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Vessel for the synthesis of 4-chloro-2,3,5,6-tetrafluoroaniline (1)

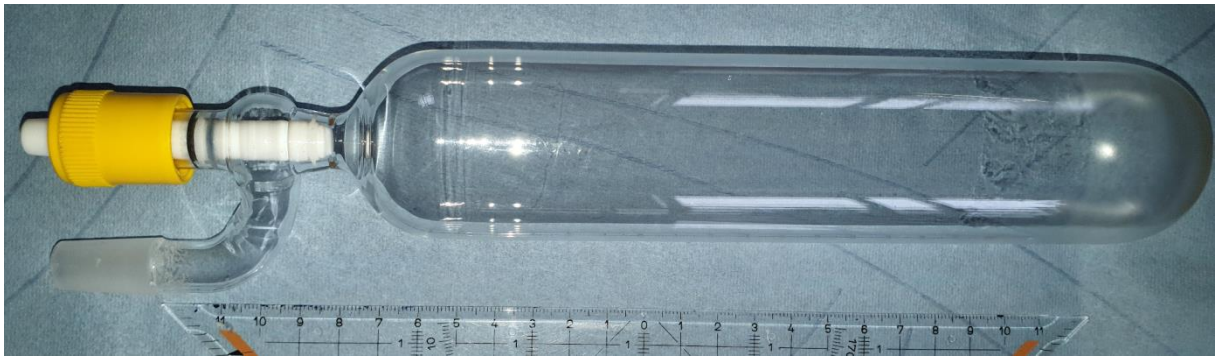


Figure S1. Photography of a reaction vessel similar to the one used for the synthesis of 4-Chloro-2,3,5,6-tetrafluoroaniline (**1**). Scale in cm. Additionally, the vessel must be surrounded by a burst protection (e.g. by placing it in a metallic container completely surrounded by non-flammable cloth) before warming up the reaction mixture above the boiling point of ammonia to prevent injuries in the event of an explosion (which we never encountered during this study).

NMR Spectra

4-Chloro-2,3,5,6-tetrafluoroaniline (1)

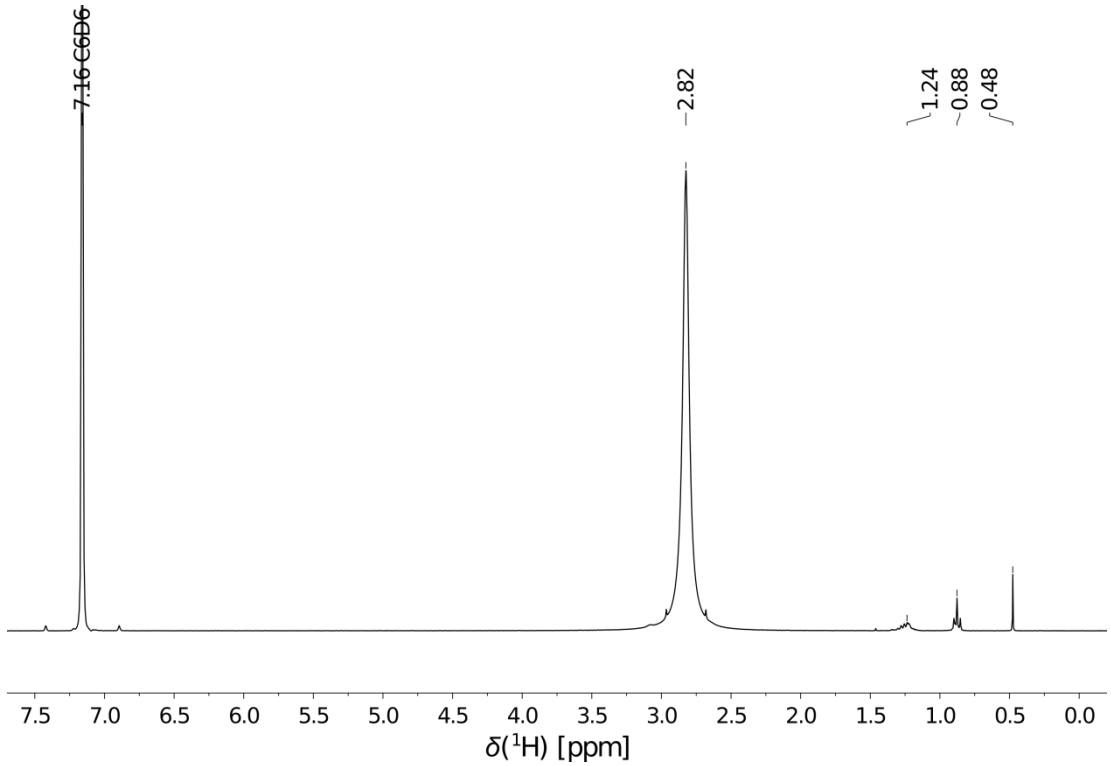


Figure S2. ^{1}H NMR spectrum (300 MHz, C_6D_6) of 4-Chloro-2,3,5,6-tetrafluoroaniline (**1**).

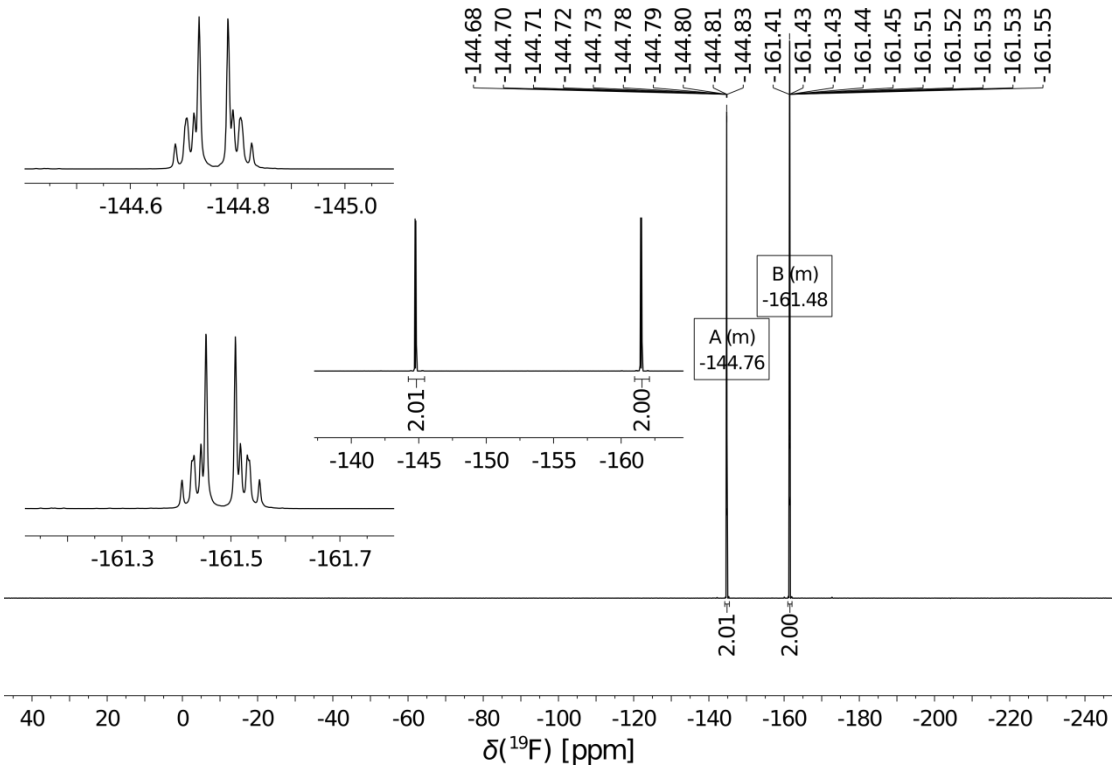


Figure S3. ^{19}F NMR spectrum (282 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroaniline (**1**).

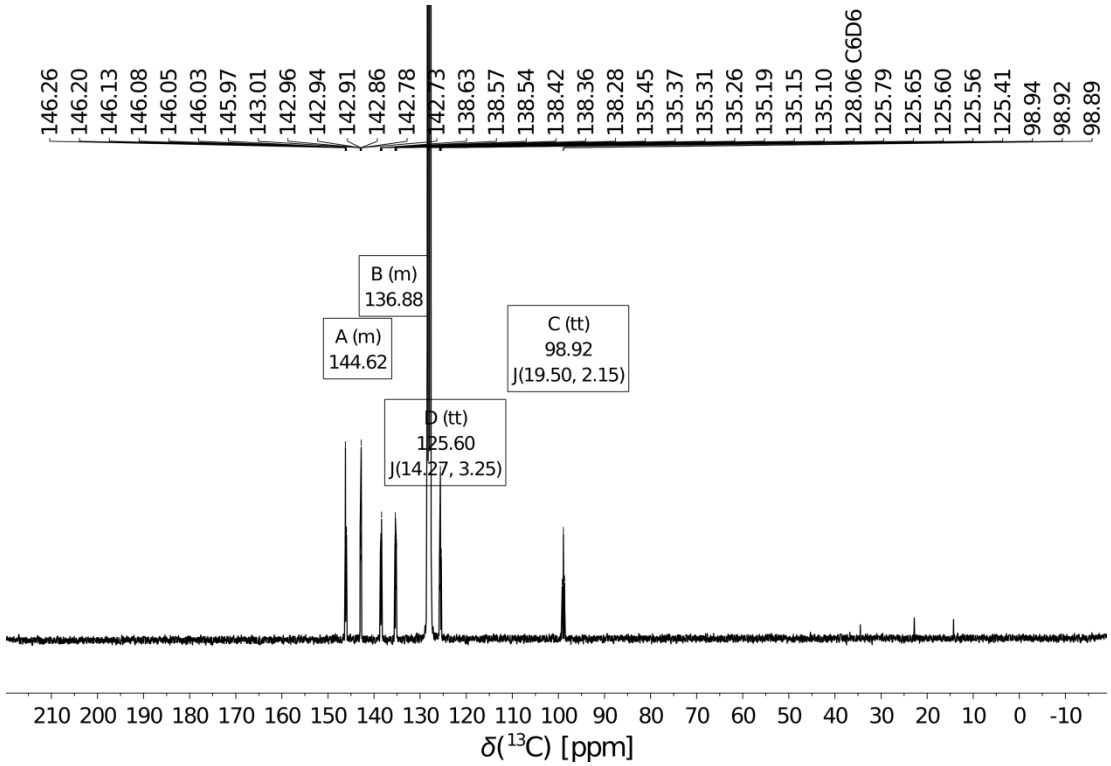


Figure S4. Full $^{13}C\{^1H\}$ NMR spectrum (75 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroaniline (**1**).

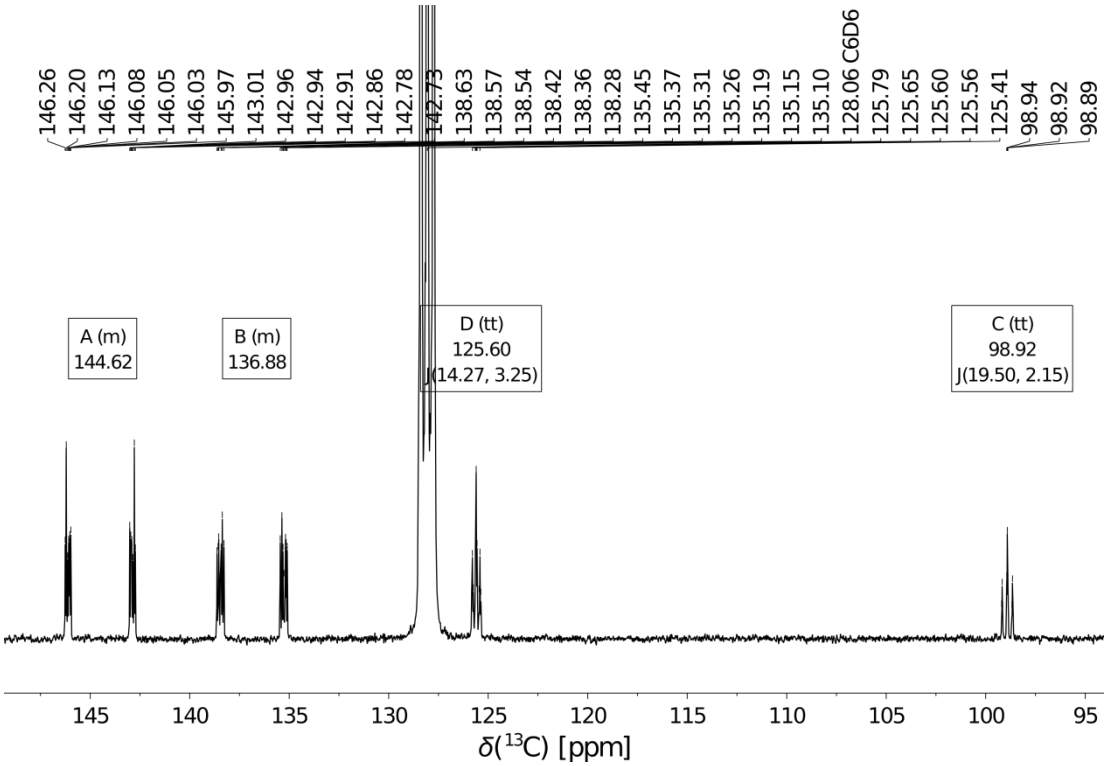


Figure S5. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroaniline (**1**).

4-Chloro-2,3,5,6-tetrafluorobromobenzene (2)

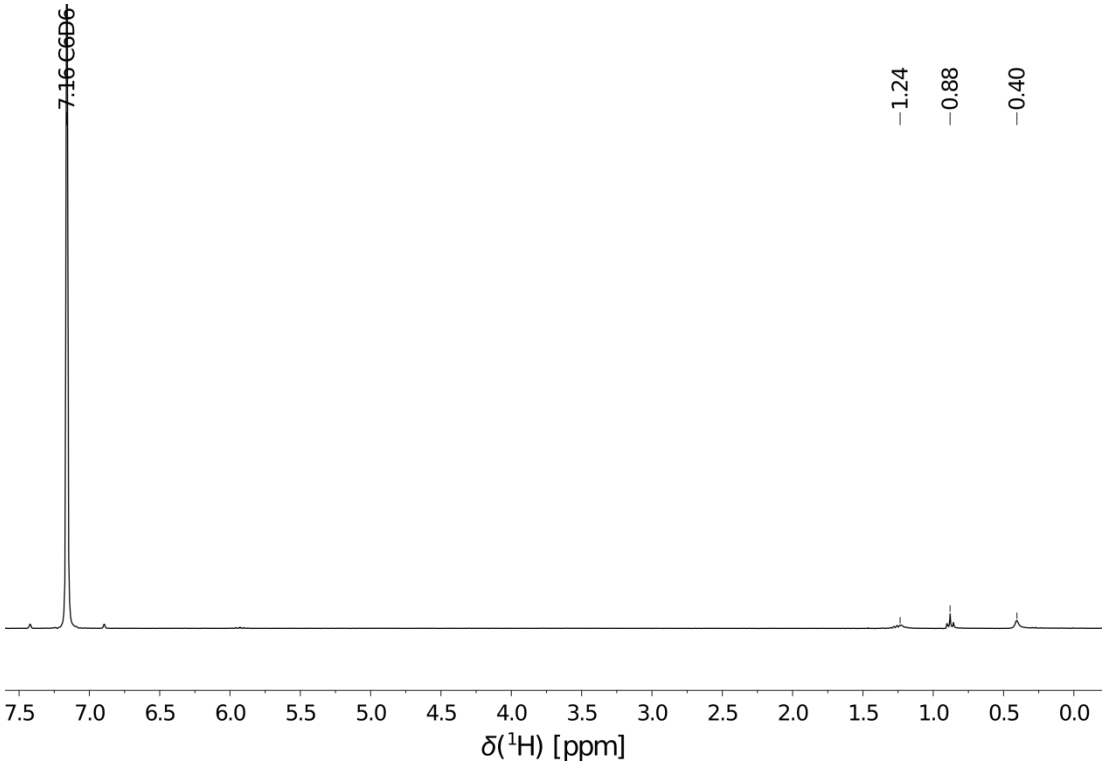


Figure S6. ^{1}H NMR spectrum (300 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluorobromobenzene (**2**).

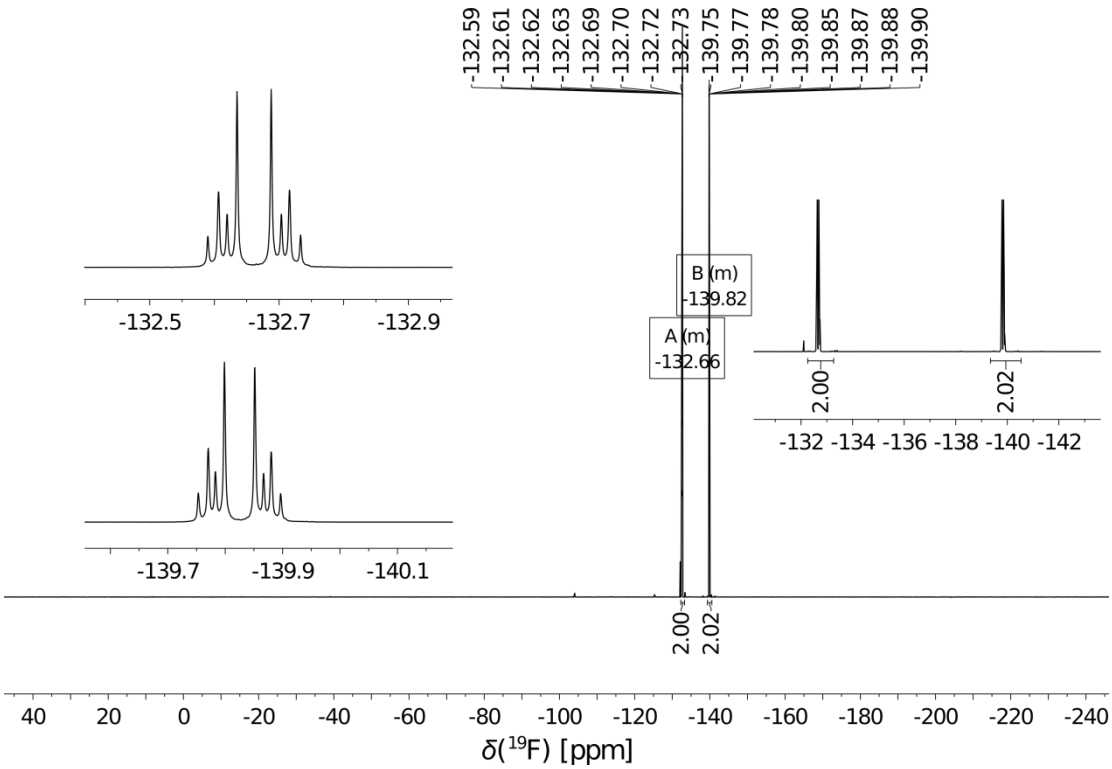


Figure S7. ^{19}F NMR spectrum (282 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluorobromobenzene (**2**).

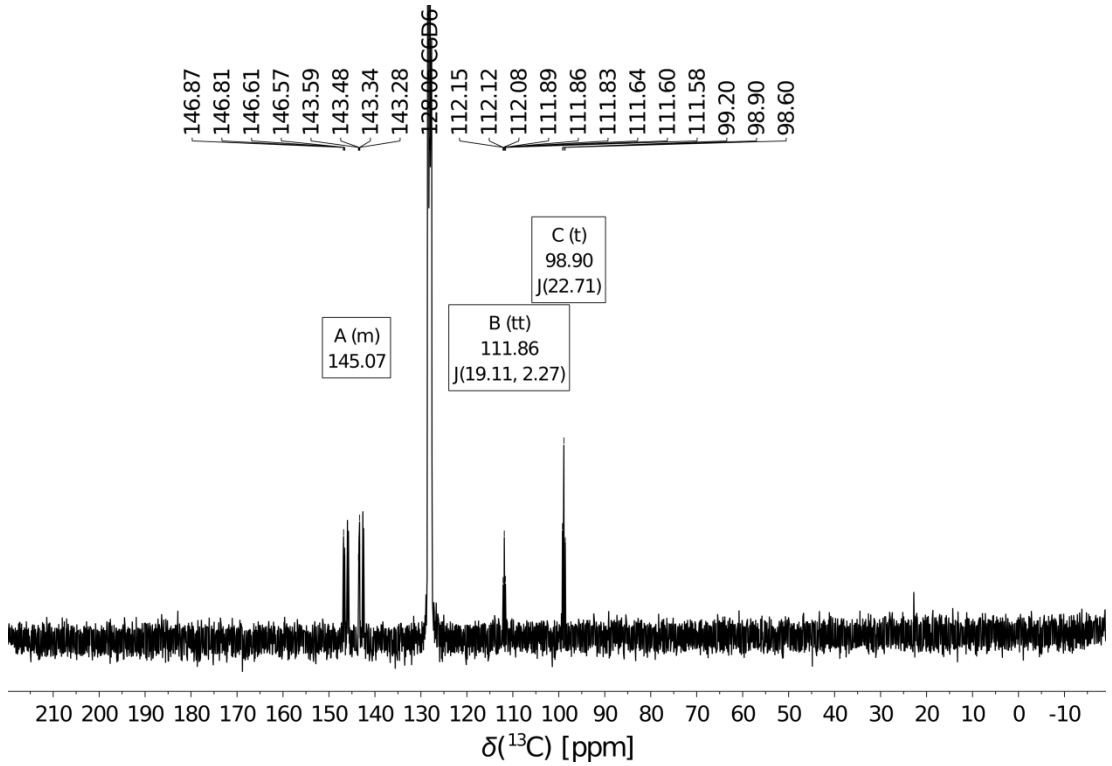


Figure S8. Full $^{13}C\{^1H\}$ NMR spectrum (75 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluorobromobenzene (**2**).

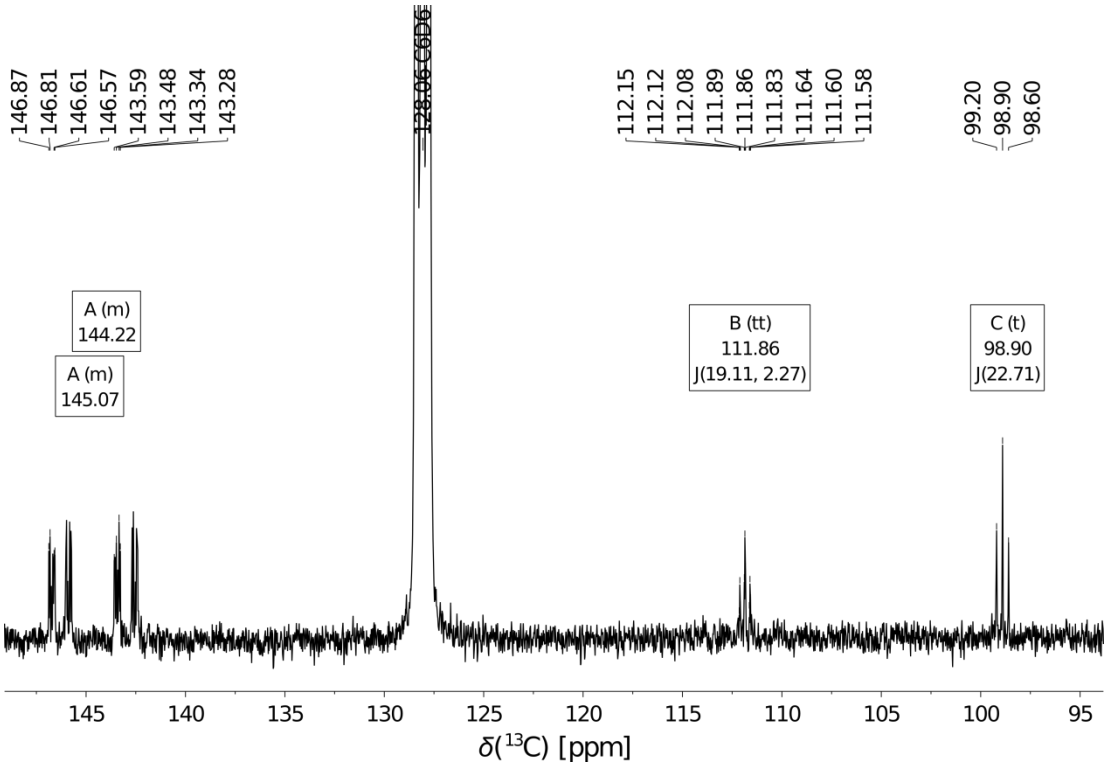


Figure S9. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluorobromobenzene (**2**).

4-Chloro-2,3,5,6-tetrafluoroiodobenzene (3)

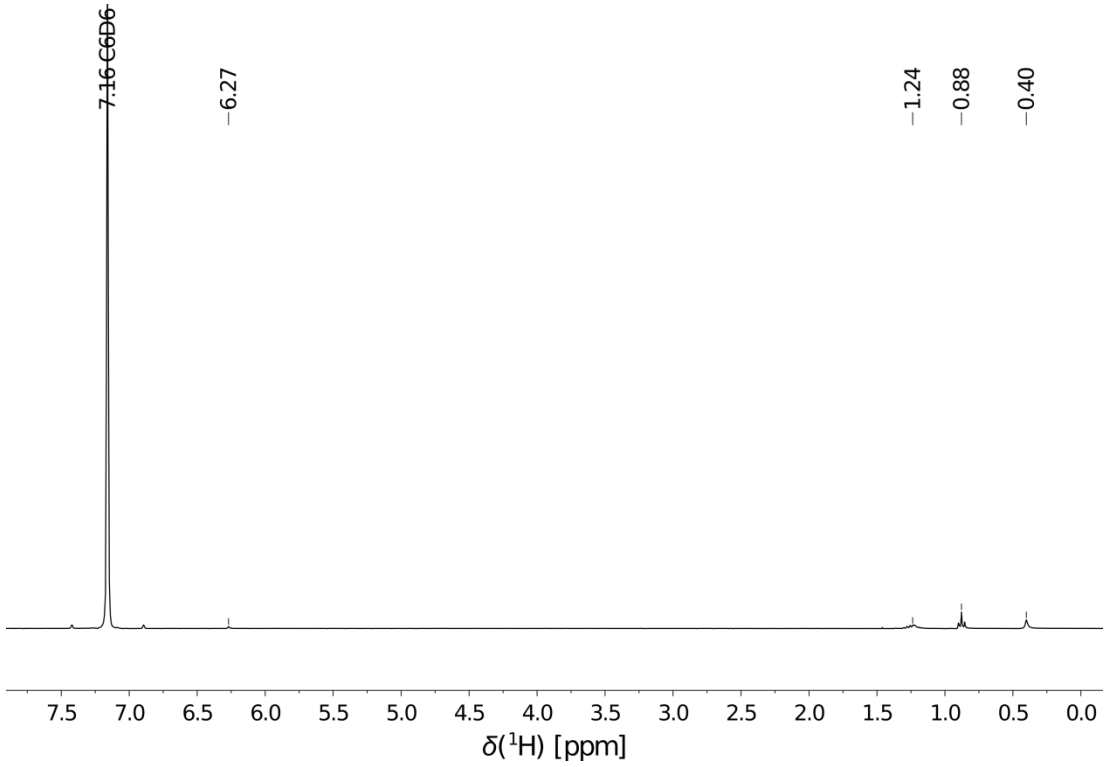


Figure S10. ^{1}H NMR spectrum (300 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroiodobenzene (**3**).

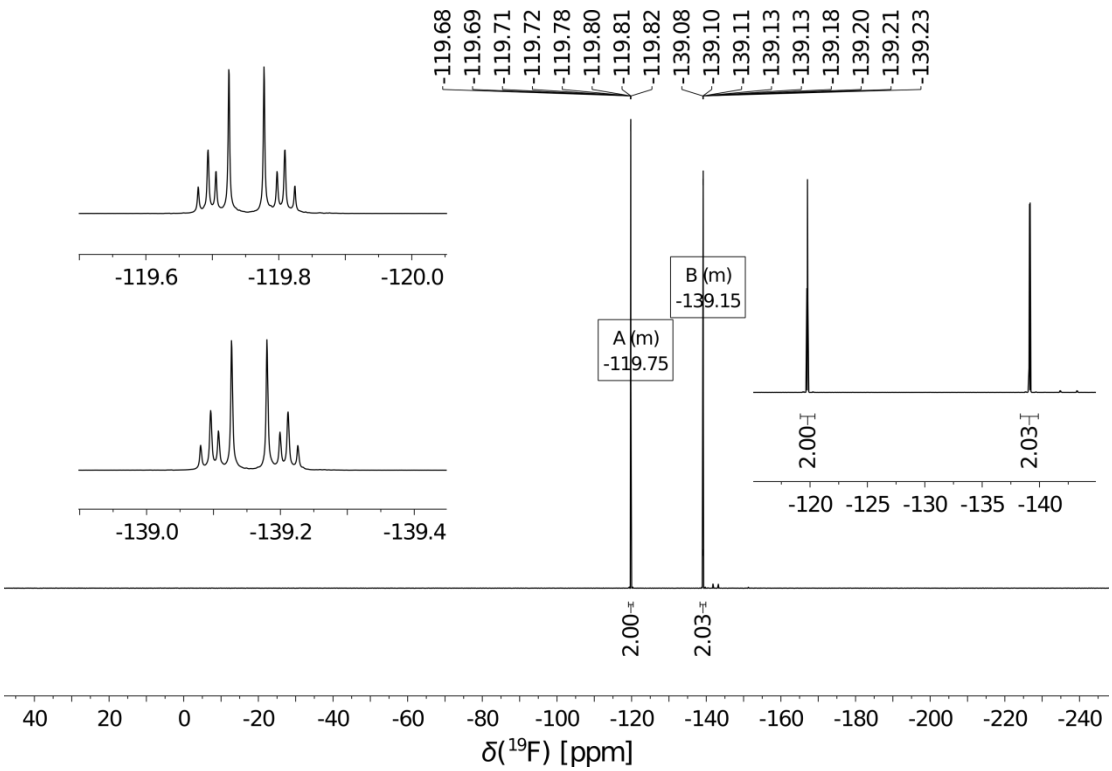


Figure S11. ^{19}F NMR spectrum (282 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroiodobenzene (**3**).

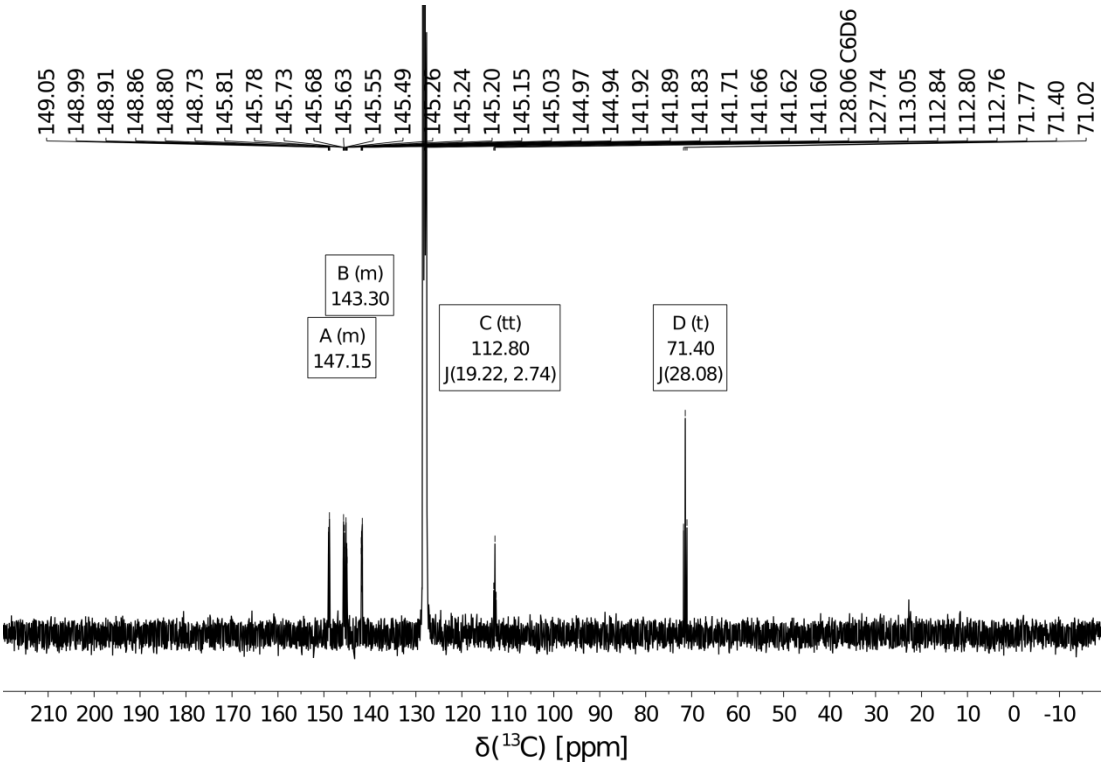


Figure S12. Full $^{13}C\{^1H\}$ NMR spectrum (75 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroiodobenzene (**3**).

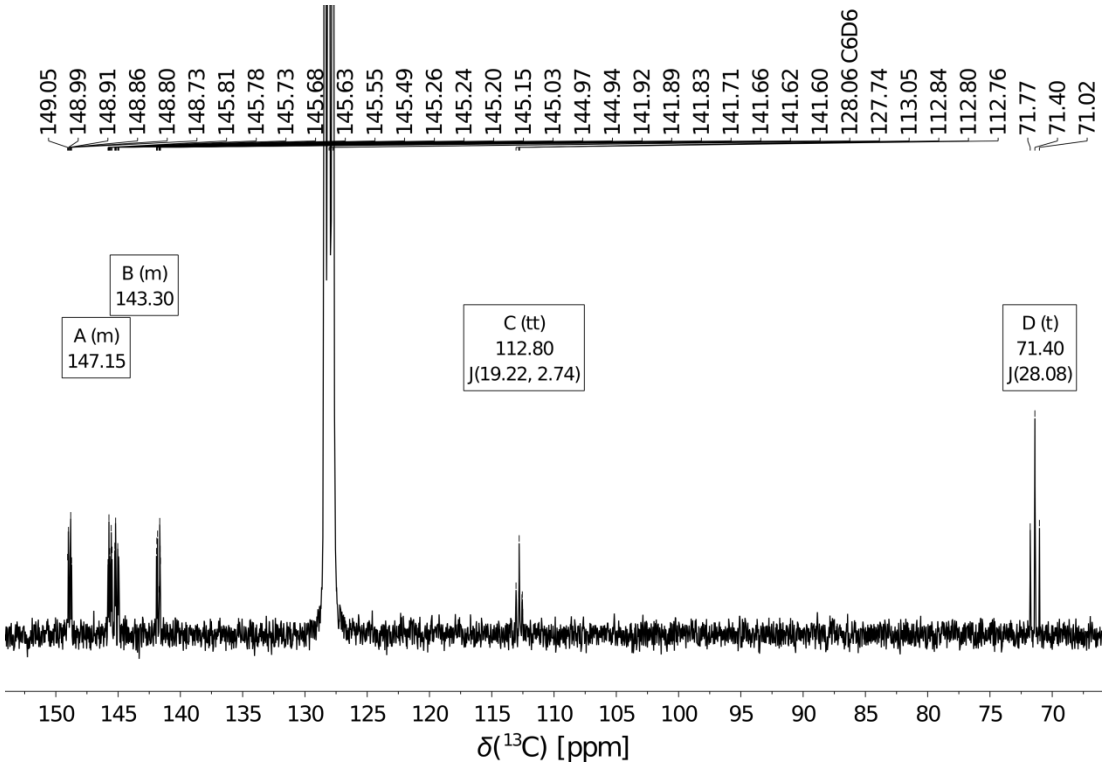


Figure S13. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of 4-chloro-2,3,5,6-tetrafluoroiodobenzene (**3**).

Bis(*para*-chlorotetrafluorophenyl)dimethylstannane (4)

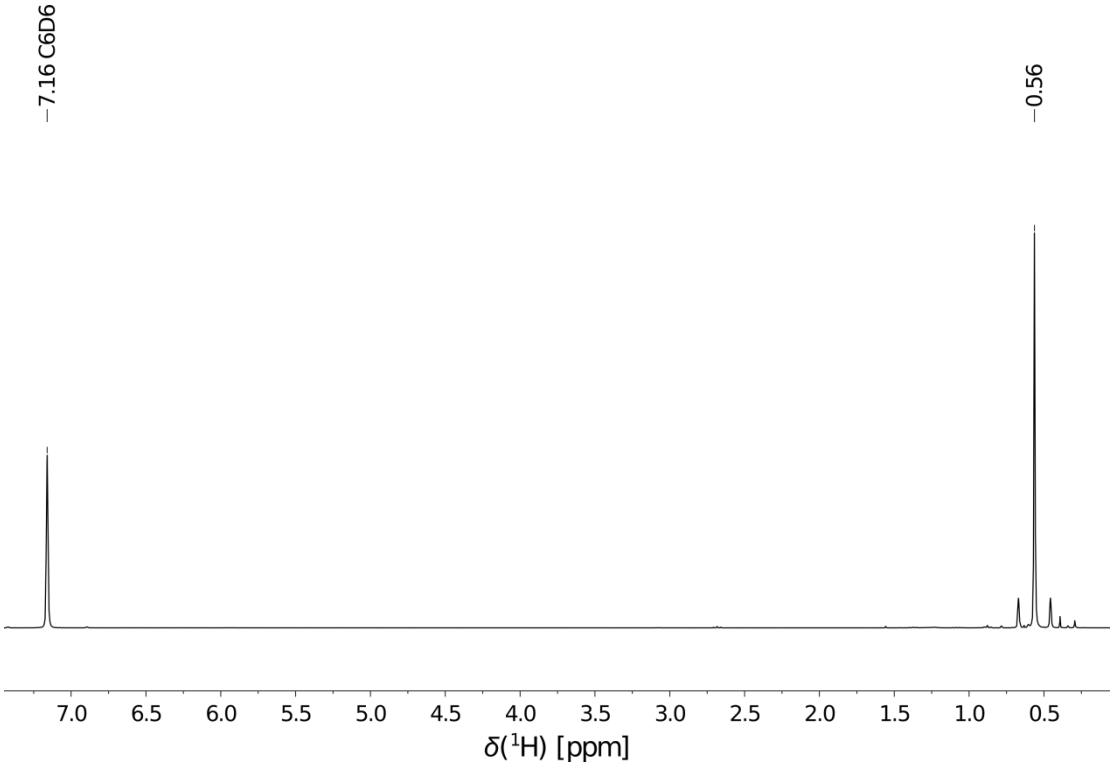


Figure S14. ^{1}H NMR spectrum (300 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)dimethylstannane (**4**).

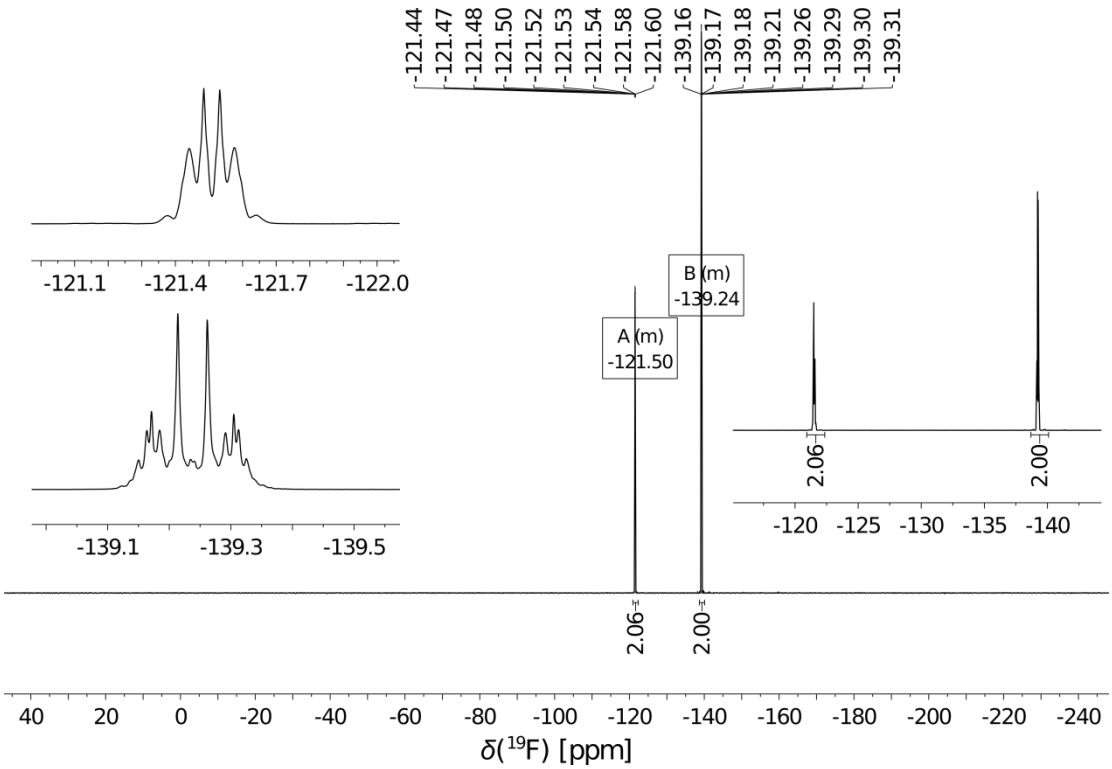


Figure S15. ^{19}F NMR spectrum (282 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)dimethylstannane (**4**).

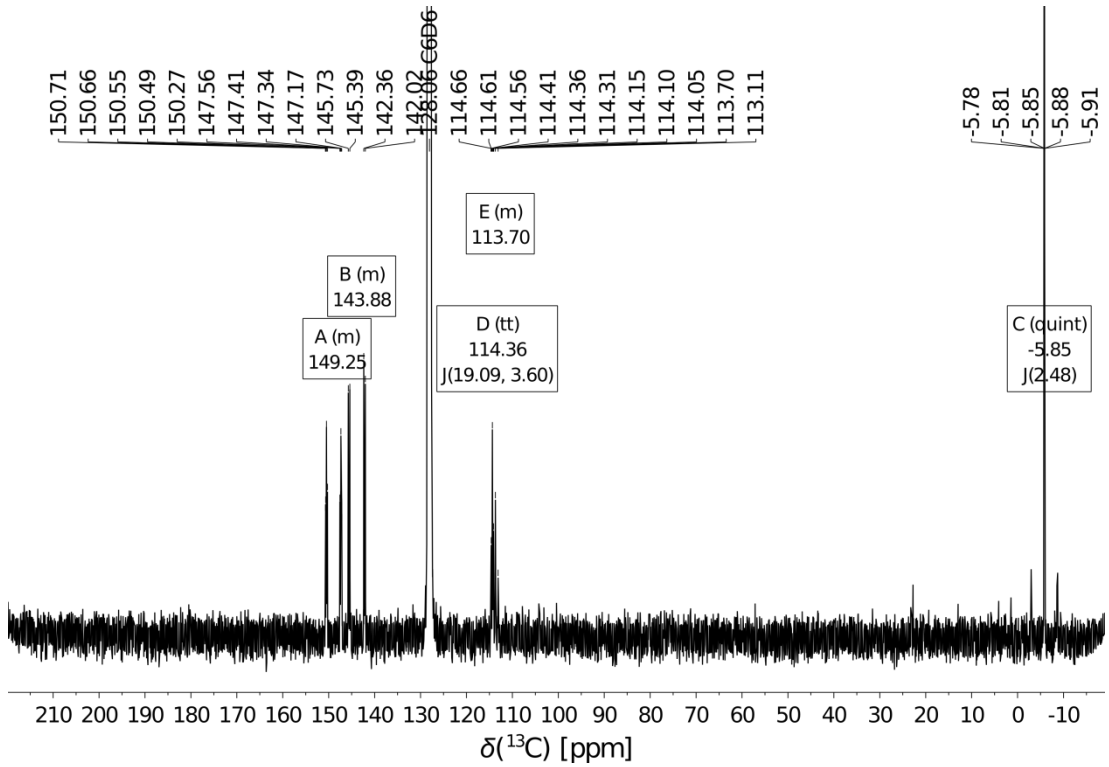


Figure S16. Full ^{13}C NMR spectrum (75 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)-dimethylstannane (**4**).

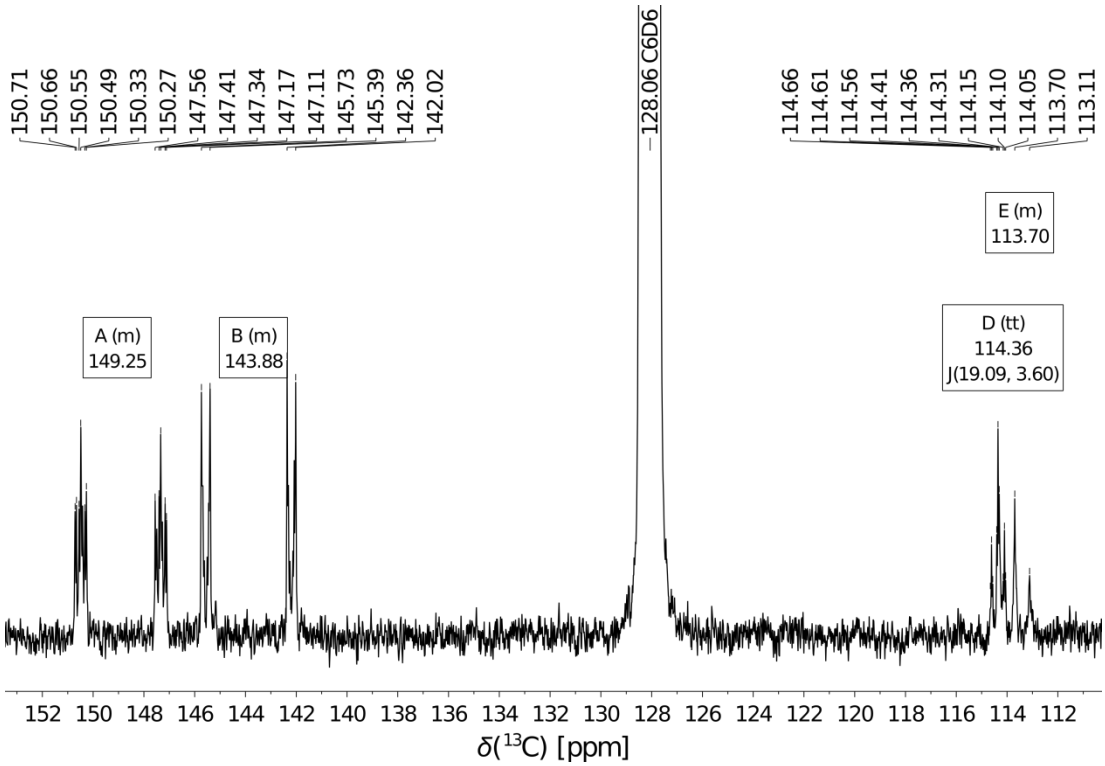


Figure S17. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)dimethylstannane (**4**) containing the signals of aromatic carbon atoms.

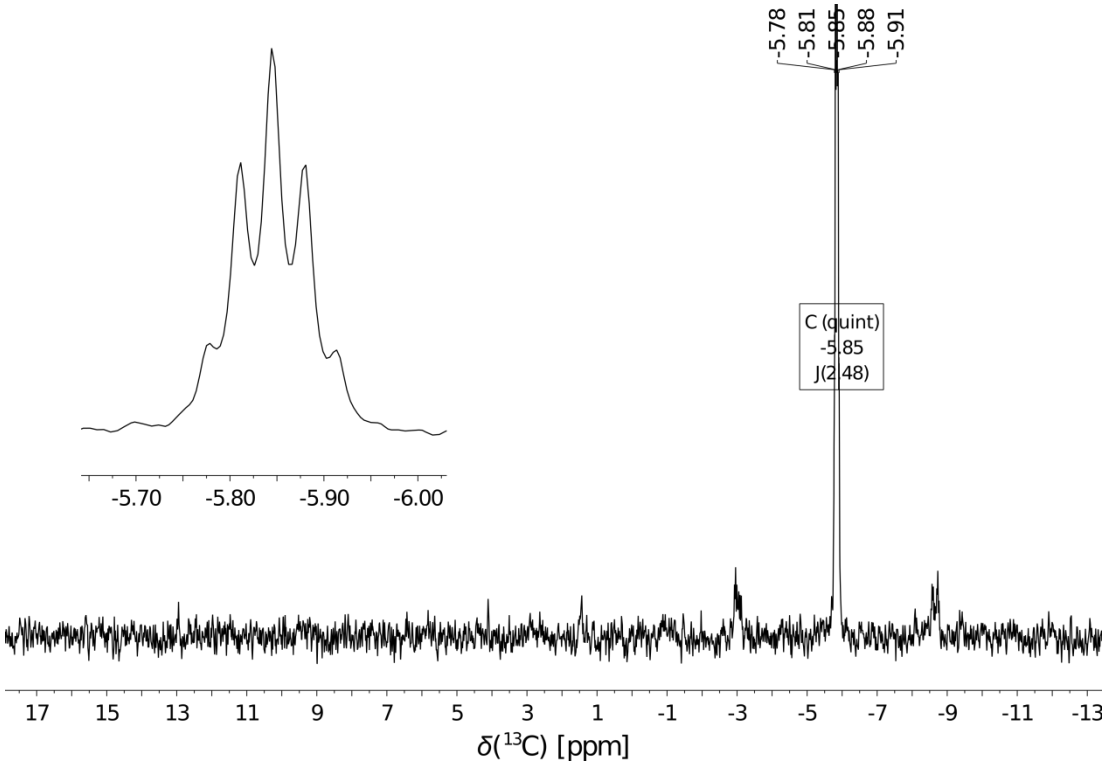


Figure S18. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)dimethylstannane (**4**) containing the signal of the aliphatic carbon atoms.

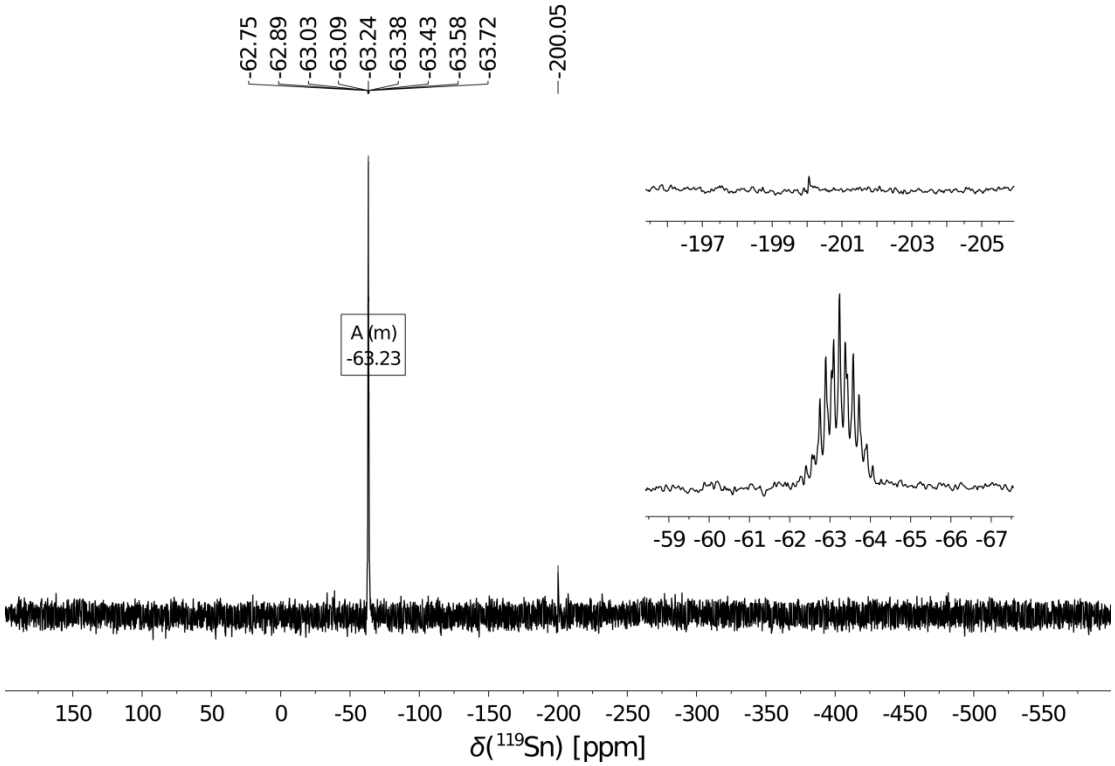


Figure S19. $^{119}Sn\{^{1}H\}$ NMR spectrum (112 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)dimethyl-stannane (**4**).

Bis(para-chlorotetrafluorophenyl)chloroborane (5)

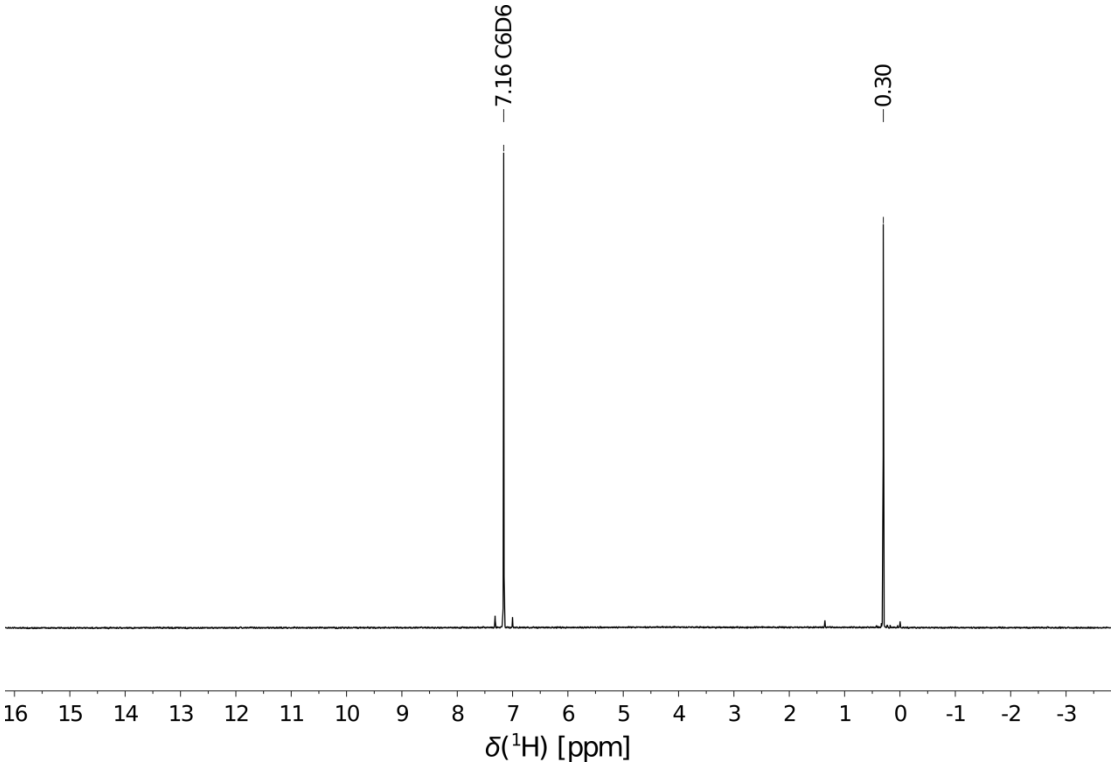


Figure S20. ^{1}H NMR spectrum (500 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)chloroborane (**5**).

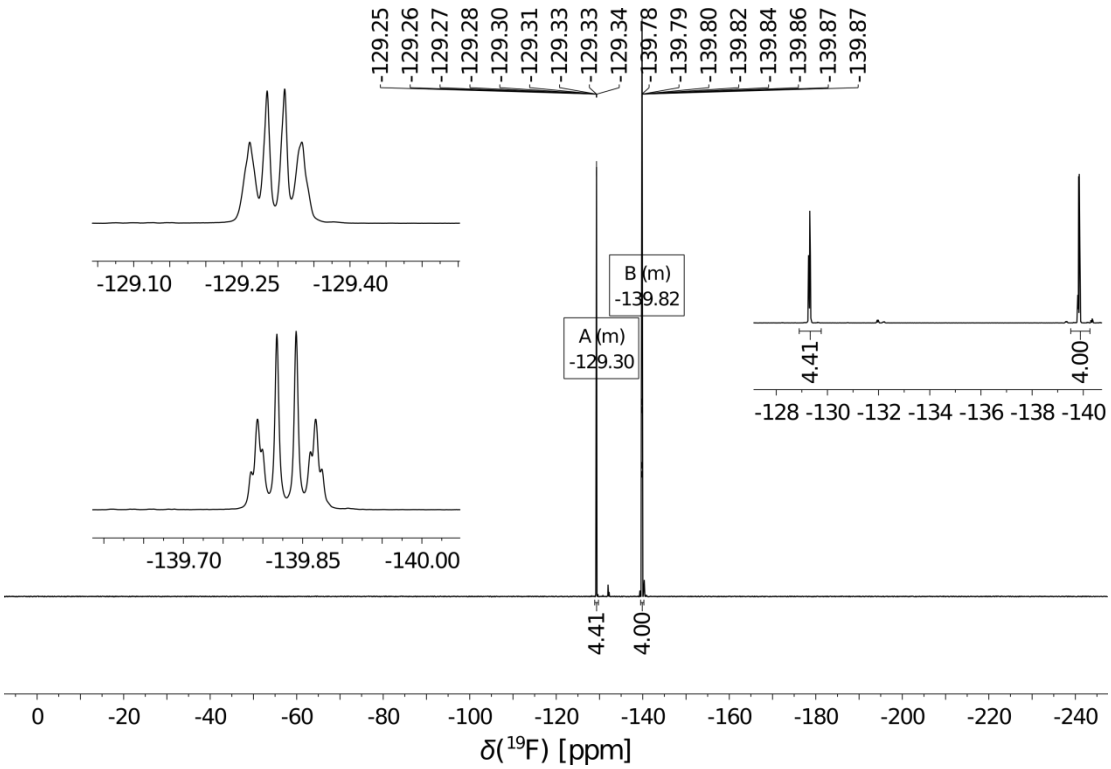


Figure S21. ^{19}F NMR spectrum (471 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)chloroborane (**5**).

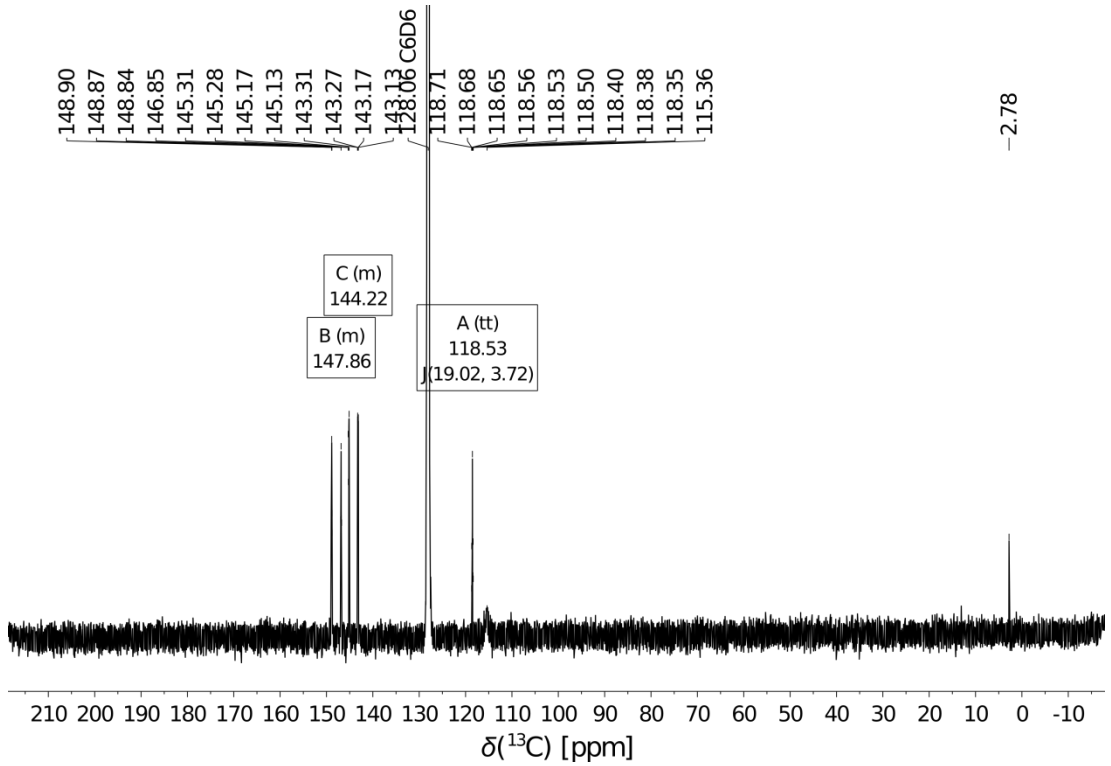


Figure S22. Full $^{13}C\{^1H\}$ NMR spectrum (126 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)chloroborane (**5**).

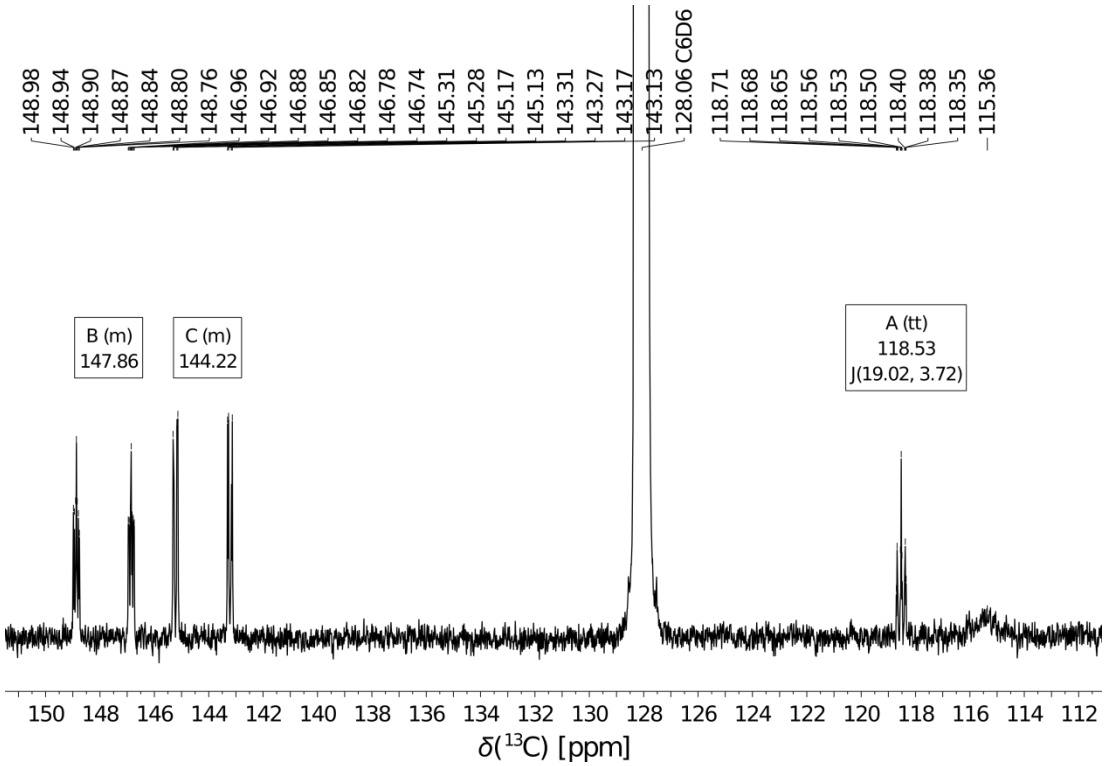


Figure S23. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)chloroborane (**5**).

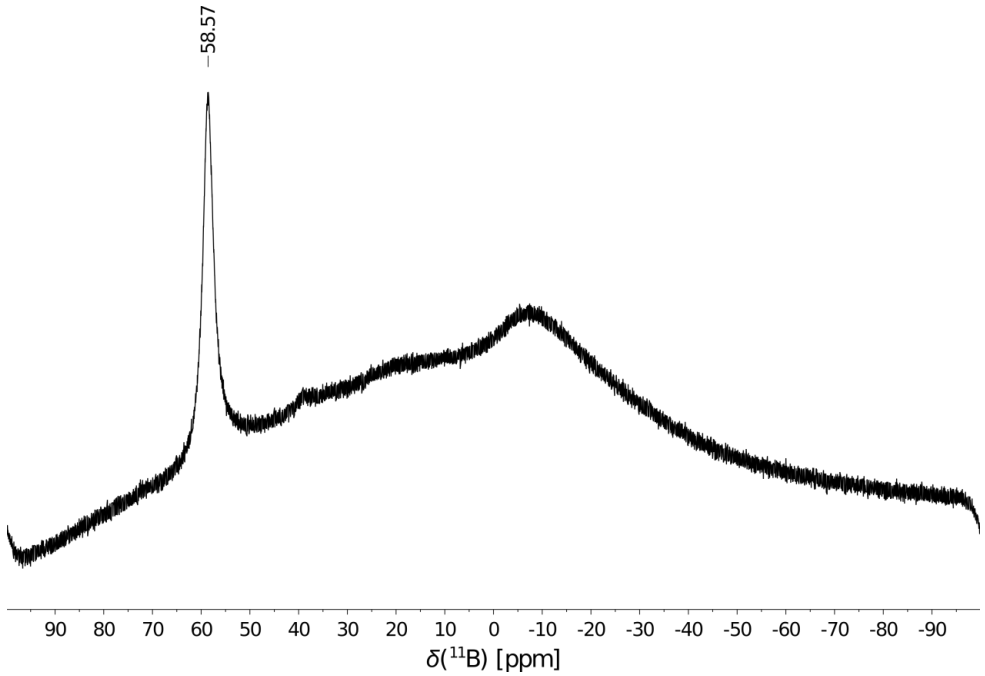


Figure S24. ^{11}B NMR spectrum (160 MHz, C_6D_6) of bis(*para*-chlorotetrafluorophenyl)chloroborane (**5**).

Reaction mixtures of the hydroborations of Ph-CH=CH$_2$, Ph-C≡CH, TMS-CH=CH$_2$ and TMS-C≡CH with bis(*para*-chlorotetrafluorophenyl)hydridoborane (6)

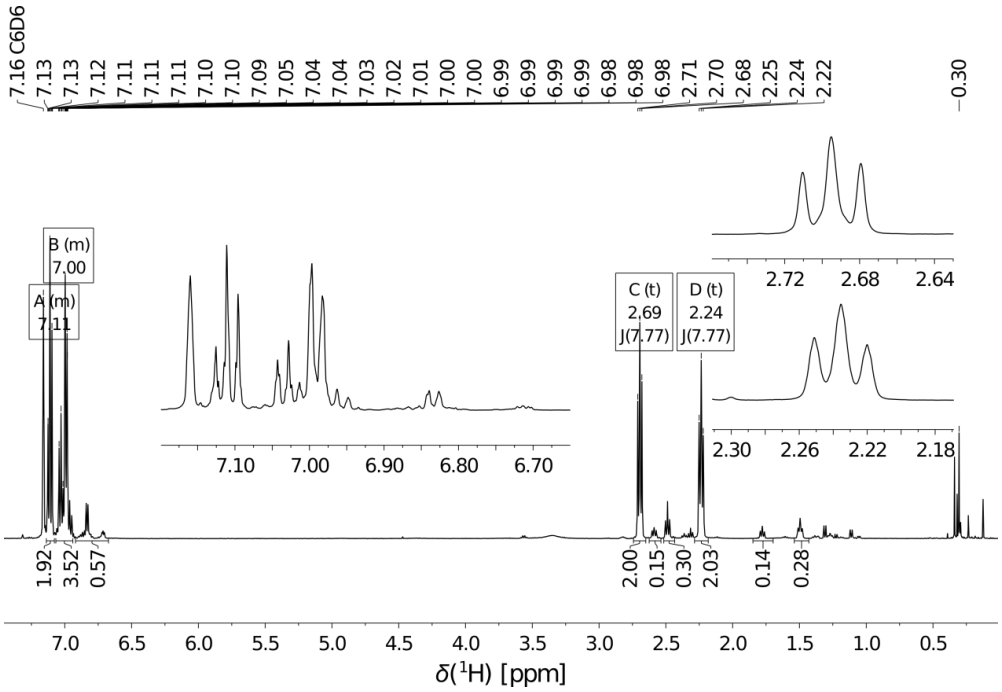


Figure S25. ^{1}H NMR spectrum (500 MHz, C_6D_6) of the hydroboration of styrene (Ph-CH=CH$_2$) with bis(*para*-chlorotetrafluorophenyl)hydridoborane (**6**) containing 2-phenyl-1-(bis(4-chloro-2,3,5,6-tetrafluorophenyl)boranyl)ethane as the main product.

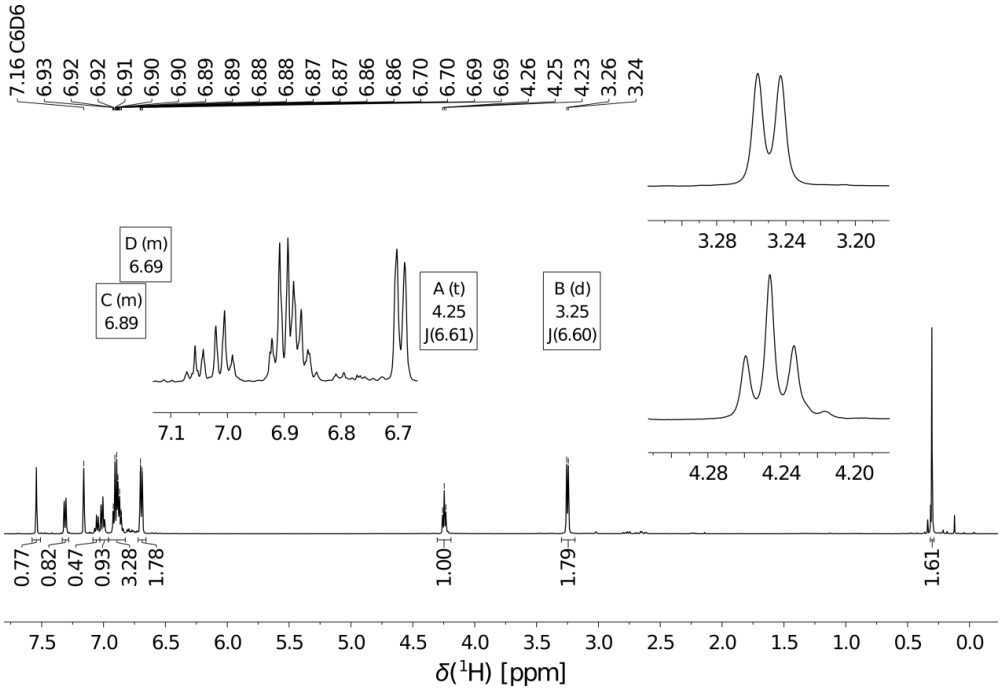


Figure S26. ^{1}H NMR spectrum (500 MHz, C_6D_6) of the hydroboration of phenylacetylene (Ph-C≡CH) with two equivalents of bis(*para*-chlorotetrafluorophenyl)hydridoborane (**6**) containing 2-phenyl-1,1-bis(bis(4-chloro-2,3,5,6-tetrafluorophenyl)boranyl)ethane as the main product.

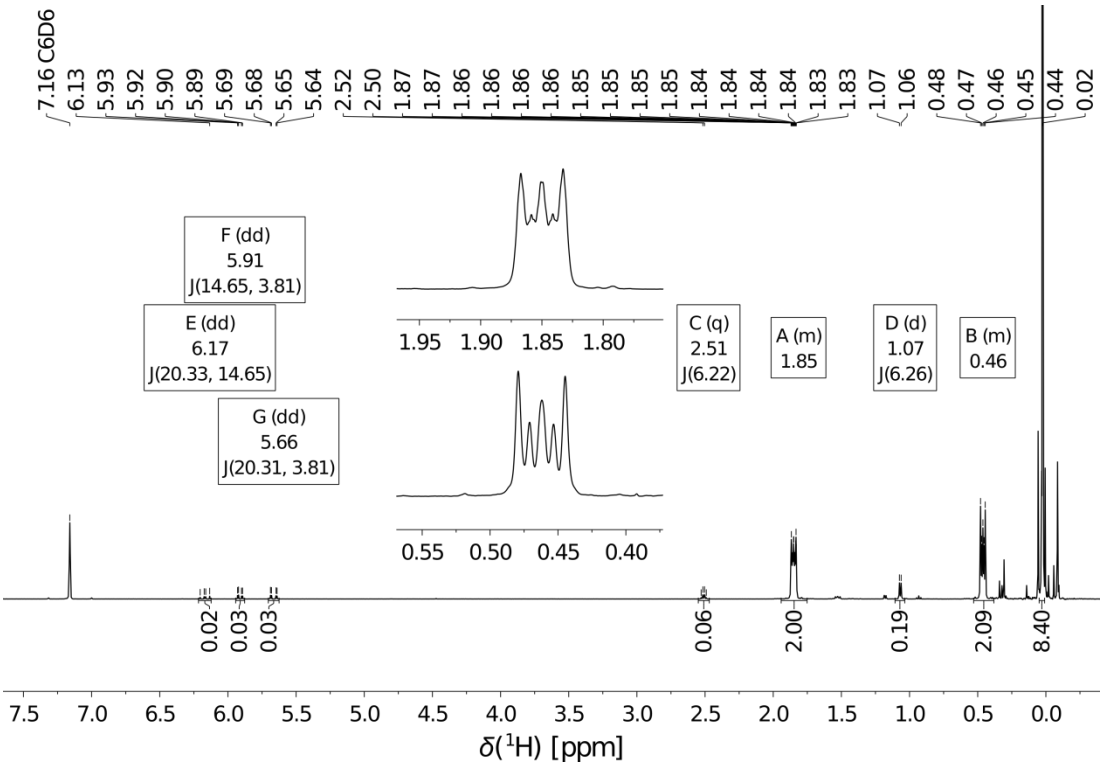


Figure S27. ^{1}H NMR spectrum (500 MHz, C_6D_6) of the hydroboration of trimethylvinylsilane (TMS-CH=CH_2) with bis(*para*-chlorotetrafluorophenyl)hydridoborane (**6**) containing 2-(trimethylsilyl)-1-(bis(4-chloro-2,3,5,6-tetrafluorophenyl)boranyl)ethane as the main product.

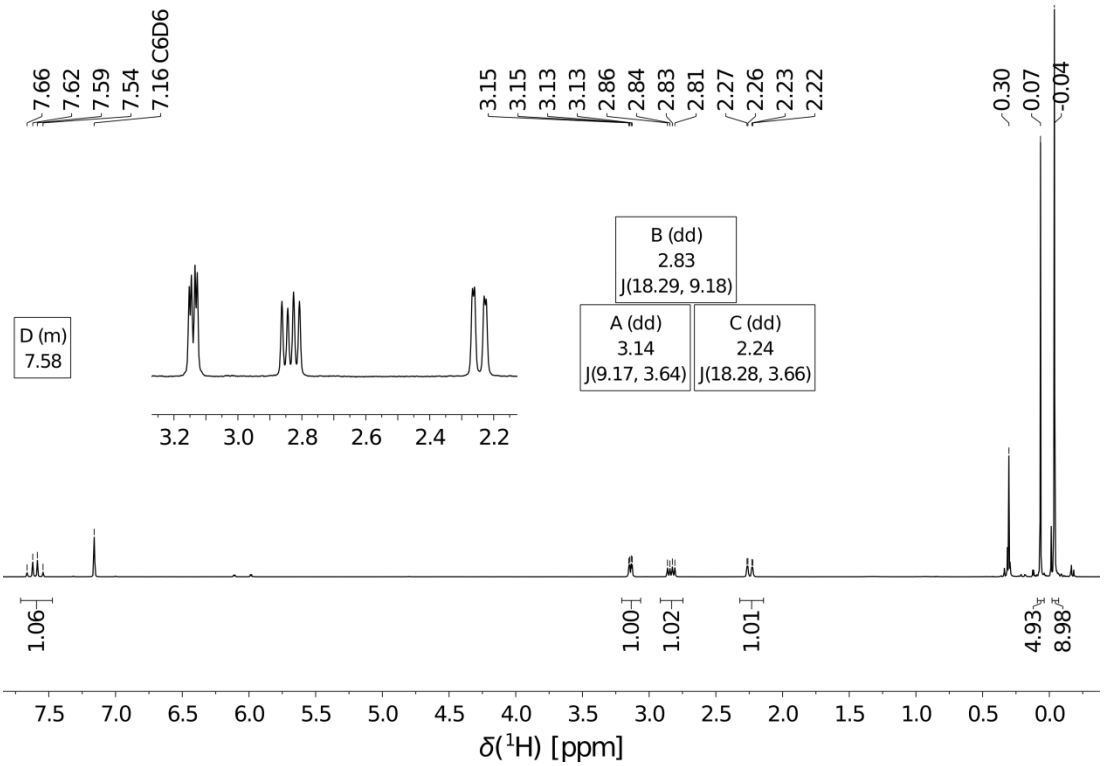


Figure S28. ^{1}H NMR spectrum (500 MHz, C_6D_6) of the hydroboration of trimethylsilylacetylene (TMS-C≡CH) with two equivalents of bis(*para*-chlorotetrafluorophenyl)hydridoborane (**6**) containing 2-(trimethylsilyl)-1,1-bis(bis(4-chloro-2,3,5,6-tetrafluorophenyl)boranyl)ethane as the main product.

Tris(*para*-chlorotetrafluorophenyl)borane (7)

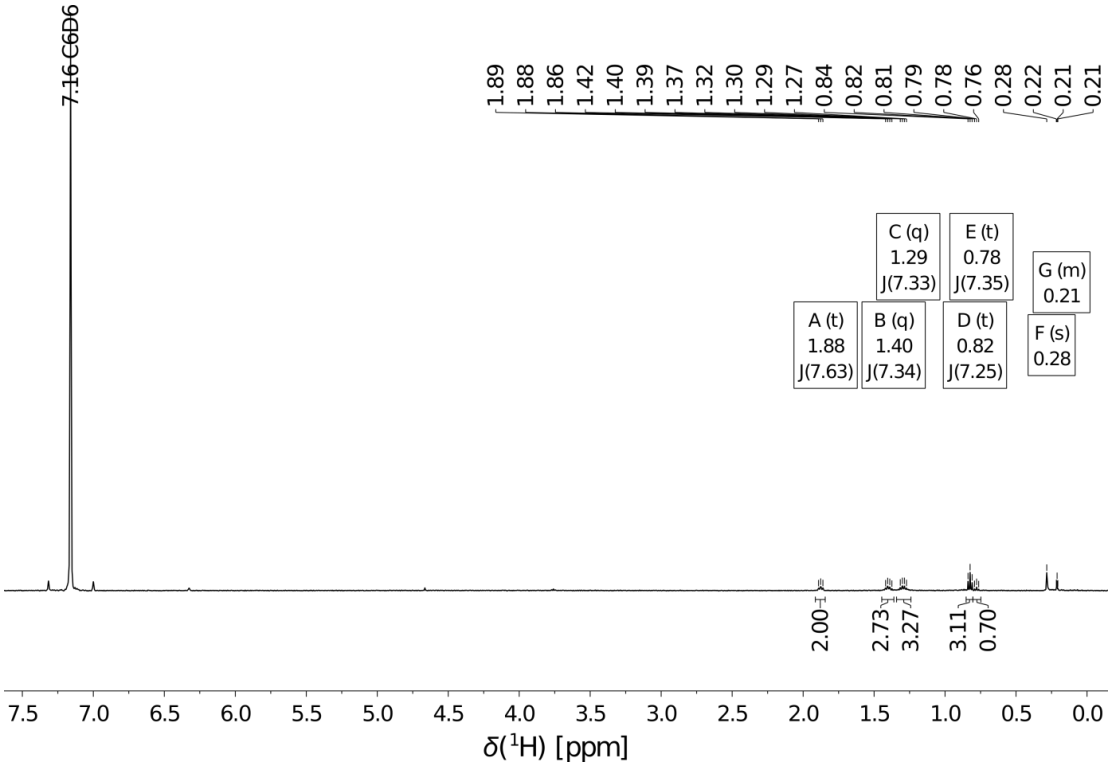


Figure S29. ^{1}H NMR spectrum (500 MHz, C_6D_6) of tris(*para*-chlorotetrafluorophenyl)borane (**7**).

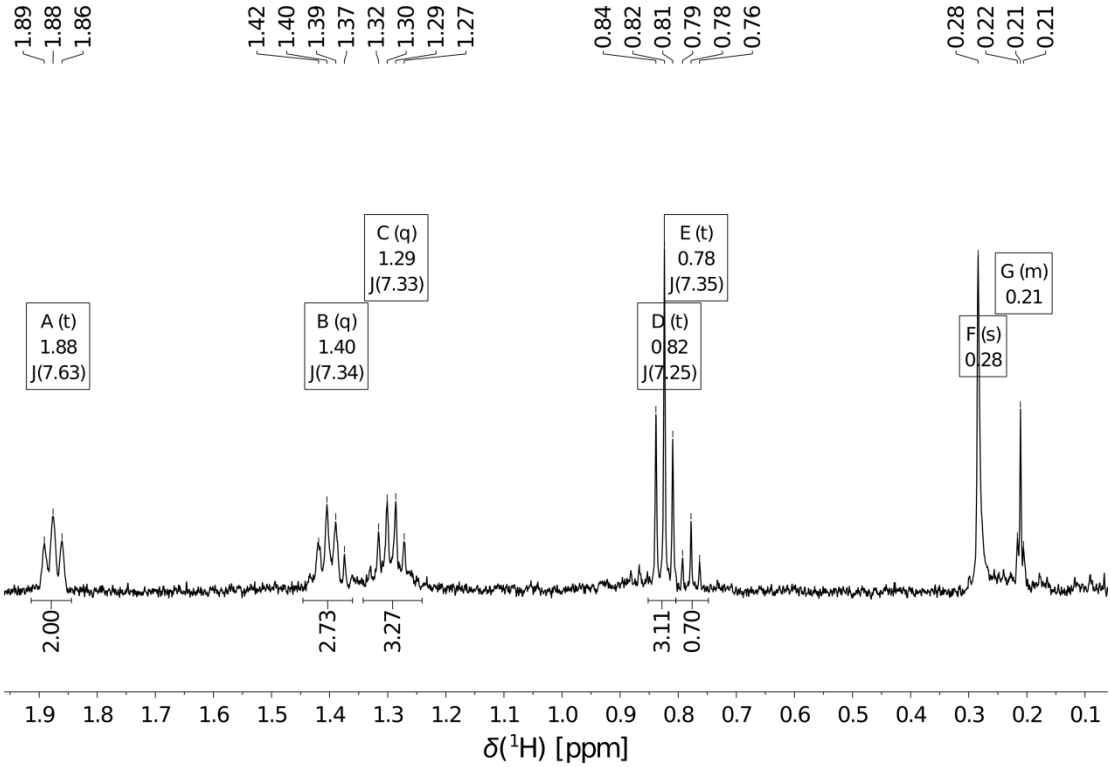


Figure S30. Excerpt of the ^{1}H NMR spectrum (500 MHz, C_6D_6) of tris(*para*-chlorotetrafluorophenyl)-borane (**7**).

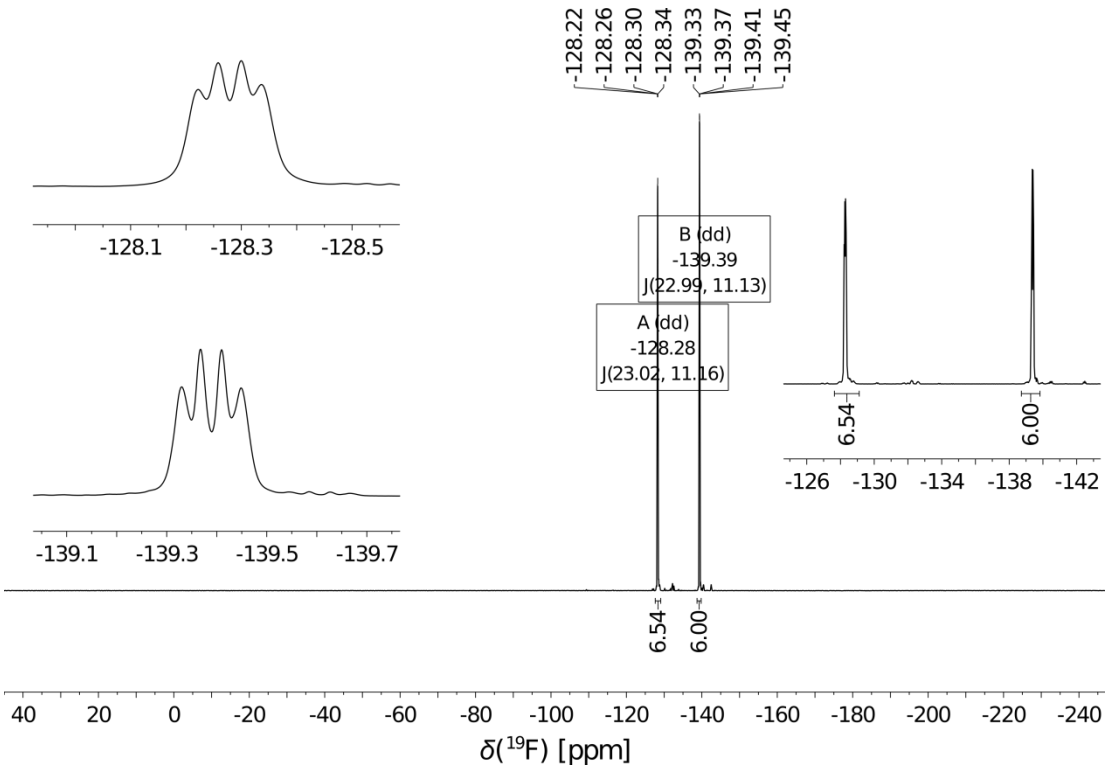


Figure S31. ^{19}F NMR spectrum (282 MHz, C_6D_6) of tris(*para*-chlorotetrafluorophenyl)borane (**7**).

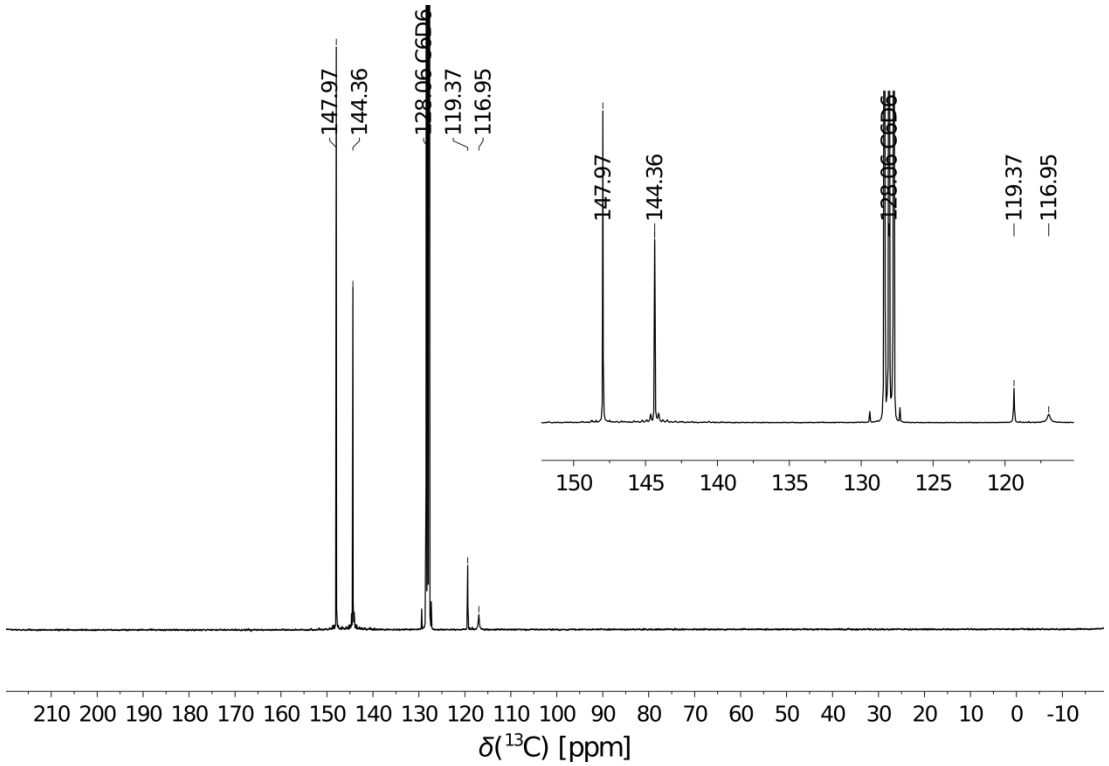


Figure S32. $^{13}C\{^{19}F\}$ NMR spectrum (75 MHz, C_6D_6) of tris(*para*-chlorotetrafluorophenyl)borane (**7**).

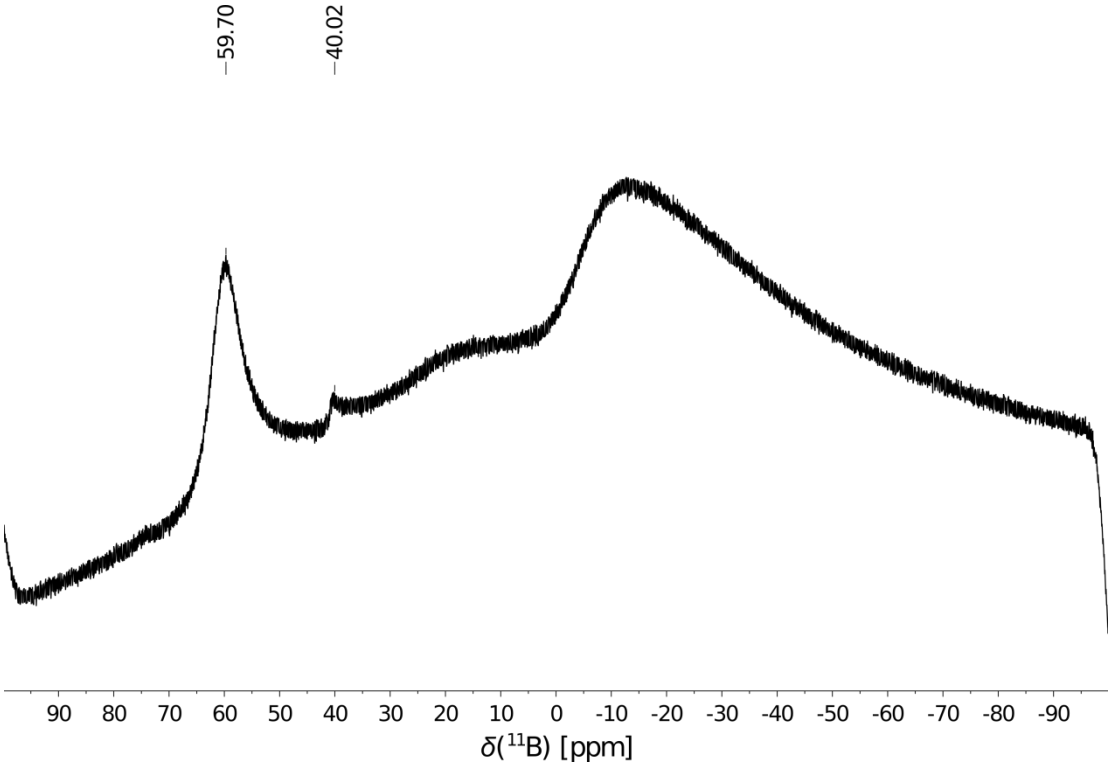


Figure S33. ^{11}B NMR spectrum (160 MHz, C_6D_6) of tris(*para*-chlorotetrafluorophenyl)borane (**7**).

2,2,6,6-Tetramethylpiperidinium tris(*para*-chlorotetrafluorophenyl)hydridoboranate ([7-H][H-TMP])

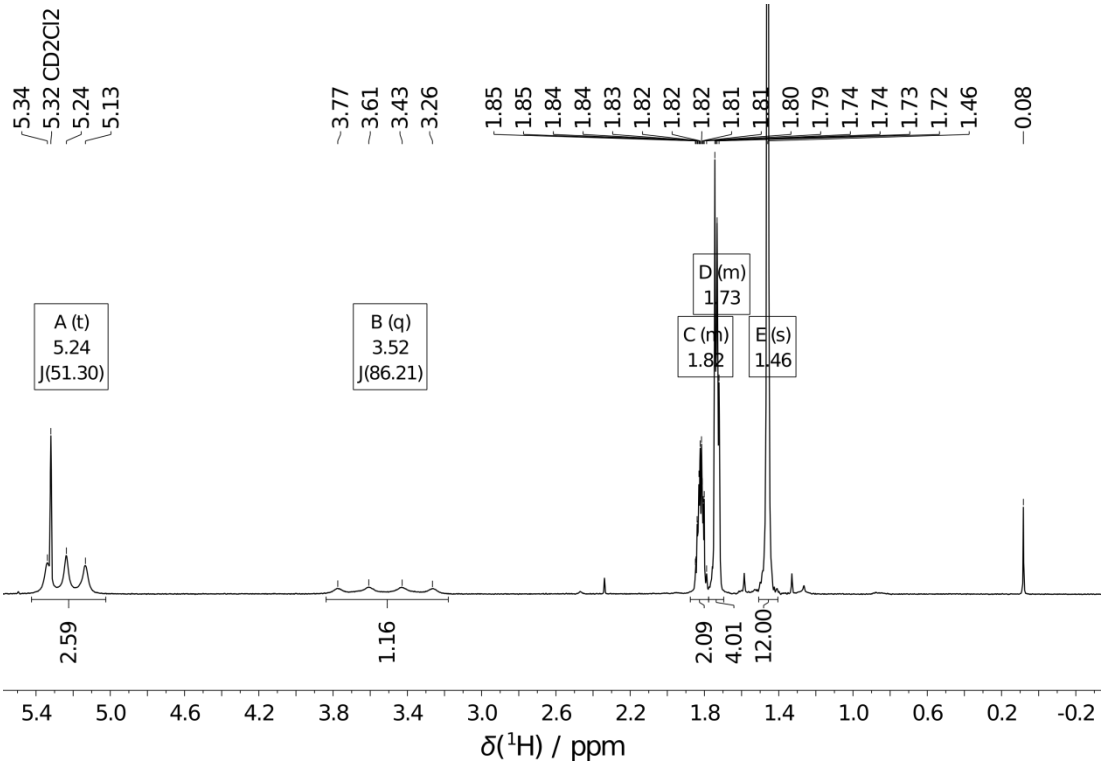


Figure S34. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of [**7**-H][H-TMP].

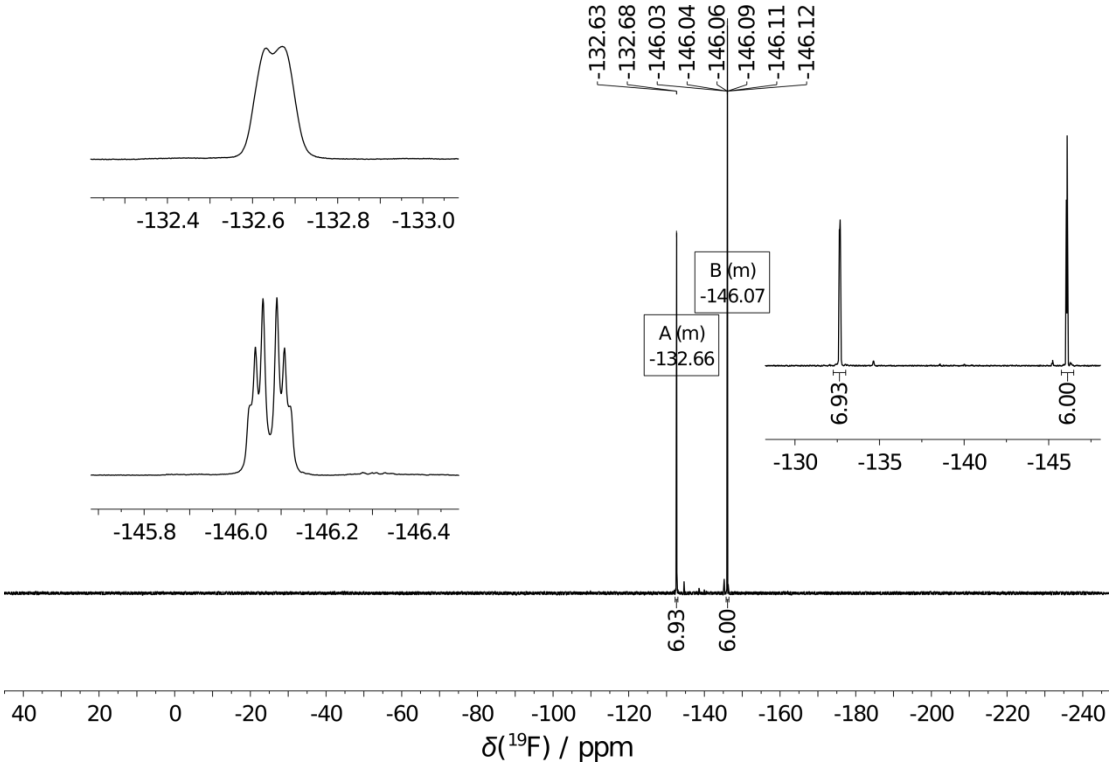


Figure S35. ^{19}F NMR spectrum (471 MHz, CD_2Cl_2) of [**7**-H][H-TMP].

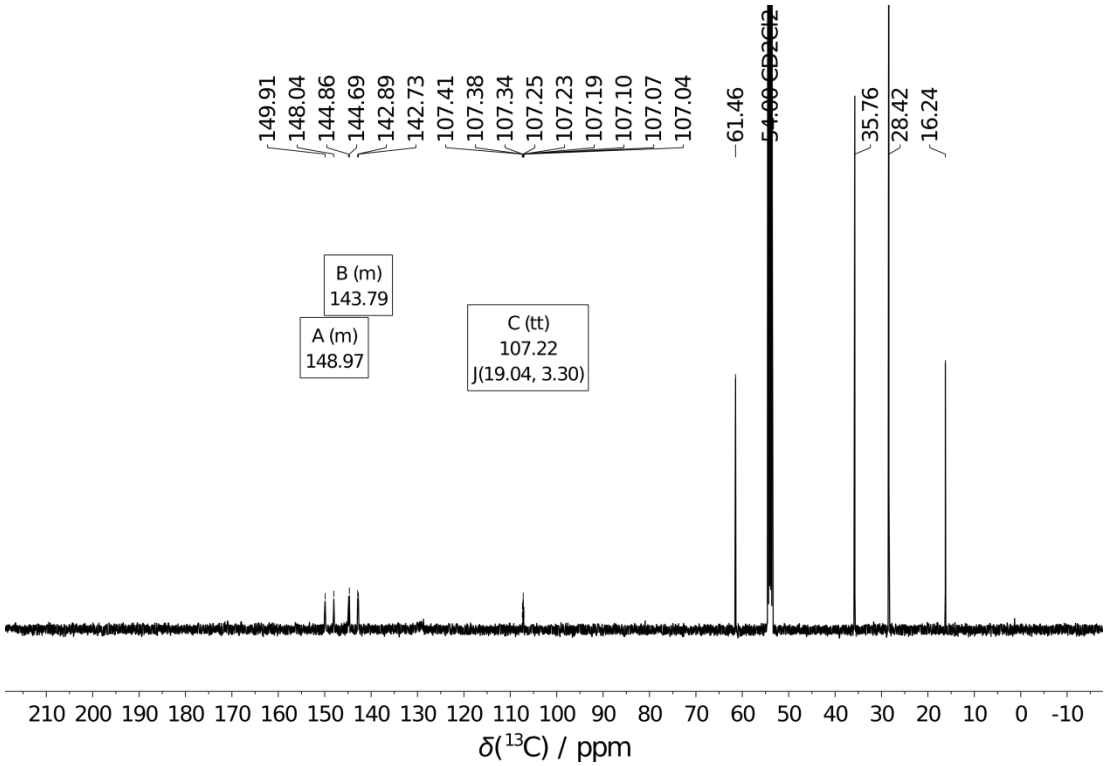


Figure S36. Full $^{13}C\{^1H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of [**7**-H][H-TMP].

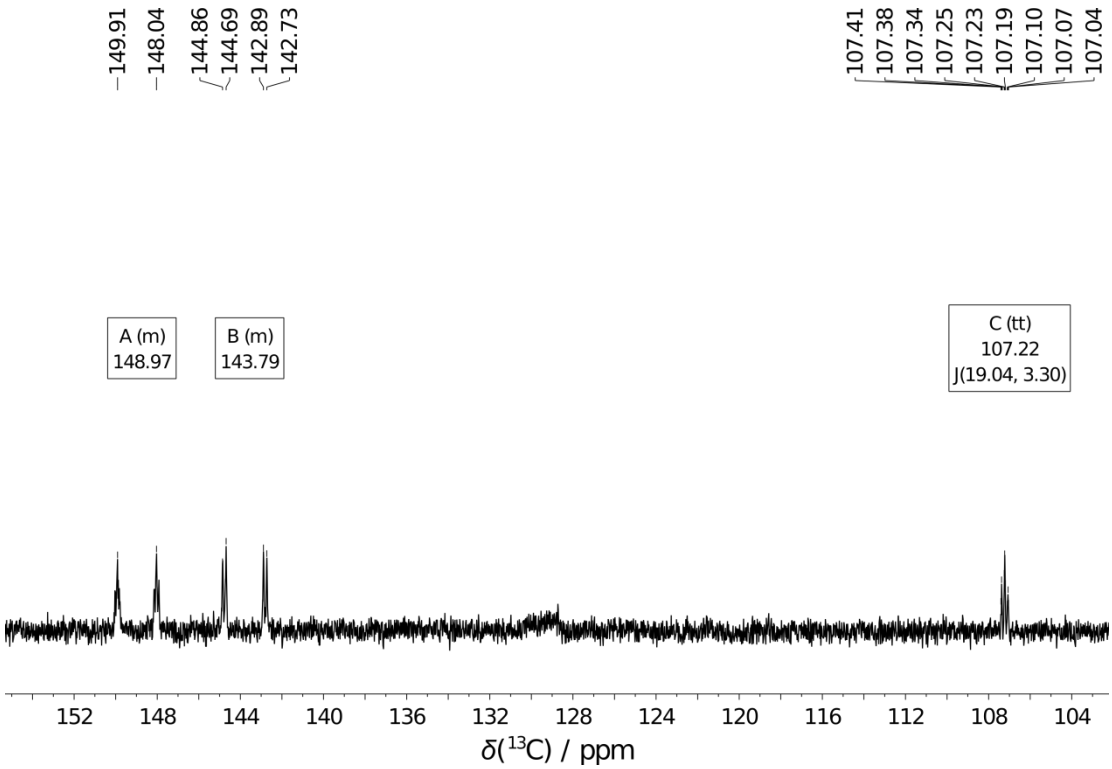


Figure S37. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of [**7**-H][H-TMP].

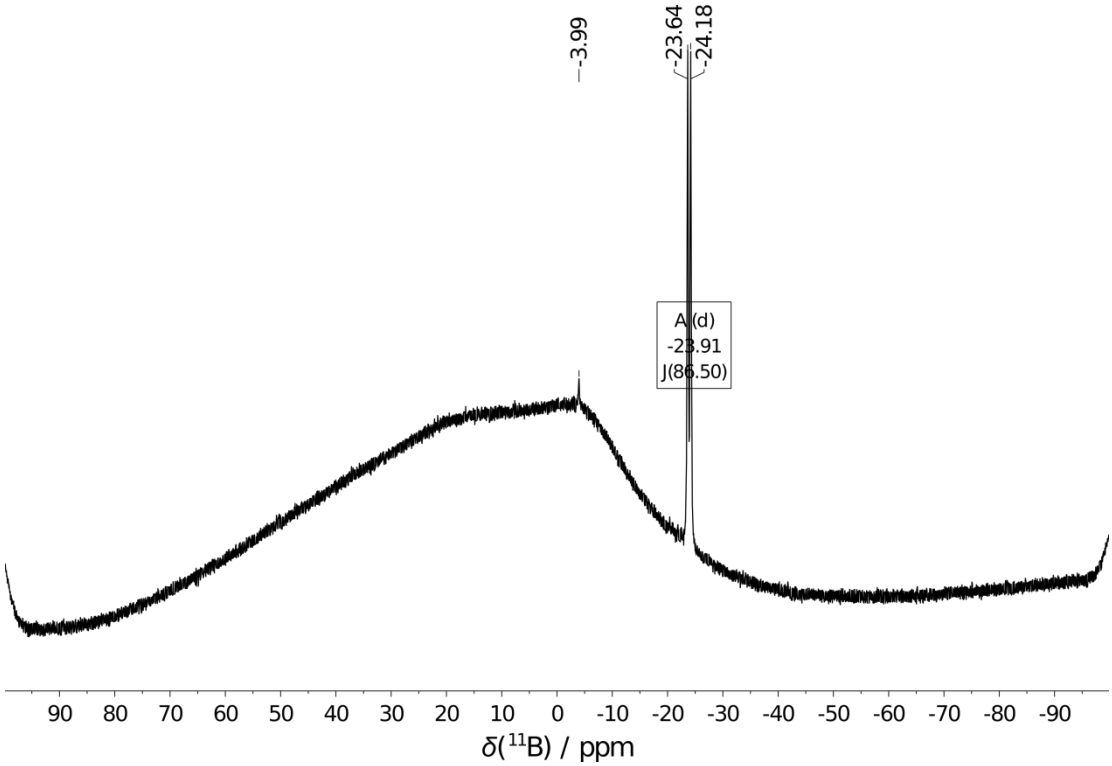


Figure S38. ^{11}B NMR spectrum (160 MHz, CD_2Cl_2) of [**7**-H][H-TMP].

1,2-Bis(bis(*para*-chlorotetrafluorophenyl)boryl)benzene (8)

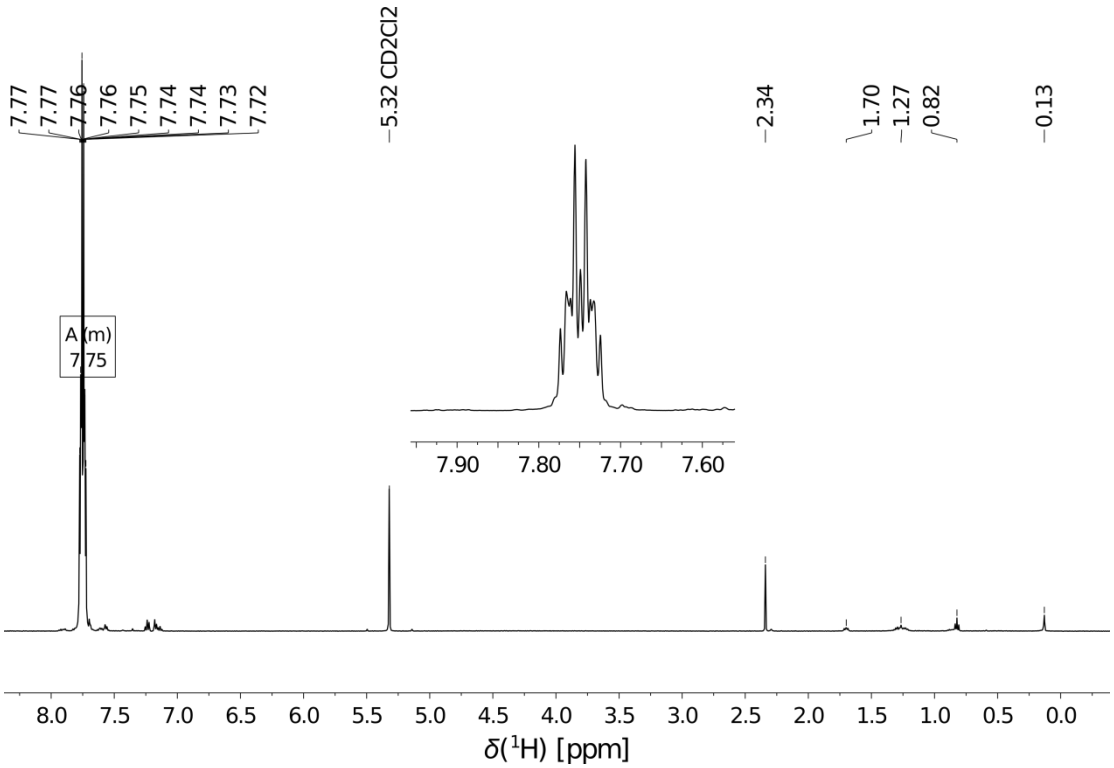


Figure S39. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of **8** containing traces of toluene.

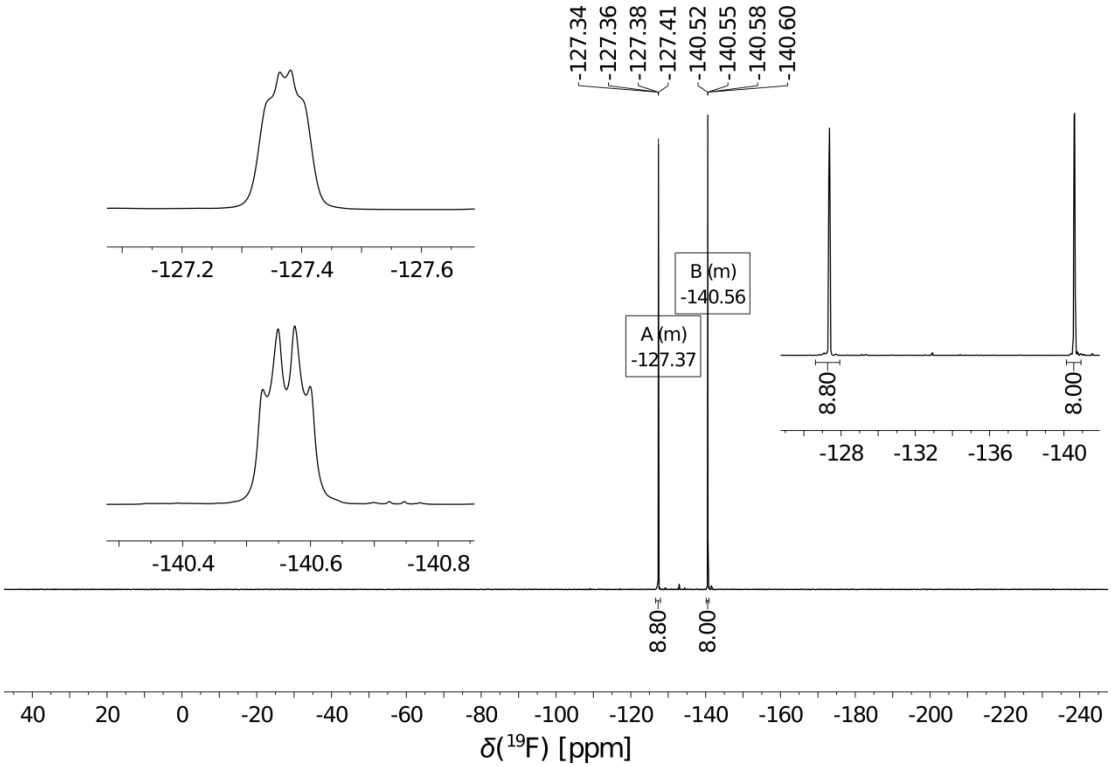


Figure S40. ^{19}F NMR spectrum (471 MHz, CD_2Cl_2) of **8**.

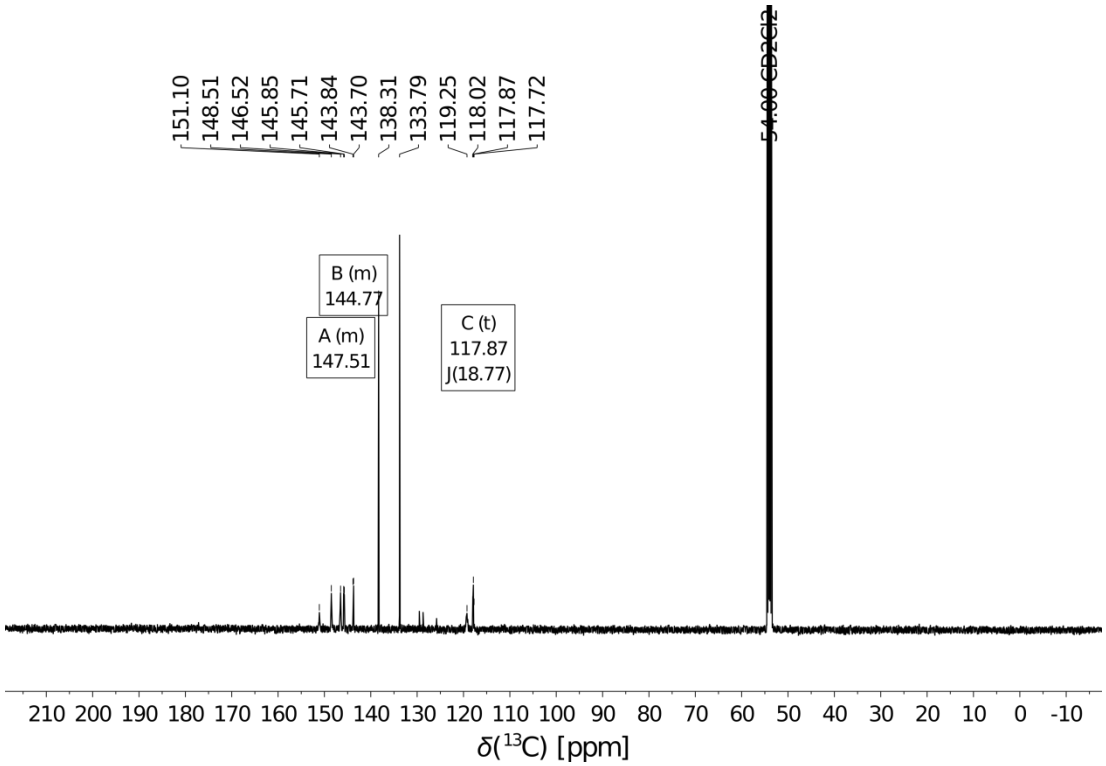


Figure S41. Full $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of **8** containing traces of toluene.

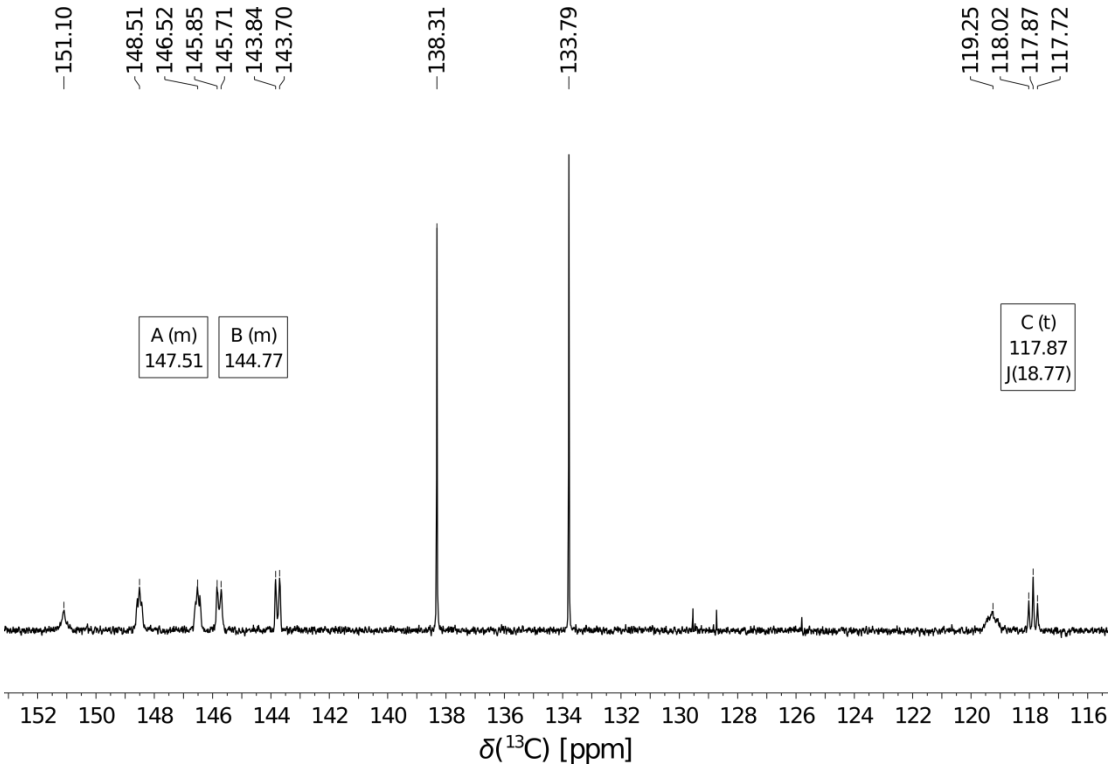


Figure S42. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of **8** containing traces of toluene.

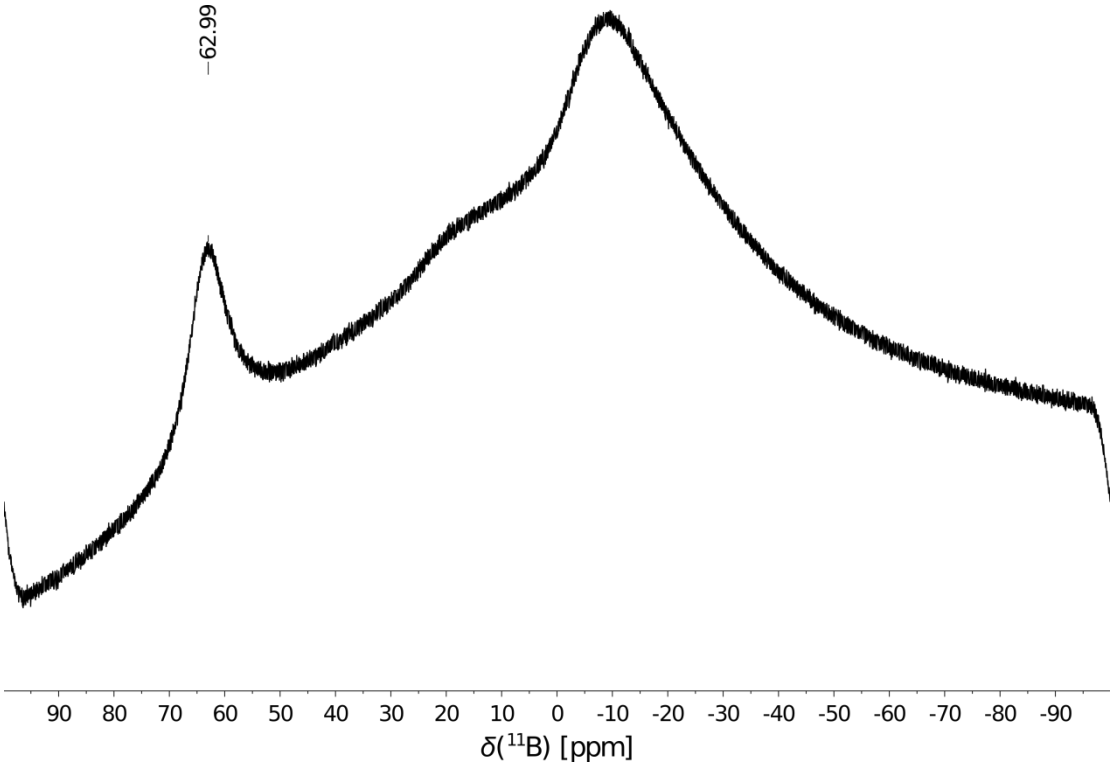


Figure S43. ^{11}B NMR spectrum (160 MHz, CD_2Cl_2) of **8**.

1,8-Bis(dichloroboryl)naphthalene

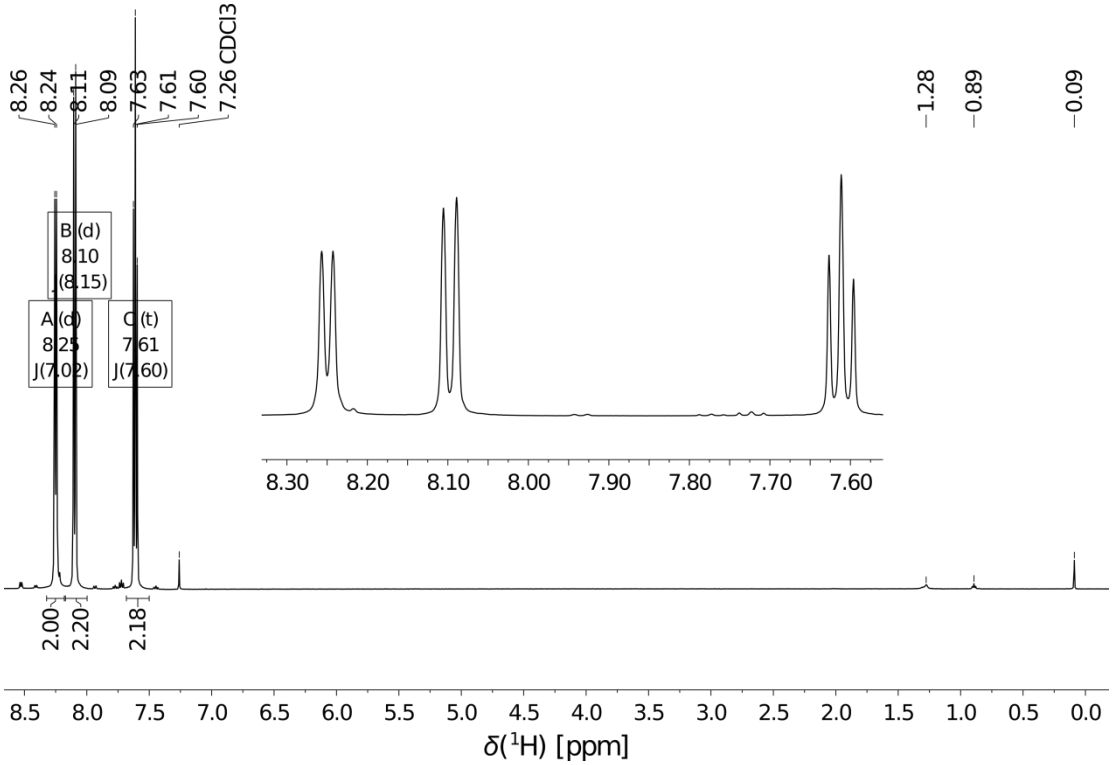


Figure S44. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of 1,8-bis(dichloroboryl)naphthalene.

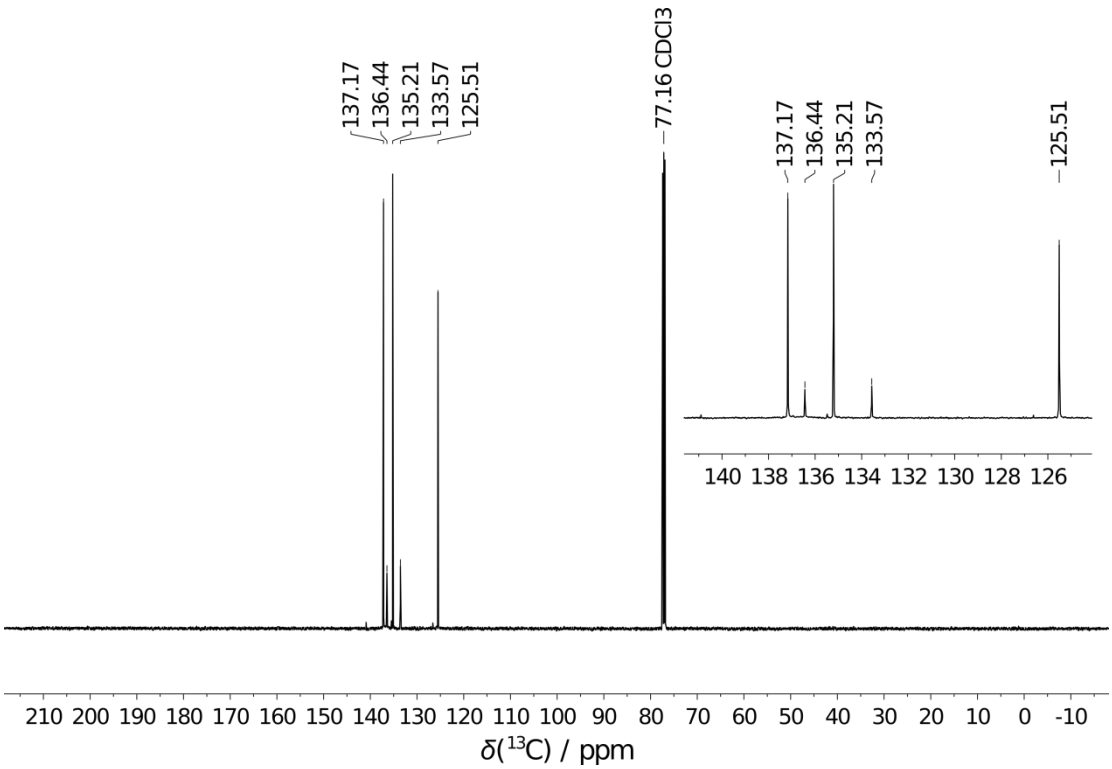


Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, $CDCl_3$) of 1,8-bis(dichloroboryl)naphthalene.

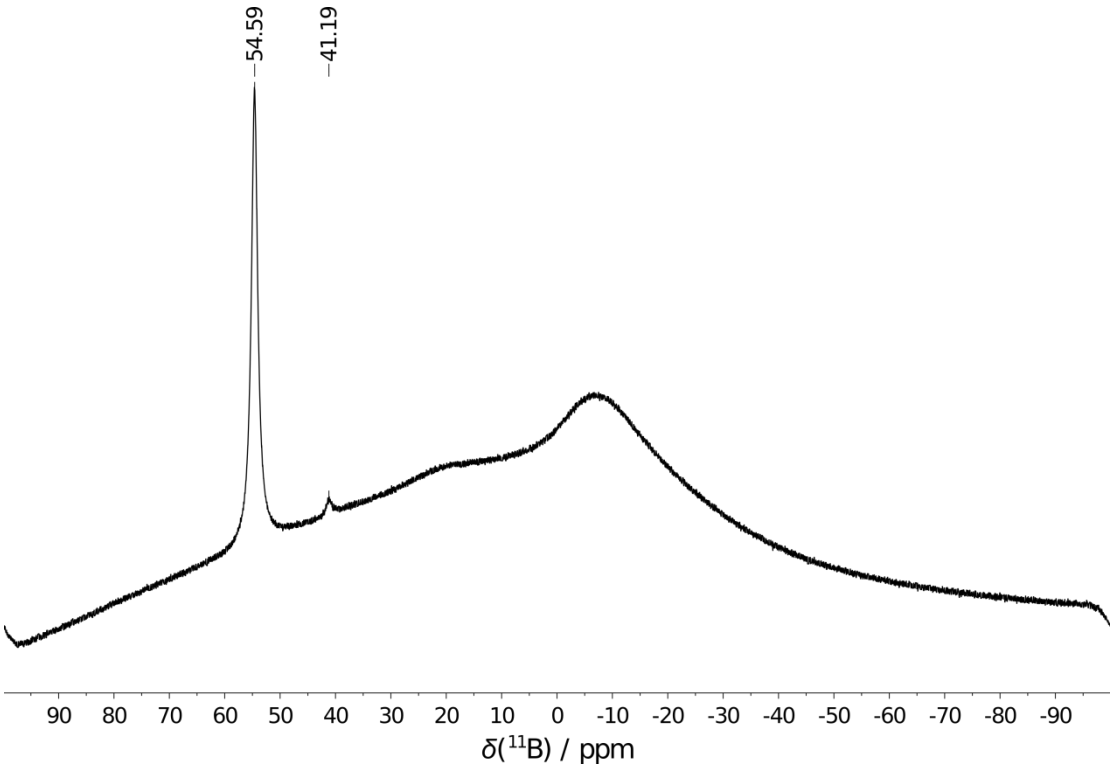


Figure S46. ^{11}B NMR spectrum (160 MHz, $CDCl_3$) of 1,8-bis(dichloroboryl)naphthalene.

1,2-Bis(bis(*para*-chlorotetrafluorophenyl)boryl)naphthalene (9)

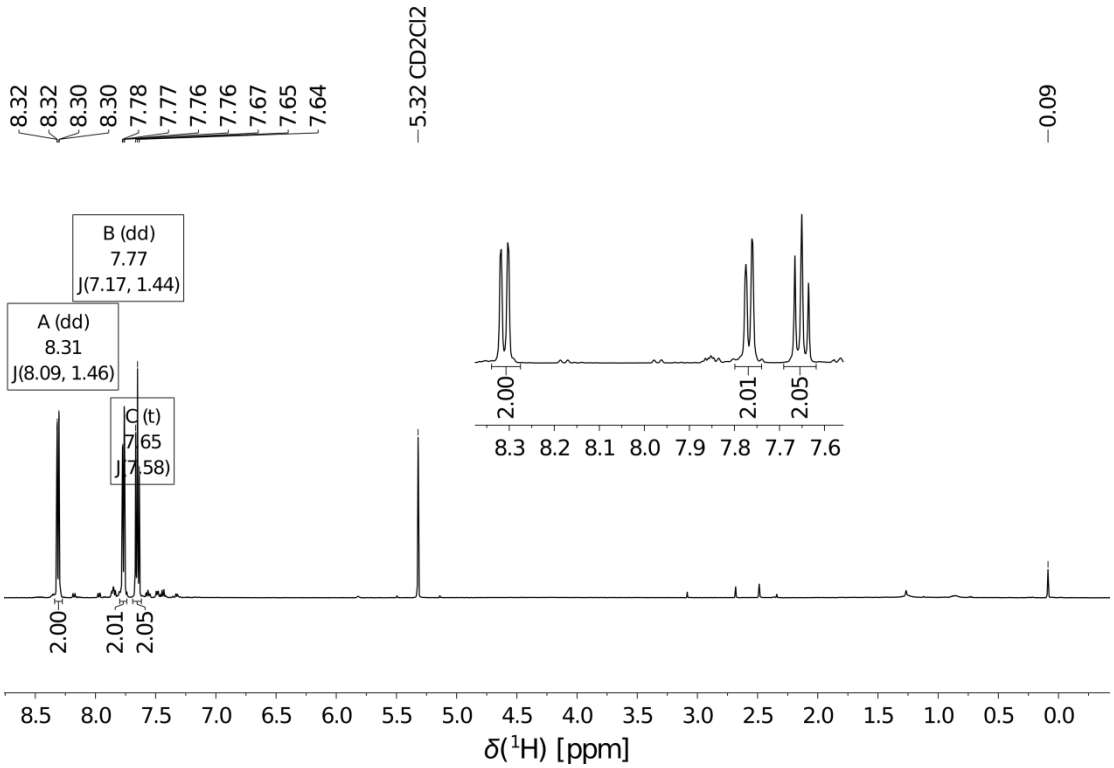


Figure S47. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of **9**.

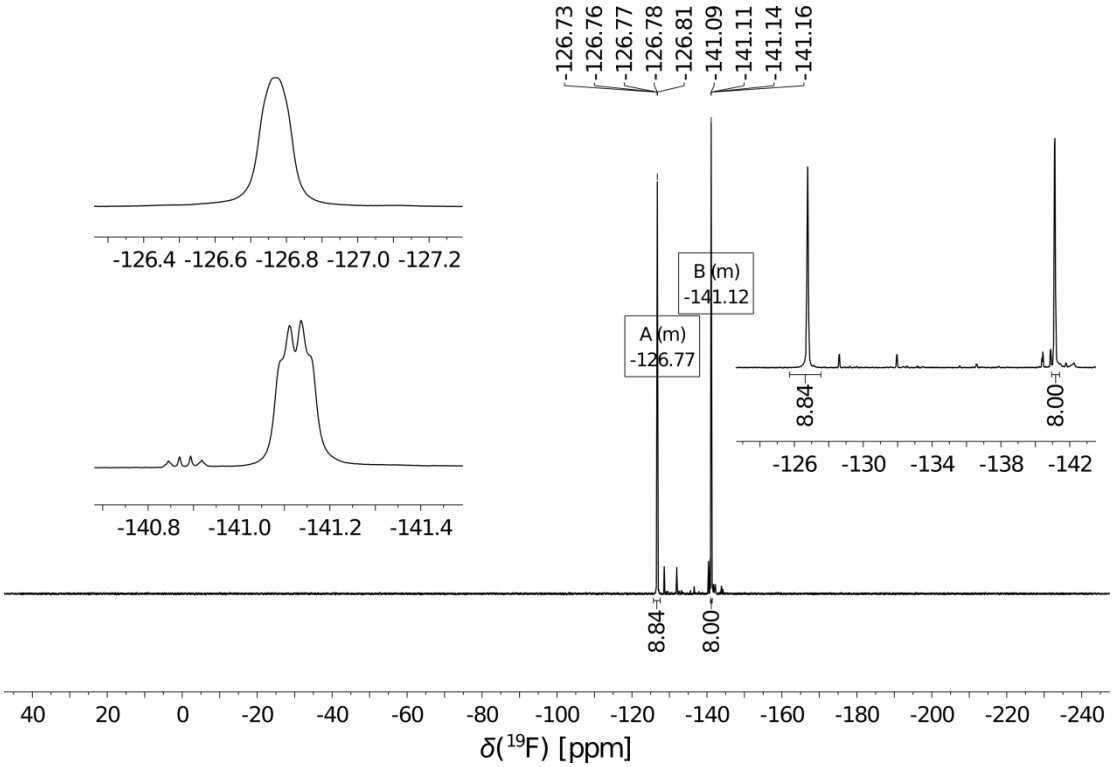


Figure S48. ^{19}F NMR spectrum (471 MHz, CD_2Cl_2) of **9**.

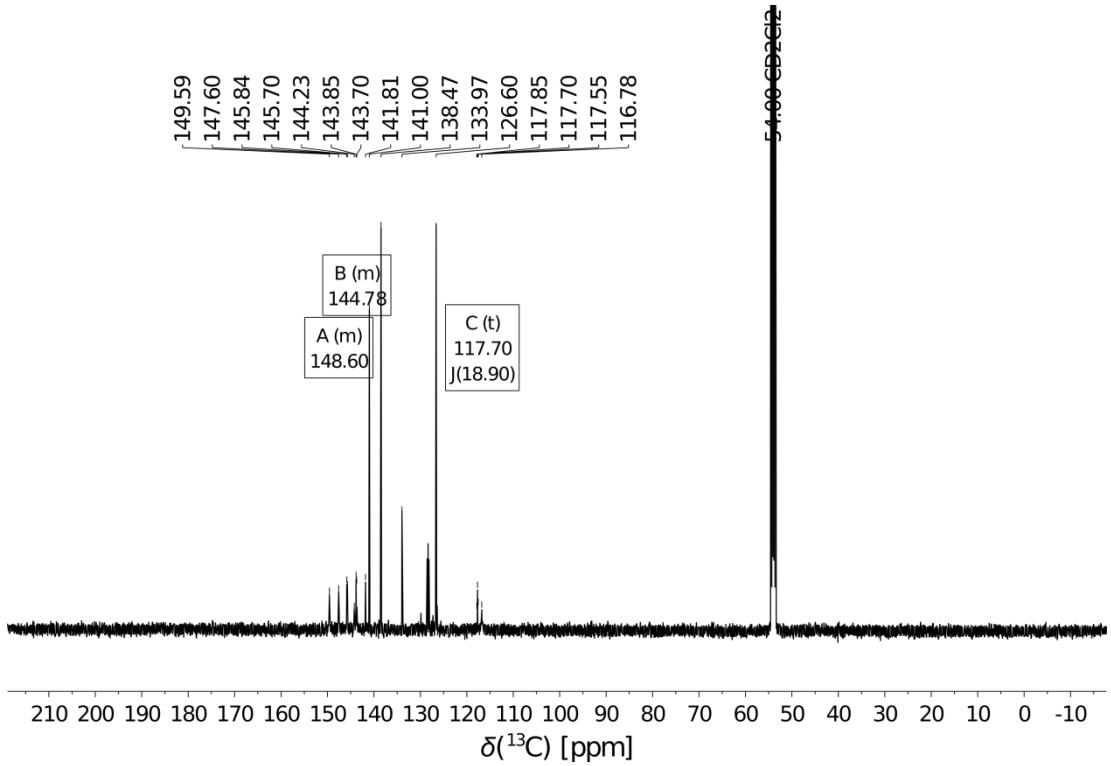


Figure S49. Full $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of **9** containing traces of C_6D_6.

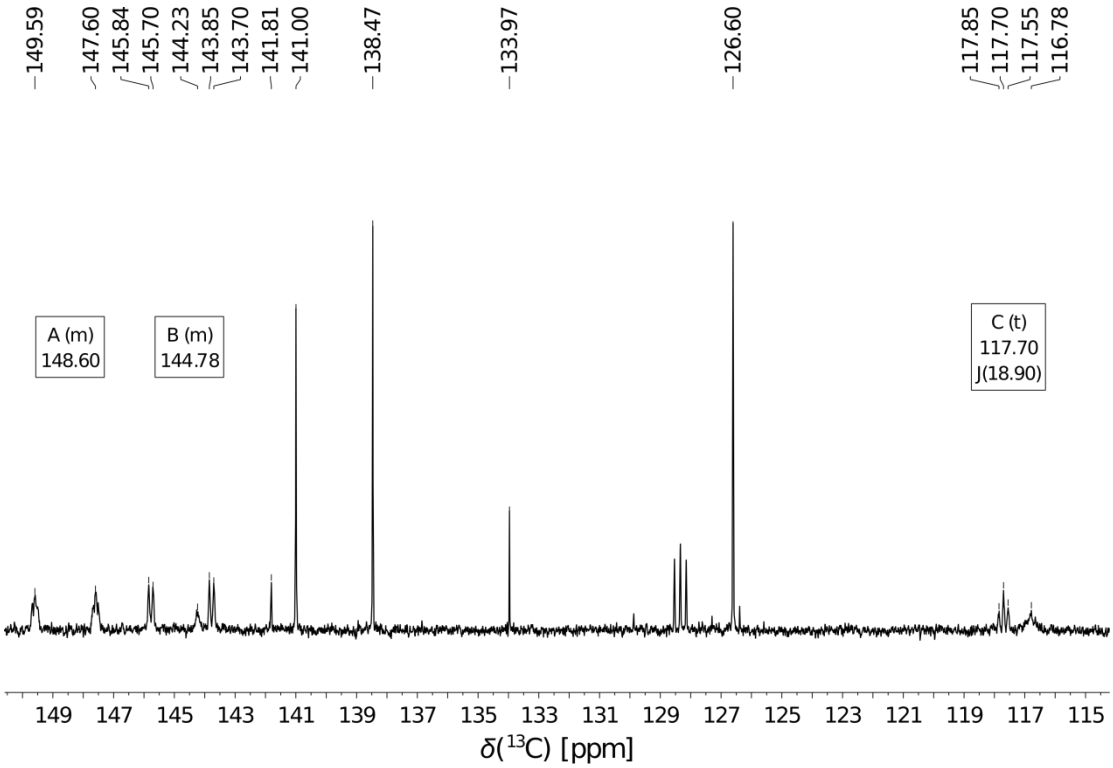


Figure S50. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of **9** containing traces of C_6D_6.

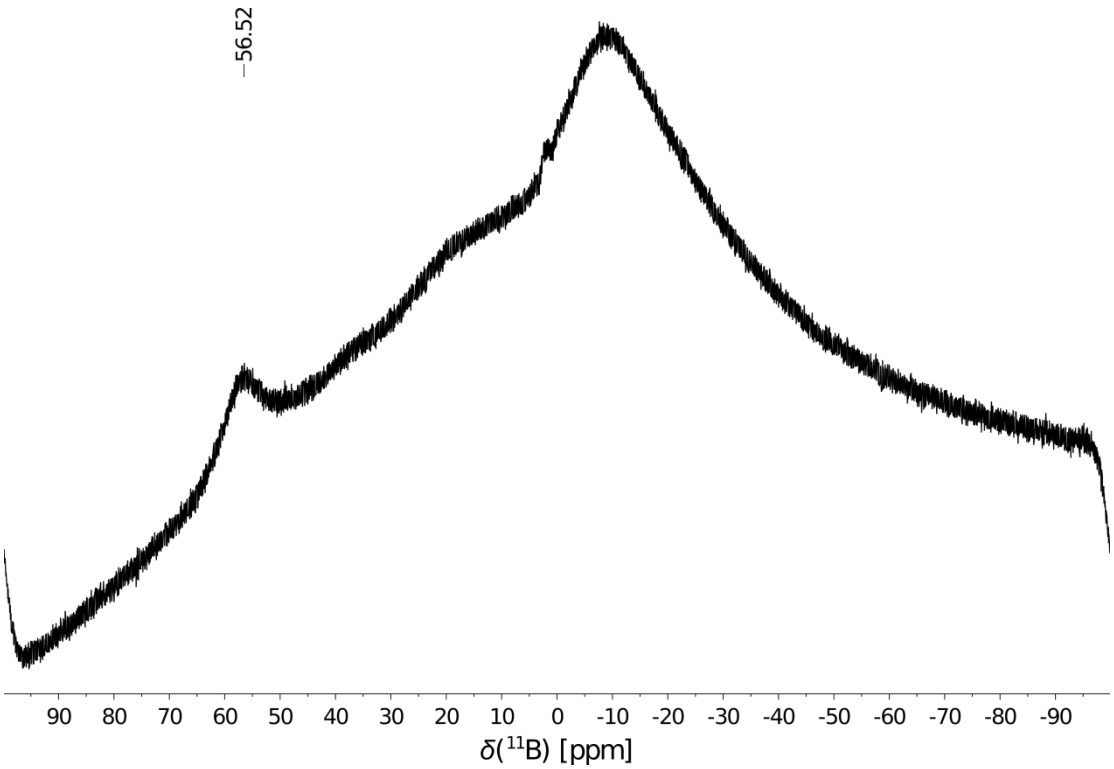


Figure S51. ^{11}B NMR spectrum (160 MHz, CD_2Cl_2) of **9**.

UV/Vis and IR spectra of tris (*para*-bhlorotetrafluorophenyl)borane (7)

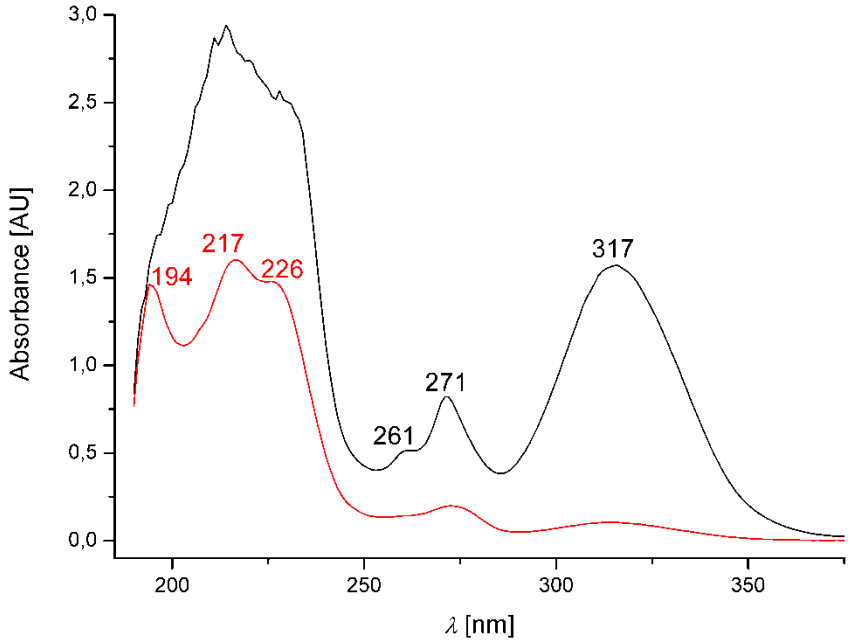


Figure S52. UV/Vis spectra of tris(*para*-chlorotetrafluorophenyl)borane (**7**) in *n*-hexane at two different concentrations (approx. range 10–200 µmol L^{-1}). Solvent background was subtracted before data processing. No significant absorption was found between 375 and 1100 nm. Recorded on a Agilent 8453 UV-vis spectrometer (Agilent Technologies, Germany), which was equipped with an eight-position cuvette holder and a diode array detector system.

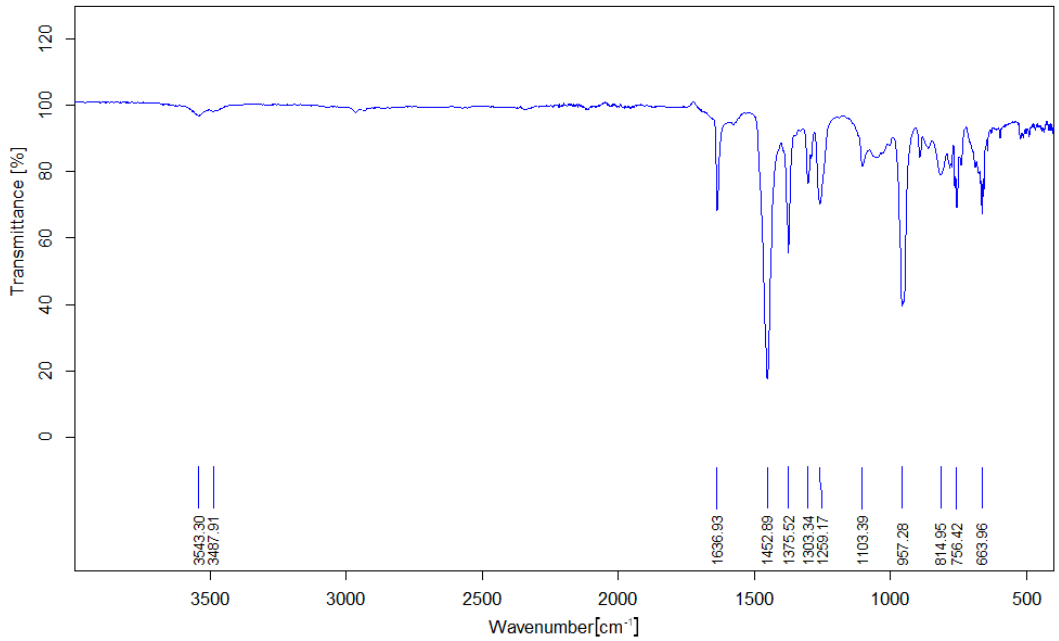


Figure S53. IR spectrum of **7** (solid state) from the evaporation of a solution in dichloromethane. Slight contamination is due to saturated hydrocarbons originating from the use of plastic syringes. Recorded on a Bruker Alpha Platinum ATR spectrometer (Bruker Corporation).

Data of the Gutmann Beckett tests

Table S1. Calculated concentration ratios [$OPEt_3$]/[R_3B] and corresponding ^{31}P NMR shifts for CD_2Cl_2 as the solvent.

[$OPEt_3$]/[(*p*-ClF_4C_6)$_3$B]	$\delta(^{31}P)$ [ppm]	[$OPEt_3$]/[(F_5C_6)$_3$B]	$\delta(^{31}P)$ [ppm]
0.110	77.49	0.103	76.96
0.330	77.50	0.303	76.97
0.667	77.51	0.625	76.98
0.990	77.52	0.971	76.99

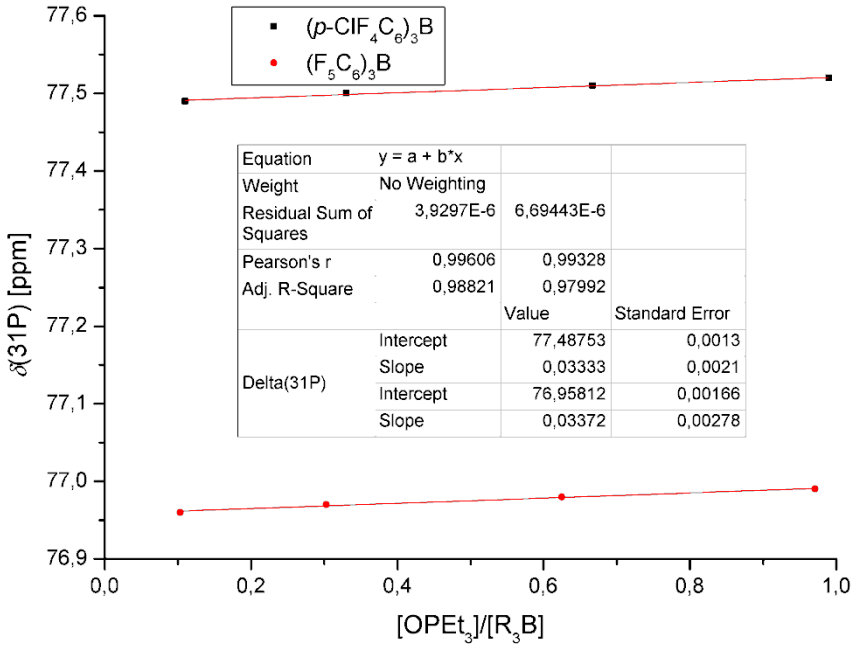


Figure S54. Graphical representation of the values presented in table S1 alongside the data of the derived linear fits (solvent: CD_2Cl_2).

Table S2. Calculated concentration ratios [$OPEt_3$)/[R_3B] and corresponding ^{31}P NMR shifts for C_6D_6 as the solvent.

[$OPEt_3$]/[(*p*-ClF_4C_6)$_3$B]	$\delta(^{31}P)$ [ppm]	[$OPEt_3$]/[(F_5C_6)$_3$B]	$\delta(^{31}P)$ [ppm]
0.120	75.73	0.0571	75.20
0.252	75.76	0.256	75.25
0.516	75.80	0.505	75.29
0.800	75.80	0.826	75.32

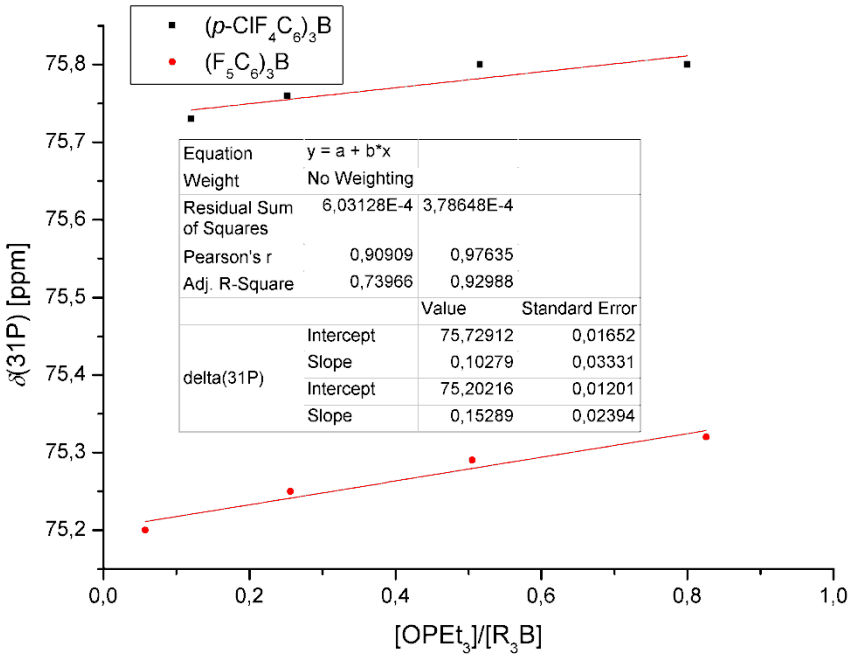


Figure S55. Graphical representation of the values presented in Table S2 alongside the data of the derived linear fits (solvent: C_6D_6).

Crystallographic Details

Single crystals were examined on a Rigaku Supernova diffractometer. Using Olex2,[1] the structures were solved with the ShelXT[2] structure solution program using Intrinsic Phasing and refined with the ShelXL[3] refinement package using Least Squares minimisation if not otherwise stated. All hydrogen atoms were refined isotropically except the carbon bonded in [**7**-H][H-TMP]. In **1** the nitrogen atom doesn't lie at the crystallographic two-fold axis and is thus disordered in ratio 1:1. In **2** the chlorine and bromine atoms share nearly the same site, ratio 1:1. The entire molecule of **3** is disordered at a center of inversion with ratio 1:1. The crystal of **4** was twinned, the ratio of the two domains was 80:20. Component 2 rotated by −180.0°around [−0.41 −0.00 0.91] (reciprocal) or [0.00 0.00 1.00] (direct). The structure of **7**·$OPEt_3$ was refined with the olex2.refine refinement package using Levenberg-Marquardt minimization. NoSpherA2 was used, an implementation of NOn-SPHERical Atom-form-factors in Olex2.[4] NoSpherA2 implementation of HAR makes use of tailor-made aspherical atomic form factors calculated on-the-fly from a Hirshfeld-partitioned electron density (ED) – not from spherical-atom form factors. The ED is calculated from a Gaussian basis set single determinant SCF wave-function - either Hartree-Fock or DFT using selected functionals – for a fragment of the crystal. This fragment can be embedded in an electrostatic crystal field by employing cluster charges. The following options were used: SOFTWARE: ORCA PARTITIONING: NoSpherA2 INT ACCURACY: Normal METHOD: M062X BASIS SET: def2-TZVPP CHARGE: 0 MULTIPLICITY: 1. The chlorine atom was refined with anharmonic thermal vibration. The two solvent toluene molecules in [**7**-H][H-TMP] are disordered with different ratios, suitable restraints were applied. Crystal was a 1:1 inversion twin. The structure could not be refined in the centrosymmetric space group $P\bar{1}$ reasonably, the cations and the toluene molecules show heavy disorder in this space group, the R_1 value increases to ca. 20%. A non-merohedral twinning could not been detected. Details of the X-ray investigation are given in Table S3–S6. CCDC 2149933−2149943 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, 42, 339–341.
2. G. M. Sheldrick, *Acta Crystallogr.* **2015**, *A71*, 3–8.
3. G. M. Sheldrick, *Acta Crystallogr.* **2015**, *C71*, 3–8.
4. F. Kleemiss, O. V. Dolomanov, M. Bodensteiner, N. Peyerimhoff, L. Midgley, L. J. Bourhis, A. Genoni, L. A. Malaspina, D. Jayatilaka, J. L. Spencer, F. White, B. Grundkötter-Stock, S. Steinhauer, D. Lentz, H. Puschmann, S. Grabowsky, *Chem. Sci.,* **2021**, *12*, 1675–1692.

Table S3. Crystallographic data of compounds **1**, **2** and **3**.

Compound	1	2	3
Empirical formula	$C_6H_2ClF_4N$	C_6F_4ClBr	C_6ClF_4I
M_r	199.54	263.42	310.41
Radiation Source	MoKα	MoKα	MoKα
λ (Å)	0.71073	0.71073	0.71073
T / K	100.0(1)	100.0(1)	95.0(1)
F(000)	392	248	284
Crystal system	monoclinic	monoclinic	monoclinic
Space group	*C*2/*c*	*C*2/*m*	$P2_1/c$
a [Å]	7.4856(2)	9.0190(5)	5.85998(13)
b [Å]	14.3043(2)	7.6651(3)	6.03279(14)
c [Å]	6.6735(2)	5.2231(2)	11.1548(3)
α [Å]	90	90	90
β [Å]	112.474(4)	97.920(5)	94.708(2)
γ [Å]	90	90	90
V [Å^3]	660.30(3)	357.64(3)	393.015(16)
Z	4	2	2
$\rho_{calcd.}$ [g cm^{-3}]	2.007	2.446	2.623
μ [mm^{-1}]	0.590	6.125	4.419
2θ range [°]	5.696 – 72.852	7.004 – 64.118	6.976 – 73.78
Index range h	$-12 \le h \le 12$	$-13 \le h \le 12$	$-9 \le h \le 9$
Index range k	$-23 \le k \le 23$	$-11 \le k \le 11$	$-10 \le k \le 9$
Index range l	$-11 \le l \le 11$	$-7 \le l \le 7$	$-18 \le l \le 18$
Refl. collect.	10105	11243	12071
Indep. refl.	1574	649	1904
R_{int}	0.0241	0.0497	0.0280
Refl. with $I>2\sigma(I)$	1439	581	1598
Data/restraints/ parameters	1574/0/65	649/0/33	1904/0/110
R_1, $I>2\sigma(I)$ / all data	0.0247 / 0.0276	0.0320 / 0.0383	0.0198 / 0.0264
wR_2, $I>2\sigma(I)$ / all data	0.0727 / 0.0747	0.0750 / 0.0789	0.0440 / 0.0470
GoF	1.067	1.109	1.069
$\rho_{max/min}$ [e Å^{-3}]	0.60/–0.21	0.97/–1.00	0.35/–0.34
CCDC	2149933	2149934	2149935

Table S4. Crystallographic data of compounds **4**, **5** and **7**·OEt_2.

Compound	4	5	7·OEt_2
Empirical formula	$C_{14}H_6Cl_2F_8Sn$	$BC_{12}Cl_3F_8$	$C_{22}H_{10}BCl_3F_{12}O$
M_r	515.78	413.28	635.46
Radiation Source	MoKα	CuKα	MoKα
λ (Å)	0.71073	1.54184	0.71073
***T* / K**	100.0(1)	100.0(1)	100.0(1)
***F*(000)**	492	1600	2512
Crystal system	triclinic	monoclinic	tetragonal
Space group	$P\bar{1}$	$P2_1/c$	$P\bar{4}2_1c$
***a* [Å]**	8.0625(3)	26.726(3)	16.90978(13)
***b* [Å]**	8.4539(3)	6.2568(6)	16.90978(13)
***c* [Å]**	12.5784(4)	16.8800(17)	16.8969(2)
α [Å]	77.556(3)	90	90
β [Å]	76.536(3)	106.138(11)	90
γ [Å]	87.824(3)	90	90
***V* [Å^3]**	814.12(5)	2711.4(5)	4831.52(10)
Z	2	8	8
$\rho_{calcd.}$ [g cm^{-3}]	2.104	2.025	1.747
μ [mm^{-1}]	1.976	7.029	0.489
2θ range [°]	5.368 – 60.052	6.886 – 151.358	4.822 – 66.25
Index range *h*	$-11 \le h \le 11$	$-33 \le h \le 33$	$-26 \le h \le 26$
Index range *k*	$-11 \le k \le 11$	$-7 \le k \le 7$	$-26 \le k \le 26$
Index range *l*	$-17 \le l \le 17$	$-20 \le l \le 20$	$-25 \le l \le 25$
Refl. collect.	19022	17368	229607
Indep. refl.	4761	6816	9187
R_{int}	0.0409	0.0443	0.0955
Refl. with *I*>2σ(*I*)	4155	5885	8075
Data/restraints/ parameters	4761/0/250	6816/0/434	9187/0/392
R_1, *I*>2σ(*I*) / all data	0.0273 / 0.0343	0.0890 / 0.0998	0.0367 / 0.0458
wR_2, *I*>2σ(*I*) / all data	0.0549 / 0.0592	0.2465 / 0.2582	0.0759 / 0.0794
GoF	1.067	1.047	1.019
$\rho_{max/min}$ [*e* Å^{-3}]	1.02/–0.46	0.70/–0.81	0.76/–0.27
Flack parameter			-0.026(15)
CCDC	2149936	2149937	2149938

Table S5. Crystallographic data of compounds **7**·$OPEt_3$, [**7**-H][H-TMP] and **8**.

Compound	**7**·$OPEt_3$	[**7**-H][H-TMP]	**8**
Empirical formula	$C_{24}H_{15}BCl_3F_{12}OP$	$C_{34}H_{29}BCl_3F_{12}N$	$C_{30}H_4B_2Cl_4F_{16}$
M_r	695.522	796.74	831.75
Radiation Source	MoKα	CuKα	CuKα
λ (Å)	0.71073	1.54184	1.54184
T / K	100.0(1)	100.0(1)	100.0(1)
F(000)	2080.1	808	812
Crystal system	trigonal	triclinic	triclinic
Space group	$R\bar{3}$	$P1$	$P\bar{1}$
a [Å]	13.13211(19)	11.2083(3)	10.6373(3)
b [Å]	13.13211(19)	11.2423(3)	12.0380(3)
c [Å]	26.3187(4)	15.8165(3)	13.5971(4)
α [Å]	90	92.226(2)	106.375(2)
β [Å]	90	101.961(2)	93.576(2)
γ [Å]	120	117.368(3)	115.075(3)
V [Å^3]	3930.65(10)	1710.74(8)	1479.57(8)
Z	6	2	2
$\rho_{calcd.}$ [g cm^{-3}]	1.763	1.547	1.867
μ [mm^{-1}]	0.517	3.272	4.827
2θ range [°]	3.9 – 90.58	5.782 – 152.782	6.93 – 152.726
Index range h	$-29 \le h \le 29$	$-13 \le h \le 14$	$-12 \le h \le 13$
Index range k	$-29 \le k \le 28$	$-14 \le k \le 13$	$-15 \le k \le 15$
Index range l	$-58 \le l \le 58$	$-19 \le l \le 19$	$-16 \le l \le 17$
Refl. collect.	124061	37565	25319
Indep. refl.	7326	12689	6101
R_{int}	0.0470	0.0392	0.0229
Refl. with $I>2\sigma(I)$	6098	11792	5631
Data/restraints/ parameters	7326/6/192	12689/548/1083	6101/0/485
R_1, $I>2\sigma(I)$ / **all data**	0.0232 / 0.0320	0.0374 / 0.0416	0.0270 / 0.0298
wR_2, $I>2\sigma(I)$ / **all data**	0.0470 / 0.0497	0.0938 / 0.0978	0.0685 / 0.0704
GoF	1.040	1.033	1.028
$\rho_{max/min}$ [e Å^{-3}]	0.41/–0.29	0.42/–0.29	0.49/–0.31
Flack parameter		0.5	
CCDC	2149939	2149940	21499341

Table S6. Crystallographic data of compounds 1,8-bis(dichloroboranyl)naphthalene and **9**.

Compound	**1,8-bis(dichloroboranyl)naphthalene**	**9**
Empirical formula	$C_{10}H_6B_2Cl_4$	$C_{34}H_6B_2Cl_4F_{16}$
M_r	289.57	881.81
Radiation Source	MoKα	CuKα
λ (Å)	0.71073	1.54184
T / K	100.0(1)	100.0(1)
F(000)	576	864
Crystal system	orthorhombic	triclinic
Space group	$P2_12_12_1$	$P\bar{1}$
a [Å]	7.0968(2)	10.7395(5)
b [Å]	9.0337(2)	12.2623(5)
c [Å]	18.3451(4)	13.9981(5)
α [Å]	90	76.888(3)
β [Å]	90	71.805(4)
γ [Å]	90	66.695(4)
V [Å^3]	1176.11(5)	1597.05(12)
Z	4	2
$\rho_{calcd.}$ [g cm^{-3}]	1.635	1.834
μ [mm^{-1}]	0.967	4.517
2θ range [°]	6.156 – 65.508	6.694 – 148.098
Index range h	$-10 \le h \le 10$	$-12 \le h \le 12$
Index range k	$-13 \le k \le 13$	$-15 \le k \le 15$
Index range l	$-27 \le l \le 27$	$-17 \le l \le 17$
Refl. collect.	29421	20974
Indep. refl.	4105	6973
R_{int}	0.0476	0.0212
Refl. with $I>2\sigma(I)$	3741	6303
Data/restraints/ parameters	4105/0/145	6973/0/530
R_1, $I>2\sigma(I)$ / all data	0.0310 / 0.0380	0.0316 / 0.0354
wR_2, $I>2\sigma(I)$ / all data	0.0650 / 0.0684	0.0872 / 0.0895
GoF	1.084	1.060
$\rho_{max/min}$ [e Å^{-3}]	0.45/–0.32	0.54/–0.36
Flack parameter	0.01(3)	
CCDC	2149942	2149943

Quantum-chemical calculation of the hydride and fluoride ion affinities

The hydride and fluoride ion affinities (HIA and FIA) were determined in accordance with the method described by Krossing *et al.* with the trimethylsilyl compounds Me_3SiY (Y = H, F) as a reference system (see equations 1 to 3).[1]

$$LA + Me_3Si{-}Y \xrightarrow{\text{(RI-)BP86/SV(P)}} LA{-}Y^- + Me_3Si^+ \quad (1)$$

$$Me_3Si{-}Y \xrightarrow{\text{G3}} Y^- + Me_3Si^+ \quad (2)$$

$$LA + Y^- \xrightarrow[\Delta H = -\,YIA]{} LA{-}Y^- \quad (3)$$

The values for the reaction enthalpy of equation 2 at the G3 level[2] of theory were taken from the publication by Krossing *et al.*.[1] For the calculation of the reaction enthalpy of (1), all structures were optimized at the (RI-)BP86/SV(P) level[3-6] of theory using TURBOMOLE 7.4.1[7, 8]. Vibrational frequencies were computed with the AOFORCE module. All structures constitute true minima and possess no imaginary frequencies. Thermal corrections to the enthalpy were obtained with the FreeH utility.

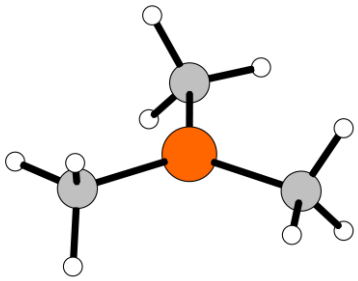
Table S7. Energetic data of the trimethylsilyl reference systems for the calculation of HIA and FIA values at the (RI-)BP86/SV(P) level of theory. The thermal energy correction was calculated at 298.15 K.

compound	Energy [h]	Thermal correction [kJ mol^{-1}]	Enthalpy [kJ mol^{-1}]
Me_3Si^+	−408.80758	298.04	−1073026.11
Me_3SiH	−409.68911	322.21	−1075316.40
Me_3SiF	−508.92748	310.86	−1335878.05

Table S8. Energetic data of the Lewis acids BCF, **7**, **8** and **9** for the calculation of HIA and FIA values at the (RI-)BP86/SV(P) level of theory. The thermal energy correction was calculated at 298.15 K.

compound	Energy [h]	Thermal correction [kJ mol^{-1}]	Enthalpy [kJ mol^{-1}]
$B(C_6F_5)_3$	−2206.75257	471.79	−5793356.29
$[B(C_6F_5)_3H]^-$	−2207,45160	492.16	−5795171.21
$[B(C_6F_5)_3F]^-$	−2306.67691	477.45	−6055701.96
$B(p\text{-}ClC_6F_4)_3$ (**7**)	−3287.79129	463.9	−8631630.96
$[B(p\text{-}ClC_6F_4)_3H]^-$	−3288.49297	485.39	−8633451.70
$[B(p\text{-}ClC_6F_4)_3F]^-$	−3387.71814	470.45	−8893982.30
$H_4C_6(1,2\text{-}(B(p\text{-}ClC_6F_4)_2))_2$ (**8**)	−4631.17063	845.84	−12158290.97
$[H_4C_6(1,2\text{-}(B(p\text{-}ClC_6F_4)_2))_2H]^-$	−4631.88155	865.97	−12160137.36
$[H_4C_6(1,2\text{-}(B(p\text{-}ClC_6F_4)_2))_2F]^-$	−4731.11609	852.50	−12420691.10
$H_6C_{10}(1,8\text{-}(B(p\text{-}ClC_6F_4)_2))_2$ (**9**)	−4784.70072	971.65	−12561258.38
$[H_6C_{10}(1,8\text{-}(B(p\text{-}ClC_6F_4)_2))_2H]^-$	−4785.41903	990.40	−12563125.53
$[H_6C_{10}(1,8\text{-}(B(p\text{-}ClC_6F_4)_2))_2F]^-$	−4884.64785	977.67	−12823663.50

Me_3Si^+



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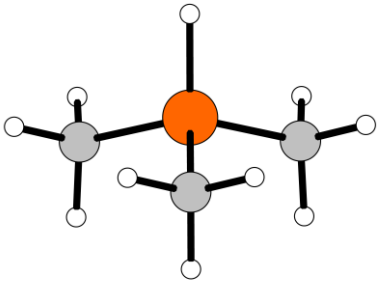
          -0.01598879    0.35642374    3.47211775    c
          -0.00006054   -0.00320928    0.00033046    si
          -3.01425465   -0.24200945   -1.74340125    c
           3.02998111   -0.11852705   -1.72851689    c
          -1.94711356    0.41558220    4.29039308    h
           1.06152160   -1.23001159    4.35604169    h
           1.01968252    2.11578011    4.01121693    h
           3.10402863    1.45531797   -3.13517903    h
           4.70608313    0.00683900   -0.47255206    h
           3.14031226   -1.89715374   -2.86022998    h
          -2.75789636   -0.47161165   -3.81303555    h
          -4.14195626   -1.86472402   -0.99943856    h
          -4.18433909    1.47730377   -1.37774658    h
```

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	34.92	0.00390	YES	YES
8	a	38.77	0.00748	YES	YES
9	a	69.65	2.68803	YES	YES
10	a	210.84	2.11984	YES	YES
11	a	211.26	2.12402	YES	YES
12	a	216.51	1.29151	YES	YES
13	a	590.98	0.00071	YES	YES
14	a	621.97	0.00139	YES	YES
15	a	622.40	0.00029	YES	YES
16	a	696.12	0.00122	YES	YES
17	a	741.26	8.27319	YES	YES
18	a	741.53	8.39950	YES	YES
19	a	817.30	83.84071	YES	YES
20	a	882.25	132.97233	YES	YES
21	a	882.41	132.68856	YES	YES
22	a	1240.76	77.09208	YES	YES
23	a	1240.83	76.99746	YES	YES
24	a	1246.99	0.01968	YES	YES
25	a	1360.39	10.84691	YES	YES
26	a	1360.86	11.45068	YES	YES
27	a	1362.38	0.49814	YES	YES
28	a	1362.55	1.02709	YES	YES
29	a	1369.00	40.08693	YES	YES
30	a	1369.97	7.23469	YES	YES
31	a	2924.84	45.99198	YES	YES
32	a	2925.03	46.02473	YES	YES
33	a	2930.03	0.03931	YES	YES
34	a	2999.70	43.42089	YES	YES
35	a	3000.03	0.32329	YES	YES
36	a	3000.13	0.78238	YES	YES
37	a	3066.49	14.30970	YES	YES
38	a	3066.79	10.63487	YES	YES
39	a	3067.60	3.85126	YES	YES

Me_3SiH



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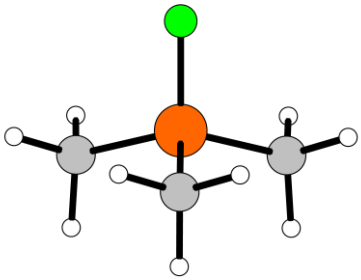
$coord
          -0.43289284    0.74985251   -0.30652084    si
          -0.46743284    0.81055102    3.28366083    c
           2.94053539    0.81006155   -1.53518914    c
          -2.17231799   -2.14127259   -1.53607812    c
          -1.78303406    3.08765329   -1.26117247    h
          -2.43591477    0.82449498    4.02525615    h
           0.50577022   -0.87463312    4.08512752    h
           0.50321412    2.52303943    4.02576026    h
           2.98516853    0.82289804   -3.63838703    h
           3.96278191    2.52311690   -0.86725028    h
           4.02052483   -0.87458096   -0.88319450    h
          -2.20912585   -2.16872827   -3.63902630    h
          -1.25175857   -3.91969306   -0.88840338    h
          -4.16551808   -2.17275972   -0.86458270    h

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection
rules
#                         cm**(-1)        km/mol         IR
RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a            150.25         0.00011      YES     YES
     8        a            163.99         0.00005      YES     YES
     9        a            165.62         0.00011      YES     YES
    10        a            197.14         0.56696      YES     YES
    11        a            198.37         0.57505      YES     YES
    12        a            231.57         0.85546      YES     YES
    13        a            595.00         1.45625      YES     YES
    14        a            602.53         7.03374      YES     YES
    15        a            603.54         7.07047      YES     YES
    16        a            667.22         0.00080      YES     YES
    17        a            684.26        11.45414      YES     YES
    18        a            684.68        11.67875      YES     YES
    19        a            833.20        17.40009      YES     YES
    20        a            833.63        16.61847      YES     YES
    21        a            856.68        70.29361      YES     YES
    22        a            889.56       162.87427      YES     YES
```

23	a	889.83	162.25261	YES	YES
24	a	1239.30	29.86095	YES	YES
25	a	1239.92	29.82629	YES	YES
26	a	1250.95	5.44550	YES	YES
27	a	1395.49	0.00118	YES	YES
28	a	1399.59	0.30250	YES	YES
29	a	1399.86	0.28297	YES	YES
30	a	1409.12	4.94364	YES	YES
31	a	1409.62	4.96243	YES	YES
32	a	1416.45	13.82765	YES	YES
33	a	2134.73	162.41460	YES	YES
34	a	2937.47	8.30321	YES	YES
35	a	2937.75	8.13007	YES	YES
36	a	2938.64	2.89349	YES	YES
37	a	3027.26	0.80470	YES	YES
38	a	3027.33	0.54760	YES	YES
39	a	3028.67	22.12874	YES	YES
40	a	3031.62	2.84826	YES	YES
41	a	3031.97	11.97371	YES	YES
42	a	3032.86	9.76990	YES	YES

Me_3SiF



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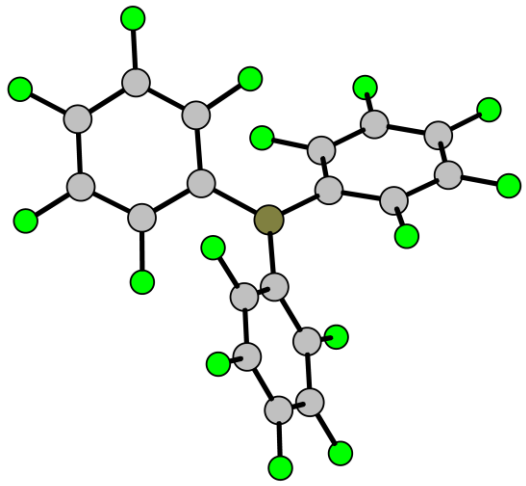
$coord
          -0.38785791    0.67107402   -0.27321083    si
          -0.45819380    0.79561098    3.28746785    c
           2.94466435    0.79678252   -1.52955236    c
          -2.16143525   -2.15298323   -1.53044534    c
          -1.86910470    3.22673216   -1.31068490    f
          -2.43411055    0.82698995    4.00721024    h
           0.50216578   -0.87854569    4.12668136    h
           0.51162995    2.51741171    4.00766275    h
           2.96693772    0.81486711   -3.63263799    h
           3.94525425    2.52297114   -0.86414260    h
           4.05745956   -0.87281493   -0.89347374    h
          -2.18975096   -2.15793568   -3.63330675    h
          -1.27172656   -3.95253890   -0.89793029    h
          -4.15593189   -2.15762116   -0.86363740    h

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection
rules
#                         cm**(-1)        km/mol          IR
RAMAN
     1                      -0.00         0.00000         -       -
     2                       0.00         0.00000         -       -
     3                       0.00         0.00000         -       -
     4                       0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a            131.33         0.00018       YES     YES
     8        a            151.66         0.00585       YES     YES
     9        a            153.77         0.00588       YES     YES
    10        a            184.22         0.13284       YES     YES
    11        a            185.57         0.10982       YES     YES
    12        a            225.30         0.09574       YES     YES
    13        a            259.34        12.17224       YES     YES
    14        a            263.20        12.08916       YES     YES
    15        a            585.80         0.02291       YES     YES
    16        a            664.84         0.00422       YES     YES
    17        a            672.51         3.43153       YES     YES
    18        a            673.46         3.50531       YES     YES
    19        a            751.14        29.98934       YES     YES
    20        a            751.92        29.30489       YES     YES
    21        a            769.96         3.56902       YES     YES
    22        a            850.81       137.46093       YES     YES
    23        a            851.37       136.74569       YES     YES
```

24	a	908.76	169.08206	YES	YES
25	a	1246.37	45.44224	YES	YES
26	a	1247.12	45.18588	YES	YES
27	a	1255.05	15.54954	YES	YES
28	a	1390.48	0.00230	YES	YES
29	a	1397.21	0.07948	YES	YES
30	a	1397.62	0.07283	YES	YES
31	a	1404.07	4.82472	YES	YES
32	a	1404.61	4.82130	YES	YES
33	a	1415.34	15.93749	YES	YES
34	a	2940.21	3.46406	YES	YES
35	a	2940.63	3.48339	YES	YES
36	a	2942.69	1.33022	YES	YES
37	a	3029.54	1.06073	YES	YES
38	a	3030.09	0.80230	YES	YES
39	a	3032.25	16.44630	YES	YES
40	a	3036.44	1.39755	YES	YES
41	a	3036.93	8.78219	YES	YES
42	a	3037.81	7.36781	YES	YES

$B(C_6F_5)_3$



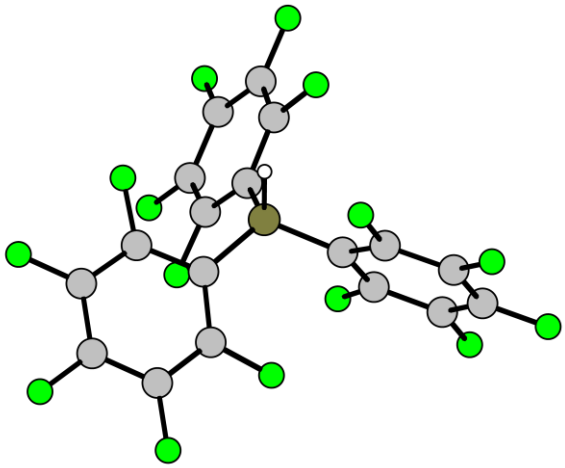
```
$coord
          0.00231502   -0.00180129    0.11931496    b
          0.00541573   -0.00526280    3.08599747    c
          2.55266219   -0.07626625   -1.41627937    c
         -2.55099332    0.08057864   -1.41228774    c
         -1.91142163    1.19356354    4.51844142    c
         -1.91565978    1.24806273    7.16876445    c
         -0.00864904   -0.04640205    8.49312533    c
          1.94643079   -1.25790699    7.16021250    c
          1.90281889   -1.24399824    4.50995181    c
          2.79032688   -1.53011224   -3.64341254    c
          5.01188463   -1.60017968   -5.08793171    c
          7.06551111   -0.07361335   -4.36947866    c
          6.92723387    1.38873928   -2.15261106    c
          4.68419248    1.37994424   -0.73901978    c
         -2.80283336    1.57680561   -3.60891252    c
         -5.02074770    1.64559565   -5.05913667    c
         -7.07369713    0.11435621   -4.34840226    c
         -6.91645527   -1.39922483   -2.16737827    c
         -4.67575164   -1.39143894   -0.74998472    c
         -3.78352361    2.45122332    3.36222428    f
         -3.74319273    2.43845850    8.43730061    f
         -0.01281387   -0.06189161   11.00783488    f
          3.76784256   -2.46616239    8.42060435    f
          3.77336699   -2.49497790    3.34407783    f
          0.87613523   -3.00962197   -4.41438496    f
          5.16555323   -3.02963897   -7.16258135    f
          9.16948919   -0.06710285   -5.74915431    f
          8.89244362    2.81820427   -1.46957864    f
          4.61527560    2.85767872    1.32344947    f
         -0.89488455    3.07533428   -4.35925863    f
         -5.18597281    3.10834165   -7.10970606    f
         -9.18141469    0.12136418   -5.72274337    f
         -8.87620260   -2.84333181   -1.49959276    f
         -4.59468430   -2.89931667    1.29053602    f

$vibrational spectrum
```

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.81	0.43543	YES	YES
8	a	23.08	0.49879	YES	YES
9	a	32.88	0.00450	YES	YES
10	a	34.67	0.02070	YES	YES
11	a	36.97	0.00373	YES	YES
12	a	38.67	0.00060	YES	YES
13	a	99.93	0.14526	YES	YES
14	a	105.13	0.12266	YES	YES
15	a	108.01	0.03380	YES	YES
16	a	126.39	0.37123	YES	YES
17	a	126.91	0.41644	YES	YES
18	a	127.87	0.05944	YES	YES
19	a	138.77	0.02632	YES	YES
20	a	144.98	0.00688	YES	YES
21	a	150.67	0.06515	YES	YES
22	a	154.83	0.00153	YES	YES
23	a	155.88	0.20548	YES	YES
24	a	158.43	0.16762	YES	YES
25	a	221.65	3.44190	YES	YES
26	a	227.79	3.79144	YES	YES
27	a	232.29	3.67940	YES	YES
28	a	263.85	0.09973	YES	YES
29	a	264.17	0.15157	YES	YES
30	a	264.30	0.24567	YES	YES
31	a	269.68	0.12280	YES	YES
32	a	270.21	0.06737	YES	YES
33	a	273.30	0.12200	YES	YES
34	a	306.86	0.11939	YES	YES
35	a	307.28	1.01961	YES	YES
36	a	310.56	0.57883	YES	YES
37	a	339.87	2.67515	YES	YES
38	a	341.01	2.55821	YES	YES
39	a	347.24	0.12492	YES	YES
40	a	350.18	0.11865	YES	YES
41	a	377.47	6.02926	YES	YES
42	a	382.92	6.58010	YES	YES
43	a	391.75	1.20881	YES	YES
44	a	394.31	1.04611	YES	YES
45	a	394.95	0.64130	YES	YES
46	a	429.85	0.48669	YES	YES
47	a	430.87	0.25152	YES	YES
48	a	431.21	0.30182	YES	YES
49	a	458.58	4.77439	YES	YES
50	a	460.14	4.07864	YES	YES
51	a	483.88	0.00422	YES	YES
52	a	509.87	0.39310	YES	YES
53	a	520.45	0.56085	YES	YES

54	a	531.13	0.48382	YES	YES
55	a	539.31	2.06038	YES	YES
56	a	563.84	3.16444	YES	YES
57	a	564.28	2.61247	YES	YES
58	a	566.92	0.02328	YES	YES
59	a	617.99	29.48504	YES	YES
60	a	620.03	28.68733	YES	YES
61	a	634.31	1.49556	YES	YES
62	a	635.28	2.32619	YES	YES
63	a	637.20	0.01725	YES	YES
64	a	662.95	20.51843	YES	YES
65	a	668.87	23.99648	YES	YES
66	a	678.13	7.83049	YES	YES
67	a	768.87	23.30457	YES	YES
68	a	771.65	22.05836	YES	YES
69	a	774.53	4.10823	YES	YES
70	a	852.05	0.11936	YES	YES
71	a	984.09	129.92797	YES	YES
72	a	984.70	57.31547	YES	YES
73	a	985.27	109.69115	YES	YES
74	a	1021.48	129.75029	YES	YES
75	a	1022.64	98.76312	YES	YES
76	a	1117.54	0.76600	YES	YES
77	a	1154.57	7.29301	YES	YES
78	a	1156.41	19.42212	YES	YES
79	a	1159.05	24.87645	YES	YES
80	a	1175.32	191.66038	YES	YES
81	a	1184.51	236.46695	YES	YES
82	a	1305.68	0.17552	YES	YES
83	a	1316.79	149.15878	YES	YES
84	a	1320.63	200.27599	YES	YES
85	a	1345.85	0.11818	YES	YES
86	a	1349.20	9.11800	YES	YES
87	a	1350.00	6.31452	YES	YES
88	a	1377.86	322.69083	YES	YES
89	a	1381.11	238.18609	YES	YES
90	a	1397.24	2.55371	YES	YES
91	a	1471.70	460.22521	YES	YES
92	a	1480.74	524.71900	YES	YES
93	a	1482.76	686.45408	YES	YES
94	a	1521.11	231.20988	YES	YES
95	a	1521.61	291.31071	YES	YES
96	a	1523.81	4.72503	YES	YES
97	a	1609.02	20.60939	YES	YES
98	a	1611.43	11.83677	YES	YES
99	a	1611.75	5.30532	YES	YES
100	a	1630.83	202.49489	YES	YES
101	a	1631.82	175.40840	YES	YES
102	a	1633.24	21.86498	YES	YES

$[B(C_6F_5)_3H]^-$



```
$coord
          -0.51640772    1.14134035   -0.45554441    b
          -0.61728508    1.15946140    2.65158449    c
           2.37006925    1.22456423   -1.59484775    c
          -2.32303170   -1.08758453   -1.64374317    c
          -2.71114665    2.22861850    3.89449987    c
          -2.93540830    2.38739759    6.53841076    c
          -0.98787620    1.43060765    8.06286625    c
           1.13735536    0.33469373    6.91706948    c
           1.26937809    0.21358224    4.26392720    c
           3.46572908   -0.53137044   -3.25845799    c
           5.88883463   -0.24469213   -4.32161941    c
           7.34870222    1.87245525   -3.68857799    c
           6.35329307    3.67396991   -2.01439344    c
           3.92133678    3.30849664   -1.01705085    c
          -3.80517655   -0.62298420   -3.80124535    c
          -5.47338899   -2.40585268   -4.85226577    c
          -5.70015320   -4.79453286   -3.72500803    c
          -4.24380038   -5.36296752   -1.58344665    c
          -2.59450044   -3.51934815   -0.61156874    c
          -4.66288543    3.17848672    2.55022362    f
          -4.98448051    3.44354932    7.62678257    f
          -1.15909874    1.56011413   10.60033696    f
           3.00858817   -0.59861569    8.37474769    f
           3.36047285   -0.89527558    3.30517405    f
           2.21111739   -2.64910685   -3.95199515    f
           6.82929311   -1.98558717   -5.92738233    f
           9.67318659    2.18125326   -4.68137169    f
           7.74171617    5.71772261   -1.39104753    f
           3.07520175    5.11974358    0.57318263    f
          -3.67699244    1.62098190   -5.00844470    f
          -6.85659546   -1.85245220   -6.92009523    f
          -7.29396948   -6.52773029   -4.69299458    f
          -4.43739144   -7.66417907   -0.50629313    f
          -1.20627497   -4.22356036    1.41415467    f
          -1.46841084    3.16880070   -1.12556635    h
```

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.09	0.01106	YES	YES
8	a	16.68	0.00514	YES	YES
9	a	21.29	0.01246	YES	YES
10	a	29.26	0.02286	YES	YES
11	a	33.50	0.02049	YES	YES
12	a	40.83	0.09646	YES	YES
13	a	95.92	0.14742	YES	YES
14	a	100.09	0.19719	YES	YES
15	a	107.44	0.11855	YES	YES
16	a	123.48	0.00373	YES	YES
17	a	124.88	0.00738	YES	YES
18	a	126.25	0.00093	YES	YES
19	a	135.66	0.01596	YES	YES
20	a	141.57	0.07225	YES	YES
21	a	144.33	0.03697	YES	YES
22	a	157.85	0.01588	YES	YES
23	a	161.62	0.05387	YES	YES
24	a	162.62	0.02991	YES	YES
25	a	218.97	1.31169	YES	YES
26	a	222.04	1.26525	YES	YES
27	a	227.45	1.83289	YES	YES
28	a	260.74	0.03969	YES	YES
29	a	263.26	0.03433	YES	YES
30	a	264.08	0.03670	YES	YES
31	a	269.16	0.04979	YES	YES
32	a	271.10	0.04602	YES	YES
33	a	272.78	0.03470	YES	YES
34	a	303.72	0.49433	YES	YES
35	a	306.04	0.72401	YES	YES
36	a	307.05	0.35399	YES	YES
37	a	336.11	1.55889	YES	YES
38	a	338.17	1.00342	YES	YES
39	a	338.32	1.46476	YES	YES
40	a	349.25	0.07508	YES	YES
41	a	362.71	0.60589	YES	YES
42	a	374.71	0.15396	YES	YES
43	a	386.63	0.06671	YES	YES
44	a	388.45	0.04985	YES	YES
45	a	390.17	0.16986	YES	YES
46	a	432.55	0.00596	YES	YES
47	a	432.90	0.06762	YES	YES
48	a	433.30	0.15275	YES	YES
49	a	453.80	1.70173	YES	YES
50	a	454.89	1.97709	YES	YES
51	a	470.59	0.01651	YES	YES
52	a	494.13	0.03100	YES	YES

53	a	502.80	0.01324	YES	YES
54	a	511.91	0.07734	YES	YES
55	a	527.43	0.53041	YES	YES
56	a	558.59	5.13858	YES	YES
57	a	559.34	4.81285	YES	YES
58	a	562.92	0.07214	YES	YES
59	a	585.22	10.07920	YES	YES
60	a	590.87	13.35415	YES	YES
61	a	626.62	0.09565	YES	YES
62	a	628.18	0.57441	YES	YES
63	a	632.22	0.09510	YES	YES
64	a	654.84	31.81158	YES	YES
65	a	662.26	4.86458	YES	YES
66	a	680.54	31.17133	YES	YES
67	a	744.42	12.19290	YES	YES
68	a	753.40	14.47375	YES	YES
69	a	769.59	1.26126	YES	YES
70	a	827.37	1.83420	YES	YES
71	a	894.04	73.20260	YES	YES
72	a	902.29	75.59096	YES	YES
73	a	964.53	109.29939	YES	YES
74	a	971.47	188.46427	YES	YES
75	a	976.64	253.74077	YES	YES
76	a	1028.07	18.38777	YES	YES
77	a	1046.62	32.37182	YES	YES
78	a	1080.46	11.79194	YES	YES
79	a	1096.36	215.82812	YES	YES
80	a	1102.41	239.75345	YES	YES
81	a	1126.32	3.75638	YES	YES
82	a	1128.56	0.97336	YES	YES
83	a	1130.21	5.17888	YES	YES
84	a	1261.45	26.43230	YES	YES
85	a	1262.72	15.51136	YES	YES
86	a	1264.11	31.39452	YES	YES
87	a	1349.24	7.51389	YES	YES
88	a	1350.72	12.66727	YES	YES
89	a	1351.37	4.36198	YES	YES
90	a	1372.95	12.56955	YES	YES
91	a	1376.23	5.29092	YES	YES
92	a	1379.59	2.05402	YES	YES
93	a	1460.55	347.75580	YES	YES
94	a	1463.59	279.30832	YES	YES
95	a	1466.12	498.34580	YES	YES
96	a	1502.39	240.93092	YES	YES
97	a	1504.91	295.11533	YES	YES
98	a	1508.32	28.99978	YES	YES
99	a	1613.62	6.61667	YES	YES
100	a	1615.85	2.36564	YES	YES
101	a	1616.23	6.38167	YES	YES
102	a	1619.26	29.14311	YES	YES
103	a	1621.75	26.94898	YES	YES
104	a	1623.98	8.66739	YES	YES
105	a	2399.37	74.56385	YES	YES

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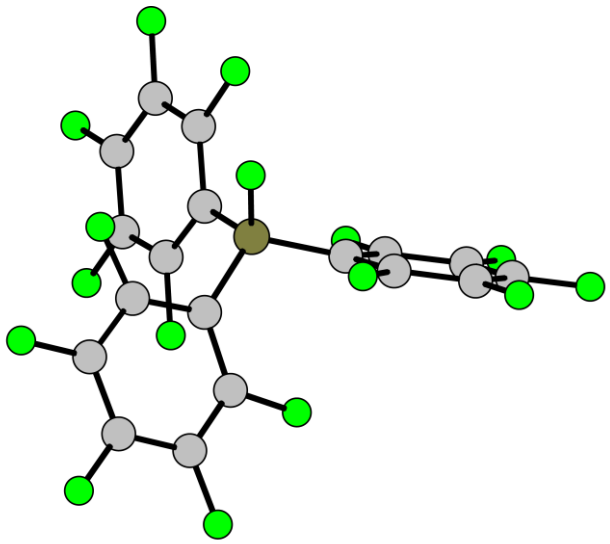

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          -2.83270607    1.93955629    3.90427083    c
          -3.07474269    2.06030512    6.54962095    c
          -1.02129791    1.35494060    8.07120941    c
           1.22470278    0.54461435    6.92081153    c
           1.37081482    0.45205394    4.26732821    c
           3.44504181   -0.55102094   -3.27507378    c
           5.88230907   -0.34347380   -4.32818616    c
           7.39561494    1.73723648   -3.70130968    c
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           6.77476946   -2.11027218   -5.93184353    f
           9.72675806    1.97902658   -4.69133588    f
           7.90817369    5.56516851   -1.40154271    f
           3.25295335    5.08356986    0.60046916    f
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          -6.87238723   -1.89970465   -6.94241665    f
          -7.31410258   -6.50567446   -4.58050647    f
          -4.44034301   -7.52078470   -0.36745005    f
          -1.21846271   -4.03101329    1.44381634    f
          -1.54069726    3.69754374   -1.20919568    f
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$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	2.66	0.01207	YES	YES
8	a	20.44	0.01154	YES	YES
9	a	25.86	0.00625	YES	YES
10	a	30.79	0.02175	YES	YES
11	a	34.38	0.02510	YES	YES
12	a	39.23	0.08212	YES	YES
13	a	95.82	0.42328	YES	YES
14	a	101.00	0.12780	YES	YES
15	a	105.43	0.21410	YES	YES
16	a	122.24	0.00158	YES	YES
17	a	124.18	0.01349	YES	YES
18	a	127.76	0.00623	YES	YES
19	a	135.40	0.07885	YES	YES
20	a	142.15	0.17843	YES	YES
21	a	147.64	0.19343	YES	YES
22	a	157.38	0.01751	YES	YES
23	a	159.87	0.15833	YES	YES
24	a	162.29	0.07494	YES	YES
25	a	205.02	2.84452	YES	YES
26	a	218.54	1.96041	YES	YES
27	a	223.79	2.09217	YES	YES
28	a	245.53	0.71470	YES	YES
29	a	248.04	0.74060	YES	YES
30	a	260.39	0.07378	YES	YES
31	a	261.94	0.06459	YES	YES
32	a	264.18	0.05087	YES	YES
33	a	271.17	0.09904	YES	YES
34	a	271.99	0.11558	YES	YES
35	a	272.28	0.03879	YES	YES
36	a	306.96	0.54619	YES	YES
37	a	307.71	0.27432	YES	YES
38	a	309.30	0.21158	YES	YES
39	a	311.99	0.91269	YES	YES
40	a	342.20	3.69458	YES	YES
41	a	344.12	2.15040	YES	YES
42	a	346.59	0.10971	YES	YES
43	a	380.25	1.15561	YES	YES
44	a	386.44	0.11351	YES	YES
45	a	386.94	0.05115	YES	YES
46	a	389.36	0.09350	YES	YES
47	a	392.24	1.57243	YES	YES
48	a	429.26	0.29102	YES	YES
49	a	433.34	0.09539	YES	YES
50	a	433.58	0.20530	YES	YES
51	a	434.63	0.18012	YES	YES
52	a	465.08	2.14947	YES	YES

53	a	465.87	1.74679	YES	YES
54	a	481.98	0.02117	YES	YES
55	a	499.44	0.08862	YES	YES
56	a	503.80	0.02143	YES	YES
57	a	513.88	0.02608	YES	YES
58	a	561.22	4.74219	YES	YES
59	a	561.78	3.49480	YES	YES
60	a	563.44	0.11261	YES	YES
61	a	598.19	35.17487	YES	YES
62	a	609.21	37.71911	YES	YES
63	a	630.20	0.31636	YES	YES
64	a	631.25	0.06738	YES	YES
65	a	633.85	0.01338	YES	YES
66	a	641.05	2.47794	YES	YES
67	a	688.73	65.92389	YES	YES
68	a	703.41	79.99524	YES	YES
69	a	745.91	3.41737	YES	YES
70	a	754.70	33.66348	YES	YES
71	a	758.85	35.53605	YES	YES
72	a	807.79	4.97571	YES	YES
73	a	911.76	10.29684	YES	YES
74	a	925.09	12.24811	YES	YES
75	a	968.76	316.88879	YES	YES
76	a	974.95	88.01769	YES	YES
77	a	980.32	146.54154	YES	YES
78	a	1009.26	1.16919	YES	YES
79	a	1084.40	51.81680	YES	YES
80	a	1088.62	281.22419	YES	YES
81	a	1091.88	360.90557	YES	YES
82	a	1128.11	0.77865	YES	YES
83	a	1131.01	0.97943	YES	YES
84	a	1131.74	1.48555	YES	YES
85	a	1263.12	54.66614	YES	YES
86	a	1264.12	63.11077	YES	YES
87	a	1265.24	8.66653	YES	YES
88	a	1348.51	7.96405	YES	YES
89	a	1349.72	5.09193	YES	YES
90	a	1350.32	5.70157	YES	YES
91	a	1370.36	25.06454	YES	YES
92	a	1373.39	18.69906	YES	YES
93	a	1381.53	0.55668	YES	YES
94	a	1458.95	318.65713	YES	YES
95	a	1463.51	486.92679	YES	YES
96	a	1465.58	553.54742	YES	YES
97	a	1506.14	185.96609	YES	YES
98	a	1507.38	237.30169	YES	YES
99	a	1510.35	13.50381	YES	YES
100	a	1615.50	13.53291	YES	YES
101	a	1616.41	6.61420	YES	YES
102	a	1618.83	2.24477	YES	YES
103	a	1622.18	53.96660	YES	YES
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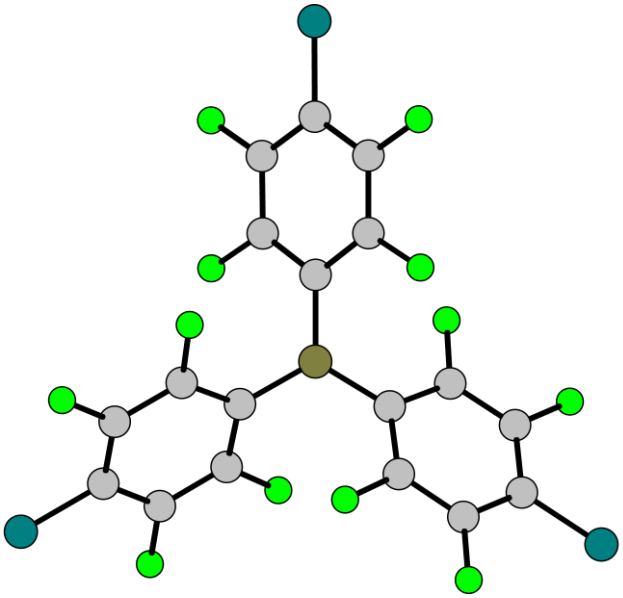

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    7.04943680    1.05129949   -2.08594481    c
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    7.21108703   -0.47004723   -4.26551546    c
   -2.80001343    1.33120774   -3.72578457    c
   -5.05442560    1.36220812   -5.11966112    c
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    4.74160013    2.61515760    1.34811757    f
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   -5.21428980    2.73211258   -7.23067119    f
   -8.87180973   -2.85602875   -1.20104555    f
   -4.55333129   -2.81614018    1.46615363    f
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$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.38	0.51359	YES	YES
8	a	18.82	0.53414	YES	YES
9	a	26.17	0.01735	YES	YES
10	a	27.45	0.00262	YES	YES
11	a	28.49	0.01003	YES	YES
12	a	32.91	0.00491	YES	YES
13	a	88.38	0.08826	YES	YES
14	a	89.26	0.08049	YES	YES
15	a	91.11	0.04500	YES	YES
16	a	122.66	0.30868	YES	YES
17	a	123.23	0.41006	YES	YES
18	a	124.28	0.06864	YES	YES
19	a	129.99	0.12723	YES	YES
20	a	131.18	0.22486	YES	YES
21	a	132.11	0.33402	YES	YES
22	a	143.19	0.08763	YES	YES
23	a	144.54	0.12210	YES	YES
24	a	144.80	0.03242	YES	YES
25	a	193.93	0.10405	YES	YES
26	a	195.22	0.09751	YES	YES
27	a	195.75	0.09915	YES	YES
28	a	214.69	2.30904	YES	YES
29	a	218.48	2.97257	YES	YES
30	a	220.13	2.93094	YES	YES
31	a	274.90	0.31146	YES	YES
32	a	276.79	0.41757	YES	YES
33	a	279.64	0.04500	YES	YES
34	a	299.91	0.23390	YES	YES
35	a	302.21	0.27157	YES	YES
36	a	303.37	0.22782	YES	YES
37	a	319.90	0.39005	YES	YES
38	a	321.79	0.32704	YES	YES
39	a	323.22	0.13808	YES	YES
40	a	333.61	0.31100	YES	YES
41	a	358.93	11.01052	YES	YES
42	a	362.10	11.36445	YES	YES
43	a	399.97	2.14971	YES	YES
44	a	401.08	2.24665	YES	YES
45	a	401.89	0.33424	YES	YES
46	a	427.08	2.58191	YES	YES
47	a	427.37	2.30116	YES	YES
48	a	427.82	0.96089	YES	YES
49	a	434.40	3.48964	YES	YES
50	a	434.72	3.29088	YES	YES
51	a	471.25	0.00275	YES	YES
52	a	504.29	1.00291	YES	YES

53	a	504.33	0.99896	YES	YES
54	a	504.57	0.01673	YES	YES
55	a	515.96	0.15089	YES	YES
56	a	576.89	2.32979	YES	YES
57	a	578.31	2.26481	YES	YES
58	a	588.09	1.91247	YES	YES
59	a	623.65	32.69245	YES	YES
60	a	624.95	35.37291	YES	YES
61	a	641.47	1.96608	YES	YES
62	a	641.99	2.01255	YES	YES
63	a	643.97	0.09482	YES	YES
64	a	665.20	19.16353	YES	YES
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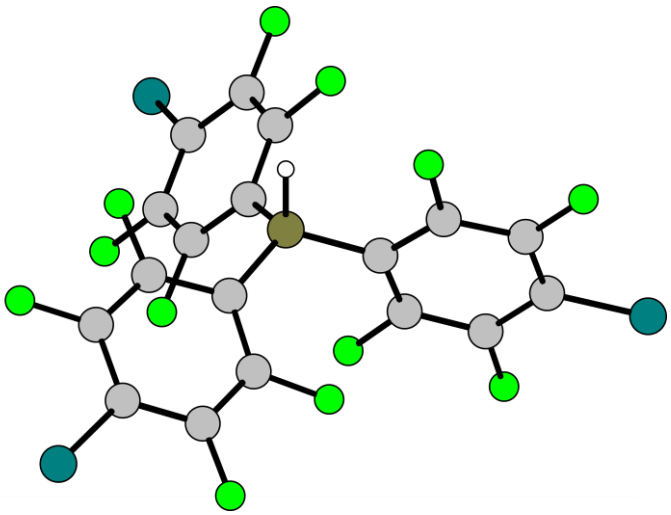
66	a	673.91	7.59983	YES	YES
67	a	750.27	38.18802	YES	YES
68	a	751.69	38.23409	YES	YES
69	a	759.43	5.21196	YES	YES
70	a	808.33	0.08469	YES	YES
71	a	879.89	59.35730	YES	YES
72	a	881.07	64.31863	YES	YES
73	a	962.66	0.03704	YES	YES
74	a	970.42	157.61535	YES	YES
75	a	974.30	111.97010	YES	YES
76	a	976.11	126.79542	YES	YES
77	a	1101.77	79.65974	YES	YES
78	a	1107.22	92.84431	YES	YES
79	a	1152.81	2.25534	YES	YES
80	a	1156.08	0.54855	YES	YES
81	a	1157.65	0.15156	YES	YES
82	a	1265.86	0.25778	YES	YES
83	a	1291.62	149.57963	YES	YES
84	a	1295.41	167.12279	YES	YES
85	a	1341.52	0.87535	YES	YES
86	a	1343.81	2.26560	YES	YES
87	a	1344.79	1.32777	YES	YES
88	a	1378.05	356.16353	YES	YES
89	a	1379.33	341.32410	YES	YES
90	a	1394.37	0.27828	YES	YES
91	a	1445.59	144.51615	YES	YES
92	a	1446.87	132.60972	YES	YES
93	a	1448.24	44.95439	YES	YES
94	a	1468.36	545.96070	YES	YES
95	a	1474.63	485.10590	YES	YES
96	a	1476.27	540.72702	YES	YES
97	a	1582.93	32.68167	YES	YES
98	a	1585.04	4.43294	YES	YES
99	a	1585.37	5.71762	YES	YES
100	a	1618.50	183.07226	YES	YES
101	a	1618.94	196.95235	YES	YES
102	a	1619.72	13.90899	YES	YES

[B(*p*-ClC$_6$F$_4$)$_3$H]$^-$



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         -7.13791125   -1.83454149   -3.45049878    c
         -6.44431656   -3.36185568   -1.39037204    c
         -4.02320687   -3.10413511   -0.32945548    c
          3.35650514   -1.15943323   -3.94381616    c
          5.29883698   -0.35374995   -5.55905817    c
          6.87924739    1.64508965   -4.80357648    c
          6.46026556    2.77081135   -2.43833360    c
          4.48455900    1.89227978   -0.88620617    c
         -0.89248880    2.26921424    3.43045423    c
         -1.32773780    3.29500883    5.83943036    c
         -0.61048626    1.90865974    7.99079340    c
          0.54110651   -0.46132910    7.66603661    c
          0.95556917   -1.40075382    5.21122570    c
         -1.42940338    1.88260769   -4.24859792    f
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         -8.08805373   -5.05523104   -0.44336830    f
         -3.49392170   -4.63358221    1.64453379    f
          1.91700038   -3.09296997   -4.79308407    f
          5.64628154   -1.47838060   -7.81292108    f
          9.30793668    2.69596019   -6.76000518    cl
          7.93633926    4.68844301   -1.65616642    f
          4.24893133    3.09312151    1.35938988    f
         -1.60636177    3.70110541    1.43978945    f
         -2.41582437    5.57841929    6.09452018    f
         -1.13119039    3.11695225   11.00728611    cl
          1.24231213   -1.82761013    9.69321986    f
          2.09119733   -3.67901266    5.07027398    f
          1.21030832   -3.55109615    0.46452537    h
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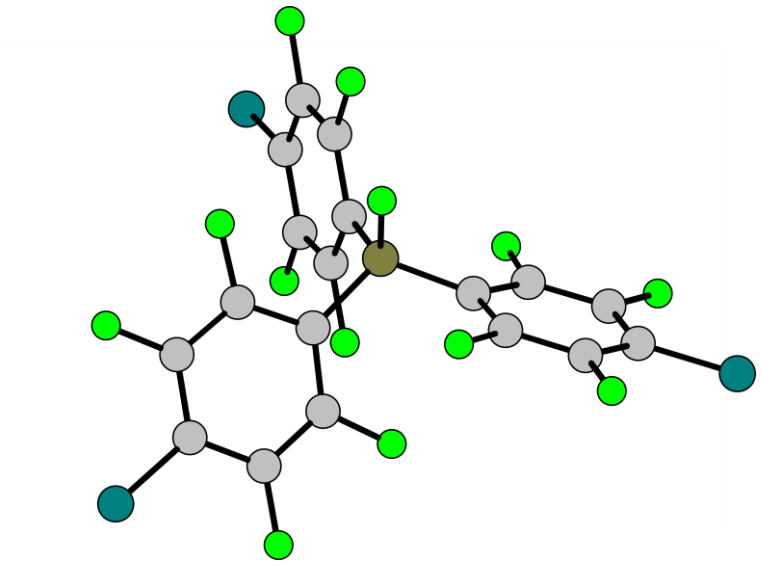
$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.97	0.00656	YES	YES
8	a	20.70	0.04637	YES	YES
9	a	23.62	0.02727	YES	YES
10	a	26.52	0.01346	YES	YES
11	a	33.80	0.05255	YES	YES
12	a	34.64	0.10990	YES	YES
13	a	83.47	0.13406	YES	YES
14	a	89.13	0.04109	YES	YES
15	a	93.99	0.05755	YES	YES
16	a	121.39	0.01425	YES	YES
17	a	122.70	0.00573	YES	YES
18	a	126.55	0.00957	YES	YES
19	a	128.62	0.01991	YES	YES
20	a	133.49	0.09335	YES	YES
21	a	137.52	0.08808	YES	YES
22	a	140.27	0.05055	YES	YES
23	a	144.94	0.07788	YES	YES
24	a	149.41	0.07812	YES	YES
25	a	191.56	0.00758	YES	YES
26	a	192.23	0.04920	YES	YES
27	a	192.35	0.00631	YES	YES
28	a	210.01	1.00110	YES	YES
29	a	214.07	0.67681	YES	YES
30	a	222.35	1.01922	YES	YES
31	a	275.68	0.00812	YES	YES
32	a	276.97	0.02334	YES	YES
33	a	279.01	0.03682	YES	YES
34	a	301.21	0.31012	YES	YES
35	a	302.83	0.29368	YES	YES
36	a	305.31	0.11067	YES	YES
37	a	318.69	0.28335	YES	YES
38	a	322.18	0.73586	YES	YES
39	a	322.48	0.52540	YES	YES
40	a	328.31	0.90798	YES	YES
41	a	340.31	1.39296	YES	YES
42	a	357.13	1.01574	YES	YES
43	a	395.19	0.27254	YES	YES
44	a	398.17	0.22863	YES	YES
45	a	399.41	0.06911	YES	YES
46	a	423.72	5.09976	YES	YES
47	a	426.01	2.78632	YES	YES
48	a	430.22	0.00552	YES	YES
49	a	432.40	0.19214	YES	YES
50	a	433.80	0.36575	YES	YES
51	a	452.09	0.01327	YES	YES
52	a	498.80	2.63490	YES	YES

53	a	499.99	2.49861	YES	YES
54	a	501.22	2.12529	YES	YES
55	a	520.57	0.39659	YES	YES
56	a	555.94	0.09027	YES	YES
57	a	561.49	0.34634	YES	YES
58	a	563.72	0.97316	YES	YES
59	a	594.85	16.37641	YES	YES
60	a	597.49	15.92244	YES	YES
61	a	632.67	0.63094	YES	YES
62	a	635.52	0.49987	YES	YES
63	a	640.75	0.69682	YES	YES
64	a	650.04	27.19471	YES	YES
65	a	663.53	2.89754	YES	YES
66	a	691.12	30.21287	YES	YES
67	a	726.97	28.09819	YES	YES
68	a	737.85	24.71658	YES	YES
69	a	752.42	3.53437	YES	YES
70	a	795.57	4.68217	YES	YES
71	a	831.53	93.64571	YES	YES
72	a	841.14	128.88291	YES	YES
73	a	930.12	13.74674	YES	YES
74	a	937.28	26.54087	YES	YES
75	a	941.81	89.12743	YES	YES
76	a	962.92	224.08934	YES	YES
77	a	972.25	104.94357	YES	YES
78	a	979.08	42.10444	YES	YES
79	a	1046.86	36.28984	YES	YES
80	a	1073.20	61.18475	YES	YES
81	a	1126.37	1.09316	YES	YES
82	a	1130.71	0.27005	YES	YES
83	a	1133.59	1.73701	YES	YES
84	a	1230.43	18.97051	YES	YES
85	a	1231.87	58.72219	YES	YES
86	a	1237.90	73.99867	YES	YES
87	a	1347.45	7.88003	YES	YES
88	a	1349.51	0.54384	YES	YES
89	a	1350.78	2.10664	YES	YES
90	a	1370.95	7.08984	YES	YES
91	a	1374.77	0.90945	YES	YES
92	a	1379.22	3.72511	YES	YES
93	a	1443.36	96.99818	YES	YES
94	a	1444.25	103.72095	YES	YES
95	a	1445.58	30.58044	YES	YES
96	a	1453.11	255.75860	YES	YES
97	a	1460.00	310.27099	YES	YES
98	a	1462.78	627.74490	YES	YES
99	a	1589.62	8.99721	YES	YES
100	a	1592.53	11.55273	YES	YES
101	a	1593.42	2.04943	YES	YES
102	a	1601.64	2.37615	YES	YES
103	a	1603.54	2.29928	YES	YES
104	a	1606.18	2.38379	YES	YES
105	a	2404.03	79.00934	YES	YES

[B(*p*-ClC$_6$F$_4$)$_3$F]$^-$



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-5.44381156	-0.11715620	-4.32018582	c
-7.19692479	-1.85714453	-3.34789465	c
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3.28585392	-0.98066422	-4.06424716	c
5.24764855	-0.14014371	-5.63941909	c
6.91661607	1.73026772	-4.75730331	c
6.56975247	2.70145991	-2.31383432	c
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-0.84269599	2.19033308	3.31160508	c
-1.32481175	3.31295528	5.66673204	c
-0.65615246	2.00873560	7.88317701	c
0.49476715	-0.37206269	7.66536050	c
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-10.20125366	-2.12080424	-4.66217511	cl
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1.75455186	-2.76875958	-5.04663492	f
5.52976184	-1.11059353	-7.97098310	f
9.37281504	2.81184799	-6.65898732	cl
8.14786310	4.47506709	-1.40553506	f
4.42034990	2.82679467	1.52791808	f
-1.49755841	3.56163532	1.25427041	f
-2.40916462	5.60779386	5.80784223	f
-1.22911521	3.33241179	10.84012909	cl
1.16426547	-1.66048043	9.75246946	f
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1.43590021	-4.02797131	0.34140437	f

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.32	0.01339	YES	YES
8	a	21.78	0.05538	YES	YES
9	a	24.29	0.02022	YES	YES
10	a	29.00	0.00268	YES	YES
11	a	33.72	0.13952	YES	YES
12	a	35.20	0.03799	YES	YES
13	a	83.29	0.14011	YES	YES
14	a	91.23	0.11413	YES	YES
15	a	94.97	0.05805	YES	YES
16	a	118.07	0.08738	YES	YES
17	a	122.61	0.00493	YES	YES
18	a	124.48	0.09252	YES	YES
19	a	126.68	0.06781	YES	YES
20	a	134.59	0.06432	YES	YES
21	a	136.19	0.30088	YES	YES
22	a	140.82	0.11681	YES	YES
23	a	144.63	0.05520	YES	YES
24	a	150.68	0.05594	YES	YES
25	a	190.52	0.34888	YES	YES
26	a	191.77	0.02074	YES	YES
27	a	192.87	0.06376	YES	YES
28	a	198.79	2.20283	YES	YES
29	a	210.99	1.17772	YES	YES
30	a	219.36	1.37229	YES	YES
31	a	233.60	0.54513	YES	YES
32	a	241.77	1.07820	YES	YES
33	a	275.48	0.06831	YES	YES
34	a	278.31	0.02148	YES	YES
35	a	279.80	0.05982	YES	YES
36	a	301.70	0.24638	YES	YES
37	a	305.41	0.10133	YES	YES
38	a	305.69	0.41652	YES	YES
39	a	308.01	0.18383	YES	YES
40	a	322.84	0.57931	YES	YES
41	a	323.68	0.30826	YES	YES
42	a	325.37	1.22004	YES	YES
43	a	350.31	3.29055	YES	YES
44	a	379.31	3.29069	YES	YES
45	a	394.90	0.08647	YES	YES
46	a	397.21	0.16277	YES	YES
47	a	397.88	0.27956	YES	YES
48	a	414.56	0.91266	YES	YES
49	a	431.70	0.26475	YES	YES
50	a	432.32	0.86244	YES	YES
51	a	433.23	0.08811	YES	YES
52	a	440.87	6.22700	YES	YES

53	a	443.16	4.54565	YES	YES
54	a	469.16	0.10226	YES	YES
55	a	499.99	3.09502	YES	YES
56	a	500.25	2.56077	YES	YES
57	a	500.84	0.64011	YES	YES
58	a	558.03	0.82982	YES	YES
59	a	561.33	0.96211	YES	YES
60	a	565.20	1.26226	YES	YES
61	a	603.19	28.69118	YES	YES
62	a	616.02	42.58203	YES	YES
63	a	636.67	0.03161	YES	YES
64	a	636.95	0.60451	YES	YES
65	a	640.78	0.43485	YES	YES
66	a	650.39	6.82235	YES	YES
67	a	682.78	59.30212	YES	YES
68	a	704.52	79.52184	YES	YES
69	a	729.44	3.51529	YES	YES
70	a	736.30	67.56076	YES	YES
71	a	741.64	57.77124	YES	YES
72	a	777.98	9.60269	YES	YES
73	a	846.25	6.65427	YES	YES
74	a	854.69	20.12134	YES	YES
75	a	924.07	0.92617	YES	YES
76	a	948.37	240.23395	YES	YES
77	a	955.17	263.00446	YES	YES
78	a	962.51	93.02573	YES	YES
79	a	973.65	47.67277	YES	YES
80	a	990.90	94.83802	YES	YES
81	a	1025.36	50.03410	YES	YES
82	a	1127.61	1.37654	YES	YES
83	a	1132.32	0.26341	YES	YES
84	a	1135.16	0.54567	YES	YES
85	a	1231.67	78.52038	YES	YES
86	a	1233.75	81.16452	YES	YES
87	a	1237.83	88.86699	YES	YES
88	a	1345.85	2.58241	YES	YES
89	a	1348.76	0.89359	YES	YES
90	a	1349.66	0.95817	YES	YES
91	a	1366.66	17.56666	YES	YES
92	a	1371.97	12.39297	YES	YES
93	a	1379.72	0.07004	YES	YES
94	a	1444.04	122.00066	YES	YES
95	a	1445.64	100.39101	YES	YES
96	a	1446.63	38.45417	YES	YES
97	a	1451.83	159.98053	YES	YES
98	a	1459.22	414.44567	YES	YES
99	a	1463.38	742.07655	YES	YES
100	a	1591.26	2.88887	YES	YES
101	a	1593.68	8.15233	YES	YES
102	a	1595.93	3.30142	YES	YES
103	a	1604.16	14.79356	YES	YES
104	a	1606.12	21.78944	YES	YES
105	a	1608.11	4.68839	YES	YES

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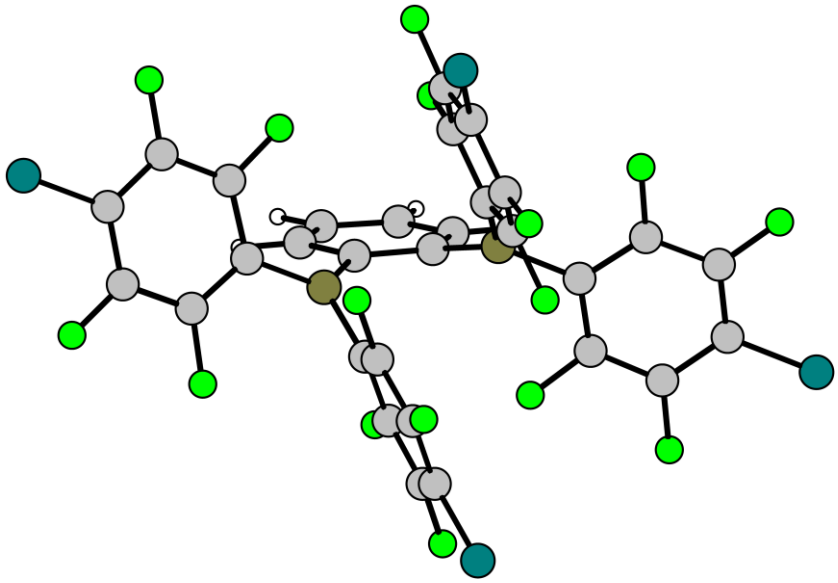

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         -2.72508871    0.94008383   -1.37765866    b
          2.72236714    0.94194367    1.37834519    b
         -1.29646237   -1.10407858   -3.02037184    c
         -5.67207622    0.64078995   -0.99458138    c
          1.29451605   -1.10708777    3.01522385    c
          5.67054058    0.64614948    0.99983928    c
          0.31424891   -0.41314444   -5.03231760    c
          1.53266436   -2.20508102   -6.56660668    c
          1.16473439   -4.79981524   -6.10204665    c
         -0.44169437   -5.56219917   -4.11848211    c
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         -7.27007978   -0.11914566   -2.99216731    c
         -9.89489993   -0.38253764   -2.71762799    c
        -11.01681121    0.07495875   -0.34686878    c
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        -14.23596749   -0.26973099    0.04513059    cl
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         -1.15792751   -4.80943647    6.09585027    c
          0.44968383   -5.56739486    4.11151762    c
          1.65508551   -3.72116080    2.64582725    c
         -2.64923916   -7.04420452    7.94508773    cl
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7.26732955	-0.10729975	3.00051954	c
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9.48560256	0.81598002	-1.69354815	c
6.87185364	1.10727815	-1.33561265	c
14.23453620	-0.26789864	-0.03315538	cl
2.66205919	-7.03048042	-7.95140538	cl
0.64015116	2.03100589	-5.61545865	f
3.00471542	-1.44834130	-8.46857313	f
-0.80584511	-8.00988611	-3.63561269	f
-3.15960699	-4.53029531	-0.76609816	f
-6.30394930	-0.54554148	-5.30273423	f
-11.31121399	-1.05539199	-4.69264325	f
-10.50459736	1.23304258	3.96952726	f
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-0.64792833	2.02262147	5.61228839	f
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0.81905480	-8.01404102	3.62748868	f
3.16483269	-4.52809108	0.75911195	f
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10.50513870	1.22389481	-3.96359056	f
5.49794409	1.77984540	-3.36029323	f

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.60	0.13215	YES	YES
8	a	9.81	0.01780	YES	YES
9	a	16.90	0.01577	YES	YES
10	a	20.91	0.22719	YES	YES
11	a	21.71	0.01613	YES	YES
12	a	27.17	0.30237	YES	YES
13	a	28.70	0.00032	YES	YES
14	a	35.79	0.11929	YES	YES
15	a	38.52	0.02206	YES	YES
16	a	44.17	0.05475	YES	YES
17	a	50.98	0.44291	YES	YES
18	a	51.58	0.12086	YES	YES
19	a	75.10	0.11966	YES	YES
20	a	89.49	0.08422	YES	YES
21	a	93.00	0.06738	YES	YES
22	a	95.58	0.40042	YES	YES
23	a	104.47	0.38920	YES	YES
24	a	121.74	0.25434	YES	YES
25	a	123.14	0.15259	YES	YES
26	a	124.27	0.02333	YES	YES
27	a	126.78	0.26055	YES	YES

28	a	130.18	0.23126	YES	YES
29	a	130.30	0.52426	YES	YES
30	a	131.86	0.09136	YES	YES
31	a	132.29	0.00063	YES	YES
32	a	140.11	0.10420	YES	YES
33	a	143.59	0.30733	YES	YES
34	a	146.26	0.00629	YES	YES
35	a	149.02	0.12014	YES	YES
36	a	193.84	0.19117	YES	YES
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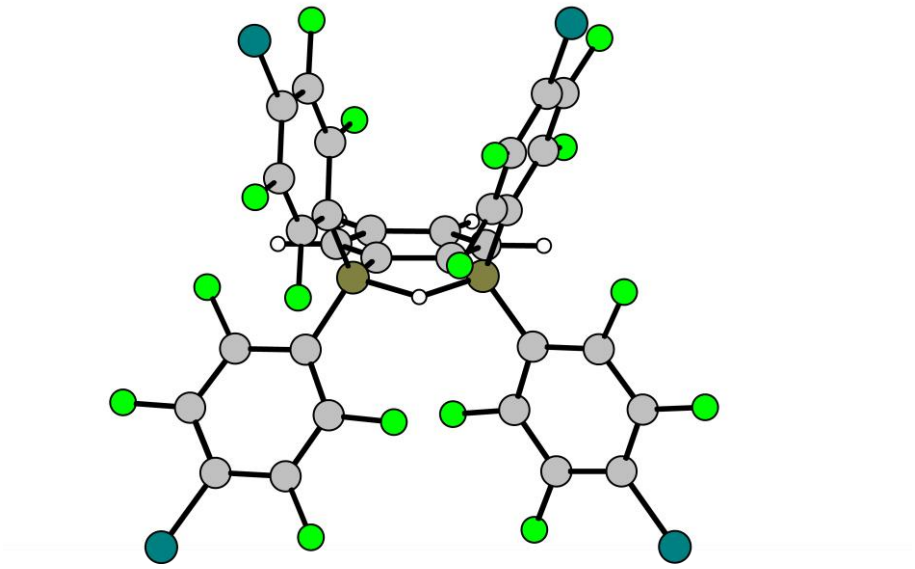

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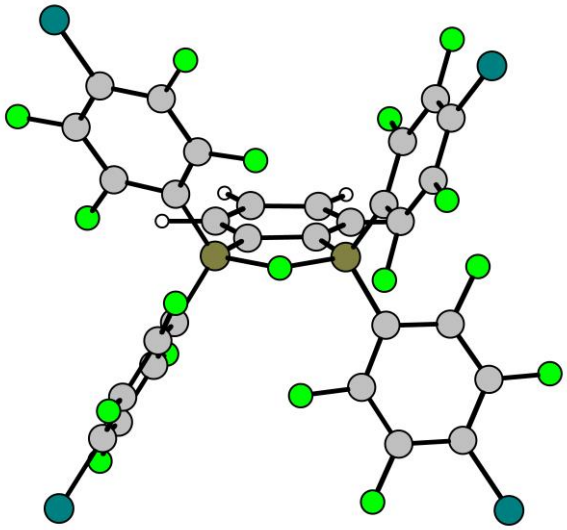

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-7.43116030	-2.69015899	3.31922839	c

-5.05017734	-2.14687104	2.26092603	c
-6.93140661	0.46372329	-3.78621473	f
-11.49220811	-0.51149374	-1.81760939	f
-12.59909689	-2.79178180	3.23457276	cl
-7.58158495	-3.73452777	5.62453029	f
-3.03813712	-2.74178396	3.70029679	f
-1.72684829	-1.75728514	-4.17605722	c
-1.36467933	-0.65933888	-6.56553361	c
-1.10211765	-2.09005335	-8.79412402	c
-1.17386771	-4.74091025	-8.67997903	c
-1.51509700	-5.91753804	-6.32259233	c
-1.78144855	-4.41699100	-4.14959480	c
-1.26594478	1.86435124	-6.85568697	f
-0.77850264	-0.91827041	-11.02116862	f
-0.84888859	-6.53767806	-11.40870092	cl
-1.58905352	-8.44715344	-6.14995283	f
-2.10745409	-5.66273474	-1.94986249	f
-4.59427334	4.33149691	-3.52207691	h
-3.37460840	8.81576195	-2.76474147	h
0.43449222	9.82756351	-0.09941263	h
2.92474813	6.33749299	1.86260742	h
0.24254679	-1.27691093	0.15500901	f

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.15	0.00383	YES	YES
8	a	14.17	0.00992	YES	YES
9	a	19.24	0.00249	YES	YES
10	a	20.17	0.03172	YES	YES
11	a	21.46	0.01850	YES	YES
12	a	22.94	0.00298	YES	YES
13	a	24.89	0.06137	YES	YES
14	a	30.82	0.01375	YES	YES
15	a	31.98	0.06075	YES	YES
16	a	50.14	0.13168	YES	YES
17	a	58.64	0.02585	YES	YES
18	a	68.88	0.04929	YES	YES
19	a	86.14	0.02455	YES	YES
20	a	92.15	0.02716	YES	YES
21	a	93.40	0.02916	YES	YES
22	a	95.87	0.03823	YES	YES
23	a	116.00	0.00014	YES	YES
24	a	122.61	0.00986	YES	YES
25	a	123.01	0.00920	YES	YES
26	a	123.39	0.01974	YES	YES
27	a	126.86	0.03402	YES	YES
28	a	131.33	0.10600	YES	YES

29	a	134.06	0.00084	YES	YES
30	a	135.19	0.00791	YES	YES
31	a	141.06	0.00004	YES	YES
32	a	145.26	0.00582	YES	YES
33	a	146.56	0.17771	YES	YES
34	a	152.38	0.24138	YES	YES
35	a	156.76	0.26951	YES	YES
36	a	191.90	0.13786	YES	YES
37	a	191.96	0.07325	YES	YES
38	a	192.70	0.04780	YES	YES
39	a	193.07	0.02461	YES	YES
40	a	198.43	1.20601	YES	YES
41	a	209.00	1.36486	YES	YES
42	a	212.32	1.70607	YES	YES
43	a	219.92	0.08074	YES	YES
44	a	222.21	0.30369	YES	YES
45	a	253.79	0.35426	YES	YES
46	a	257.94	1.01043	YES	YES
47	a	269.31	0.23125	YES	YES
48	a	276.16	0.00771	YES	YES
49	a	277.45	0.09056	YES	YES
50	a	278.20	0.16330	YES	YES
51	a	281.18	0.16125	YES	YES
52	a	303.85	0.09171	YES	YES
53	a	304.34	0.39521	YES	YES
54	a	304.88	0.08713	YES	YES
55	a	308.62	0.45831	YES	YES
56	a	320.50	0.33483	YES	YES
57	a	321.05	1.42578	YES	YES
58	a	322.53	0.15047	YES	YES
59	a	324.90	0.08077	YES	YES
60	a	340.18	4.14889	YES	YES
61	a	351.87	0.15314	YES	YES
62	a	370.11	0.09410	YES	YES
63	a	375.81	1.71483	YES	YES
64	a	395.23	0.23495	YES	YES
65	a	396.05	0.88281	YES	YES
66	a	397.32	0.46635	YES	YES
67	a	398.54	0.07892	YES	YES
68	a	420.96	11.40230	YES	YES
69	a	424.09	0.29436	YES	YES
70	a	431.12	3.96631	YES	YES
71	a	431.72	0.27542	YES	YES
72	a	432.21	0.30173	YES	YES
73	a	432.33	0.20864	YES	YES
74	a	441.70	41.23489	YES	YES
75	a	445.45	2.91929	YES	YES
76	a	454.02	0.20987	YES	YES
77	a	460.22	51.32908	YES	YES
78	a	464.61	14.05131	YES	YES
79	a	500.34	0.09852	YES	YES
80	a	501.28	2.27725	YES	YES
81	a	502.25	0.65104	YES	YES
82	a	502.52	1.84465	YES	YES
83	a	506.08	0.65703	YES	YES
84	a	544.94	100.96198	YES	YES
85	a	568.07	0.60644	YES	YES

86	a	571.97	12.65675	YES	YES
87	a	574.40	0.02594	YES	YES
88	a	580.79	37.37066	YES	YES
89	a	610.38	152.22479	YES	YES
90	a	622.90	9.60681	YES	YES
91	a	631.48	1.37251	YES	YES
92	a	636.50	62.64574	YES	YES
93	a	637.80	33.10448	YES	YES
94	a	639.70	6.61739	YES	YES
95	a	642.43	4.02318	YES	YES
96	a	644.32	1.38626	YES	YES
97	a	656.87	0.31537	YES	YES
98	a	675.88	1.81262	YES	YES
99	a	691.56	39.56520	YES	YES
100	a	702.16	178.06383	YES	YES
101	a	706.17	4.98386	YES	YES
102	a	718.37	4.56013	YES	YES
103	a	727.45	5.76217	YES	YES
104	a	742.79	58.07035	YES	YES
105	a	748.01	19.14910	YES	YES
106	a	757.16	18.67402	YES	YES
107	a	769.39	3.24200	YES	YES
108	a	778.54	27.49382	YES	YES
109	a	819.34	47.24291	YES	YES
110	a	854.71	2.42563	YES	YES
111	a	857.30	67.31779	YES	YES
112	a	870.43	7.37048	YES	YES
113	a	875.64	7.64301	YES	YES
114	a	876.05	2.29245	YES	YES
115	a	935.02	5.38947	YES	YES
116	a	958.39	100.43508	YES	YES
117	a	961.77	46.07965	YES	YES
118	a	964.33	171.23442	YES	YES
119	a	965.37	121.44902	YES	YES
120	a	966.78	3.77276	YES	YES
121	a	970.99	160.72870	YES	YES
122	a	977.48	22.88226	YES	YES
123	a	1006.56	104.44507	YES	YES
124	a	1009.77	71.46830	YES	YES
125	a	1040.82	3.38833	YES	YES
126	a	1075.90	23.39611	YES	YES
127	a	1132.19	0.09374	YES	YES
128	a	1133.18	1.26880	YES	YES
129	a	1138.74	1.16993	YES	YES
130	a	1140.03	0.01502	YES	YES
131	a	1140.45	6.50992	YES	YES
132	a	1159.31	15.05339	YES	YES
133	a	1192.90	29.77444	YES	YES
134	a	1239.90	124.25384	YES	YES
135	a	1242.23	5.28026	YES	YES
136	a	1249.42	135.21702	YES	YES
137	a	1251.98	53.10113	YES	YES
138	a	1255.14	31.49171	YES	YES
139	a	1333.31	0.33598	YES	YES
140	a	1343.97	1.61829	YES	YES
141	a	1344.35	0.62558	YES	YES
142	a	1348.06	3.22982	YES	YES

143	a	1349.07	0.22053	YES	YES
144	a	1374.82	18.57388	YES	YES
145	a	1376.34	1.04775	YES	YES
146	a	1384.07	35.41614	YES	YES
147	a	1385.09	11.73258	YES	YES
148	a	1427.47	21.18562	YES	YES
149	a	1446.28	15.80655	YES	YES
150	a	1447.26	232.25097	YES	YES
151	a	1447.71	25.10366	YES	YES
152	a	1447.97	30.16133	YES	YES
153	a	1450.93	0.61096	YES	YES
154	a	1458.93	9.51753	YES	YES
155	a	1460.69	518.72449	YES	YES
156	a	1464.46	280.24369	YES	YES
157	a	1469.26	809.44263	YES	YES
158	a	1568.05	0.26799	YES	YES
159	a	1592.70	9.88197	YES	YES
160	a	1593.14	4.51172	YES	YES
161	a	1594.43	3.49713	YES	YES
162	a	1595.52	8.53565	YES	YES
163	a	1603.68	1.57403	YES	YES
164	a	1609.72	32.31737	YES	YES
165	a	1610.08	16.07330	YES	YES
166	a	1611.42	5.19349	YES	YES
167	a	1612.05	24.12543	YES	YES
168	a	3065.08	4.36448	YES	YES
169	a	3082.74	48.07945	YES	YES
170	a	3100.96	29.74001	YES	YES
171	a	3110.20	19.10729	YES	YES

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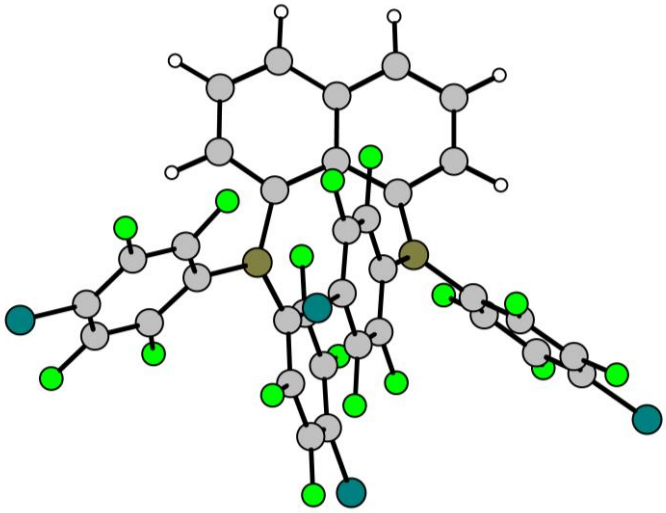

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          1.20636236   -2.87479875    0.42480561    b
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-3.78409021	-3.95121974	2.61600219	f
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0.65550879	-2.44003688	-5.09022534	f
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-8.66336424	-4.52280619	-5.57284328	cl
3.84284104	-5.25564474	3.77693621	h
3.86847137	-5.15793889	8.45986788	h
1.31662164	-1.86521695	10.74495501	h
-1.35565864	1.71718273	10.76252529	h
-3.90046483	5.03735033	8.50957289	h
-3.85647429	5.19484317	3.82904894	h

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.98	0.06717	YES	YES
8	a	9.84	0.07701	YES	YES
9	a	13.33	0.08876	YES	YES
10	a	23.81	0.19513	YES	YES
11	a	25.01	0.12908	YES	YES
12	a	27.85	0.14098	YES	YES
13	a	29.97	0.00046	YES	YES
14	a	35.43	0.04992	YES	YES
15	a	43.47	0.00281	YES	YES
16	a	48.00	0.46365	YES	YES
17	a	55.17	0.09464	YES	YES
18	a	55.72	0.01509	YES	YES
19	a	71.83	0.03636	YES	YES
20	a	77.01	0.21858	YES	YES
21	a	93.50	0.47444	YES	YES
22	a	98.94	0.01216	YES	YES
23	a	101.91	0.15693	YES	YES
24	a	108.01	0.16359	YES	YES
25	a	122.91	0.08172	YES	YES

26	a	126.72	0.39585	YES	YES
27	a	128.16	0.26020	YES	YES
28	a	128.85	0.13817	YES	YES
29	a	131.84	0.00478	YES	YES
30	a	132.43	0.01681	YES	YES
31	a	137.42	0.00320	YES	YES
32	a	138.59	0.07516	YES	YES
33	a	143.64	0.00405	YES	YES
34	a	150.83	0.08968	YES	YES
35	a	156.50	1.00379	YES	YES
36	a	177.49	0.01660	YES	YES
37	a	189.47	0.08237	YES	YES
38	a	190.05	0.53988	YES	YES
39	a	195.00	0.07441	YES	YES
40	a	195.19	0.03542	YES	YES
41	a	197.11	0.04993	YES	YES
42	a	197.25	0.11386	YES	YES
43	a	222.06	0.18891	YES	YES
44	a	224.76	0.08250	YES	YES
45	a	226.03	5.47651	YES	YES
46	a	229.90	2.37235	YES	YES
47	a	241.91	3.57247	YES	YES
48	a	254.34	2.22060	YES	YES
49	a	276.68	0.00653	YES	YES
50	a	278.11	0.05711	YES	YES
51	a	280.10	0.10651	YES	YES
52	a	280.15	0.03304	YES	YES
53	a	302.69	0.12597	YES	YES
54	a	303.42	0.04412	YES	YES
55	a	305.56	0.08981	YES	YES
56	a	305.83	0.14340	YES	YES
57	a	321.79	0.39517	YES	YES
58	a	322.26	0.22370	YES	YES
59	a	323.23	0.31025	YES	YES
60	a	323.90	0.02072	YES	YES
61	a	335.77	0.43484	YES	YES
62	a	346.03	5.36226	YES	YES
63	a	366.01	0.45776	YES	YES
64	a	374.11	4.25890	YES	YES
65	a	398.37	0.24465	YES	YES
66	a	398.54	1.33166	YES	YES
67	a	404.44	0.43808	YES	YES
68	a	404.62	2.78285	YES	YES
69	a	409.84	0.22848	YES	YES
70	a	415.68	0.17548	YES	YES
71	a	426.25	8.79197	YES	YES
72	a	430.11	1.75224	YES	YES
73	a	430.36	0.95029	YES	YES
74	a	432.72	0.02255	YES	YES
75	a	433.99	6.50079	YES	YES
76	a	450.65	2.89900	YES	YES
77	a	462.27	2.06403	YES	YES
78	a	464.42	0.73982	YES	YES
79	a	470.22	1.65047	YES	YES
80	a	502.07	4.03605	YES	YES
81	a	503.40	0.41858	YES	YES
82	a	504.17	1.31793	YES	YES

83	a	504.24	0.33332	YES	YES
84	a	505.25	4.77442	YES	YES
85	a	514.31	0.27953	YES	YES
86	a	519.47	8.43347	YES	YES
87	a	544.59	0.12823	YES	YES
88	a	565.58	16.85273	YES	YES
89	a	575.54	7.65526	YES	YES
90	a	579.02	0.36947	YES	YES
91	a	592.26	1.07654	YES	YES
92	a	593.28	3.04623	YES	YES
93	a	601.28	23.67132	YES	YES
94	a	628.97	8.52314	YES	YES
95	a	634.70	7.61437	YES	YES
96	a	639.56	1.85278	YES	YES
97	a	640.97	0.06323	YES	YES
98	a	642.37	2.08273	YES	YES
99	a	643.01	0.19840	YES	YES
100	a	649.76	19.04930	YES	YES
101	a	656.80	42.87087	YES	YES
102	a	661.37	2.05033	YES	YES
103	a	675.80	6.95210	YES	YES
104	a	696.00	74.55103	YES	YES
105	a	709.12	6.90535	YES	YES
106	a	733.78	2.49785	YES	YES
107	a	745.58	0.38735	YES	YES
108	a	746.88	17.27350	YES	YES
109	a	758.12	33.17639	YES	YES
110	a	763.11	0.00662	YES	YES
111	a	779.09	18.35166	YES	YES
112	a	782.67	0.00224	YES	YES
113	a	785.99	57.35848	YES	YES
114	a	825.00	16.97418	YES	YES
115	a	847.58	6.65555	YES	YES
116	a	867.26	11.85474	YES	YES
117	a	876.64	4.32848	YES	YES
118	a	880.70	117.51715	YES	YES
119	a	913.29	0.00233	YES	YES
120	a	931.12	3.81835	YES	YES
121	a	941.76	1.23803	YES	YES
122	a	967.34	75.10439	YES	YES
123	a	968.03	1.02903	YES	YES
124	a	970.20	197.45129	YES	YES
125	a	972.76	2.90539	YES	YES
126	a	975.37	15.06481	YES	YES
127	a	976.61	173.75522	YES	YES
128	a	980.03	7.23603	YES	YES
129	a	1046.43	11.65199	YES	YES
130	a	1061.25	42.35348	YES	YES
131	a	1070.24	0.76401	YES	YES
132	a	1080.29	222.64846	YES	YES
133	a	1106.97	0.35514	YES	YES
134	a	1124.95	5.50557	YES	YES
135	a	1148.55	1.23979	YES	YES
136	a	1149.36	1.60967	YES	YES
137	a	1152.18	2.44547	YES	YES
138	a	1153.57	28.03161	YES	YES
139	a	1157.36	8.62245	YES	YES

140	a	1163.40	2.81262	YES	YES
141	a	1208.67	6.70790	YES	YES
142	a	1233.79	2.21302	YES	YES
143	a	1239.38	65.30711	YES	YES
144	a	1272.12	110.13225	YES	YES
145	a	1272.31	131.07585	YES	YES
146	a	1283.58	235.20344	YES	YES
147	a	1284.56	52.17814	YES	YES
148	a	1338.77	0.68057	YES	YES
149	a	1339.22	0.93549	YES	YES
150	a	1341.83	3.30693	YES	YES
151	a	1342.51	4.76644	YES	YES
152	a	1345.39	48.83127	YES	YES
153	a	1351.28	0.42307	YES	YES
154	a	1368.07	0.44664	YES	YES
155	a	1371.09	232.52317	YES	YES
156	a	1372.41	5.87724	YES	YES
157	a	1377.62	84.68234	YES	YES
158	a	1387.70	98.24761	YES	YES
159	a	1409.88	16.08797	YES	YES
160	a	1445.28	86.79820	YES	YES
161	a	1446.95	92.72332	YES	YES
162	a	1447.04	70.46621	YES	YES
163	a	1449.66	199.98893	YES	YES
164	a	1450.95	72.91893	YES	YES
165	a	1458.95	2.91258	YES	YES
166	a	1463.67	147.42780	YES	YES
167	a	1465.79	777.77650	YES	YES
168	a	1475.08	741.70433	YES	YES
169	a	1510.95	33.74957	YES	YES
170	a	1557.76	70.74487	YES	YES
171	a	1582.82	20.08835	YES	YES
172	a	1582.93	15.36759	YES	YES
173	a	1585.43	22.68104	YES	YES
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175	a	1599.40	36.24642	YES	YES
176	a	1603.29	9.89638	YES	YES
177	a	1613.98	111.38222	YES	YES
178	a	1614.50	77.59587	YES	YES
179	a	1618.62	41.49539	YES	YES
180	a	1618.72	140.85437	YES	YES
181	a	3089.73	0.12467	YES	YES
182	a	3091.50	3.49473	YES	YES
183	a	3101.10	7.08916	YES	YES
184	a	3101.53	13.84569	YES	YES
185	a	3116.80	23.29412	YES	YES
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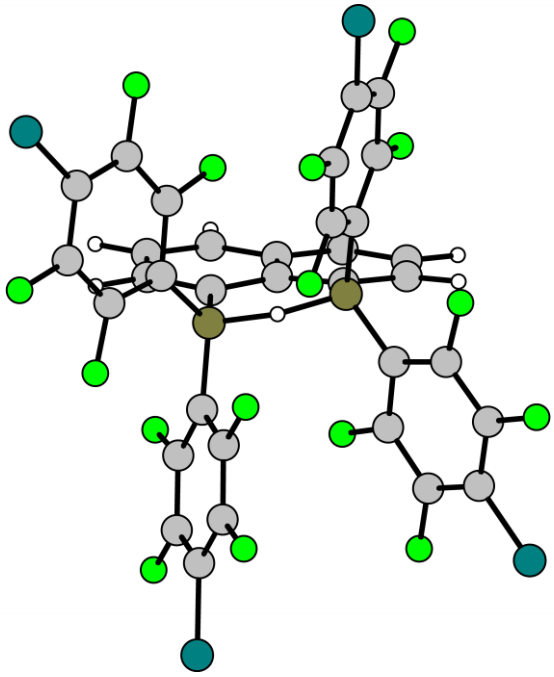

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5.16871274	1.57902033	-1.19097657	f
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$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.17	0.01116	YES	YES
8	a	12.12	0.06211	YES	YES
9	a	19.89	0.00610	YES	YES
10	a	20.87	0.00425	YES	YES
11	a	22.16	0.00427	YES	YES
12	a	25.61	0.01206	YES	YES
13	a	28.09	0.02968	YES	YES
14	a	35.57	0.00777	YES	YES
15	a	39.29	0.00297	YES	YES
16	a	49.07	0.04214	YES	YES
17	a	55.25	0.06895	YES	YES
18	a	59.53	0.02559	YES	YES
19	a	84.36	0.00034	YES	YES
20	a	93.09	0.00820	YES	YES

21	a	94.10	0.00611	YES	YES
22	a	98.40	0.00622	YES	YES
23	a	100.26	0.28522	YES	YES
24	a	118.87	0.14836	YES	YES
25	a	119.48	0.00583	YES	YES
26	a	121.60	0.04316	YES	YES
27	a	123.71	0.00200	YES	YES
28	a	129.82	0.03076	YES	YES
29	a	130.58	0.01607	YES	YES
30	a	134.57	0.05667	YES	YES
31	a	142.43	0.04051	YES	YES
32	a	143.38	0.30620	YES	YES
33	a	146.93	0.00174	YES	YES
34	a	148.30	0.06622	YES	YES
35	a	148.99	0.03653	YES	YES
36	a	170.55	1.16218	YES	YES
37	a	185.98	0.70459	YES	YES
38	a	191.85	0.40178	YES	YES
39	a	193.11	0.03354	YES	YES
40	a	193.47	0.10470	YES	YES
41	a	194.09	0.02170	YES	YES
42	a	201.28	1.56747	YES	YES
43	a	214.49	0.60001	YES	YES
44	a	217.51	0.00648	YES	YES
45	a	221.25	0.90833	YES	YES
46	a	221.42	0.89817	YES	YES
47	a	249.58	0.06749	YES	YES
48	a	255.20	0.15287	YES	YES
49	a	278.19	0.04185	YES	YES
50	a	278.57	0.00506	YES	YES
51	a	280.08	0.03242	YES	YES
52	a	280.10	0.02349	YES	YES
53	a	306.71	0.12191	YES	YES
54	a	307.55	0.00093	YES	YES
55	a	308.92	0.28866	YES	YES
56	a	310.60	0.11733	YES	YES
57	a	322.95	1.99828	YES	YES
58	a	324.96	0.04419	YES	YES
59	a	325.27	0.01941	YES	YES
60	a	325.63	0.14842	YES	YES
61	a	345.06	0.97661	YES	YES
62	a	350.41	0.11520	YES	YES
63	a	357.48	4.95481	YES	YES
64	a	361.97	0.19583	YES	YES
65	a	393.33	0.33114	YES	YES
66	a	393.43	0.01004	YES	YES
67	a	395.57	0.04114	YES	YES
68	a	395.86	0.03482	YES	YES
69	a	414.70	0.63728	YES	YES
70	a	420.33	0.00229	YES	YES
71	a	421.82	17.42942	YES	YES
72	a	432.64	0.28838	YES	YES
73	a	433.44	0.38034	YES	YES
74	a	434.27	0.00972	YES	YES
75	a	434.93	0.01551	YES	YES
76	a	449.23	3.27498	YES	YES
77	a	459.30	1.93977	YES	YES

78	a	472.65	0.74697	YES	YES
79	a	482.97	0.19696	YES	YES
80	a	491.38	1.65977	YES	YES
81	a	501.45	2.56979	YES	YES
82	a	501.62	0.60772	YES	YES
83	a	501.78	3.09408	YES	YES
84	a	504.19	0.44282	YES	YES
85	a	512.15	0.38942	YES	YES
86	a	526.72	35.96156	YES	YES
87	a	562.02	1.07189	YES	YES
88	a	562.63	6.66765	YES	YES
89	a	567.59	0.57436	YES	YES
90	a	568.01	30.01227	YES	YES
91	a	579.96	19.22557	YES	YES
92	a	601.00	24.68015	YES	YES
93	a	605.28	2.76213	YES	YES
94	a	623.12	1.27007	YES	YES
95	a	636.29	0.91061	YES	YES
96	a	636.48	0.28812	YES	YES
97	a	637.92	4.79172	YES	YES
98	a	639.11	0.69112	YES	YES
99	a	639.34	0.91882	YES	YES
100	a	643.73	58.89674	YES	YES
101	a	651.74	12.46030	YES	YES
102	a	672.24	3.00067	YES	YES
103	a	684.19	21.02241	YES	YES
104	a	695.60	129.18443	YES	YES
105	a	711.50	0.47013	YES	YES
106	a	726.86	2.26874	YES	YES
107	a	737.62	44.15559	YES	YES
108	a	737.85	0.92533	YES	YES
109	a	749.53	12.42604	YES	YES
110	a	755.26	16.13807	YES	YES
111	a	774.74	1.37581	YES	YES
112	a	780.72	68.09487	YES	YES
113	a	787.14	0.06780	YES	YES
114	a	809.09	10.00186	YES	YES
115	a	832.83	33.18387	YES	YES
116	a	855.38	17.81368	YES	YES
117	a	858.57	0.01187	YES	YES
118	a	861.96	110.49966	YES	YES
119	a	884.78	0.00215	YES	YES
120	a	899.49	3.39284	YES	YES
121	a	925.22	6.01515	YES	YES
122	a	947.64	0.36592	YES	YES
123	a	948.09	67.57593	YES	YES
124	a	953.58	0.56151	YES	YES
125	a	961.03	111.84065	YES	YES
126	a	961.86	15.69775	YES	YES
127	a	967.51	90.26535	YES	YES
128	a	968.12	259.41983	YES	YES
129	a	990.99	13.88242	YES	YES
130	a	1010.44	0.00029	YES	YES
131	a	1018.71	0.11871	YES	YES
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137	a	1137.27	0.00388	YES	YES
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152	a	1340.59	0.65474	YES	YES
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154	a	1348.63	50.71341	YES	YES
155	a	1351.73	1.35141	YES	YES
156	a	1370.08	42.55554	YES	YES
157	a	1374.23	7.12612	YES	YES
158	a	1374.95	78.07778	YES	YES
159	a	1381.66	0.28900	YES	YES
160	a	1383.37	2.01290	YES	YES
161	a	1411.57	0.37887	YES	YES
162	a	1447.82	402.46207	YES	YES
163	a	1449.58	16.86565	YES	YES
164	a	1449.96	119.88255	YES	YES
165	a	1450.73	40.78624	YES	YES
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167	a	1453.26	2.98018	YES	YES
168	a	1456.29	258.17556	YES	YES
169	a	1459.47	268.99431	YES	YES
170	a	1466.62	869.31556	YES	YES
171	a	1506.18	12.87273	YES	YES
172	a	1572.61	1.50114	YES	YES
173	a	1589.07	6.19168	YES	YES
174	a	1589.21	0.70588	YES	YES
175	a	1590.96	1.59296	YES	YES
176	a	1592.60	13.32665	YES	YES
177	a	1596.37	0.11722	YES	YES
178	a	1605.39	7.39846	YES	YES
179	a	1605.45	37.70379	YES	YES
180	a	1608.99	15.07467	YES	YES
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182	a	1610.31	20.17792	YES	YES
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184	a	3060.46	0.10853	YES	YES
185	a	3061.04	1.35433	YES	YES
186	a	3069.72	12.97421	YES	YES
187	a	3070.82	51.61824	YES	YES
188	a	3088.23	75.19788	YES	YES
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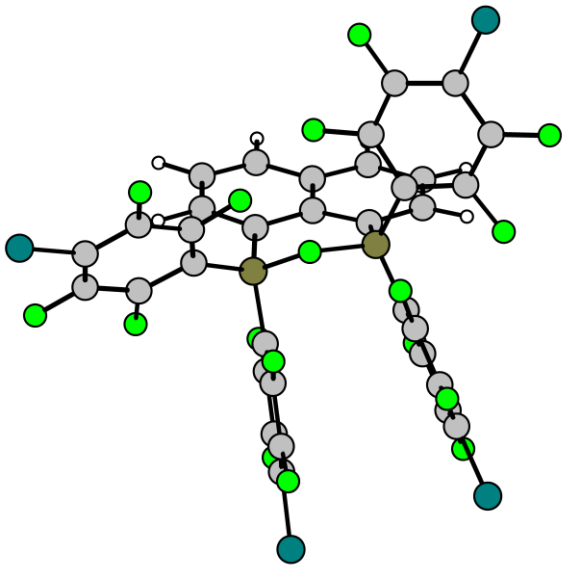

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-10.70845666	-4.90109806	-2.80195890	f
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1.70687328	6.69354685	7.92377958	h
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$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.99	0.00444	YES	YES
8	a	17.24	0.00758	YES	YES
9	a	19.93	0.00628	YES	YES
10	a	21.49	0.01333	YES	YES
11	a	24.11	0.04271	YES	YES
12	a	26.28	0.03068	YES	YES
13	a	32.32	0.00176	YES	YES
14	a	32.83	0.06942	YES	YES
15	a	33.63	0.01103	YES	YES
16	a	46.70	0.06728	YES	YES
17	a	51.16	0.03400	YES	YES
18	a	54.22	0.02413	YES	YES
19	a	84.15	0.00791	YES	YES
20	a	89.40	0.05099	YES	YES

21	a	94.64	0.04097	YES	YES
22	a	96.00	0.06755	YES	YES
23	a	99.82	0.03708	YES	YES
24	a	117.99	0.04512	YES	YES
25	a	122.65	0.02712	YES	YES
26	a	123.98	0.01773	YES	YES
27	a	124.72	0.01038	YES	YES
28	a	126.75	0.11936	YES	YES
29	a	129.74	0.01227	YES	YES
30	a	137.98	0.00222	YES	YES
31	a	140.41	0.01377	YES	YES
32	a	143.01	0.01465	YES	YES
33	a	145.02	0.11969	YES	YES
34	a	148.65	0.03943	YES	YES
35	a	150.35	0.05521	YES	YES
36	a	161.09	0.41296	YES	YES
37	a	176.32	0.95550	YES	YES
38	a	191.63	0.09783	YES	YES
39	a	192.77	0.00294	YES	YES
40	a	193.24	0.03340	YES	YES
41	a	193.45	0.01972	YES	YES
42	a	202.89	1.06765	YES	YES
43	a	213.88	0.50448	YES	YES
44	a	216.54	0.85224	YES	YES
45	a	221.64	1.57735	YES	YES
46	a	224.89	0.03243	YES	YES
47	a	240.67	0.07853	YES	YES
48	a	246.16	1.15845	YES	YES
49	a	274.79	0.92141	YES	YES
50	a	276.68	0.01675	YES	YES
51	a	278.81	0.39151	YES	YES
52	a	279.22	0.01237	YES	YES
53	a	281.01	0.27407	YES	YES
54	a	304.90	0.02131	YES	YES
55	a	305.82	0.14690	YES	YES
56	a	306.18	0.20198	YES	YES
57	a	309.55	0.09278	YES	YES
58	a	322.18	1.76095	YES	YES
59	a	322.92	0.05779	YES	YES
60	a	324.24	1.24654	YES	YES
61	a	325.13	0.34375	YES	YES
62	a	338.60	0.66849	YES	YES
63	a	352.01	0.09148	YES	YES
64	a	359.27	1.96509	YES	YES
65	a	366.42	1.67812	YES	YES
66	a	393.08	1.86971	YES	YES
67	a	394.83	0.51110	YES	YES
68	a	394.96	0.28238	YES	YES
69	a	395.53	1.03796	YES	YES
70	a	397.41	0.13877	YES	YES
71	a	413.55	0.26362	YES	YES
72	a	427.43	1.34749	YES	YES
73	a	431.51	0.40309	YES	YES
74	a	432.14	0.06026	YES	YES
75	a	432.80	0.22066	YES	YES
76	a	432.99	1.15920	YES	YES
77	a	436.48	1.33013	YES	YES

78	a	444.50	11.98627	YES	YES
79	a	459.07	3.01237	YES	YES
80	a	468.72	0.22107	YES	YES
81	a	471.55	16.01118	YES	YES
82	a	484.10	17.82893	YES	YES
83	a	500.65	1.39432	YES	YES
84	a	501.47	1.26246	YES	YES
85	a	502.06	1.09292	YES	YES
86	a	502.26	1.10157	YES	YES
87	a	511.67	0.18580	YES	YES
88	a	532.34	10.84030	YES	YES
89	a	560.17	41.89839	YES	YES
90	a	566.80	69.61352	YES	YES
91	a	568.75	19.95779	YES	YES
92	a	575.51	4.39874	YES	YES
93	a	576.96	20.70865	YES	YES
94	a	583.45	26.51358	YES	YES
95	a	609.63	98.25296	YES	YES
96	a	623.51	52.92834	YES	YES
97	a	631.08	13.70421	YES	YES
98	a	636.27	0.87456	YES	YES
99	a	638.80	0.96359	YES	YES
100	a	640.31	6.41558	YES	YES
101	a	643.57	0.74552	YES	YES
102	a	645.50	9.94728	YES	YES
103	a	657.12	1.23653	YES	YES
104	a	672.72	56.76957	YES	YES
105	a	683.76	53.47344	YES	YES
106	a	702.94	54.76648	YES	YES
107	a	704.70	45.04128	YES	YES
108	a	719.98	72.29691	YES	YES
109	a	727.27	12.07159	YES	YES
110	a	738.78	29.02222	YES	YES
111	a	747.16	20.76241	YES	YES
112	a	750.15	15.69696	YES	YES
113	a	776.32	43.65442	YES	YES
114	a	778.87	28.26581	YES	YES
115	a	784.24	1.55395	YES	YES
116	a	804.21	4.01213	YES	YES
117	a	821.77	27.19274	YES	YES
118	a	838.00	25.05621	YES	YES
119	a	853.20	16.89851	YES	YES
120	a	857.52	3.59582	YES	YES
121	a	869.17	43.40278	YES	YES
122	a	878.94	1.95600	YES	YES
123	a	897.19	1.03004	YES	YES
124	a	929.82	9.50448	YES	YES
125	a	947.44	0.30361	YES	YES
126	a	951.45	92.13292	YES	YES
127	a	954.86	2.51312	YES	YES
128	a	960.38	59.84603	YES	YES
129	a	965.98	57.79130	YES	YES
130	a	968.33	205.02371	YES	YES
131	a	969.36	150.29378	YES	YES
132	a	999.27	61.96601	YES	YES
133	a	1011.96	81.94026	YES	YES
134	a	1032.13	87.96969	YES	YES

135	a	1036.11	3.77370	YES	YES
136	a	1079.79	8.74960	YES	YES
137	a	1096.06	2.37981	YES	YES
138	a	1134.76	1.23618	YES	YES
139	a	1136.20	1.05712	YES	YES
140	a	1139.13	0.63702	YES	YES
141	a	1140.52	7.22427	YES	YES
142	a	1142.06	0.12145	YES	YES
143	a	1144.57	10.68183	YES	YES
144	a	1205.19	0.42576	YES	YES
145	a	1224.04	2.51722	YES	YES
146	a	1229.65	14.67197	YES	YES
147	a	1243.00	89.32597	YES	YES
148	a	1246.87	68.76673	YES	YES
149	a	1247.54	18.95778	YES	YES
150	a	1253.59	166.04093	YES	YES
151	a	1340.19	0.49040	YES	YES
152	a	1342.59	2.12678	YES	YES
153	a	1345.68	0.89985	YES	YES
154	a	1346.41	1.41128	YES	YES
155	a	1347.83	10.97729	YES	YES
156	a	1352.00	14.78702	YES	YES
157	a	1372.76	3.45945	YES	YES
158	a	1376.37	1.85261	YES	YES
159	a	1378.91	14.41605	YES	YES
160	a	1380.40	12.55398	YES	YES
161	a	1383.63	21.40334	YES	YES
162	a	1413.26	4.21100	YES	YES
163	a	1445.72	25.10334	YES	YES
164	a	1447.71	168.07568	YES	YES
165	a	1449.30	16.90302	YES	YES
166	a	1450.33	91.55143	YES	YES
167	a	1451.41	23.61457	YES	YES
168	a	1455.83	282.56240	YES	YES
169	a	1460.00	133.82365	YES	YES
170	a	1464.91	226.10463	YES	YES
171	a	1468.19	933.52946	YES	YES
172	a	1509.40	5.06629	YES	YES
173	a	1575.21	0.85576	YES	YES
174	a	1590.80	7.69361	YES	YES
175	a	1592.43	4.14121	YES	YES
176	a	1593.35	15.06368	YES	YES
177	a	1593.93	1.74288	YES	YES
178	a	1599.29	1.38640	YES	YES
179	a	1609.42	14.38387	YES	YES
180	a	1610.22	40.14921	YES	YES
181	a	1610.87	11.85343	YES	YES
182	a	1611.62	12.16577	YES	YES
183	a	1612.43	10.06692	YES	YES
184	a	3062.07	1.02423	YES	YES
185	a	3064.50	3.57568	YES	YES
186	a	3070.91	29.51671	YES	YES
187	a	3084.21	50.89254	YES	YES
188	a	3090.80	63.43997	YES	YES
189	a	3102.99	31.14814	YES	YES

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Selected distances and angles of the calculated ions $[7\text{-H}]^-$, $[7\text{-F}]^-$, $[8\text{-H}]^-$, $[8\text{-F}]^-$, $[9\text{-H}]^-$ and $[9\text{-F}]^-$

Table S9. Selected distances [Å] and angles [°] derived from the above described quantum-chemical calculations. X = H or F.

	$[7\text{-H}]^-$	$[7\text{-F}]^-$	$[8\text{-H}]^-$	$[8\text{-F}]^-$	$[9\text{-H}]^-$	$[9\text{-F}]^-$
$r_{B\text{-}X}$	1.238	1.425	1.414/1.400	1.608/1.607	1.388/1.389	1.595/1.592
$r_{B\cdots B}$	-	-	2.458	2.709	2.636	2.794
$r_{C(ipso)\cdots C(ipso)}$	-	-	1.417	1.423	2.503	2.528
$r_{C(para)\cdots C(para)}$	-	-	1.408	1.407	2.492	2.478
$<_{B,X,B}$	-	-	121.7	114.9	143.3	122.5