Supporting Information for:

An Intermolecular FLP System derived from an NHC-coordinated Trisilacyclopropylidene

Benedikt J. Guddorf,[a] Alexander Hepp,[a] Constantin Daniliuc,[b] Douglas W. Stephan,*[c] and Felicitas Lips*[a]

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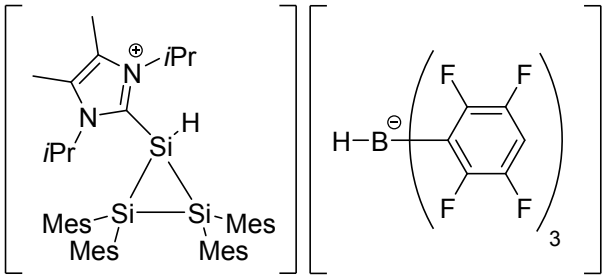
1. Characterization of compounds 1-4

Compound **1**



FT-IR ($\tilde{\nu}$/cm^{-1}, KBr-pellet, intensitiy in brackets): 3092 (vw), 3019 (m), 2980 (s), 2951 (s), 2920 (s), 2857 (m), 2729 (vw), 2511 (vw), 2372 (m), 2344 (w), 2143 (m), 1798 (vw), 1659 (vw), 1622 (m), 1601 (s), 1560 (w), 1545 (m), 1470 (vs), 1458 (vs), 1423 (vs), 1396 (s), 1377 (s), 1350 (m), 1317 (w), 1288 (m), 1223 (vs), 1161 (vs), 1115 (w), 1084 (m), 1055 (w), 1026 (m), 947 (m), 918 (vs), 889 (s), 866 (w), 849 (m), 831 (m), 814 (m), 793 (m), 745 (m), 729 (w), 712 (s), 692 (w), 675 (w), 625 (m), 613 (m), 594 (m), 567 (w), 548 (m), 411 (w).

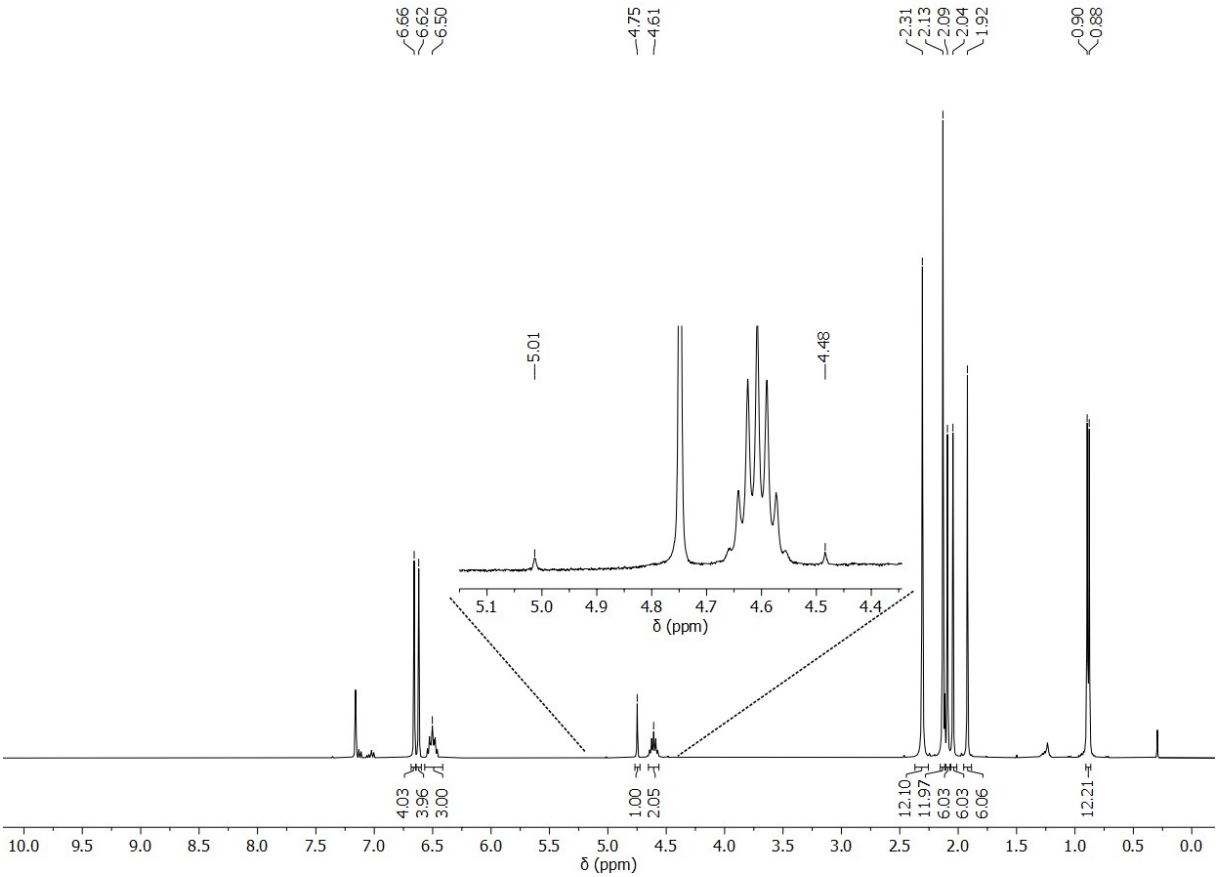


Figure S1. ^{1}H-NMR spectrum of compound **1** in C_6D_6 at 300 K. Zoomed area shows the ^{29}Si satellites of the Si–H signal at δ = 4.75 ppm with a characteristic coupling constant of $^{1}J_{SiH}$ = 212 Hz. (* hexane, ** silicon grease).

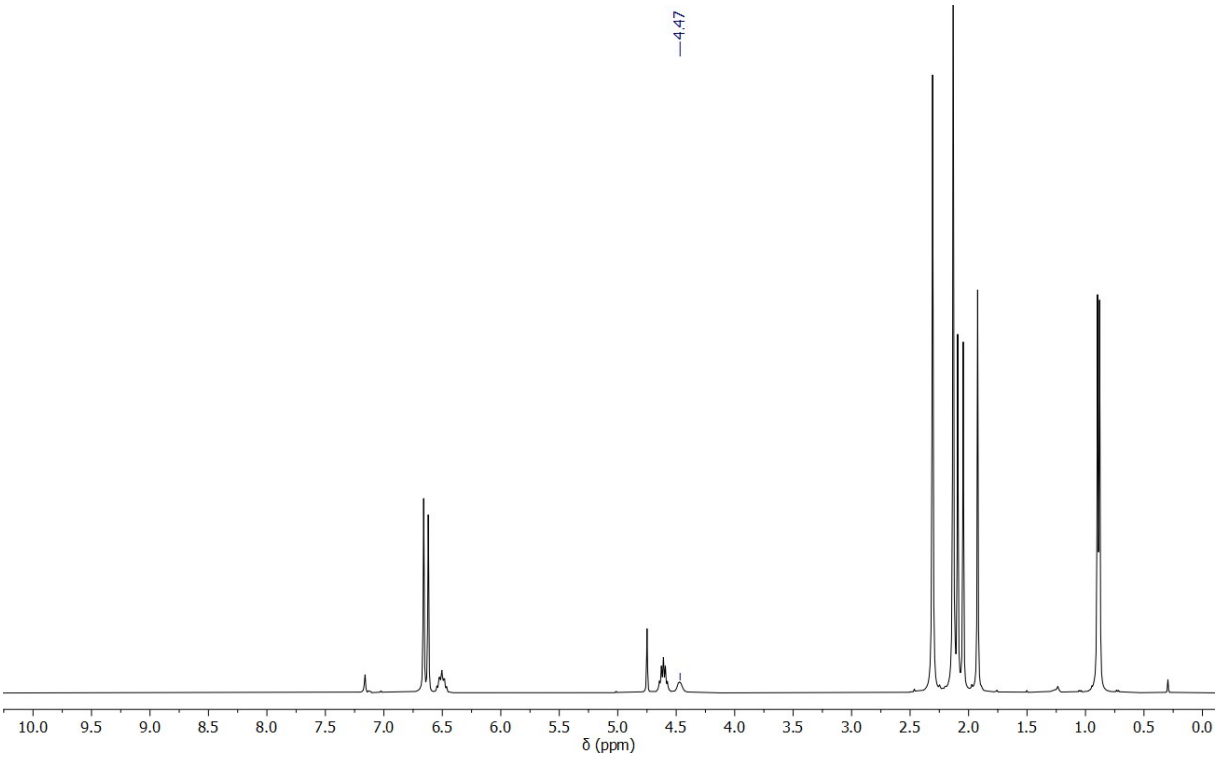


Figure S2. $^{1}H\{^{11}B\}$-NMR spectrum of compound **1** in C_6D_6 at 300 K.

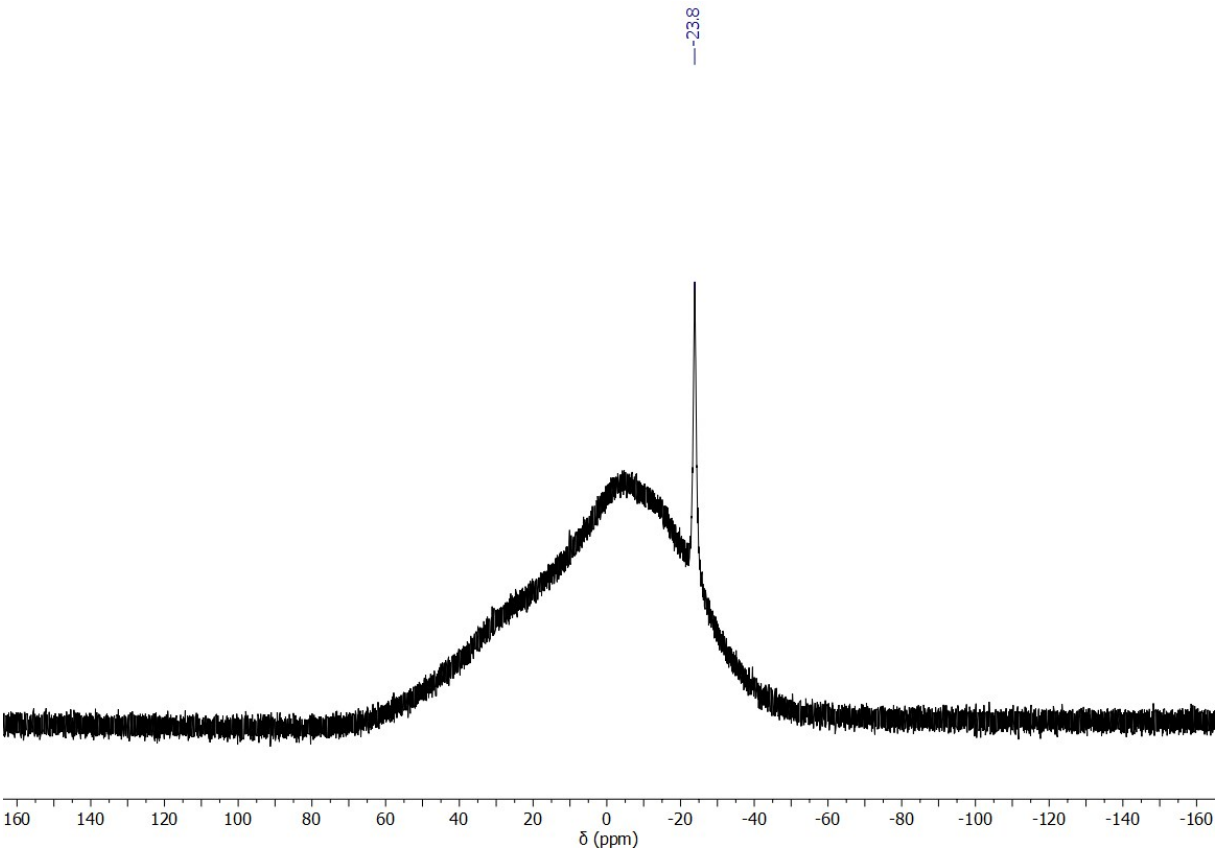


Figure S3. $^{11}B\{^{1}H\}$-NMR spectrum of compound **1** in C_6D_6 at 300 K.

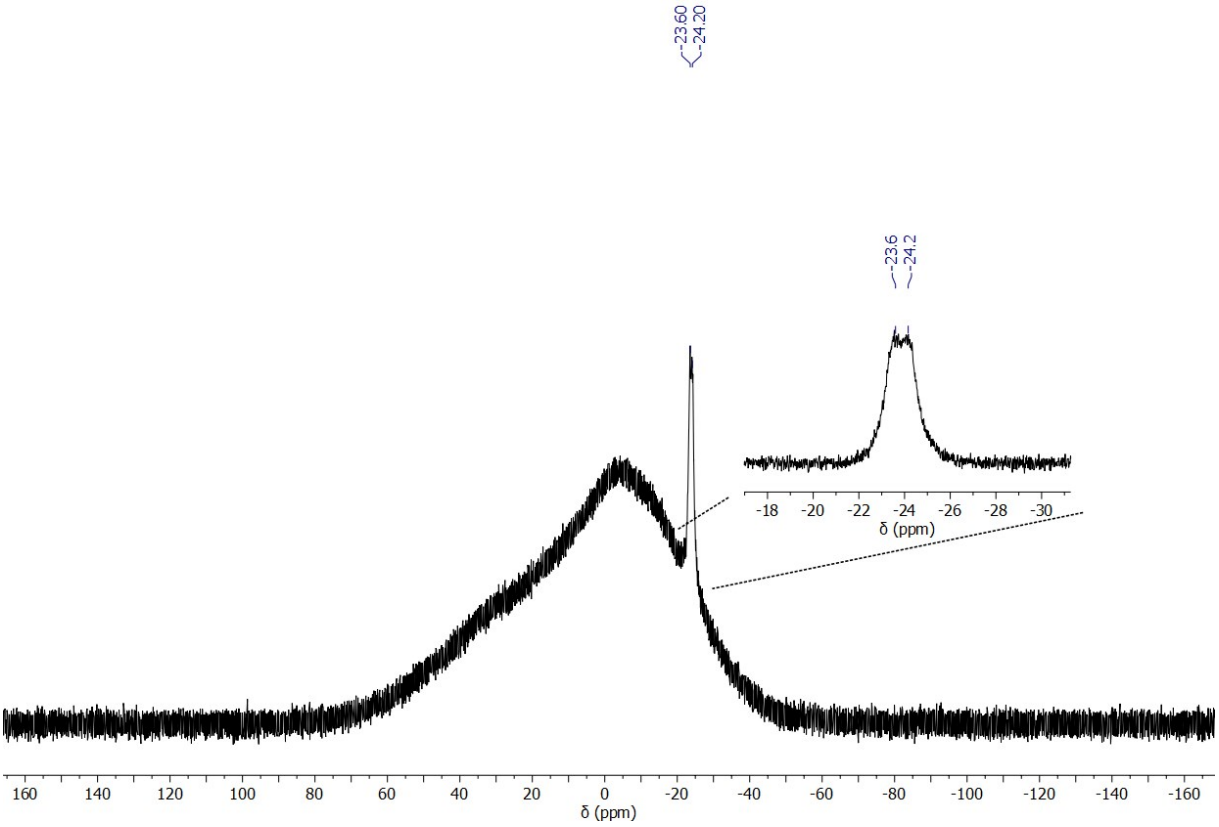


Figure S4. ^{11}B-NMR spectrum of compound **1** in C_6D_6 at 300 K.

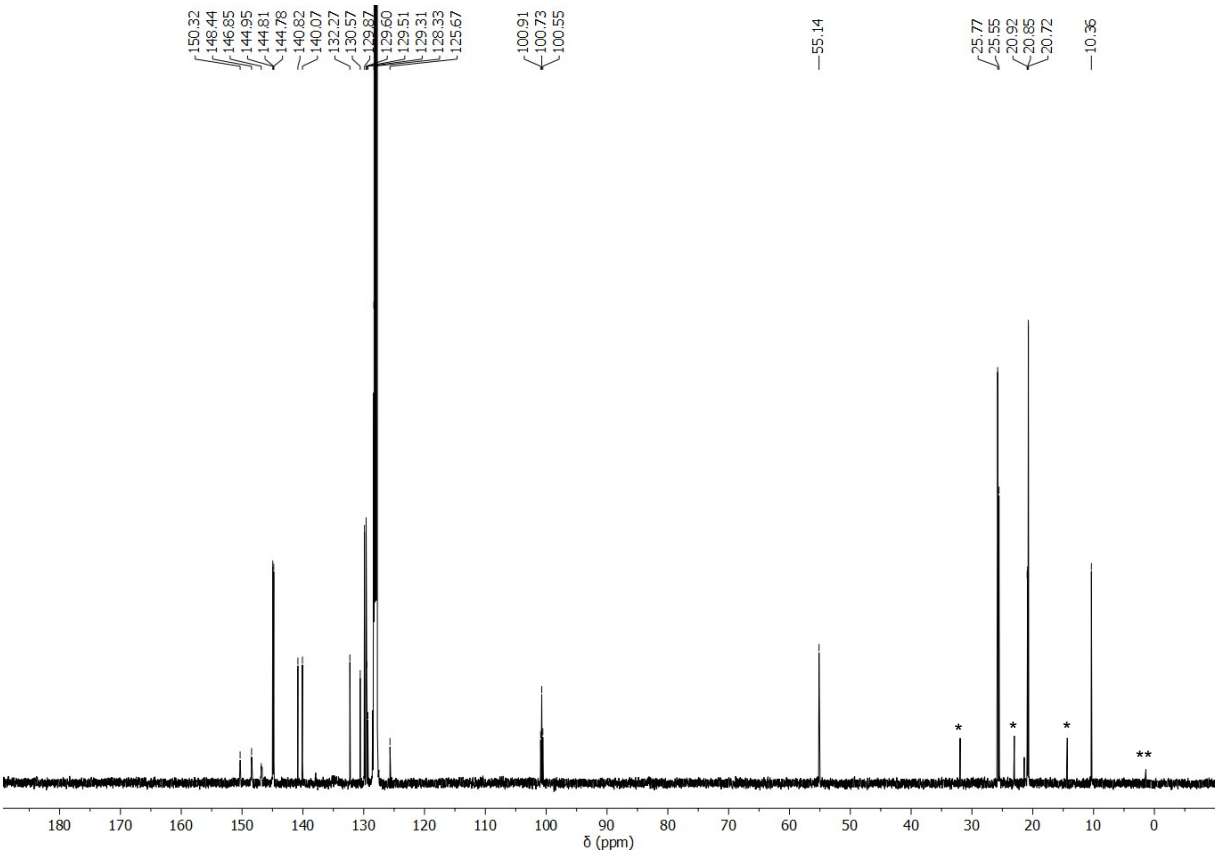


Figure S5. ^{13}C{^{1}H}-NMR spectrum of compound **1** in C_6D_6 at 300 K (* hexane, ** silicon grease).

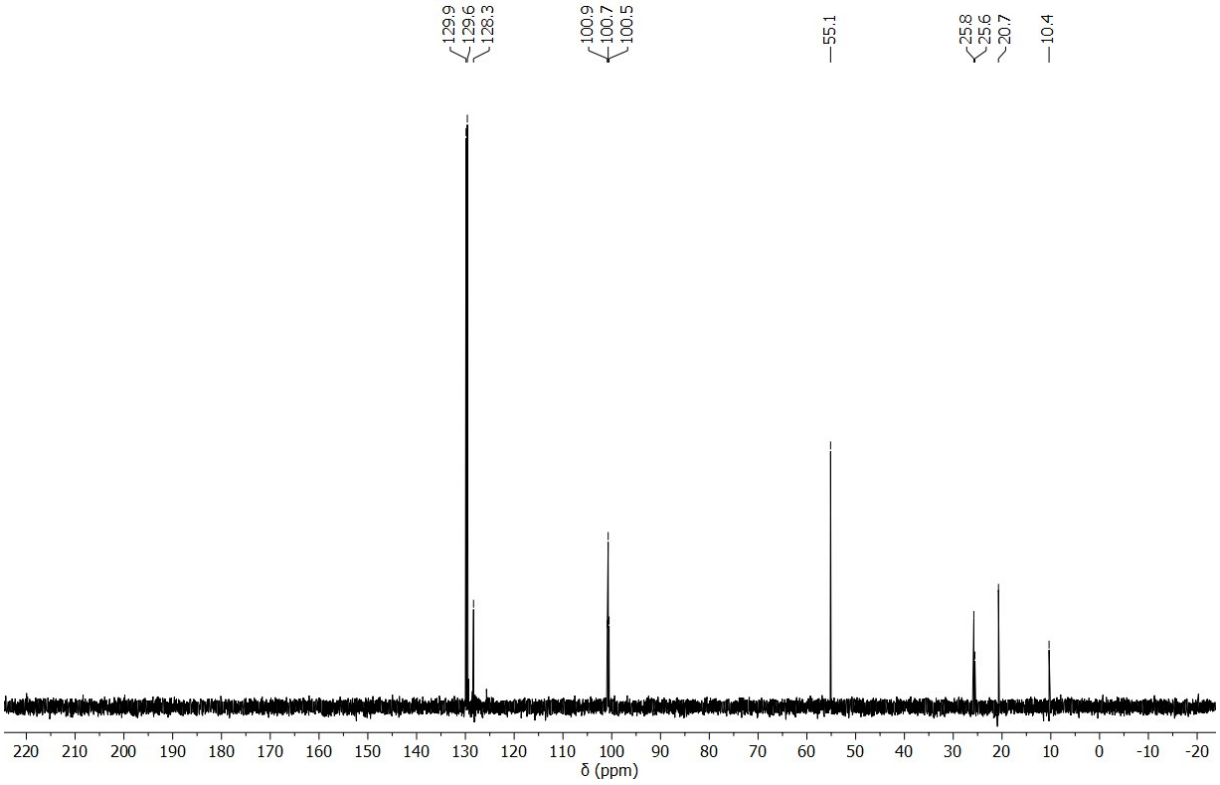


Figure S6. $^{13}C\{^{1}H\}$Dept135-NMR spectrum of compound **1** in C_6D_6 at 300 K.

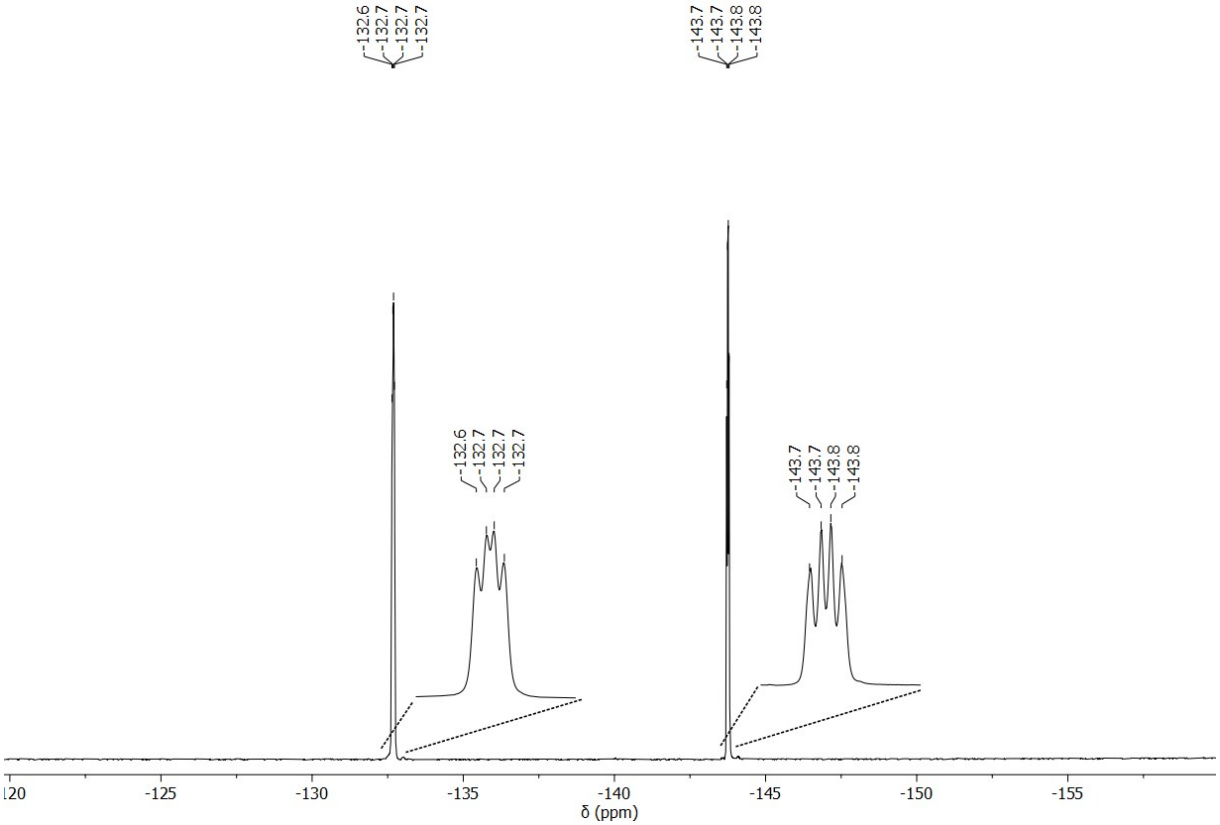


Figure S7. $^{19}F\{^{1}H\}$-NMR spectrum of compound **1** in C_6D_6 at 300 K.

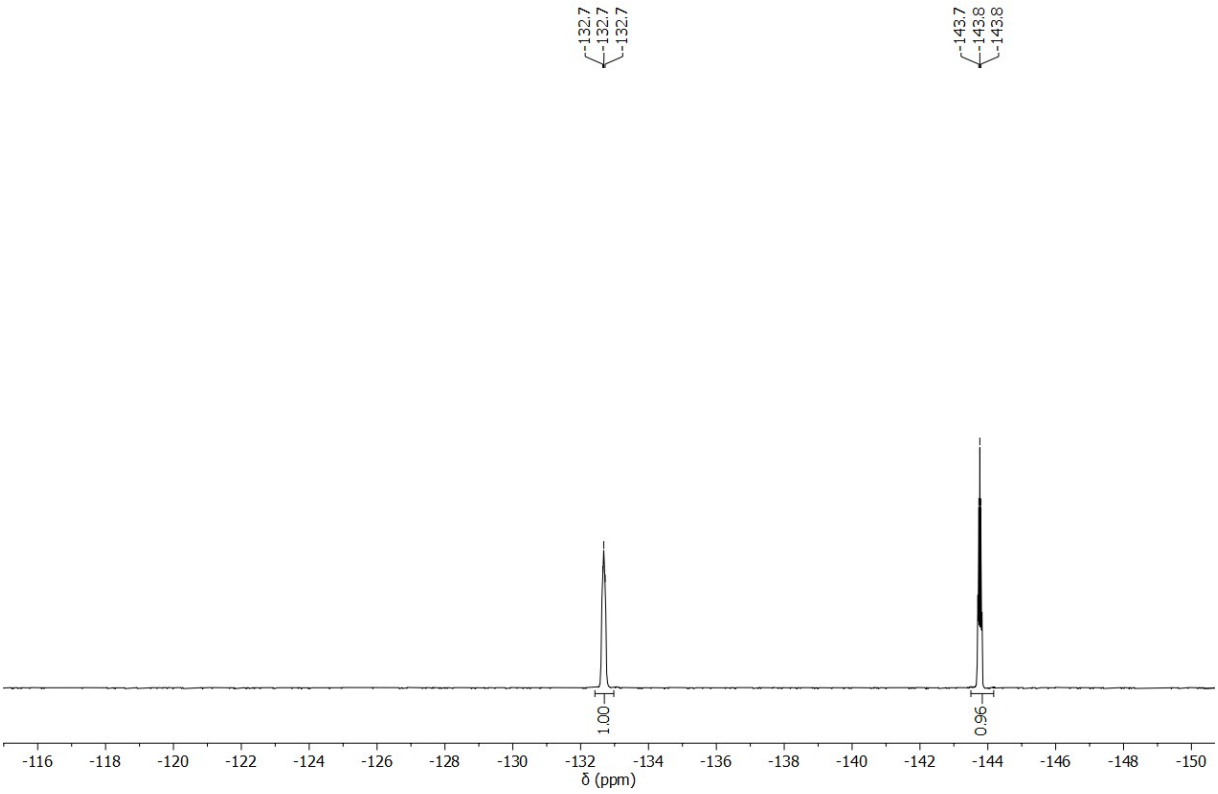


Figure S8. ^{19}F-NMR spectrum of compound **1** in C_6D_6 at 300 K.

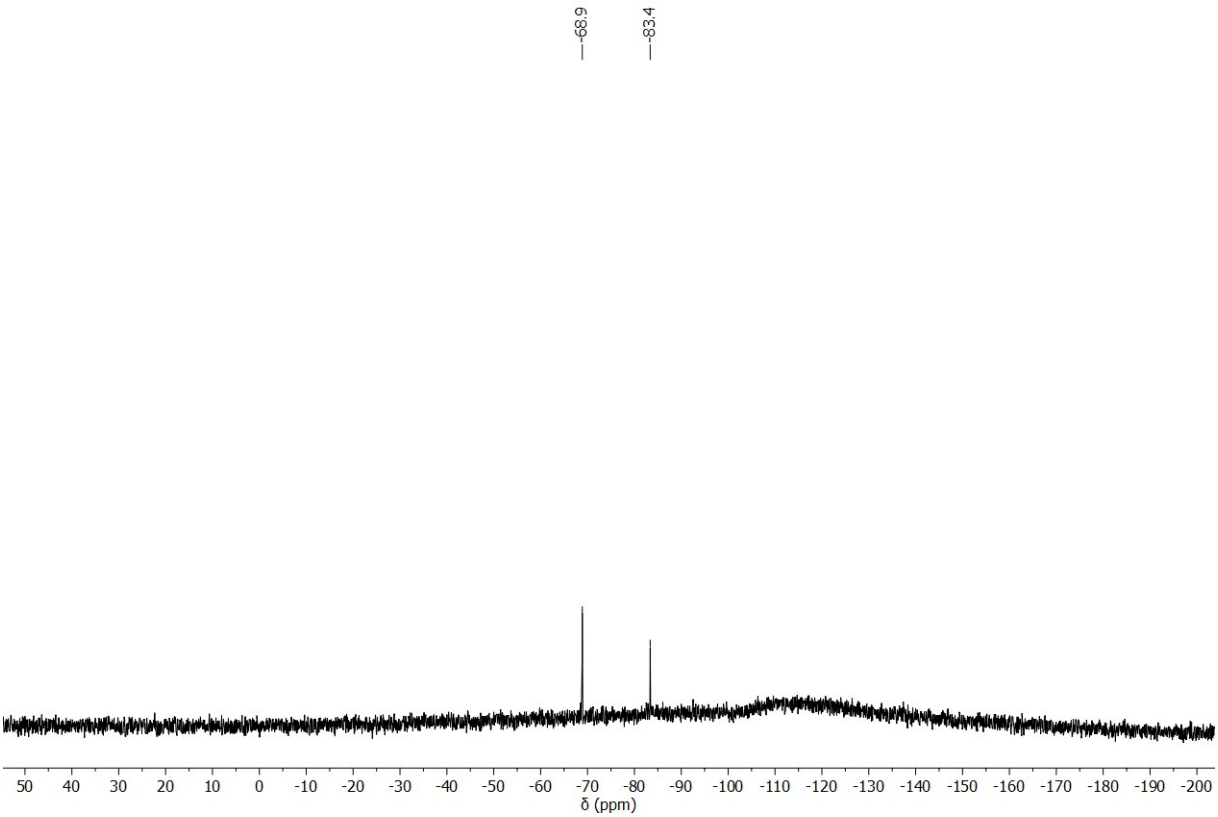


Figure S9. ^{29}Si{^{1}H}IG-NMR spectrum of compound **1** in C_6D_6 at 300 K.

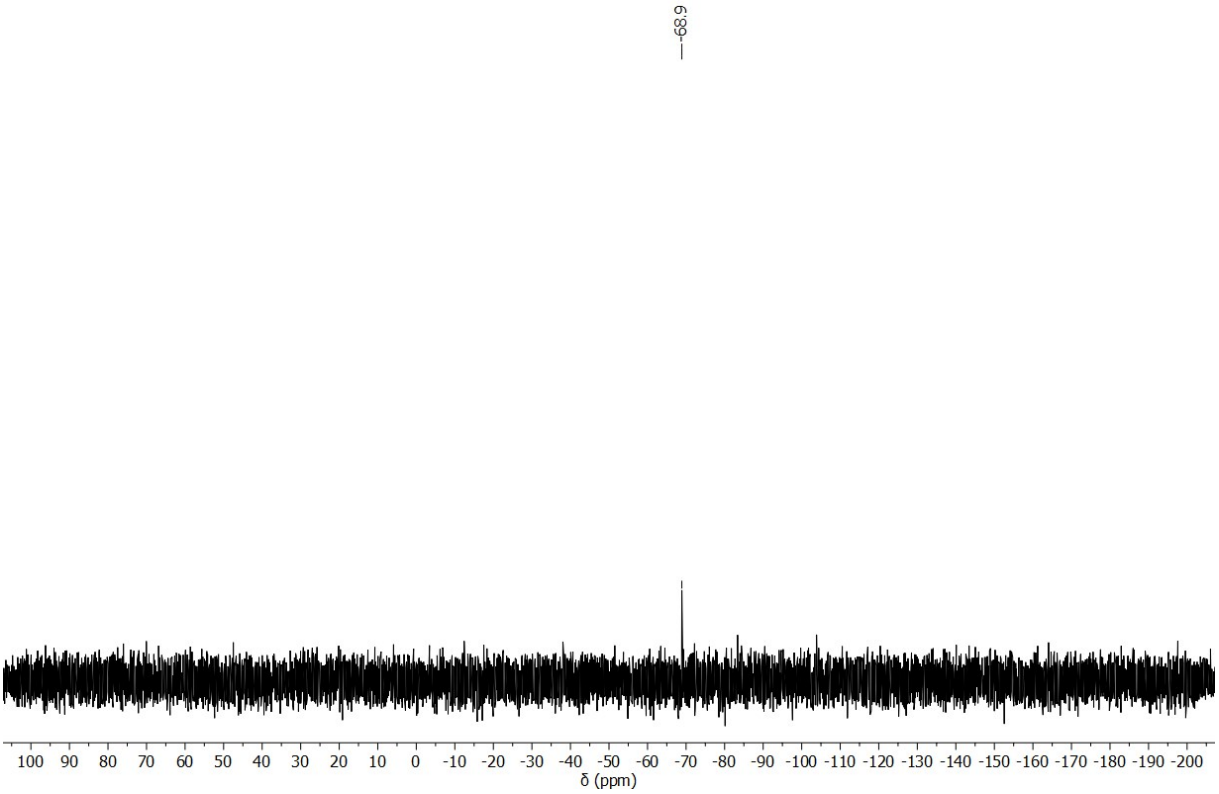


Figure S10. $^{29}Si\{^{1}H\}$Dept19.5-NMR spectrum of compound **1** in C_6D_6 at 300 K.

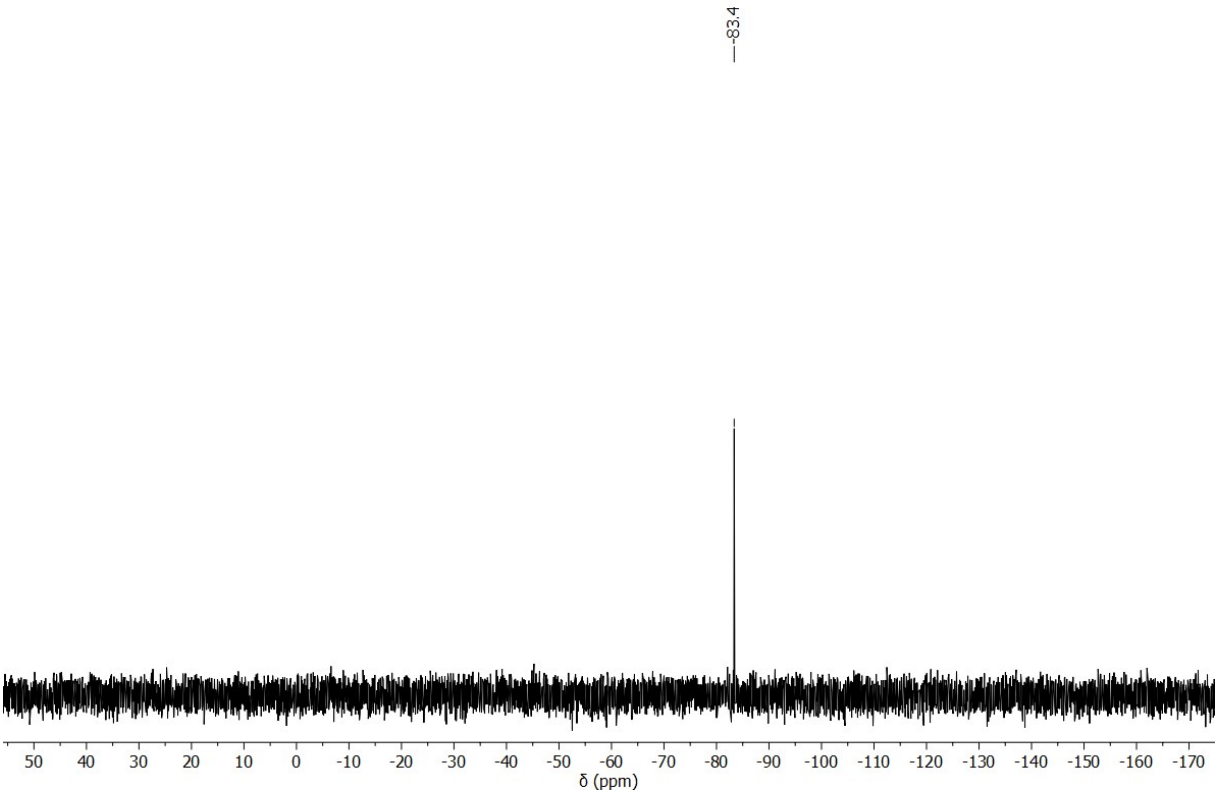


Figure S11. $^{29}Si\{^{1}H\}$Dept90-NMR spectrum of compound **1** in C_6D_6 at 300 K.

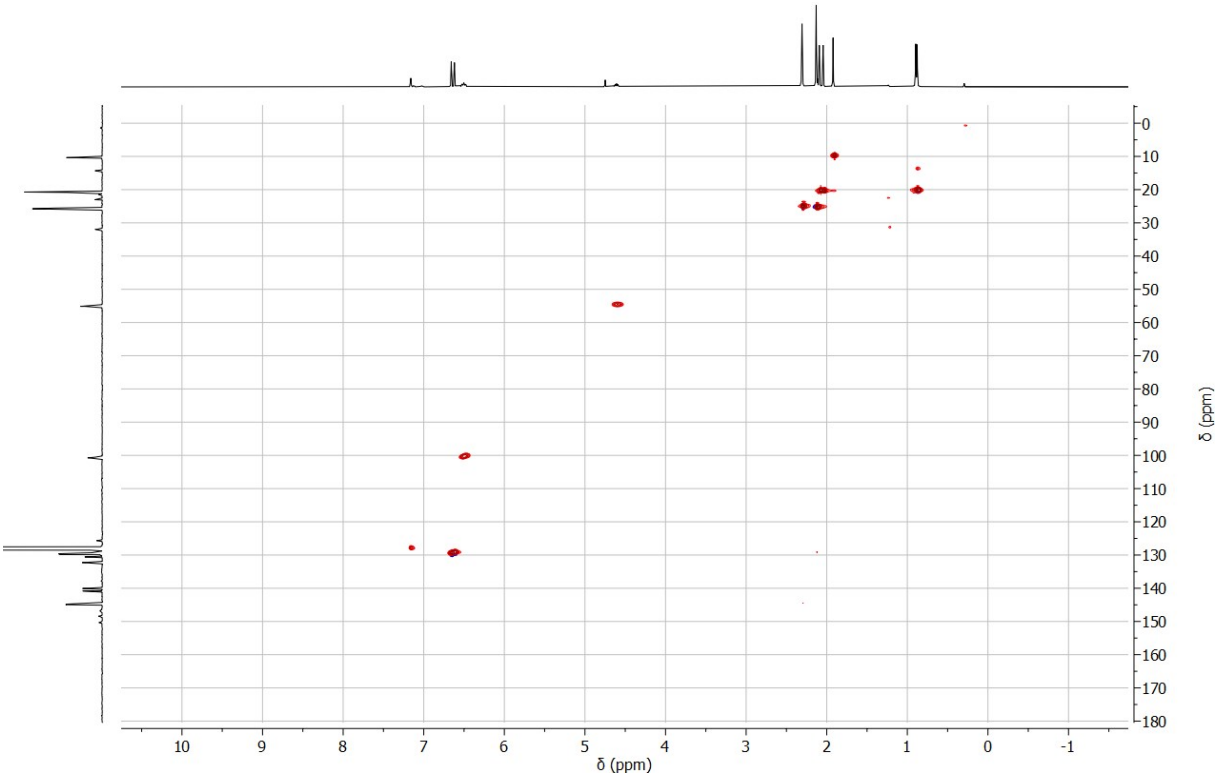


Figure S12. $^{1}H,^{13}C$-HSCQ-NMR spectrum of compound **1** in C_6D_6 at 300 K.

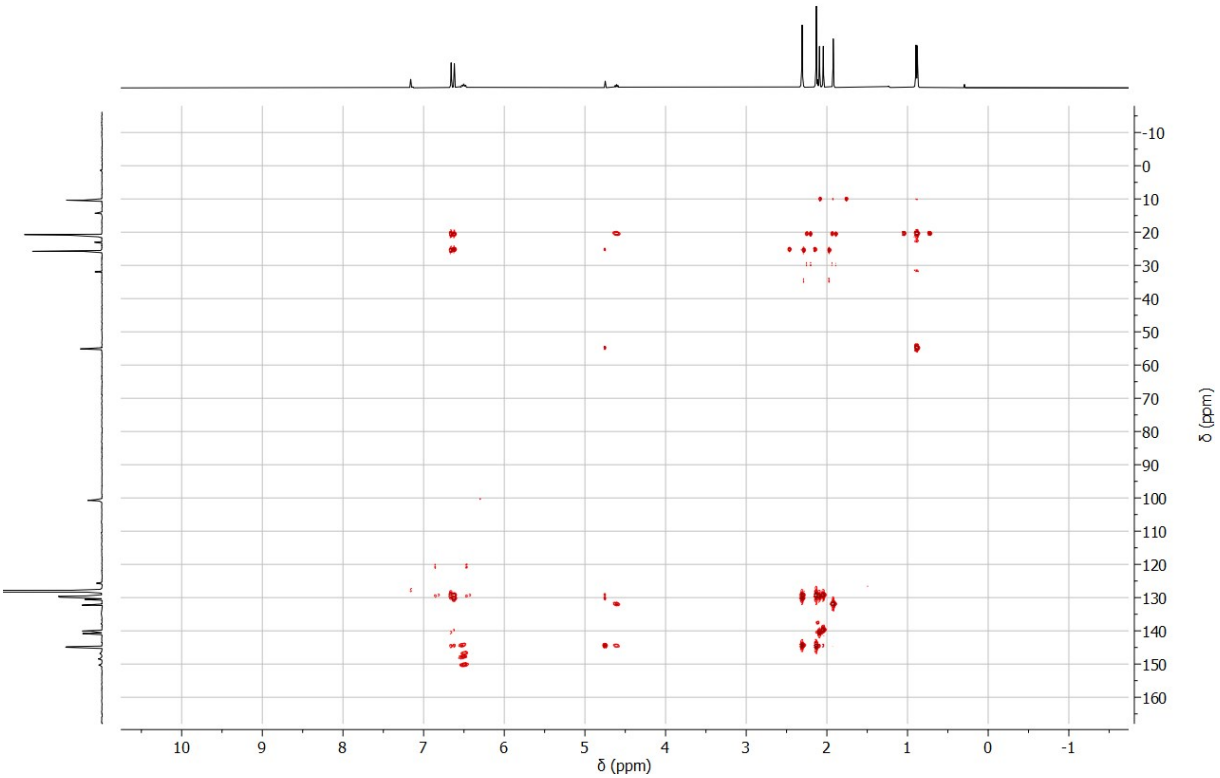


Figure S13. $^{1}H,^{13}C$-HMBC-NMR spectrum of compound **1** in C_6D_6 at 300 K.

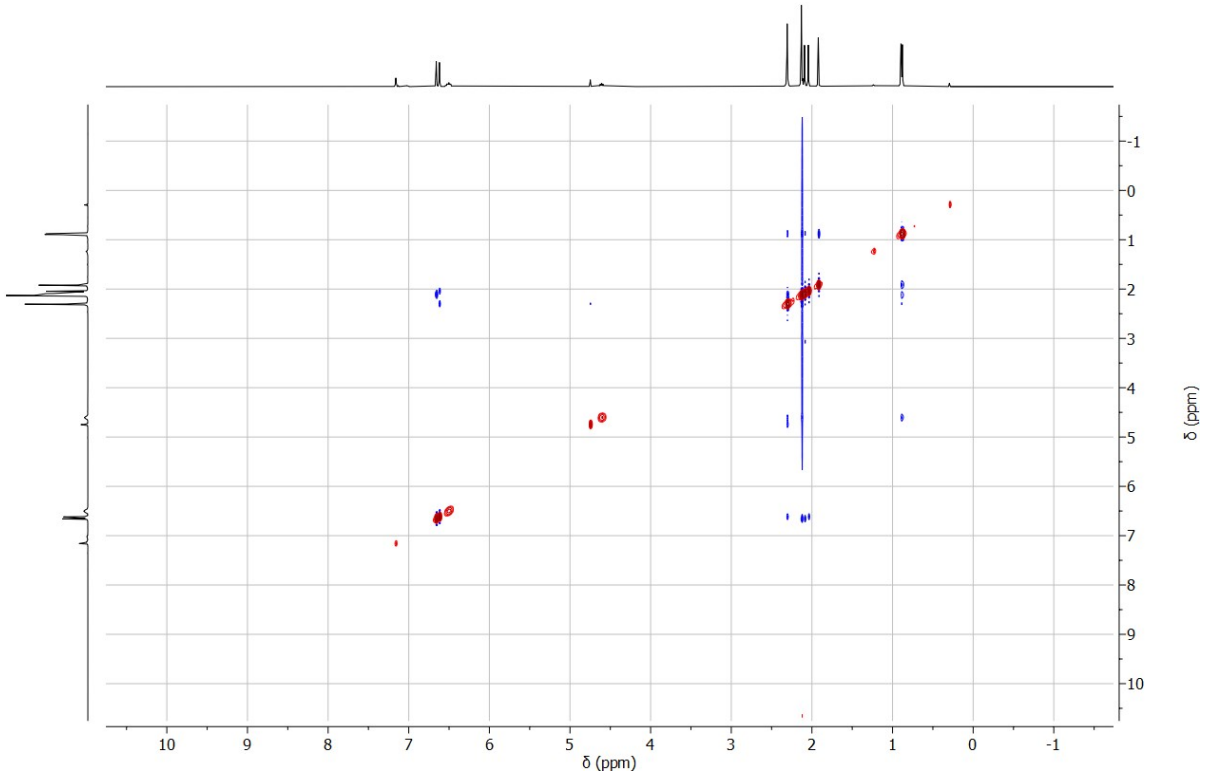


Figure S14. ^{1}H,^{1}H-ROESY-NMR spectrum of compound **1** in C_6D_6 at 300 K.

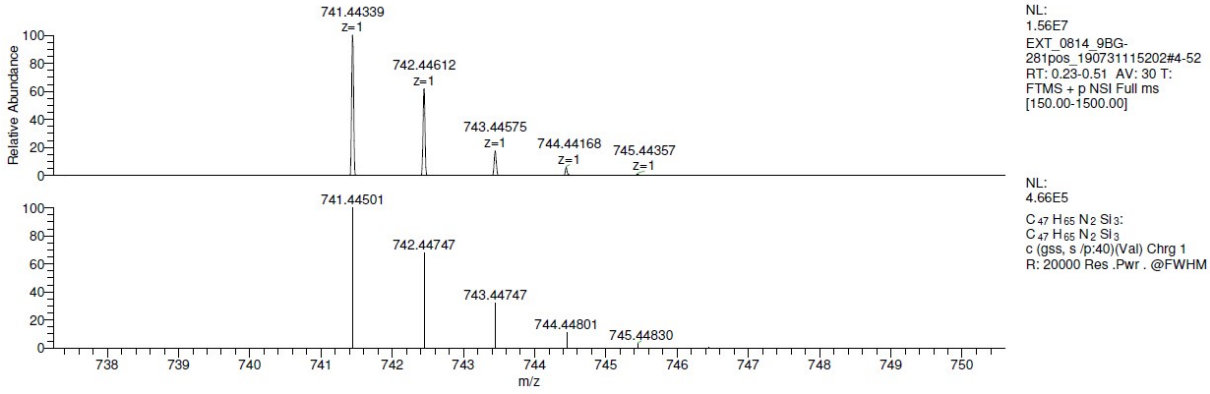


Figure S15. ESI-MS spectrum (positive mode, THF) of compound **1**.

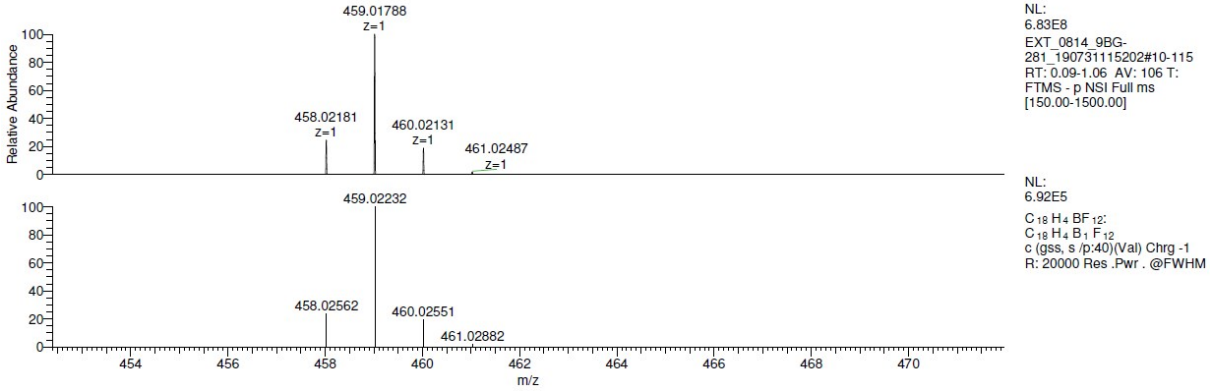


Figure S16. ESI-MS spectrum (negative mode, THF) of compound **1**.

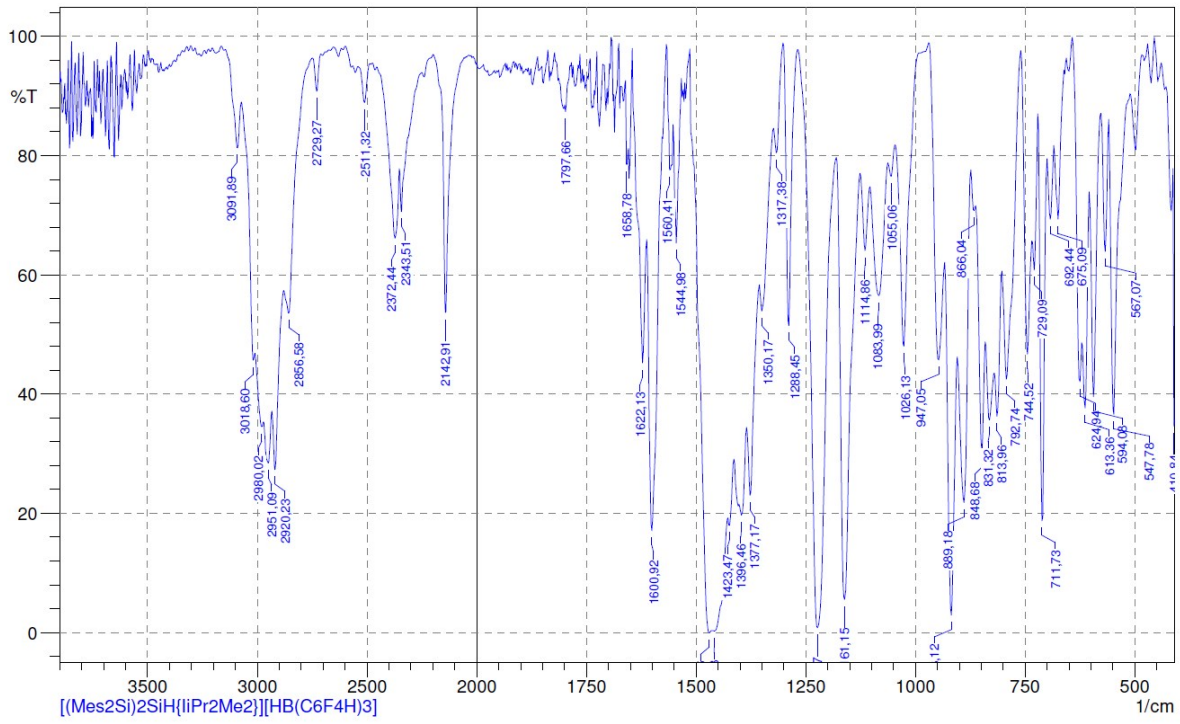
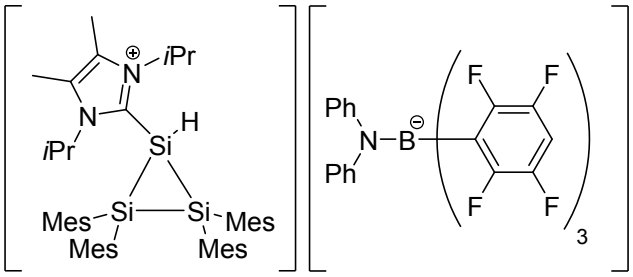


Figure S17. FT-IR spectrum (KBr-pellet) of compound **1**.

Compound **2**



FT-IR ($\tilde{\nu}$/cm^{-1}, KBr-pellet, intensitiy in brackets): 3084 (m), 3048 (m), 2978 (vs), 2955 (vs), 2920 (vs), 2859 (s),2131 (m), 1601 (vs), 1587 (vs), 1545 (w), 1487 (vs), 1468 (vs), 1447 (vs), 1406 (s), 1393 (s), 1377 (s), 1350 (w), 1337 (w), 1289 (vs), 1260 (s), 1223 (vs), 1215 (vs), 1207 (w), 1163 (Vs), 1111 (vw), 1094 (w), 1032 (s), 1007 (w), 993 (m), 939 (w), 916 (s), 905 (s), 889 (s), 849 (m), 824 (m), 779 (m), 750 (s), 696 (vs), 656 (vw), 633 (m), 615 (s), 596 (w), 569 (wv), 550 (m), 500 (vw), 411 (m).

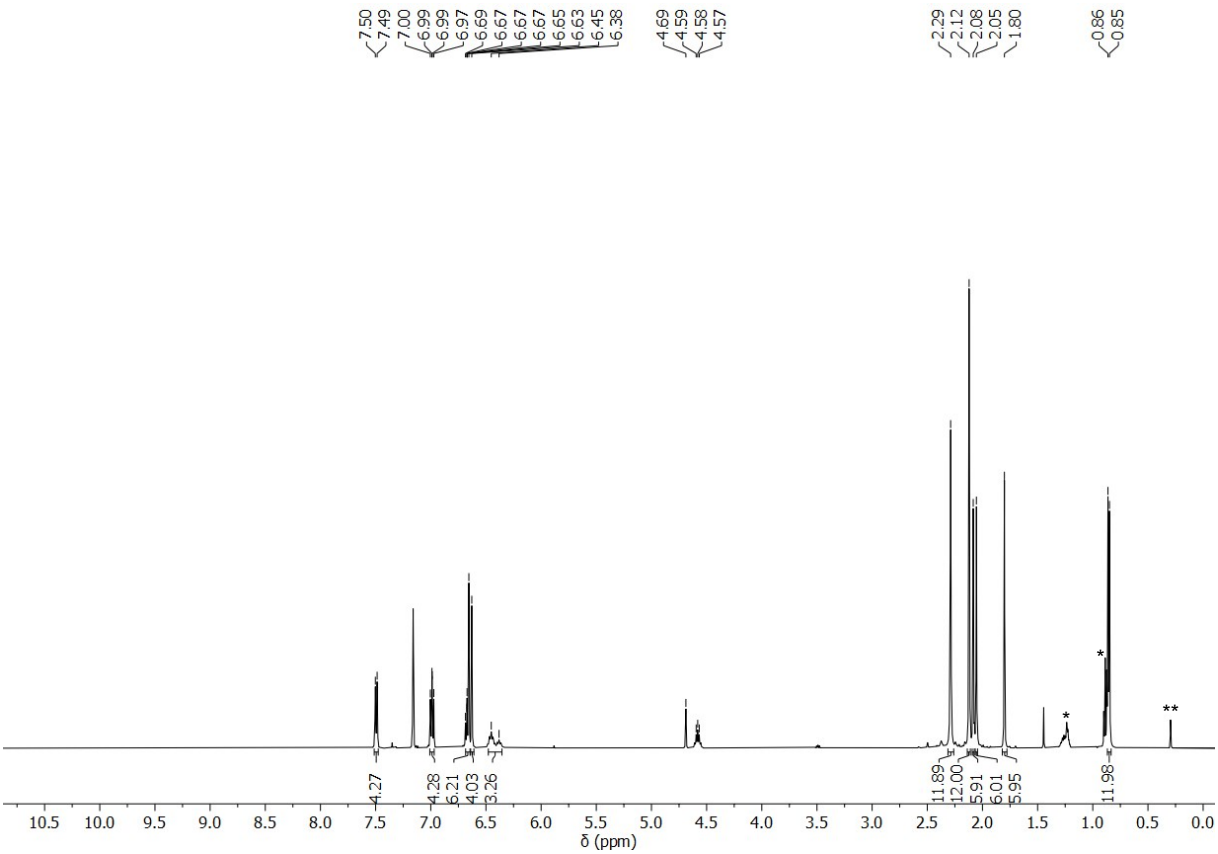


Figure S18. ^{1}H-NMR spectrum of compound **2** in C_6D_6 at 300 K (* hexane, ** silicon grease).

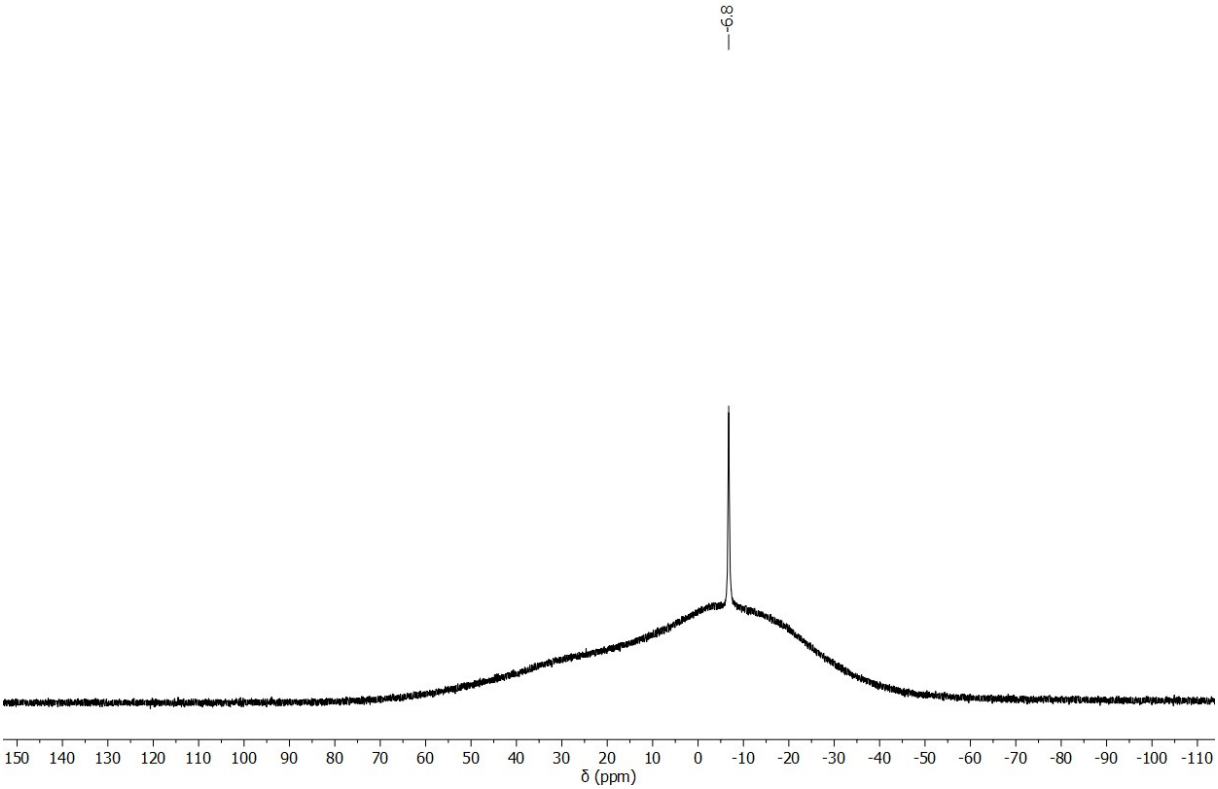


Figure S19. $^{11}B\{^{1}H\}$-NMR spectrum of compound **2** in C_6D_6 at 300 K.

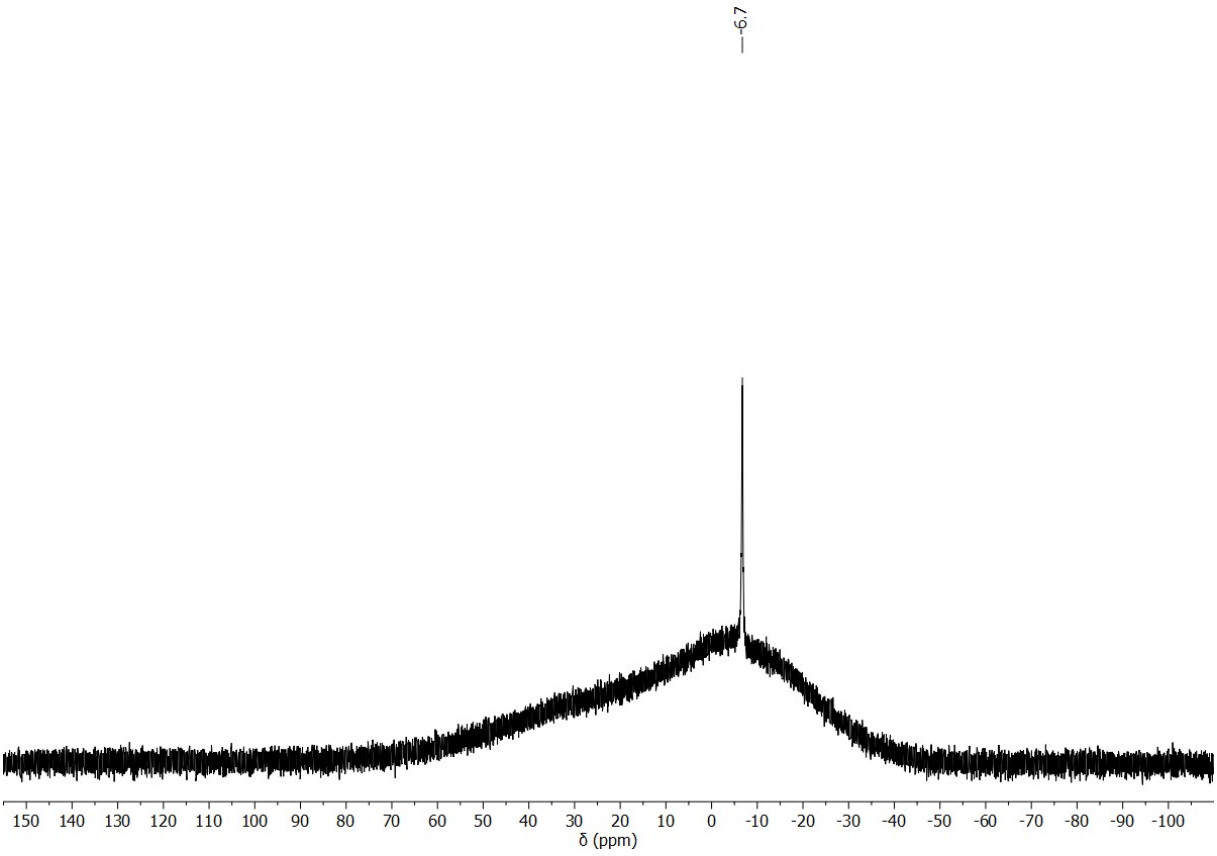


Figure S20. ^{11}B-NMR spectrum of compound **2** in C_6D_6 at 300 K.

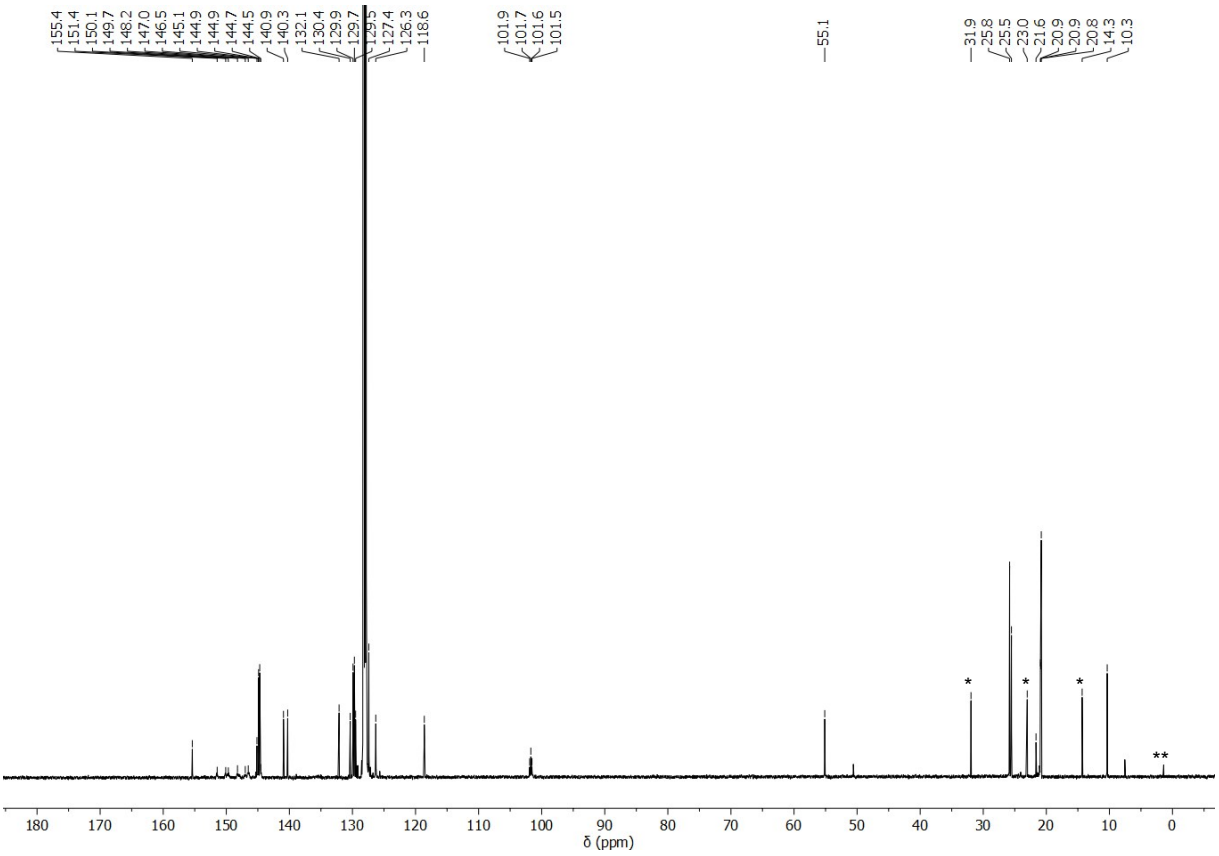


Figure S21. $^{13}C\{^{1}H\}$-NMR spectrum of compound **2** in C_6D_6 at 300 K (* hexane, ** silicon grease).

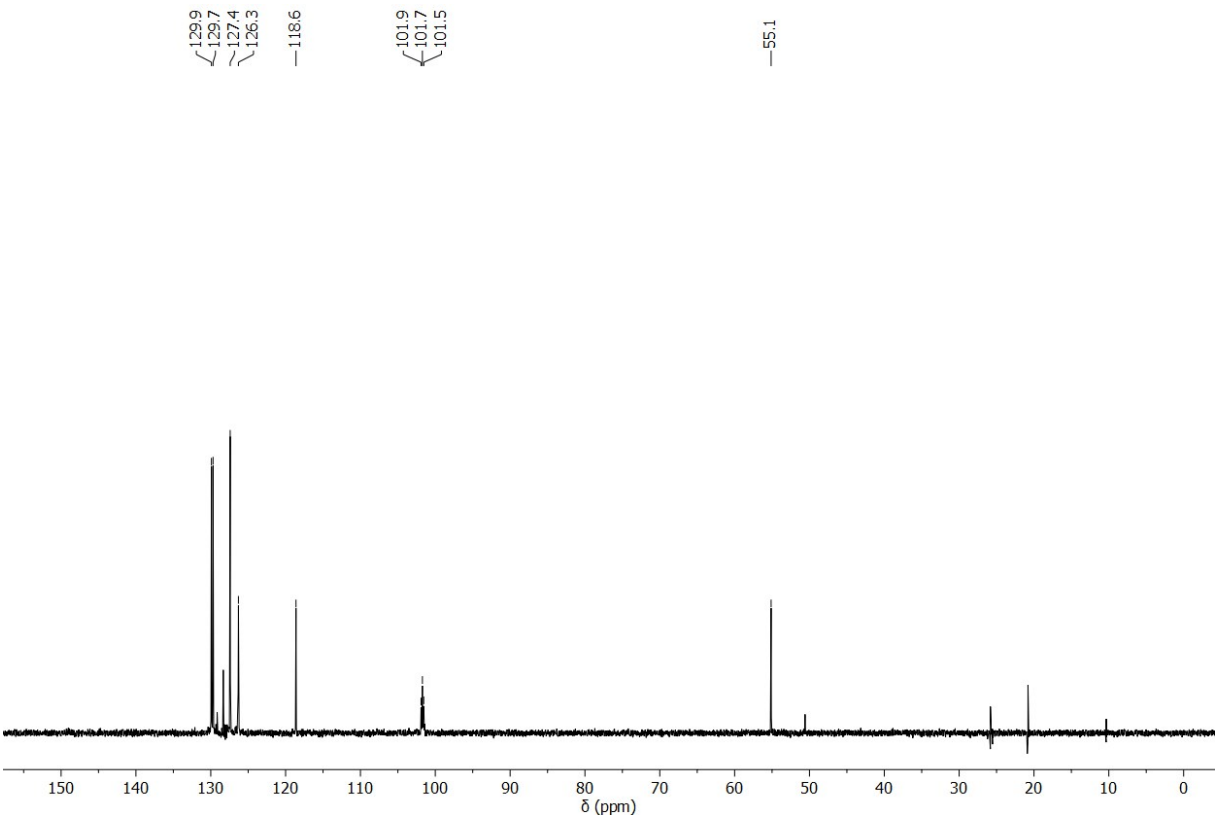


Figure S22. $^{13}C\{^{1}H\}$Dept135-NMR spectrum of compound **2** in C_6D_6 at 300 K.

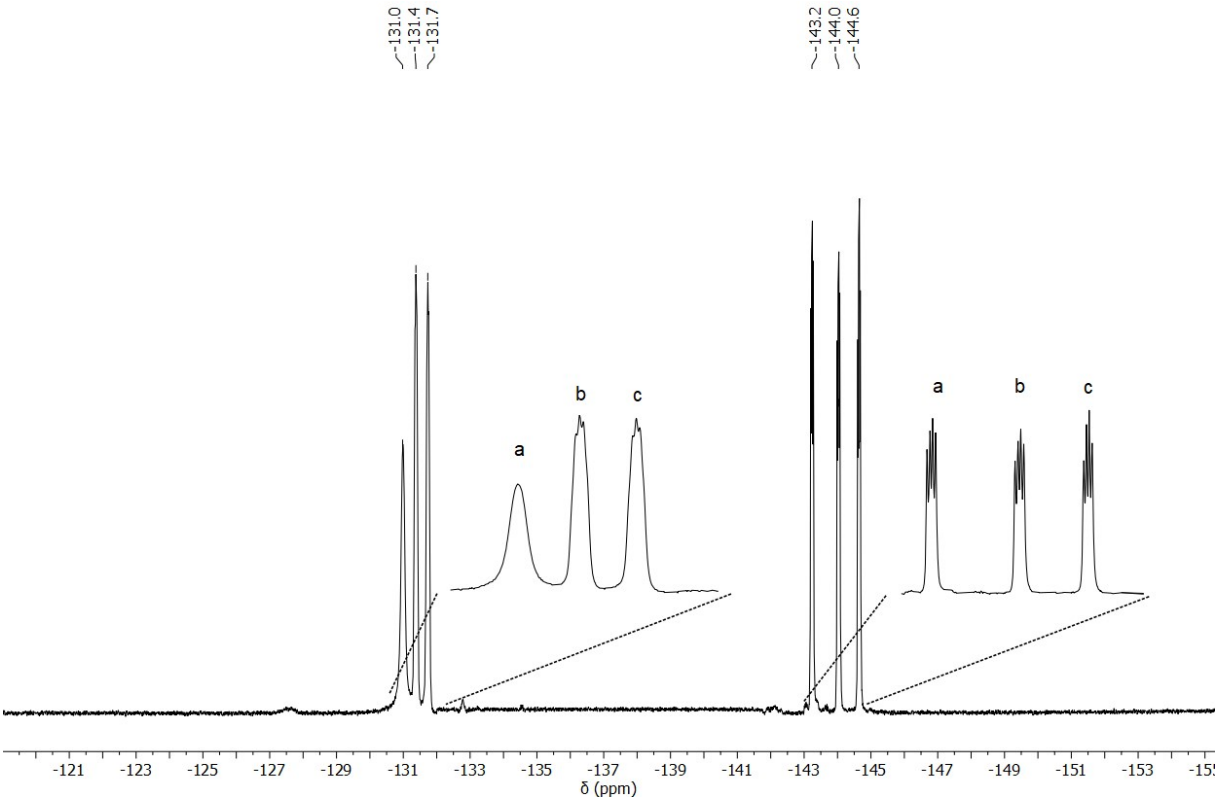


Figure S23. $^{19}F\{^{1}H\}$-NMR spectrum of compound **2** in C_6D_6 at 300 K.

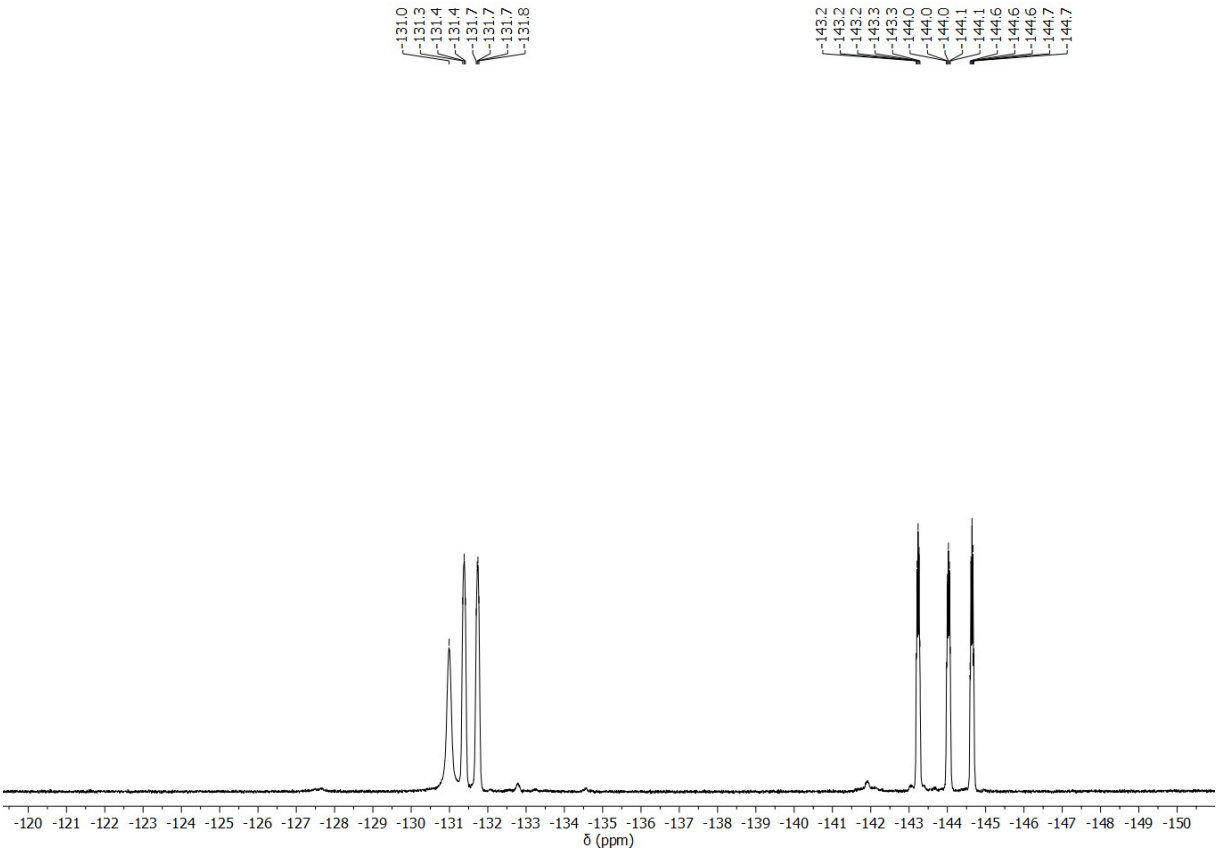


Figure S24. ^{19}F-NMR spectrum of compound **2** in C_6D_6 at 300 K.

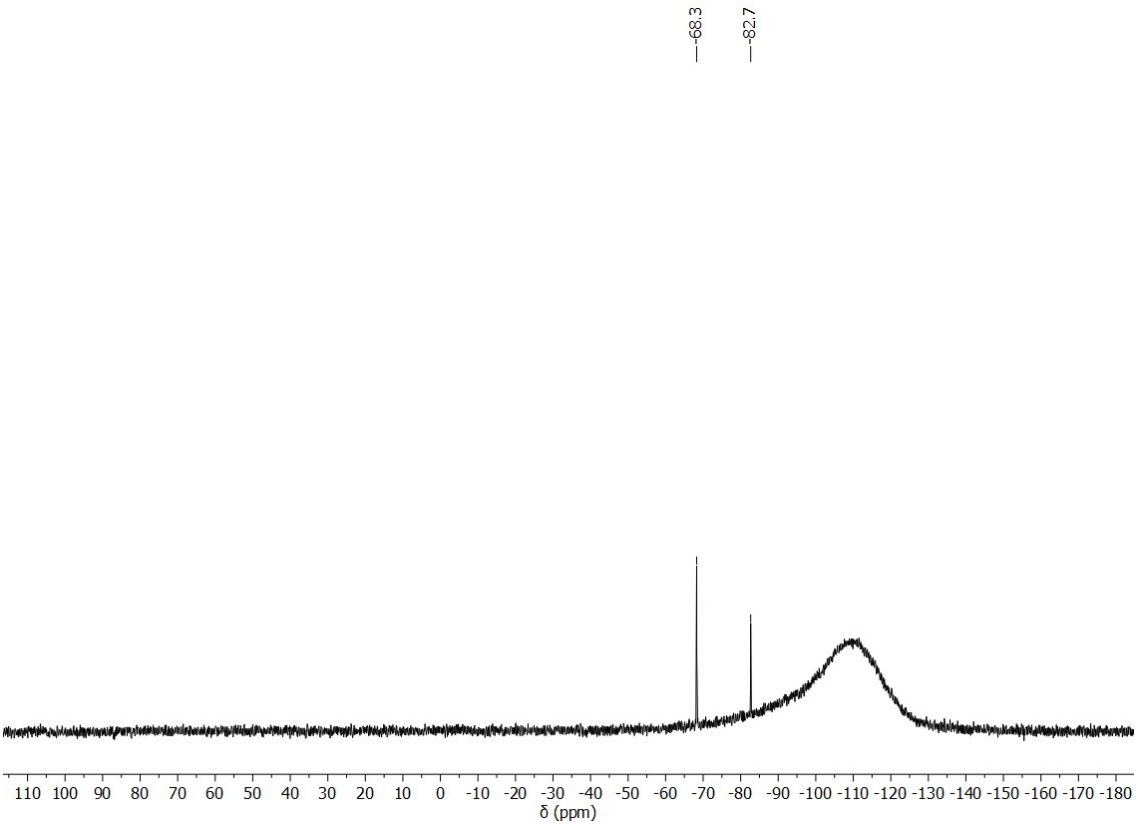


Figure S25. $^{29}Si\{^{1}H\}$IG-NMR spectrum of compound **2** in C_6D_6 at 300 K.

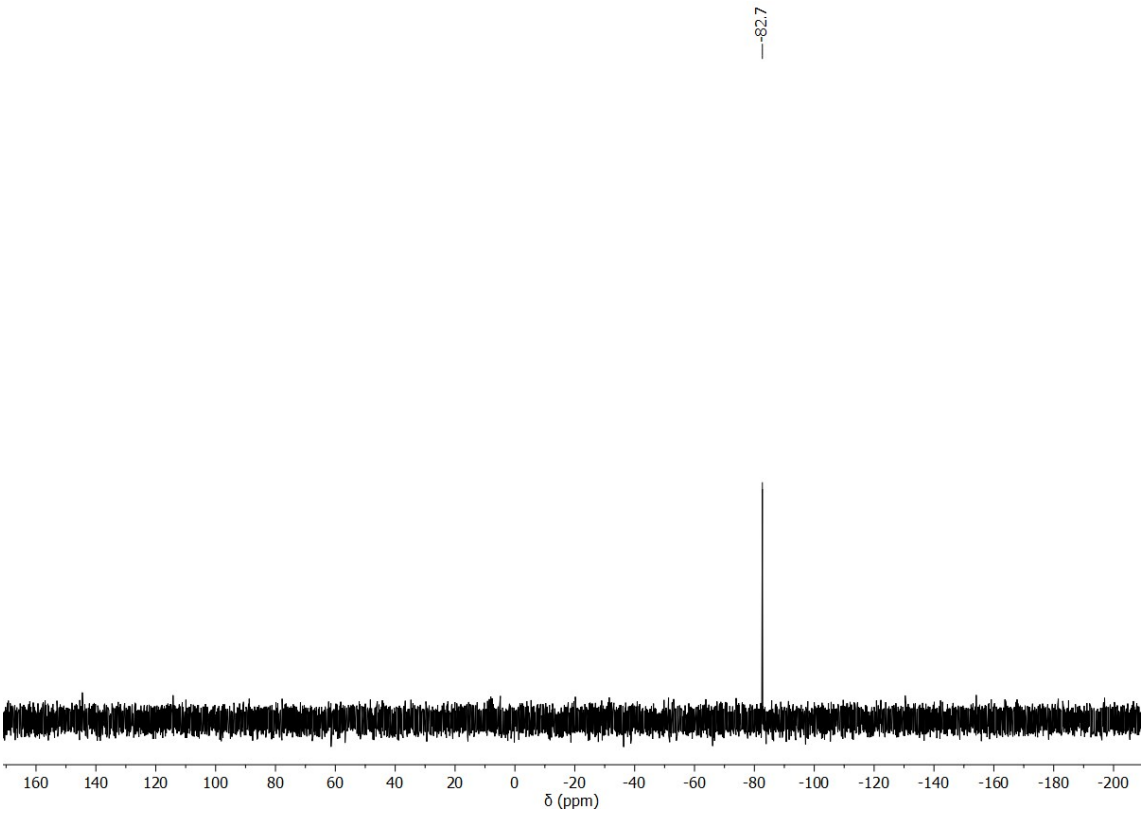


Figure S26. $^{29}Si\{^{1}H\}$Dept90-NMR spectrum of compound **2** in C_6D_6 at 300 K.

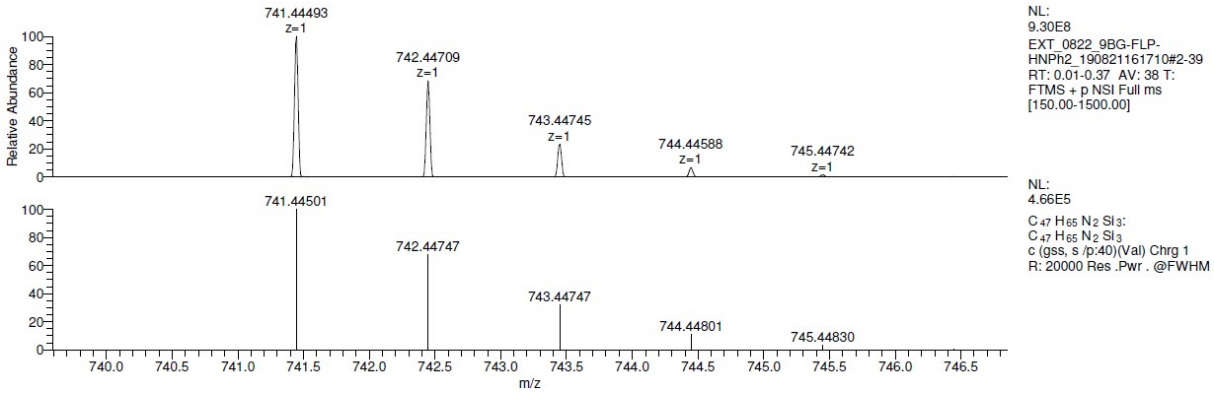


Figure S27. ESI-MS spectrum (positive mode, THF) of compound **2**.

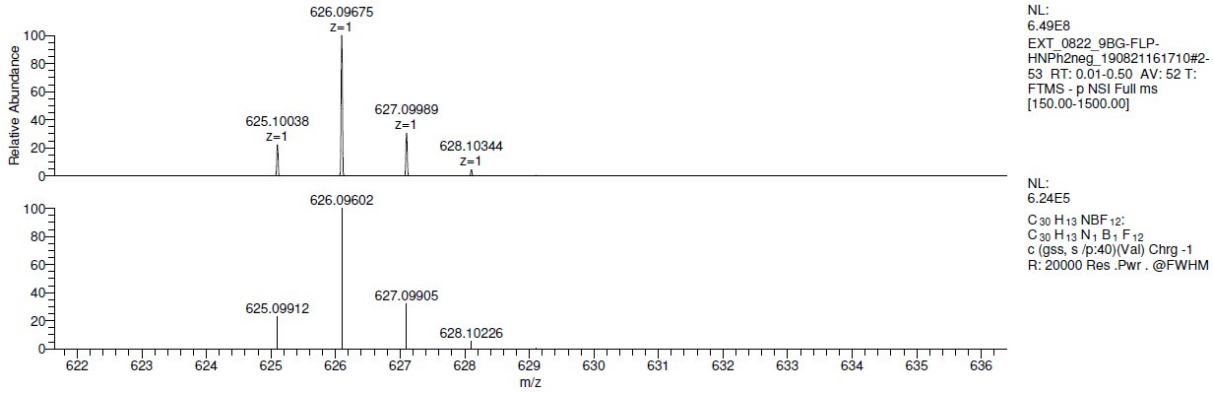


Figure S28. ESI-MS spectrum (negative mode, THF) of compound **2**.

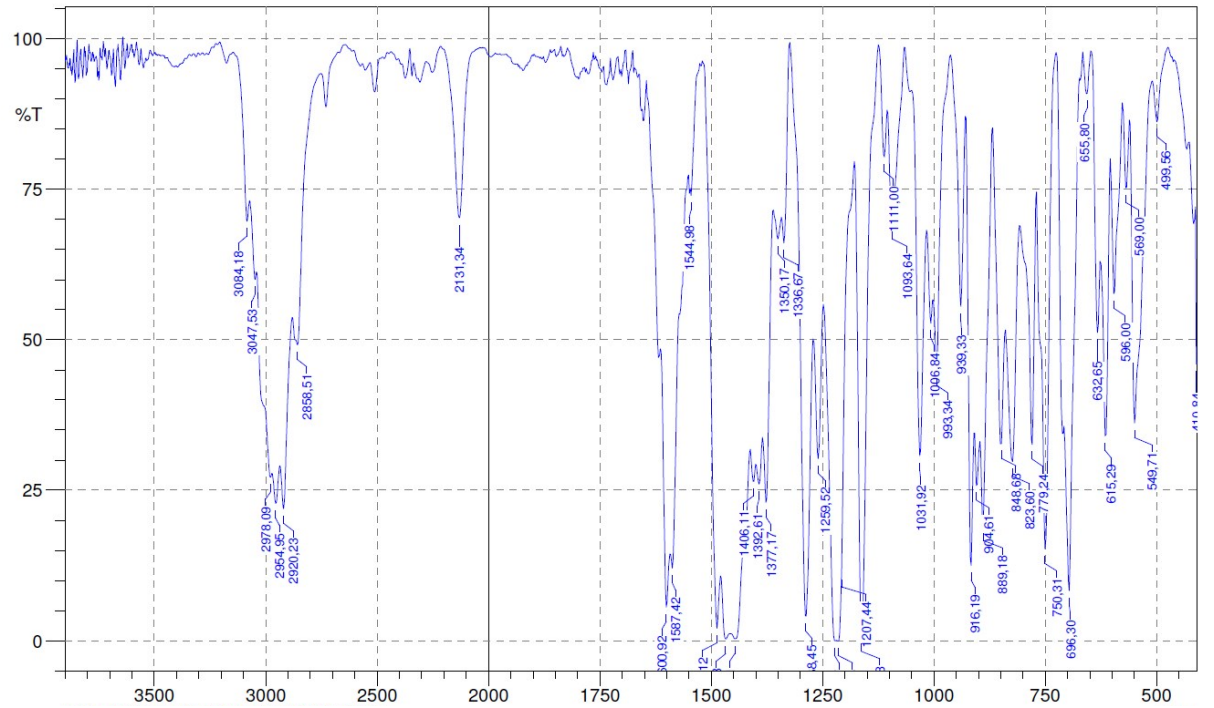
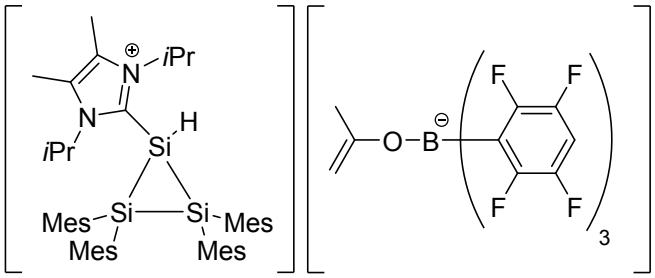


Figure S29. FT-IR spectrum (KBr-pellet) of compound **2**.

Compound **3**



FT-IR ($\tilde{\nu}$/cm^{-1}, KBr-pellet, intensitiy in brackets): 3088 (vw), 3007 (w), 2990 (w), 2965 (w), 2947 (w), 2918 (w), 2855 (vw), 2143 (w), 1601 (m), 1587 (m), 1560 (w), 1545 (w), 1487 (m), 1462 (vs), 1395 (m), 1375 (m), 1327 (vw), 1288 (m), 1261 (vw), 1217 (s), 1163 (m), 1092 (vw), 1030 (w), 993 (w), 945 (vw), 916 (m), 905 (w), 887 (w), 849 (m), 829 (w), 779 (w), 748 (m), 694 (m), 631 (w), 615 (m), 598 (w), 550 (w), 536 (w).

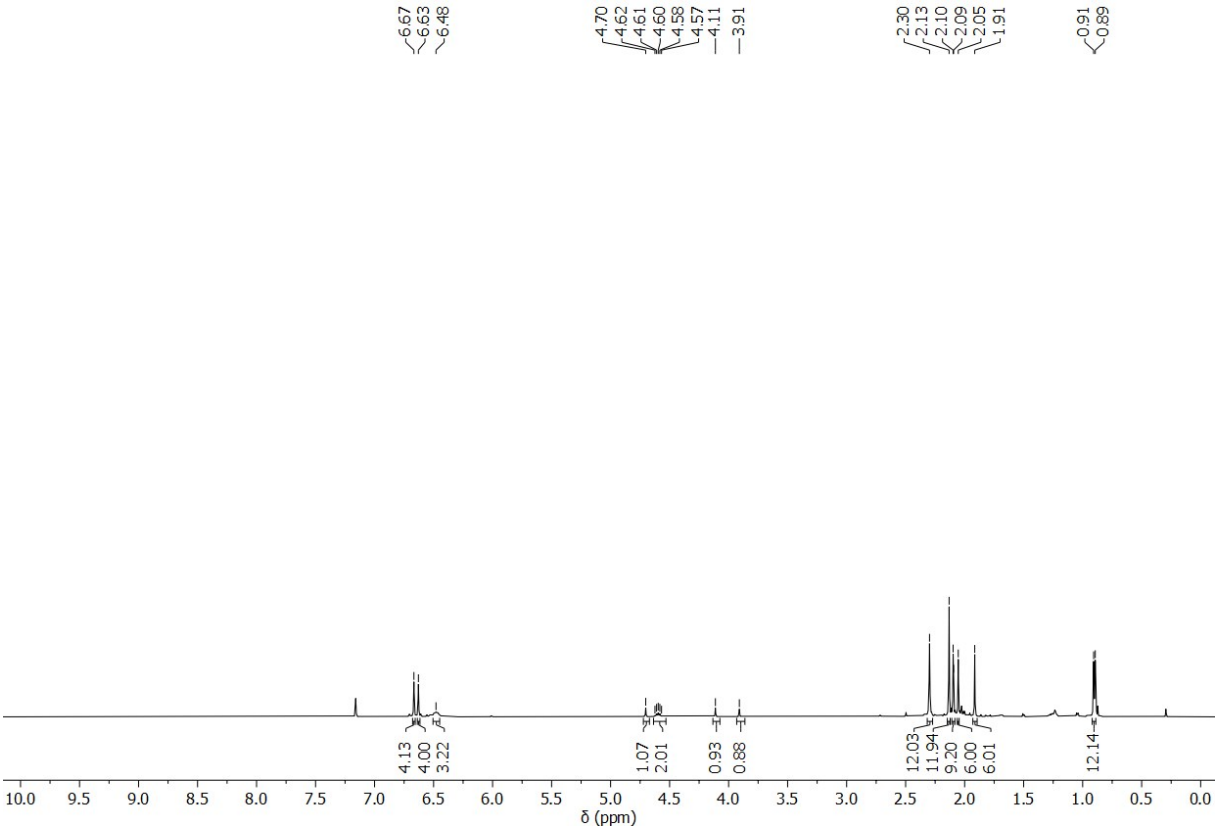


Figure S30. ^{1}H-NMR spectrum of compound **3** in C_6D_6 at 300 K.

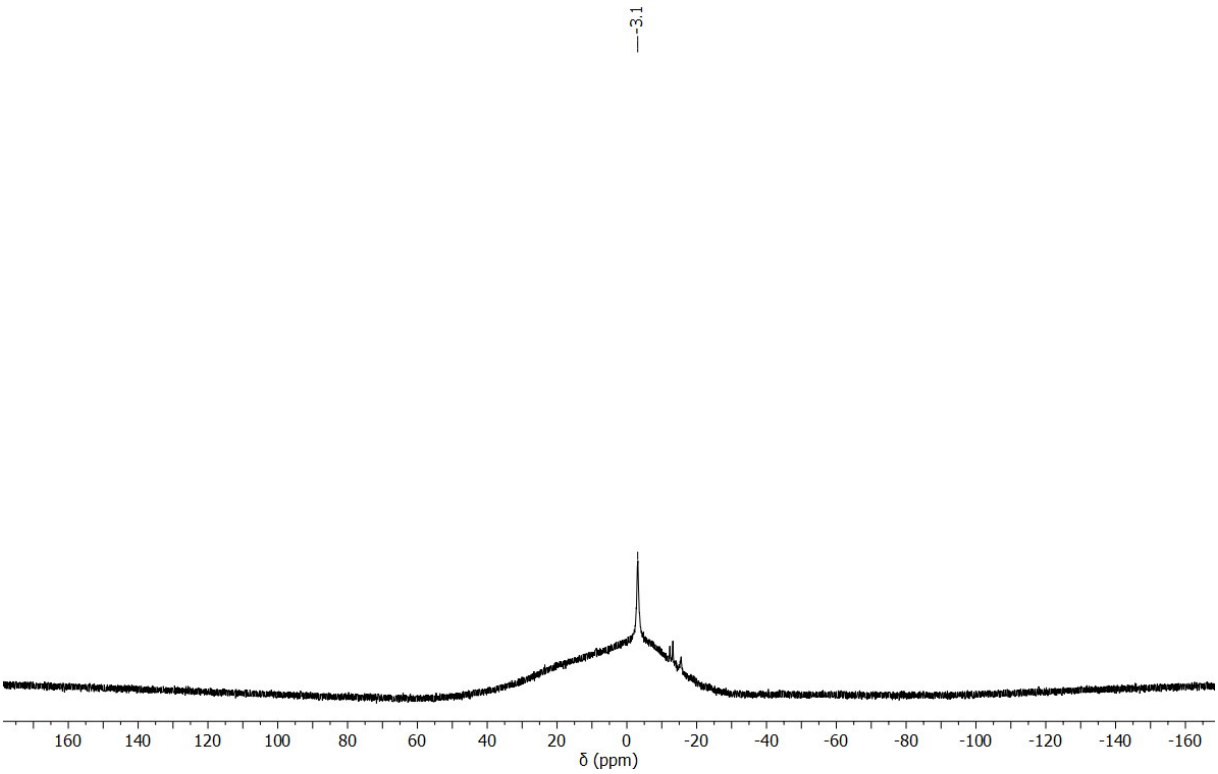


Figure S31. $^{11}B\{^{1}H\}$-NMR spectrum of compound **3** in C_6D_6 at 300 K.

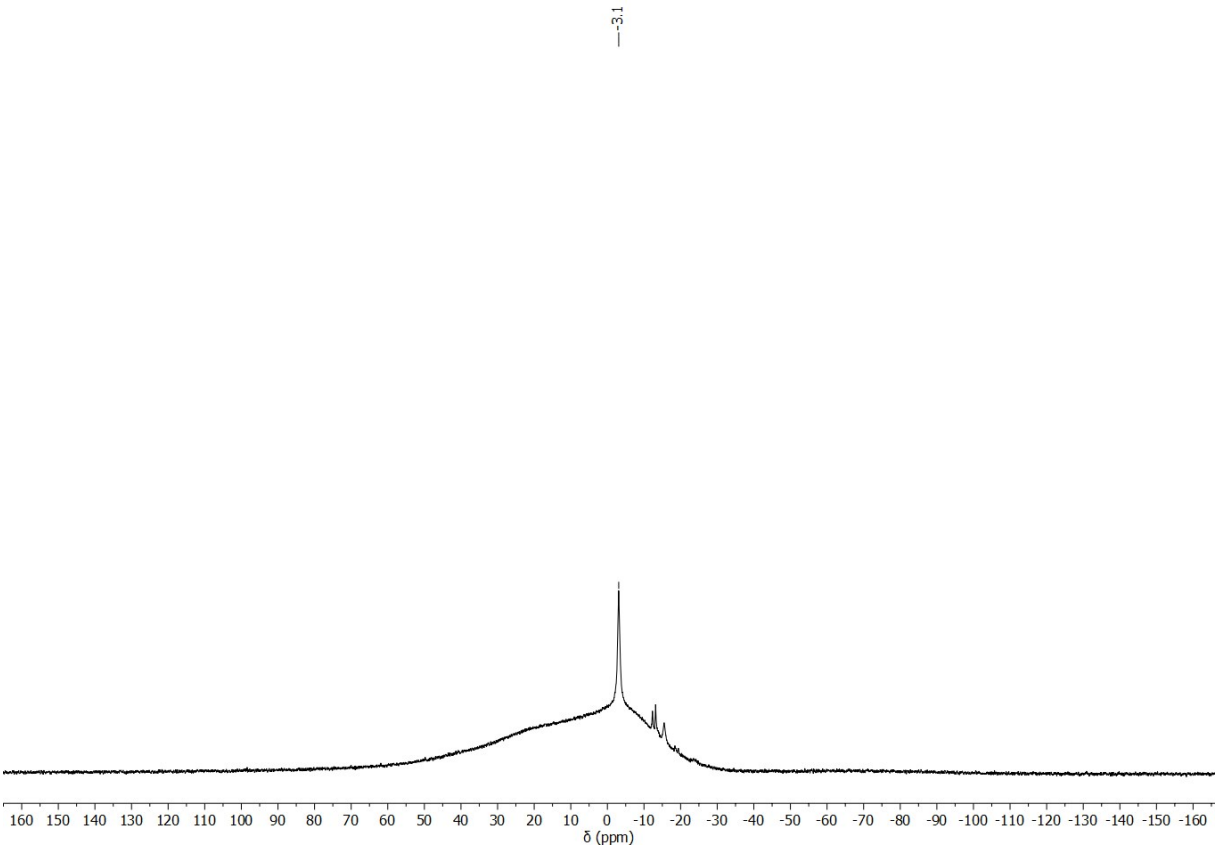


Figure S32. ^{11}B-NMR spectrum of compound **3** in C_6D_6 at 300 K.

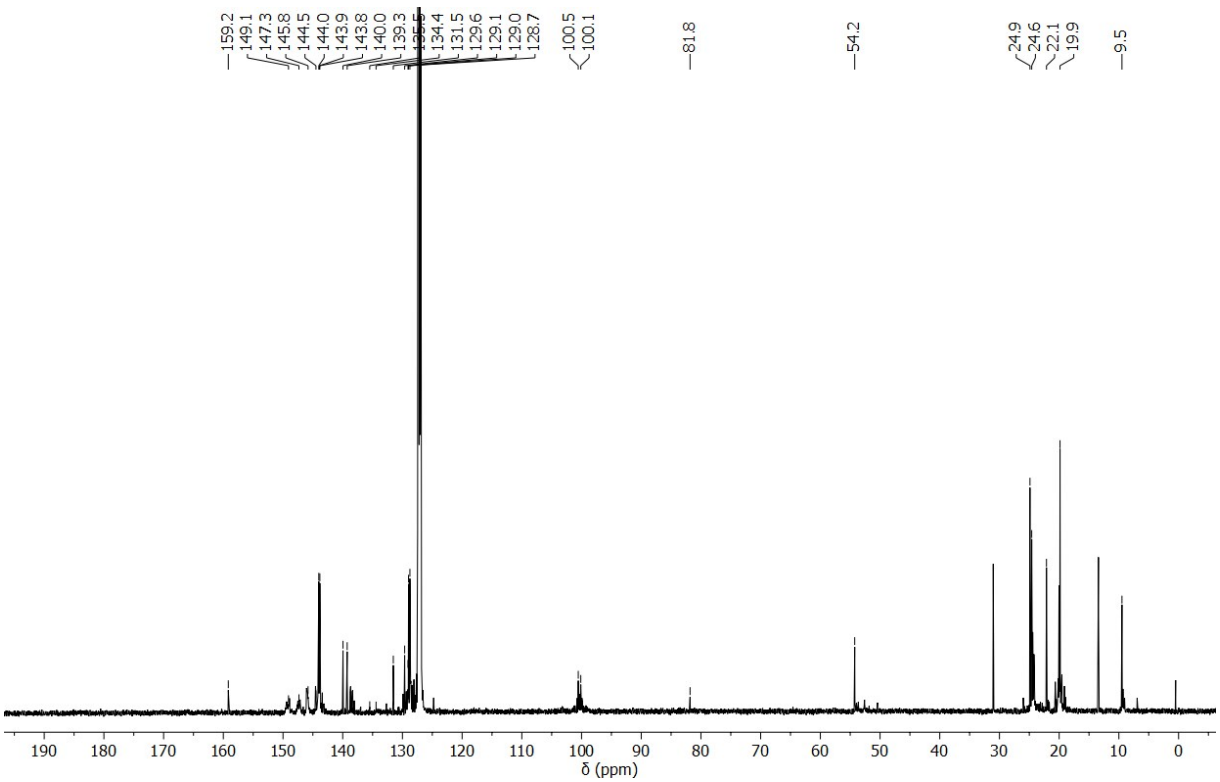


Figure S33. $^{13}C\{^{1}H\}$-NMR spectrum of compound **3** in C_6D_6 at 300 K.

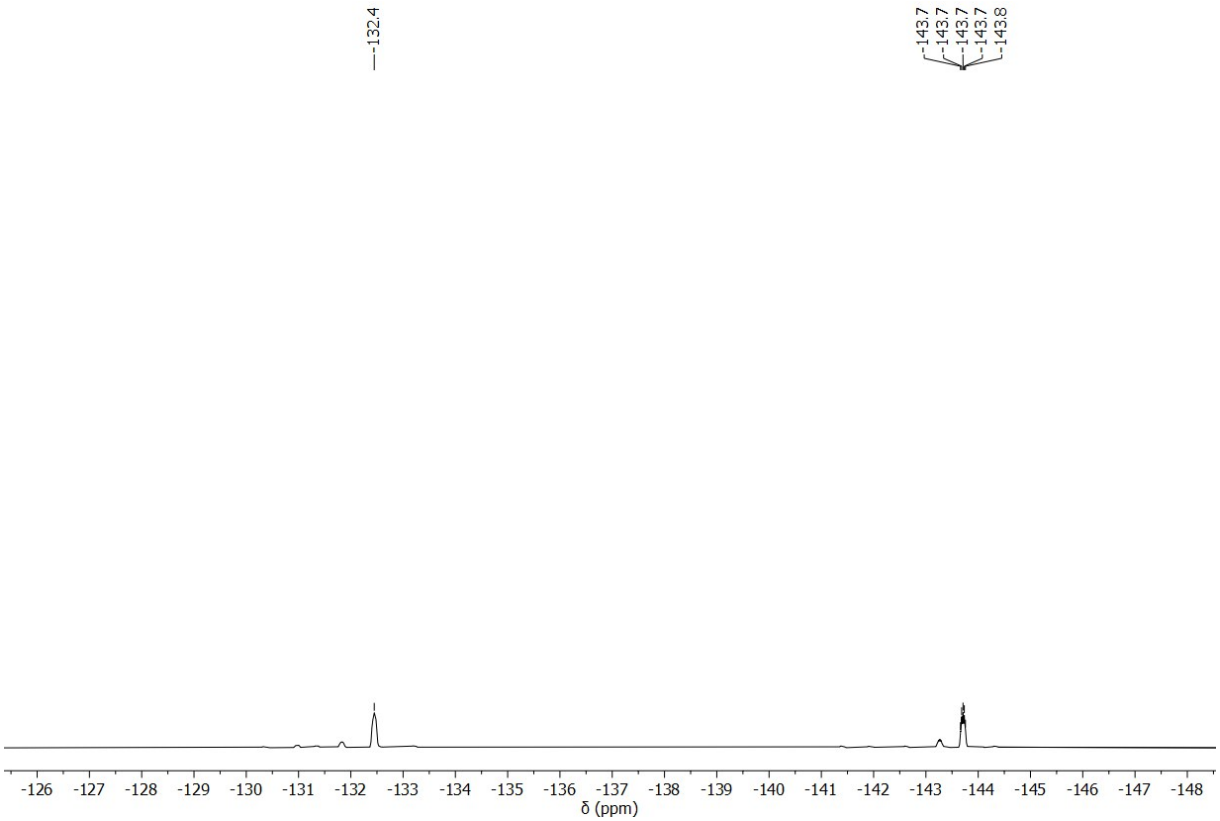


Figure S34. $^{19}F\{^{1}H\}$-NMR spectrum of compound **3** in C_6D_6 at 300 K.

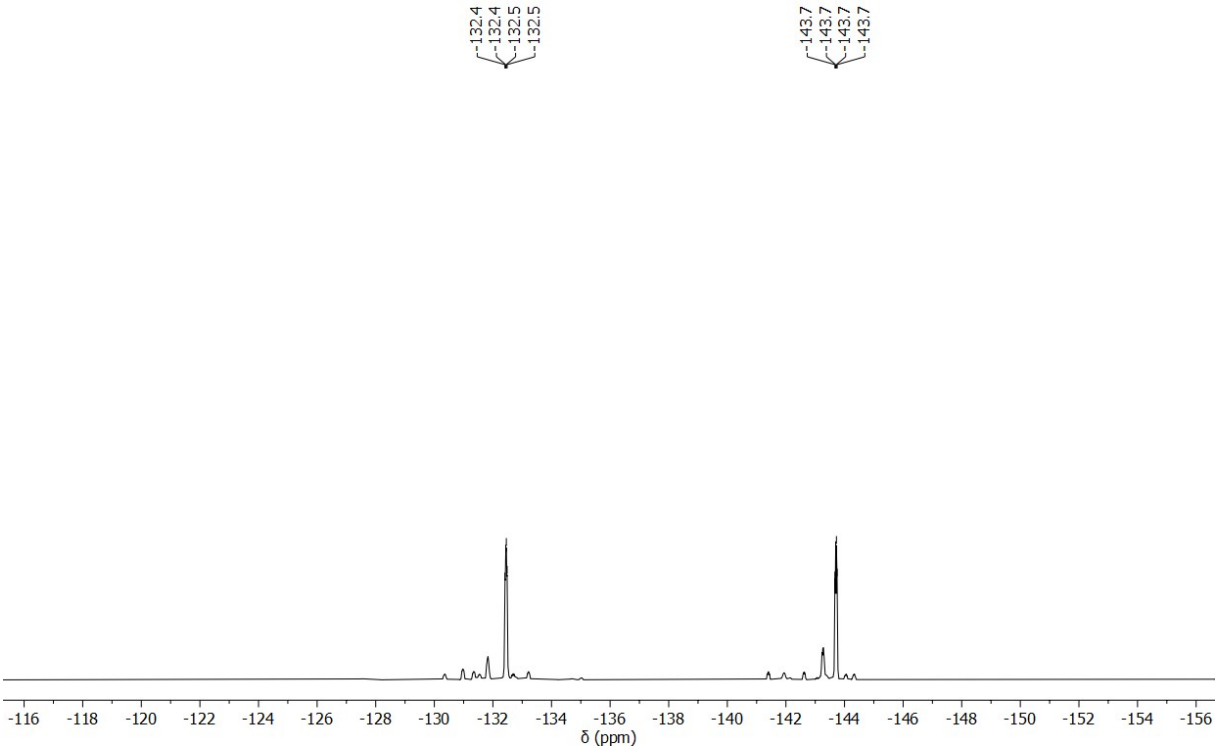


Figure S35. ^{19}F-NMR spectrum of compound **3** in C_6D_6 at 300 K.

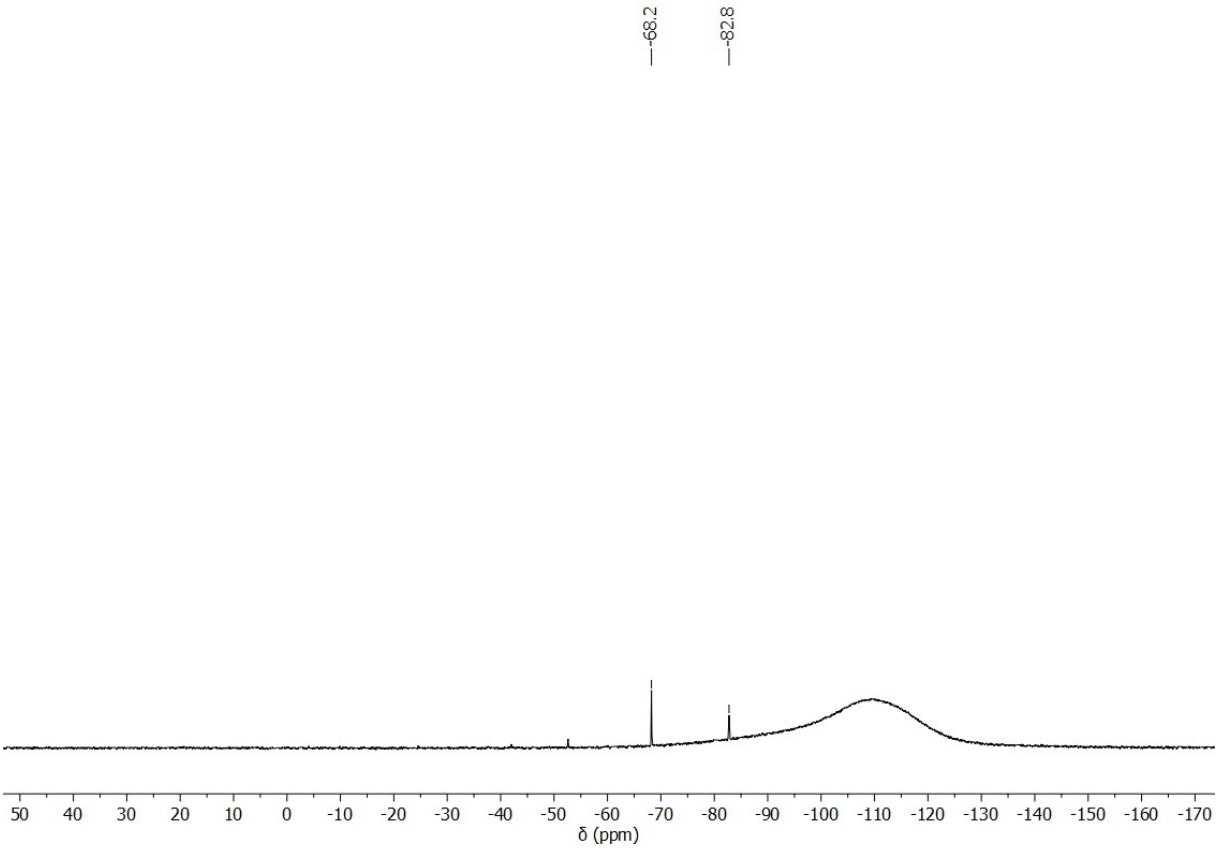


Figure S36. ^{29}Si{^{1}H}IG-NMR spectrum of compound **3** in C_6D_6 at 300 K.

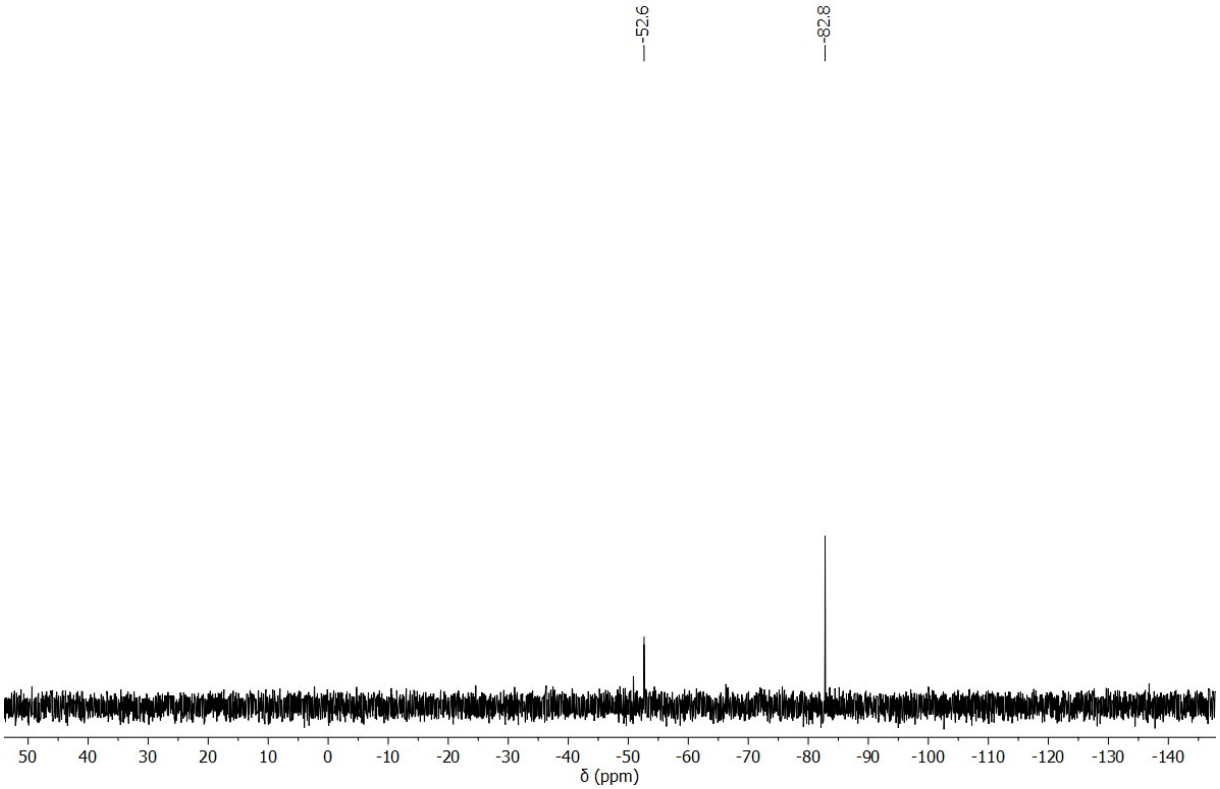


Figure S37. $^{29}Si\{^{1}H\}$Dept90-NMR spectrum of compound **3** in C_6D_6 at 300 K.

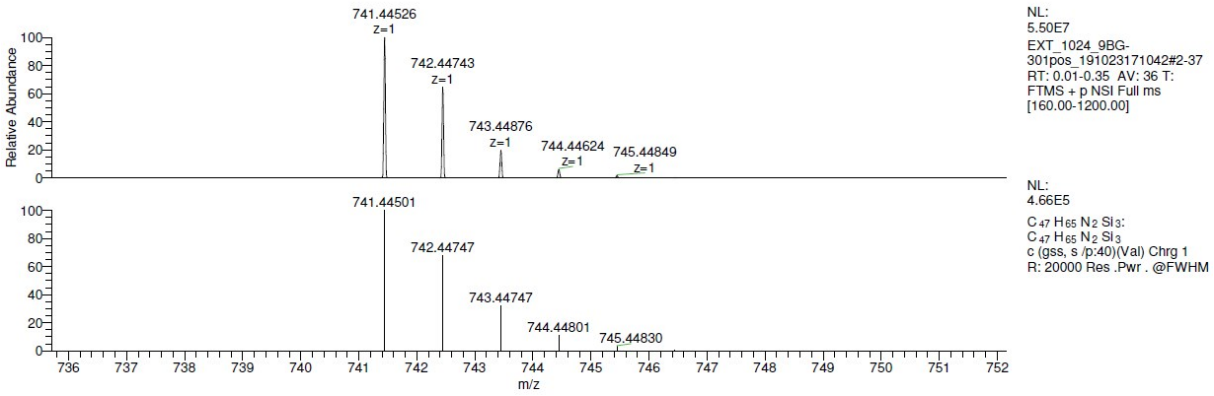


Figure S38. ESI-MS spectrum (positive mode, THF) of compound **3**.

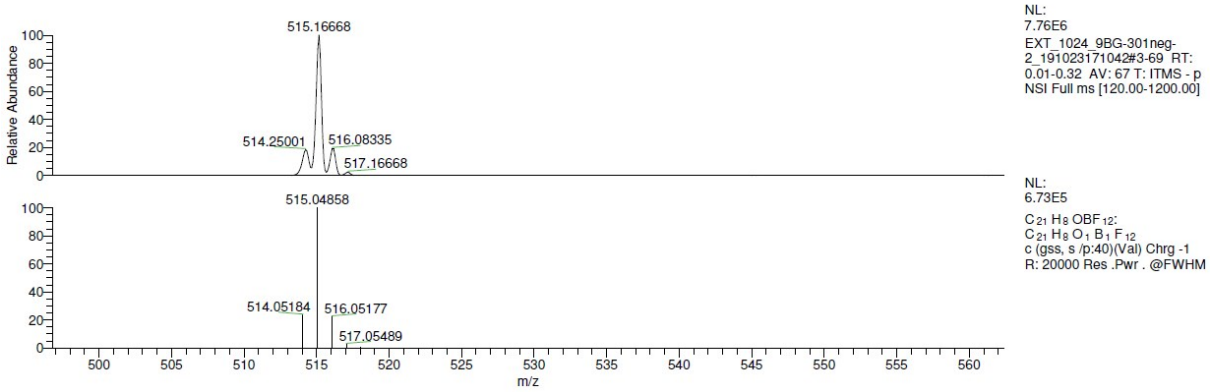


Figure S39. ESI-MS spectrum (negative mode, THF) of compound **3**.

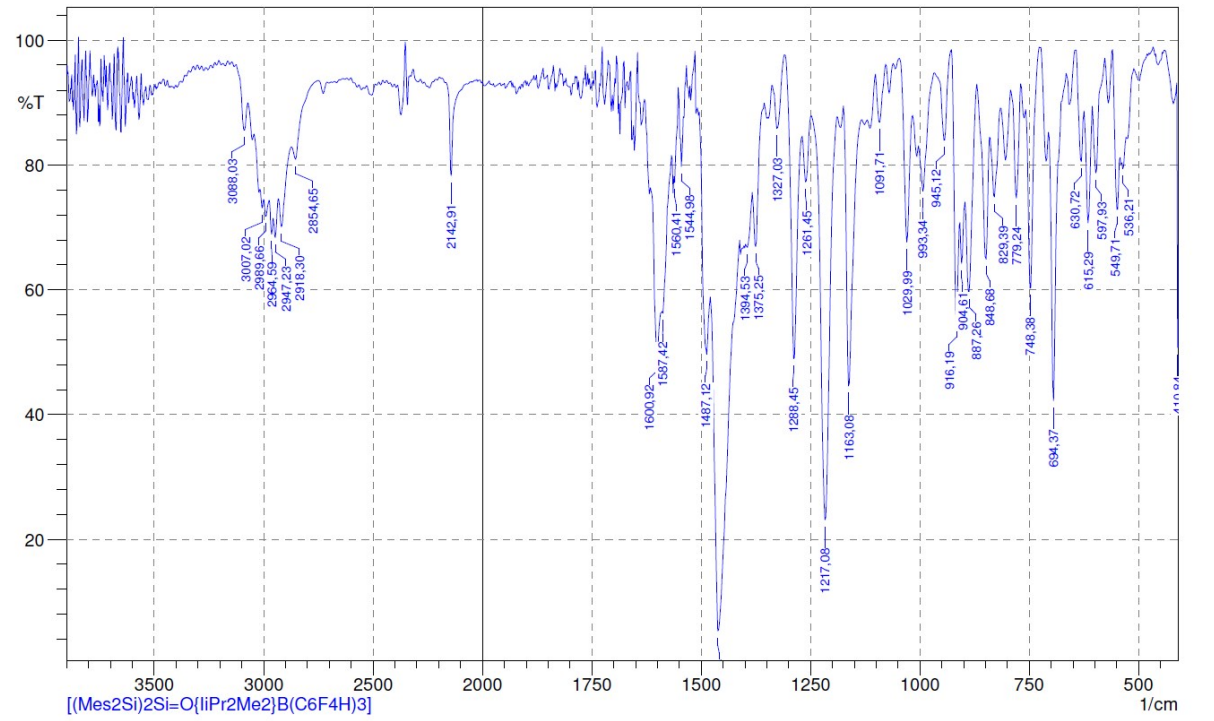
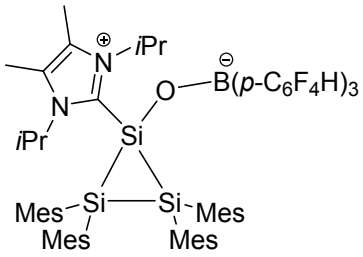


Figure S40. FT-IR spectrum (KBr-pellet) of compound **3**.

Compound **4**



FT-IR ($\tilde{\nu}$/cm^{-1}, KBr-pellet, intensitiy in brackets): 3090 (m), 3019 (m), 2986 (m), 2953 (m), 2918 (m), 2870 (w), 2729 (vw), 1651 (w), 1626 (w), 1601 (s), 1545 (w), 1470 (vs), 1462 (vs), 1404 (m), 1373 (s), 1350 (w), 1292 (vw), 1225 (vw), 1163 (vs), 1123 (w), 1076 (vs), 1028 (m), 974 (vw), 922 (m), 908 (m), 893 (m), 876 (m), 831 (m), 787 (m), 750 (m), 712 (m), 692 (m), 679 (w), 644 (vw), 634 (vw), 611 (w), 596 (vw), 550 (m), 521 (vw), 482 (vw), 453 (vw).

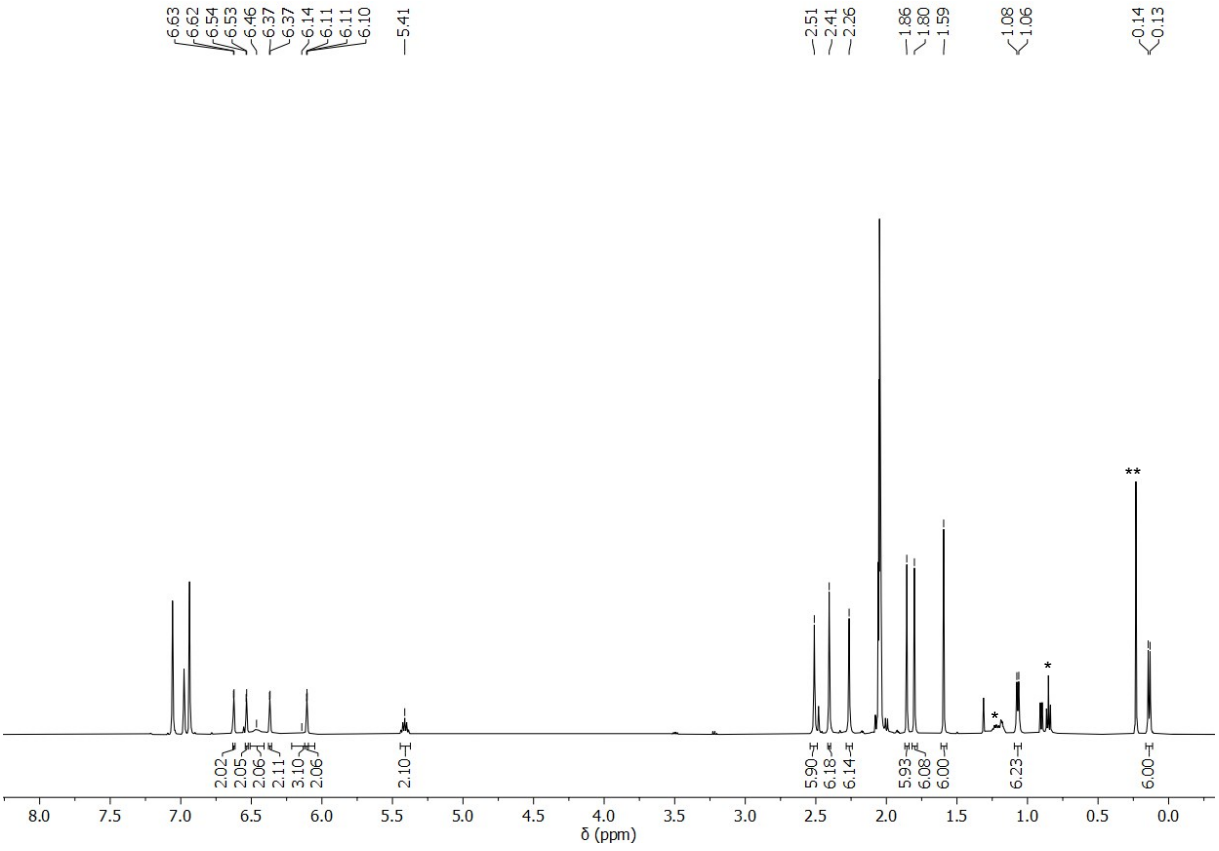


Figure S41. ^{1}H-NMR spectrum of compound **4** in C_6D_6 at 300 K (* hexane, ** silicon grease).

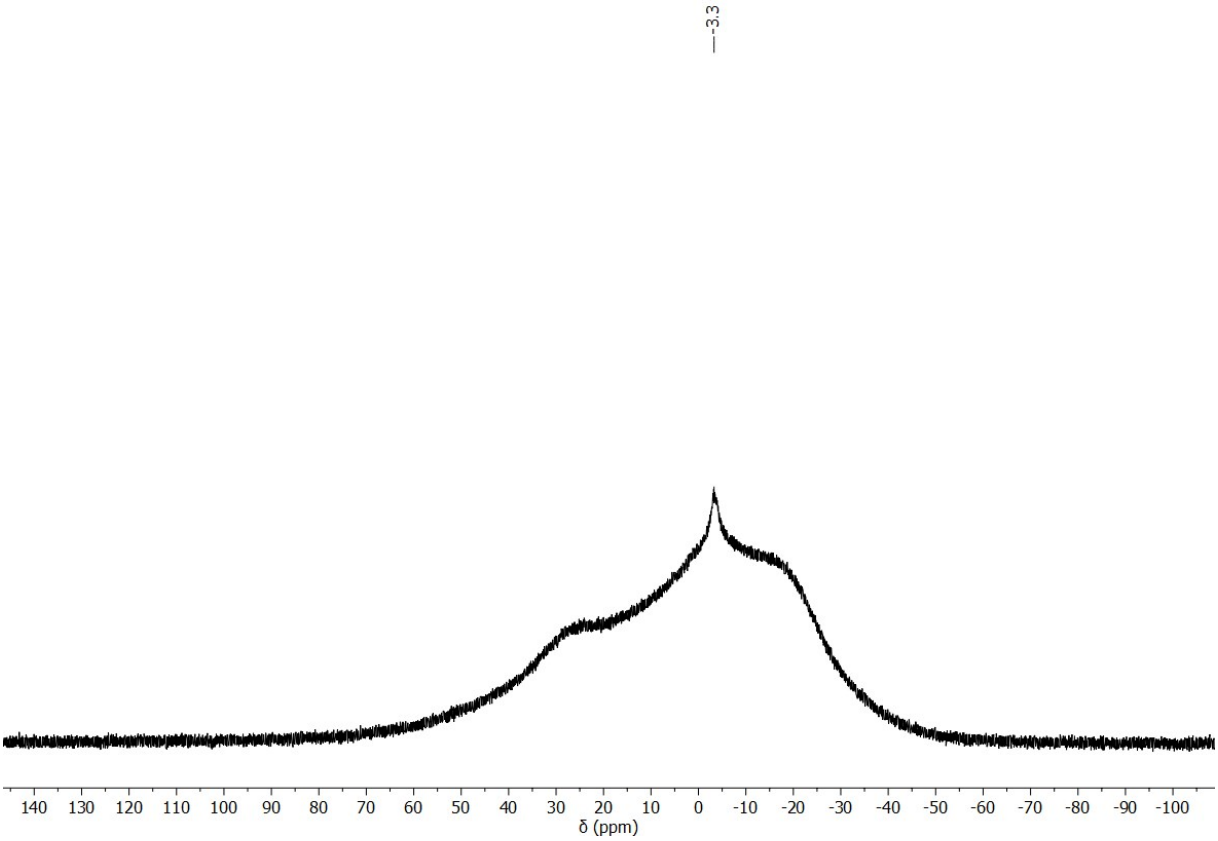


Figure S42. $^{11}B\{^{1}H\}$-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

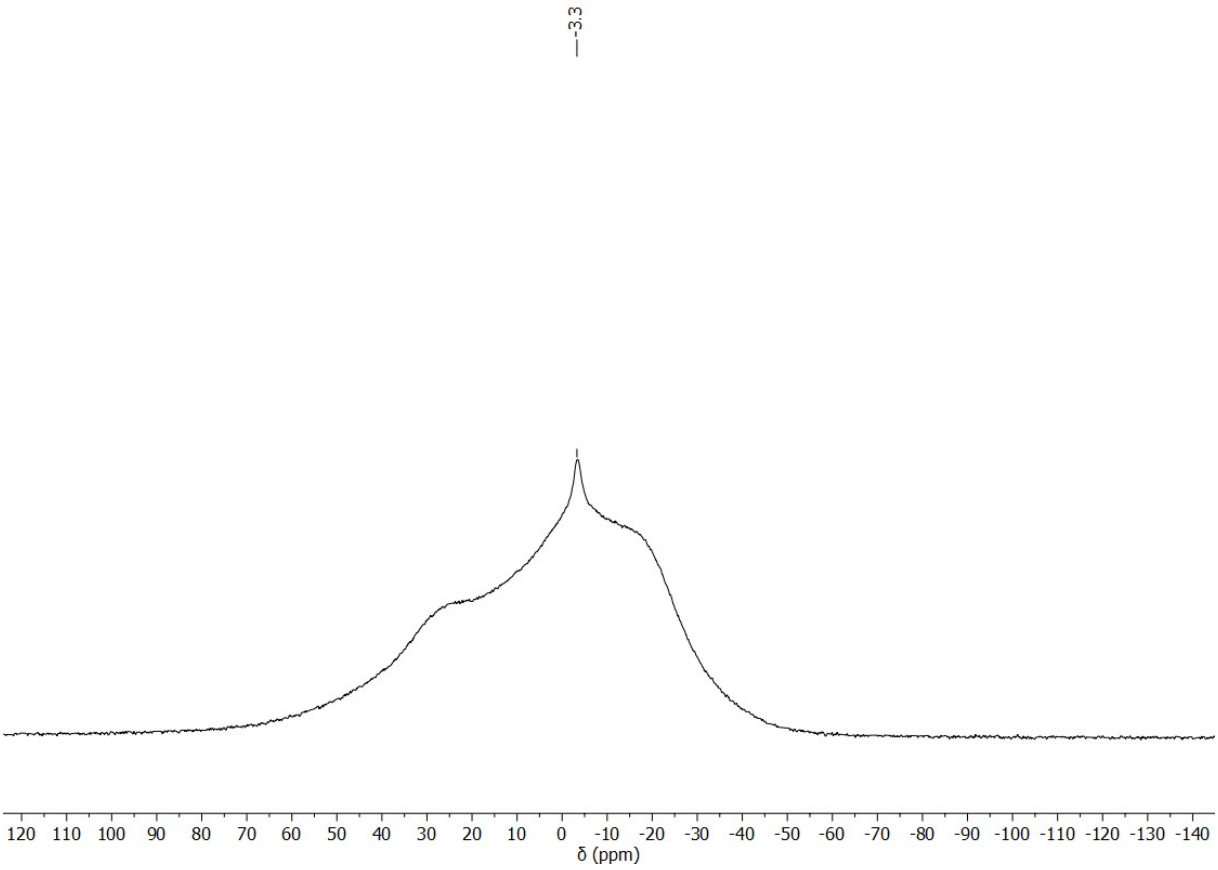


Figure S43. ^{11}B-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

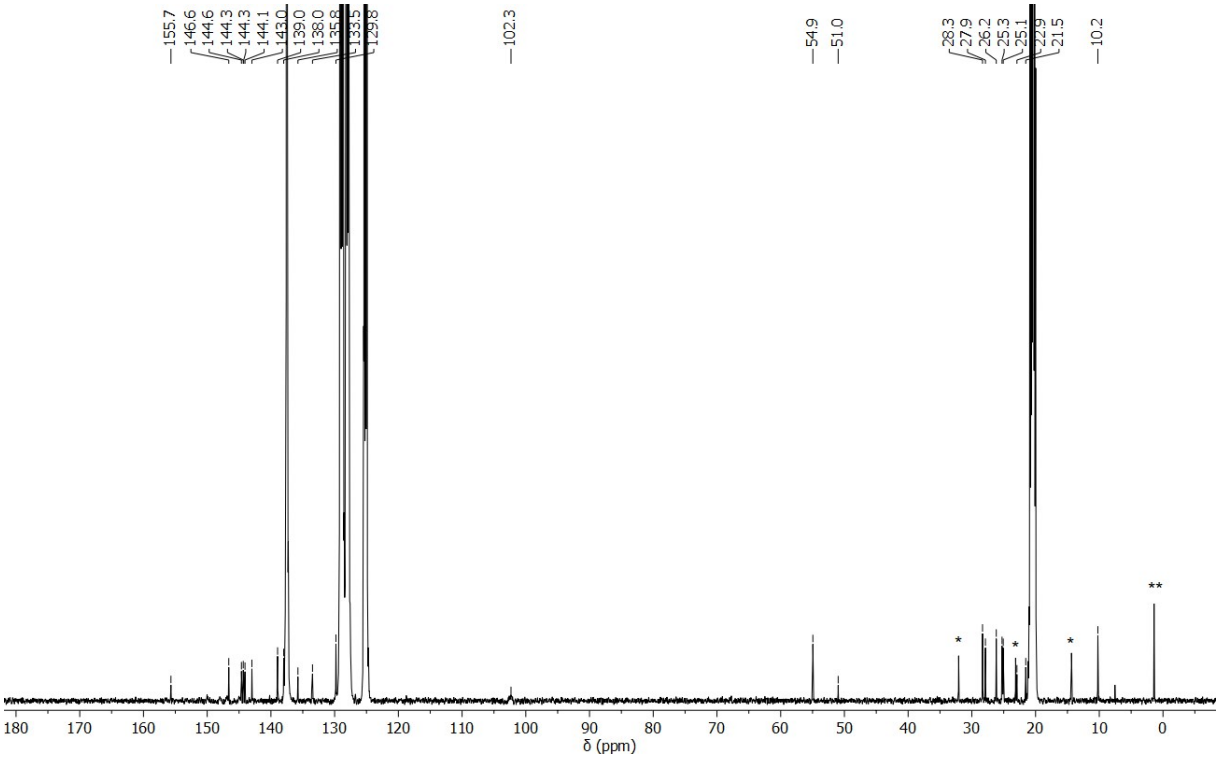


Figure S44. $^{13}C\{^{1}H\}$-NMR spectrum of compound **4** in toluene-d_8 at 300 K (* hexane, ** silicon grease).

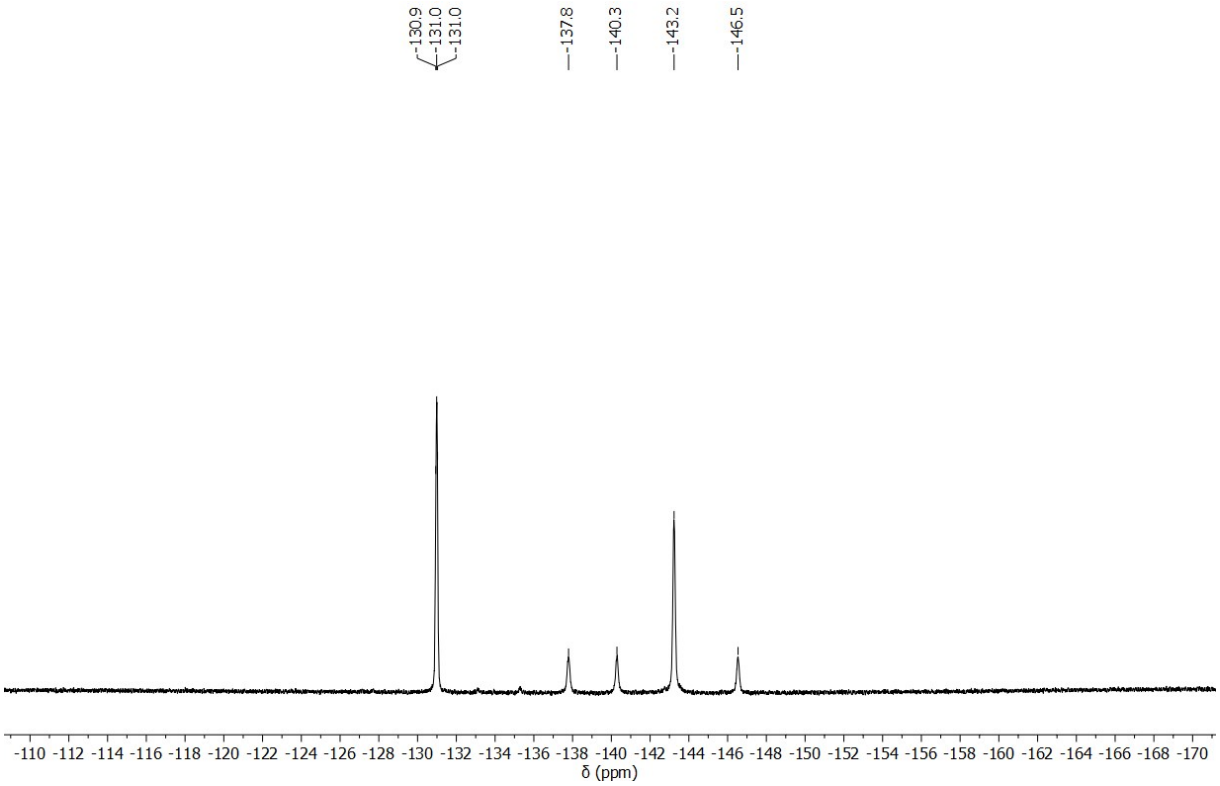


Figure S45. $^{19}F\{^{1}H\}$-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

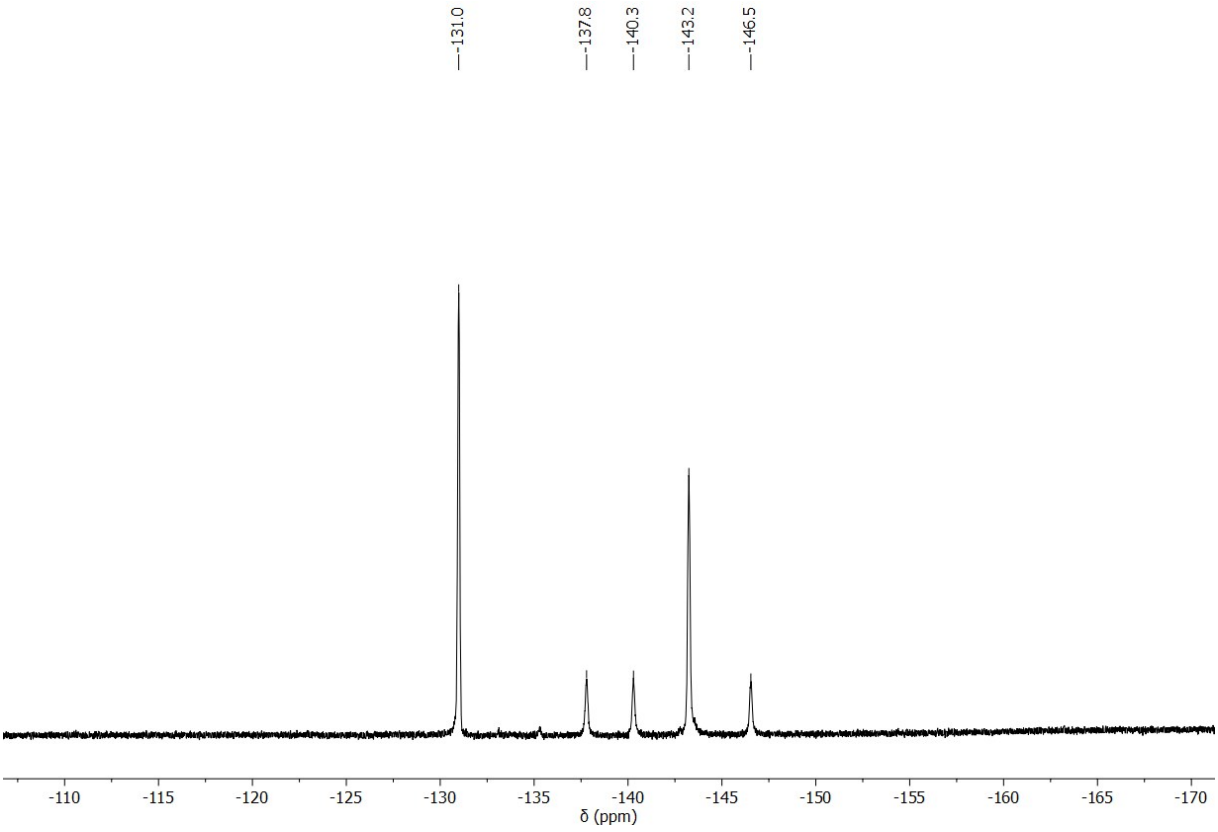


Figure S46. ^{19}F-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

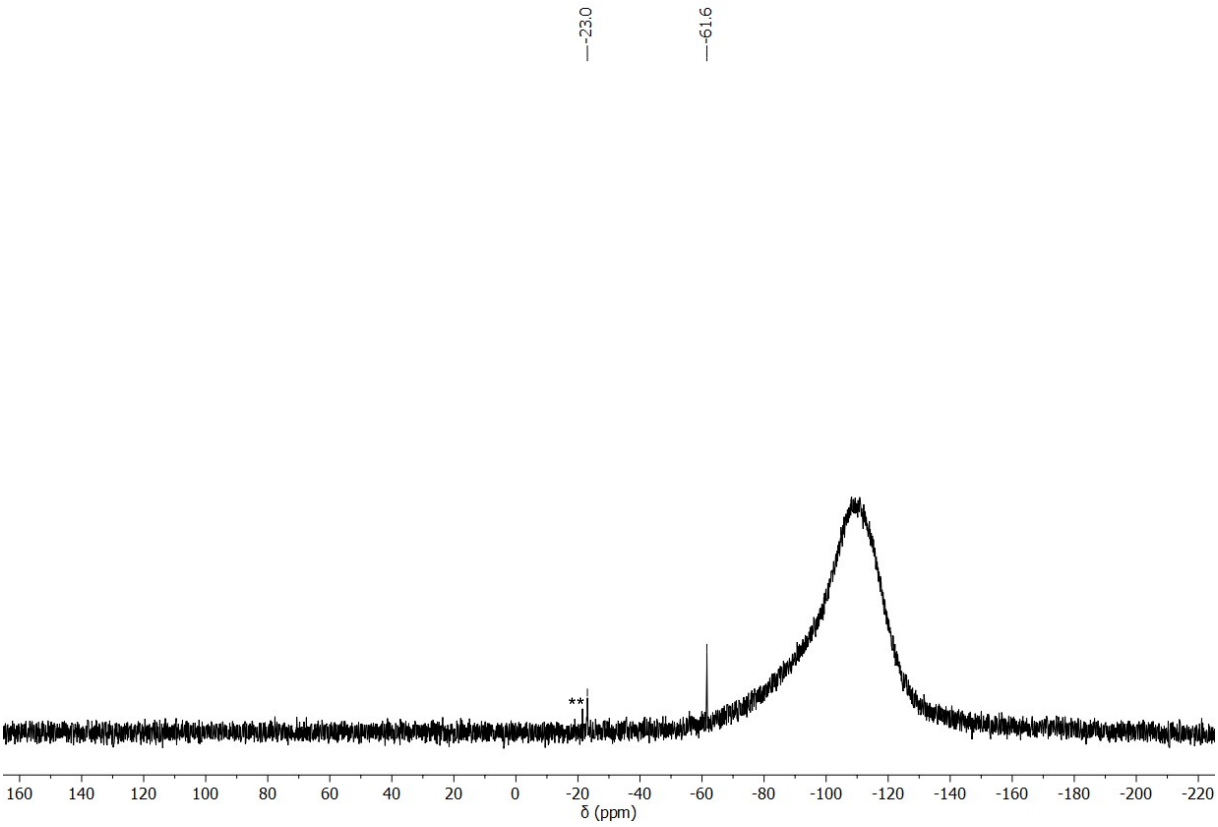


Figure S47. ^{29}Si{^{1}H}IG-NMR spectrum of compound **4** in toluene-d_8 at 300 K (** silicon grease).

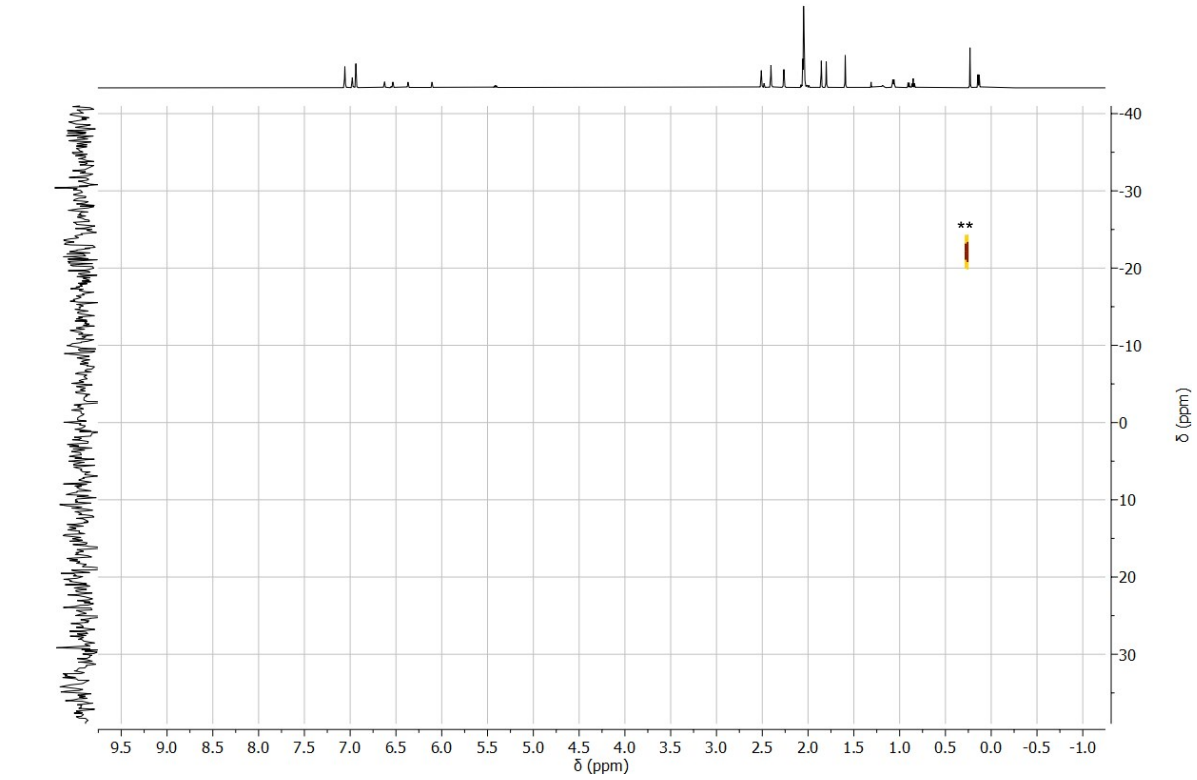


Figure S48. $^{1}H,^{29}Si\{/\}$HSQC-NMR spectrum of compound **4** in toluene-d_8 at 300 K (** silicon grease).

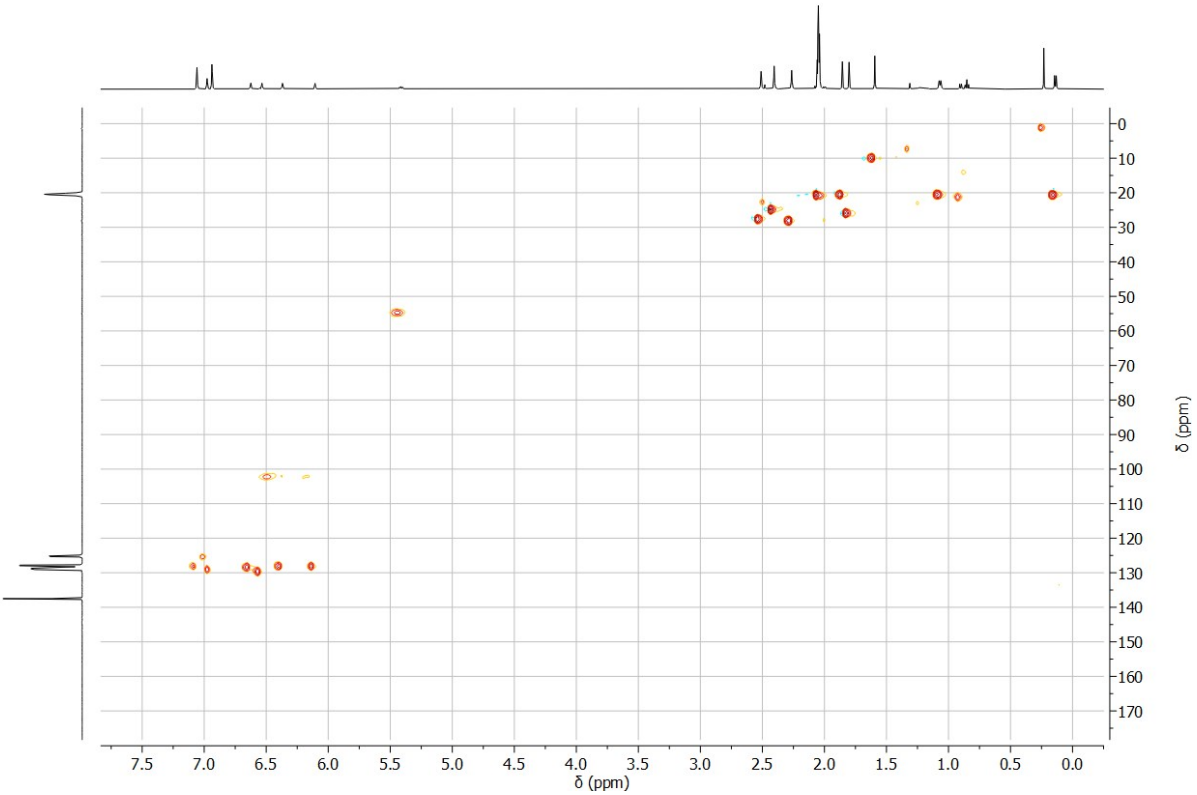


Figure S49. $^{1}H,^{13}C$-HSCQ-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

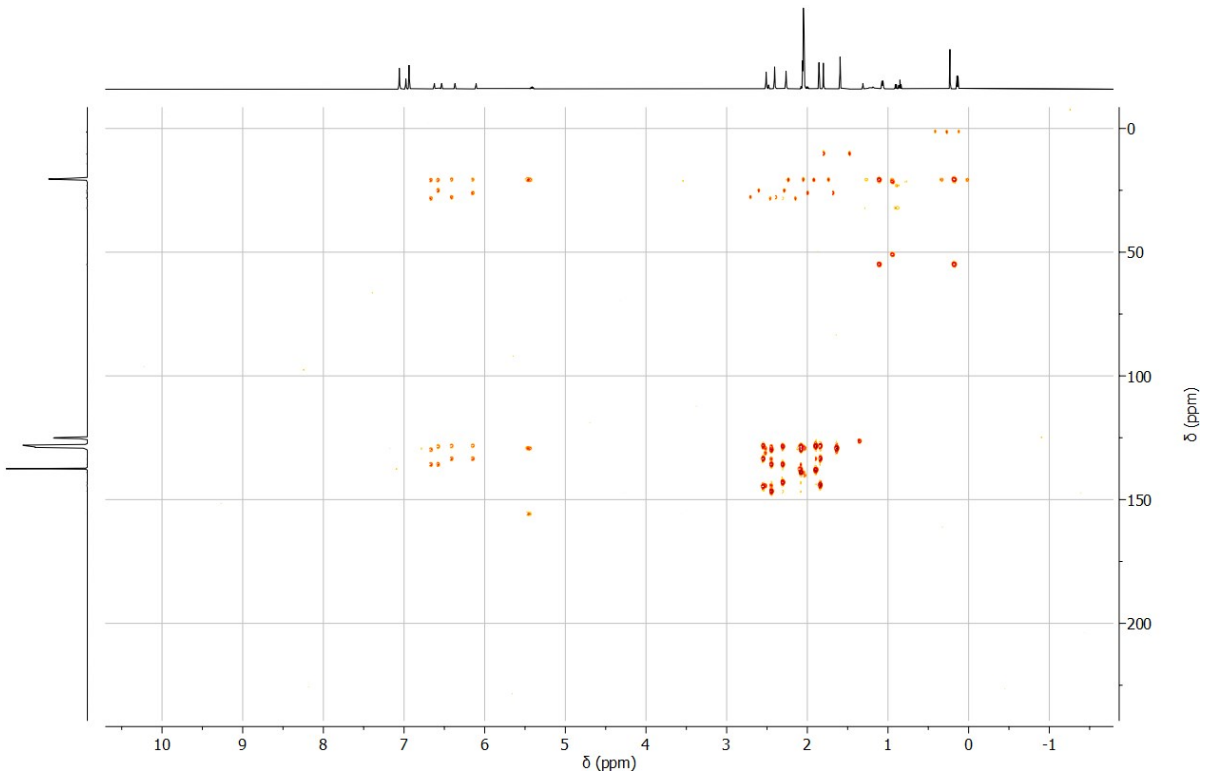


Figure S50. $^{1}H,^{13}C$-HMBC-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

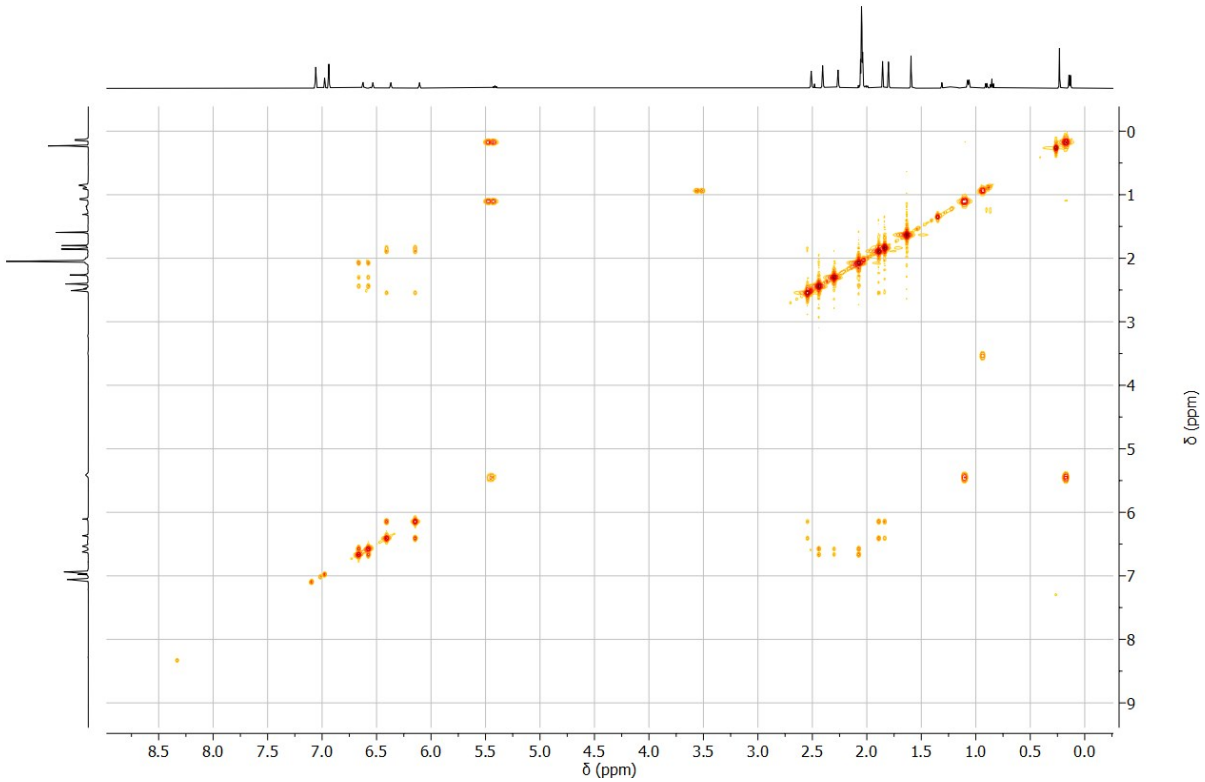


Figure S51. $^{1}H,^{1}H$-COSY-NMR spectrum of compound **4** in toluene-d_8 at 300 K.

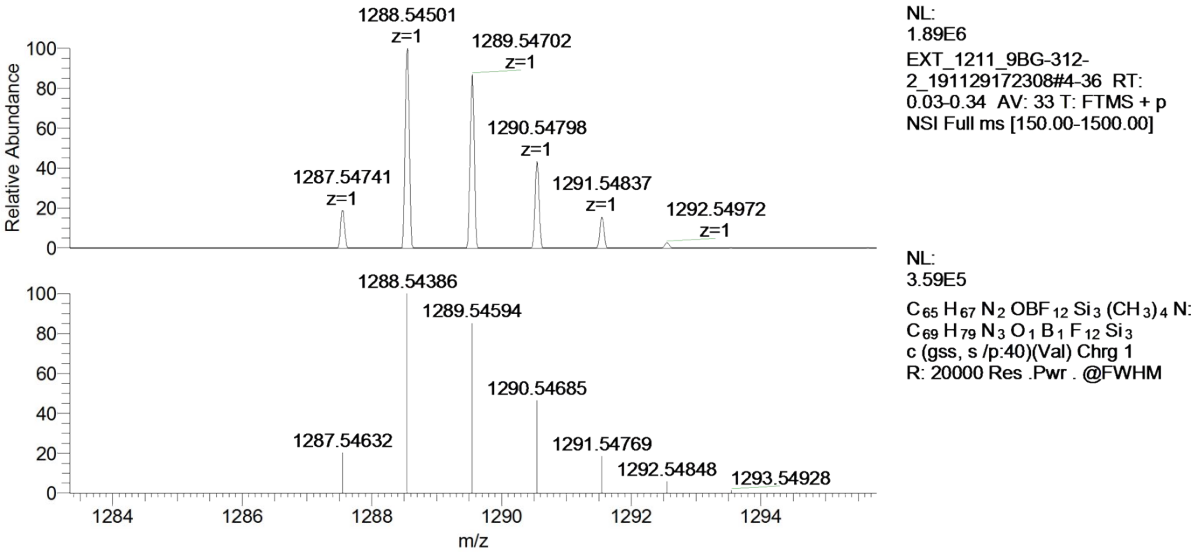


Figure S52. ESI-MS spectrum (positive mode, THF) of compound **3**.

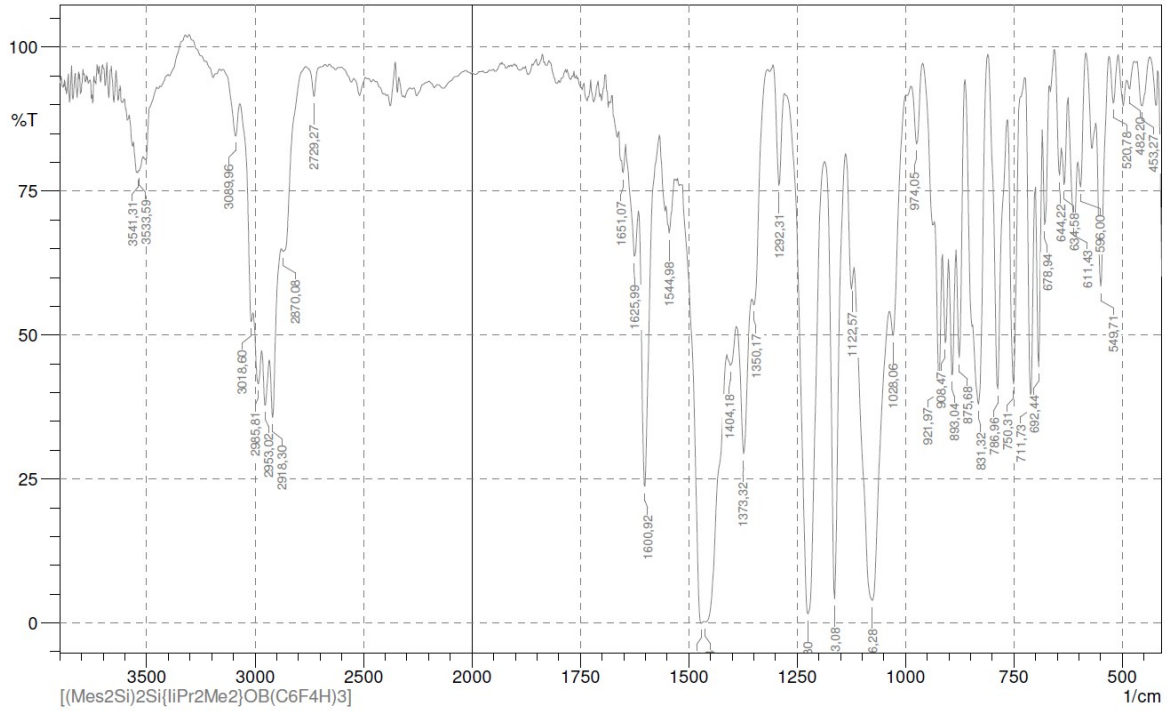


Figure S53. FT-IR spectrum (KBr-pellet) of compound **4**.

2. X-ray crystallographic data and collection parameters

A colorless needle-like specimen of $C_{68}H_{74}BF_{12}N_2OSi_3$, approximate dimensions 0.038 mm x 0.083 mm x 0.219 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

A total of 474 frames were collected. The total exposure time was 3.56 hours. The frames were integrated with the Bruker SAINT software package[S1] using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 51547 reflections to a maximum θ angle of 25.35° (0.83 Å resolution), of which 12199 were independent (average redundancy 4.226, completeness = 99.9%, R_{int} = 14.63%, R_{sig} = 11.77%) and 8179 (67.05%) were greater than $2\sigma(F^2)$. The final cell constants of $\underline{a}$ = 12.0609(7) Å, $\underline{b}$ = 12.8451(9) Å, $\underline{c}$ = 22.3125(14) Å, α = 85.936(2)°, β = 75.667(2)°, γ = 84.697(2)°, volume = 3330.7(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 4707 reflections above 20 σ(I) with 5.007° < 2θ < 52.96°. Data were corrected for absorption effects using the multi-scan method (SADABS).[S2,S3] The ratio of minimum to maximum apparent transmission was 0.901. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9680 and 0.9940.

The structure was solved and refined using the Bruker SHELXTL Software Package,[S4-S6] using the space group P-1, with Z = 2 for the formula unit, $C_{68}H_{74}BF_{12}N_2OSi_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 830 variables converged at R1 = 8.12%, for the observed data and wR2 = 16.52% for all data. The goodness-of-fit was 1.049. The largest peak in the final difference electron density synthesis was 0.383 $e^-/Å^3$ and the largest hole was -0.371 $e^-/Å^3$ with an RMS deviation of 0.077 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.255 g/cm^3 and F(000), 1318 e^-.

The structure contains one disordered hexane solvent molecule that was treated with PART instructions (75% and 25% occupancy) and refined with SIMU, SAME and SADI restraints. Another solvent molecule was treated with the Platon SQUEEZE routine.[S7]

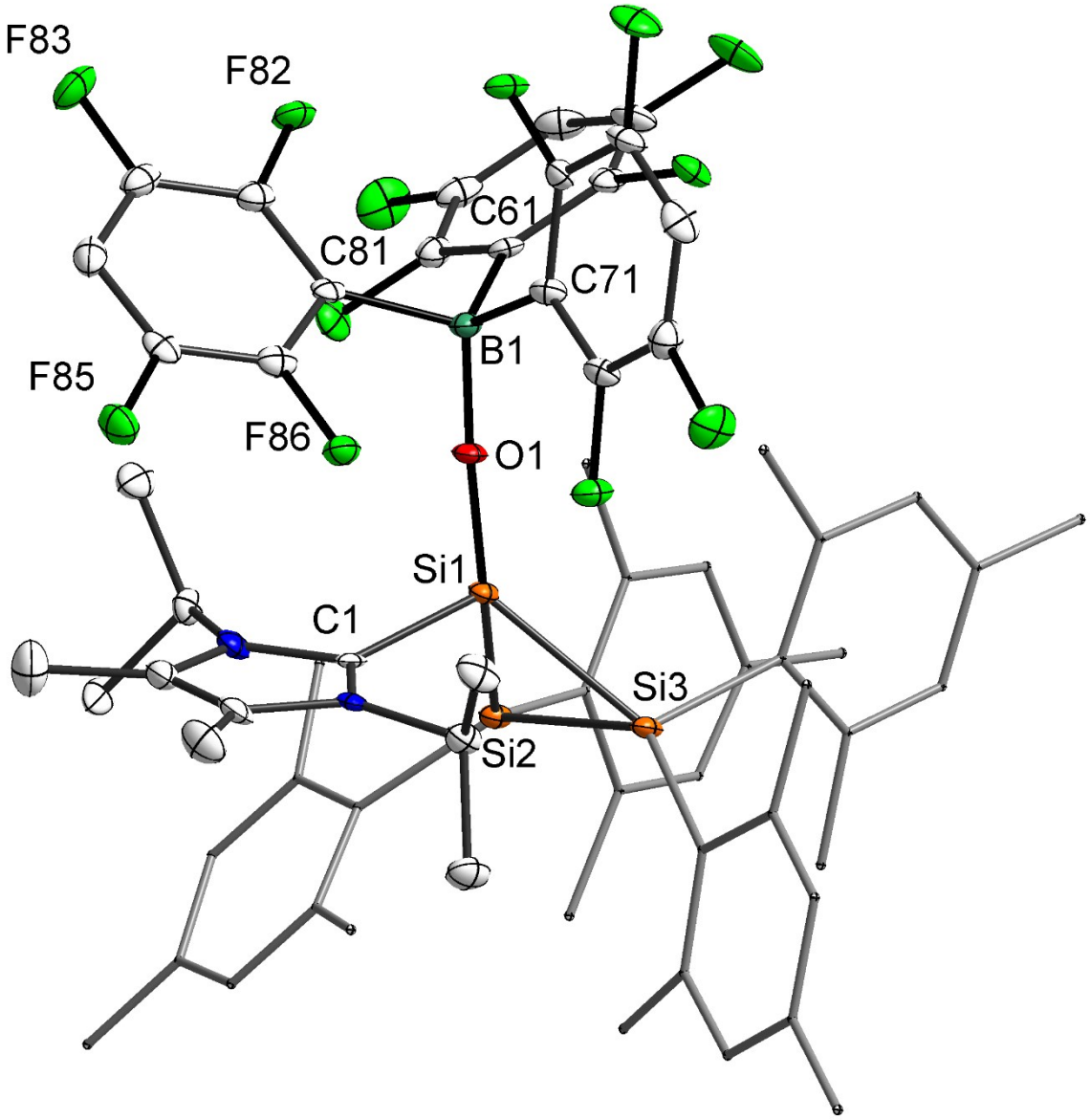


Figure S54. Molecular structure of **4**.

Selected bond length (Å):

Si1−C1 1.955(4), Si1−O1 1.588(3), B1−O1 1.487(6), Si1−Si3 2.377(2), Si1−Si2 2.381(2), Si2−Si3 2.427(2), B1−C61 1.660(6), B1−C71 1.660(6), B1−C81 1.660(6).

Selected angles (°):

Si1-O1-B1 173.0(3), O1-Si1-C1 102.82(16), O1-B1-C61 106.1(3), O1-B1-C71 114.5(3), O1-B1-C81 109.8(3), C1-Si1-Si3 112.25(12), C1-Si1-Si2 103.74(13), O1-Si1-Si2 135.27(12), O1-Si1-Si3 135.48(12), Si3-Si1-Si2 61.34(5)

Table S1. Crystallographic information of **4**·solvent.

Compound	**4**·solvent
Empirical formula	$C_{68}H_{74}BF_{12}N_2OSi_3$
Formula weight /g·mol^{-1}	1258.37
Crystal color, shape	colorless, needle-like specimen
Crystal size / mm^3	0.038x0.083x0.219
Crystal system	triclinic
Space group	$P\bar{1}$
a / Å *b* / Å *c* / Å	12.0609(7) 12..8451(9) 22.3125(14)
α / ° β / ° γ / °	85.936(2) 75.667(2) 84.697(2)
V / Å^3	3330.7(4)
Z	2
T / K	100(2)
Completeness to θ 25.24°/ %	99.9
ρ_{calc} / g·cm^{-3}	1.255
μ(Mo) / mm^{-1}	0.147
2 θ range / °	5.01-52.96
Reflections measured	51547
Independent reflections	12199
R(int)	0.1463
Ind. reflections ($I > 2\sigma(I)$)	4707
Parameters	830
Restraints	826
R_1 ($I > 2\ \sigma(I)$)	0.0812
wR_2 (all data)	0.1652
GooF (all data)	1.049
Max. peak/hole / e$^-$·Å^{-3}	0.077/-0.371
Absorption correction type	multi-scan
Min. /Max. transmission	0.9680/0.9940

3.Calculation of the Proton affinity (PA) of A

Geometry optimizations and frequency analysis were performed on the TPSS-D3/def2-TZVP level of theory[S8] for **A** and [**A**-H]$^+$ using Turbomole.[S9] This was done once in the gas phase and once with COSMO.[S10] The obtained coordinates were used for single point calculations on the B97-D-D3/def2-TZVP level of theory[S11] in the gas phase and with the application of COSMO.

Table S2. Calculated compounds **A** and [**A-H**]$^+$ in the gas phase and with COSMO at the TPSS-D3/def2-TZVP level of theory.

	TPSS-D3/def2-TZVP Gas phase		**TPSS-D3/def2-TZVP COSMO**	
	A	**[A-H]$^+$**	**A**	**[A-H]$^+$**
Energy /Hartree	-2808.925522446	-2809.37970174	-2808.945421091	-2809.437290508
ZPE correction	0.9800544	0.9907698000	0.9783645	0.9882665
$E_{corrected}$ /Hartree	-2807.945468100	-2808.38893194	-2807.967056591	-2808.449024008
PA /Hartree	-0.44346384		-0.481967417	
PA /kJ/mol	1164.31		1265.41	

Table S3. Calculated compounds **A** and [**A-H**]$^+$ in the gas phase and with COSMO at the B97-D3/def2-TZVP level of theory.

	B97-D/ def2-TZVP Gas phase		**B97-D/ Def2-TZVP COSMO**	
	A	**[A-H]$^+$**	**A**	**[A-H]$^+$**
Energy /Hartree	-2807.068063062	-2807.523941845	-2807.087533197	-2807.581815800
PA /Hartree	-0.455878783		-0.494282603	
PA /kJ/mol	1196.91		1297.74	

4. Calculated model compound of 4

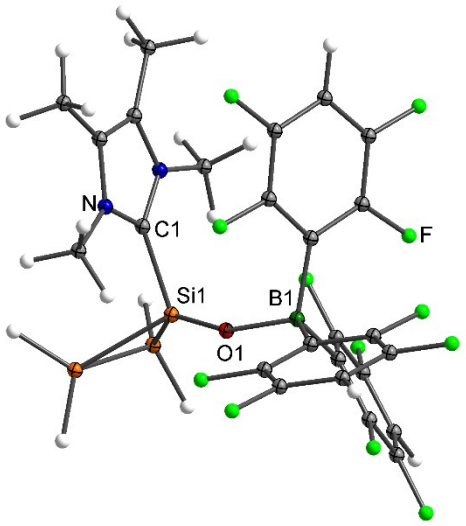


Table S4. Comparison of bond lengths/Å and angles/° in **4** and the calculated model compound.

	4	**Model compound**
Si1-O1-B1	173.0(3)	143.098
Si1−O1	1.588(3)	1.5919
B1−O1	1.487(6)	1.5027
Si1−C1	1.955(4)	1.9098
Si1−Si2	2.381(2)	2.3328
Si1−Si3	2.377(2)	2.3176
Si2−Si3	2.427(2)	2.3600
Si2-Si1-Si3	61.34(5)	60.991

5. References

[S1] Bruker VENTURE and (2012) SAINT (Version 8.27a). Bruker AXS Inc., Madison, Wisconsin, USA.

[S2] An Empirical Correction for Absorption Anisotropy, Blessing, R. H. (1995). Acta Cryst., A51, 33–38.

[S3] Sheldrick, G.M., SADABS (2012/1) 'Siemens Area Detector Absorption Correction' Universität Göttingen, Göttingen, Germany.

[S4] Sheldrick, G.M., (2002). SHELXTL. Version 6.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

[S5] Sheldrick, G. M., (1997). SHELXS97. Universität Göttingen: Göttingen, Germany.

[S6] Sheldrick, G. M., SHELXL2014 structure refinement program.

[S7] a) P. v. d. Sluis, A. L. Spek, *Acta Crystallogr., Sect. A: Found. Crystallogr.* 1990, **46**, 194–201; b) A. L. Spek, *Acta Cryst.* 2015, **C71**, 9–18.

[S8] J. Tao, J. P. Perdew, V. N. Staroverov, G. E. Scuseria, *Phys. Rev. Lett.* 2003, **91** (14), 146401, 1–4.

[S9] TURBOMOLE V7.3, 2018, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

[S10] A. Schäfer, A. Klamt, D. Sattel, J. C. F. Lohrenz, F. Eckert, *Phys. Chem. Chem. Phys.* 2000*,* **2** (10)*, 2187–2193.*

[S11] A. D. Becke, *J. Chem. Phys.* 1997, **107** (2), 8554–8560.

6. Cartesian Coordinates of all compounds

Cartesian Coordinates of compound [**A-H**]$^+$

Si	3.0290631	7.6359405	6.3218759
Si	3.7892294	6.3836938	4.4704730
Si	2.5745747	8.4173809	4.1463430
N	1.3630746	8.1471869	8.6355022
N	1.2060534	6.0571178	8.0510502
C	1.8296478	7.2241997	7.7456854
C	0.4577873	7.5541480	9.5094228
C	0.3487961	6.2370322	9.1318634
C	1.8421409	9.5597067	8.6448939
H	2.3236518	9.6718833	7.6692816
C	0.6978669	10.5713579	8.7146437
H	1.0981356	11.5536732	8.4508777
H	-0.0941619	10.3267881	8.0015310
H	0.2677602	10.6483054	9.7145018
C	2.9016029	9.7563396	9.7299569
H	3.3066782	10.7697539	9.6583502
H	2.4815012	9.6289035	10.7318982
H	3.7228099	9.0461379	9.6006996
C	1.5289969	4.7778837	7.3602475
H	2.1974644	5.0894612	6.5529557
C	0.3042187	4.1212469	6.7265961
H	0.6566495	3.3445870	6.0432528
H	-0.3459521	3.6538275	7.4700811
H	-0.2787725	4.8416747	6.1474838
C	2.3039085	3.8419054	8.2882589
H	2.6280713	2.9744175	7.7085289
H	3.1875844	4.3387375	8.6971703
H	1.6896518	3.4799503	9.1165337
C	-0.2413871	8.2510387	10.6288273
H	0.4429253	8.8731267	11.2108444
H	-1.0578360	8.8856569	10.2698899
H	-0.6695349	7.5077876	11.3042673
C	-0.5439846	5.1866709	9.7025631
H	-1.3881482	4.9766986	9.0376186
H	-0.0177426	4.2479542	9.8869303
H	-0.9502828	5.5343261	10.6543075
C	2.9908583	4.6769061	4.2688591

C	1.9150840	4.3664866	3.4043328
C	1.4822380	3.0409919	3.2827964
H	0.6581535	2.8238190	2.6058390
C	2.0743189	1.9947797	3.9900671
C	3.1356513	2.3090276	4.8435959
H	3.6224192	1.5129356	5.4047154
C	3.6071844	3.6151967	4.9885554
C	1.2018846	5.4075439	2.5839507
H	1.8793593	6.1989679	2.2550083
H	0.7427312	4.9554421	1.7006317
H	0.4048457	5.8946572	3.1551486
C	1.6105307	0.5714502	3.8168461
H	0.5755777	0.5301000	3.4661274
H	2.2322990	0.0525632	3.0767985
H	1.6852618	0.0116243	4.7542616
C	4.7817058	3.8426212	5.9085328
H	4.6566378	4.7549233	6.5057622
H	4.9076328	2.9983469	6.5918112
H	5.7097525	3.9623247	5.3406503
C	5.6210930	6.2598698	4.0387090
C	6.7016005	6.6098185	4.8821926
C	8.0121589	6.4550242	4.4226194
H	8.8314064	6.7285419	5.0849310
C	8.3036141	5.9719224	3.1448805
C	7.2300923	5.6529210	2.3122556
H	7.4250327	5.3000201	1.3011970
C	5.9054643	5.7879359	2.7321543
C	6.5097177	7.1789569	6.2648498
H	5.8015973	6.5886901	6.8552935
H	7.4621591	7.2093820	6.8008222
H	6.1179789	8.2016879	6.2194357
C	9.7275637	5.7897905	2.6869511
H	9.8118681	5.8941260	1.6013734
H	10.3936235	6.5167559	3.1608485
H	10.0913748	4.7887731	2.9510073
C	4.8112530	5.4514416	1.7483146
H	3.9777123	6.1638612	1.8171562
H	5.1916698	5.4843409	0.7238703
H	4.3957527	4.4540727	1.9274303
C	0.8930717	8.5624071	3.3115389
C	-0.3463628	8.3544450	3.9577044
C	-1.5364420	8.5605583	3.2575108
H	-2.4823106	8.3927092	3.7695351
C	-1.5487102	8.9606785	1.9184084
C	-0.3193128	9.1313028	1.2797592
H	-0.2992617	9.4116147	0.2283185
C	0.8927670	8.9383035	1.9466801
C	-0.4331711	7.8836058	5.3867313
H	-0.0070973	8.6166594	6.0806049
H	-1.4732954	7.7049194	5.6738815
H	0.1231412	6.9507654	5.5284382
C	-2.8455227	9.2061208	1.1913429
H	-2.7461536	9.0003358	0.1216979
H	-3.6509369	8.5845207	1.5933626
H	-3.1532326	10.2540441	1.2974364
C	2.1789440	9.1151018	1.1787016
H	2.8839500	8.3014609	1.3939176
H	1.9920228	9.1192924	0.1016934
H	2.6804290	10.0522932	1.4442777
C	3.5614818	10.0286141	4.0434868
C	2.9869941	11.1627859	4.6853209
C	3.6994725	12.3567083	4.7617189
H	3.2403236	13.2107874	5.2570793
C	4.9762465	12.4929264	4.2031698

C	5.5020453	11.3998042	3.5209372
H	6.4714847	11.4942473	3.0345683
C	4.8195300	10.1797771	3.4189477
C	1.5817016	11.1379261	5.2326633
H	1.3786448	10.2115644	5.7832505
H	1.4073495	11.9874938	5.8986268
H	0.8454925	11.1842123	4.4223693
C	5.7419732	13.7848787	4.3268737
H	5.1043703	14.6460969	4.1013136
H	6.1167384	13.9170053	5.3494115
H	6.6005662	13.8030829	3.6504276
C	5.4583514	9.1098228	2.5717092
H	4.8011768	8.2499987	2.4428072
H	5.6923678	9.5120036	1.5795650
H	6.3940015	8.7491177	3.0098889
H	4.0163091	8.5328813	6.9651348

Cartesian Coordinates of the model compound of **4**

B	7.9246522	7.1502892	17.5587192
O	7.6954538	8.5034495	16.9466640
C	6.5304551	6.2872997	17.5123963
C	9.1590468	6.5090781	16.6750305
C	8.2476165	7.3444335	19.1819054
N	7.0148796	11.3864522	18.8739598
C	8.1893250	10.9050932	18.3904243
C	7.1732174	11.8733073	20.1613217
C	5.7303013	11.3191501	18.1679987
N	9.0941082	11.0988984	19.3835756
C	8.4946828	11.6878354	20.4871042
C	10.4869790	10.6462541	19.3606512
Si	8.3530969	9.9398882	16.7506088
Si	7.9593541	11.5762905	15.1353580
Si	10.1426396	10.7760467	15.5383326
H	10.5411927	9.9043756	14.4065488
H	11.3017943	11.5370828	16.0766684
H	7.4197934	11.3330860	13.7753593
H	7.5056534	12.8922888	15.6620771
C	6.0426809	12.4154153	20.9629108
C	9.2350141	11.9600886	21.7490064
H	5.7804591	10.5282505	17.4207569
H	5.3126593	11.6296659	21.1872633
H	5.5260733	13.2251461	20.4367307
H	6.4142533	12.8079764	21.9111106
H	10.0831723	12.6342111	21.5853349
H	9.6207606	11.0308554	22.1840147
H	8.5684649	12.4226971	22.4789015
H	10.7135328	10.2836279	18.3606151
C	9.0242970	5.5342641	15.6837091
C	10.4348567	7.0715293	16.7461658
F	7.8367107	4.9232335	15.4601802
C	10.0796332	5.1437767	14.8574667
F	9.8667326	4.1884514	13.9225332
C	11.3341364	5.7227759	14.9653153
C	11.4957740	6.7058044	15.9309619
H	12.1511795	5.4223379	14.3205485
F	12.6974034	7.3195662	16.0778465
F	10.6879059	8.0542053	17.6680209
C	6.5143812	5.0054110	18.0682282
C	5.2948314	6.7328771	17.0399442
F	7.6733650	4.4836458	18.5508787
C	5.3748014	4.2154792	18.1454352
F	5.4493454	2.9784791	18.6931630
C	4.1593042	4.6824513	17.6639597
C	4.1405241	5.9533948	17.1121863
H	3.2622367	4.0772673	17.7158037
F	2.9736072	6.4556110	16.6340150
F	5.1452954	7.9643957	16.4817419
C	7.3697101	8.1132736	19.9545068
C	9.2962895	6.7743614	19.9104670
F	10.1764918	5.9352795	19.3234430

C	9.4958153	7.0179714	21.2699065
F	10.5514673	6.4489915	21.8985629
C	8.6320745	7.8279459	21.9937379
C	7.5523221	8.3657303	21.3095248
H	8.7759590	7.9998390	23.0538343
F	6.6523538	9.1406123	21.9781281
F	6.2484960	8.6426163	19.3882792
H	5.5149821	12.2785757	17.6910560
H	4.9521507	11.0722218	18.8900661
H	10.6135374	9.8325071	20.0780428
H	11.1440863	11.4801035	19.6156820