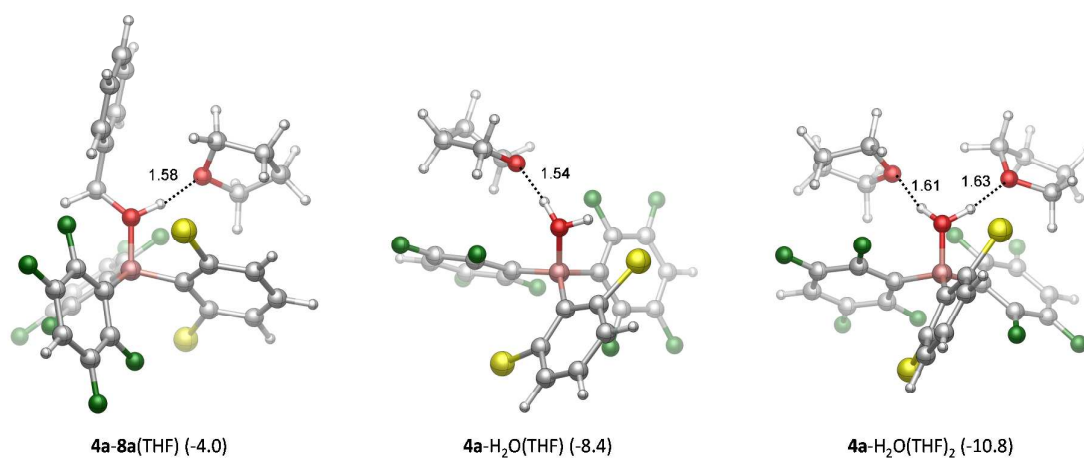


Figure S51 Most stable forms of **4a-8a(THF)**, **4a-H₂O(THF)** and **4a-H₂O(THF)₂** complexes. Gibbs free energy of THF association is indicated in parenthesis (in kcal/mol; for $T = 25\text{ }^{\circ}\text{C}$, $c = 1\text{ mol/dm}^3$, solvent = THF). For **4a-H₂O(THF)₂**, the computed free energy change is relative to **4a-H₂O** + 2THF. Computed O...H bond lengths are given in Å.

The stability of these solvated species of course varies with the nature of the borane (see Figures S52 and S53). As expected, adducts of borane **1a** are extremely stable, whereas those of chlorinated boranes **1e** and **4a** are found to be considerably less stable. Interestingly, we find notable difference in the relative stabilities of THF solvated water adducts of boranes **1e** and **4a** (**4a-H₂O(THF)₂** is 2.7 kcal/mol less stable than **1e-H₂O(THF)₂**) implying that the former borane might be less sensitive to water impurity in catalytic reactions.

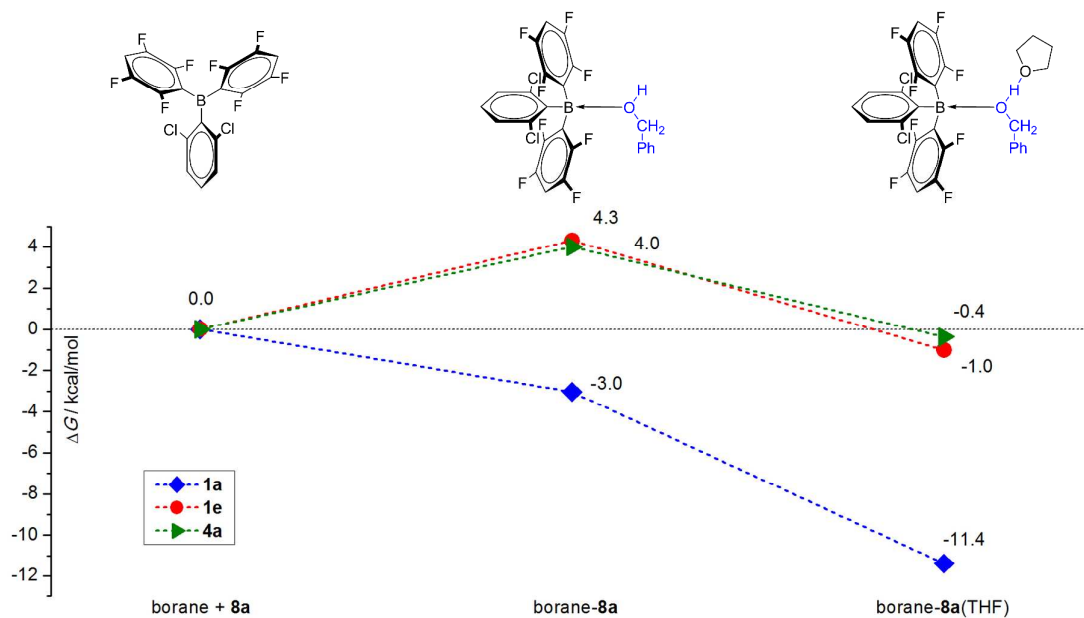


Figure S52 Stabilization effect of H-bonded THF on the **4a-8a** adduct. The reported Gibbs free energies are relative to dissociation limits (borane + **8a** and borane + **8a** + THF, respectively).

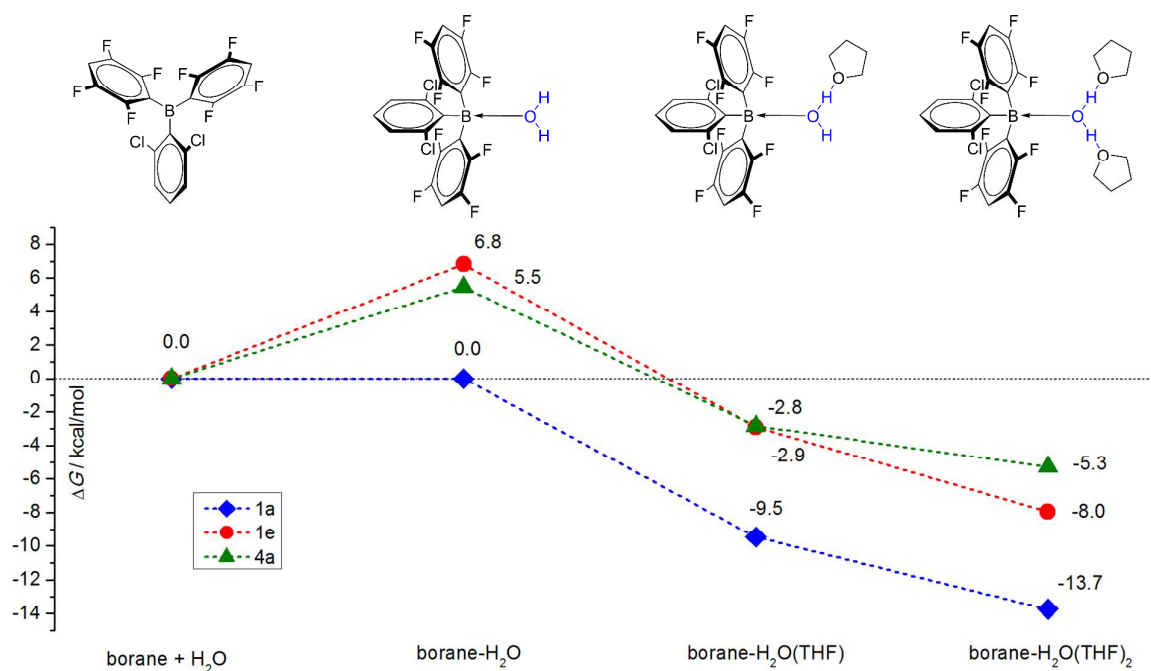


Figure S53 Stabilization effect of H-bonded THF on the **4a**-H₂O adduct. The reported Gibbs free energies are relative to dissociation limits (borane + H₂O, borane + H₂O + THF and borane + H₂O + 2THF respectively).

On the mechanism of catalytic hydrogenation

The mechanism of catalytic hydrogenation of carbonyl compounds using borane **4a** was investigated computationally. In these calculations, benzaldehyde was used as a prototype substrate and we aimed to identify and characterize the main elementary steps of the catalytic cycle.

The envisioned catalytic cycle is initiated by heterolytic H₂ splitting, which may occur via two alternative pathways corresponding to H₂ activation by the **4a**/THF and **4a**/**5** pairs. Transition states located for the two scenarios are depicted in Figure S54. According to the computed free energies, H₂ activation by **4a**/THF is clearly favored kinetically.¹²

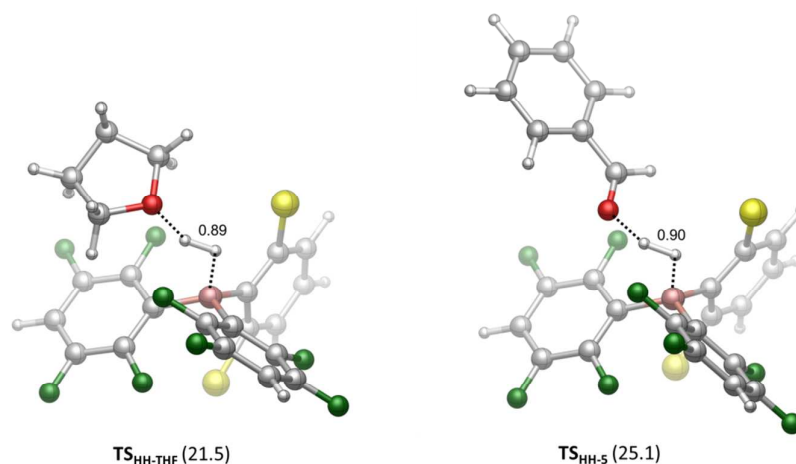


Figure S54 Transition states of heterolytic H_2 splitting by **4a**/THF and **4a**/**5** pairs. Relative Gibbs free energies are given in parenthesis (in kcal/mol; with respect to **4a** + **5** + THF + H_2 reactants; for $T = 50^\circ\text{C}$). Computed H-H bond lengths are given in Å.

The product state of transition state $\text{TS}_{\text{HH-THF}}$ corresponds to the $[\mathbf{4aH}][\text{THF-H}]^+$ ion pair lying at 16.0 kcal/mol in free energy (see Figure S55). This intermediate can be stabilized considerably by association of an additional solvent molecule yielding the $[\mathbf{4aH}][\text{THF-H-THF}]^+$ species. In this ion pair, the proton is solvated by two THF molecules via strong H-bonds, nevertheless, the H_2 splitting step remains rather endergonic.

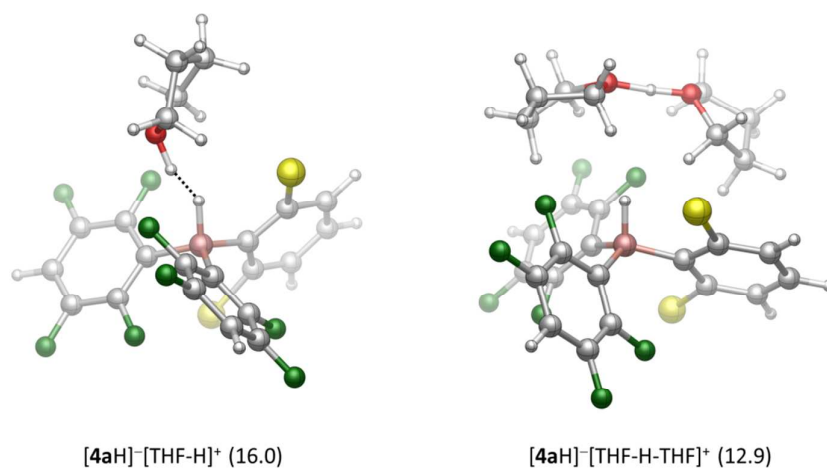


Figure S55 Intermediates $[\mathbf{4aH}][\text{THF-H}]^+$ and $[\mathbf{4aH}][\text{THF-H-THF}]^+$.

The substrate molecule can similarly associate with $[\mathbf{4aH}][\text{THF-H}]^+$ resulting in the $[\mathbf{4aH}][\text{THF-H-5}]^+$ ion pair (see Figure S56). This step corresponds to substrate activation and it occurs via transition state TS_{act} lying at 22.0 kcal/mol.¹³ The $[\mathbf{4aH}][\text{THF-H-5}]^+$ intermediate involves a highly electrophilic substrate as the proton is shifted to the carbonyl oxygen. Consequently, hydride transfer from $[\mathbf{4aH}]^-$ can easily occur (see TS_{hydr} in Figure S56) yielding the alcohol product (**8a**) and regenerating the borane. The free energy of transition state TS_{hydr} is predicted to be 21.1 kcal/mol.

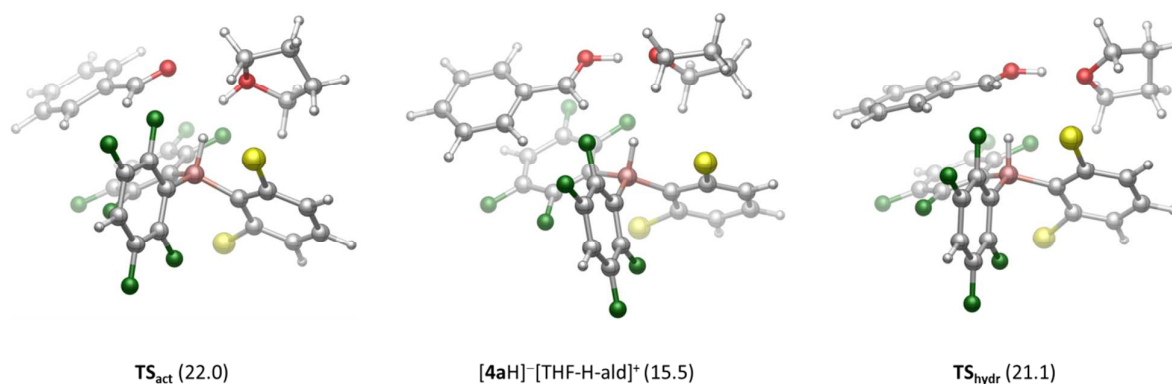


Figure S56 Substrate activation and hydride transfer steps of the catalytic cycle.

The free energy diagram of the entire catalytic cycle is shown in Figure S57. It is apparent that the transition states associated with the three basic steps of the cycle (H_2 cleavage, substrate activation and hydride transfer) are found to have very similar free energies, therefore none of these steps can be identified as rate-determining in the catalytic process. Our results, however, provide solid support for the mechanism proposed previously by Stephan and Ashley, which considers the borane/ether pair to induce H_2 splitting and Brønsted acid activation of the substrate.

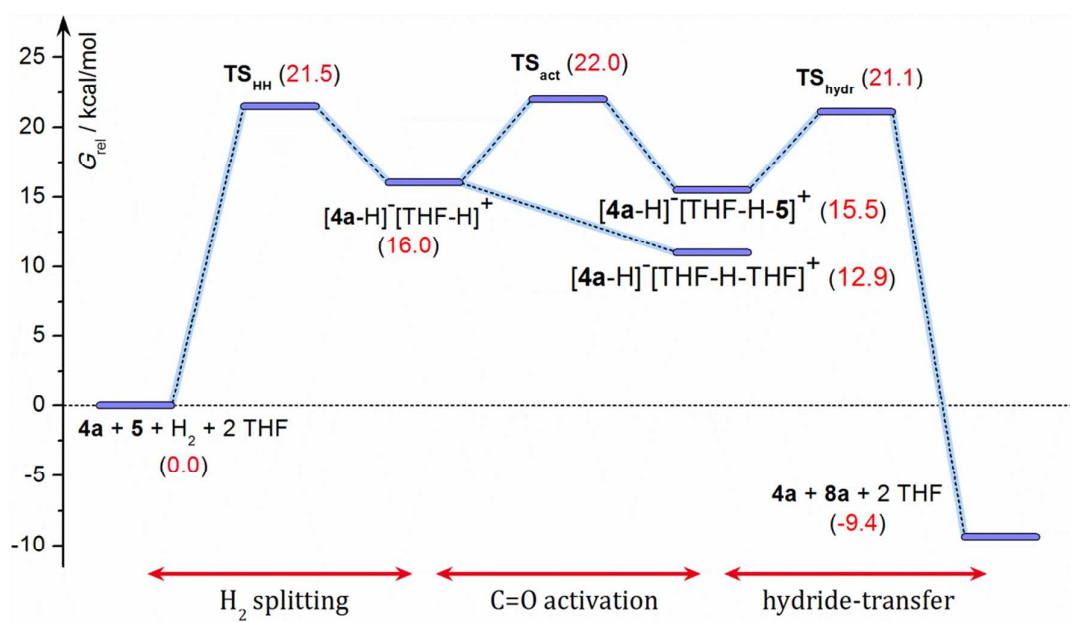


Figure S35 Gibbs free energy diagram computed for the entire catalytic cycle.

Total energy data of the calculated structures

The energy data computed for the ω B97XD/6-311G(d,p) optimized geometries of the structures discussed in the manuscript and the Supporting Information are listed in Table S1.

Table S1: Energy data (in a.u. at $T = 298.15$ K) computed for ω B97XD/6-311G(d,p) optimized structures.^a

structures	E_0	E_0'	$G_{298.15\text{ K}}^0$	$G_{\text{THF}}^{\text{sol}}$	$G_{\text{THF}, 298.15\text{ K}}^0$
5	-345.5355	-345.5649	-345.4553	-345.5471	-345.4933
8a	-346.7426	-346.7749	-346.6419	-346.7549	-346.6834
THF ^b	-232.4378	-232.4599	-232.3485	-232.4443	-232.3718
H ₂ O	-76.4234	-76.4383	-76.4192	-76.4299	-76.4377
1a	-2208.2096	-2208.4145	-2208.1131	-2208.2150	-2208.3205
[1aH] ⁻	-2208.9226	-2209.1292	-2208.8205	-2208.9659	-2209.0675
1e	-4010.0559	-4010.2496	-4009.9712	-4010.0665	-4010.1726
[1eH] ⁻	-4010.7657	-4010.9582	-4010.6743	-4010.8137	-4010.9118
4b	-2892.4173	-2892.5729	-2892.2920	-2892.4327	-2892.4600
[4bH] ⁻	-2893.1154	-2893.2715	-2892.9827	-2893.1743	-2893.1947
4a	-2432.8170	-2432.9649	-2432.6796	-2432.8322	-2432.8398
[4aH] ⁻	-2433.5109	-2433.6599	-2433.3662	-2433.5716	-2433.5730
[4aH] ⁻ iso	-2433.5107	-2433.6595	-2433.3653	-2433.5715	-2433.5717
4d	-2693.9610	-2694.0959	-2693.8174	-2693.9788	-2693.9672
[4dH] ⁻	-2694.6487	-2694.7844	-2694.4979	-2694.7137	-2694.6955
4c	-2234.3604	-2234.4877	-2234.2052	-2234.3781	-2234.3471
[4cH] ⁻	-2235.0437	-2235.1724	-2234.8812	-2235.1108	-2235.0740
1a-5	-2553.7773	-2554.0081	-2553.5774	-2553.7947	-2553.8227
1a-THF	-2440.6841	-2440.9040	-2440.4709	-2440.6982	-2440.7017
1a-8a	-2554.9942	-2555.2226	-2554.7681	-2555.0094	-2555.0087
1a-H₂O	-2284.6655	-2284.8746	-2284.5432	-2284.6744	-2284.7582
1e-5	-4355.6128	-4355.8324	-4355.4238	-4355.6355	-4355.6631
1e-THF	-4242.5170	-4242.7255	-4242.3158	-4242.5360	-4242.5402
1e-8a	-4356.8234	-4357.0426	-4356.6130	-4356.8433	-4356.8491
1e-H₂O	-4086.5006	-4086.6999	-4086.3892	-4086.5145	-4086.5995
4a-5	-2778.3751	-2778.5491	-2778.1330	-2778.4016	-2778.3305
4a-THF	-2665.2802	-2665.4430	-2665.0250	-2665.3019	-2665.2066
4a-8a	-2779.5861	-2779.7597	-2779.3226	-2779.6097	-2779.5168
4a-H₂O	-2509.2649	-2509.4186	-2509.1005	-2509.2825	-2509.2687
1a-8a(THF)	-2787.4715	-2787.7166	-2787.1322	-2787.4911	-2787.3938
1e-8a(THF)	-4589.3027	-4589.5384	-4588.9744	-4589.3251	-4589.2294
4a-8a(THF)	-3012.0631	-3012.2532	-3011.6824	-3012.0892	-3011.8955
1a-H₂O(THF)	-2517.1438	-2517.3706	-2516.9084	-2517.1566	-2517.1451
1e-H₂O(THF)	-4318.9765	-4319.1931	-4318.7547	-4318.9949	-4318.9867
4a-H₂O(THF)	-2741.7391	-2741.9097	-2741.4646	-2741.7607	-2741.6538
1a-H₂O(THF)₂	-2749.6097	-2749.8545	-2749.2642	-2749.6274	-2749.5236
1e-H₂O(THF)₂	-4551.4455	-4551.6796	-4551.1120	-4551.4690	-4551.3666
4a-H₂O(THF)₂	-2974.2095	-2974.3959	-2973.8207	-2974.2349	-2974.0294

^a Notation: E_0 and E_0' refer to electronic energies computed at ω B97XD/6-311G(d,p) and ω B97XD/6-311++G(3df,3pd) level of DFT; G^0 and G_{sol}^0 denote gas-phase and solution-phase Gibbs free energies obtained from ω B97XD/6-311G(d,p) calculations (sol = THF, $T = 298.15$ K). The last column is obtained as $G_{\text{sol}}^0 = E_0' + (G^0 - E_0) + (G_{\text{sol}}^0 - E_0) + \Delta G_{\text{conc}}$. The relative stabilities (at $T = 298.15$ K) discussed in the manuscript and in the SI are obtained from these values. The value ΔG_{conc} corresponds to concentration correction to the free energy when switching from $p = 1$ atm (ideal gas standard state) to $c = 1$ mol/dm³ (standard concentration in solution phase, where $\Delta G_{\text{conc}} = 0.00302$ a.u.).

^b In case of THF the value ΔG_{conc} corresponds to concentration correction to the free energy when switching from $p = 1$ atm (ideal gas standard state) to $c = 12.2$ mol/dm³ (estimated concentration in liquid phase, where $\Delta G_{\text{conc}} = 0.00538$ a.u.).

Table S2: Energy data (in a.u. at $T = 323.15$ K) computed for ω B97XD/6-311G(d,p) optimized structures.^a

structures	E_0	E_0'	$G_{323.15\text{ K}}^0$	$G_{\text{THF}}^{\text{soliv}}$	$G_{\text{THF}, 323.15\text{ K}}^0$
5	-345.5355	-345.5649	-345.4584	-345.5471	-345.4962
THF ^b	-232.4378	-232.4599	-232.3513	-232.4443	-232.3742
TS _{HH-THF}	-2666.4365	-2666.6008	-2666.1786	-2666.4587	-2666.3618
TS _{HH-5}	-2779.5230	-2779.6980	-2779.2782	-2779.5511	-2779.4781
[4aH][THF-H] ⁺	-2666.4376	-2666.6030	-2666.1780	-2666.4680	-2666.3705
[4aH][THF-H-THF] ⁺	-2898.9117	-2899.0922	-2898.5396	-2898.9447	-2898.7497
[4aH]-[THF-H-5] ⁺	-3012.0111	-3012.2023	-3011.6466	-3012.0440	-3011.8676
TS _{act}	-3011.9989	-3012.1901	-3011.6346	-3012.0337	-3011.8573
TS _{hydr}	-3012.0051	-3012.1962	-3011.6387	-3012.0373	-3011.8587
8a	-346.7426	-346.7749	-346.6454	-346.7549	-346.6866
H ₂	-1.1761	-1.1766	-1.1787	-1.1756	-1.1755

^a Notation: E_0 and E_0' refer to electronic energies computed at ω B97XD/6-311G(d,p) and ω B97XD/6-311++G(3df,3pd) level of DFT; G^0 and G_{sol}^0 denote gas-phase and solution-phase Gibbs free energies obtained from ω B97XD/6-311G(d,p) calculations (sol = THF, $T = 298.15$ K). The last column is obtained as $G_{\text{sol}}^0 = E_0' + (G^0 - E_0) + (G_{\text{sol}}^0 - E_0) + \Delta G_{\text{conc}}$. The relative stabilities (at $T = 323.15$ K) discussed in the manuscript and in the SI are obtained from these values. The value ΔG_{conc} corresponds to concentration correction to the free energy when switching from $p = 1$ atm to $c = 1$ mol/dm³ (where $\Delta G_{\text{conc}} = 0.00327$ a.u.).

^b In case of THF the value ΔG_{conc} corresponds to concentration correction to the free energy when switching from $p = 1$ atm to $c = 11.9$ mol/dm³ (estimated concentration in liquid phase, where $\Delta G_{\text{conc}} = 0.00580$ a.u.).

References:

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- ² a) Chai, J.-D.; Head-Gordon, M., *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620; b) Chai, J.-D.; Head-Gordon, M. *J. Chem. Phys.* **2008**, *128*, 084106; c) Grimme, S. *J. Comput. Chem.* **2006**, *27*, 1787-1799.
- ³ For the 6-311G(d,p) and 6-311++G(3df,3pd) basis sets, see: a) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650-654; b) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* **1980**, *72*, 5639-5648. c) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. v. R. *J. Comp. Chem.* **1983**, *4*, 294-301; d) Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984**, *80*, 3265-3269.
- ⁴ Tomasi, J.; Mennucci, B.; Cancès, E. *J. Mol. Struct. (Theochem)* **1999**, *464*, 211-226.
- ⁵ Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378-6396.
- ⁶ *Gaussian 09, Revision A.02*, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.J.; Heyd, J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.
- ⁷ Ashley, A. E.; Herrington, T. J.; Wildgoose, G. G.; Zaher, H.; Thompson, A. L.; Rees, N. H.; Krämar, T.; O'Hare, D. *J. Am. Chem. Soc.* **2011**, *133*, 14727-14740.

⁸ In addition to the reported structures, several low-lying isomeric forms of these complexes differing in the relative orientation of acid/base partners could be identified computationally, however, they are not discussed here.

⁹ See: Scott, D. J.; Fuchter, M. J.; Ashley, A. E. *Angew. Chem. Int. Ed.* **2014**, *53*, 10218-10386.

¹⁰ The electron density of Cl and F substituents involved in H-bond is higher in **4a** as compared to those in **1e**.

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¹² The computed Gibbs free energies corresponds to $T = 323.15$ K, $c = 1$ mol/dm³ for reaction components, $c_{\text{THF}} = 11.9$ mol/dm³.

¹³ An alternative substrate activation pathway involving an THF \leftrightarrow **5** exchange in the dissociated form of the [THF-H-THF]⁺ species was also examined, but it was found to be less favored kinetically

Cartesian coordinates of the calculated structures

Cartesian coordinates of ω B97XD/6-311G(d,p) optimized geometries are given below in standard XYZ format (units are in Å). First line indicates total number of atoms, second line is molecule name (as defined above, see also Table S1).

14

5

C	1.989893	0.464961	0.000023
O	2.832437	-0.394446	-0.000036
C	0.529305	0.211975	0.000011
C	-0.358059	1.285438	-0.000003
C	0.043764	-1.096290	0.000016
C	-1.727818	1.056715	-0.000010
H	0.027245	2.300832	-0.000007
C	-1.322311	-1.324054	0.000005
H	0.755013	-1.914240	0.000027
C	-2.207256	-0.247733	-0.000007
H	-2.419752	1.890716	-0.000020
H	-1.703850	-2.338495	0.000007
H	-3.276249	-0.429004	-0.000015
H	2.272983	1.539690	0.000096

16

8a

C	-0.518288	-1.293649	0.000916
C	-1.873236	-0.996561	0.002079
C	-2.295088	0.329184	0.001041
C	-1.351937	1.347528	-0.001227
C	0.007039	1.049503	-0.002733
C	0.432527	-0.273563	-0.001772
H	-0.194663	-2.330914	0.002214
H	-2.602014	-1.799473	0.004153
H	-3.353441	0.564129	0.002201
H	-1.672741	2.383462	-0.001770
H	0.746723	1.839461	-0.004286
C	1.898486	-0.629476	-0.005021
H	2.109839	-1.235174	-0.898477
H	2.109308	-1.254941	0.874788
O	2.682100	0.543516	0.008104
H	3.603176	0.287529	-0.003355

13

THF

C	1.158015	0.428657	-0.134003
O	0.000008	1.243623	-0.000004

C	-1.158008	0.428672	0.134008
C	-0.728773	-0.990837	-0.231338
C	0.728757	-0.990849	0.231336
H	1.517675	0.472767	-1.170849
H	1.942670	0.820941	0.518019
H	-1.517655	0.472782	1.170859
H	-1.942666	0.820967	-0.518004
H	-1.340029	-1.754971	0.251595
H	-0.781897	-1.140163	-1.313898
H	0.781880	-1.140182	1.313895
H	1.340003	-1.754988	-0.251601

3

H₂O

O	0.000000	0.000000	0.117661
H	0.000000	0.754832	-0.470644
H	0.000000	-0.754832	-0.470644

34

1a

B	0.000000	0.000000	0.000002
C	0.000000	0.000000	1.564862
C	-0.758890	-0.908030	2.301102
C	0.758890	0.908030	2.301102
C	-0.778400	-0.915660	3.684242
C	0.778400	0.915660	3.684242
C	0.000000	0.000000	4.376462
C	0.000000	1.355210	-0.782428
C	0.758890	1.538800	-1.936928
C	-0.758890	2.446830	-0.364178
C	0.778400	2.732820	-2.635108
C	-0.778400	3.648480	-1.049128
C	0.000000	3.790130	-2.188228
C	0.000000	-1.355210	-0.782428
C	0.758890	-2.446830	-0.364178
C	-0.758890	-1.538800	-1.936928
C	0.778400	-3.648480	-1.049128
C	-0.778400	-2.732820	-2.635108
C	0.000000	-3.790130	-2.188228
F	1.530280	1.798950	1.676632
F	1.527740	1.783970	4.350952
F	0.000000	0.000000	5.698182
F	-1.527740	-1.783970	4.350952
F	-1.530280	-1.798950	1.676632
F	1.530280	-2.351480	0.719622
F	1.527740	-4.660020	-0.630518
F	0.000000	-4.934770	-2.849088

F	-1.527740	-2.876050	-3.720438
F	-1.530280	-0.552530	-2.396258
F	1.530280	0.552530	-2.396258
F	1.527740	2.876050	-3.720438
F	0.000000	4.934770	-2.849088
F	-1.527740	4.660020	-0.630518
F	-1.530280	2.351480	0.719622

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[1aH]⁻

B	0.000000	0.000000	0.817733
C	-0.021449	1.570986	0.365573
C	0.730565	2.493807	1.082130
C	-0.749366	2.106249	-0.687261
C	0.755167	3.850495	0.798605
C	-0.757816	3.457099	-1.003572
C	0.000000	4.337595	-0.253455
C	1.371238	-0.766918	0.365573
C	2.198748	-0.404155	-0.687261
C	1.794418	-1.879591	1.082130
C	3.372844	-1.072262	-1.003572
C	2.957043	-2.579242	0.798605
C	3.756467	-2.168798	-0.253455
C	-1.349790	-0.804068	0.365573
C	-2.524983	-0.614216	1.082130
C	-1.449383	-1.702094	-0.687261
C	-3.712210	-1.271254	0.798605
C	-2.615028	-2.384838	-1.003572
C	-3.756467	-2.168798	-0.253455
F	-0.397633	-1.944755	-1.486174
F	-2.653172	-3.243147	-2.030847
F	-4.891063	-2.815436	-0.544602
F	-4.814942	-1.051420	1.526593
F	-2.558718	0.250144	2.107200
F	1.883024	0.628017	-1.486174
F	4.135233	-0.676141	-2.030847
F	1.495990	2.090843	2.107200
F	4.883771	-2.828067	-0.544602
F	1.062728	-2.340987	2.107200
F	3.318028	-3.644152	1.526593
F	-1.482062	3.919287	-2.030847
F	0.007292	5.643503	-0.544602
F	1.496914	4.695573	1.526593
F	-1.485391	1.316738	-1.486174
H	0.000000	0.000000	2.026420

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1e

B	0.000000	0.000000	-0.560913
C	0.000000	0.000000	1.020126
C	1.163940	-0.248986	1.732273
C	-1.163940	0.248986	1.732273
C	1.185211	-0.256131	3.124909
C	-1.185211	0.256131	3.124909
C	0.000000	0.000000	3.822126
C	-0.659394	-1.201996	-1.311219
C	-1.358355	-1.028083	-2.507322
C	-0.645334	-2.497091	-0.791678
C	-2.001377	-2.066176	-3.154769
C	-1.263376	-3.561890	-1.424892
C	-1.947203	-3.341157	-2.609990
C	0.659394	1.201996	-1.311219
C	0.645334	2.497091	-0.791678
C	1.358355	1.028083	-2.507322
C	1.263376	3.561890	-1.424892
C	2.001377	2.066176	-3.154769
C	1.947203	3.341157	-2.609990
F	0.000000	2.764336	0.341134
F	1.210094	4.783083	-0.909888
F	2.549935	4.345179	-3.221412
F	2.668672	1.857821	-4.282241
F	1.458426	-0.181281	-3.056786
F	-1.458426	0.181281	-3.056786
F	-2.668672	-1.857821	-4.282241
F	-2.549935	-4.345179	-3.221412
F	-1.210094	-4.783083	-0.909888
F	0.000000	-2.764336	0.341134
Cl	2.604137	-0.598130	0.821099
Cl	2.650719	-0.578500	3.975473
Cl	0.000000	0.000000	5.547373
Cl	-2.650719	0.578500	3.975473
Cl	-2.604137	0.598130	0.821099

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[1eH]⁻

B	-0.529022	-0.069245	-0.723579
C	-1.288909	1.352914	-0.458337
C	1.057816	-0.078455	-0.293290
C	-1.340954	-1.373483	-0.175278
C	1.621555	0.647795	0.761489
C	2.997316	0.718888	0.993409
C	3.870076	0.002849	0.178225
C	3.349072	-0.801468	-0.832613
C	1.969030	-0.836881	-1.041209

C	-2.399191	1.563382	0.346403
C	-3.042597	2.787751	0.456384
C	-2.571795	3.874169	-0.257897
C	-1.463660	3.716530	-1.071923
C	-0.856821	2.474253	-1.157125
C	-0.970757	-2.178812	0.890683
C	-1.678272	-3.309349	1.277230
C	-2.818301	-3.669944	0.584757
C	-3.233655	-2.892820	-0.483291
C	-2.495999	-1.775823	-0.836376
Cl	0.582272	1.450983	1.911527
Cl	1.373731	-1.922566	-2.272826
F	-1.272431	-4.051826	2.314382
F	-4.340532	-3.232254	-1.155955
F	-2.961485	-1.058414	-1.869416
F	-4.108410	2.934182	1.253363
F	-0.998648	4.762285	-1.766011
F	0.215124	2.390100	-1.959782
F	-2.896323	0.575799	1.108867
F	0.115853	-1.894060	1.626238
H	-0.531700	-0.161028	-1.927440
Cl	3.639461	1.680566	2.290611
Cl	5.585954	0.092916	0.433548
Cl	4.431082	-1.739005	-1.817946
F	-3.514930	-4.754002	0.943215
F	-3.178151	5.062532	-0.162195

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4b

B	-0.177020	0.008096	0.134910
C	1.246645	-0.598914	0.443275
C	2.255566	-0.581242	-0.517294
C	1.545662	-1.165243	1.675656
C	3.515563	-1.110380	-0.253689
C	2.792981	-1.692114	1.966535
C	3.776980	-1.663246	0.993240
C	-1.392558	-0.962511	-0.042352
C	-2.665384	-0.635474	0.426796
C	-1.249465	-2.221301	-0.625624
C	-3.731285	-1.511509	0.322548
C	-2.317972	-3.095345	-0.748884
C	-3.565970	-2.748135	-0.271753
C	-0.330692	1.562760	0.024556
C	0.417885	2.434269	0.814619
C	-1.185048	2.148466	-0.909950
C	0.307720	3.810313	0.690527
C	-1.285445	3.521165	-1.050645

C	-0.541844	4.363746	-0.246219
F	1.250670	1.959983	1.741256
F	1.033207	4.599777	1.481989
F	-2.106326	4.030090	-1.969002
F	-1.913076	1.382653	-1.725092
F	-2.879236	0.537516	1.025687
F	-4.923933	-1.156051	0.799561
F	-2.131934	-4.280264	-1.329599
F	-0.070902	-2.611428	-1.110516
Cl	1.875146	0.086045	-2.080795
Cl	4.772937	-1.098716	-1.449458
Cl	0.308949	-1.172580	2.913969
H	-4.399677	-3.431851	-0.361098
H	-0.623843	5.437593	-0.349266
H	4.758382	-2.072050	1.195161
H	2.994427	-2.117231	2.940873

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[4bH]⁻

B	0.243007	0.024293	0.766377
C	-0.089664	1.569580	0.353132
C	-1.007685	-1.019829	0.571523
C	1.644581	-0.542569	0.150166
C	-2.010059	-0.942475	-0.410658
C	-3.106110	-1.805322	-0.438795
C	-3.227132	-2.818110	0.496967
C	-2.233022	-2.974399	1.442665
C	-1.161358	-2.094165	1.456481
C	0.554121	2.323049	-0.619953
C	0.262052	3.658638	-0.850194
C	-0.704016	4.314063	-0.113636
C	-1.364690	3.588227	0.858704
C	-1.056535	2.257132	1.080403
C	1.771192	-1.517478	-0.829618
C	3.001409	-1.992300	-1.261439
C	4.178007	-1.502921	-0.733115
C	4.082364	-0.524265	0.238063
C	2.847886	-0.064098	0.660170
Cl	-1.870867	0.220782	-1.709638
Cl	0.068564	-2.439240	2.671362
F	3.049133	-2.941846	-2.214416
F	5.206755	-0.015203	0.776503
F	2.843527	0.899423	1.596486
F	0.923699	4.326490	-1.813819
F	-2.316071	4.186849	1.599356
F	-1.748051	1.622131	2.041914
F	1.480145	1.767246	-1.421640

F	0.685734	-2.046823	-1.420267
H	0.418684	0.089201	1.960772
Cl	-4.367051	-1.669872	-1.648092
H	-4.081280	-3.481857	0.468237
H	-2.286834	-3.775391	2.168683
H	-0.937069	5.354430	-0.293375
H	5.138597	-1.867195	-1.070200

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4a

B	0.000000	0.000000	0.182214
C	0.000000	0.000000	1.757217
C	-1.177472	-0.099668	2.492729
C	1.177472	0.099668	2.492729
C	-1.201348	-0.096619	3.877494
C	1.201348	0.096619	3.877494
C	0.000000	0.000000	4.565418
C	0.364764	1.319276	-0.579802
C	1.115742	1.303293	-1.755101
C	0.000000	2.573157	-0.091369
C	1.486159	2.468409	-2.402880
C	0.352702	3.742703	-0.746184
C	1.102272	3.698964	-1.904603
C	-0.364764	-1.319276	-0.579802
C	0.000000	-2.573157	-0.091369
C	-1.115742	-1.303293	-1.755101
C	-0.352702	-3.742703	-0.746184
C	-1.486159	-2.468409	-2.402880
C	-1.102272	-3.698964	-1.904603
F	0.730975	-2.679715	1.018097
F	0.034955	-4.916314	-0.246742
F	-2.217419	-2.399105	-3.515385
F	-1.527641	-0.143814	-2.272053
F	1.527641	0.143814	-2.272053
F	2.217419	2.399105	-3.515385
F	-0.034955	4.916314	-0.246742
F	-0.730975	2.679715	1.018097
Cl	-2.696138	-0.187178	1.621425
Cl	2.696138	0.187178	1.621425
H	1.384017	4.611228	-2.413367
H	-1.384017	-4.611228	-2.413367
H	0.000000	0.000000	5.648630
H	2.143939	0.165534	4.404445
H	-2.143939	-0.165534	4.404445

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[4aH]⁻

B	-0.005677	0.232161	-0.634347
C	-1.375253	-0.597735	-0.310968
C	-0.002447	1.791422	-0.129744
C	1.355575	-0.564302	-0.206209
C	-0.712586	2.346752	0.942720
C	-0.736186	3.698544	1.261818
C	0.006322	4.588680	0.505814
C	0.775038	4.106463	-0.540037
C	0.756918	2.747804	-0.822443
C	-1.486941	-1.726574	0.490390
C	-2.679382	-2.414575	0.656045
C	-3.834494	-2.001019	0.023834
C	-3.753930	-0.878890	-0.778395
C	-2.554748	-0.206854	-0.938014
C	2.154453	-0.267643	0.889704
C	3.330061	-0.948625	1.168014
C	3.762860	-1.979695	0.359330
C	2.980075	-2.305601	-0.731479
C	1.810998	-1.613692	-0.997612
Cl	-1.619048	1.320803	2.059312
Cl	1.820159	2.250700	-2.142994
F	4.058718	-0.605076	2.247267
F	3.362703	-3.310738	-1.542791
F	1.102398	-2.007308	-2.069134
F	-2.715533	-3.499446	1.453182
F	-4.857757	-0.438658	-1.412179
F	-2.564818	0.879427	-1.728474
F	-0.430458	-2.189251	1.182724
F	1.805273	0.702407	1.751816
H	0.013286	0.288012	-1.842224
H	-1.323681	4.038207	2.105444
H	-0.000601	5.647200	0.740244
H	1.388072	4.770700	-1.136066
H	-4.766742	-2.533095	0.153621
H	4.676425	-2.516362	0.575026

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[4aH]iso

B	-0.016835	0.251226	-0.640064
C	-1.199431	-0.820077	-0.254085
C	-0.378734	1.723175	-0.016344
C	1.505899	-0.266696	-0.346282
C	-0.728589	1.947094	1.322344
C	-1.132984	3.166454	1.845388
C	-1.187930	4.271199	1.011701
C	-0.817105	4.136382	-0.314839
C	-0.421526	2.891249	-0.788812

C	-1.078993	-1.970782	0.515290
C	-2.136419	-2.837118	0.745499
C	-3.387820	-2.591047	0.217835
C	-3.541242	-1.450750	-0.546187
C	-2.472997	-0.598745	-0.771643
C	2.482721	0.394452	0.387315
C	3.781856	-0.081229	0.511360
C	4.177655	-1.249243	-0.104583
C	3.230205	-1.923642	-0.852233
C	1.942258	-1.435714	-0.967198
Cl	-0.608536	0.633017	2.492786
Cl	0.077330	2.873615	-2.482966
F	4.672332	0.613291	1.245267
F	3.572216	-3.066443	-1.477594
F	1.086927	-2.149539	-1.719550
F	-1.944267	-3.932411	1.505289
F	-4.745285	-1.169072	-1.080532
F	-2.711308	0.483863	-1.530783
F	0.086922	-2.286970	1.105290
F	2.218344	1.550613	1.020694
H	-0.079227	0.332442	-1.843854
H	-1.389545	3.243332	2.894443
H	-1.503988	5.234086	1.397192
H	-0.828500	4.986263	-0.985457
H	-4.215725	-3.262516	0.398671
H	5.187791	-1.622252	-0.007517

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4d

B	-0.339758	0.019636	0.230282
C	1.223321	0.008902	0.465522
C	2.092240	-0.470432	-0.512410
C	1.786505	0.471454	1.647752
C	3.469738	-0.486200	-0.313565
C	3.152846	0.461456	1.874009
C	3.993340	-0.019093	0.884695
C	-1.055660	1.390654	0.001355
C	-2.335050	1.664267	0.496591
C	-0.431505	2.449993	-0.656721
C	-2.964961	2.883461	0.361758
C	-1.046559	3.682161	-0.824023
C	-2.308993	3.903495	-0.315319
C	-1.111048	-1.340940	0.242661
C	-0.742696	-2.411825	1.061999
C	-2.185010	-1.585637	-0.613173
C	-1.385417	-3.634168	1.060486
C	-2.839068	-2.806062	-0.649779

C	-2.445187	-3.830979	0.186831
F	0.271813	-2.249934	1.922230
F	-3.851838	-2.979742	-1.503692
F	-2.595650	-0.639651	-1.458694
F	-2.982729	0.703915	1.171577
F	-0.400285	4.649287	-1.480585
F	0.785954	2.296520	-1.176118
Cl	1.402054	-1.011464	-2.017848
Cl	4.556753	-1.075898	-1.532269
Cl	0.722274	1.051859	2.910956
H	-2.768137	4.874033	-0.454185
H	-2.972703	-4.775404	0.143859
H	5.064782	-0.033859	1.035727
H	3.555439	0.822334	2.811230
H	-3.952048	3.025316	0.780465
H	-1.053331	-4.413645	1.732760

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[4dH]⁻

B	0.220683	-0.060534	-0.664964
C	1.575733	-0.959086	-0.510570
C	-1.095223	-0.687777	0.093490
C	0.431534	1.527136	-0.353807
C	-1.094929	-1.467576	1.254425
C	-2.223206	-2.067165	1.796016
C	-3.451382	-1.878941	1.194617
C	-3.527764	-1.067903	0.075210
C	-2.377781	-0.480712	-0.451157
C	2.776395	-0.561581	0.058521
C	3.912476	-1.362794	0.072381
C	3.897432	-2.622051	-0.484948
C	2.716539	-3.072685	-1.064290
C	1.613996	-2.240251	-1.061432
C	-0.056600	2.217396	0.744471
C	0.114175	3.586626	0.919717
C	0.800441	4.336458	-0.008430
C	1.321662	3.690784	-1.124502
C	1.126153	2.330043	-1.258664
Cl	0.376594	-1.699069	2.197121
Cl	-2.572342	0.589349	-1.822978
F	-0.398301	4.178405	2.018820
H	1.877014	4.229012	-1.882298
F	1.667988	1.748269	-2.350916
F	5.039604	-0.896130	0.650110
H	2.644096	-4.055252	-1.513425
F	0.488850	-2.728168	-1.629332
F	2.888206	0.632124	0.667191

F	-0.725905	1.574663	1.717813
H	-0.025292	-0.133617	-1.846704
H	-2.138365	-2.667392	2.692813
H	-4.346907	-2.335663	1.595190
Cl	-5.112071	-0.820128	-0.634147
H	4.793287	-3.229551	-0.459214
H	0.923769	5.400550	0.149066

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4c

B	-0.041054	-0.067663	0.108174
C	0.728052	-1.439205	-0.020760
C	0.673785	-2.206474	-1.180709
C	1.502052	-1.951663	1.016266
C	1.344718	-3.410312	-1.319733
C	2.182228	-3.154854	0.925019
C	2.099134	-3.881078	-0.254525
C	0.780588	1.263388	0.135432
C	0.416450	2.356914	0.927744
C	1.963012	1.417298	-0.587226
C	1.151870	3.520166	1.014403
C	2.715038	2.582055	-0.534688
C	2.315852	3.632172	0.264802
C	-1.602990	-0.084679	0.202779
C	-2.307357	-1.092509	0.866709
C	-2.389395	0.884069	-0.419574
C	-3.685876	-1.147081	0.933090
C	-3.773692	0.847075	-0.385648
C	-4.425465	-0.163659	0.291775
F	-1.620470	-2.050349	1.503729
F	-4.469135	1.798454	-1.016002
F	-1.814223	1.873585	-1.104705
F	-0.692708	2.268384	1.676312
F	3.829579	2.671845	-1.266183
F	2.397142	0.442045	-1.384594
Cl	-0.250041	-1.594918	-2.539997
Cl	1.583736	-1.049539	2.517743
H	2.920402	4.529821	0.293026
H	-5.507937	-0.170734	0.308906
H	2.628039	-4.822123	-0.344798
H	2.763366	-3.514751	1.763920
H	0.813567	4.321087	1.657743
H	-4.163607	-1.950280	1.477635
H	1.278938	-3.964350	-2.246943

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[4cH]⁻

B	0.033260	-0.149075	0.730618
C	-1.581512	-0.189484	0.488568
C	0.851067	-1.426209	0.105155
C	0.723055	1.283913	0.359978
C	0.511963	-2.185973	-1.022392
C	1.193742	-3.317946	-1.450716
C	2.313383	-3.740626	-0.755449
C	2.741916	-3.008876	0.339190
C	2.019550	-1.889885	0.729853
C	-2.339842	0.738978	-0.208858
C	-3.725455	0.673048	-0.301614
C	-4.427815	-0.345575	0.302952
C	-3.715615	-1.307229	1.010953
C	-2.340127	-1.198645	1.082426
C	1.550897	1.537396	-0.722579
C	2.153352	2.770870	-0.946943
C	1.941790	3.826571	-0.089265
C	1.107886	3.630066	1.006177
C	0.533113	2.387604	1.191641
Cl	-0.825822	-1.702563	-2.070125
Cl	2.703432	-1.009813	2.101707
F	2.950100	2.928239	-2.025378
H	0.898723	4.426856	1.708947
F	-0.282719	2.256449	2.260758
F	-4.384127	1.620063	-1.003376
H	-4.213335	-2.133685	1.502632
F	-1.695649	-2.163267	1.775439
F	-1.751716	1.751043	-0.870887
F	1.805202	0.580654	-1.632163
H	0.140653	-0.260165	1.930993
H	0.850701	-3.847731	-2.330539
H	2.858066	-4.622124	-1.074815
H	3.629498	-3.294348	0.889752
H	-5.506407	-0.378515	0.213934
H	2.418535	4.778870	-0.284873

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C	-0.181915	1.250441	1.101599
C	-1.485194	1.537307	1.486257
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C	-1.834958	2.588919	2.312584
C	0.481632	3.154225	2.475782
C	-0.836518	3.409855	2.810153
C	1.569714	0.108905	-0.652952
C	1.810965	1.126019	-1.571219

C	2.633774	-0.757399	-0.440823
C	3.000149	1.262429	-2.265228
C	3.843854	-0.651665	-1.111029
C	4.026286	0.361206	-2.035059
C	-0.177788	-1.464832	0.731822
C	-0.291207	-1.732015	2.090650
C	-0.273780	-2.579041	-0.095305
C	-0.497555	-3.008559	2.595166
C	-0.487024	-3.866108	0.363117
C	-0.599653	-4.081326	1.727210
F	-0.176628	-0.758299	2.997790
F	-0.596379	-3.209228	3.904910
F	-0.581262	-4.887627	-0.483202
F	-0.154588	-2.427361	-1.428039
F	0.879527	2.065586	-1.804930
F	3.169435	2.252796	-3.138588
F	4.827936	-1.513501	-0.870811
F	2.549482	-1.745674	0.459125
B	0.141021	0.003635	0.111338
O	-0.889188	0.254434	-1.115365
C	-1.972870	-0.288687	-1.342161
H	-2.334692	-1.079983	-0.678022
C	-2.783147	0.100794	-2.468946
C	-4.002047	-0.551320	-2.679956
C	-2.355205	1.116662	-3.334974
C	-4.795192	-0.189490	-3.756366
H	-4.320690	-1.335117	-2.000901
C	-3.152752	1.470690	-4.406432
H	-1.406500	1.606041	-3.148402
C	-4.368096	0.818700	-4.614389
H	-5.741027	-0.687634	-3.928772
H	-2.834809	2.253555	-5.083817
H	-4.988835	1.101825	-5.456847
F	-0.803186	-5.305105	2.195310
F	5.176141	0.475400	-2.687926
F	-2.496799	0.744592	1.070798
F	-3.105860	2.810470	2.637882
F	-1.141683	4.425109	3.607807
F	1.446843	3.928014	2.961852
F	2.083977	1.893220	1.390420

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O	-0.293298	0.058902	2.016714
C	-0.126179	-1.068344	2.937952
C	-0.992117	1.164812	2.662865
C	-0.953070	-0.673524	4.145785

H	-0.473589	-1.962383	2.427550
H	0.936620	-1.135144	3.160333
C	-0.853623	0.853250	4.136061
H	-0.515503	2.086056	2.339456
H	-2.032223	1.143710	2.332808
H	-1.990870	-0.990456	4.017001
H	-0.562088	-1.123125	5.058336
H	0.121259	1.182053	4.502411
H	-1.633576	1.337369	4.723641
C	0.490554	-1.410347	-0.022573
C	-0.054178	-2.239955	-0.998319
C	1.718184	-1.837431	0.478994
C	0.547008	-3.420231	-1.414068
C	2.347010	-3.009765	0.099638
C	1.751764	-3.812081	-0.859271
C	1.048379	1.141999	0.020591
C	1.890030	1.830544	0.879938
C	1.325193	1.313163	-1.332202
C	2.910380	2.662962	0.440112
C	2.330612	2.128650	-1.815267
C	3.131257	2.815804	-0.915729
C	-1.616251	0.388181	-0.096764
C	-2.029585	1.535406	-0.760669
C	-2.643180	-0.488822	0.241085
C	-3.352709	1.771330	-1.116155
C	-3.970579	-0.293470	-0.085332
C	-4.328226	0.851547	-0.781064
F	-2.359722	-1.602664	0.942412
F	-4.899873	-1.178513	0.263303
F	-5.595488	1.066664	-1.106366
F	-3.687926	2.885322	-1.759022
F	-1.168952	2.507921	-1.076442
F	1.772817	1.719659	2.217253
F	0.585227	0.658180	-2.237332
F	2.537776	2.258334	-3.121605
F	4.103318	3.606656	-1.352677
F	3.680570	3.305054	1.315365
F	-1.195571	-1.930588	-1.616840
F	2.362813	-1.094003	1.395416
F	3.509814	-3.364730	0.638403
F	2.333384	-4.939642	-1.243699
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B	-0.100890	0.051344	0.405743

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C	-1.056173	0.302210	-0.555101
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C	-1.536359	1.586440	-0.788584
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C	-2.792163	1.846888	-1.311582
C	-3.210550	-0.502513	-1.387294
C	-3.639056	0.793675	-1.607557
C	1.094549	-1.375819	0.010110
C	1.151311	-2.012599	-1.226143
C	1.878420	-1.955291	0.999818
C	1.906788	-3.153038	-1.454480
C	2.639687	-3.097084	0.819796
C	2.652568	-3.702441	-0.425093
C	1.440464	1.219317	0.196734
C	2.073557	1.826077	1.268199
C	1.902009	1.625096	-1.051171
C	3.071829	2.778988	1.144649
C	2.893700	2.573537	-1.229044
C	3.484756	3.157961	-0.119641
B	0.316883	0.036628	0.259321
H	0.492253	0.230720	2.420595
O	-0.230613	0.050812	1.803904
C	-1.128078	-0.971853	2.323991
H	-0.877628	-1.076849	3.380924
H	-0.903779	-1.909501	1.813507
C	-2.566775	-0.576301	2.132215
C	-3.512187	-1.568057	1.889132
C	-2.965924	0.755823	2.190310
C	-4.845153	-1.230891	1.693768
H	-3.202537	-2.604996	1.816014
C	-4.296365	1.092290	1.982399
H	-2.229947	1.533478	2.358940
C	-5.238234	0.100573	1.732439
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H	-4.596070	2.133582	2.004920
H	-6.273756	0.367021	1.557120
F	1.919343	-3.724945	-2.652924
F	0.467533	-1.542753	-2.269121
F	3.354436	-3.605113	1.818875
F	1.931907	-1.397198	2.231969
F	1.367714	1.093955	-2.154328
F	3.283304	2.926981	-2.447878
F	3.629533	3.320653	2.221916
F	1.736702	1.501322	2.547404
F	4.438075	4.067236	-0.268701
F	3.374554	-4.795427	-0.629616
F	-1.636394	-1.998112	-0.607571
F	-4.028693	-1.523503	-1.623755
F	-0.809952	2.661487	-0.455822

F	-3.205198	3.098383	-1.492835
F	-4.859328	1.025296	-2.071753

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1a-H₂O

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C	-0.448285	3.638117	-0.850486
C	1.497344	3.620113	0.543780
C	0.633118	4.301966	-0.298459
C	-1.446993	-0.630549	0.281134
C	-1.636653	-1.507062	-0.779558
C	-2.602428	-0.296232	0.972357
C	-2.879800	-2.021957	-1.119627
C	-3.860782	-0.782580	0.676991
C	-3.997206	-1.662009	-0.385692
C	1.254530	-0.928511	0.295152
C	1.535561	-2.085257	1.003138
C	2.096590	-0.683995	-0.782364
C	2.573884	-2.949700	0.711794
C	3.149153	-1.520995	-1.119768
C	3.392538	-2.658169	-0.366738
F	0.749902	-2.426295	2.065905
F	2.787841	-4.036809	1.443405
F	3.923315	-1.245087	-2.161646
F	1.898457	0.372844	-1.573059
F	-0.612507	-1.876071	-1.552977
F	-3.006390	-2.855669	-2.144071
F	-4.921811	-0.420256	1.387502
F	-2.527999	0.588161	2.007253
B	-0.006878	0.019683	0.663819
H	-0.810677	0.433648	2.654068
H	0.115158	-0.845403	2.678791
O	0.017573	0.052870	2.327805
F	-5.188386	-2.149813	-0.697470
F	4.397361	-3.463716	-0.677462
F	-1.710855	1.722681	-1.135504
F	-1.276091	4.284499	-1.664669
F	0.844063	5.580574	-0.575935
F	2.543992	4.248173	1.069567
F	2.139596	1.665605	1.611894

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C	1.213012	-0.134421	-0.310646
C	2.013714	-0.766396	0.653783

C	1.916728	0.453335	-1.371823
C	3.408824	-0.695780	0.660216
C	3.311999	0.545309	-1.396622
C	4.061394	-0.004583	-0.357891
C	-1.236733	1.070628	-0.938626
C	-1.005491	2.405715	-0.631320
C	-2.218092	0.856136	-1.899577
C	-1.683082	3.465100	-1.205611
C	-2.921202	1.887820	-2.504673
C	-2.656294	3.200423	-2.154333
C	-1.113896	-1.576951	-0.295074
C	-2.354137	-1.856511	0.268309
C	-0.532954	-2.626696	-0.993867
C	-2.963719	-3.096383	0.191128
C	-1.113279	-3.881526	-1.100577
C	-2.334633	-4.120622	-0.496694
F	-3.050771	-0.895780	0.898426
F	-4.150255	-3.307595	0.756782
F	-0.507155	-4.853154	-1.776352
F	0.638991	-2.465830	-1.620206
F	-0.038335	2.730795	0.253545
F	-1.405986	4.720270	-0.864087
F	-3.845812	1.625953	-3.422709
F	-2.509050	-0.374392	-2.329812
Cl	1.278223	-1.756329	1.897699
Cl	1.079631	1.003054	-2.794558
B	-0.426783	-0.114399	-0.163009
O	-0.774233	0.308714	1.365828
C	-0.098914	0.936958	2.186193
H	0.927961	1.225604	1.942461
C	-0.634762	1.298710	3.474072
C	-1.943776	0.942103	3.826416
C	0.176695	2.009736	4.363745
C	-2.429762	1.302264	5.068896
H	-2.549505	0.387698	3.119350
C	-0.319253	2.367118	5.606603
H	1.188003	2.277686	4.076692
C	-1.618906	2.012758	5.953878
H	-3.438852	1.033060	5.355436
H	0.300101	2.918299	6.303084
H	-2.006969	2.292398	6.926741
F	-2.904903	-5.315801	-0.585363
F	-3.323304	4.195004	-2.724521
Cl	4.126405	1.332056	-2.702077
Cl	5.782194	0.134547	-0.351603
Cl	4.335629	-1.450573	1.910415

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C	-1.224417	-0.259466	0.235831
C	-2.169099	0.743696	0.513220
C	-1.768857	-1.452652	-0.257921
C	-3.516505	0.651590	0.171113
C	-3.112366	-1.575048	-0.637404
C	-3.983510	-0.506208	-0.450845
C	1.478118	-1.083712	0.068896
C	2.384196	-1.751789	0.875674
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C	3.366052	-2.598642	0.380854
C	2.607062	-2.127308	-1.835009
C	3.478417	-2.789837	-0.983636
C	0.961909	1.425942	-0.119121
C	0.360965	2.130851	-1.161265
C	2.247692	1.864199	0.190644
C	0.946291	3.223007	-1.784253
C	2.865607	2.954878	-0.397218
C	2.203531	3.647824	-1.394442
F	-0.831608	1.775995	-1.644312
F	0.309260	3.859310	-2.761107
F	2.772428	4.693368	-1.978134
F	4.088024	3.323765	-0.024665
F	2.986925	1.203833	1.100188
F	2.363666	-1.614725	2.217329
F	4.203447	-3.216889	1.209836
F	4.412620	-3.594375	-1.474302
F	2.702207	-2.302190	-3.148613
F	0.807932	-0.697768	-2.156061
Cl	-1.687594	2.196252	1.362249
Cl	-4.613889	1.948093	0.491863
Cl	-5.633931	-0.625404	-0.940238
Cl	-3.711749	-3.043113	-1.326181
Cl	-0.827553	-2.920338	-0.327309
O	0.376061	0.107544	2.144807
C	1.005046	1.073610	3.044560
C	-0.338239	-0.922655	2.901850
C	0.293844	0.838763	4.359000
H	2.062645	0.828835	3.096130
H	0.856420	2.059945	2.612046
C	0.074525	-0.675014	4.337750
H	-0.043668	-1.890794	2.502674
H	-1.404407	-0.758126	2.742949
H	-0.661609	1.368806	4.380125
H	0.899249	1.171064	5.202260
H	-0.694836	-1.007352	5.034457

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H	1.004692	-1.200607	4.562229
B	0.377284	0.031943	0.530000

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C	0.970565	-0.646858	-0.149650
C	1.479887	-1.474257	0.861112
C	1.878758	-0.347475	-1.167660
C	2.831209	-1.807444	0.963125
C	3.238050	-0.659620	-1.108703
C	3.726566	-1.357971	-0.007063
C	-1.658196	-0.984976	-0.869605
C	-2.957509	-0.529571	-1.069679
C	-1.380251	-2.219835	-1.445766
C	-3.921588	-1.221002	-1.776826
C	-2.319784	-2.951523	-2.161337
C	-3.596412	-2.449404	-2.330724
C	-0.951416	0.378406	1.460024
C	-0.107826	1.264004	2.123350
C	-2.052247	-0.042968	2.196329
C	-0.331702	1.730749	3.406930
C	-2.312723	0.396071	3.485767
C	-1.449554	1.290689	4.095348
B	-0.580314	-0.084585	-0.055790
H	-0.134093	1.331769	-1.695273
O	-0.557078	1.363388	-0.822571
C	-1.245579	2.633610	-0.611023
H	-2.244047	2.549852	-1.034154
H	-1.323483	2.752777	0.466794
C	-0.444730	3.718649	-1.263163
C	0.755982	4.149330	-0.697197
C	-0.875898	4.272522	-2.466100
C	1.511967	5.123770	-1.330637
H	1.093600	3.714188	0.236183
C	-0.119013	5.251831	-3.098395
H	-1.810287	3.940382	-2.907657
C	1.075248	5.675593	-2.531186
H	2.443116	5.455961	-0.887083
H	-0.462133	5.681751	-4.031998
H	1.667667	6.438290	-3.023211
F	-5.146784	-0.726112	-1.926709
F	-3.339590	0.645607	-0.538449
F	-1.996614	-4.127008	-2.690184
F	-0.173284	-2.782556	-1.339933
F	-2.900395	-0.950112	1.707626
F	-3.377876	-0.044659	4.146315
F	0.508440	2.590245	3.975171

F	0.996592	1.724555	1.509170
Cl	1.315329	0.337311	-2.693488
Cl	0.385093	-2.236168	1.980069
F	-1.689101	1.719699	5.326315
F	-4.502004	-3.133799	-3.015442
Cl	3.408401	-2.771481	2.274740
Cl	5.411380	-1.708106	0.127291
Cl	4.318065	-0.194840	-2.376414

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1e-H₂O

C	1.078298	-0.090574	-0.257200
C	1.976507	-0.935384	-0.915545
C	1.648625	0.710220	0.742653
C	3.358269	-0.904291	-0.725065
C	3.027203	0.780562	0.959420
C	3.890501	-0.007950	0.198747
C	-1.338138	-1.360637	-0.110442
C	-2.510714	-1.767009	-0.731752
C	-0.954833	-2.135930	0.976076
C	-3.265048	-2.855662	-0.342418
C	-1.679959	-3.237617	1.409135
C	-2.838345	-3.602176	0.745219
C	-1.274335	1.368902	-0.422594
C	-2.422512	1.568906	0.333735
C	-0.770734	2.501919	-1.057215
C	-3.036686	2.805957	0.458203
C	-1.355586	3.752206	-0.958400
C	-2.501018	3.903591	-0.193460
F	-2.977498	0.566112	1.022929
F	-4.131709	2.945986	1.198125
F	-0.829839	4.802250	-1.580089
F	0.352852	2.419329	-1.779075
F	-2.988914	-1.050742	-1.786962
F	-4.377797	-3.186675	-0.986456
F	-1.269493	-3.945513	2.453705
F	0.143056	-1.839593	1.674652
Cl	1.376811	-2.200841	-1.992619
Cl	0.633347	1.578597	1.855976
O	-0.575497	-0.113018	-2.281791
B	-0.521390	-0.051844	-0.617001
H	-0.077451	-0.878462	-2.618965
H	-1.501328	-0.204039	-2.549387
F	-3.078741	5.091414	-0.085680
F	-3.537067	-4.653744	1.145806
Cl	4.409833	-1.951669	-1.609631

Cl	5.597269	0.092744	0.426636
Cl	3.680217	1.830360	2.164376

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4a-5

C	-0.436496	-0.098771	-1.846265
C	0.011468	-1.253744	-2.514109
C	-0.978818	0.861151	-2.716819
C	0.008249	-1.422437	-3.890414
C	-0.998867	0.730358	-4.099775
C	-0.486912	-0.409164	-4.691188
C	-0.423519	1.530132	0.432007
C	0.563332	2.475245	0.173807
C	-1.426503	1.950006	1.298345
C	0.575458	3.738176	0.735261
C	-1.433199	3.215718	1.867490
C	-0.431088	4.124835	1.597203
C	-1.224661	-1.067578	0.585935
C	-0.902963	-1.463296	1.880479
C	-2.361177	-1.659335	0.048827
C	-1.627733	-2.417739	2.573044
C	-3.099774	-2.612034	0.733961
C	-2.737075	-3.009951	2.003952
F	0.126616	-0.894460	2.535555
F	-1.251629	-2.756750	3.811754
F	-4.177598	-3.146741	0.151917
F	-2.802818	-1.313010	-1.168003
F	1.553655	2.190419	-0.702892
F	1.561859	4.587518	0.430725
F	-2.431351	3.555640	2.687020
F	-2.463517	1.157734	1.591616
Cl	0.594425	-2.661437	-1.615961
Cl	-1.788839	2.303504	-2.127215
H	-0.439195	5.111138	2.040449
H	-3.312243	-3.750962	2.541909
H	-0.499362	-0.519342	-5.768660
H	-1.432145	1.519716	-4.699494
H	0.375977	-2.345371	-4.318915
B	-0.341240	0.035617	-0.216774
O	1.176072	-0.357989	0.216088
C	2.205776	-0.331317	-0.460442
H	2.155228	-0.072684	-1.522555
C	3.488536	-0.641748	0.125597
C	3.583059	-0.993447	1.478350

C	4.629721	-0.585620	-0.679077
C	4.823053	-1.285969	2.014887
H	2.681117	-1.032959	2.077820
C	5.868730	-0.878749	-0.132735
H	4.539661	-0.311337	-1.724820
C	5.960774	-1.227440	1.210711
H	4.910741	-1.560462	3.058909
H	6.759501	-0.836745	-0.747151
H	6.930208	-1.457157	1.638252

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4a-THF

C	-1.251568	-1.284114	-0.516362
C	-2.631139	-1.174777	-0.255544
C	-0.946855	-2.356690	-1.368383
C	-3.614714	-1.936776	-0.860918
C	-1.903766	-3.137612	-2.008923
C	-3.244835	-2.911075	-1.772630
C	1.390879	-0.354300	-0.187194
C	1.749529	0.021736	-1.478871
C	2.453016	-0.635916	0.657678
C	3.060467	0.085274	-1.910290
C	3.775649	-0.582102	0.241629
C	4.097435	-0.222305	-1.049307
C	-0.530210	1.343526	0.057103
C	-1.375495	1.882017	-0.912361
C	0.199314	2.293250	0.770881
C	-1.533694	3.248529	-1.093471
C	0.046638	3.659623	0.608268
C	-0.833630	4.157948	-0.328923
F	-2.069783	1.099783	-1.742789
F	-2.376579	3.683724	-2.033397
F	0.773431	4.494088	1.358199
F	1.131092	1.901305	1.661755
F	0.785970	0.309293	-2.366947
F	3.324297	0.440388	-3.170351
F	4.744877	-0.877268	1.114526
F	2.251550	-0.979242	1.949043
Cl	-3.244729	-0.037623	0.949692
Cl	0.702129	-2.908870	-1.645065
H	5.127113	-0.176751	-1.376235
H	-0.957762	5.222521	-0.472178
H	-3.997799	-3.509280	-2.270999
H	-1.582301	-3.927553	-2.674507
H	-4.654396	-1.764116	-0.616902
O	-0.358235	-0.723398	1.758149
C	-0.512331	0.076108	2.969919

C	-0.352714	-2.152339	2.071477
C	-1.025993	-0.922885	3.983751
H	0.468767	0.463825	3.231878
H	-1.198867	0.886007	2.735410
C	-0.277050	-2.195410	3.583620
H	-1.284748	-2.569950	1.689806
H	0.495755	-2.600804	1.559027
H	-2.105118	-1.058480	3.876288
H	-0.810512	-0.601599	5.002912
H	0.762603	-2.147761	3.913636
H	-0.731389	-3.104130	3.978503
B	-0.191709	-0.258652	0.208450

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4a-8a

C	0.169754	-0.161337	1.790033
C	0.674996	0.776758	2.704861
C	-0.487722	-1.224784	2.421236
C	0.434808	0.739481	4.070809
C	-0.752322	-1.308684	3.778314
C	-0.309739	-0.294584	4.608311
H	0.849494	1.512906	4.703628
H	-1.282819	-2.164562	4.173870
H	-0.509872	-0.331443	5.671938
C	1.542414	-0.942875	-0.442869
C	1.636254	-1.179645	-1.811006
C	2.511288	-1.577230	0.327979
C	2.594851	-1.995270	-2.380163
C	3.485013	-2.398276	-0.228404
C	3.536518	-2.622059	-1.587049
H	4.295312	-3.260126	-2.018972
C	0.280131	1.531217	-0.353588
C	-0.807969	2.320406	0.009629
C	1.232533	2.165189	-1.142488
C	-0.957941	3.635770	-0.391754
C	1.098972	3.485316	-1.549274
C	0.001239	4.236463	-1.182405
H	-0.100590	5.265235	-1.499868
B	0.357282	-0.007405	0.164400
H	-1.253691	-1.503870	-0.104311
O	-1.045329	-0.622474	-0.454797
C	-1.872682	-0.301192	-1.608982
H	-1.427936	-0.764204	-2.486868
H	-1.825572	0.779872	-1.715681
C	-3.263413	-0.800837	-1.356363
C	-4.086454	-0.166822	-0.424742
C	-3.728534	-1.928422	-2.028164

C	-5.358870	-0.657603	-0.174405
H	-3.721281	0.707380	0.101147
C	-5.005542	-2.417795	-1.779099
H	-3.090350	-2.423818	-2.753196
C	-5.819861	-1.782831	-0.851243
H	-5.994959	-0.160374	0.548532
H	-5.361935	-3.293546	-2.308692
H	-6.815823	-2.162873	-0.654677
F	2.611691	-2.169853	-3.705239
F	0.777945	-0.569835	-2.652286
F	4.380493	-2.978231	0.574876
F	2.559948	-1.420524	1.655166
F	2.354044	1.537396	-1.508933
F	2.054558	4.033590	-2.303200
F	-2.038157	4.322169	-0.007710
F	-1.776318	1.806281	0.791589
Cl	-0.959406	-2.687685	1.516442
Cl	1.783646	2.039756	2.192154

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4a-H₂O

C	0.172771	1.799340	0.048202
C	-0.567800	2.425705	-0.967147
C	1.095719	2.665333	0.655815
C	-0.461876	3.774567	-1.283858
C	1.240015	4.012121	0.372102
C	0.433027	4.575844	-0.600667
H	-1.075711	4.180818	-2.076721
H	1.979628	4.601190	0.897700
H	0.520469	5.628106	-0.841046
C	-1.419316	-0.472262	0.229576
C	-1.616879	-1.513773	-0.668445
C	-2.556945	-0.058130	0.906217
C	-2.864257	-2.085690	-0.872544
C	-3.809032	-0.611275	0.720646
C	-3.974671	-1.643197	-0.181381
H	-4.945293	-2.091725	-0.342965
C	1.295643	-0.706521	0.166845
C	1.481053	-1.918198	0.827697
C	2.240529	-0.401295	-0.805889
C	2.552555	-2.754512	0.564627
C	3.315252	-1.233824	-1.081373
C	3.486803	-2.417908	-0.394834
H	4.322967	-3.069209	-0.609886
Cl	2.274710	2.057303	1.848235
Cl	-1.651191	1.525111	-2.012857
F	0.590423	-2.328962	1.742252

F	2.673674	-3.900569	1.240516
F	4.190749	-0.879045	-2.025544
F	2.138292	0.716150	-1.536004
F	-0.609364	-1.972297	-1.416918
F	-2.988308	-3.075642	-1.757601
F	-4.849851	-0.145932	1.413557
F	-2.461668	0.968732	1.802900
B	0.021626	0.230051	0.502735
H	0.800480	0.730338	2.491567
H	-0.783646	0.740653	2.468064
O	0.007761	0.271083	2.164528

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1a-8a(THF)

C	1.267050	0.604530	0.638228
C	1.995850	-0.523581	0.999318
C	1.949528	1.803813	0.775914
C	3.291155	-0.492184	1.472915
C	3.250313	1.885708	1.255406
C	3.926056	0.731953	1.601972
C	-1.237967	-0.584327	0.701691
C	-1.158261	-0.954167	2.039989
C	-2.368537	-1.046665	0.035298
C	-2.098689	-1.766419	2.660221
C	-3.329742	-1.854239	0.617814
C	-3.187609	-2.229286	1.942631
C	-1.017392	1.774725	-0.397423
C	-1.515509	2.191426	-1.622193
C	-1.389850	2.564651	0.685794
C	-2.300540	3.327019	-1.776124
C	-2.169566	3.700416	0.579538
C	-2.628679	4.087630	-0.670039
B	-0.187415	0.409138	-0.069358
H	-0.016319	-1.336856	-1.457299
O	0.150731	-0.346308	-1.420114
C	1.145207	0.096820	-2.375538
H	0.796792	-0.264718	-3.344246
H	1.089561	1.183140	-2.382787
C	2.543694	-0.372243	-2.074326
C	2.836562	-1.730966	-1.963179
C	3.564374	0.559354	-1.911223
C	4.124076	-2.144999	-1.655422
H	2.046329	-2.462754	-2.090876
C	4.857574	0.144592	-1.617558
H	3.342799	1.618951	-1.988776
C	5.136667	-1.208246	-1.478585
H	4.338902	-3.201439	-1.545890

H	5.640274	0.880546	-1.474600
H	6.138938	-1.532887	-1.225516
F	-1.963689	-2.100238	3.939580
F	-0.156627	-0.537335	2.814019
F	-4.377969	-2.284497	-0.086844
F	-2.571124	-0.725324	-1.253470
F	-0.979283	2.222421	1.914812
F	-2.484310	4.418193	1.653862
F	-2.742503	3.682541	-2.980886
F	-1.263703	1.508134	-2.752554
C	-0.327006	-3.795914	-0.621364
O	-0.294597	-2.833839	-1.698720
C	-1.251577	-3.176515	-2.720234
C	-2.191452	-4.172483	-2.060818
C	-1.251257	-4.908169	-1.101908
H	-0.712681	-3.295449	0.269437
H	0.695468	-4.119400	-0.425214
H	-1.738792	-2.256285	-3.041831
H	-0.712517	-3.621149	-3.562931
H	-2.975106	-3.647708	-1.511803
H	-2.666427	-4.834077	-2.785658
H	-1.774665	-5.387350	-0.274213
H	-0.684557	-5.674144	-1.638021
F	-3.379414	5.175173	-0.800812
F	-4.091882	-3.010867	2.518871
F	1.402111	2.964581	0.391420
F	3.866572	3.063113	1.338913
F	5.185078	0.790417	2.019350
F	3.940751	-1.614445	1.771635
F	1.448568	-1.743683	0.846874

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1e-8a(THF)

C	0.615528	-0.946329	0.086129
C	0.938787	-2.034496	-0.741020
C	1.596623	-0.611917	1.038210
C	2.195092	-2.653721	-0.722939
C	2.837611	-1.249756	1.116723
C	3.155570	-2.247691	0.199445
C	-1.753015	-0.229810	-1.282029
C	-1.237807	0.084375	-2.536163
C	-3.093758	-0.592129	-1.283194
C	-1.958831	0.033432	-3.711451
C	-3.857494	-0.666471	-2.442911
C	-3.289595	-0.353365	-3.663342
C	-1.592516	-0.326629	1.450699
C	-1.794668	-1.638017	1.869875

C	-2.089674	0.630850	2.318589
C	-2.413267	-1.983035	3.058513
C	-2.713546	0.336454	3.520830
C	-2.875911	-0.983584	3.897482
B	-0.803721	-0.079820	0.038755
H	0.667385	1.508700	-0.419823
O	-0.271735	1.432909	-0.066754
C	-1.043853	2.549461	-0.585152
H	-1.175399	2.422586	-1.659595
H	-2.011628	2.500032	-0.094988
C	-0.317374	3.830258	-0.292546
C	0.200687	4.584217	-1.341225
C	-0.121821	4.258389	1.020770
C	0.902025	5.756870	-1.087254
H	0.064519	4.245113	-2.362891
C	0.585916	5.424548	1.275057
H	-0.518420	3.670792	1.839017
C	1.099334	6.175458	0.221962
H	1.298738	6.338555	-1.911325
H	0.734313	5.751310	2.297790
H	1.649179	7.087649	0.423559
F	-1.395905	0.345788	-4.875670
F	0.053985	0.451177	-2.645267
F	-5.135327	-1.026746	-2.383626
F	-3.737705	-0.903943	-0.155319
F	-1.981028	1.944144	2.037569
F	-3.153108	1.314164	4.310342
F	-2.573724	-3.258935	3.395373
F	-1.403838	-2.653780	1.089894
Cl	1.302063	0.628119	2.233817
Cl	-0.232283	-2.746731	-1.811723
C	2.942751	2.814643	-0.379460
O	2.097623	1.828695	-0.978363
C	2.915079	0.966181	-1.782863
C	4.337306	1.050588	-1.197394
C	4.210430	2.051462	-0.034859
H	2.414124	3.228483	0.478309
H	3.127232	3.617253	-1.103425
H	2.479004	-0.029837	-1.737088
H	2.877441	1.314106	-2.818998
H	4.694188	0.078100	-0.856294
H	5.037634	1.412632	-1.952163
H	4.078023	1.529602	0.913401
H	5.078001	2.705994	0.055834
F	-3.472548	-1.288460	5.043133
F	-4.009134	-0.412157	-4.775609
Cl	2.578005	-3.925267	-1.830080

Cl	4.715585	-2.988876	0.223332
Cl	3.984541	-0.841216	2.347336

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4a-8a(THF)

C	-0.339553	-0.316898	1.611707
C	-0.799934	-1.405729	2.374293
C	0.451333	0.579097	2.357327
C	-0.448925	-1.627428	3.701295
C	0.813729	0.393747	3.684315
C	0.374976	-0.731870	4.356494
H	-0.841280	-2.496480	4.212462
H	1.421777	1.138333	4.181317
H	0.647736	-0.894222	5.392248
C	-1.259578	-1.235617	-0.884604
C	-0.516735	-2.406546	-1.013231
C	-2.436893	-1.210184	-1.621706
C	-0.907667	-3.481280	-1.785529
C	-2.852278	-2.287007	-2.397891
C	-2.095622	-3.434837	-2.490349
H	-2.419445	-4.269185	-3.097323
C	-1.560897	1.362646	-0.043807
C	-2.718841	1.419039	0.727661
C	-1.290724	2.518146	-0.758753
C	-3.526589	2.539543	0.802515
C	-2.085001	3.652774	-0.696874
C	-3.216625	3.680471	0.088928
H	-3.842839	4.560431	0.139513
B	-0.670758	-0.009590	0.022711
H	1.532342	-0.188567	-0.055985
O	0.794821	0.232964	-0.593540
C	1.127195	0.119513	-2.001013
H	1.052091	-0.925490	-2.302626
H	0.381663	0.702587	-2.533963
C	2.520448	0.634634	-2.222489
C	3.536479	-0.249182	-2.573639
C	2.820496	1.984684	-2.040096
C	4.837710	0.205993	-2.749305
H	3.309292	-1.302876	-2.697092
C	4.121171	2.438387	-2.208125
H	2.033697	2.671918	-1.755819
C	5.131905	1.550378	-2.562830
H	5.621186	-0.490372	-3.025555
H	4.346859	3.488896	-2.064951
H	6.146612	1.908013	-2.696262
F	-0.132559	-4.569218	-1.847758
F	0.649435	-2.525764	-0.345074

F	-4.001820	-2.194926	-3.071179
F	-3.241977	-0.142221	-1.621262
F	-0.210654	2.600657	-1.564159
F	-1.739339	4.729302	-1.412466
F	-4.620611	2.510266	1.569138
F	-3.107479	0.339170	1.420244
Cl	1.049807	2.088519	1.665819
Cl	-1.935595	-2.590036	1.750322
C	3.970818	0.061951	0.826358
O	2.831871	-0.778006	0.617187
C	2.834357	-1.839994	1.587970
C	3.861819	-1.443178	2.659679
C	4.195781	0.016945	2.327494
H	3.730827	1.049032	0.433129
H	4.825381	-0.342485	0.271024
H	1.822004	-1.925231	1.979800
H	3.094456	-2.773798	1.084296
H	3.456587	-1.559257	3.665360
H	4.756851	-2.064900	2.581590
H	3.500886	0.697947	2.822653
H	5.212851	0.295198	2.606918

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1a-H₂O(THF)

F	-2.517678	0.194112	-2.187226
F	-4.781729	-1.228459	-2.116427
F	-5.103018	-3.203856	-0.269813
F	-3.112461	-3.728513	1.496057
F	-0.851866	-2.341341	1.444909
F	-0.214563	2.597407	-1.956966
F	-0.991511	4.912377	-0.930312
F	-1.885321	5.068059	1.635008
F	-1.968259	2.825444	3.166423
F	-1.162016	0.481261	2.163970
F	0.837921	-2.617525	-1.194597
F	2.969718	-3.835391	-0.169417
F	4.425782	-2.635997	1.788037
F	3.730848	-0.155411	2.649900
F	1.650371	1.097860	1.625651
O	0.110147	-0.004071	-2.009085
C	-1.569112	-1.019947	-0.387988
C	-2.625170	-0.790794	-1.257493
C	-3.812371	-1.499002	-1.248012
C	-3.976925	-2.503554	-0.308238
C	-2.957557	-2.768535	0.590385
C	-1.783030	-2.031280	0.538614
C	-0.651269	1.420147	0.065911

C	-0.637272	2.592476	-0.671839
C	-1.038797	3.821879	-0.169522
C	-1.495038	3.903614	1.132969
C	-1.537663	2.756628	1.911580
C	-1.124118	1.555173	1.366774
C	1.102843	-0.714383	0.182483
C	1.520443	-1.974029	-0.240070
C	2.619886	-2.634242	0.280211
C	3.362019	-2.027705	1.281199
C	3.000362	-0.767685	1.722082
C	1.895417	-0.137434	1.166372
B	-0.243830	-0.069739	-0.470284
H	0.998887	0.458042	-2.211982
H	-0.597416	0.393404	-2.529983
C	3.371128	0.009109	-2.703501
O	2.353469	0.999380	-2.460446
C	2.835259	2.017375	-1.553212
C	4.314657	1.712799	-1.344695
C	4.390219	0.203984	-1.593109
H	3.800722	0.193409	-3.692584
H	2.892467	-0.971957	-2.697341
H	2.644102	2.989792	-2.006191
H	2.268169	1.940296	-0.622477
H	4.923919	2.250594	-2.075444
H	4.648907	1.994538	-0.345830
H	4.084984	-0.345834	-0.702144
H	5.386050	-0.133890	-1.880519

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1e-H₂O(THF)

F	-1.506771	2.540928	1.647887
F	-1.695055	4.986637	0.654910
F	0.714465	3.673402	-3.160013
F	0.887193	1.194604	-2.205345
F	-0.490012	-2.502090	1.215675
F	-2.343174	-4.242472	0.449059
F	-4.010812	-1.125874	-2.644304
F	-2.235383	0.654936	-1.852812
O	-0.479840	0.138457	1.850049
C	1.453872	-0.273418	0.217347
C	1.968265	-1.245460	-0.653916
C	3.302769	-1.666048	-0.616603
C	4.191199	-1.086520	0.286899
C	3.744062	-0.063346	1.118801
C	2.403974	0.321023	1.058845
C	-0.286737	1.739156	-0.232671
C	-0.941145	2.760685	0.438826

C	-1.054716	4.053867	-0.045748
C	-0.488887	4.370087	-1.267583
C	0.175478	3.385466	-1.980441
C	0.261806	2.107588	-1.455437
C	-1.252527	-0.832519	-0.277298
C	-1.346043	-2.112838	0.262378
C	-2.284061	-3.048060	-0.134759
C	-3.180330	-2.723183	-1.139398
C	-3.128987	-1.463579	-1.708030
C	-2.185308	-0.545992	-1.265291
B	-0.130458	0.201878	0.303762
H	-0.025425	0.813302	2.370109
H	-1.471557	0.127467	2.072995
Cl	1.957447	1.680784	2.088552
Cl	0.982455	-1.947812	-1.905440
C	-3.937707	0.594066	1.609616
O	-2.923835	-0.011408	2.436875
C	-3.383318	-1.266074	2.978496
C	-4.868580	-1.329568	2.645842
C	-4.953627	-0.508980	1.356883
H	-4.368517	1.435456	2.158933
H	-3.459980	0.969297	0.704188
H	-3.174688	-1.269538	4.048911
H	-2.822459	-2.076368	2.504607
H	-5.216778	-2.355481	2.524033
H	-5.457533	-0.858031	3.436739
H	-4.653746	-1.112871	0.498149
H	-5.951187	-0.113943	1.164201
F	-4.104332	-3.595156	-1.521497
F	-0.584637	5.601193	-1.752676
Cl	3.875130	-2.900856	-1.682368
Cl	5.834914	-1.609837	0.358967
Cl	4.852612	0.703712	2.201726

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4a-H₂O(THF)

F	0.122640	2.510679	-1.094095
F	-1.376677	4.642391	-0.618403
F	-4.463224	1.983176	1.729275
F	-2.985349	-0.164097	1.277480
F	0.172194	1.242362	2.260398
F	2.423400	1.050972	3.612993
F	3.998170	-2.220267	0.625927
F	1.731379	-2.074844	-0.743056
O	0.200021	-0.072575	-1.718249
C	-1.389894	-1.613831	-0.455143
C	-2.248123	-1.769225	-1.552905

C	-3.010740	-2.894344	-1.818778
C	-2.955226	-3.959032	-0.936972
C	-2.175046	-3.855642	0.199907
C	-1.432508	-2.704117	0.426109
C	-1.386785	1.056797	0.024237
C	-1.029640	2.326928	-0.408947
C	-1.791040	3.455496	-0.161666
C	-2.966130	3.361301	0.555589
C	-3.340498	2.116007	1.018213
C	-2.564577	0.996112	0.760027
C	0.850937	-0.381413	0.661986
C	1.086818	0.383529	1.798329
C	2.263492	0.285135	2.530730
C	3.265903	-0.583314	2.151991
C	3.051290	-1.363723	1.032818
C	1.872956	-1.262270	0.317272
B	-0.475474	-0.263258	-0.280559
H	-0.426402	0.203204	-2.398854
H	1.068405	0.440901	-1.776158
Cl	-0.602689	-2.673233	1.975178
Cl	-2.500788	-0.442140	-2.714705
C	3.131664	1.842921	-1.029106
O	2.495524	0.971868	-1.983318
C	3.452417	0.058367	-2.557058
C	4.739455	0.260817	-1.766074
C	4.619628	1.718978	-1.316697
H	2.727599	2.844266	-1.169513
H	2.887439	1.496665	-0.020495
H	3.577197	0.321061	-3.611707
H	3.050207	-0.952361	-2.480555
H	4.766785	-0.407722	-0.903744
H	5.625917	0.069955	-2.371740
H	5.226937	1.948533	-0.440566
H	4.910410	2.394992	-2.125493
H	-3.536994	-4.853544	-1.122389
H	-2.145443	-4.656504	0.926780
H	-3.641495	-2.926221	-2.697179
H	-3.568648	4.235946	0.758642
H	4.181273	-0.662108	2.722425

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1a-H₂O(THF)₂

F	-0.376667	1.011171	2.716337
F	-1.029031	3.490929	3.384210
F	-0.776471	5.519853	1.596720
F	0.178274	5.008204	-0.895935
F	0.864086	2.526492	-1.588065

F	2.943944	1.629218	1.026160
F	5.466836	1.185631	0.322796
F	6.089546	-0.805498	-1.415299
F	4.111624	-2.366021	-2.442796
F	1.567772	-1.946732	-1.742436
F	-2.270710	-0.306328	0.413097
F	-3.415183	-2.219868	1.859393
F	-1.888846	-4.053022	3.170571
F	0.819677	-3.882280	3.038162
F	1.988395	-1.967170	1.644281
O	-0.189536	0.029118	-1.409842
C	0.223286	1.634938	0.504746
C	-0.239366	1.952865	1.774494
C	-0.578803	3.243298	2.156606
C	-0.445368	4.281041	1.251010
C	0.042669	4.016897	-0.017718
C	0.377536	2.717379	-0.355521
C	2.129055	-0.101408	-0.374955
C	3.173521	0.650354	0.141248
C	4.501473	0.431558	-0.197038
C	4.823365	-0.583071	-1.080813
C	3.813970	-1.373091	-1.606659
C	2.505631	-1.118180	-1.240174
C	-0.079077	-1.054447	0.916382
C	-1.456539	-1.183053	1.038619
C	-2.083482	-2.159789	1.787352
C	-1.311369	-3.094513	2.457157
C	0.066763	-3.004393	2.383451
C	0.653726	-1.993708	1.630474
B	0.559914	0.128119	-0.019850
H	-0.915421	0.691470	-1.544036
H	-0.529903	-0.870988	-1.667028
C	-1.159048	-3.474373	-1.591622
O	-1.404096	-2.148691	-2.097183
C	-2.807624	-1.924595	-2.281881
C	-3.502284	-3.029373	-1.500307
C	-2.507656	-4.185565	-1.638960
H	-0.778103	-3.386761	-0.570353
H	-0.393476	-3.939478	-2.212497
H	-3.037069	-0.922003	-1.916082
H	-3.035513	-1.980154	-3.352621
H	-3.619276	-2.740588	-0.454793
H	-4.488772	-3.264245	-1.901633
H	-2.641772	-4.688240	-2.600454
H	-2.606223	-4.929586	-0.847917
C	-2.969196	2.348477	-0.925344
O	-2.112283	1.724682	-1.880881

C	-2.818052	1.684543	-3.121156
C	-4.311991	1.566791	-2.755402
C	-4.338983	1.752632	-1.223295
H	-2.582875	2.120412	0.066066
H	-2.949576	3.434512	-1.081993
H	-2.609191	2.603023	-3.678857
H	-2.432396	0.836650	-3.689030
H	-4.891687	2.339625	-3.262190
H	-4.725602	0.600681	-3.048632
H	-4.433111	0.790886	-0.714818
H	-5.154425	2.394811	-0.889563

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1e-H₂O(THF)₂

F	-2.921090	0.774887	-0.483460
F	-3.928115	2.833053	-1.840426
F	0.415035	4.210301	-2.991085
F	1.444072	2.191660	-1.633504
F	0.245241	-2.242488	1.470903
F	-0.770711	-4.674901	1.128471
F	-2.872650	-3.255472	-2.828198
F	-1.863317	-0.831819	-2.522221
O	-0.762660	0.346763	1.289119
C	1.488619	-0.050684	-0.039205
C	2.175381	-0.655572	-1.102476
C	3.523943	-1.004803	-1.047090
C	4.258952	-0.713391	0.100892
C	3.645711	-0.019016	1.139855
C	2.291620	0.320390	1.042429
C	-0.690526	1.337856	-1.033271
C	-2.056482	1.591752	-1.109800
C	-2.610100	2.652238	-1.801265
C	-1.769086	3.539832	-2.454337
C	-0.401191	3.348193	-2.390720
C	0.110626	2.268473	-1.681694
C	-0.777909	-1.397092	-0.489084
C	-0.519703	-2.445951	0.385528
C	-1.029712	-3.723380	0.230364
C	-1.842063	-4.000176	-0.854774
C	-2.108629	-2.996775	-1.770558
C	-1.578612	-1.729312	-1.575172
B	-0.157209	0.084615	-0.129322
H	-1.540493	-0.218124	1.565668
H	-0.963824	1.302154	1.498452
Cl	1.663881	1.327866	2.328913
Cl	1.348616	-0.921234	-2.613827
C	-3.840494	-1.484859	1.427470

O	-2.717161	-1.042857	2.210765
C	-2.440910	-1.974328	3.274737
C	-3.314673	-3.190116	2.990583
C	-4.507781	-2.566612	2.263130
H	-4.472480	-0.620557	1.226115
H	-3.470107	-1.880202	0.477360
H	-1.372919	-2.192908	3.270439
H	-2.708455	-1.496815	4.222553
H	-2.792186	-3.894494	2.340440
H	-3.594700	-3.716501	3.903495
H	-5.056334	-3.280896	1.648400
H	-5.203844	-2.122213	2.979908
C	-0.745076	3.903052	1.248480
O	-1.356977	2.782551	1.916453
C	-1.399682	3.005263	3.336061
C	-0.492583	4.202021	3.589085
C	-0.664550	5.003757	2.297052
H	-1.362274	4.160665	0.387149
H	0.248405	3.601899	0.902400
H	-2.435585	3.213337	3.621626
H	-1.070051	2.091190	3.835002
H	0.545928	3.879848	3.701129
H	-0.778851	4.756949	4.483048
H	0.158138	5.692951	2.105775
H	-1.595598	5.576396	2.324268
F	-2.359001	-5.212805	-1.012961
F	-2.273198	4.571107	-3.121326
Cl	4.295635	-1.792224	-2.379611
Cl	5.919990	-1.176721	0.215381
Cl	4.575921	0.411509	2.535592

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4a-H₂O(THF)₂

F	2.564235	-0.550422	-1.438593
F	4.925812	-0.027400	-0.346803
F	2.896258	0.434390	3.867779
F	0.547271	-0.151567	2.828875
F	-0.660147	1.859306	1.069555
F	-2.847083	2.464327	2.459576
F	-4.399336	-1.944651	1.958204
F	-2.238795	-2.583669	0.596893
O	-0.004889	0.443027	-1.247498
C	0.041472	-2.138189	-0.868360
C	-0.489392	-2.404861	-2.137273
C	-0.321364	-3.599743	-2.822869
C	0.373237	-4.634211	-2.222941
C	0.833061	-4.475743	-0.927769

C	0.643190	-3.262772	-0.282974
C	1.427457	-0.355073	0.632756
C	2.601086	-0.321616	-0.114355
C	3.840357	-0.046877	0.440014
C	3.965786	0.225299	1.786535
C	2.819630	0.195032	2.555397
C	1.586429	-0.092492	1.988723
C	-1.335887	-0.391812	0.761322
C	-1.570162	0.882309	1.271516
C	-2.696829	1.214664	1.996162
C	-3.678030	0.271427	2.236170
C	-3.479491	-1.000487	1.744013
C	-2.332701	-1.322686	1.024103
B	0.005775	-0.674882	-0.128994
H	0.582519	1.225673	-1.072050
H	-0.894241	0.809584	-1.496812
Cl	1.115077	-3.251310	1.413185
Cl	-1.544571	-1.247926	-2.952868
C	2.182739	2.742641	-2.346206
O	1.420433	2.593785	-1.143001
C	2.156771	3.127039	-0.026821
C	3.577440	3.406440	-0.539028
C	3.631627	2.687275	-1.893671
H	1.937483	3.705015	-2.811684
H	1.893397	1.933331	-3.017147
H	1.652239	4.029963	0.324783
H	2.127372	2.380812	0.767180
H	3.731604	4.479965	-0.670721
H	4.335451	3.039992	0.153880
H	4.306403	3.171700	-2.600474
H	3.946930	1.650701	-1.777098
C	-3.537754	1.456919	-1.479538
O	-2.175205	1.769231	-1.803776
C	-1.979104	3.182880	-1.752282
C	-2.934065	3.660567	-0.670540
C	-4.141468	2.731579	-0.864927
H	-3.522449	0.613186	-0.788296
H	-4.057809	1.150662	-2.391140
H	-0.925608	3.356967	-1.528725
H	-2.221458	3.619917	-2.729531
H	-2.485291	3.516934	0.312094
H	-3.193374	4.714729	-0.778446
H	-4.863453	3.179712	-1.551226
H	-4.655353	2.524477	0.074294
H	1.322116	-5.287355	-0.405361
H	0.519880	-5.571421	-2.745897
H	-0.750565	-3.714048	-3.809590

H	4.929893	0.436703	2.228359
H	-4.564028	0.517991	2.805097

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TS_{HH-THF}

C	0.848182	-0.158729	0.852954
C	2.045295	0.543917	0.780295
C	0.812364	-1.176911	1.798386
C	3.143925	0.247042	1.566928
C	1.905147	-1.484266	2.596814
C	3.088469	-0.780764	2.486214
C	-0.760027	1.827860	-0.001153
C	-0.829311	2.730563	-1.066847
C	-1.041548	2.402970	1.245463
C	-1.091251	4.085566	-0.923704
C	-1.308324	3.749234	1.435587
C	-1.319114	4.597966	0.341158
C	-1.605868	-0.784758	-0.296424
C	-2.946559	-0.465318	-0.119973
C	-1.354527	-2.094308	-0.690206
C	-3.958255	-1.399539	-0.307996
C	-2.347694	-3.034081	-0.883862
C	-3.672764	-2.692729	-0.691322
F	-3.326250	0.764176	0.240140
F	-5.227418	-1.029358	-0.116343
F	-2.021853	-4.275420	-1.258728
F	-0.079821	-2.486861	-0.889647
F	2.181147	1.537871	-0.118017
F	4.275785	0.944833	1.406232
F	1.804744	-2.473666	3.486999
F	-0.298963	-1.889615	1.995785
O	1.831996	-0.742224	-2.110771
C	2.750006	-1.704969	-1.538734
C	2.536575	0.216109	-2.940490
C	4.114732	-1.053332	-1.678860
H	2.437365	-1.895950	-0.514548
H	2.667509	-2.627161	-2.119104
C	3.971624	-0.292871	-2.999668
H	2.461055	1.191488	-2.458410
H	2.039072	0.247025	-3.909711
H	4.294824	-0.357796	-0.856558
H	4.920381	-1.787878	-1.692528
H	4.686317	0.523855	-3.101312
H	4.103109	-0.972345	-3.845788
H	0.032496	0.296852	-1.388948
H	0.758313	-0.210193	-1.440794
B	-0.377011	0.255409	-0.131559

Cl	-0.620677	2.181345	-2.733894
Cl	-1.152100	1.389002	2.674431
H	-1.517029	4.118912	2.430887
H	-1.524004	5.653516	0.471922
H	-1.122785	4.722688	-1.797588
H	3.939179	-1.020551	3.109285
H	-4.462291	-3.417164	-0.837121

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TS_{HH-5}

C	-0.987310	1.789670	0.267566
C	-1.459079	2.277501	1.494850
C	-0.708649	2.796050	-0.664807
C	-1.588119	3.625433	1.792727
C	-0.823229	4.155082	-0.410508
C	-1.255316	4.569983	0.836527
C	-2.003808	-0.493245	-0.856698
C	-3.322325	-0.060344	-0.832147
C	-1.746704	-1.591282	-1.668445
C	-4.316760	-0.687111	-1.571362
C	-2.724307	-2.224233	-2.412389
C	-4.030215	-1.774641	-2.370099
C	-0.106575	-0.644659	1.153984
C	-0.613122	-1.826885	1.679642
C	1.075232	-0.196451	1.732505
C	0.020309	-2.508395	2.709256
C	1.724282	-0.867646	2.751975
C	1.197252	-2.039236	3.257198
F	-1.762196	-2.341581	1.231872
F	-0.522833	-3.635736	3.175837
F	2.866401	-0.375948	3.244743
F	1.646242	0.943335	1.284398
F	-3.690064	0.982933	-0.080328
F	-5.569169	-0.224945	-1.503543
F	-2.402480	-3.276336	-3.172672
F	-0.492554	-2.076516	-1.736039
Cl	-2.004324	1.173946	2.746361
Cl	-0.207325	2.387119	-2.313104
H	-4.806092	-2.262741	-2.943851
H	1.688660	-2.572761	4.059250
H	-1.352159	5.626217	1.056353
H	-0.586124	4.870945	-1.186465
H	-1.959854	3.924065	2.764050
C	2.790973	0.244308	-1.163377
C	4.226200	0.058185	-1.263473
C	5.048008	1.184774	-1.348175
C	4.779911	-1.227264	-1.263268

C	6.422488	1.028433	-1.434866
H	4.606622	2.175949	-1.341858
C	6.151658	-1.376534	-1.350449
H	4.122386	-2.085420	-1.193091
C	6.969058	-0.250216	-1.436025
H	7.066756	1.896526	-1.499201
H	6.591304	-2.366405	-1.350543
H	8.044104	-0.372954	-1.502643
H	0.753257	-0.219418	-0.931393
O	1.995927	-0.689259	-1.080948
H	0.047925	0.330052	-1.052664
B	-0.794984	0.206412	-0.043117
H	2.409494	1.275353	-1.159404

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[4aH]⁻[THF-H]⁺

C	-1.285401	-0.766290	0.479450
C	-2.512834	-0.123416	0.405603
C	-1.279129	-1.937594	1.226518
C	-3.660122	-0.593888	1.018598
C	-2.417982	-2.427603	1.848317
C	-3.624720	-1.762029	1.753197
C	-0.030401	-0.008527	-1.868518
C	0.556730	1.070163	-2.541693
C	-0.645664	-0.924658	-2.732702
C	0.509668	1.275129	-3.912120
C	-0.726347	-0.761786	-4.108846
C	-0.154931	0.351513	-4.700504
C	1.439391	-0.590586	0.364441
C	2.365919	-1.381563	-0.299001
C	1.814081	-0.180362	1.634916
C	3.586659	-1.723142	0.267408
C	3.025170	-0.503957	2.215921
C	3.933596	-1.287276	1.530867
F	2.103817	-1.857717	-1.521388
F	4.438032	-2.487717	-0.423754
F	3.314748	-0.053898	3.444799
F	0.958101	0.580390	2.366257
F	-2.619186	1.030257	-0.298038
F	-4.804115	0.092811	0.900602
F	-2.345129	-3.565318	2.546763
F	-0.161651	-2.665502	1.343876
O	-0.735377	2.729608	1.299334
C	-1.367805	3.633310	0.306565
C	0.422148	3.389324	1.936774
C	-0.488472	4.871232	0.309707
H	-1.395368	3.089032	-0.634599

H	-2.376657	3.800486	0.676920
C	0.143541	4.858650	1.705539
H	0.428459	3.059939	2.971120
H	1.314614	3.035689	1.419484
H	-1.071949	5.771739	0.119523
H	0.281145	4.786088	-0.459662
H	-0.555485	5.237634	2.455048
H	1.059233	5.447116	1.759326
H	-0.019890	1.089887	0.055394
H	-0.443877	1.838941	0.827293
B	0.014501	-0.111571	-0.244255
Cl	1.499339	2.285902	-1.648864
Cl	-1.318400	-2.424917	-2.116778
H	-1.223368	-1.514797	-4.706381
H	-0.208987	0.488438	-5.773696
H	0.995274	2.137773	-4.349082
H	-4.512486	-2.146681	2.236040
H	4.883738	-1.556660	1.971126

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[4aH]⁻[THF-H-THF]⁺

B	-0.575449	0.229653	0.055021
C	-0.252762	1.810379	0.338689
C	0.051410	2.429614	1.559233
C	-0.247134	2.711339	-0.740230
C	0.361803	3.777112	1.701285
C	0.048096	4.063989	-0.648658
C	0.365918	4.599759	0.588532
H	0.579400	4.172811	2.684985
H	0.015239	4.684261	-1.535260
H	0.593744	5.654422	0.687501
C	-0.083886	-0.852212	1.177446
C	-0.896717	-1.652928	1.971673
C	1.270246	-1.112035	1.313708
C	-0.388090	-2.632357	2.816483
C	1.800975	-2.076532	2.144883
C	0.970604	-2.864364	2.915500
H	1.362397	-3.624897	3.576373
C	-2.127223	0.011870	-0.386984
C	-3.194086	0.753792	0.100991
C	-2.462970	-0.951771	-1.324507
C	-4.496468	0.563328	-0.334140
C	-3.755214	-1.160672	-1.772452
C	-4.795285	-0.397495	-1.280711
H	-5.810914	-0.550867	-1.618398
H	0.102345	-0.054494	-0.915291
Cl	-0.653313	2.152352	-2.369150

Cl	0.016111	1.528164	3.071208
F	2.165586	-0.387899	0.587227
F	3.137793	-2.257352	2.175581
F	-1.232373	-3.364172	3.550757
F	-2.224476	-1.494635	1.973189
F	-1.499568	-1.748887	-1.845123
F	-2.993074	1.686854	1.043485
F	-5.479426	1.316835	0.175555
F	-3.994925	-2.111496	-2.688981
O	3.745999	0.532889	-1.615059
C	4.756282	0.551640	-0.561218
C	2.767817	1.623070	-1.423036
C	4.722538	1.988810	-0.078531
H	4.451827	-0.150411	0.216099
H	5.694783	0.243432	-1.018702
C	3.234203	2.342218	-0.168267
H	1.787712	1.163630	-1.322686
H	2.819163	2.233557	-2.323878
H	5.319329	2.623280	-0.738989
H	5.114770	2.077901	0.934458
H	3.051687	3.413868	-0.235946
H	2.693059	1.962276	0.697316
O	2.785768	-1.564885	-2.232637
C	2.780622	-2.727768	-1.355456
C	1.580993	-1.539927	-3.063352
C	1.381801	-3.301286	-1.498022
H	3.549277	-3.410661	-1.725017
H	3.032870	-2.396916	-0.350696
C	1.034577	-2.949441	-2.946442
H	1.891036	-1.251390	-4.066861
H	0.887551	-0.809502	-2.640416
H	0.689278	-2.799923	-0.818490
H	1.360171	-4.372468	-1.297469
H	1.543776	-3.621080	-3.643733
H	-0.035435	-2.976843	-3.139330
H	3.278319	-0.473092	-1.857817

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[4aH]⁻[THF-H-5]⁺

B	0.766107	0.204401	0.253532
C	0.969327	1.653972	-0.464022
C	2.100109	-0.256536	1.082249
C	-0.665218	0.076164	1.040163
C	1.632295	2.718261	0.132549
C	1.825527	3.932074	-0.508330
C	1.347113	4.145060	-1.787286
C	0.673191	3.108882	-2.401185

C	0.502152	1.904265	-1.743156
C	3.266236	-0.593004	0.375944
C	4.427043	-1.097305	0.943307
C	4.474686	-1.284923	2.314422
C	3.380756	-0.928487	3.082572
C	2.244468	-0.417330	2.467366
C	-1.129002	-1.185521	1.404540
C	-2.368485	-1.416773	1.975423
C	-3.233592	-0.369510	2.215336
C	-2.807589	0.896692	1.867504
C	-1.557961	1.108823	1.301349
Cl	3.352315	-0.332838	-1.372940
Cl	0.982275	0.095903	3.583251
F	-0.183830	0.940106	-2.423824
F	0.174820	3.267328	-3.636693
F	2.475085	4.915702	0.124477
F	2.095092	2.603962	1.383925
F	-0.352653	-2.267051	1.192732
F	-2.744300	-2.671288	2.256451
F	-3.627045	1.939143	2.051755
F	-1.262288	2.379681	0.990559
H	1.491117	5.093465	-2.286104
H	5.280752	-1.323250	0.317169
H	5.367508	-1.681026	2.782997
H	3.403439	-1.027760	4.160004
H	-4.210131	-0.533076	2.649025
H	0.677691	-0.615618	-0.645604
O	0.406236	-3.340918	-1.798095
C	1.440401	-3.545809	-0.805226
C	2.695841	-3.865056	-1.618637
C	2.379056	-3.370519	-3.049763
C	1.025966	-2.680449	-2.919014
H	1.550729	-2.630902	-0.223313
H	1.100484	-4.352379	-0.158743
H	3.556596	-3.349611	-1.192499
H	2.905825	-4.935139	-1.618822
H	3.134408	-2.680111	-3.424219
H	2.310652	-4.212163	-3.740727
H	1.131235	-1.616505	-2.687247
H	0.368925	-2.817148	-3.777962
H	-0.858831	-2.952109	-1.470729
O	-1.877132	-2.640928	-1.321046
C	-2.005840	-1.392277	-1.380653
H	-1.121960	-0.783456	-1.589103
C	-3.267397	-0.743292	-1.198727
C	-4.421874	-1.463328	-0.853777
C	-5.601887	-0.782263	-0.635841

C	-5.634486	0.609005	-0.755512
C	-4.495059	1.326256	-1.097886
C	-3.305292	0.652461	-1.319184
H	-4.365944	-2.539515	-0.743953
H	-6.499227	-1.323245	-0.361899
H	-6.562298	1.138020	-0.569851
H	-4.527713	2.405371	-1.171234
H	-2.401482	1.191344	-1.578599

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TS_{act}

C	-0.757818	0.066547	0.885002
C	-1.289876	-1.188416	1.152379
C	-1.620567	1.118295	1.169501
C	-2.550145	-1.408736	1.668522
C	-2.887517	0.923893	1.704231
C	-3.372057	-0.339746	1.964390
C	1.995039	-0.350574	1.133451
C	3.227784	-0.631676	0.517584
C	2.018002	-0.601661	2.515076
C	4.341235	-1.161499	1.153246
C	3.104133	-1.146294	3.192714
C	4.268505	-1.440818	2.507546
C	1.071298	1.627469	-0.424666
C	1.504511	2.684585	0.364650
C	1.005116	1.893824	-1.783235
C	1.840528	3.921583	-0.158427
C	1.333788	3.124825	-2.327673
C	1.757633	4.158418	-1.517730
F	1.591489	2.526484	1.692470
F	2.245620	4.899581	0.660374
F	1.245815	3.306272	-3.653571
F	0.630878	0.927784	-2.656538
F	-0.537993	-2.291502	0.891107
F	-2.981584	-2.661806	1.862681
F	-3.665095	1.988790	1.935754
F	-1.274235	2.390653	0.927129
O	0.690089	-2.961862	-1.405080
C	1.686829	-3.581656	-0.496296
C	1.254716	-2.718023	-2.747941
C	2.900978	-3.813035	-1.383694
H	1.847667	-2.887330	0.324920
H	1.207735	-4.492182	-0.144399
C	2.350350	-3.759775	-2.817185
H	0.426198	-2.842828	-3.437802
H	1.618571	-1.690997	-2.755530
H	3.372397	-4.769695	-1.159925

H	3.632488	-3.021031	-1.227827
H	1.936099	-4.726297	-3.113673
H	3.114328	-3.475238	-3.540214
H	0.689222	-0.610630	-0.733159
H	0.268679	-2.141530	-1.039764
B	0.731687	0.168324	0.214463
Cl	3.472196	-0.284922	-1.202534
Cl	0.662414	-0.186908	3.553870
H	3.030865	-1.317199	4.258855
H	5.121710	-1.857401	3.029067
H	5.251740	-1.334896	0.593828
H	-4.369211	-0.488083	2.353960
H	2.016050	5.123168	-1.932134
C	-2.053900	-0.574068	-1.938380
O	-1.538850	-1.663637	-2.089324
H	-1.466075	0.343948	-2.104168
C	-3.449765	-0.371996	-1.518949
C	-3.922876	0.927385	-1.347340
C	-4.277120	-1.463180	-1.249676
C	-5.221383	1.140036	-0.906218
H	-3.261959	1.768361	-1.533750
C	-5.572828	-1.250110	-0.812077
H	-3.879244	-2.463553	-1.373408
C	-6.042619	0.051044	-0.640417
H	-5.585546	2.148506	-0.754523
H	-6.218519	-2.092810	-0.594542
H	-7.055808	0.215030	-0.290570

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TS_{hydr}

B	-0.081777	0.472078	0.207632
C	-0.981101	1.789146	-0.145442
C	1.308559	0.962137	0.930409
C	-0.884158	-0.776610	0.876380
C	-1.486609	2.597134	0.866649
C	-2.225165	3.741749	0.622116
C	-2.495545	4.144952	-0.672130
C	-2.002976	3.368654	-1.699320
C	-1.262987	2.228408	-1.429078
C	2.301864	1.606623	0.172487
C	3.514211	2.063275	0.668722
C	3.805974	1.875080	2.008898
C	2.869203	1.263241	2.821663
C	1.656856	0.840150	2.286502
C	-0.192531	-1.933355	1.226237
C	-0.799889	-3.065439	1.735031
C	-2.171154	-3.115388	1.891918

C	-2.893413	-2.005973	1.506150
C	-2.264134	-0.873145	1.007700
Cl	2.057460	1.927447	-1.546997
Cl	0.556132	0.150934	3.469666
F	-0.818408	1.545342	-2.516557
F	-2.238325	3.712683	-2.973860
F	-2.685738	4.463693	1.650058
F	-1.278555	2.257901	2.145079
F	1.148030	-1.979646	1.078208
F	-0.051450	-4.132463	2.051782
F	-4.231208	-2.026953	1.585630
F	-3.070077	0.134493	0.636920
H	-3.073268	5.037054	-0.870713
H	4.210564	2.565735	0.009286
H	4.747084	2.220071	2.420360
H	3.059152	1.123048	3.877803
H	-2.661188	-3.996489	2.282486
H	0.276007	-0.012029	-0.867179
O	3.384864	-1.168917	-1.459569
C	3.928140	-1.435562	-0.142099
C	5.367283	-0.944439	-0.208092
C	5.714165	-1.105995	-1.690040
C	4.406754	-0.712345	-2.359758
H	3.316965	-0.912338	0.590530
H	3.863158	-2.512587	0.033669
H	5.414292	0.107232	0.082680
H	6.022806	-1.513723	0.451350
H	6.545870	-0.476696	-2.008577
H	5.960981	-2.146928	-1.917028
H	4.312419	0.371976	-2.468035
H	4.244458	-1.188315	-3.328481
H	2.081369	-1.689515	-1.811551
O	1.160064	-2.149961	-1.898280
C	0.197387	-1.403728	-2.252200
H	0.395047	-0.453782	-2.744890
C	-1.145666	-1.912083	-2.158948
C	-1.373981	-3.178270	-1.600200
C	-2.668726	-3.633453	-1.448594
C	-3.738070	-2.828308	-1.835968
C	-3.517095	-1.575114	-2.395882
C	-2.222948	-1.115065	-2.565223
H	-0.533379	-3.776184	-1.272436
H	-2.852343	-4.603665	-1.004242
H	-4.752979	-3.177380	-1.685320
H	-4.353553	-0.949803	-2.680387
H	-2.038968	-0.130642	-2.972737

2			
H ₂			
H	0.000000	0.000000	0.372200
H	0.000000	0.000000	-0.372200