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Electronic Supplementary Information

H_2 Activation By A Highly Electron-Deficient Aralkylated Organoborane

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Contents

Page

1. Mass spectrometry
   - 1.1 [TMPH][HB(CH(C_6F_5)$_2$)$_3$] (**2**) – ES+ 2
   - 1.2 [TMPH][HB(CH(C_6F_5)$_2$)$_3$] (**2**) – ES– 3

2. X-ray diffraction
   - 2.1 Tris[bis(pentafluorophenyl)methyl]borane, B(CH(C_6F_5)$_2$)$_3$ (**1**) 4

3. NMR spectroscopy
   - 3.1 Bis(pentafluorophenyl)methyl chloride, CHCl(C_6F_5)$_2$
     - ^{1}H, ^{19}F 5
   - 3.2 Tris[bis(pentafluorophenyl)methyl]borane, B(CH(C_6F_5)$_2$)$_3$ (**1**)
     - ^{1}H, ^{19}F, ^{11}B 6
     - ^{13}C 7
   - 3.3 [TMPH][HB(CH(C_6F_5)$_2$)$_3$] (**2**)
     - ^{1}H, ^{19}F 8
     - ^{11}B, ^{11}B (hydride region) 9
     - ^{13}C 10
   - 3.4 Polymerised THF
     - ^{1}H 10

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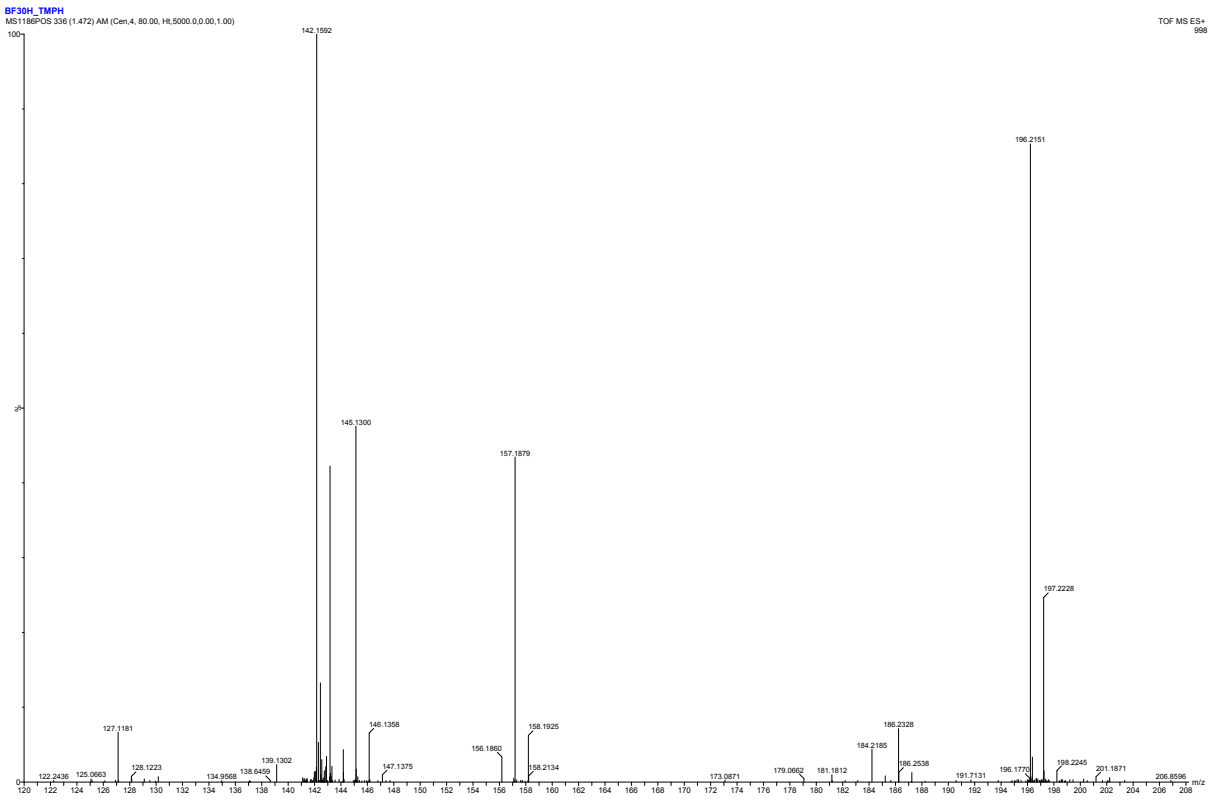
1. Mass spectrometry

1.1 (**2**) [TMPH][HB(CH(C_6F_5)$_2$)$_3$] – ES+



Elemental Composition Report:

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0; Element prediction: Off; Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

94 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 9-9 H: 0-200 N: 0-10 O: 0-20 Na: 0-1

Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
142.1592	142.1596	-0.4	-2.8	0.5	130.7	0.0	C9 H20 N

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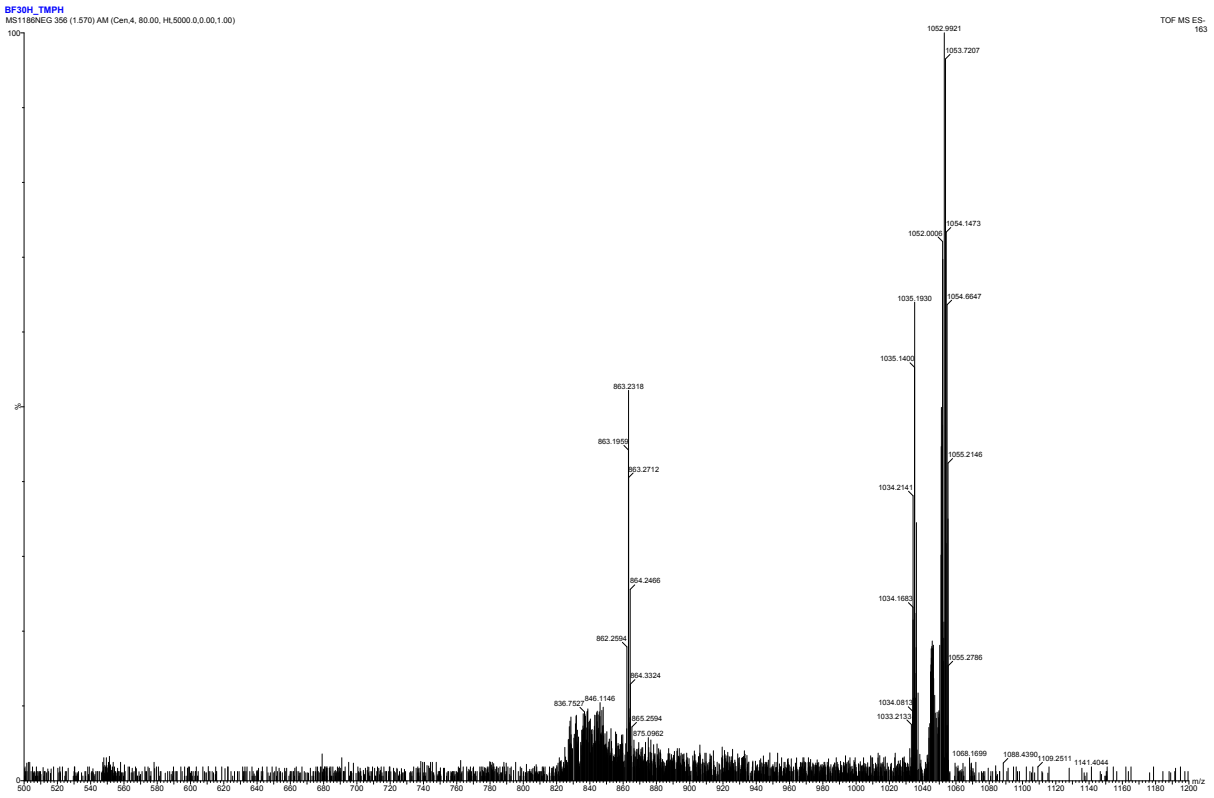
1.3 (**2**) [TMPH][HB(CH(C_6F_5)$_2$)$_3$] – ES–



Elemental Composition Report:

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0; Element prediction: Off; Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

461 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 39-39 H: 0-200 N: 0-10 O: 0-20 Na: 0-1 F: 30-30 11B: 1-1

Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1052.9921	1052.9927	-0.6	-0.6	23.5	107.7	0.0	C39 H4 F30 11B

2. X-ray diffraction

Crystal data and structure refinement for $B(CH(C_6F_5)_2)_3$, (**1**)

Formula	$C_{39}H_3BF_{30}\cdot 1.5(C_7H_8)$	
Formula weight	1190.43	
Temperature	173 K	
Diffractometer, wavelength	OD Xcalibur 3, 0.71073 Å	
Crystal system, space group	Monoclinic, P $2_1/c$	
Unit cell dimensions	a = 24.3971(7) Å	α = 90°
	b = 12.6719(3) Å	β = 92.764(3)°
	c = 14.5724(5) Å	γ = 90°
Volume, Z	4499.9(2) $Å^3$, 4	
Density (calculated)	1.757 Mg/m^3	
Absorption coefficient	0.189 mm^{-1}	
F(000)	2348	
Crystal colour / morphology	Colourless plates	
Crystal size	0.48 x 0.44 x 0.14 mm^3	
θ range for data collection	2.98 to 32.78°	
Index ranges	$-27 \le h \le 36$, $-18 \le k \le 17$, $-21 \le l \le 15$	
Reflns collected / unique	50254 / 15102 [R(int) = 0.0437]	
Reflns observed [$F>4\sigma(F)$]	10074	
Absorption correction	Analytical	
Max. and min. transmission	0.973 and 0.927	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15102 / 126 / 753	
Goodness-of-fit on F^2	1.043	
Final R indices [$F>4\sigma(F)$]	R_1 = 0.0878, wR_2 = 0.2337	
R indices (all data)	R_1 = 0.1244, wR_2 = 0.2535	
Largest diff. peak, hole	0.457, –0.440 $eÅ^{-3}$	
Mean and maximum shift/error	0.000 and 0.001	

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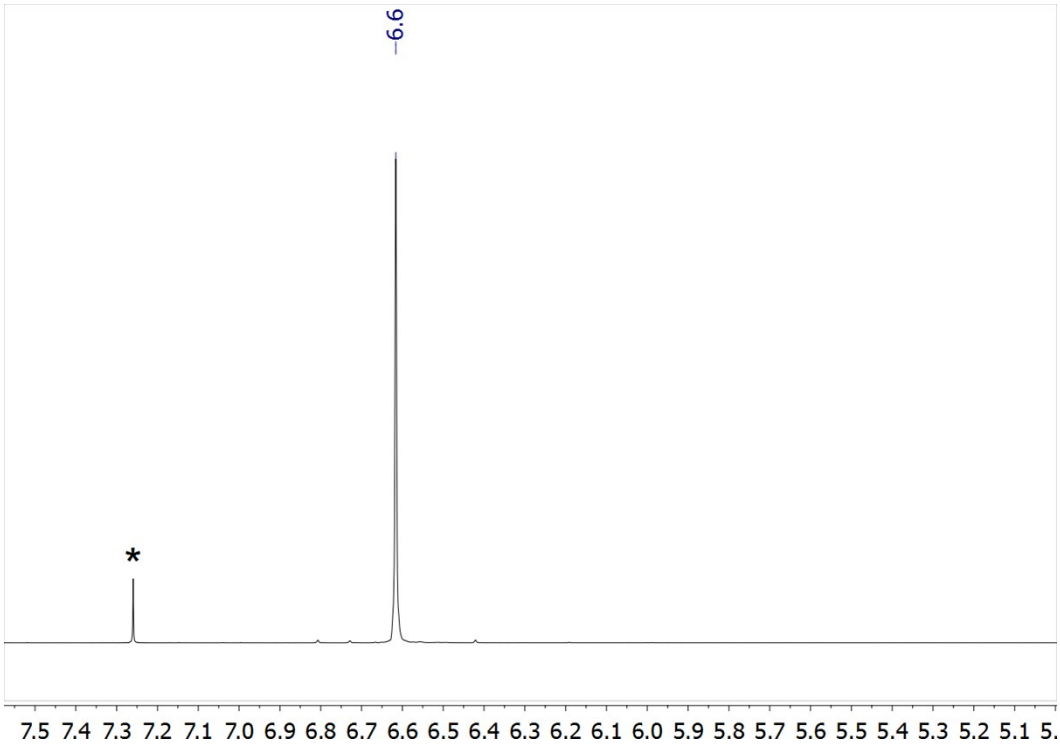
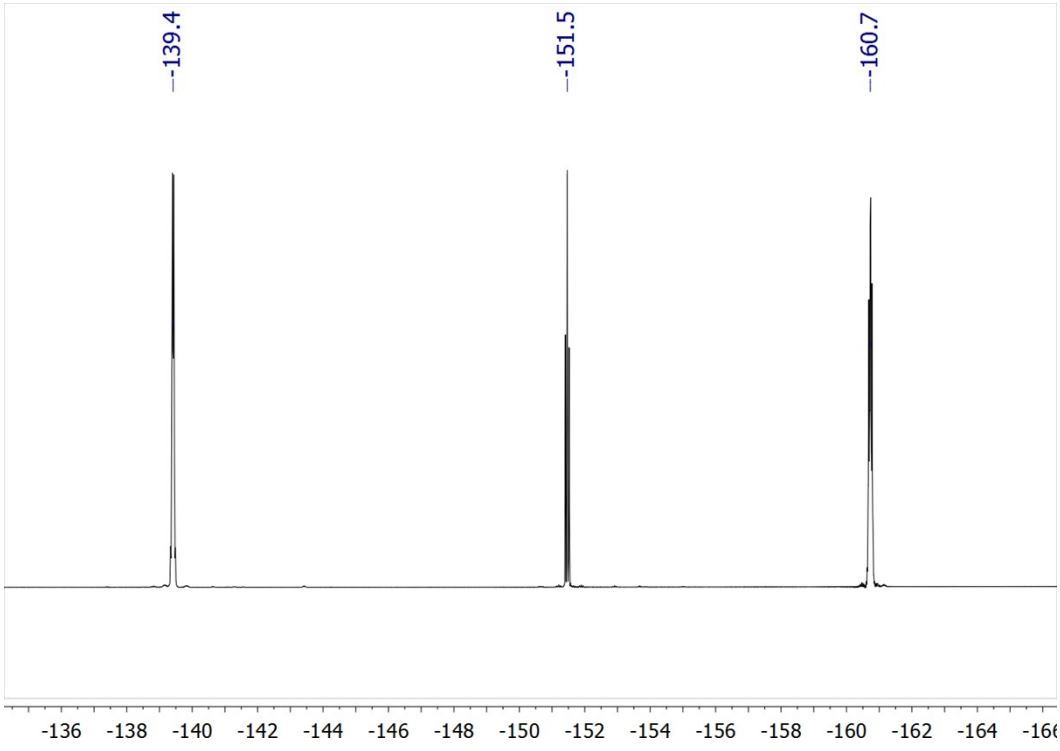
3. NMR

3.1 Bis(pentafluorophenyl)methyl chloride, $CHCl(C_6F_5)_2$

- ^1H NMR ($CDCl_3$, * indicates solvent peak)

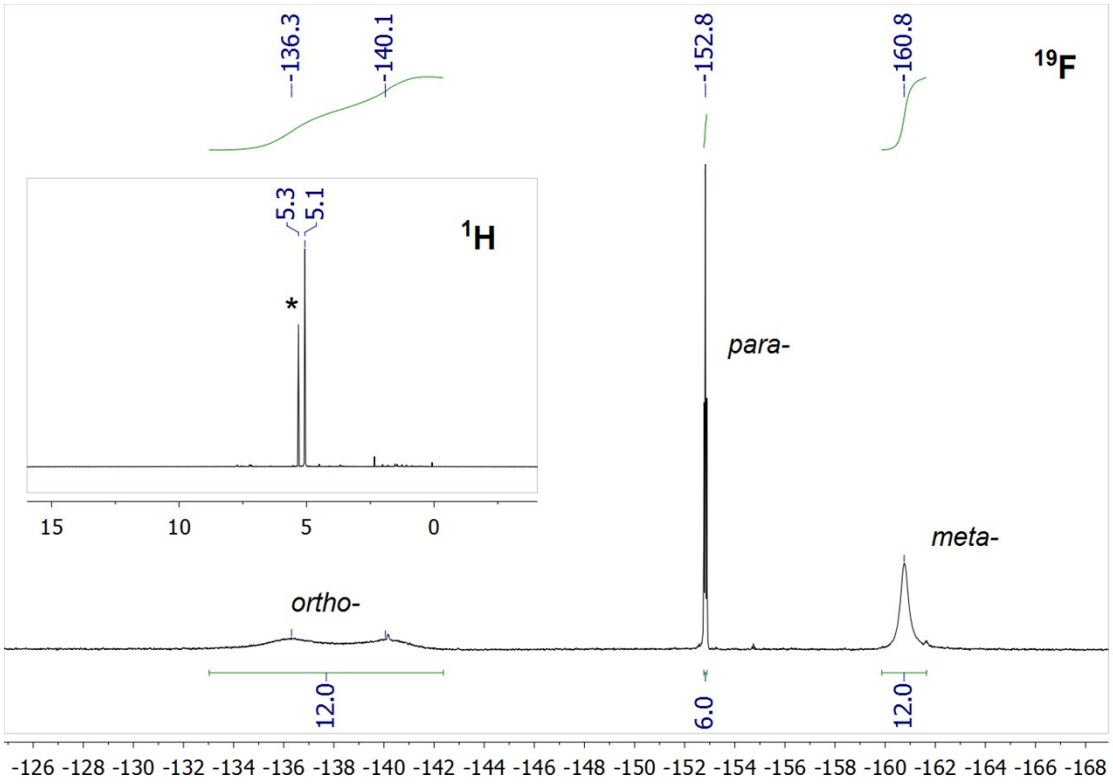


- ^{19}F NMR ($CDCl_3$)

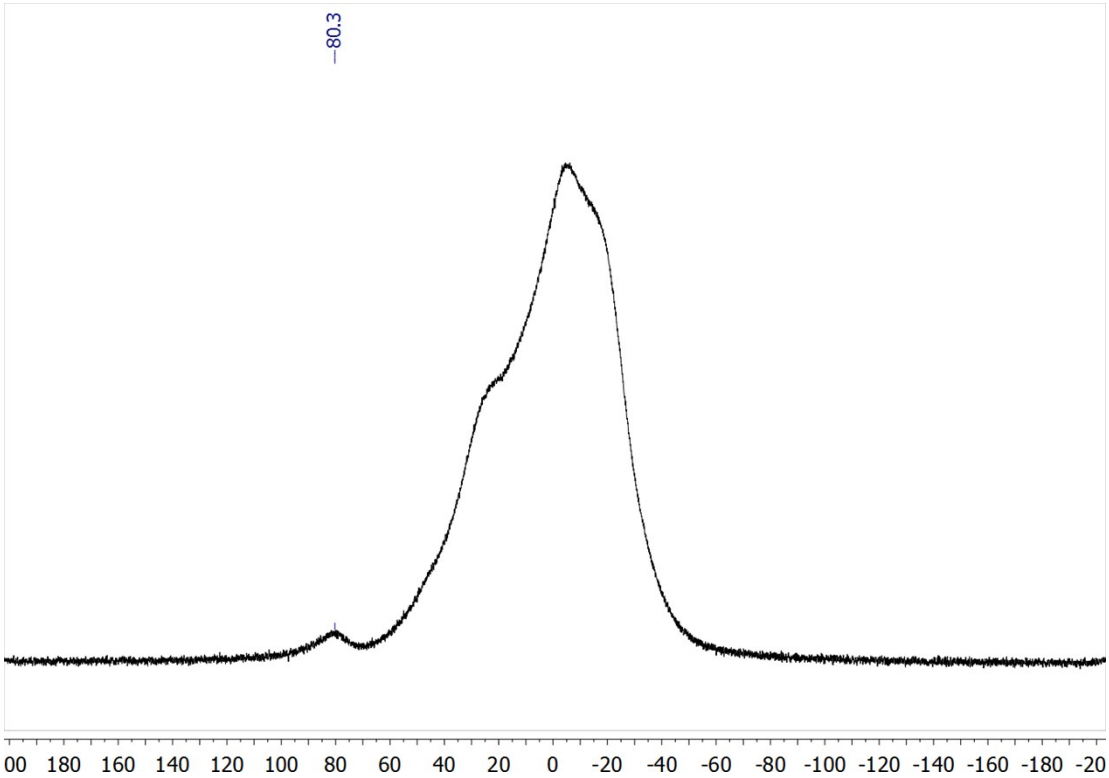


3.2 Tris[bis(pentafluorophenyl)methyl]borane, $B(CH(C_6F_5)_2)_3$ (**1**)

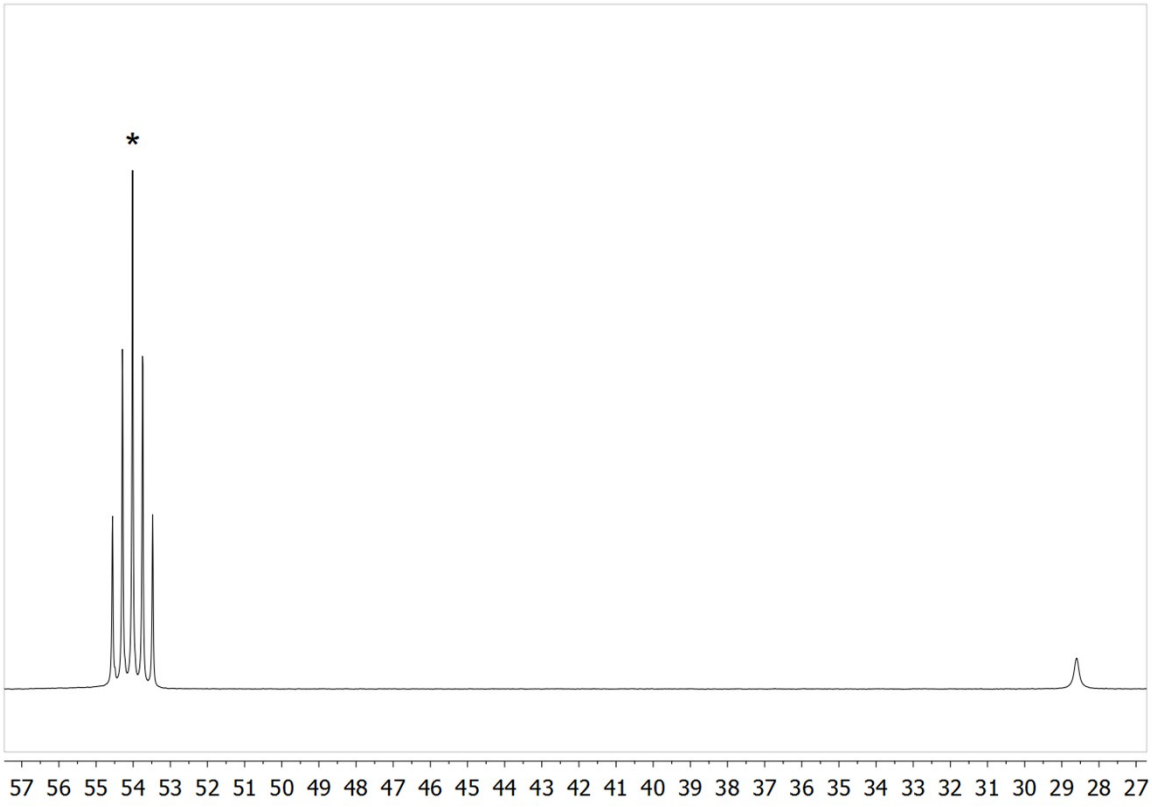
- ^{1}H, ^{19}F NMR (CD_2Cl_2, * indicates solvent peak)



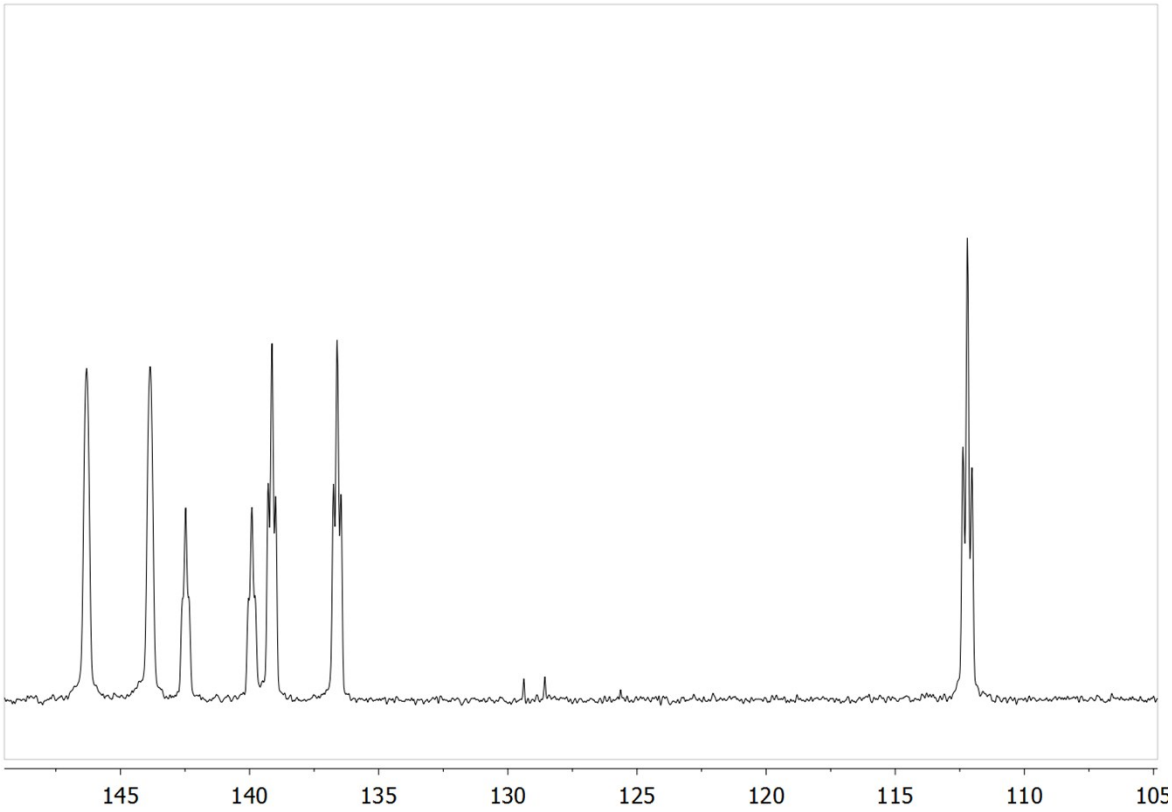
- ^{11}B $\{^{1}H\}$NMR (CD_2Cl_2)



- ^{13}C {^{1}H}NMR (CD_2Cl_2, aliphatic region, * indicates solvent peak)

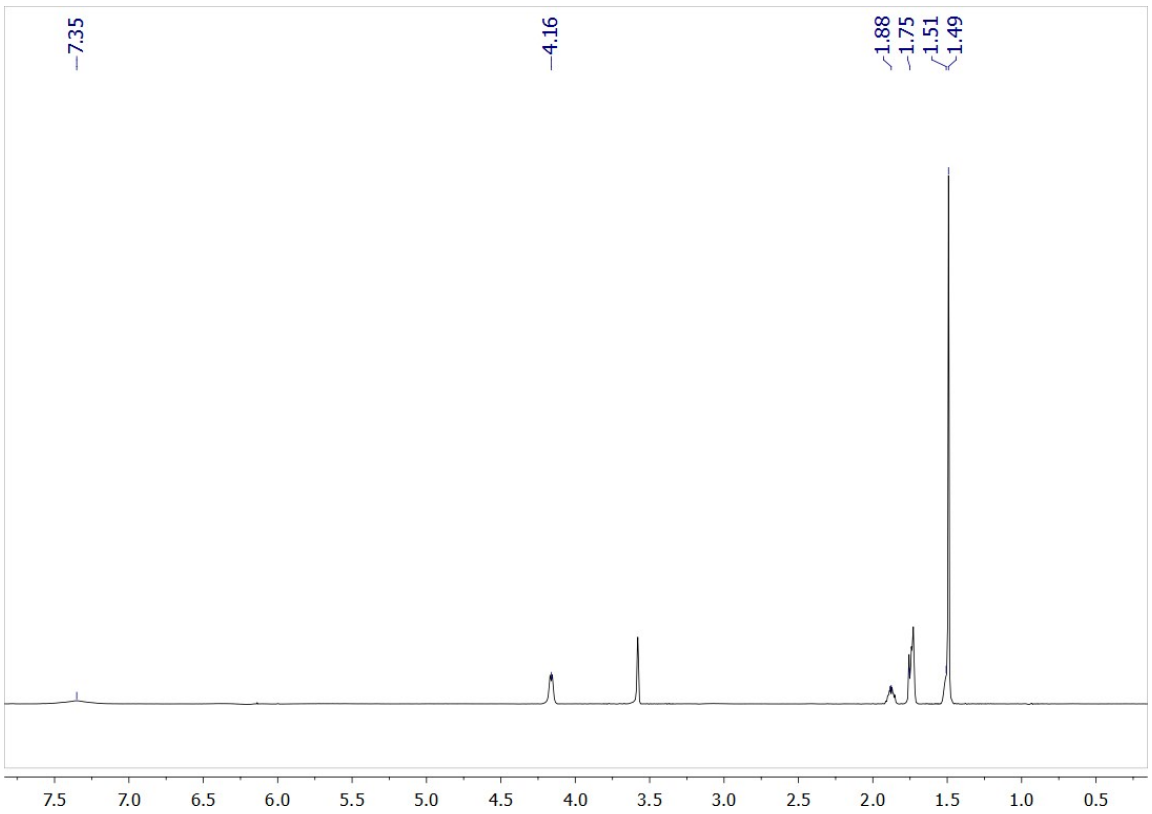


- ^{13}C {^{1}H} NMR (CD_2Cl_2, aromatic region)

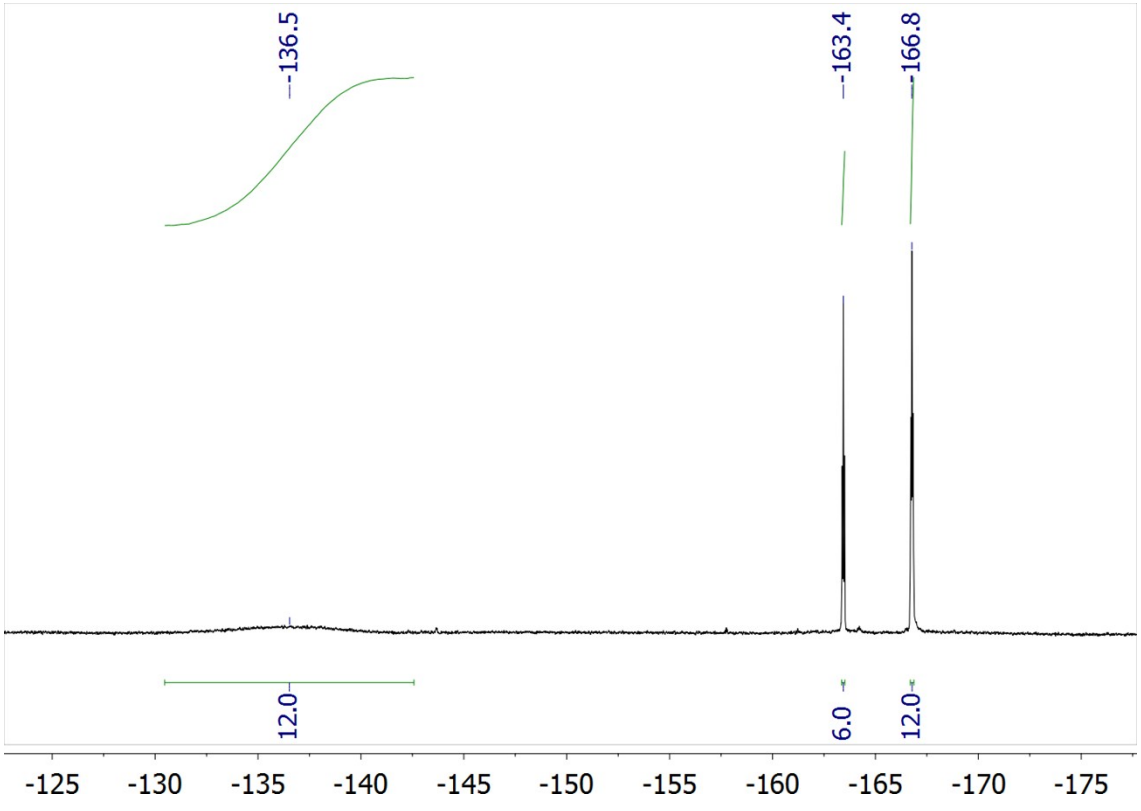


3.3 $[TMPH][HB(CH(C_6F_5)_2)_3]$ (**2**)

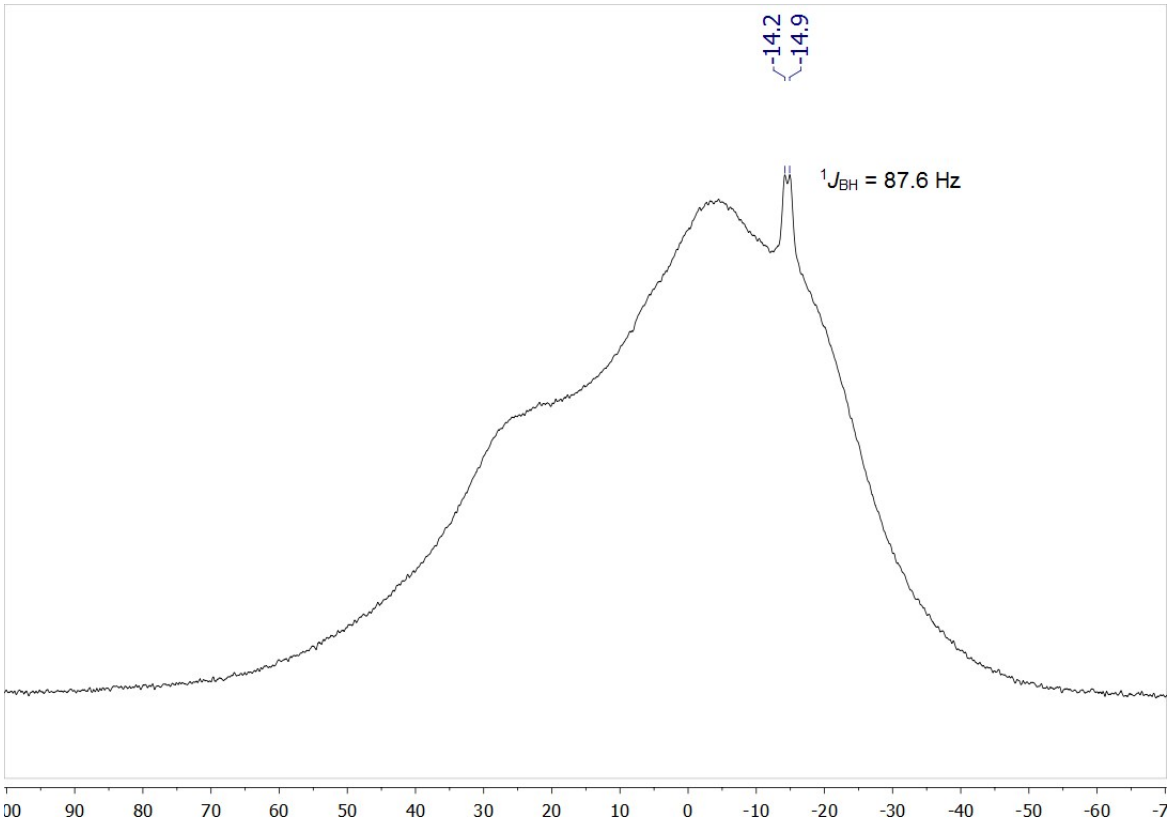
- ^1H NMR (THF-d_8)



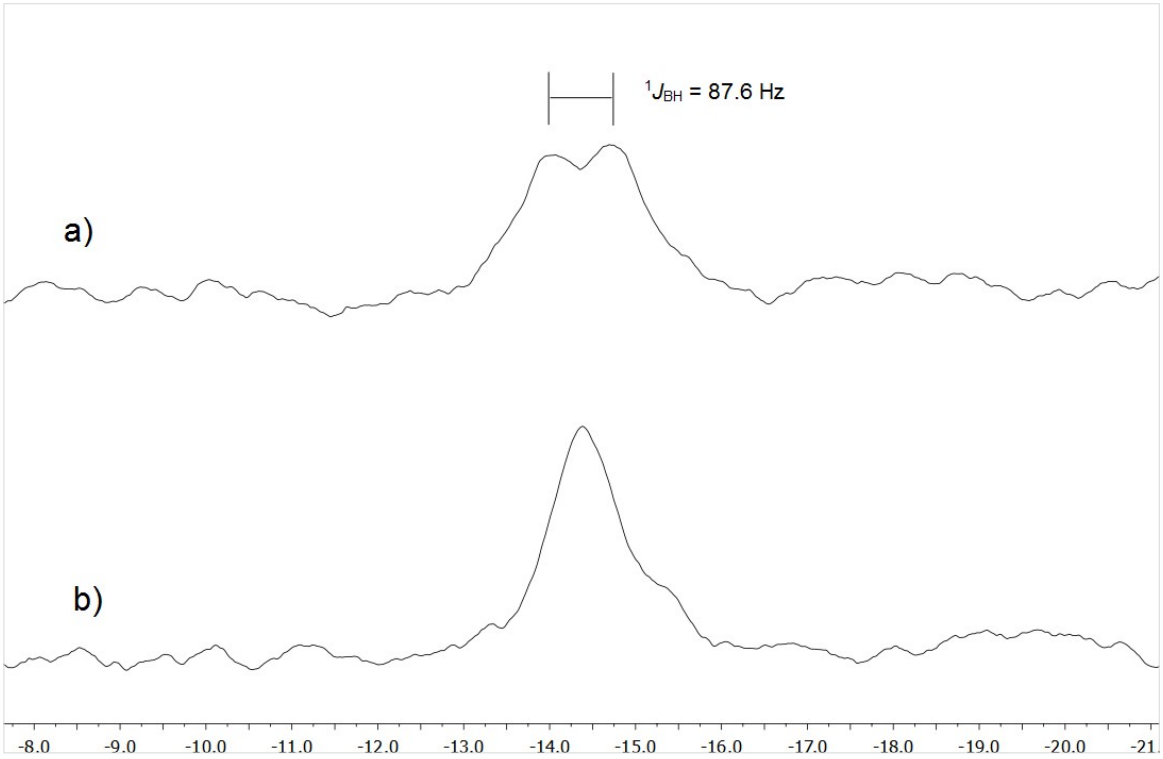
- ^{19}F NMR (THF-d_8)



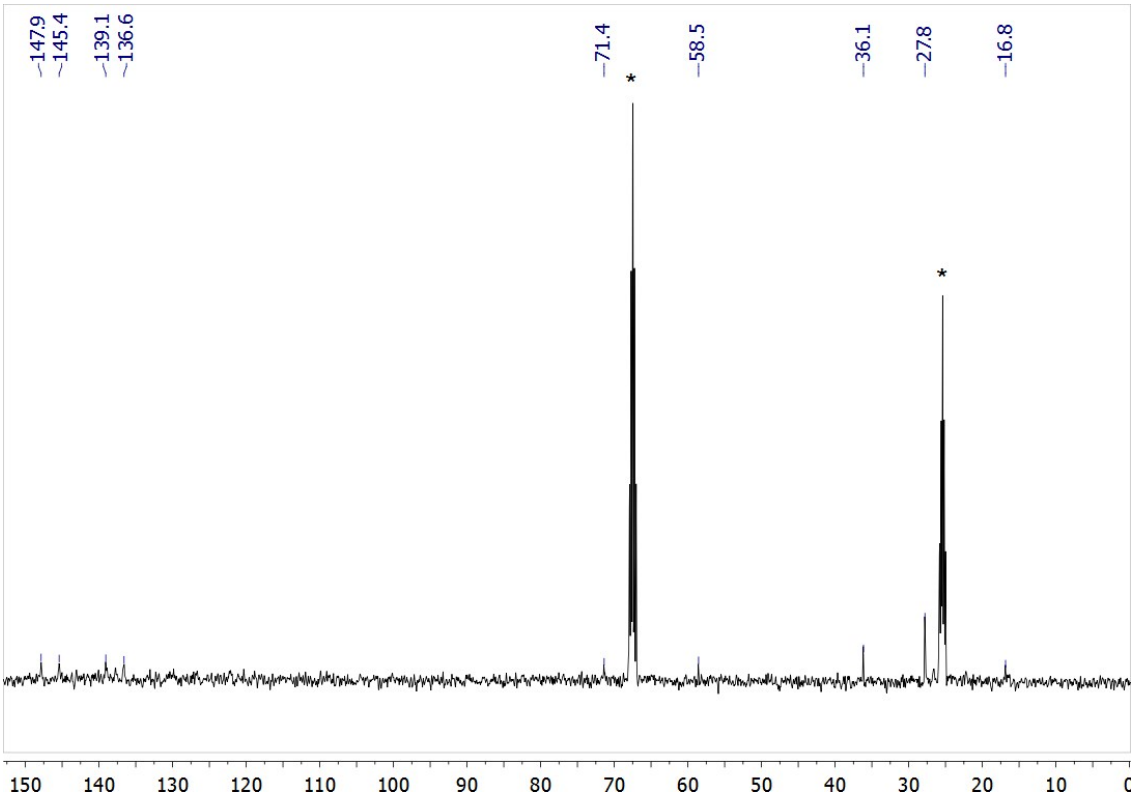
- ^{11}B NMR (THF-d_8)



- a) ^{11}B NMR and b) $^{11}B\{^1H\}$ NMR (THF-d_8) (borohydride region)



- ^{13}C {^{1}H}NMR (THF-d_8, * indicates solvent peak)



3.4 Polymerised THF solvent formed with $B(CH(C_6F_5)_2)_3$ under H_2 (THF, * indicates solvent peak)