Supplementary Information

Complexation of Boron and Aluminum with a Bidentate Hydroxy-BN-naphthalene Ligand

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Abstract: The isoelectronic relationship of 1,2-azaborinine (B=N structural motif) and benzene (C=C) is well documented. Upon deprotonation of the former, the anionic 1,2-azaboratabenzene is obtained, which is isosteric with pyridine (C=N) and has a similar capability as an aromatic *N*-donor. We present the complexation of boron and aluminum precursors with a κ^2-*N*,*O*-donating 8-hydroxy-BN-naphthalene ligand (**H_2(BQ)**, **1**). Six chelate complexes with 1:1 and 2:1 stoichiometries were isolated and characterized by X-ray diffraction analysis and NMR spectroscopy. Comparing the isosteric dimethylaluminum complexes of **H_2(BQ)** and an 8-hydroxyquinoline (**HQ'**, **2**) as reference allowed us to quantify the influence of such a formal substitution of carbon by boron on the structure and the electronic properties: While the structural parameters of the ligands were similar, the electropositive boron atom affected the electron density distributions within the complexes substantially. As the consequence, the Al–N bond was significantly shortened and the aluminum atom showed a different coordination geometry than in the quinoline analog. Moreover, strong hypsochromic shifts of both the absorption and the emission were observed. The results highlight that the differences between CN and BN polyaromatic complexes are more distinct than between equally charged BN and CC congeners.

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1. Investigation of the Hydrolytic Stabilities

The hydrolytic stability of **Li[Me$_2$Al(BQ)]** (**4**) and **[Me$_2$Al(BQ)]$_2$** (**3**) was investigated by NMR and IR spectroscopy as well as mass spectrometry. Using dry THF-d_8 or benzene-d_6 as solvents, we did not observe decomposition products of **4** in the respective ^{1}H NMR spectra. Moreover, crystalline samples could be stored in a glove box for an infinite time without signs of degradation. Also, the **[Me$_2$Al(BQ)]$^-$** anion was detected as the only species by electrospray ionization mass spectrometry (ESI-MS). However, the addition of 1% water in non-dried THF (0.1 mL) both induced the reprotonation of the azaborinine nitrogen atom and the cleavage of the Al-CH$_3$ bonds. In fact, the subsequent crystallization from *n*-hexane revealed that the complex of the NH-protonated ligand with aluminum via the phenolate **[Al(H(BQ))$_3$(THF)]$_2$** was formed (Figure **S1**). Such solid-state molecular structure involving a pentacoordinate aluminum has been reported for a similar complex of phenol and aluminum.[1] An IR spectrum and the melting point could not be obtained, as rapid hydrolysis was found under the conditions in our laboratories.

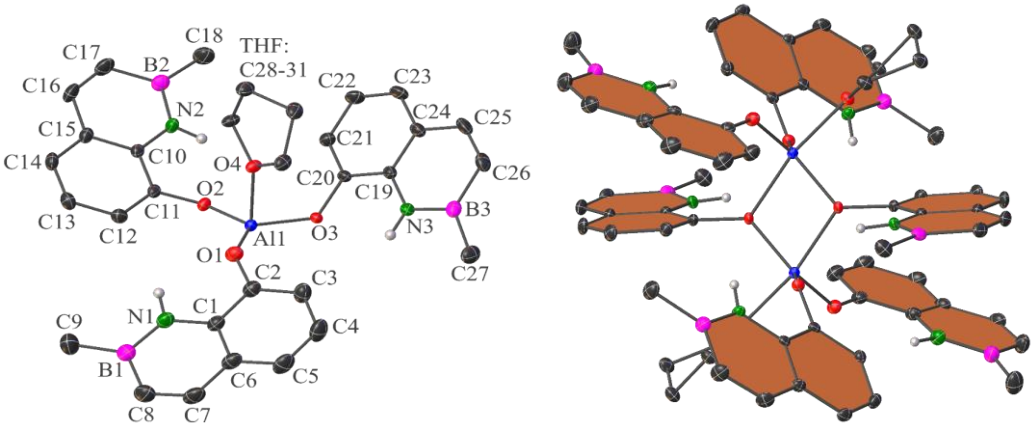


Figure S1. Molecular structure of the monomeric unit and the dimer of **[Al(H(BQ))$_3$(THF)]$_2$**.

In contrast, solid samples of **3** were prone to hydrolysis, so that O-H stretching vibrations were absent in the IR spectrum, and a thermal stability up to 210 °C was observed. Moreover, it was possible to record a high-resolution mass spectrum of this compound, showing **[MeAl(Q′)]$^+$** as the fragment with the highest relative intensity. However, a strongly donating solvent such as THF induced a decomposition, presumably by coordinating to the aluminum atom and breaking the trigonal-bipyramidal coordination.

2. Crystallography

Table S1: Crystal Data and Structure Refinements.

Complex	**([Li(THF)$_2$(diox)$_{0.5}$][Et$_2$B(BQ)])$_2$**
CCDC	2259514
Empirical formula	$C_{46}H_{76}B_4Li_2N_2O_8$
Formula weight	842.20
Temperature/K	100.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.796(3)
b/Å	14.727(4)
c/Å	17.458(4)
α/°	90
β/°	103.832(12)
γ/°	90
Volume/Å^3	2445.6(12)
Z	2
ϱ_{calc}g/cm^3	1.144
μ/mm^{-1}	0.074
F(000)	912.0
Crystal size/mm^3	0.1 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.806 to 51.36
Index ranges	-9 ≤ h ≤ 11, -17 ≤ k ≤ 17, -21 ≤ l ≤ 21
Reflections collected	10969
Independent reflections	4594 [R_{int} = 0.0880, R_{sigma} = 0.1200]
Data/restraints/parameters	4594/0/283
Goodness-of-fit on F^2	1.012
Final R indexes [I>=2σ (I)]	R_1 = 0.0770, wR_2 = 0.1986
Final R indexes [all data]	R_1 = 0.1120, wR_2 = 0.2302
Largest diff. peak/hole / e Å^{-3}	0.41/-0.52

Complex	**[Li(THF)$_3$][Ph$_2$B(BQ)]**
CCDC	2259522
Empirical formula	$C_{33}H_{42}B_2LiNO_4$
Formula weight	545.23
Temperature/K	100.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.6018(8)
b/Å	20.7780(12)
c/Å	16.8289(9)
α/°	90
β/°	90.789(2)
γ/°	90
Volume/Å^3	6154.3(6)
Z	8
ϱ_{calc}g/cm^3	1.177
μ/mm^{-1}	0.074
F(000)	2336.0
Crystal size/mm^3	0.42 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.86 to 56.646

Index ranges	$-22 \le h \le 23$, $-27 \le k \le 27$, $-22 \le l \le 22$
Reflections collected	338940
Independent reflections	15347 [R_{int} = 0.0825, R_{sigma} = 0.0261]
Data/restraints/parameters	15347/0/935
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0646, wR_2 = 0.1533
Final R indexes [all data]	R_1 = 0.0757, wR_2 = 0.1619
Largest diff. peak/hole / e Å^{-3}	0.72/-0.38

Complex	**$([Na(THF)_2][B(BQ)_2])_2$**
CCDC	2259516
Empirical formula	$C_{26}H_{32}B_3N_2NaO_4$
Formula weight	491.95
Temperature/K	119.99
Crystal system	triclinic
Space group	P-1
a/Å	11.1607(19)
b/Å	11.892(2)
c/Å	12.316(2)
α/°	117.706(6)
β/°	92.755(6)
γ/°	110.342(6)
Volume/Å^3	1313.0(4)
Z	2
ϱ_{calc}g/cm^3	1.244
μ/mm^{-1}	0.095
F(000)	520.0
Crystal size/mm^3	0.6 × 0.3 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.822 to 56.712
Index ranges	$-13 \le h \le 14$, $-15 \le k \le 15$, $-16 \le l \le 16$
Reflections collected	36401
Independent reflections	6557 [R_{int} = 0.0508, R_{sigma} = 0.0353]
Data/restraints/parameters	6557/0/327
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0503, wR_2 = 0.1180
Final R indexes [all data]	R_1 = 0.0690, wR_2 = 0.1288
Largest diff. peak/hole / e Å^{-3}	0.53/-0.39

Complex	**$[Li(THF)_3][Me_2Al(BQ)]$**
CCDC	2259515
Empirical formula	$C_{23}H_{38}AlBLiNO_4$
Formula weight	437.27
Temperature/K	100.00
Crystal system	monoclinic
Space group	Cc
a/Å	17.801(3)
b/Å	8.5125(13)
c/Å	18.438(4)
α/°	90
β/°	114.105(13)
γ/°	90
Volume/Å^3	2550.4(8)
Z	4
ϱ_{calc}g/cm^3	1.139

μ/mm^{-1}	0.106
F(000)	944.0
Crystal size/mm^3	0.3 × 0.2 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.84 to 61.138
Index ranges	-25 ≤ h ≤ 25, -12 ≤ k ≤ 12, -26 ≤ l ≤ 26
Reflections collected	35381
Independent reflections	7388 [R_{int} = 0.0504, R_{sigma} = 0.0436]
Data/restraints/parameters	7388/2/432
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0370, wR_2 = 0.0769
Final R indexes [all data]	R_1 = 0.0487, wR_2 = 0.0811
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.22

Complex	**[Li(THF)$_3$][Ph$_2$Al(BQ)]**
CCDC	2259521
Empirical formula	$C_{33}H_{42}AlBLiNO_4$
Formula weight	561.40
Temperature/K	100.00
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	17.6861(10)
b/Å	9.5637(6)
c/Å	18.7543(19)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	3172.2(4)
Z	4
$\rho_{calc}g/cm^3$	1.176
μ/mm^{-1}	0.100
F(000)	1200.0
Crystal size/mm^3	0.14 × 0.05 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.606 to 61.08
Index ranges	-25 ≤ h ≤ 22, -13 ≤ k ≤ 13, -26 ≤ l ≤ 26
Reflections collected	69045
Independent reflections	9687 [R_{int} = 0.0627, R_{sigma} = 0.0417]
Data/restraints/parameters	9687/1/371
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0599, wR_2 = 0.1621
Final R indexes [all data]	R_1 = 0.0760, wR_2 = 0.1761
Largest diff. peak/hole / e $Å^{-3}$	0.96/-0.43

Complex	**[Li(THF)$_3$][Al(BQ)$_2$]**
CCDC	2259518
Empirical formula	$C_{30}H_{40}AlB_2LiN_2O_5$
Formula weight	564.18
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
a/Å	10.070(3)
b/Å	10.701(3)
c/Å	15.809(5)
α/°	85.336(11)

β/°	81.473(12)
γ/°	64.072(9)
Volume/Å^3	1515.0(8)
Z	2
ϱ_{calc}g/cm^3	1.237
μ/mm^{-1}	0.108
F(000)	600.0
Crystal size/mm^3	0.56 × 0.2 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.232 to 56.706
Index ranges	-12 ≤ h ≤ 13, -14 ≤ k ≤ 14, -21 ≤ l ≤ 21
Reflections collected	29381
Independent reflections	7543 [R_{int} = 0.0730, R_{sigma} = 0.0675]
Data/restraints/parameters	7543/0/372
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0559, wR_2 = 0.1095
Final R indexes [all data]	R_1 = 0.0918, wR_2 = 0.1236
Largest diff. peak/hole / e Å^{-3}	0.37/-0.32

Complex	**[Me$_2$Al(Q')]**
CCDC	2259520
Empirical formula	$C_{12}H_{14}AlNO$
Formula weight	215.22
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
a/Å	9.537(3)
b/Å	9.792(2)
c/Å	12.638(3)
α/°	88.302(9)
β/°	73.190(10)
γ/°	81.824(9)
Volume/Å^3	1118.1(5)
Z	4
ϱ_{calc}g/cm^3	1.279
μ/mm^{-1}	0.153
F(000)	456.0
Crystal size/mm^3	0.223 × 0.161 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.718 to 61.088
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -18 ≤ l ≤ 18
Reflections collected	71748
Independent reflections	6824 [R_{int} = 0.0508, R_{sigma} = 0.0272]
Data/restraints/parameters	6824/0/277
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0353, wR_2 = 0.1045
Final R indexes [all data]	R_1 = 0.0381, wR_2 = 0.1076
Largest diff. peak/hole / e Å^{-3}	0.50/-0.34

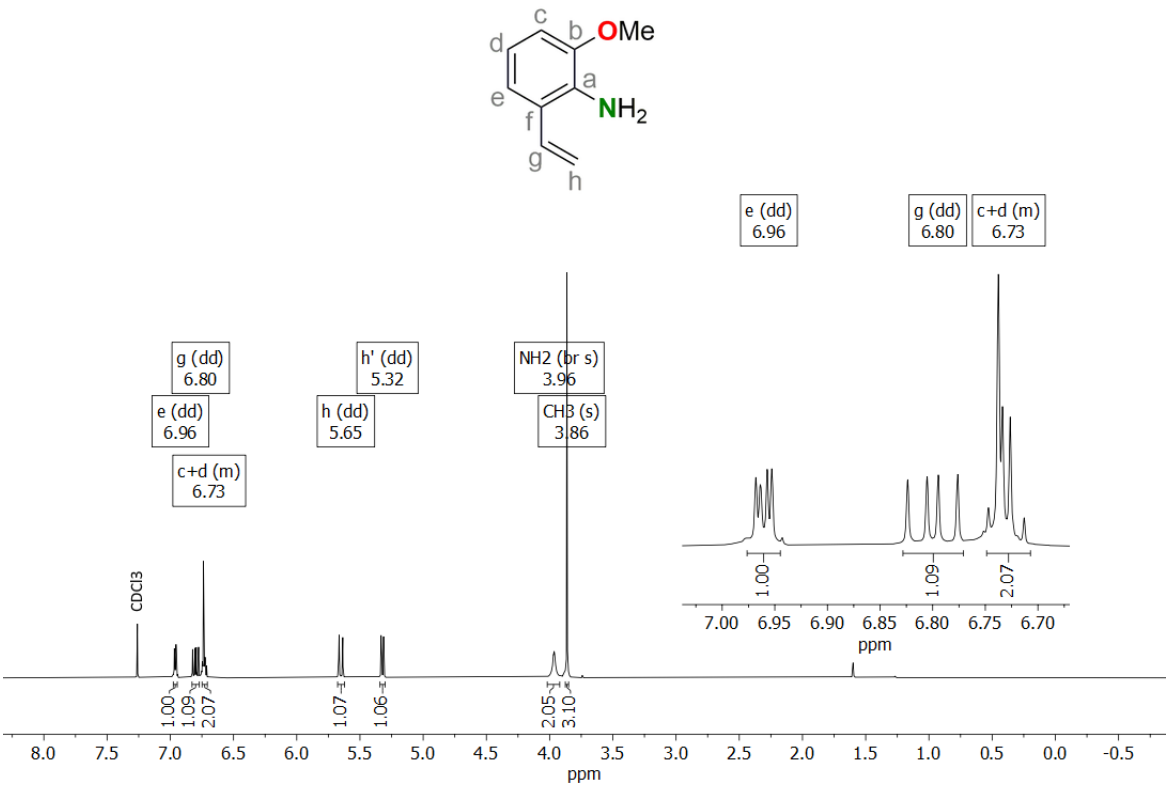
Complex	**[Al(H(BQ))$_3$](THF)]$_2$**
CCDC	2259519
Empirical formula	$C_{62}H_{70}Al_2B_6N_6O_8$
Formula weight	1146.06
Temperature/K	119.99
Crystal system	triclinic

Space group	P-1
a/Å	11.3152(7)
b/Å	11.7091(6)
c/Å	13.0761(8)
α/°	95.048(2)
β/°	113.613(2)
γ/°	105.874(2)
Volume/Å^3	1488.02(15)
Z	1
ϱ_{calc}g/cm^3	1.279
μ/mm^{-1}	0.110
F(000)	604.0
Crystal size/mm^3	0.4 × 0.3 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.078 to 58.258
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 12, -17 ≤ l ≤ 17
Reflections collected	44252
Independent reflections	7986 [R_{int} = 0.0364, R_{sigma} = 0.0265]
Data/restraints/parameters	7986/0/394
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0435, wR_2 = 0.1112
Final R indexes [all data]	R_1 = 0.0556, wR_2 = 0.1185
Largest diff. peak/hole / e Å^{-3}	0.45/-0.33

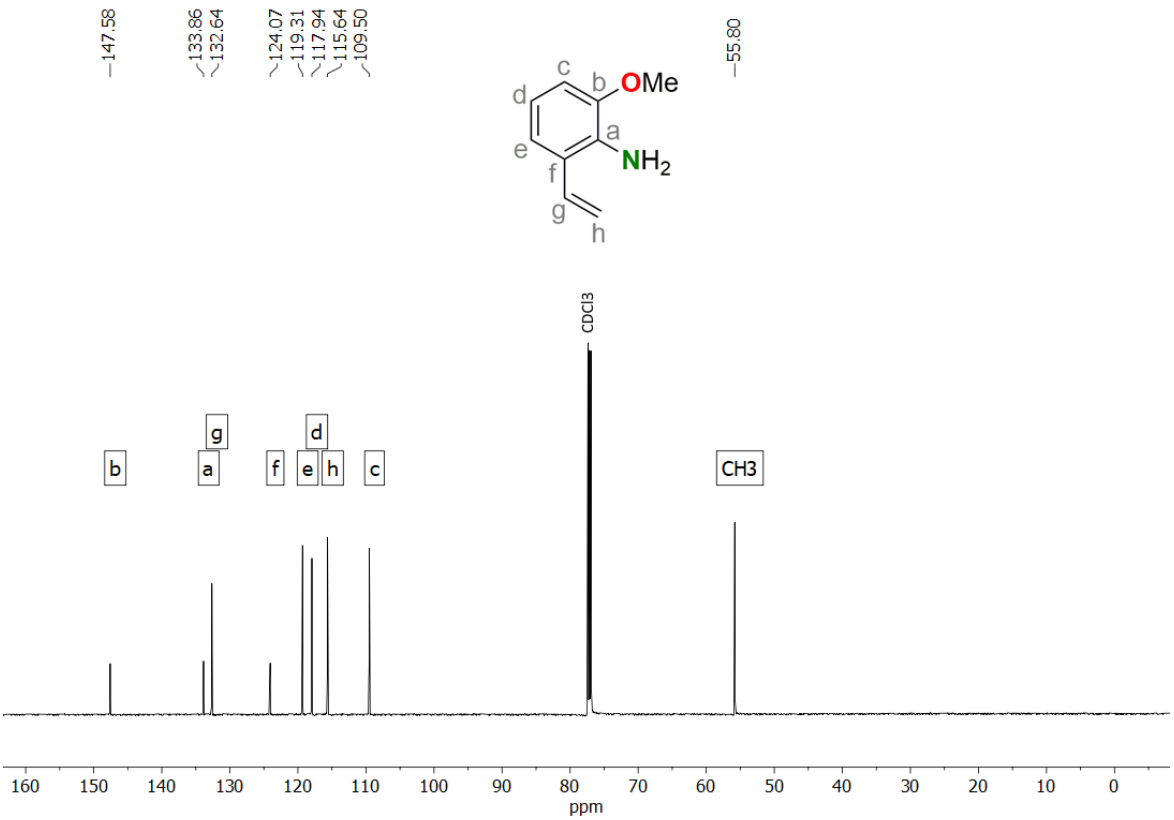
3. NMR Spectra

3.1. 2-Methoxy-6-vinylaniline (6)

^{1}H NMR (601 MHz, $CDCl_3$)

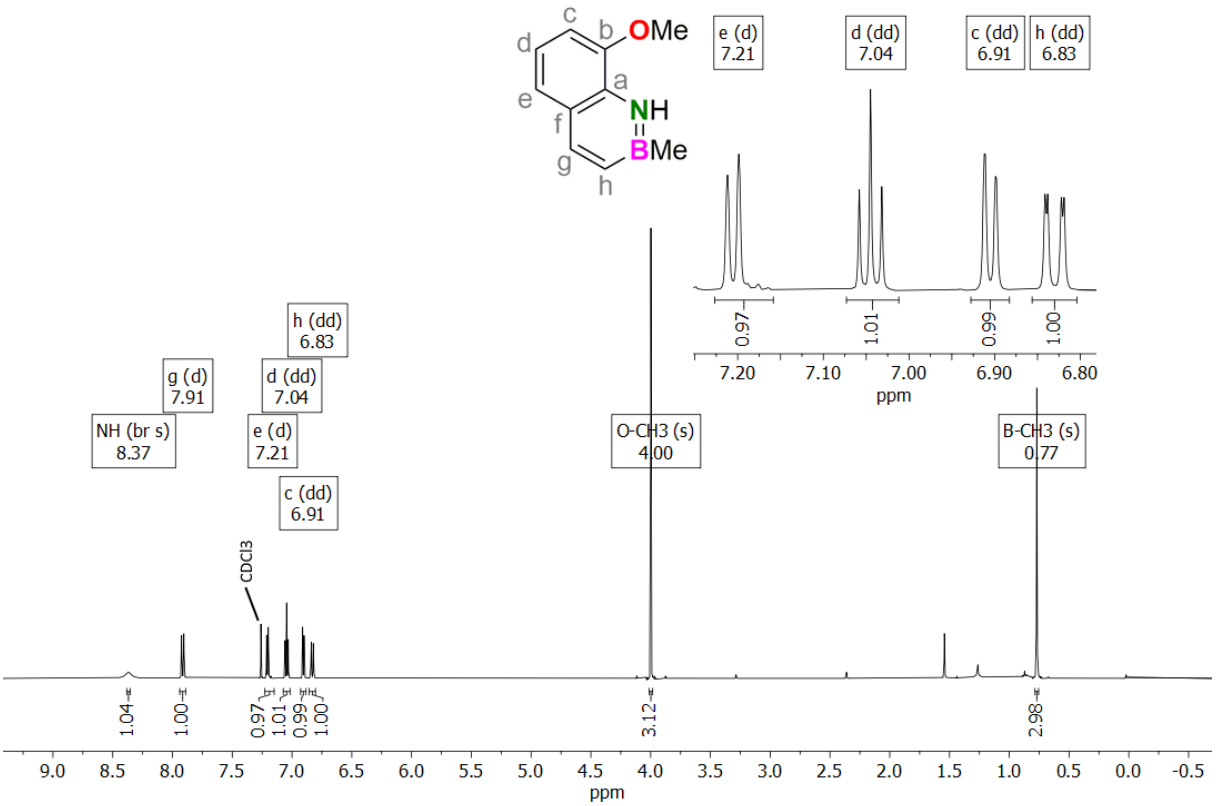


^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$)

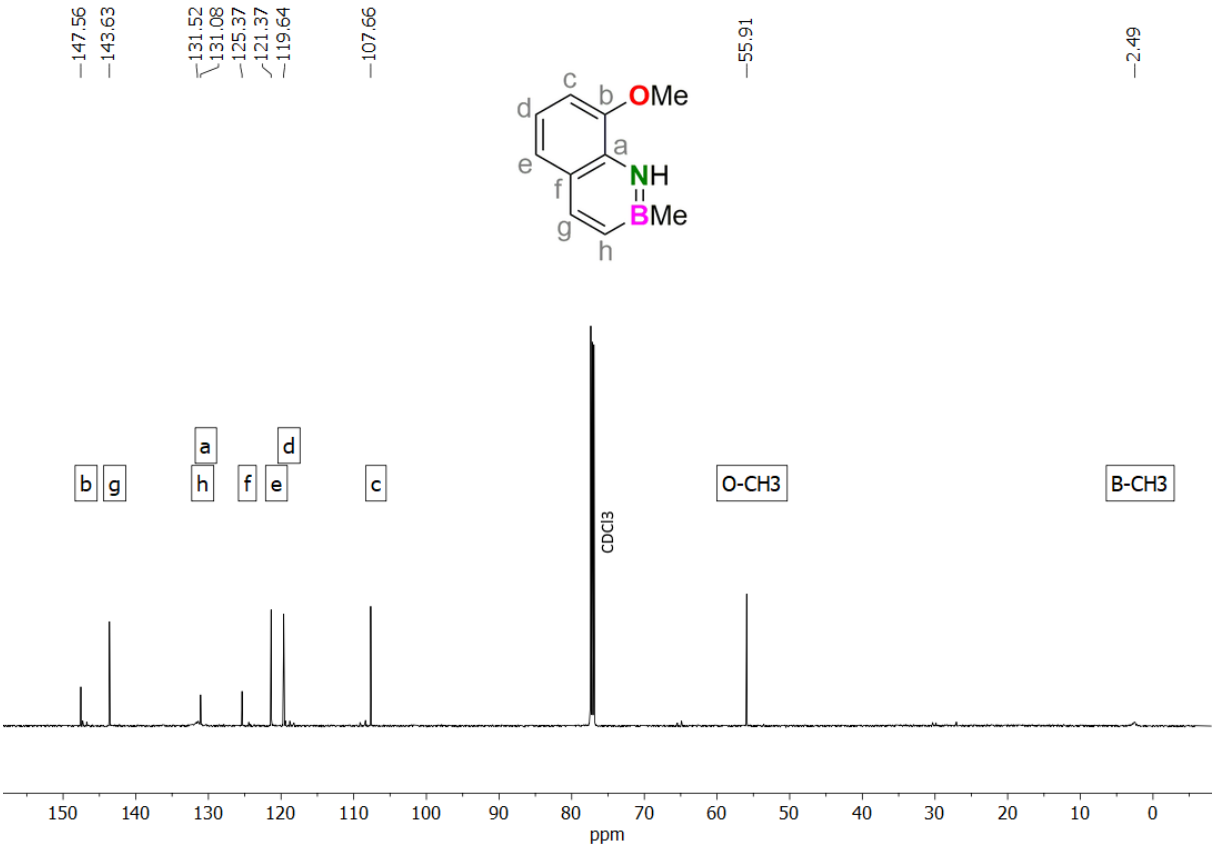


3.2. 8-Methoxy-2-methyl-1,2-dihydro-1-aza-2-boranaphthalene (7)

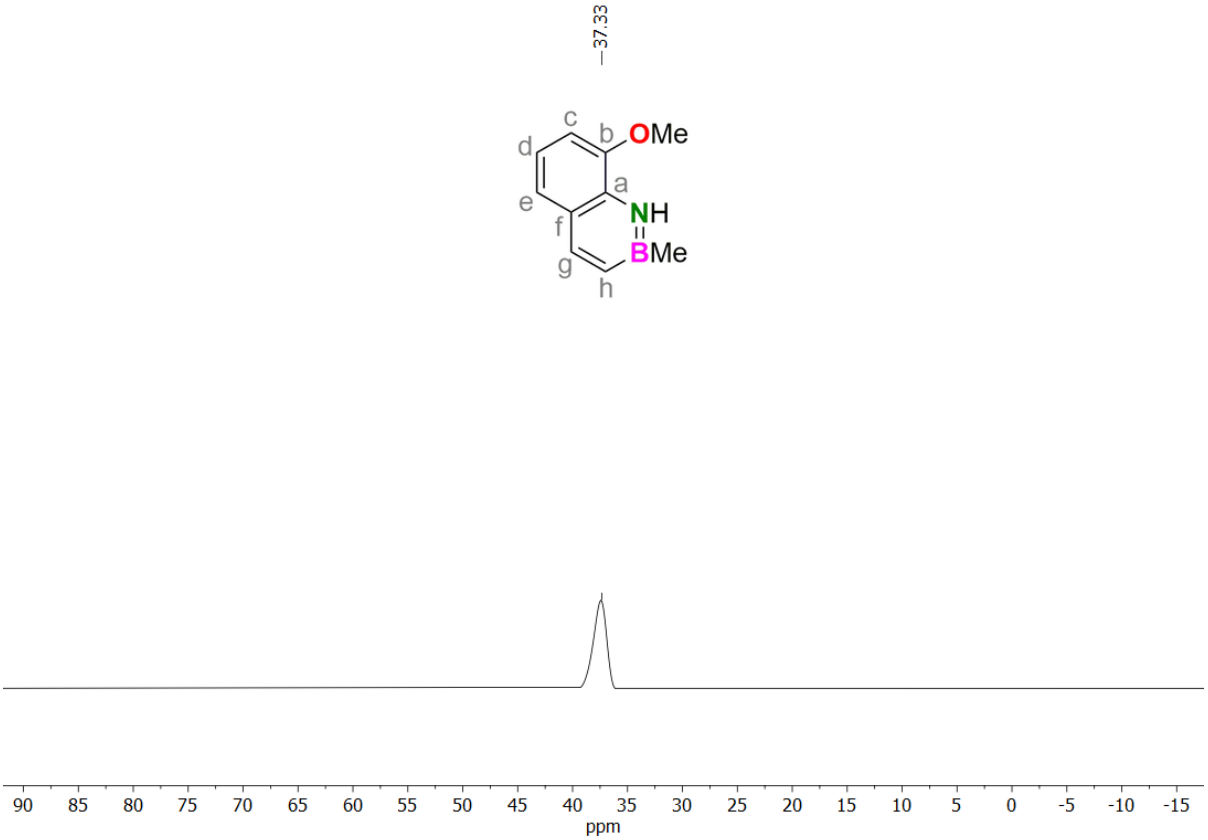
^{1}H NMR (601 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$)

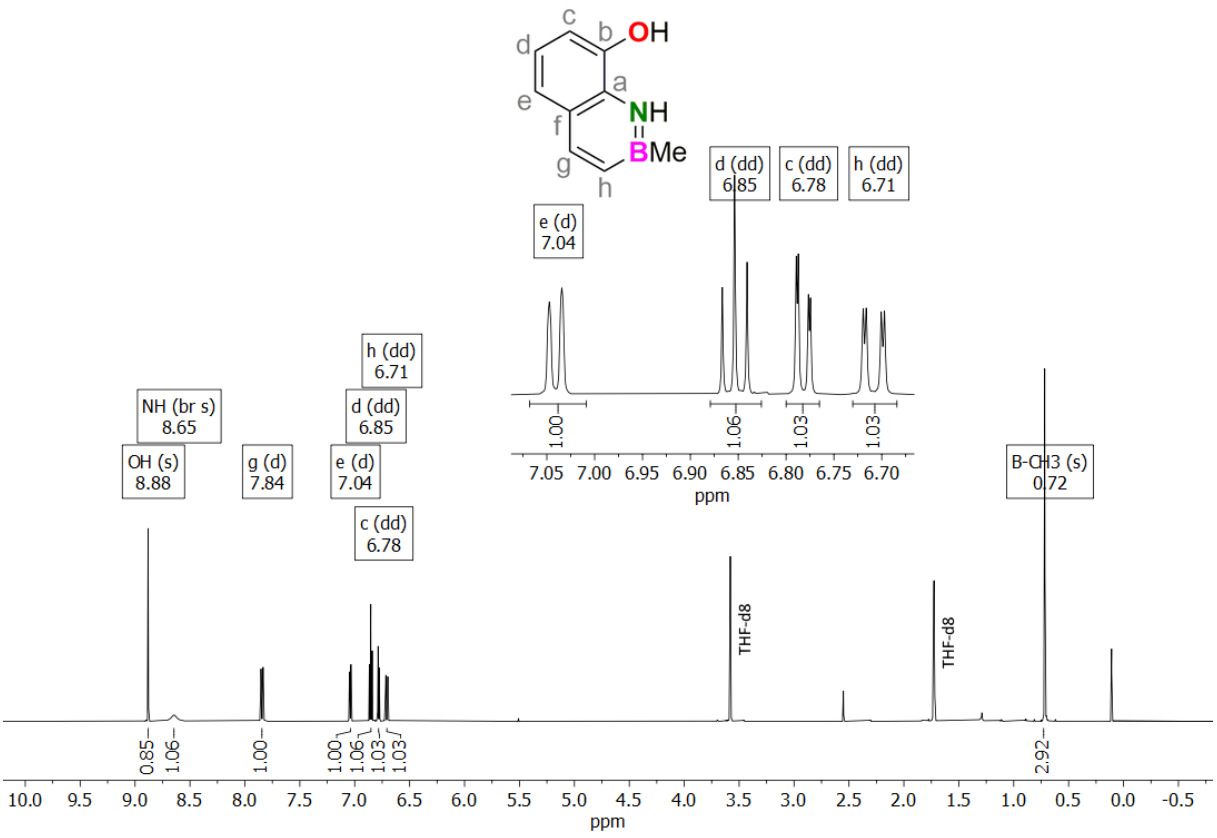


$^{11}B\{^{1}H\}$ NMR (193 MHz, $CDCl_3$)

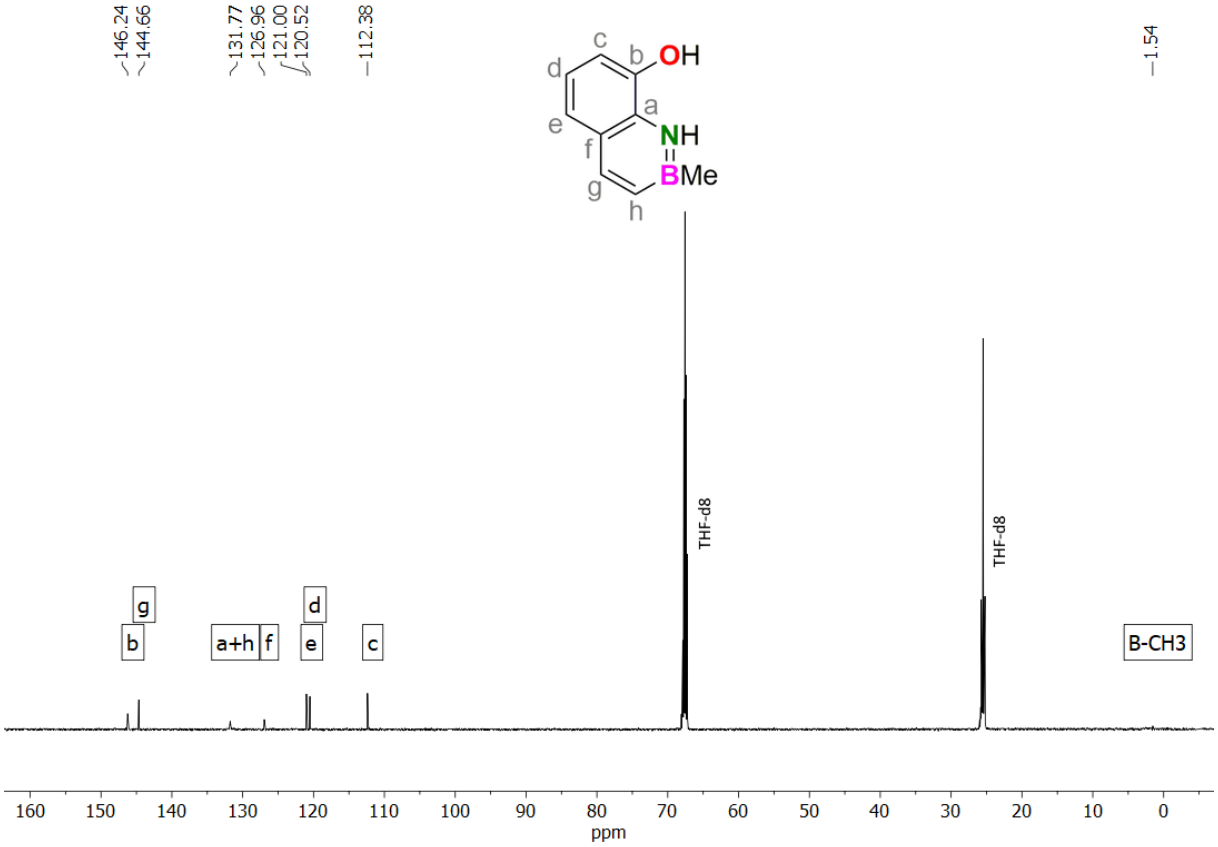


3.3. 8-Hydroxy-2-methyl-1,2-dihydro-1-aza-2-boranaphthalene (1)

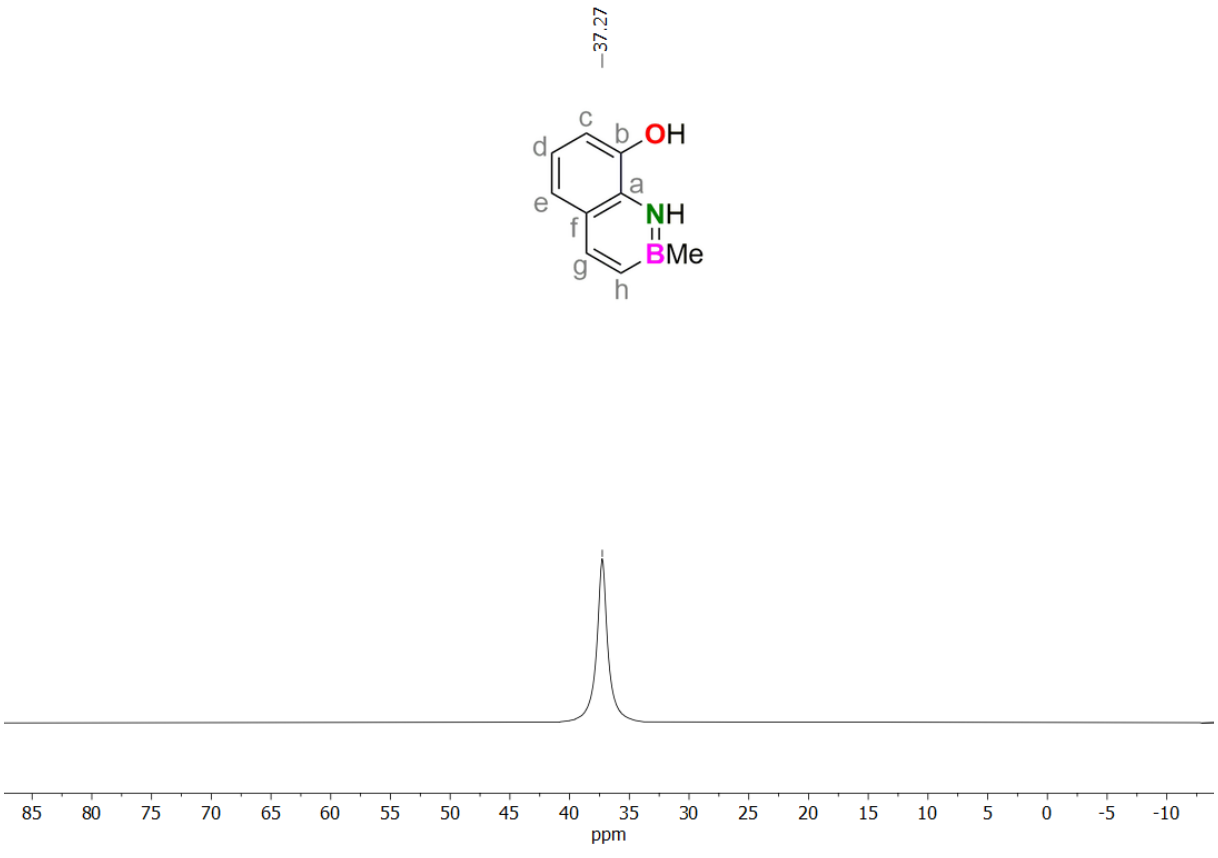
^{1}H NMR (601 MHz, THF-d_8)



$^{13}C\{^{1}H\}$ NMR (151 MHz, THF-d_8)

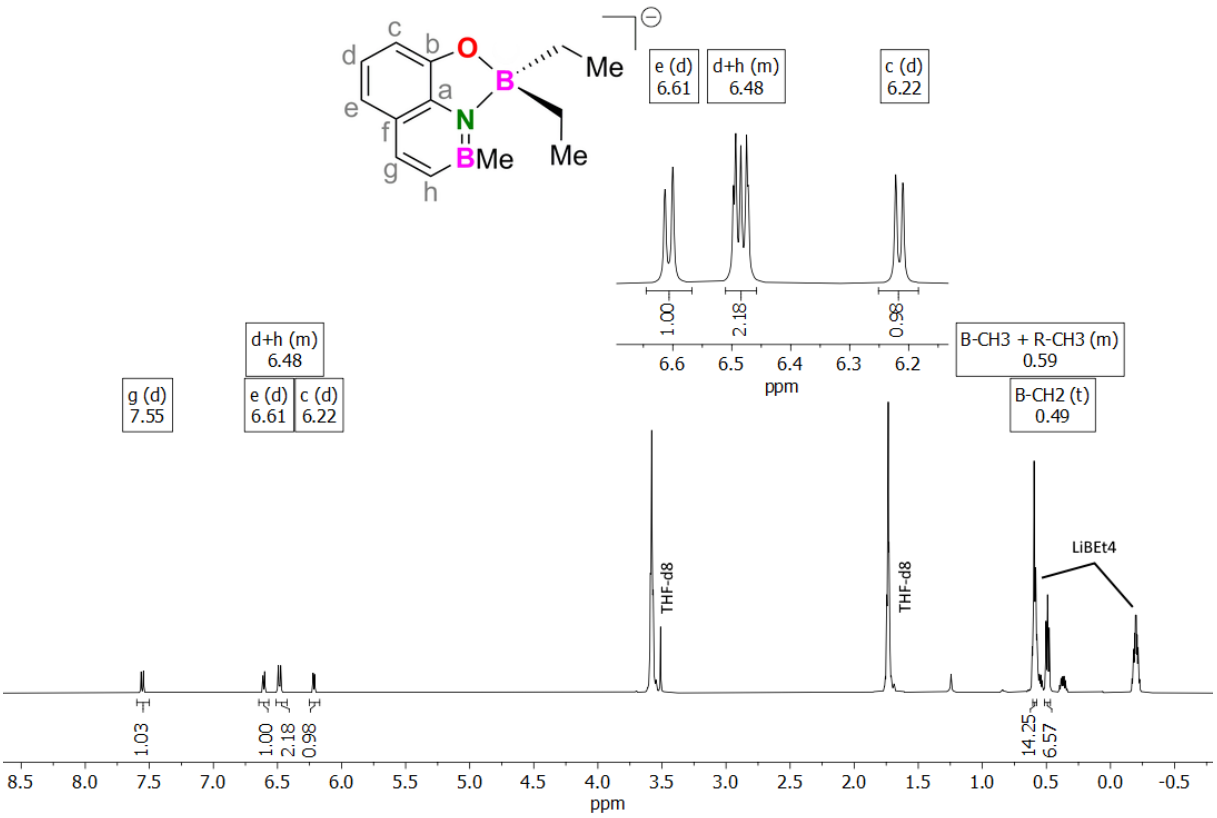


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

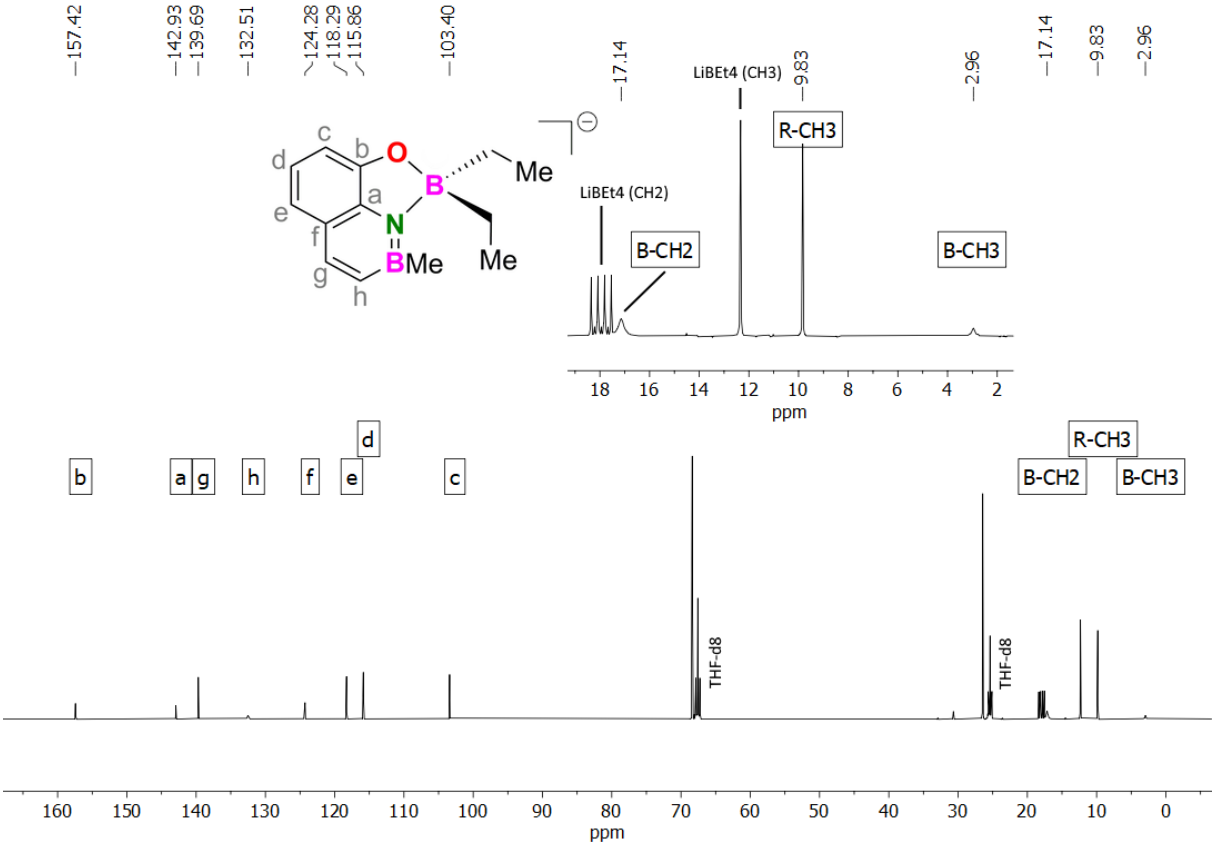


3.4. Li[Et$_2$B(BQ)]) (9)

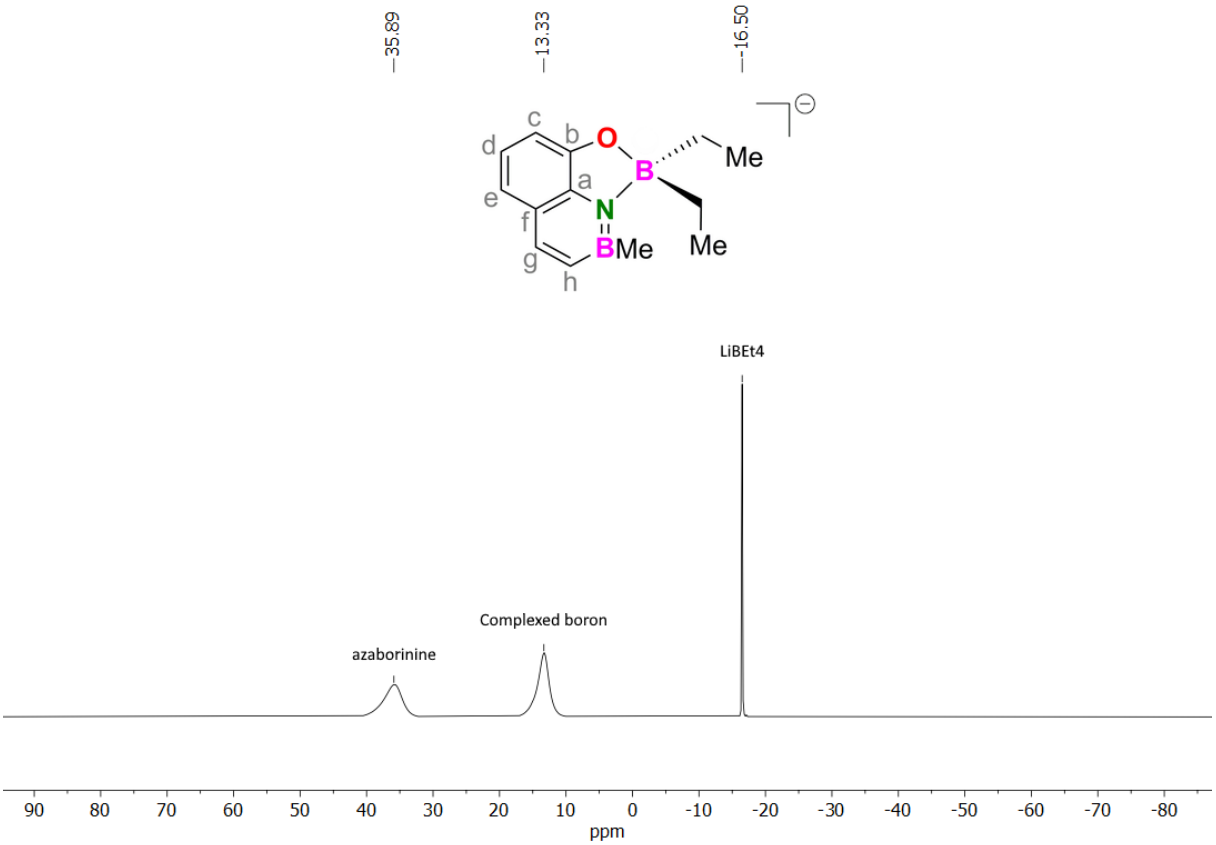
^{1}H NMR (601 MHz, THF-d_8)



^{13}C{^{1}H} NMR (151 MHz, THF-d_8)

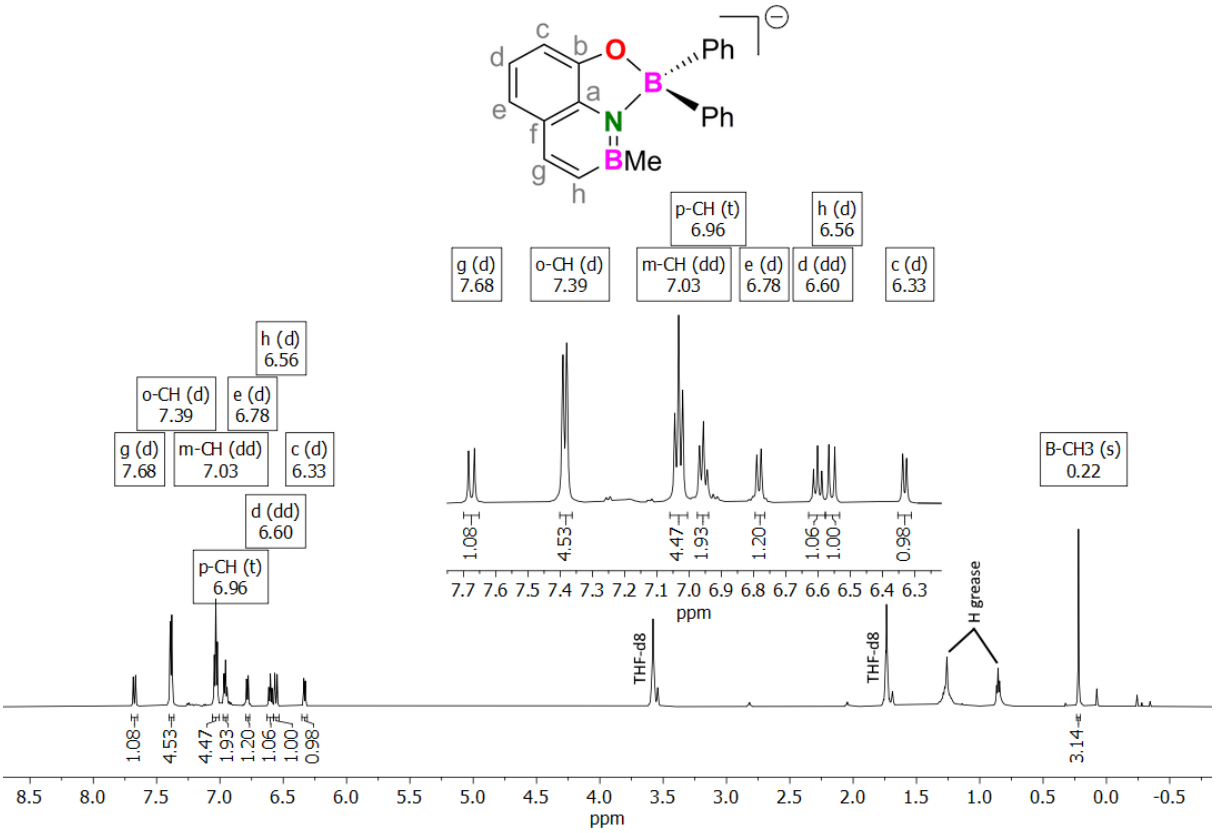


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

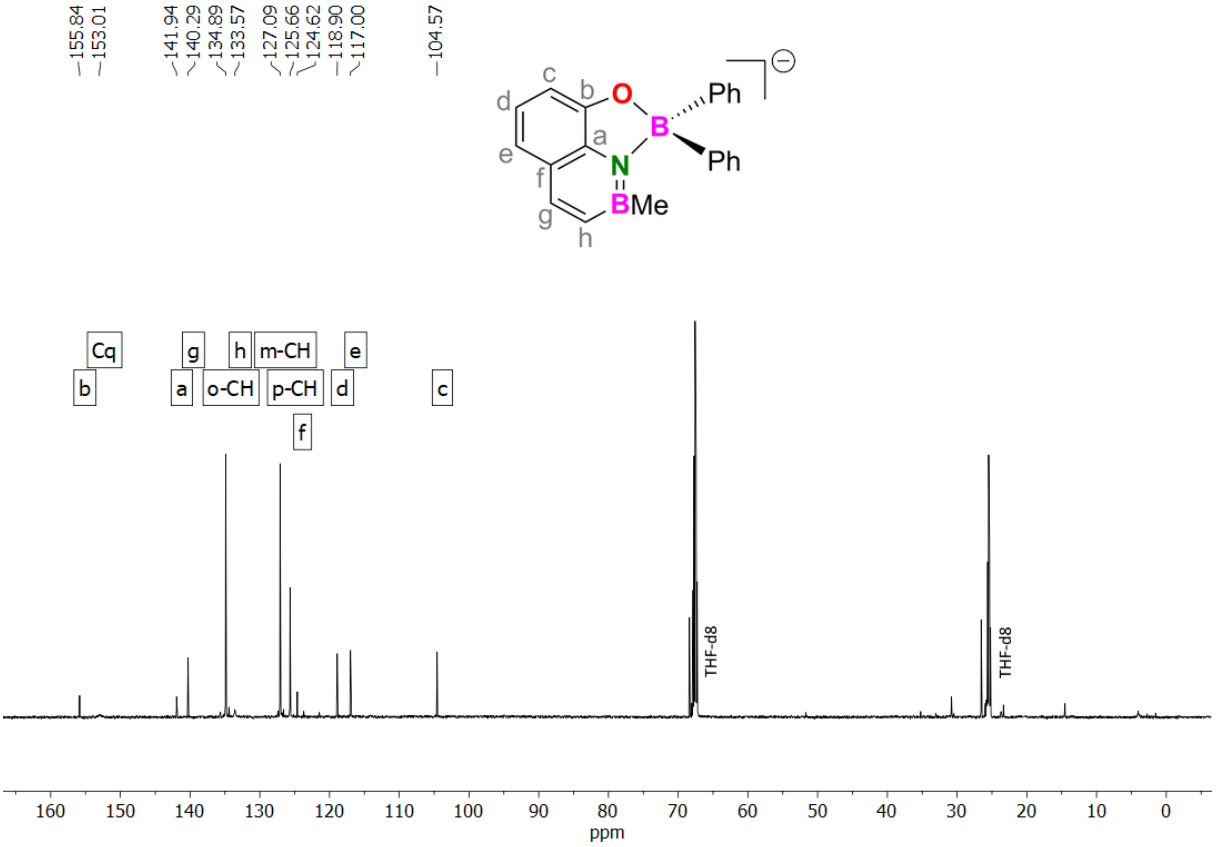


3.5. Li[Ph$_2$B(BQ)]) (10)

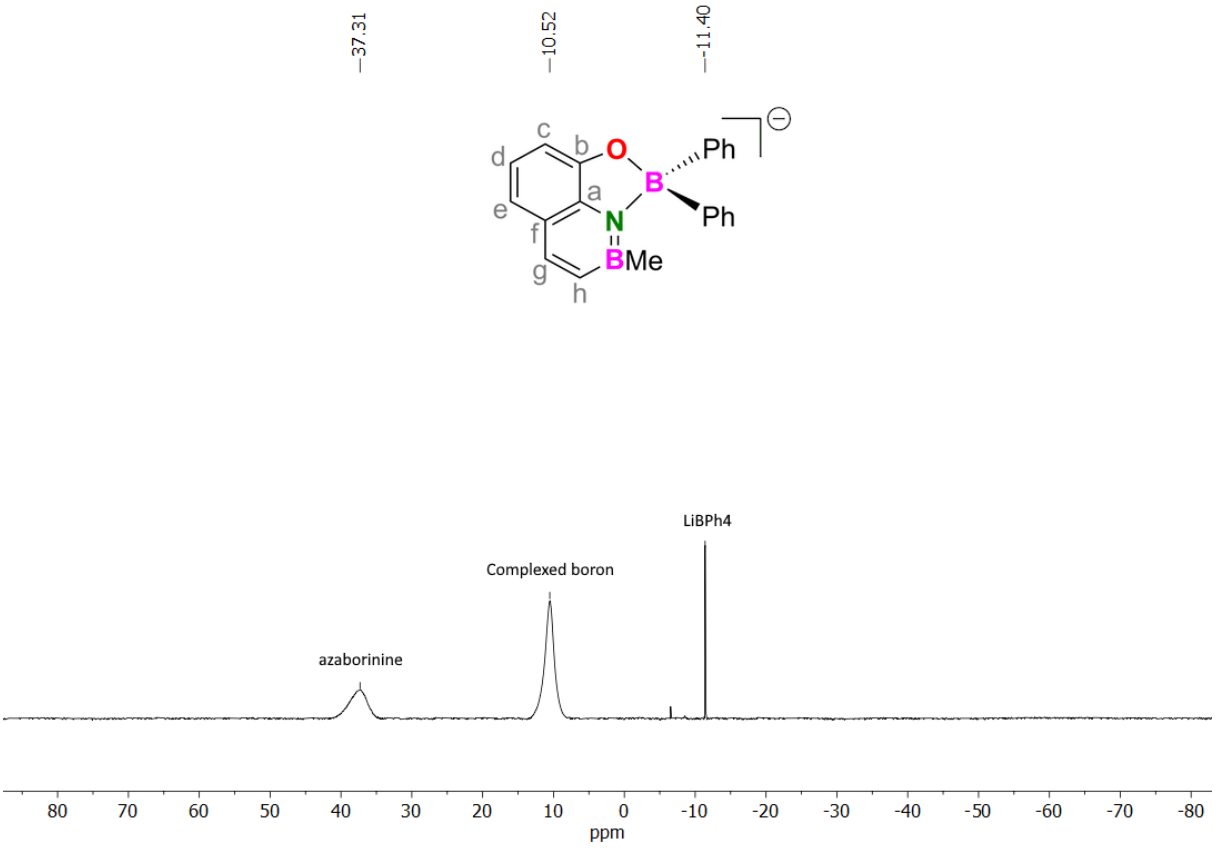
^{1}H NMR (601 MHz, THF-d_8)



$^{13}C\{^{1}H\}$ NMR (151 MHz, THF-d_8)

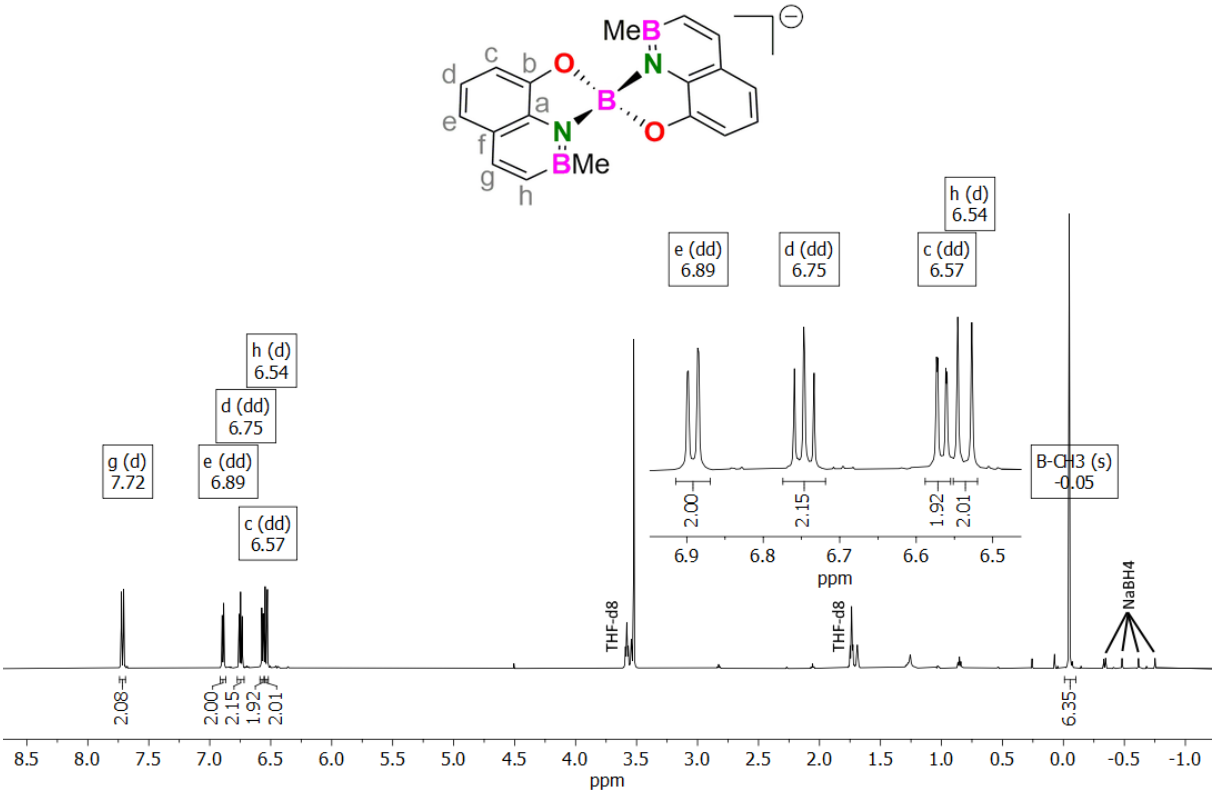


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

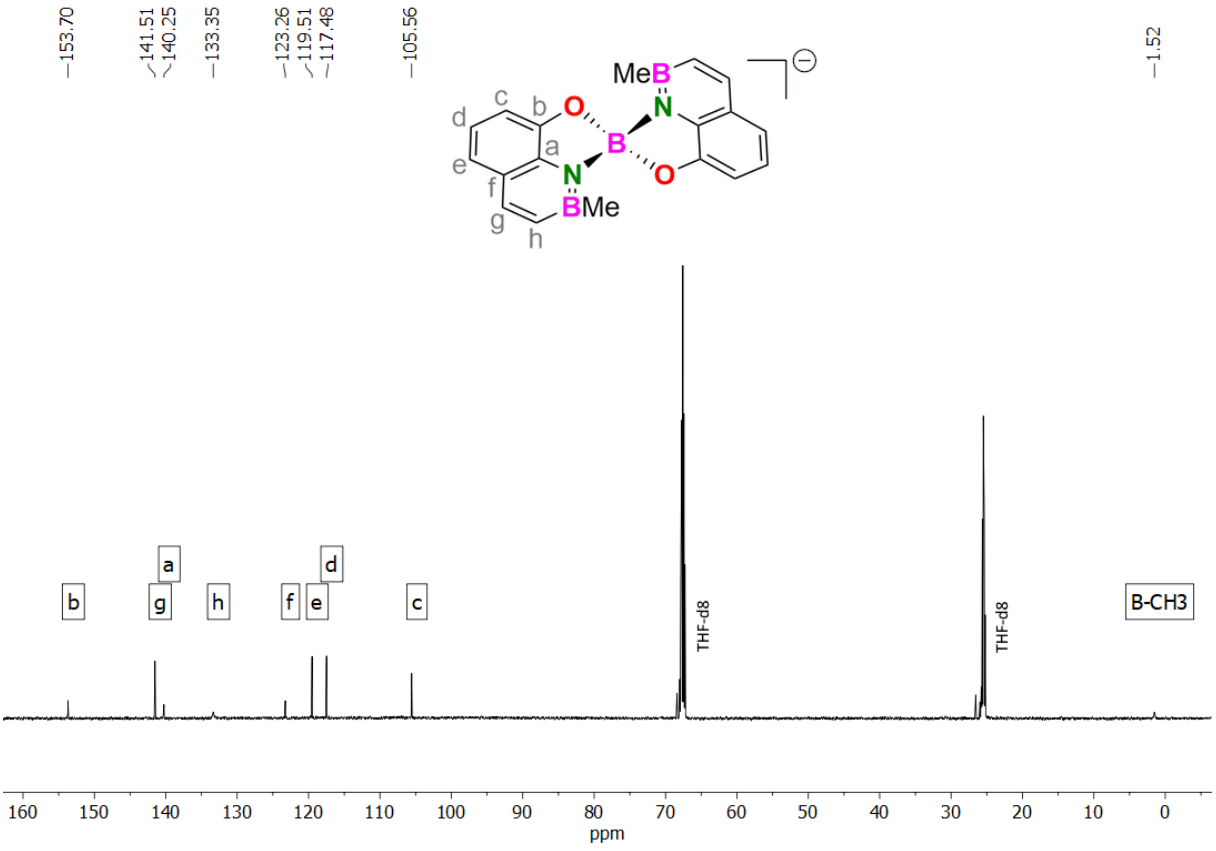


3.6. Na[B(BQ)$_2$] (11)

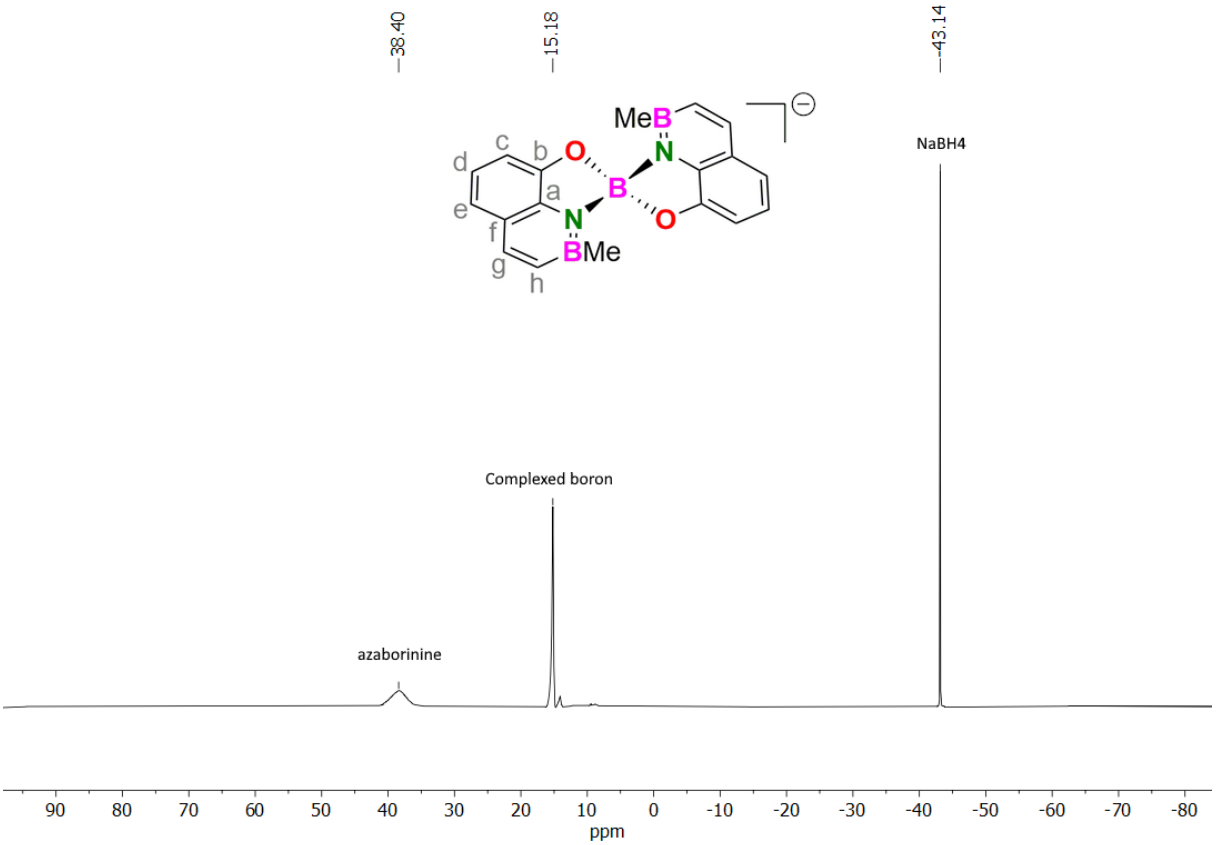
^{1}H NMR (601 MHz, THF-d_8)



^{13}C{^{1}H} NMR (151 MHz, THF-d_8)

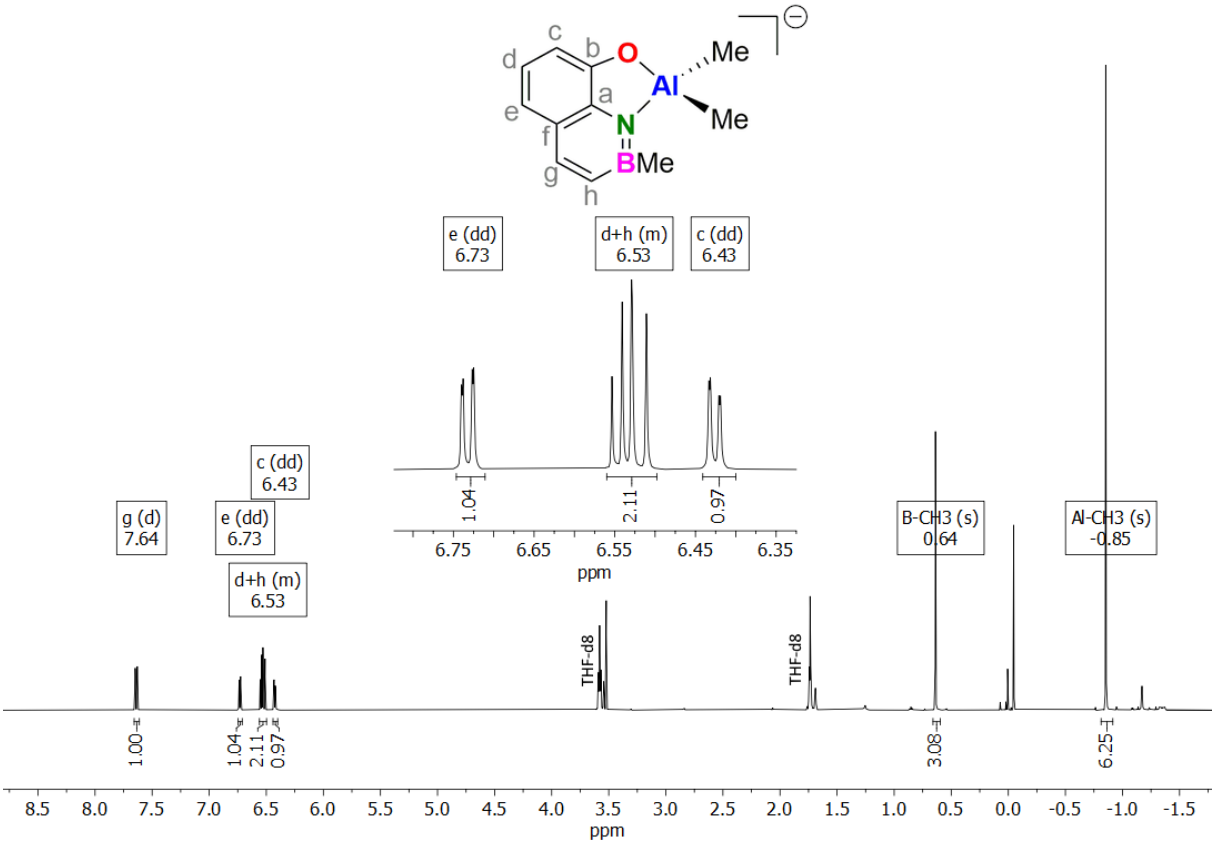


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

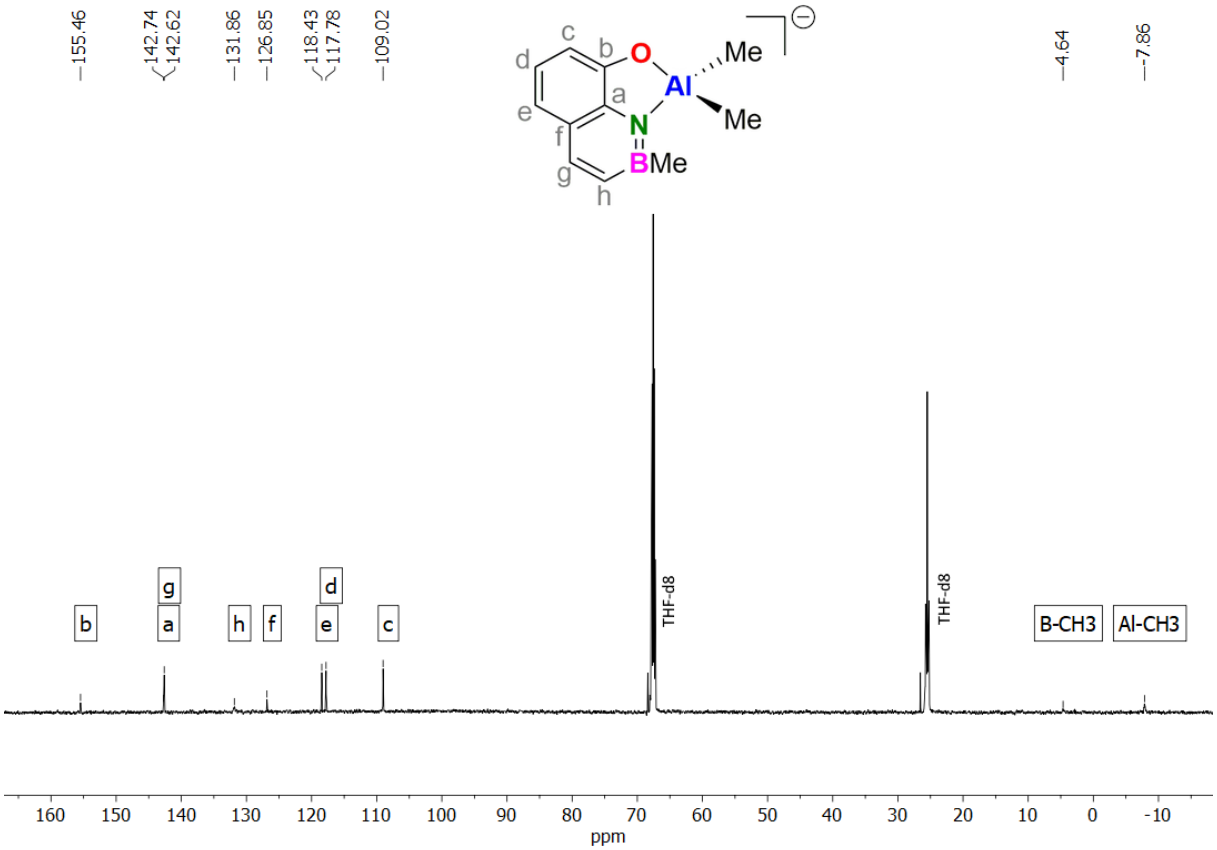


3.7. Li[Me$_2$Al(BQ)]) (4)

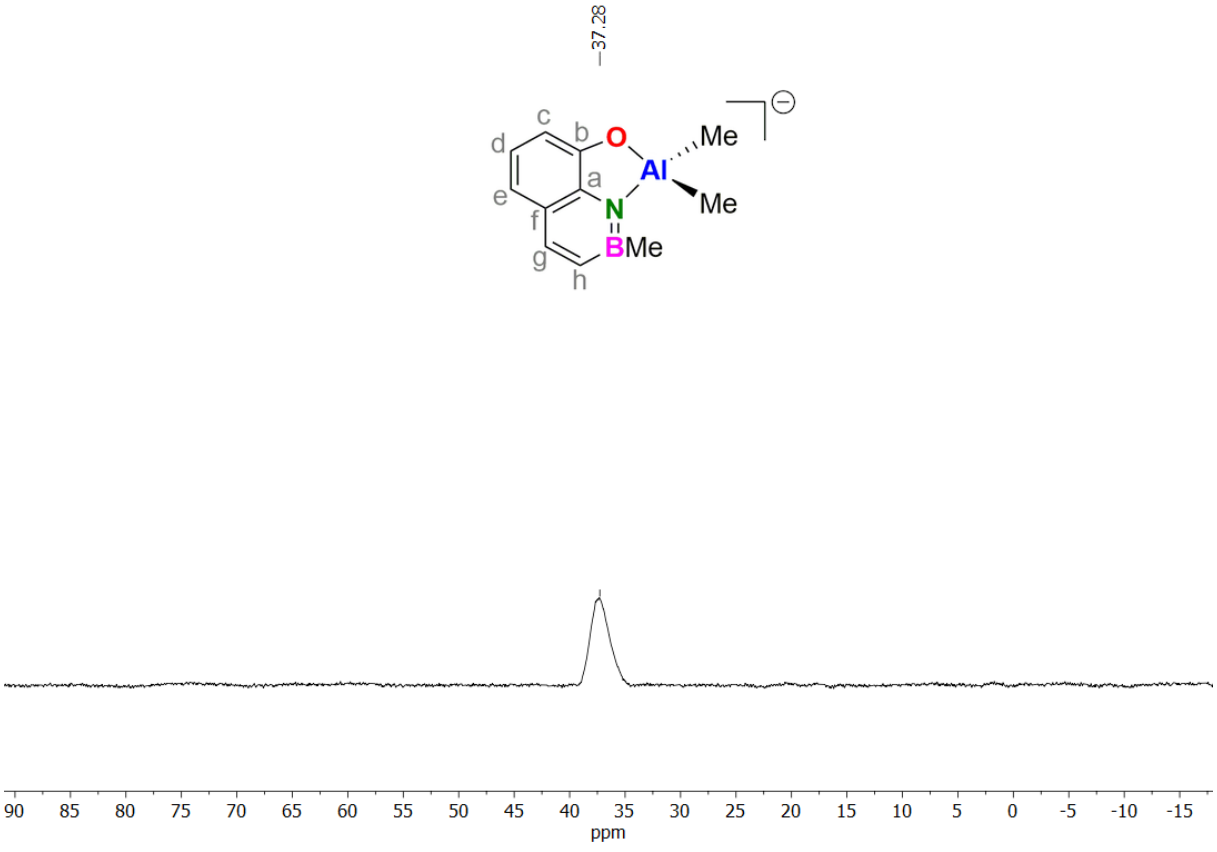
^{1}H NMR (601 MHz, THF-d_8)



$^{13}C\{^{1}H\}$ NMR (151 MHz, THF-d_8)

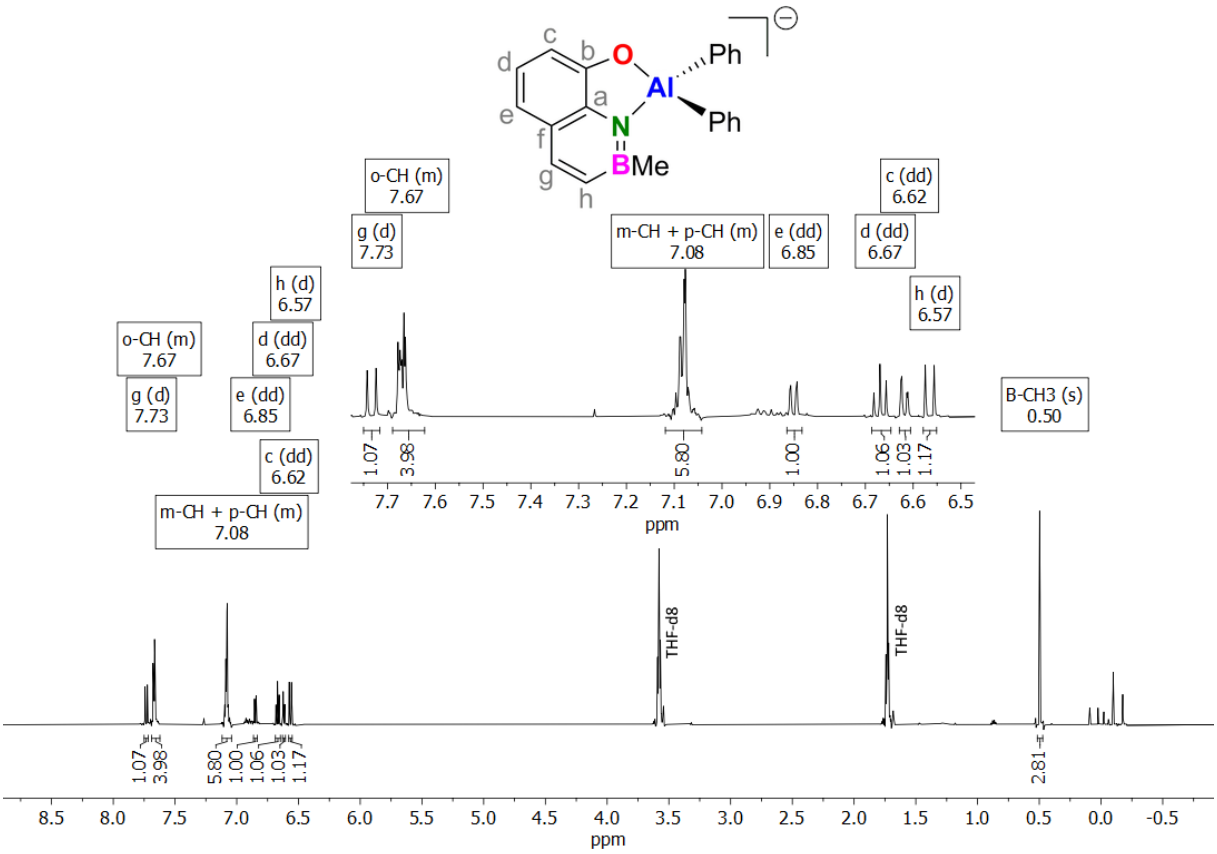


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

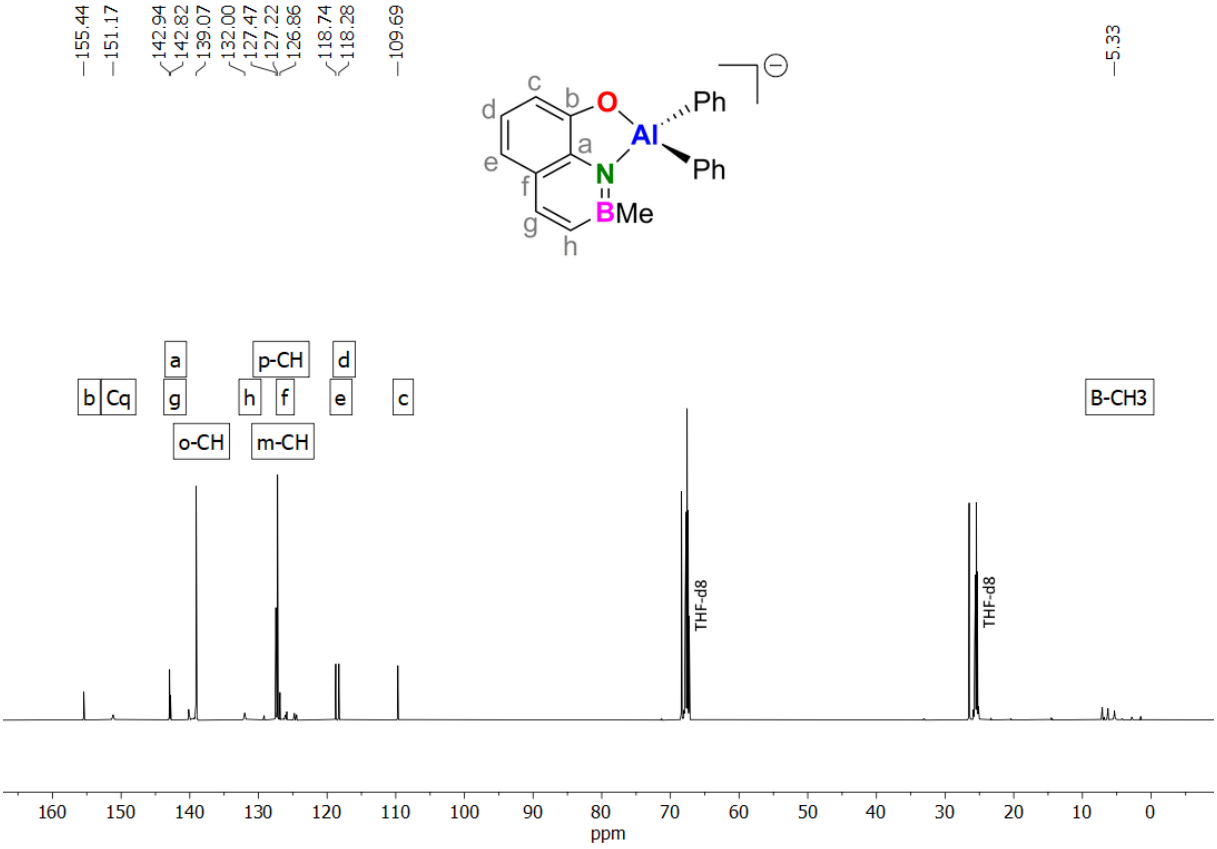


3.8. Li[Ph$_2$Al(BQ)]) (12)

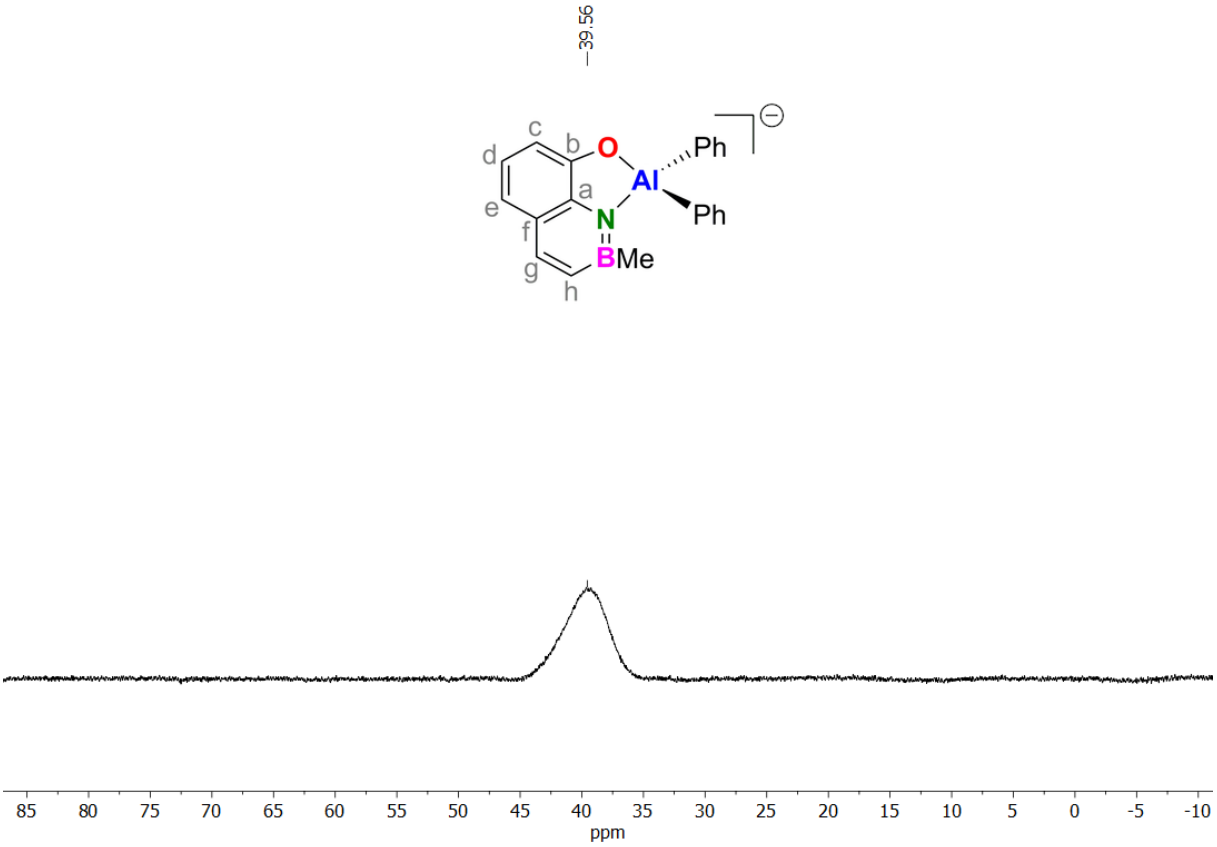
^{1}H NMR (601 MHz, THF-d_8)



^{13}C{^{1}H} NMR (151 MHz, THF-d_8)

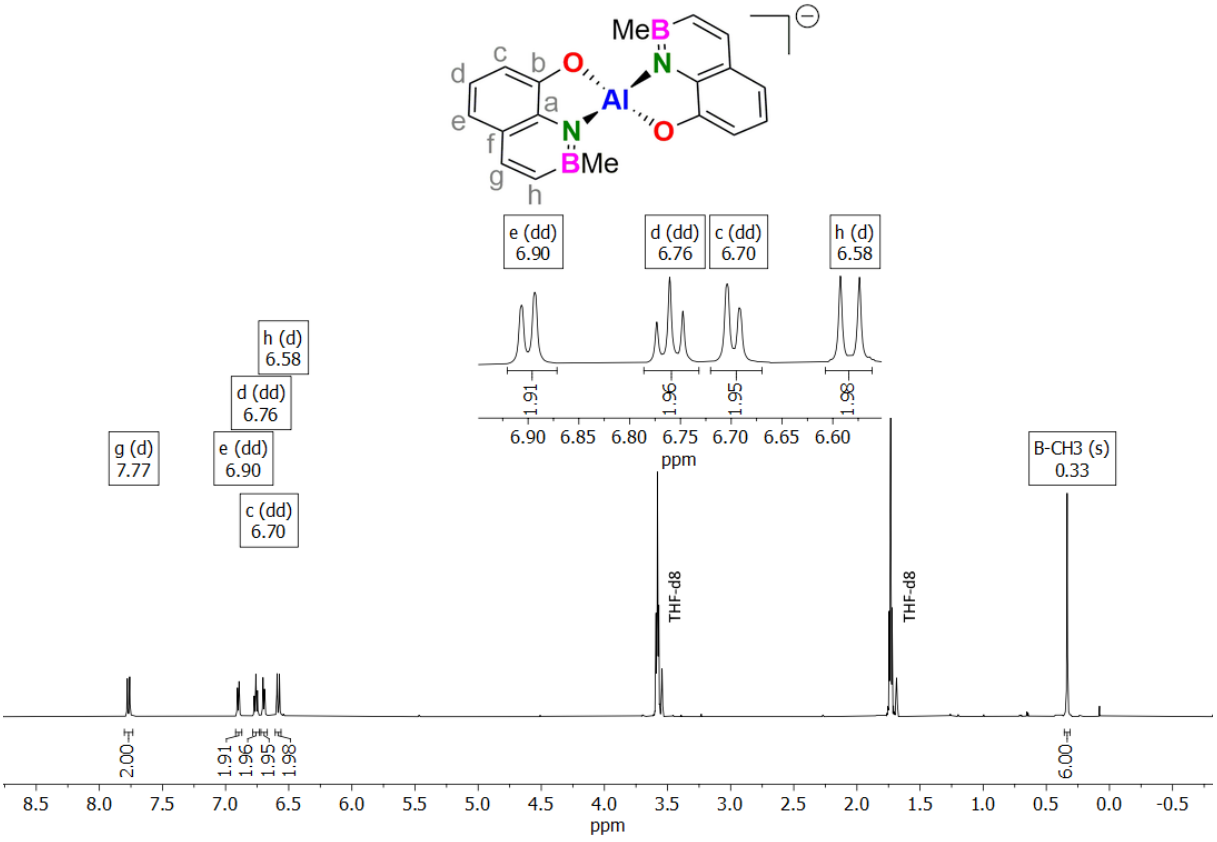


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

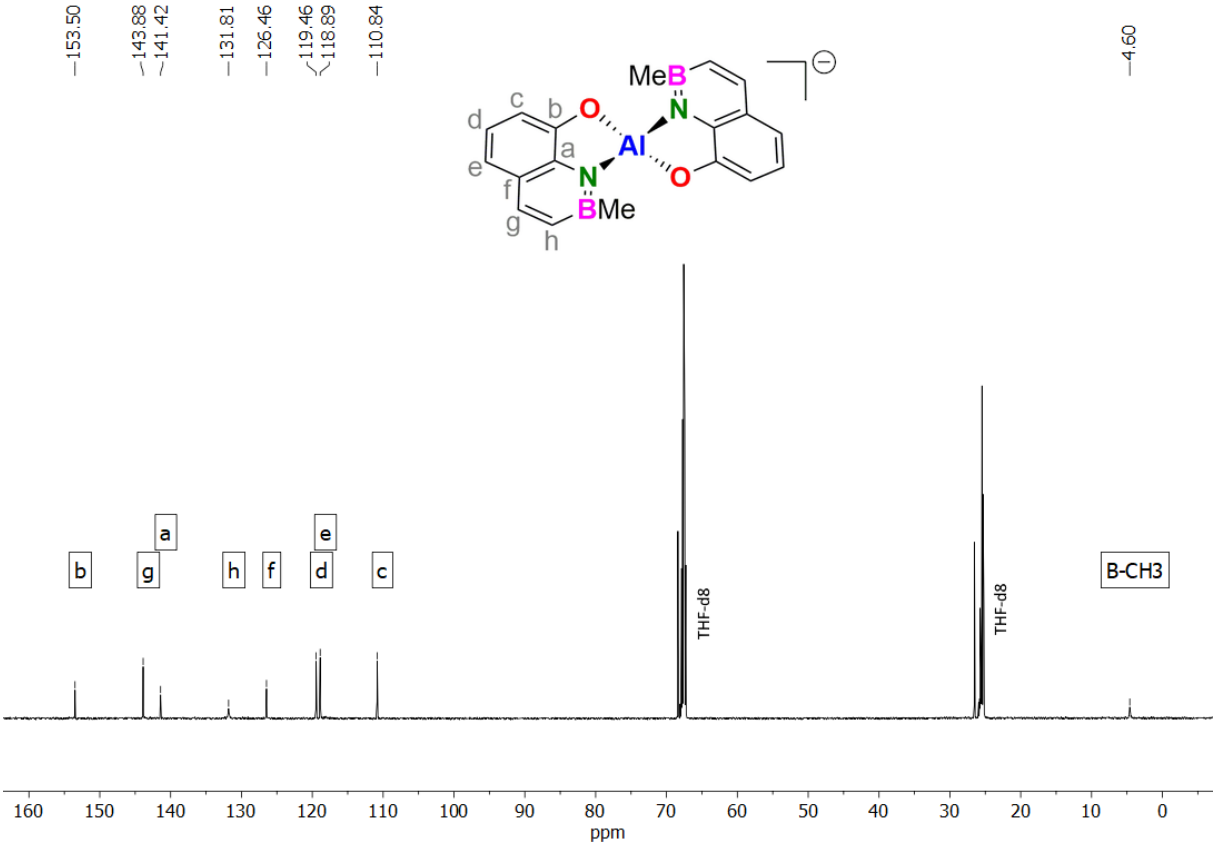


3.9. Li[Al(BQ)$_2$] (13)

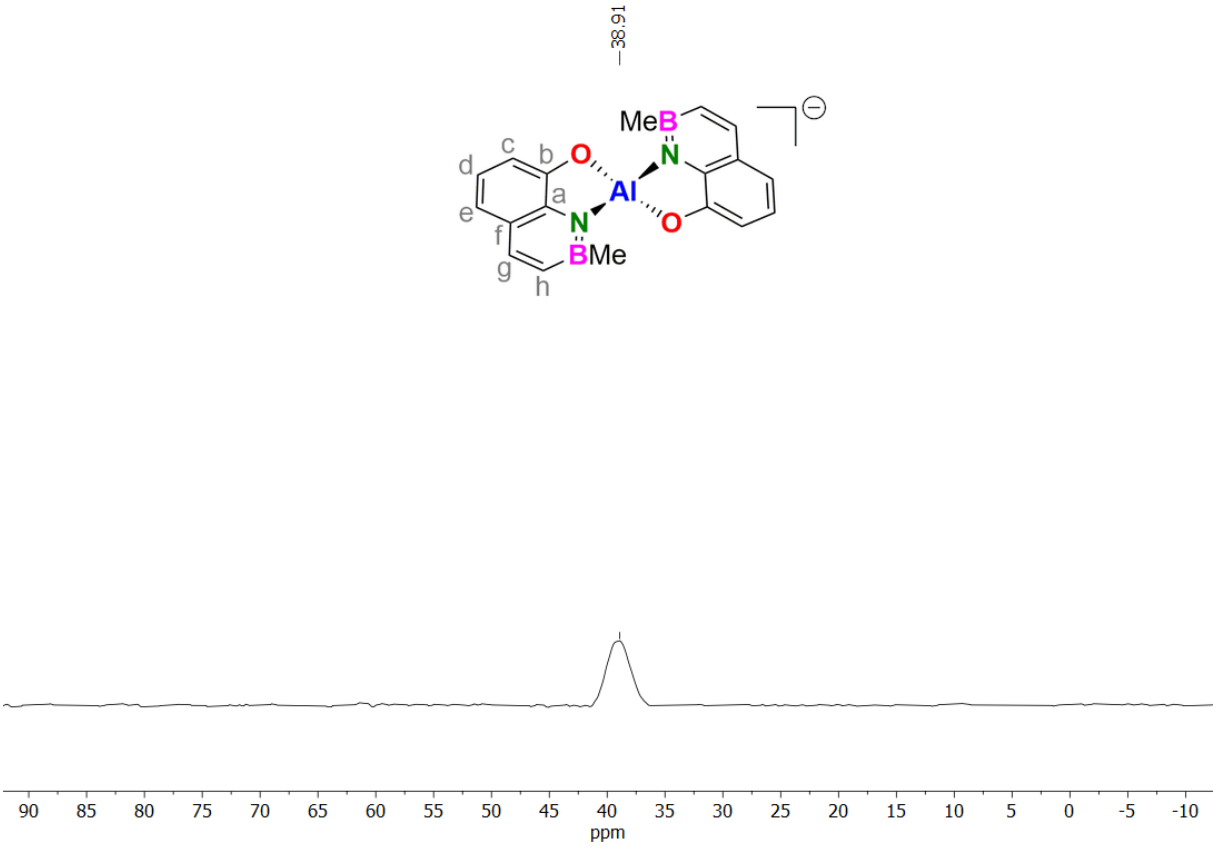
^{1}H NMR (601 MHz, THF-d_8)



$^{13}C\{^{1}H\}$ NMR (151 MHz, THF-d_8)

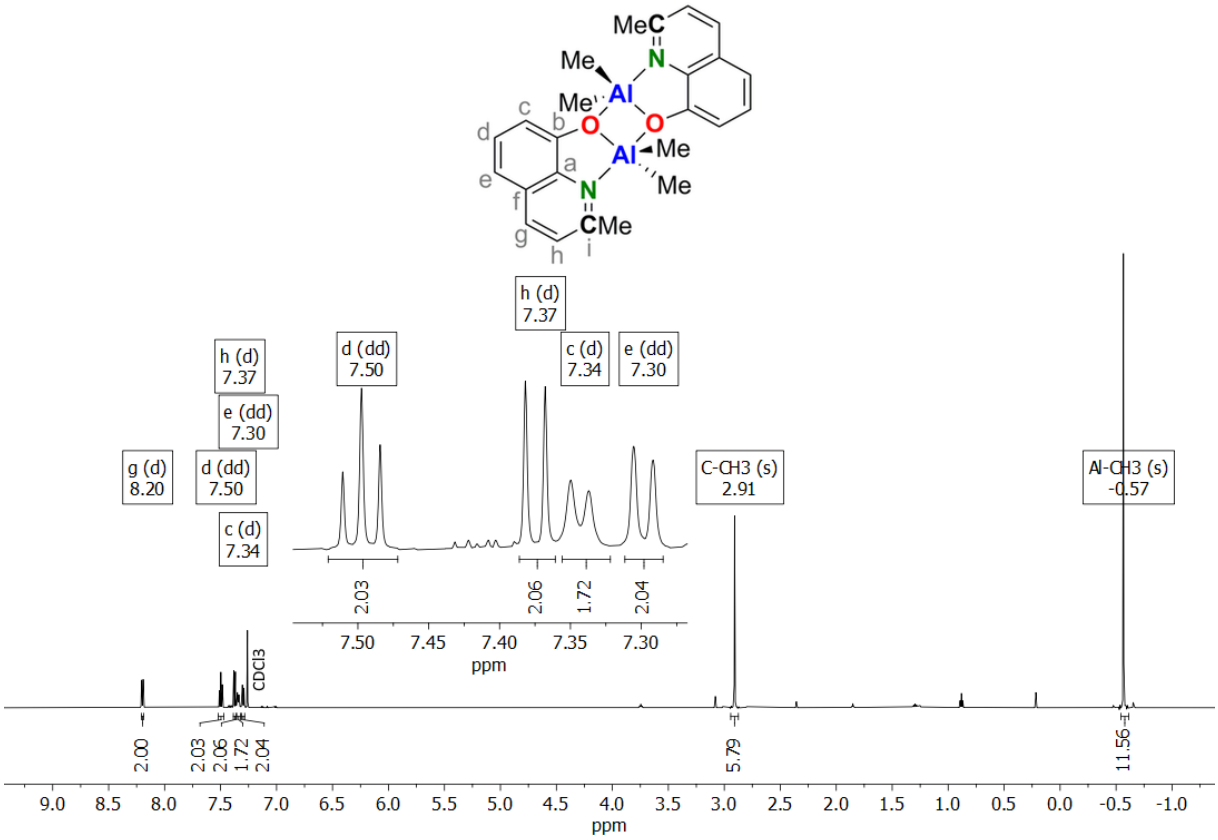


$^{11}B\{^{1}H\}$ NMR (193 MHz, THF-d_8)

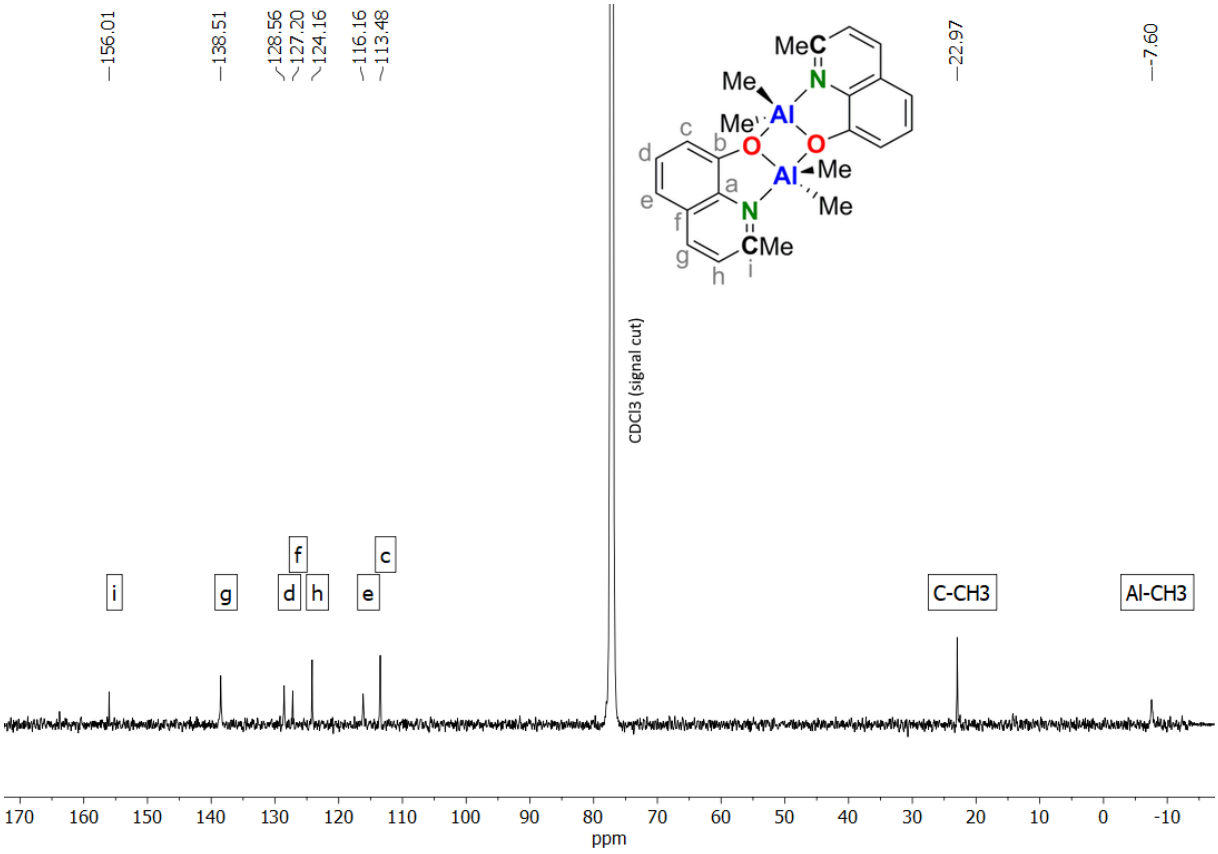


3.10. $[Me_2Al(Q')]_2$ (3)

^1H NMR (601 MHz, $CDCl_3$)



$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$)



4. Optical Spectroscopy

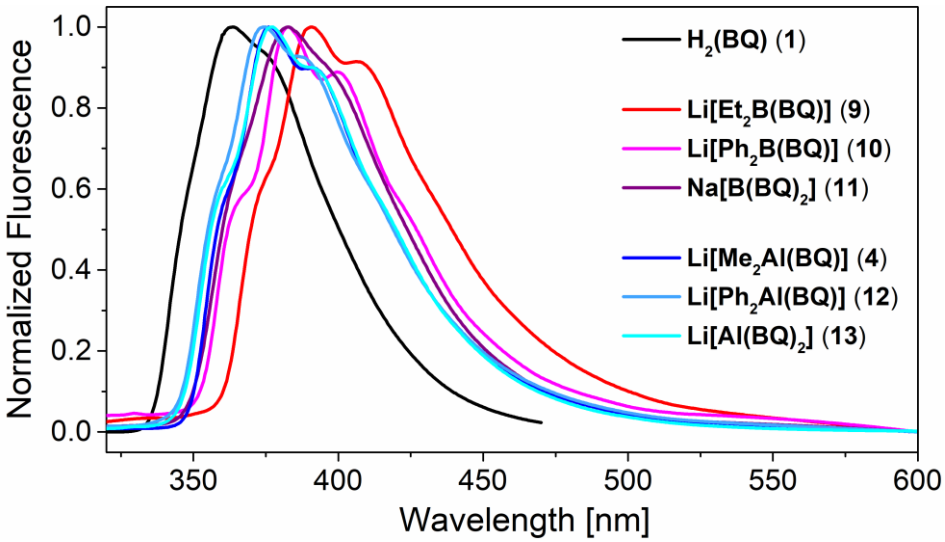


Figure S2. Fluorescence emission spectra of **H_2(BQ)** and its complexes with boron and aluminum in THF solutions.

5. Calculations

Table S2. Coordinates of the geometry-optimized structures.

Li[Me$_2$Al(BQ)] (**4**)			
Energy: –522269.7252143			
Charge: 0			
Multiplicity: 1			
Atom	X	Y	Z
C	-1.06675	1.91504	0.21772
C	-0.99552	0.54344	0.09050
C	0.10911	2.69059	0.25006
C	1.33397	2.06454	0.15145
C	1.42725	0.65494	0.02936
C	0.25117	-0.11427	-0.00601
C	0.37989	-1.54478	-0.14568
C	1.59351	-2.14585	-0.23802
B	2.87763	-1.29312	-0.18581
N	2.70147	0.11507	-0.05258
C	4.33219	-1.91965	-0.27875
O	2.53198	2.74102	0.14218
Al	3.97758	1.50839	0.16077
C	5.18026	1.54468	1.70561
C	4.85001	2.16025	-1.58118
H	-2.03637	2.40918	0.29810
H	-1.90825	-0.05595	0.06467
H	0.06661	3.77543	0.36632
H	-0.55129	-2.12227	-0.17455
H	1.61624	-3.23562	-0.34342
H	4.49931	-2.65286	0.52922
H	5.15204	-1.18330	-0.22013
H	4.46242	-2.47811	-1.22211
H	5.67077	2.52608	1.82550
H	5.98392	0.79354	1.62053
H	4.26477	2.06285	-2.52348
H	5.71507	1.50041	-1.74960
H	5.30246	3.17677	-1.56379
H	4.63932	1.33277	2.64244
Li	3.15786	3.40831	-1.38667

[Me$_2$Al(BQ)]$^-$ (**14**)			
Energy: –517571.4593898			
Charge: –1			
Multiplicity: 1			
Atom	X	Y	Z
C	-1.01759	1.95972	0.20629
C	-0.98565	0.58557	0.11585
C	0.17444	2.71533	0.20830
C	1.40470	2.08214	0.11909
C	1.44688	0.65170	0.02116
C	0.25543	-0.09582	0.02095
C	0.36098	-1.52628	-0.07923
C	1.56601	-2.15275	-0.17203
B	2.85854	-1.31213	-0.17307
N	2.70465	0.09456	-0.07226
C	4.30655	-1.97309	-0.27419
O	2.57311	2.71995	0.11561
Al	3.99728	1.55794	-0.05256
C	5.18489	1.58083	1.54582
C	4.95045	1.79271	-1.78571
H	-1.97743	2.47902	0.27799
H	-1.91066	0.00228	0.11459
H	0.15374	3.80465	0.28021
H	-0.58136	-2.09072	-0.07856
H	1.56745	-3.24752	-0.24657
H	4.37788	-2.66303	-1.13430
H	4.52418	-2.58310	0.62193
H	5.12081	-1.23690	-0.37149
H	5.73156	2.53779	1.63667
H	5.95005	0.78402	1.50149
H	5.75117	1.04346	-1.92662
H	5.43163	2.78545	-1.86197
H	4.26468	1.69856	-2.64607
H	4.62351	1.43841	2.48569

[Me$_2$Al(Q′)]$_2$ (3)			
Energy: –1051651.7114221			
Charge: 0			
Multiplicity: 1			
Atom	X	Y	Z
C	-3.87082	-2.69737	0.10197
C	-3.89183	-4.09400	-0.12682
C	-2.72043	-4.76357	-0.36051
N	-1.44386	-2.75844	-0.18114
C	-2.60224	-2.08044	0.05885
C	-2.46676	-0.67905	0.28078
C	-3.59505	0.06851	0.54080
C	-4.86358	-0.55545	0.58040
C	-5.01510	-1.90324	0.36706
Al	0.26332	-1.34141	-0.14443
O	-1.22182	-0.19440	0.22503
C	3.64564	3.08225	0.01166
C	3.65277	4.49492	0.10216
C	2.47341	5.17313	0.25619
N	1.21235	3.15029	0.23140
C	2.38002	2.46204	0.08328
C	2.25904	1.04382	0.01162
C	3.39966	0.28243	-0.12723
C	4.66471	0.91016	-0.20064
C	4.80163	2.27475	-0.13514
Al	-0.48812	1.72258	0.28423
O	1.01619	0.55669	0.09323
C	-1.48486	-4.06546	-0.37639
C	0.72469	-1.49298	-2.06465
C	1.17771	-2.20054	1.39181
C	-1.08888	2.17289	2.12247
C	-1.30714	2.34077	-1.40723
C	1.24273	4.46882	0.31992
H	-2.71787	-5.83975	-0.53551
H	-3.50217	1.13859	0.72127
H	-5.74014	0.06032	0.78934
H	-5.99866	-2.37380	0.40101
H	2.46074	6.26056	0.33539
H	3.32017	-0.80272	-0.17382
H	5.55119	0.28309	-0.31080
H	5.78313	2.74750	-0.19125
H	0.06285	-0.82629	-2.64646
H	0.61561	-2.49825	-2.50369
H	1.75590	-1.16131	-2.27492
H	1.84054	-1.49996	1.92626
H	1.80034	-3.06269	1.09351
H	0.45225	-2.57899	2.13331
H	-1.96116	2.85227	2.13388
H	-0.30198	2.66121	2.72255
H	-1.39468	1.26796	2.67395
H	-0.63667	2.12444	-2.25823
H	-1.51124	3.42435	-1.43501
H	-2.26066	1.83025	-1.62405
H	-4.84522	-4.62674	-0.11326
C	-0.04807	5.21788	0.47280
C	-0.19854	-4.81013	-0.57966
H	4.60269	5.03187	0.05442
H	-0.37295	-5.76153	-1.09934

[Me$_2$Al(Q′)] (15)			
Energy: –525816.2632290			
Charge: 0			
Multiplicity: 1			
Atom	X	Y	Z
C	-0.98862	1.91709	0.20545
C	-0.96980	0.54259	0.13878
C	0.19122	2.69238	0.17253
C	1.42943	2.08139	0.07173
C	1.45667	0.65034	0.00435
C	0.27673	-0.12313	0.03420
C	0.45265	-1.52456	-0.04856
C	1.71277	-2.06070	-0.15065
C	2.84824	-1.21809	-0.17052
N	2.70229	0.09680	-0.09382
C	4.23975	-1.76926	-0.26676
O	2.58680	2.71259	0.03165
Al	4.07082	1.63321	-0.07904
C	5.09479	1.54591	1.59832
C	4.95443	1.70880	-1.83509
H	-1.94683	2.43446	0.28641
H	-1.89205	-0.03880	0.16405
H	0.14723	3.78030	0.22580
H	-0.42411	-2.17597	-0.03288
H	1.85650	-3.13906	-0.21784
H	4.22809	-2.84834	-0.46425
H	4.78671	-1.59463	0.67275
H	4.79939	-1.26923	-1.07069
H	4.45732	1.30882	2.46663
H	5.57618	2.51583	1.81328
H	5.90591	0.79776	1.56660
H	4.25658	1.49985	-2.66331
H	5.80137	1.00695	-1.92632
H	5.36819	2.71644	-2.01546

H	0.26308	-5.03259	0.39513
H	0.51741	-4.21091	-1.15428
H	-0.77526	4.63327	1.04821
H	-0.48804	5.42243	-0.51587
H	0.11704	6.18110	0.97406

6. References

1. Mohammadnezhad, G.; Amini, M.M.; Khavasi, H.R.; Plass, W. Structural and spectroscopic characterizations of aluminum phenoxide. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2016**, *157*, 238-243, doi:https://doi.org/10.1016/j.saa.2016.01.009.