

Electronic Supplementary Information

N=N Bond Cleavage in Diazirines by a Cyclic Diborane(4) Compound

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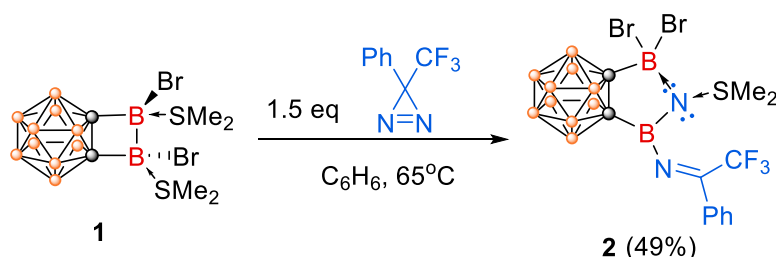
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Experimental Section

General Procedure. All reactions were carried out under a dry argon atmosphere with the rigid exclusion of air and moisture using standard Schlenk line and glovebox techniques. All organic solvents were dried and distilled by standard methods prior to use. NMR spectra were acquired on a Bruker DPX 500 NMR spectrometer (^1H : 500 MHz, ^{11}B : 160 MHz, $^{13}\text{C}\{^1\text{H}\}$: 125 MHz, ^{19}F : 470 MHz, ^{31}P : 202 MHz) or on a Bruker DPX 400 NMR spectrometer (^1H : 400 MHz, $^{13}\text{C}\{^1\text{H}\}$: 100 MHz) at 298 K. All chemical shifts were reported in δ unit with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external $\text{BF}_3\cdot\text{OEt}_2$ (0.00 ppm) for boron chemical shifts, to external CFCl_3 (0.00 ppm) for fluorine chemical shifts, to external 85% H_3PO_4 (0.00 ppm) for phosphorus chemical shifts. The data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, sept = septet, m = multiplet or unresolved, br = broad), coupling constant, integration, and assignment. Mass spectra were obtained on a Bruker Solarix 9.4T ICR Mass Spectrometer or a Thermo Scientific Q Exactive Focus Orbitrap Mass Spectrometer. Carborane-fused diboracycle **1** was prepared according to literature procedures.¹ All other chemicals were purchased from either Aldrich, J&K, TCI or Acros Chemical Co. and used as received unless otherwise specified.



Synthesis of 2. To a benzene solution (6 mL) of 1,2-[$\text{B}_2\text{Br}_2(\text{SMe}_2)_2$]-1,2- $\text{C}_2\text{B}_{10}\text{H}_{10}$ (**1**; 90 mg, 0.2 mmol) was added a benzene solution (5 mL) of 3-phenyl-3-(trifluoromethyl)-3H-diazirine (TPD) (56 mg, 0.3 mmol) at room temperature. The reaction mixture was heated at 65 °C overnight. The reaction mixture was allowed to slowly cool down to room temperature, from which colorless block shaped crystals of **2** were obtained. After removal of volatiles in vacuo, the residue was washed by cold toluene (2 mL) and then dissolved in DCM. The resulting solution was stored in a freezer at -30 °C overnight to give **2** as colorless crystals suitable for X-ray analyses (57 mg, 49%).

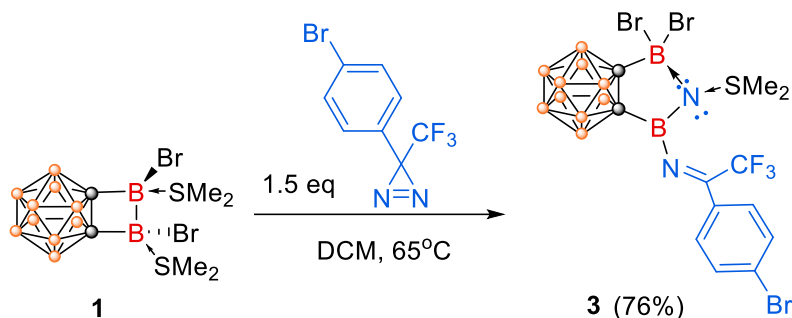
^1H NMR (500 MHz, CD_2Cl_2): δ 7.91 (d, $^3J_{\text{HH}} = 8.3$ Hz, 2H), 7.75 (t, $^3J_{\text{HH}} = 7.5$ Hz, 1H), 7.63 (t, $^3J_{\text{HH}} = 7.8$ Hz, 2H) (phenyl *H*), 2.99 (s, 3H), 2.94 ppm (s, 3H) ($\text{S}(\text{CH}_3)_2$).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CD_2Cl_2): δ 154.35 (q, $^2J_{\text{CF}} = 33.9$ Hz, $\text{N}=\text{C}-\text{CF}_3$), 135.63, 130.21, 129.80, 129.79, 128.82 (aromatic C), 118.21 (q, $^1J_{\text{CF}} = 285.8$ Hz, CF_3), 31.38, 30.87 ($\text{N}(\text{CH}_3)_2$).

^{11}B NMR (128 MHz, CD_2Cl_2): δ 29.13 (s, 1B, *exo-B*), -0.25 (s, 1B, *exo-B*), -1.73 (d, $^1J_{\text{BH}} = 157.6$ Hz, 1B, cage B), -2.98 (d, $^1J_{\text{BH}} = 148.3$ Hz, 1B, cage B), -6.12 (d, $^1J_{\text{BH}} = 148.0$ Hz, 2B, cage B), -9.84 to -11.90 ppm (m, 6B, cage B).

^{19}F NMR (470 MHz, CD_2Cl_2): δ -66.65 (s, 3F).

HRMS (ESI-MS) calc. for $\text{C}_{12}\text{H}_{21}\text{B}_{12}\text{Br}_2\text{F}_3\text{N}_2\text{S}$ $[\text{M}+\text{H}]^+$: 571.31509. Found: 571.31675.



Synthesis of 3. To a dichloromethane (DCM) solution (6 mL) of 1,2-[B₂Br₂(SMe₂)₂]-1,2-C₂B₁₀H₁₀ (**1**; 67 mg, 0.15 mmol) was added a DCM solution (5 mL) of 3-(4-bromophenyl)-3-(trifluoromethyl)-3H-diazirine (60 mg, 0.23 mmol) at room temperature. The reaction mixture was heated at 65 °C overnight. The reaction mixture was allowed to slowly cool down to room temperature. After removal of volatiles in vacuo, the residue was washed by cold ether (2 mL) and then dissolved in DCM. The light-pink solution was stored in a freezer at -30 °C overnight to afford **3** as a white solid (75 mg, 76%).

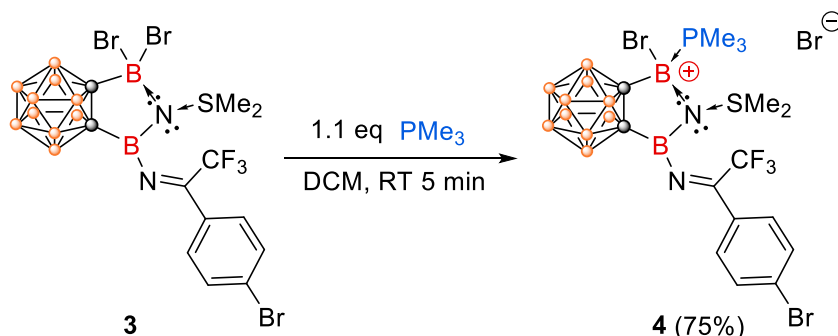
¹H NMR (500 MHz, CD₂Cl₂): δ 7.78 (s, 4H, aromatic *H*), 2.99 (s, 3H, S(CH₃)₂), 2.96 ppm (s, 3H, S(CH₃)₂).

¹³C{¹H} NMR (100 MHz, CD₂Cl₂): δ 153.65 (m, ²J_{CF} = 35.3 Hz, N=C-CF₃), 133.70, 131.34, 131.11, 127.92 (aromatic C), 118.16 (m, ¹J_{CF} = 285.9 Hz, CF₃), 32.09, 31.52 ppm (N(CH₃)₂).

¹¹B NMR (128 MHz, CD₂Cl₂): δ 29.63 (s, 1B, *exo*-B), -0.44 (s, 1B, *exo*-B), -1.75 (d, ¹J_{BH} = 150.4 Hz, 1B, cage B), -3.08 (d, ¹J_{BH} = 168.8 Hz, 1B, cage B), -6.28 (d, ¹J_{BH} = 146.4 Hz, 2B, cage B), -10.06 to -12.18 ppm (m, 6B, cage B).

¹⁹F NMR (470 MHz, CD₂Cl₂): δ -66.81 (s, 3F).

HRMS (APCI-positive mode) calc. for C₁₂H₂₀B₁₂Br₃F₃N₂S [M-Br]⁺: 571.08389. Found: 571.08159.



Synthesis of 4. To a DCM solution (6 mL) of **3** (65 mg, 0.1 mmol) was added a toluene solution (0.11 mL) of trimethylphosphine (9 mg, 0.11 mmol) at room temperature and the mixture was stirred at room temperature for 5 minutes. The resultant solution was then filtered and concentrated to *ca.* 1 mL. This solution was kept in a freezer at -30 °C overnight to give **4** as colorless crystals (55 mg, 75%).

¹H NMR (400 MHz, CD₂Cl₂): δ 7.79 (s, 4H, aromatic *H*), 3.62 (brs, 3H, S(CH₃)₂), 3.28 (s, 3H, S(CH₃)₂), 1.94 ppm (d, ²J_{PH} = 11.9 Hz, 9H, P(CH₃)₃).

¹¹B NMR (128 MHz, CD₂Cl₂): 31.82 (brs, 1B, *exo*-B), -0.98 (br, m, 3B, cage B), -5.99 (br, m, 3B, cage B), -10.78 ppm (br, m, 3B, cage B), the signal of the *exo*-sp³B falls in the range of those of cage Bs.

¹⁹F NMR (470 MHz, CD₂Cl₂): δ -66.80 (s, 3F, CF₃).

³¹P NMR (162 MHz, CD₂Cl₂): δ -12.73 ppm (m, P(CH₃)₃).

Noted that it was not feasible to take the ¹³C NMR spectrum, HRMS and elemental analyses since **4** was thermally unstable.

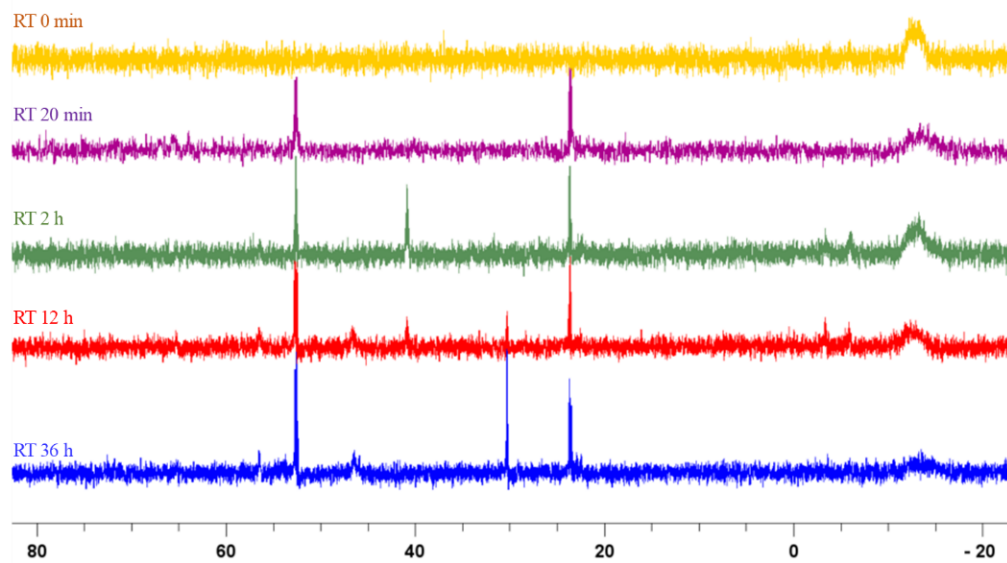


Figure S1. Time dependent ^{31}P NMR spectra of **4** in CD_2Cl_2 .

Crystal Data

X-ray Structure Determination. Single crystals were immersed in Paraton-*N* oil and were sealed under argon in thin-walled glass capillaries. The data were collected at 297 K (for **2**) or 245 K (for **4**) on a Bruker D8 Venture X-Ray Diffractometer using Mo-K α radiation. An empirical absorption correction was applied using the SADABS program.² All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F^2 using the SHELXTL program package.³ All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and refinement are given in Table S1.

Details of the crystal structures were deposited in the Cambridge Crystallographic Data Centre with CCDC 2324682 for **2** and 2324683 for **4**.

Table S1. Crystal Data and Summary of Data Collection and Refinement.

Compound	2 ·C ₆ H ₆	4 ·1.5CH ₂ Cl ₂
Formula	C ₁₈ H ₂₇ B ₁₂ Br ₂ F ₃ N ₂ S	C _{16.5} H ₃₂ B ₁₂ Br ₃ F ₃ N ₂ PSCl ₃
M _w	650.01	854.27
Crystal size (mm ³)	0.50 x 0.40 x 0.30	0.40 x 0.30 x 0.20
Crystal system	Orthorhombic	Monoclinic
Space Group	Pbca	C2/c
a, Å	10.0967(4)	16.7138(19)
b, Å	23.8308(10)	35.995(4)
c, Å	24.3101(11)	13.3816(16)
β , deg	90	118.474(3)
V, Å ³	5849.3(4)	7076.6(15)
Z	8	8
D_{calcd} Mg/m ³	1.476	1.604
Radiation (Å)	0.71073	0.71073
2 θ range, deg	5.244 to 50.498	4.696 to 50.500
μ , mm ⁻¹	2.876	3.782
F(000)	528	3352
No. of obsd reflns	5294	6398
No. of params refnd	343	368
Goodness of fit	1.058	1.044
R1	0.0553	0.0840
wR2	0.1190	0.2148

Computational Details

Geometry optimizations were carried out with the Gaussian16 program, Revision C.01⁴ at the M06-2X⁵-D3⁶⁻⁷/6-311G(d,p) level of density functional theory. Frequency calculations were made to determine the characteristics of all stationary points as energy minimum or transition states and obtain thermal corrections. Intrinsic reaction coordinates (IRC)⁸⁻⁹ were calculated to confirm that transition states lead to relevant intermediates. The solvent effect of benzene was taken into consideration by performing single-point solvation energy calculations with the conductor-like polarizable continuum model (CPCM)¹⁰⁻¹³ using UAKS radii. The natural bond orbital (NBO)¹⁴ calculations were performed at the B3LYP¹⁵⁻¹⁶⁺-D3⁶⁻⁷/6-311+G(d,p) level of density functional theory.

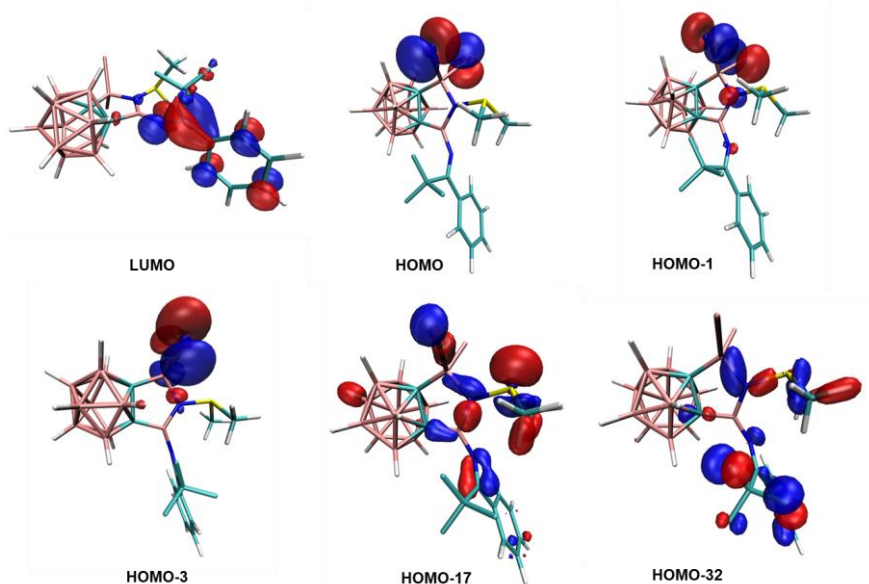


Figure S2. Plots of selected molecular orbitals of **2** calculated at the B3LYP-D3/6-311+G(d,p) level of theory (isovalue 0.04 a. u.).

Table S2. Occupancy of lone-pairs of **2** at the B3LYP-D3/6-311+G(d,p) level of theory.

LP	Occupancy	%p	%s
LP S1	1.96	51.72	48.27
LP(σ) N1	1.74	99.94	0.04
LP(π) N1	1.68	96.80	3.19

Table S3. Hyperconjugation stabilization energy calculated for **2** at the B3LYP-D3/6-311+G(d,p) level of theory.

donor NBOs	acceptor NBOs	$E^{(2)}_{ij}$ / kcal mol ⁻¹
LP(σ) N1	LP* B13	175.45
BD B14–N1	LP* B13	134.11
LP(π) N1	LP* B14	52.80
LP(σ) N1	BD* B14–N1	34.97
BD S1–N1	LP* B13	18.69
LP S1	BD* B14–N1	5.69

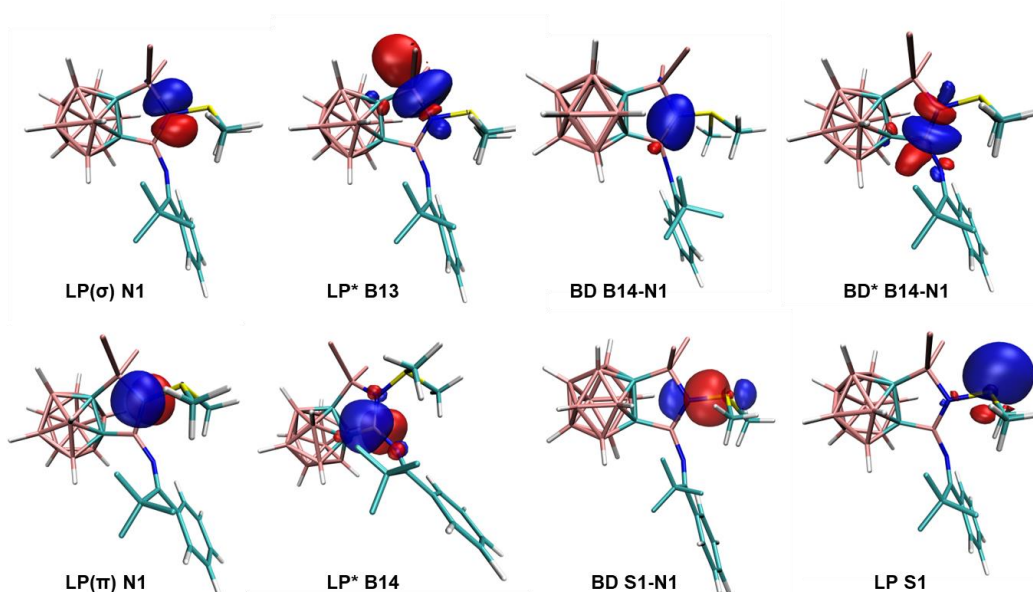


Figure S3. Plots of selected natural bond orbitals of **2** at the B3LYP-D3/6-311+G(d,p) level of theory (isovalue 0.04 a. u.).

Cartesian coordinates:

1				B	-2.57756600	-1.46519500	0.84467500
Br	1.21419200	1.80815500	1.66740000	H	-2.43235500	-2.47687200	1.44049900
C	-1.26727900	0.82376200	0.02639200	B	-2.57778300	-1.42940000	-0.91779400
B	-2.57967300	1.46059700	-0.84603300	H	-2.42367500	-2.41169500	-1.55347100
H	-2.43714600	2.47248000	-1.44192800	B	-1.72541100	0.02833700	-1.42404300
B	-2.58195600	1.42552300	0.91659800	H	-0.98843600	0.04702500	-2.33786600
H	-2.43078900	2.40835400	1.55222400	B	-4.01408900	-0.89515800	-0.02238500
B	-1.72806700	-0.03106800	1.42426300	H	-5.01156000	-1.52884300	-0.03863200
H	-0.99289500	-0.04649400	2.33977100	B	-3.46779400	0.02951100	-1.43555500
B	-4.01691400	0.88786400	0.01919400	H	-4.04217400	0.05582100	-2.46761900
H	-5.01620200	1.51859300	0.03322000	B	0.37454100	-0.87738500	-0.05820100
B	-3.47019200	-0.03607700	1.43409600	S	1.03466700	1.74910700	-1.57356400
H	-4.04647300	-0.06440300	2.46496200	C	2.82873500	1.62304700	-1.41088800
B	0.37297700	0.87711600	0.06133000	H	3.06645500	0.56207500	-1.48474700
Br	1.21909300	-1.80235200	-1.66651000	H	3.28657700	2.16497600	-2.23677500
S	1.03682000	-1.75052200	1.57400000	H	3.13890300	2.02738600	-0.44853400
C	-1.26546600	-0.82650900	-0.02534100	C	0.78033900	3.51538600	-1.27731800
C	2.83115000	-1.62205000	1.41089500	H	-0.29688900	3.66574000	-1.21151400
H	3.06859400	-0.56083600	1.47995600	H	1.25738600	3.80583600	-0.34294600
H	3.28894700	-2.16080600	2.23882400	H	1.18332300	4.06817500	-2.12431300
H	3.14087900	-2.02949900	0.44966400				
C	0.78740800	-3.51756300	1.27573700	SMe₂			
H	-0.28893000	-3.66998700	1.20022300	S	0.00000000	0.66585500	-0.00000800
H	1.27461000	-3.80793300	0.34642800	C	-1.37218000	-0.51691100	0.00000100
H	1.18339100	-4.06931200	2.12685700	H	-2.29632700	0.05948100	-0.00005000

H	-1.34632700	-1.14246600	-0.89292100	H	0.93634500	-3.21681400	1.41529400
H	-1.34637700	-1.14238800	0.89298000	H	2.42909700	-2.92518000	0.47588900
C	1.37218000	-0.51691100	0.00001000	H	2.49941000	-3.09486200	2.27001400
H	2.29632700	0.05948000	-0.00002800	C	3.30120400	-0.31179100	1.39551900
H	1.34636800	-1.14239200	0.89298500	H	3.20901800	0.77356300	1.36388000
H	1.34633600	-1.14246100	-0.89291500	H	3.90632400	-0.61171600	2.24922500
Diazirine				H	3.71372000	-0.68100300	0.45812100
F	2.99636500	0.07748500	0.00002800	B	-1.93086900	-1.65567500	1.04533900
F	1.68596700	-1.25693200	-1.07730900	H	-1.49695100	-2.51883100	1.72757000
F	1.68593100	-1.25692000	1.07733900	B	-1.98407800	-1.81017300	-0.71467200
C	0.71493300	0.59648600	-0.00001000	H	-1.58639900	-2.77969100	-1.25658100
C	1.78104300	-0.46828700	0.00001200	B	-1.56641400	-0.23123900	-1.40867700
C	-0.71983600	0.21589800	-0.00000800	H	-0.87019000	-0.08717300	-2.34474500
C	-1.12508500	-1.12150400	-0.00003800	B	-3.48683400	-1.58699700	0.20335800
H	-0.39607000	-1.92053000	-0.00006600	H	-4.27448600	-2.46146400	0.30433400
C	-2.47658300	-1.43898000	-0.00003300	B	-3.24914600	-0.70408200	-1.32398300
H	-2.77785900	-2.47948900	-0.00005600	H	-3.83844900	-0.94947300	-2.31691300
C	-3.43786300	-0.43471300	0.00000100	B	0.72903400	-0.42609000	-0.03264000
H	-4.49093500	-0.68835000	0.00000500	Br	0.90411700	2.97146300	0.03525400
C	-3.03951500	0.89612500	0.00003000	TS1			
H	-3.77922400	1.68726700	0.00005800	Br	1.58499100	-0.66567900	1.84664100
C	-1.68927200	1.22192900	0.00002500	C	-1.00987700	-0.80051100	-0.01170100
H	-1.39406700	2.26396900	0.00004900	B	-2.33784600	-1.63344600	0.62345200
N	1.10548600	1.87591700	0.60601800	H	-2.17329300	-2.70584600	1.08286000
N	1.10549100	1.87589900	-0.60607300	B	-2.19191700	-1.34220900	-1.11219100
A				H	-1.90252200	-2.20629000	-1.85935600
Br	1.77407400	-1.10877300	-1.61011200	B	-1.42065800	0.22872800	-1.32767000
C	-1.33557900	0.79781900	-0.06973800	H	-0.58054300	0.43699900	-2.13403300
B	-2.78775400	0.97067200	-0.92597800	B	-3.73635100	-1.03409100	-0.30102600
H	-2.92825100	1.91494100	-1.61712700	H	-4.67916800	-1.71799400	-0.49687700
B	-2.73796800	1.12289900	0.83199100	B	-3.14547000	0.12084100	-1.51765600
H	-2.83275800	2.17258100	1.36066700	H	-3.62204700	0.25929300	-2.58923000
B	-1.48756300	0.01606700	1.42864800	B	0.65139700	-0.69930700	-0.05470700
H	-0.73406500	0.31796200	2.28494900	C	-1.16442500	0.83508700	0.25621000
B	-3.98127500	0.11963200	0.07191600	B	-2.44231200	1.50772300	-0.64995500
H	-5.11557800	0.44772300	0.07753200	H	-2.32022500	2.60143300	-1.08077400
B	-3.16282900	-0.45728100	1.54232300	B	-2.58930400	1.22018600	1.08680200
H	-3.68013200	-0.52696800	2.60158900	H	-2.57793500	2.11370300	1.85749500
B	0.19053300	1.21597800	-0.04707800	B	-1.66140900	-0.24481100	1.48324800
S	1.63286600	-0.96846000	1.62230900	H	-1.02871900	-0.32639200	2.46348900
C	-0.87056700	-0.79939700	0.04753800	B	-3.88930200	0.71819600	-0.01569300
C	1.91771700	-2.74345200	1.41945800	H	-4.93143700	1.27456500	-0.01080900
				B	-3.39350700	-0.35707900	1.30535400

H	-4.05998100	-0.56373000	2.25777800	H	0.01803800	3.60772500	0.29739300
B	0.41630600	0.92335600	0.18225000	C	-3.01905700	1.75999600	-0.98501400
Br	1.65323800	-1.71722700	-1.40658600	H	-3.70489700	2.58951800	-1.14539800
S	1.49904900	2.46820700	0.17550300	H	-3.17599700	0.98137900	-1.73065900
C	0.62843400	3.43453500	-1.09592000	H	-3.10183100	1.33502300	0.01466900
H	1.27494100	4.26201500	-1.38146600				
H	0.39368000	2.80016800	-1.94968500	C			
H	-0.28656500	3.80737500	-0.63953800	Br	-0.50979600	-1.94684100	-1.41411600
C	2.92768200	1.82436000	-0.74129500	C	1.59629000	0.30517300	-1.23407400
H	3.63327900	2.63877300	-0.89294400	B	1.33938100	1.15156200	-2.68873600
H	3.36044000	1.04640000	-0.11227900	H	0.87723100	0.57100900	-3.60411000
H	2.58829200	1.38868100	-1.67940700	B	2.96843300	0.80494300	-2.10785800
B				H	3.64274200	-0.01571500	-2.61843700
Br	-1.49104900	-2.07311100	-1.04284000	B	2.93551100	0.86798400	-0.34901100
C	1.00125600	-0.66363100	0.25986900	H	3.52567900	0.10370900	0.30915000
B	2.29780900	-1.69499400	-0.07843100	B	2.56665100	2.43467700	-2.68072300
H	2.08608900	-2.84998900	-0.17377800	H	3.01817600	2.85667600	-3.68726000
B	2.16461800	-0.85445800	1.47056900	B	3.55506100	2.24081700	-1.21793100
H	1.86283500	-1.41952600	2.45925800	H	4.70798300	2.49134600	-1.16090900
B	1.44400000	0.73264600	1.16869500	B	1.02553900	-1.05570100	-0.52104800
H	0.64215200	1.24069300	1.86354300	C	1.32866200	1.26649500	0.06541600
B	3.71498900	-0.87708600	0.60456500	B	2.50178900	2.48941700	0.19883500
H	4.63647900	-1.49032400	1.01646500	H	2.84382300	2.82978700	1.27898900
B	3.17420200	0.62830000	1.38346000	B	0.87612100	2.84617400	-0.38795500
H	3.66777300	1.08323700	2.35479600	H	0.10898800	3.42777200	0.29247600
B	-0.66193600	-0.62668500	0.06990100	B	0.31073300	1.43352900	-1.28993100
C	1.21997300	0.80751000	-0.51666900	H	-0.78146800	1.01073600	-1.22154400
B	2.51775000	1.69124200	0.11759800	B	2.28115200	3.47538800	-1.26066500
H	2.42826000	2.86950700	0.16937200	H	2.53037500	4.63007700	-1.25383600
B	2.64604400	0.85219000	-1.43290600	B	0.90819700	2.81066100	-2.16852000
H	2.64054500	1.44860000	-2.45103300	H	0.15568200	3.46843900	-2.79822900
B	1.64775500	-0.62628900	-1.33277900	B	0.66516600	0.12684900	0.98137800
H	0.96676000	-0.98001300	-2.22471400	Br	2.42129100	-2.45128900	-0.06243800
B	3.93028100	0.68490600	-0.22556100	S	1.33290100	-0.15553100	2.81598400
H	4.99206000	1.17163800	-0.40023000	C	3.13667800	-0.27940300	2.82381400
B	3.38204900	-0.74066900	-1.13972700	H	3.41487000	-0.48711900	3.85659600
H	4.02754800	-1.26552500	-1.97713800	H	3.46198700	-1.06883300	2.15075900
B	-0.32802900	0.86389500	-0.67323900	H	3.53064300	0.68729900	2.51788600
Br	-1.72078600	-0.35343200	1.79821200	C	0.86463200	-1.87208500	3.17195600
S	-1.32666400	2.36984500	-1.23465500	H	1.30760800	-2.13614700	4.13125100
C	-1.04071700	3.35106700	0.27996600	H	-0.22063000	-1.89573000	3.24786600
H	-1.65261900	4.24789600	0.20732800	H	1.21895800	-2.51984300	2.37272800
H	-1.30873200	2.74701900	1.14698500	F	-1.65186400	2.58668200	2.19168200
				F	-3.72731000	2.16106400	1.77202000

F	-2.42068000	2.82374200	0.19018700	S	1.32518700	0.08647900	2.86844600
C	-2.15718700	0.61421800	1.01230500	C	3.12001000	-0.13392400	2.87639200
C	-2.49017900	2.07662700	1.28993300	H	3.39526900	-0.28432300	3.91980000
C	-3.02174900	-0.14103900	0.06297300	H	3.40013800	-0.98522100	2.26133300
C	-3.39716800	0.38909600	-1.17140100	H	3.56590400	0.78564600	2.50373700
H	-3.06104100	1.37024600	-1.47772600	C	0.77437000	-1.57298100	3.35519400
C	-4.18773600	-0.36680700	-2.02656200	H	1.18593100	-1.77176400	4.34373900
H	-4.46347200	0.03622100	-2.99284800	H	-0.31221100	-1.54034500	3.40276500
C	-4.61381200	-1.63620800	-1.65150400	H	1.11577800	-2.30085200	2.62269200
H	-5.22438000	-2.22322800	-2.32691500	F	-1.66901300	2.80502500	1.99884500
C	-4.25688200	-2.15336300	-0.41158000	F	-3.72975700	2.34449000	1.54214600
H	-4.58857400	-3.14023300	-0.11468400	F	-2.35612600	2.84748700	-0.04186500
C	-3.46005400	-1.40741200	0.44396900	C	-2.14101200	0.72051500	1.00343100
H	-3.16187000	-1.81491000	1.40272500	C	-2.47343200	2.20439700	1.12321300
N	-0.77995700	0.25812400	1.28103400	C	-2.98397500	-0.11299500	0.09361700
N	-1.59018900	-0.08743100	2.16811900	C	-3.37023100	0.32698600	-1.17303000
				H	-3.05984100	1.29506100	-1.54166200
TS2				C	-4.14143800	-0.49816400	-1.98111200
Br	-0.53784800	-2.00511200	-1.39366400	H	-4.42659900	-0.16074500	-2.96967000
C	1.60218800	0.18981500	-1.23730300	C	-4.53905900	-1.75157900	-1.52957100
B	1.38216400	0.93785500	-2.74983800	H	-5.13779400	-2.39178300	-2.16639000
H	0.91296000	0.30421100	-3.62560300	C	-4.17103600	-2.18122600	-0.25967300
B	2.99735100	0.58131400	-2.13150800	H	-4.48316400	-3.15422800	0.09875100
H	3.64383100	-0.29734900	-2.57813100	C	-3.39400900	-1.36407700	0.54923000
B	2.95394300	0.76165500	-0.37997100	H	-3.08988700	-1.69801900	1.53387100
H	3.51119000	0.02395100	0.33472000	N	-0.76976300	0.39727600	1.30680500
B	2.65021800	2.17857900	-2.81755500	N	-1.61556300	0.13225600	2.22683700
H	3.12304200	2.51332600	-3.84679500				
B	3.62035000	2.05381600	-1.33446900	D			
H	4.78008600	2.27125300	-1.28326400	Br	-0.67195000	-1.84696100	-2.16244900
B	1.00486300	-1.15172700	-0.55321300	S	-1.61479000	1.76758300	-2.31911100
C	1.35321700	1.23279600	-0.01159100	C	-1.58145900	0.42859000	0.53825100
B	2.56206300	2.42690800	0.04956900	C	-3.35697500	1.31700500	-2.49803600
H	2.90191900	2.82995000	1.10838700	H	-3.39302900	0.26936900	-2.78799000
B	0.95394600	2.79471900	-0.57673900	H	-3.90912000	1.48167200	-1.57694200
H	0.20030400	3.43897100	0.06008800	H	-3.74966000	1.93315400	-3.30610900
B	0.34611000	1.34451400	-1.38444300	C	-1.72269700	3.55119400	-1.98784800
H	-0.75670200	0.95690900	-1.29362500	H	-0.70853000	3.84808200	-1.70978500
B	2.38556100	3.32034500	-1.47457500	H	-2.03211200	4.05616600	-2.90136100
H	2.67174100	4.46431400	-1.54084300	H	-2.42121500	3.72659800	-1.17165300
B	0.99861900	2.63993700	-2.34923300	B	-3.13567000	0.85183800	1.07208200
H	0.27434700	3.27536800	-3.03189300	H	-3.68425300	1.73354400	0.50830500
B	0.63530500	0.28418000	1.04783600	B	-1.71467500	1.19854400	2.05719300
Br	2.29802300	-2.50504800	0.13604100	H	-1.29700800	2.29768200	2.13069400

B	-0.54852300	-0.11250500	1.81111000	B	3.24990700	-1.40250100	0.83196400
H	0.61092600	0.02780700	1.69052700	H	3.06100500	-2.42727800	1.37427200
B	-3.16755900	0.50488700	2.80406500	B	2.46768300	0.03838500	1.47436900
H	-3.83903100	1.15115700	3.52898000	H	1.71692100	0.06064500	2.37758100
B	-1.55817500	-0.08494900	3.26386500	B	4.71355800	-0.89334000	-0.02142000
H	-1.05965600	0.12394300	4.31261300	H	5.66212700	-1.59550000	-0.06237700
B	-0.86835000	1.18971700	-0.63757700	B	4.22380100	-0.05837700	1.46981400
Br	1.06625800	-3.01061200	0.33526900	H	4.79922000	-0.15372000	2.49630500
C	-1.32278800	-1.20747300	0.75730700	B	0.38485700	-1.27186700	0.00797400
B	-1.28363600	-1.60737200	2.41456600	Br	0.22949800	-3.11661000	0.77479200
H	-0.56375300	-2.47377900	2.75200500	S	0.60173600	3.49648700	-0.47752600
B	-2.69632700	-1.96295800	1.41290800	C	2.09844300	0.96667400	0.08355400
H	-2.93293000	-3.06390900	1.06000200	C	-0.98768100	4.02104000	0.21490300
B	-2.85288400	-0.66533300	0.21514600	H	-0.80976700	4.25018600	1.26455800
H	-3.15329000	-0.87700600	-0.89909200	H	-1.30198100	4.91827200	-0.31525500
B	-2.89836400	-1.23084600	3.01770200	H	-1.72643800	3.22910000	0.13100300
H	-3.36691100	-1.85568800	3.90302400	C	0.18967300	3.12804000	-2.21441900
B	-3.87277000	-0.64990800	1.64616900	H	1.10979400	2.76209600	-2.66981300
H	-5.03163100	-0.84684000	1.53391100	H	-0.57926400	2.35670500	-2.25617400
B	-0.37798200	-1.95204600	-0.27059000	H	-0.12610400	4.05601300	-2.68801800
F	0.89354000	3.90069500	0.84789800	B	3.43943400	1.45472900	1.00322500
F	2.99609200	3.44665700	1.05701500	H	3.32541200	2.43665900	1.65238600
F	1.52680500	2.34510300	2.19014300	B	3.44559100	1.55267000	-0.75771700
C	1.69549100	1.91654800	-0.15782900	H	3.33350200	2.60626500	-1.29188200
C	1.77389000	2.91032800	0.99243800	B	2.48036100	0.21902400	-1.39748000
C	2.63174600	0.73612300	-0.13454700	H	1.75754500	0.37346500	-2.30873100
C	3.36170900	0.34883000	0.98885700	B	4.83823100	0.87261300	0.08571900
H	3.27932100	0.89577500	1.91912300	H	5.86571200	1.45473200	0.11837700
C	4.21117300	-0.75164800	0.91943900	B	4.23070200	0.10720700	-1.40179000
H	4.77884900	-1.04194500	1.79543300	H	4.80712300	0.13616600	-2.43222700
C	4.33661500	-1.47037600	-0.26291600	B	0.72309100	1.69329600	0.14047600
H	5.00074500	-2.32527900	-0.31113200	F	-1.14445900	1.12830800	3.10093900
C	3.60762500	-1.08559700	-1.38473400	F	-2.91156400	-0.06760900	2.79906800
H	3.70042400	-1.63977600	-2.31127700	F	-2.83418900	1.96736900	2.06192100
C	2.76245600	0.01245300	-1.32135000	C	-1.59338000	0.36355600	0.88849700
H	2.20580900	0.34545900	-2.19044500	C	-2.11775800	0.84085500	2.24839400
N	1.24112400	2.44322700	-1.41536000	C	-2.69314400	0.04267600	-0.07561800
N	0.37999500	1.71452200	-0.65530200	C	-3.24693000	-1.23185200	0.01603700
E				H	-2.83228200	-1.94917700	0.71612300
Br	-0.39117600	-1.27035800	-1.90099400	C	-4.28885900	-1.58971500	-0.82673700
C	1.94883900	-0.68151200	-0.01064500	H	-4.70568900	-2.58718000	-0.76785200
B	3.23698200	-1.30063400	-0.93120600	C	-4.77915700	-0.67842600	-1.75613400
H	3.02442700	-2.25215800	-1.59297100	H	-5.58616500	-0.96347700	-2.41986400
				C	-4.23181200	0.59665300	-1.83753700

H	-4.61222200	1.30662500	-2.56170100	F	-2.49220600	2.86616600	1.06387800
C	-3.19233700	0.96058000	-0.99050700	C	-1.49944800	0.84718500	0.33944800
H	-2.76425200	1.95265000	-1.06911600	C	-1.76143400	1.82566700	1.48350900
N	-0.38092000	1.03424800	0.54959000	C	-2.75256200	0.29117400	-0.26070900
N	-0.35938900	-0.33582700	0.98571200	C	-3.45100200	-0.69814100	0.42556700
TS3				H	-3.06851400	-1.08034600	1.36460700
Br	-0.71250800	-2.00276100	-1.59728200	C	-4.60847400	-1.22380500	-0.13200400
C	1.74497100	-1.06918200	-0.04352900	H	-5.14150900	-2.01154900	0.38549000
B	2.84258200	-1.95274300	-0.98738500	C	-5.06816300	-0.75542100	-1.35815900
H	2.43552600	-2.89107500	-1.57023800	H	-5.96664500	-1.17516000	-1.79412100
B	2.94468500	-1.95223200	0.77485500	C	-4.37160400	0.24205700	-2.03209500
H	2.60501500	-2.89103400	1.39531700	H	-4.72465500	0.59892200	-2.99176300
B	2.44897000	-0.36002500	1.35996900	C	-3.21026500	0.76868500	-1.48298800
H	1.75707800	-0.16601100	2.29008300	H	-2.63764500	1.51850800	-2.01564900
B	4.41557200	-1.74807300	-0.18541900	N	-0.41087500	1.17216200	-0.55516400
H	5.23238100	-2.59981400	-0.23050100	N	-0.35124700	0.07262100	0.57018400
B	4.16251700	-0.75906800	1.27280100	F			
H	4.77829900	-0.88896000	2.27162400	Br	-0.82557100	-2.40483500	-0.96698300
B	0.11336100	-1.32095100	0.10889500	C	1.72421900	-1.13156200	0.01914800
Br	-0.36669600	-2.50797900	1.67494600	B	2.67146800	-2.25625200	-0.81797300
S	1.48158900	3.40343100	-0.21856200	H	2.17340800	-3.27546800	-1.13047500
C	2.14968200	0.53902600	-0.06734300	B	2.97839000	-1.88136800	0.88056300
C	0.05146000	4.43403200	0.19767300	H	2.67941000	-2.63790000	1.73162100
H	0.00654100	4.53828400	1.27795600	B	2.59943800	-0.17431500	1.13311300
H	0.21878900	5.40427200	-0.26785400	H	2.02754100	0.26116300	2.06686800
H	-0.86085500	3.97677900	-0.18051900	B	4.32813300	-1.96314900	-0.26095000
C	1.25985900	3.41956500	-2.03292100	H	5.11500400	-2.84225800	-0.20845700
H	1.94345700	2.69386400	-2.46617500	B	4.27654600	-0.67132200	0.95719900
H	0.22894000	3.15643600	-2.26536000	H	5.00487700	-0.60093300	1.88366300
H	1.50445500	4.42140400	-2.38126300	B	0.12786400	-1.22848600	0.33285500
B	3.61282300	0.83664400	0.74976000	Br	-0.32145700	-1.70648800	2.24303000
H	3.71418300	1.85797700	1.33572800	S	1.35077000	3.21131400	0.21286700
B	3.52739300	0.83013800	-1.00962100	C	2.13935300	0.42251500	-0.41017800
H	3.60969400	1.85094900	-1.59947800	C	-0.01314400	4.27560500	-0.35497900
B	2.30203900	-0.35770300	-1.51428500	H	-0.62623200	4.55497400	0.49342300
H	1.52154000	-0.14476000	-2.36899400	H	0.44523700	5.16243400	-0.78619300
B	4.83437200	-0.02922300	-0.19999800	H	-0.60306500	3.75111400	-1.10593500
H	5.94264300	0.37445200	-0.26288100	C	2.42314500	3.54813100	-1.22068200
B	4.01364800	-0.75879400	-1.60498800	H	3.38001300	3.06366100	-1.07344200
H	4.52606400	-0.87951300	-2.66197700	H	1.94598200	3.18929200	-2.13185700
B	0.87752200	1.46930000	-0.06595600	H	2.55532600	4.62805000	-1.25081500
F	-0.61358700	2.32508200	1.98178800	B	3.70071900	0.79172600	0.15258600
F	-2.40518000	1.23458700	2.47630700	H	3.92390200	1.88814300	0.53499400

B	3.39838700	0.41721300	-1.54990500	B	3.47680400	1.92731400	-0.08751900
H	3.41025000	1.24448800	-2.39058700	H	3.39760400	3.08782900	0.10406300
B	2.10156900	-0.78403900	-1.61910500	B	3.36640100	1.26375000	-1.73608900
H	1.22926200	-0.74213700	-2.40487800	H	3.20844300	1.97488600	-2.66297000
B	4.77787500	-0.30889700	-0.71057600	B	2.37352500	-0.21672600	-1.66377500
H	5.88101200	0.01700000	-0.98089400	H	1.54816200	-0.46892800	-2.46220600
B	3.78029200	-1.28756700	-1.80980700	B	4.81205400	0.97575900	-0.75828100
H	4.15792600	-1.66516300	-2.86262000	H	5.83567800	1.49336500	-1.03684700
B	0.80371000	1.30789700	-0.24543300	B	4.12321200	-0.34115200	-1.73575600
F	-0.87310000	2.57886600	1.62487200	H	4.63529400	-0.76543400	-2.71034000
F	-2.73451300	1.56588300	1.85593400	B	0.61287800	1.45691800	-0.70849700
F	-2.53807100	3.06656600	0.32404200	F	-0.51622300	3.18912200	0.45940900
C	-1.49661300	0.98093000	-0.06356200	F	-2.13703600	2.38683800	1.63906900
C	-1.91112100	2.06247100	0.94487800	F	-2.54906600	3.32074700	-0.26642800
C	-2.70865900	0.22910100	-0.54432200	C	-1.53766700	1.20467400	-0.31287800
C	-3.42975200	-0.60880300	0.30428400	C	-1.70418800	2.55149300	0.40019600
H	-3.09883200	-0.77173600	1.32216900	C	-2.78104500	0.39477100	-0.45886200
C	-4.54271500	-1.27800500	-0.18323900	C	-3.33371200	-0.22092900	0.66178800
H	-5.08885600	-1.94963200	0.46712400	H	-2.85926000	-0.12314600	1.63072300
C	-4.94454900	-1.10169400	-1.50301900	C	-4.47802800	-0.99224100	0.51239000
H	-5.81231900	-1.63022500	-1.87905800	H	-4.90452800	-1.48913300	1.37440500
C	-4.22915000	-0.25632800	-2.34271900	C	-5.06640000	-1.13342200	-0.73992700
H	-4.53483500	-0.12373400	-3.37304600	H	-5.95774600	-1.73890600	-0.85072500
C	-3.10743200	0.40816300	-1.86484700	C	-4.51114200	-0.50876800	-1.85157200
H	-2.51921700	1.03779900	-2.52072300	H	-4.96625600	-0.62625800	-2.82705400
N	-0.43798100	1.10592900	-1.06552000	C	-3.36107300	0.25645200	-1.71579800
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Br	-0.35174900	-2.23882200	-0.91093500	N	-0.29022900	0.57876500	0.02655200
C	1.97285300	-0.44062300	0.01129700	H			
B	3.19376900	-1.40410300	-0.64224200	Br	-0.88540700	-2.66107800	0.69714800
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B	3.31708100	-0.74686300	0.99570900	B	2.74462700	-2.48004400	0.26816900
H	3.15117300	-1.43059600	1.93948100	H	2.35411300	-3.39961500	0.89162500
B	2.55530100	0.84749100	0.99698000	B	3.14283100	-0.94405300	1.04922100
H	1.83927000	1.26165100	1.83493200	H	3.02588100	-0.80480300	2.21269700
B	4.71205800	-0.66505400	-0.09092600	B	2.56711500	0.35654700	0.00617300
H	5.66864400	-1.32800500	0.10564200	H	1.98811300	1.31436400	0.36520900
B	4.30450200	0.73239300	0.93250100	B	4.39240500	-1.82332000	0.15568100
H	4.94694500	1.07750400	1.85994300	H	5.28800900	-2.34092400	0.72409100
B	0.39165100	-0.85834800	0.29858700	B	4.27013900	-0.05488400	-0.00176400
Br	-0.00808400	-1.19270600	2.23103700	H	5.05643200	0.70212400	0.44866400
C	2.10407500	1.12434300	-0.63076500	B	0.16131000	-0.97817000	0.67088600

Br	-0.00234100	0.07271400	2.36419500	C	1.98190300	-0.65138000	-0.08011300
C	1.94747600	-0.42537100	-1.38229900	B	3.12506500	-1.86057000	-0.44456000
B	3.45641300	0.29745600	-1.53962900	H	2.86111000	-2.97127800	-0.15551900
H	3.52845500	1.29275300	-2.16893900	B	3.44257800	-0.65365200	0.80294100
B	3.06730300	-1.25201300	-2.32549000	H	3.39409600	-0.93315000	1.94553900
H	2.87567700	-1.30513400	-3.48747600	B	2.69310100	0.84683100	0.29042800
B	1.93759000	-2.13606800	-1.26697100	H	2.11848600	1.54382200	1.03407400
H	0.99686500	-2.71033600	-1.67465400	B	4.70058100	-1.03691200	-0.37726900
B	4.58686400	-1.06279600	-1.43695300	H	5.67489200	-1.61704700	-0.04787900
H	5.61765500	-1.03062000	-2.01128100	B	4.41625900	0.65457500	0.08818100
B	3.64097300	-2.56232500	-1.27439100	H	5.15541300	1.29418000	0.75141200
H	3.97917400	-3.59694300	-1.72977700	B	0.45069300	-0.83735000	0.52074000
B	0.50220300	0.01760300	-1.62793600	Br	0.36886300	-0.90593000	2.51951300
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C	-2.92049800	-0.09113000	-0.64268500	B	2.20038400	-1.10444700	-1.74279500
C	-3.38967600	0.34227400	0.59514000	H	1.30526300	-1.60232900	-2.31035200
H	-2.80273100	1.03030400	1.19244900	B	4.71469400	0.24250900	-1.61307600
C	-4.59977000	-0.14746600	1.06729100	H	5.69599300	0.58166900	-2.17570600
H	-4.96419800	0.17025700	2.03586200	B	3.92474800	-1.31632700	-1.94570100
C	-5.33303300	-1.04898400	0.30311500	H	4.32212700	-2.09013800	-2.74327300
H	-6.27516900	-1.43092800	0.67747900	B	0.49576900	0.82950800	-1.33811400
C	-4.85957700	-1.46909700	-0.93532600	F	-1.22810900	3.06111300	-1.24756100
H	-5.42915600	-2.17615100	-1.52510700	F	-2.97905100	2.47012000	-0.14101400
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H	-3.24883500	-1.33547700	-2.36098300	C	-1.54644600	0.70140100	-0.92968300
N	-0.79257500	-0.46745300	-1.97276100	C	-2.16487100	2.10297400	-1.12925800
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S	0.63525400	3.65078600	0.80249600	C	-3.12015200	-0.41244100	0.67411300
C	1.99537100	4.13600500	-0.29344700	H	-2.64617200	0.12952800	1.48624800
H	2.44468800	5.07095400	0.04187400	C	-4.15288500	-1.30105200	0.93838800
H	2.75573600	3.35339800	-0.33414200	H	-4.49637400	-1.44131500	1.95561200
H	1.57709900	4.28002800	-1.28936300	C	-4.73411700	-2.01841100	-0.10208700
C	1.58858400	3.39977600	2.32107800	H	-5.53534200	-2.71726500	0.10566200
H	2.29184400	2.57259600	2.20530400	C	-4.28621100	-1.84509700	-1.40733400
H	2.12006700	4.31275000	2.59024400	H	-4.73825800	-2.40620200	-2.21595300
H	0.88075700	3.15021400	3.10998000	C	-3.24752100	-0.96351100	-1.67647900
				H	-2.85862900	-0.84111600	-2.67997400
				N	-0.63242200	0.40089300	-2.01166500
				N	-0.30869100	0.65123500	-0.06103000
TS4				S	-0.42480600	2.30651900	1.43246300
Br	-0.42939900	-2.46563300	-0.19767200				

C	0.65177400	3.54011500	0.64132200	C	-4.08609200	-1.47465800	0.67528200
H	0.07305800	4.45060100	0.50021600	H	-4.45353600	-1.78340400	1.64605300
H	1.51665500	3.71387900	1.27712600	C	-4.60704300	-2.04115600	-0.48235500
H	0.98572600	3.17147800	-0.32780400	H	-5.38549100	-2.79142300	-0.41275700
C	0.36366100	2.25579700	3.06382000	C	-4.12895800	-1.64560700	-1.72791800
H	1.37005300	1.84693400	3.00463200	H	-4.53588400	-2.08417900	-2.63085200
H	0.37296900	3.29266600	3.40624600	C	-3.11843800	-0.69895800	-1.81808900
H	-0.25633100	1.64668800	3.71331300	H	-2.70667000	-0.39880000	-2.77374800
I				N	-0.68247200	0.91796400	-1.94840300
Br	-0.37122600	-2.28033700	-0.63900000	N	-0.27692400	0.74962900	0.23782900
C	2.01304800	-0.47343200	-0.10963100	S	-0.42811400	1.62624200	1.80151000
B	3.21779200	-1.60332900	-0.49561700	C	-0.13617900	3.38026100	1.42215400
H	3.01136900	-2.73098700	-0.22319600	H	-1.05195300	3.83029700	1.06722700
B	3.46738800	-0.40272100	0.77987200	H	0.14515800	3.82929600	2.37261300
H	3.43200000	-0.71253200	1.91911900	H	0.66960700	3.47078300	0.69361500
B	2.66402300	1.07252000	0.26888700	C	0.98589200	1.43832700	2.97506100
H	2.08740400	1.82457100	0.94877100	H	1.67471500	0.66169200	2.67559000
B	4.75266300	-0.70740400	-0.40072100	H	1.48968200	2.39888700	3.03199900
H	5.75133400	-1.24946600	-0.07916000	H	0.50355500	1.16186100	3.91122500
B	4.39024500	0.95846800	0.08996100	TS5			
H	5.08946700	1.61966000	0.77557600	Br	-0.38263500	-2.31969000	-0.36926600
B	0.47528400	-0.82255200	0.42412600	C	2.00636900	-0.46964400	-0.12720700
Br	0.31525100	-1.49326300	2.34047700	B	3.16227300	-1.63183600	-0.55999600
C	1.99186700	0.73749900	-1.23859400	H	2.96201900	-2.74568300	-0.23196600
B	3.40244400	1.70077300	-1.19197100	B	3.52525600	-0.38905800	0.64650400
H	3.28817900	2.85655200	-1.40280600	H	3.57015700	-0.65219900	1.79692200
B	3.15288200	0.50561900	-2.46208500	B	2.70425500	1.07732700	0.13813900
H	2.88201400	0.83904700	-3.55878200	H	2.19593600	1.86544000	0.83071600
B	2.26722100	-0.85928900	-1.78977600	B	4.71142400	-0.75957000	-0.61658900
H	1.41865700	-1.37896200	-2.39964400	H	5.72452700	-1.30530000	-0.35089100
B	4.71239200	0.59323800	-1.61650600	B	4.41007000	0.92833500	-0.16643100
H	5.67852600	0.98766900	-2.16938900	H	5.16849900	1.60464700	0.43678600
B	3.99636200	-0.98875700	-1.98014300	B	0.50303200	-0.76709700	0.52953700
H	4.43211500	-1.73101600	-2.78751600	Br	0.46191800	-1.30418300	2.49849600
B	0.45647700	1.05731500	-1.25519700	C	1.91307000	0.69922500	-1.29902100
F	-1.43144900	3.30752500	-0.97291000	B	3.33766800	1.63838500	-1.39732200
F	-2.80940900	2.50523900	0.48389000	H	3.22569400	2.78755400	-1.64397100
F	-3.20096200	2.29654100	-1.62729300	B	2.97656900	0.40056100	-2.59626200
C	-1.51148700	0.90295700	-0.79445100	H	2.62774500	0.69611600	-3.68191000
C	-2.24028800	2.27163000	-0.72013500	B	2.12497900	-0.92080700	-1.80567500
C	-2.58482600	-0.15203000	-0.65609600	H	1.22637000	-1.45248200	-2.32830300
C	-3.08196200	-0.51888200	0.58955200	B	4.59706900	0.49390400	-1.87613600
H	-2.66820800	-0.09543400	1.49825000	H	5.52354500	0.85211400	-2.51491000

B	3.83356300	-1.08769100	-2.12238000	C	-0.61068500	-2.86794400	-1.60553900
H	4.19514400	-1.86784200	-2.93105000	H	-0.87928600	-3.92439400	-1.61475000
B	0.37976300	1.03828200	-1.22045200	H	-1.48947900	-2.22708700	-1.55530900
F	-1.68008000	3.30488000	-1.08848900	H	0.00347700	-2.62476200	-2.47236700
F	-2.80303100	2.45991600	0.55259100	C	-2.73965900	0.03407500	0.24372400
F	-3.47153900	2.20656000	-1.48491300	C	-2.68182800	0.12652100	1.77842300
C	-1.62132600	0.90416400	-0.88812400	C	-4.07674100	0.01852400	-0.39314200
C	-2.39535200	2.24201900	-0.71432300	C	-5.26096600	-0.05919700	0.34651700
C	-2.60385600	-0.21430900	-0.72598900	H	-5.24133500	-0.10906100	1.42686200
C	-3.14300000	-0.53115600	0.51729200	C	-6.48593900	-0.07269100	-0.30793900
H	-2.80036200	-0.02021400	1.41078100	H	-7.40007400	-0.13173100	0.26937900
C	-4.07478900	-1.55398600	0.61694900	C	-6.53918900	-0.00457000	-1.69478000
H	-4.47156900	-1.82874300	1.58622500	H	-7.49735400	-0.00983700	-2.20026300
C	-4.48316100	-2.23583000	-0.52522600	C	-5.36231400	0.07988700	-2.43564700
H	-5.20645500	-3.03826100	-0.44358900	H	-5.40292400	0.14613600	-3.51578000
C	-3.96374300	-1.89258600	-1.76903400	C	-4.13764200	0.09157500	-1.78958400
H	-4.28268500	-2.42397900	-2.65728900	H	-3.21327900	0.17514700	-2.34856000
C	-3.02059300	-0.87981300	-1.87387100	B	-0.27882900	0.08323900	-0.20939900
H	-2.57560600	-0.61374000	-2.82473500	N	-1.66872900	-0.05528500	-0.40708800
N	-0.74853000	0.95895900	-1.95181200	B	1.28786600	1.73195500	1.26800700
N	-0.25327000	0.74887600	0.27774500	H	1.08522300	0.99114000	2.15836500
S	-0.31274800	1.73479300	1.73887300	B	2.88873900	2.28221500	0.76378200
C	-0.04626700	3.44259700	1.18315300	H	3.81687800	1.93666900	1.40128500
H	-0.96704800	3.84623100	0.78997200	B	2.94941100	2.26183900	-1.00485500
H	0.23296600	3.99220000	2.07996900	H	3.91863300	1.90214700	-1.56936000
H	0.75767300	3.47088800	0.44685900	B	1.38554500	1.69853900	-1.60331500
C	1.14101500	1.67412000	2.88645200	H	1.23825300	0.93430100	-2.48699100
H	1.82357400	0.87065900	2.64954500	B	0.07050000	2.87111300	0.65828900
H	1.64155800	2.63687300	2.83295600	H	-0.97042000	2.91067800	1.21731800
H	0.68204700	1.49506000	3.85765000	B	1.63612000	3.45097900	1.26389700
2				H	1.71603700	4.03429600	2.28756600
S	0.45156300	-2.59113900	-0.17640300	B	2.66605700	3.78758600	-0.14663100
Br	3.04238800	-1.26109400	1.58667600	H	3.49027400	4.63390500	-0.12774700
Br	3.17724200	-1.29479300	-1.71792500	B	1.73602800	3.41686800	-1.61666200
F	-1.42457300	0.18583000	2.21114100	H	1.88698800	3.97537000	-2.64628700
F	-3.23307600	-0.97614000	2.32278000	B	0.13218400	2.85239700	-1.10819200
F	-3.33657900	1.18371900	2.24381900	H	-0.86633600	2.87674900	-1.73849300
C	2.05898100	1.11182200	-0.13612100	B	0.92920400	4.15402000	-0.21114500
C	0.45711800	1.46921200	-0.19533700	H	0.50574900	5.25657400	-0.23838700
C	-0.67488700	-2.89177900	1.19869900	B	2.19982700	-0.51003400	-0.11030100
H	-0.77917900	-3.97168200	1.30409600	N	0.70344900	-0.96239700	-0.16525800
H	-0.18027300	-2.47204800	2.07487500				
H	-1.63937600	-2.42132500	1.02446200				

NMR Figures

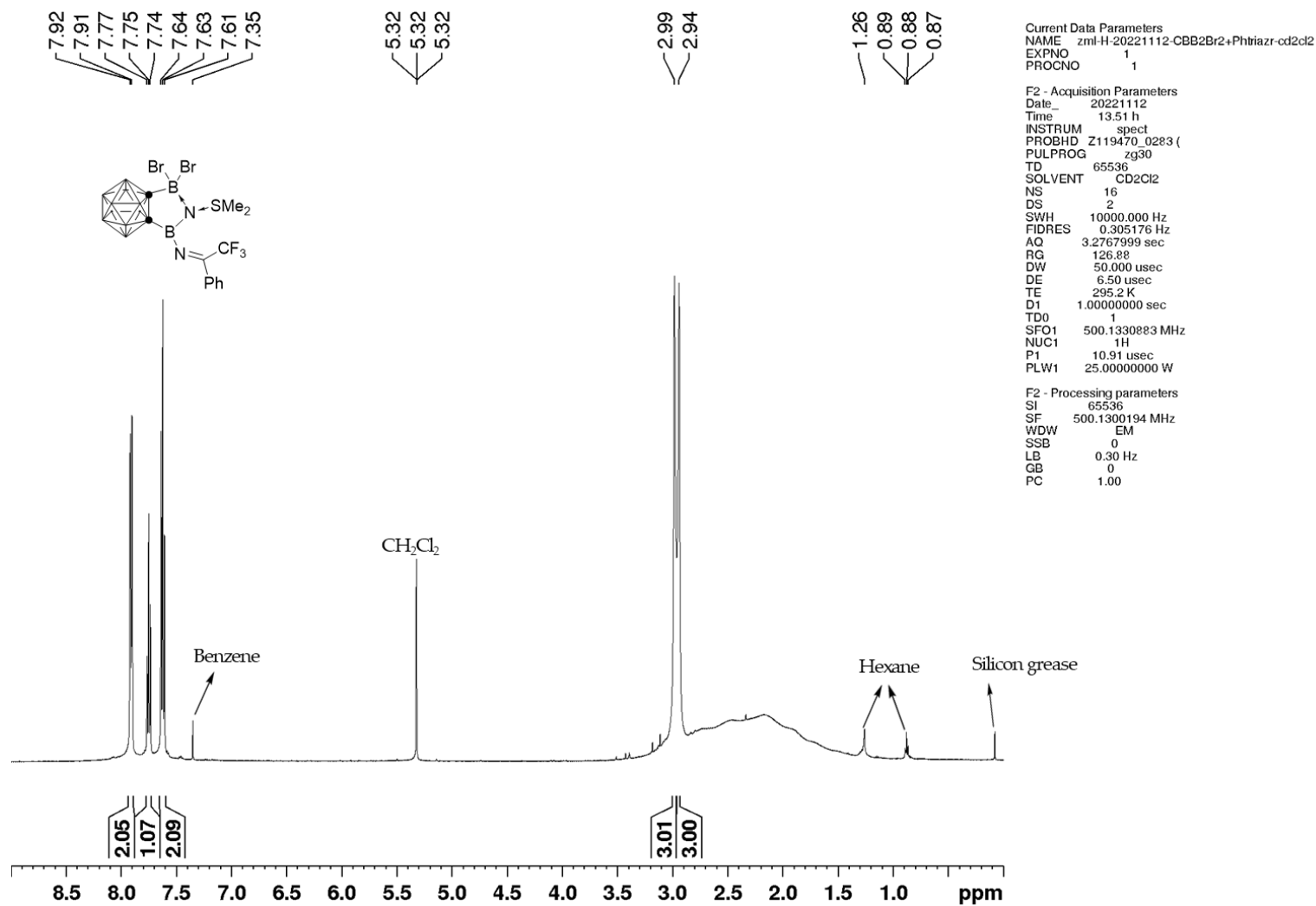


Figure S4. ¹H NMR spectrum of compound 2 in CD₂Cl₂.

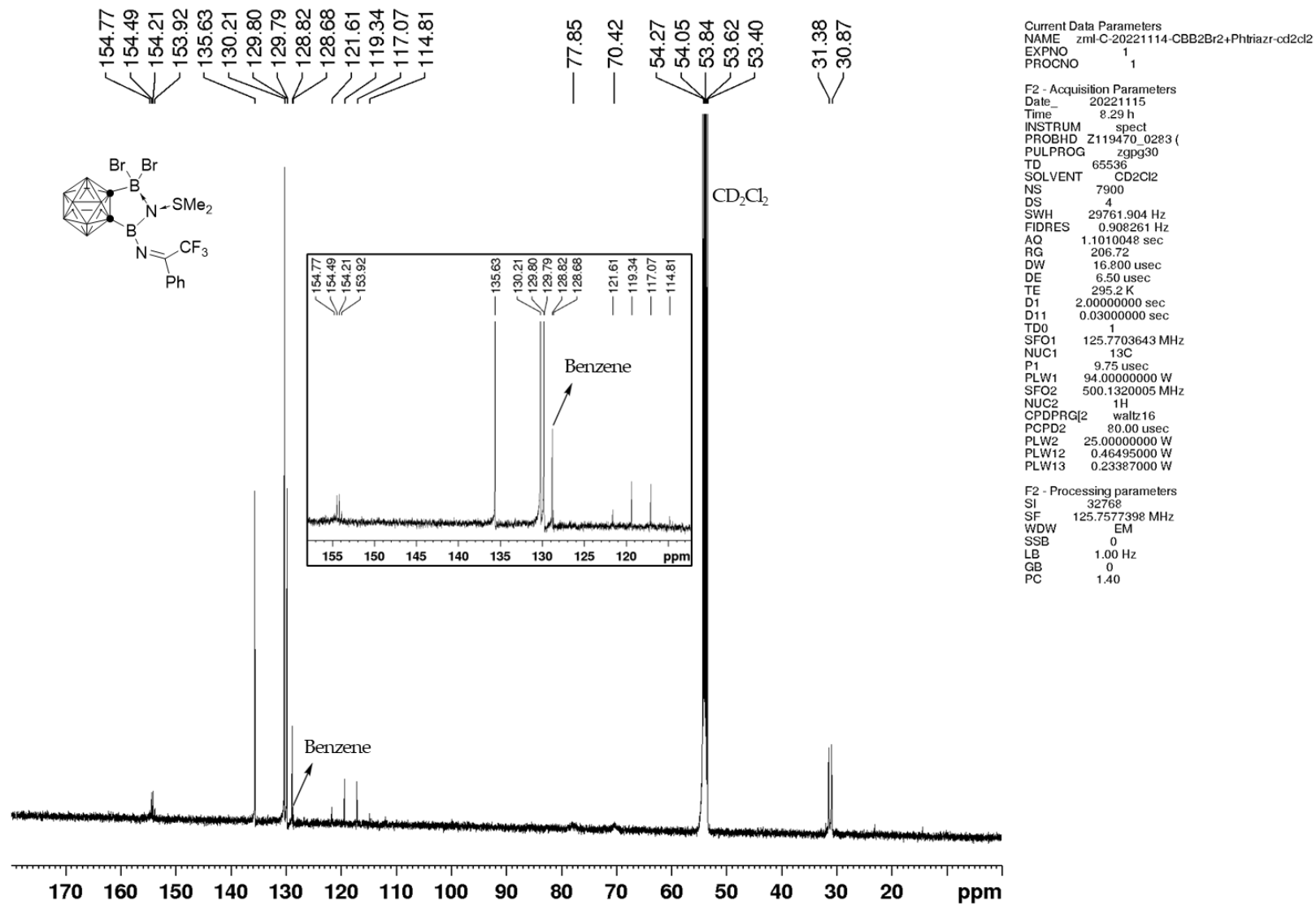


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2** in CD_2Cl_2 .

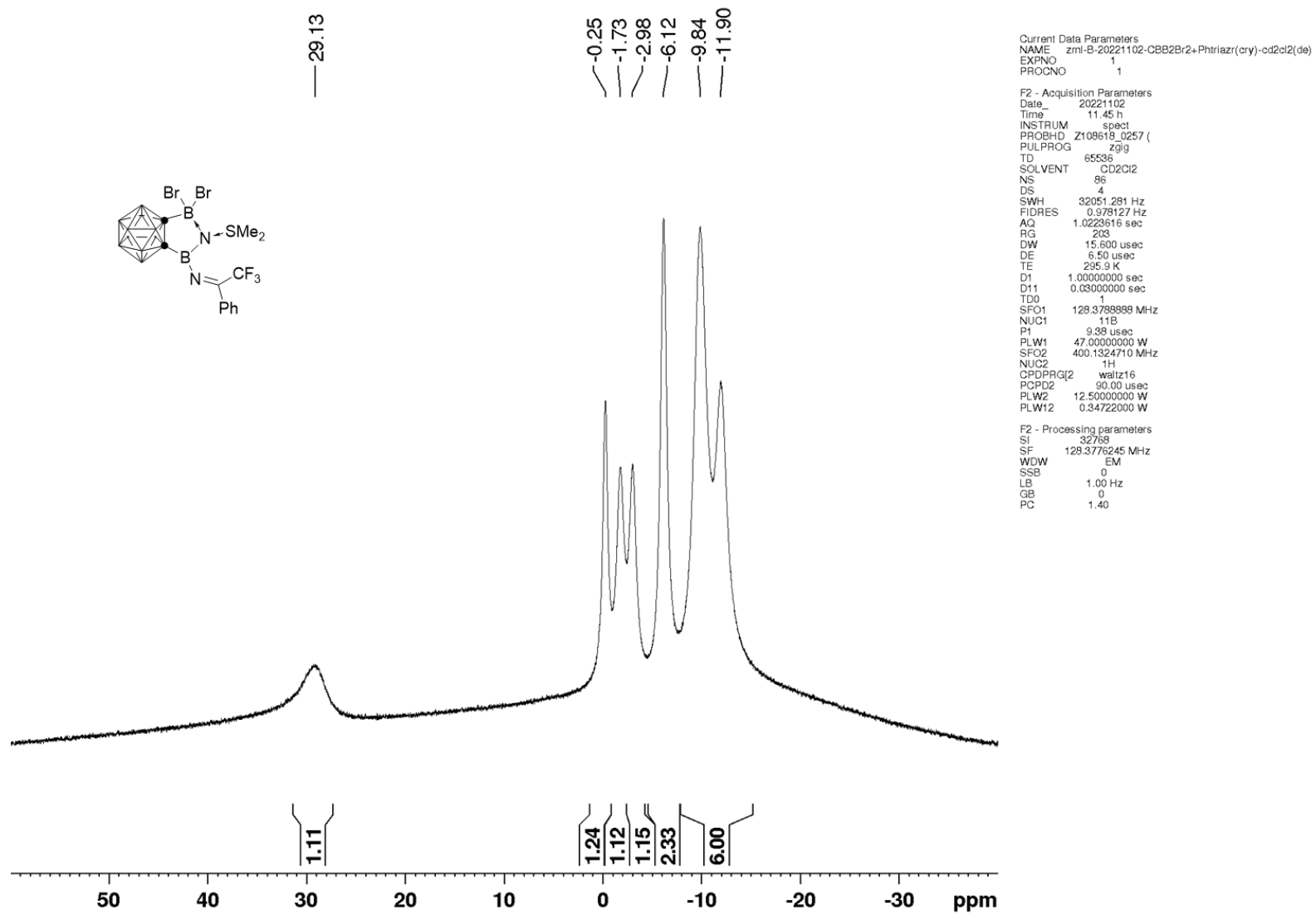


Figure S6. ¹¹B{¹H} NMR spectrum of compound **2** in CD₂Cl₂.

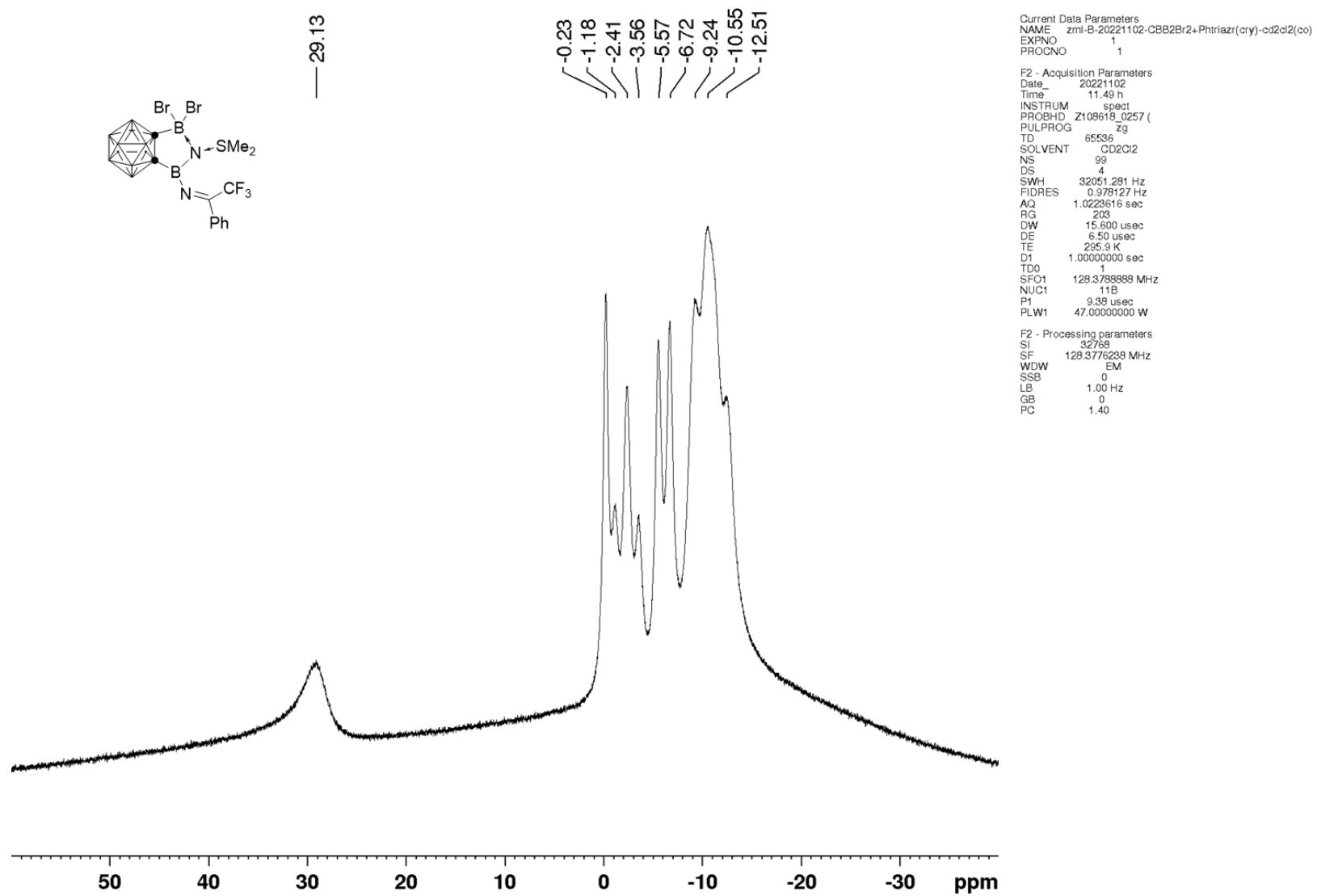
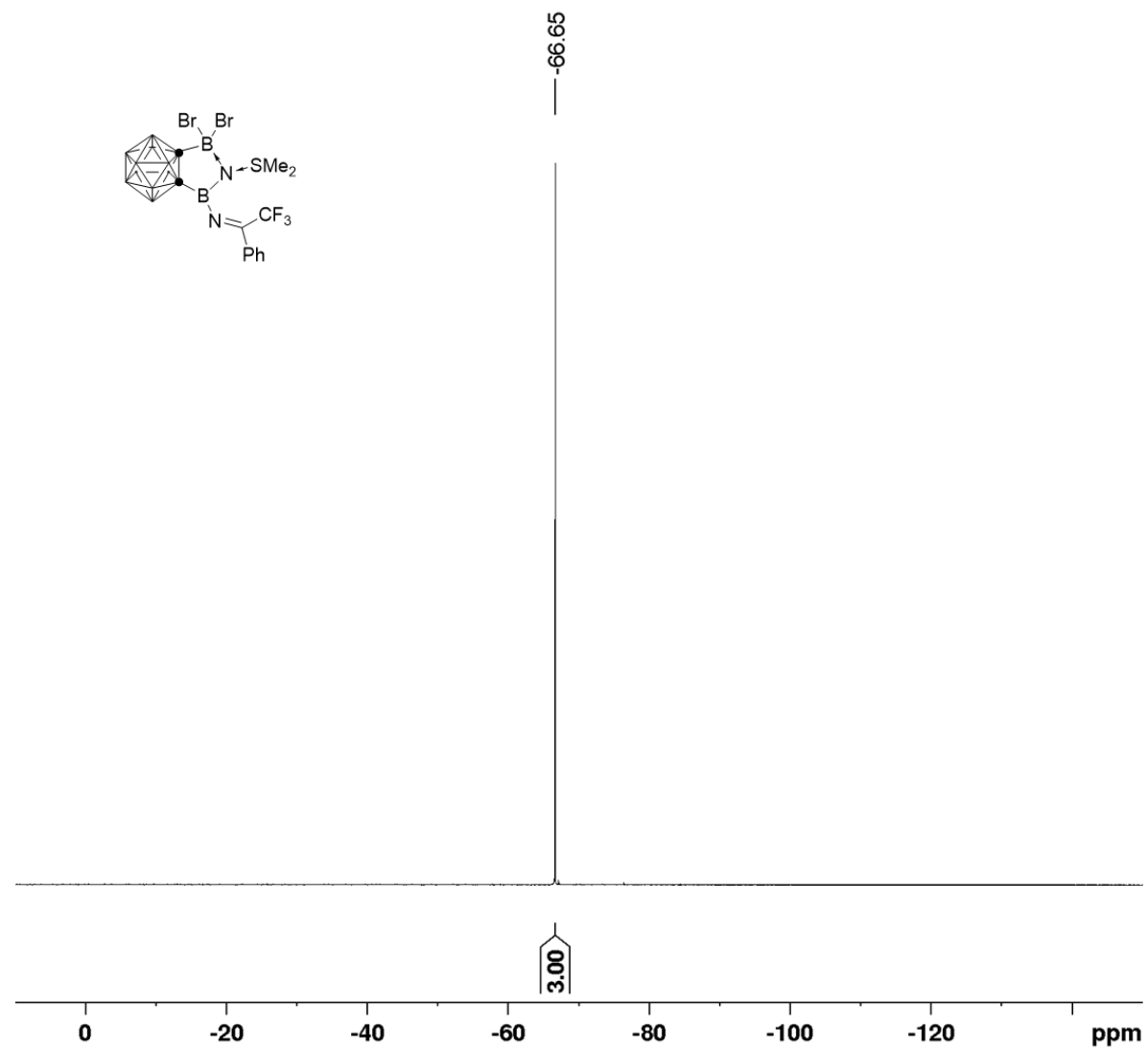


Figure S7. ¹¹B NMR spectrum of compound 2 in CD₂Cl₂.



Current Data Parameters
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 PROCNO 1

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 Time 13.39 h
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 PULPROG zgpg30
 TD 131072
 SOLVENT CD2Cl2
 NS 16
 DS 4
 SWH 113636.367 Hz
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 AQ 0.5767168 sec
 RG 206.72
 DW 4.400 usec
 DE 6.50 usec
 TE 295.2 K
 D1 1.00000000 sec
 TD0 1
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 NUC1 19F
 P1 15.00 usec
 PLW1 47.23500061 W

F2 - Processing parameters
 SI 65536
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S8. ¹⁹F{¹H} NMR spectrum of compound 2 in CD₂Cl₂.

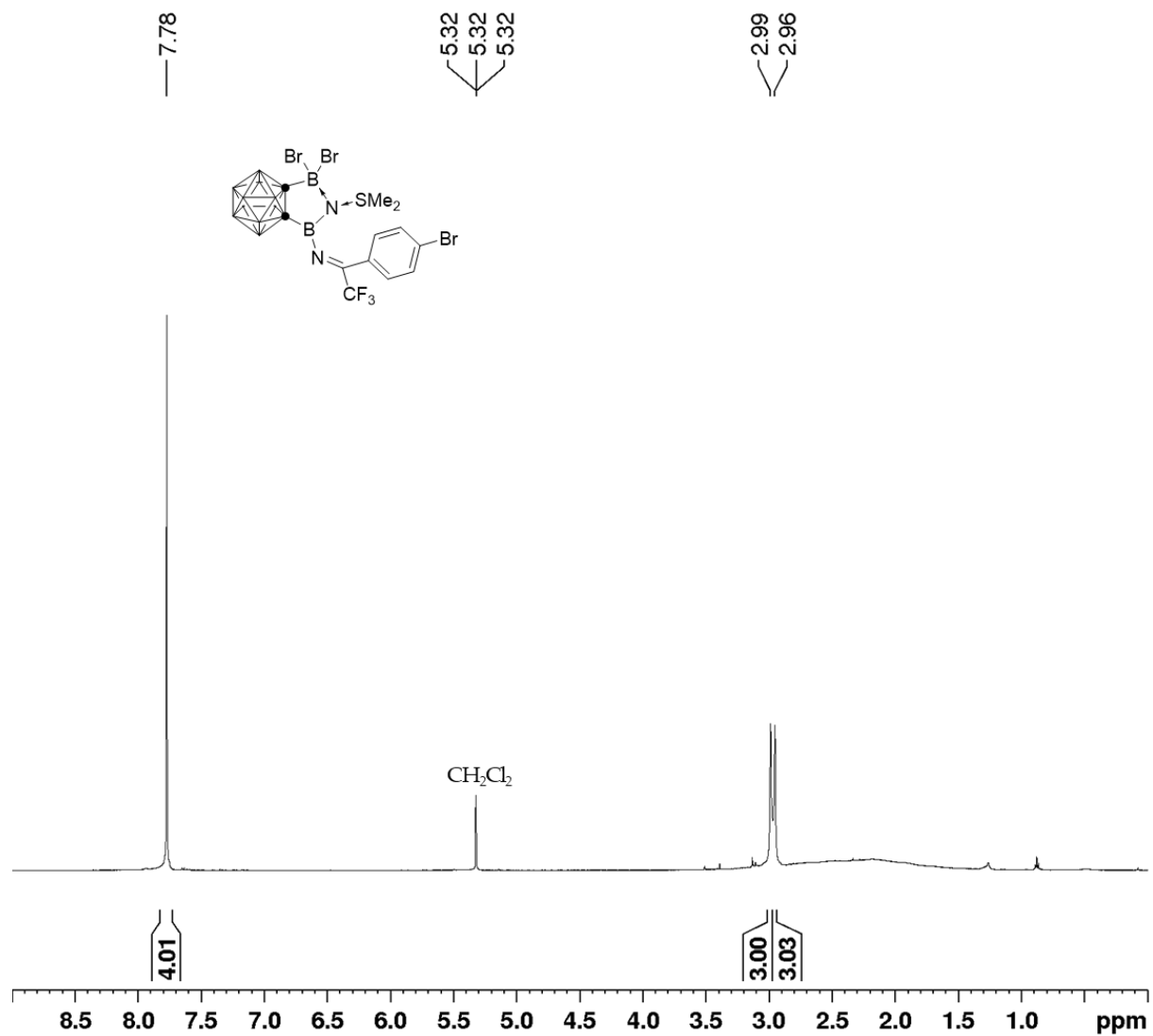


Figure S9. ¹H NMR spectrum of compound 3 in CD₂Cl₂.

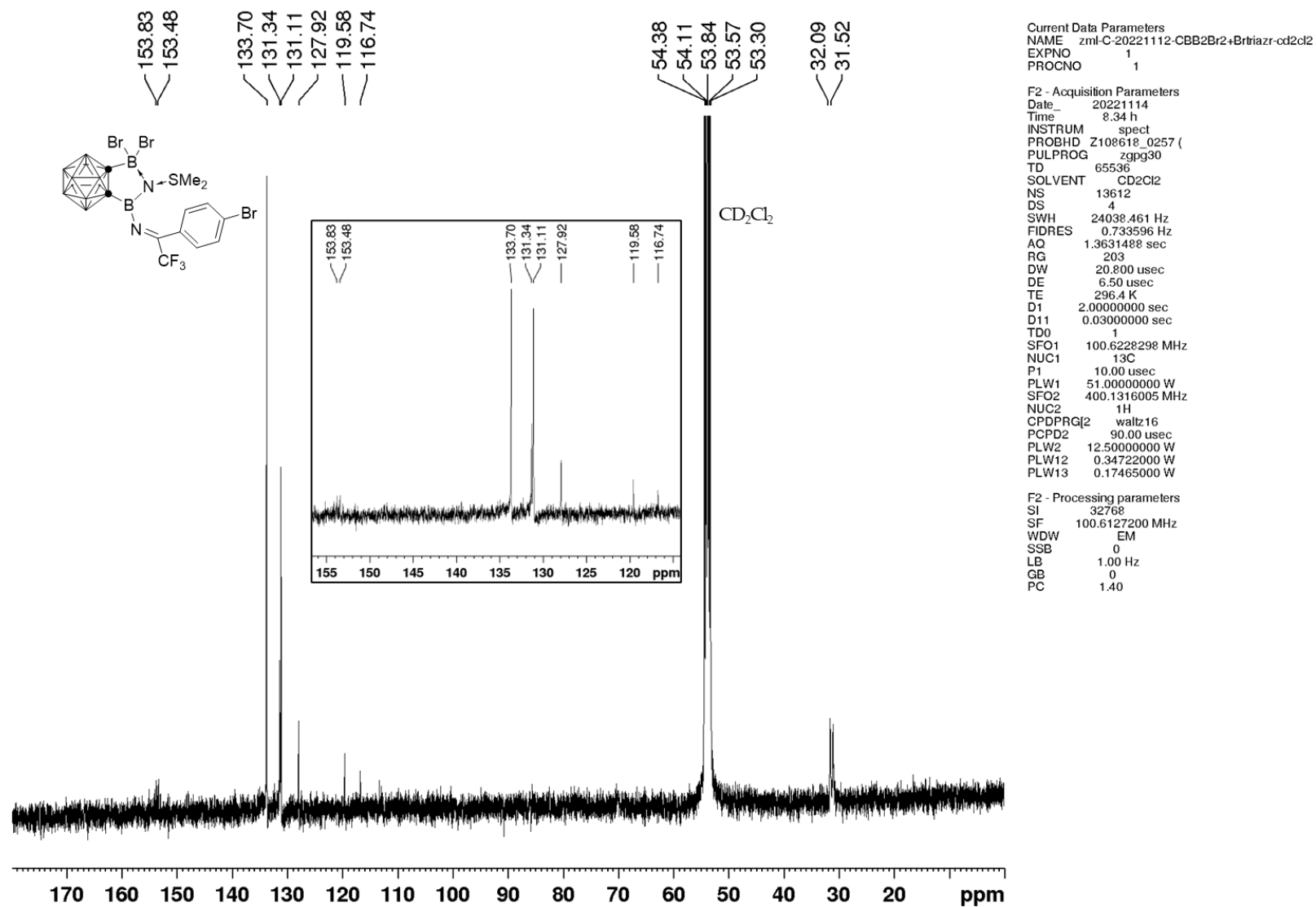


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3** in CD_2Cl_2 .

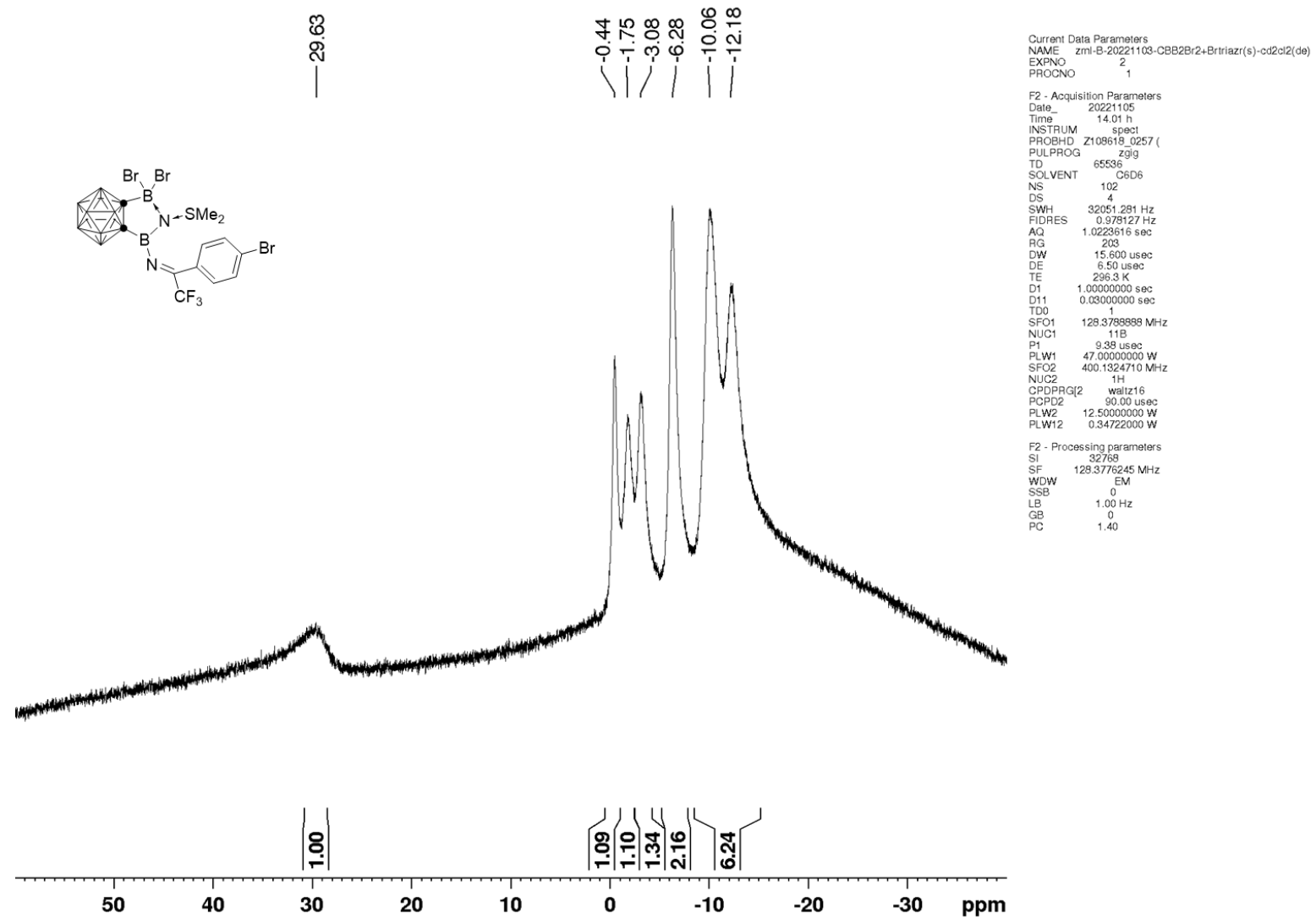
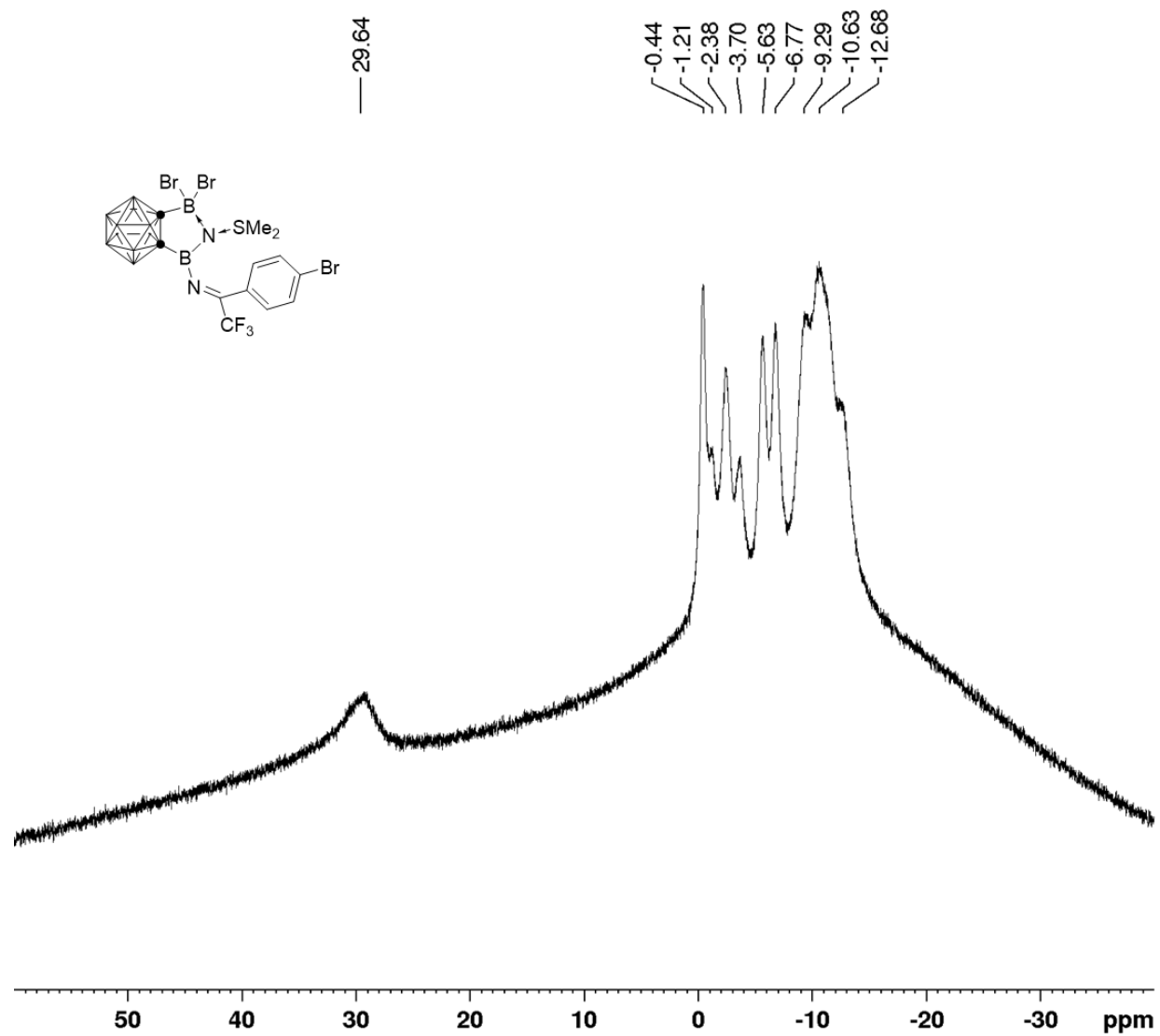


Figure S11. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound 3 in CD_2Cl_2 .

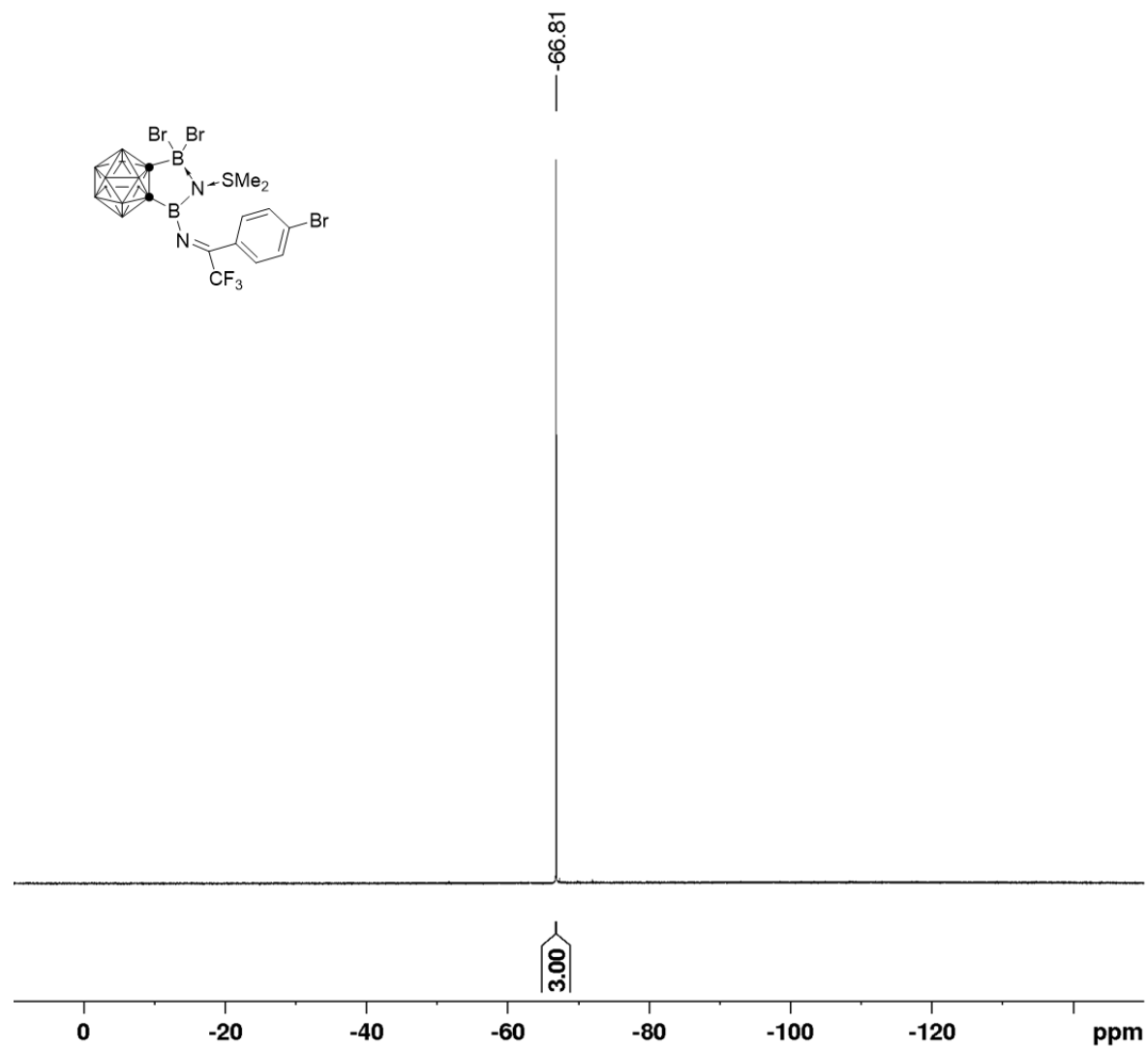


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 PROCNO 1

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 TD 65536
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 NS 136
 DS 4
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 DW 15.600 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.0000000 sec
 TD0 1
 SFO1 128.378898 MHz
 NUC1 11B
 P1 9.98 usec
 PLW1 47.0000000 W

F2 - Processing parameters
 SI 32768
 SF 128.3776233 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S12. ^{11}B NMR spectrum of compound **3** in CD_2Cl_2 .



Current Data Parameters
 NAME zml-F-20221112-CBB2Br2+Brtriazr-cd2cl2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20221112
 Time 13.42 h
 INSTRUM spect
 PROBHD Z119470_0283 (
 PULPROG zgpg30
 TD 131072
 SOLVENT CD2Cl2
 NS 16
 DS 4
 SWH 113636.367 Hz
 FIDRES 1.733953 Hz
 AQ 0.5767168 sec
 RG 206.72
 DW 4.400 usec
 DE 6.50 usec
 TE 295.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 470.5453180 MHz
 NU1 19F
 P1 15.00 usec
 PLW1 47.23500061 W

F2 - Processing parameters
 SI 65536
 SF 470.5923772 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S13. ¹⁹F{¹H} NMR spectrum of compound 3 in CD₂Cl₂.

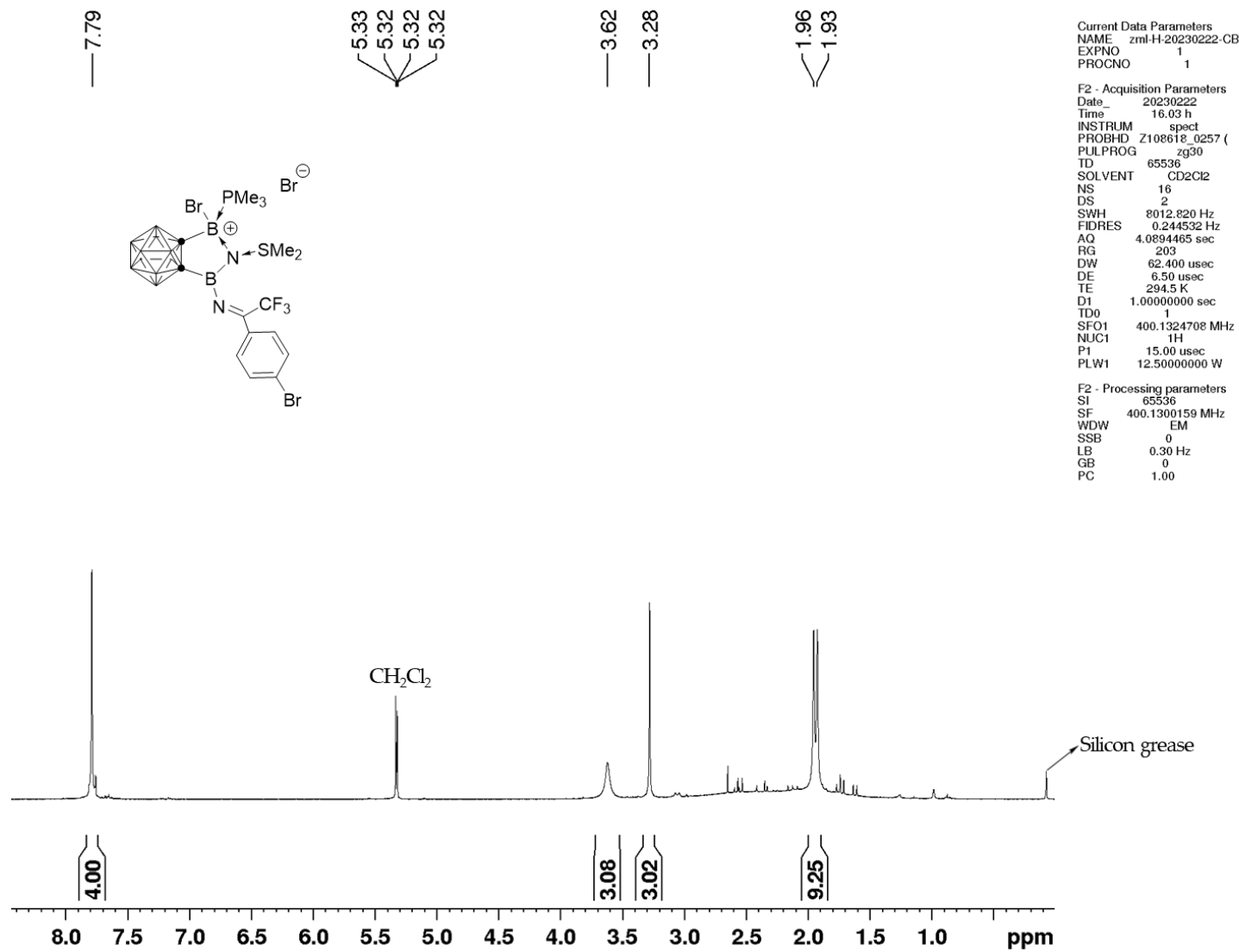


Figure S14. ¹H NMR spectrum of compound 4 in CD₂Cl₂.

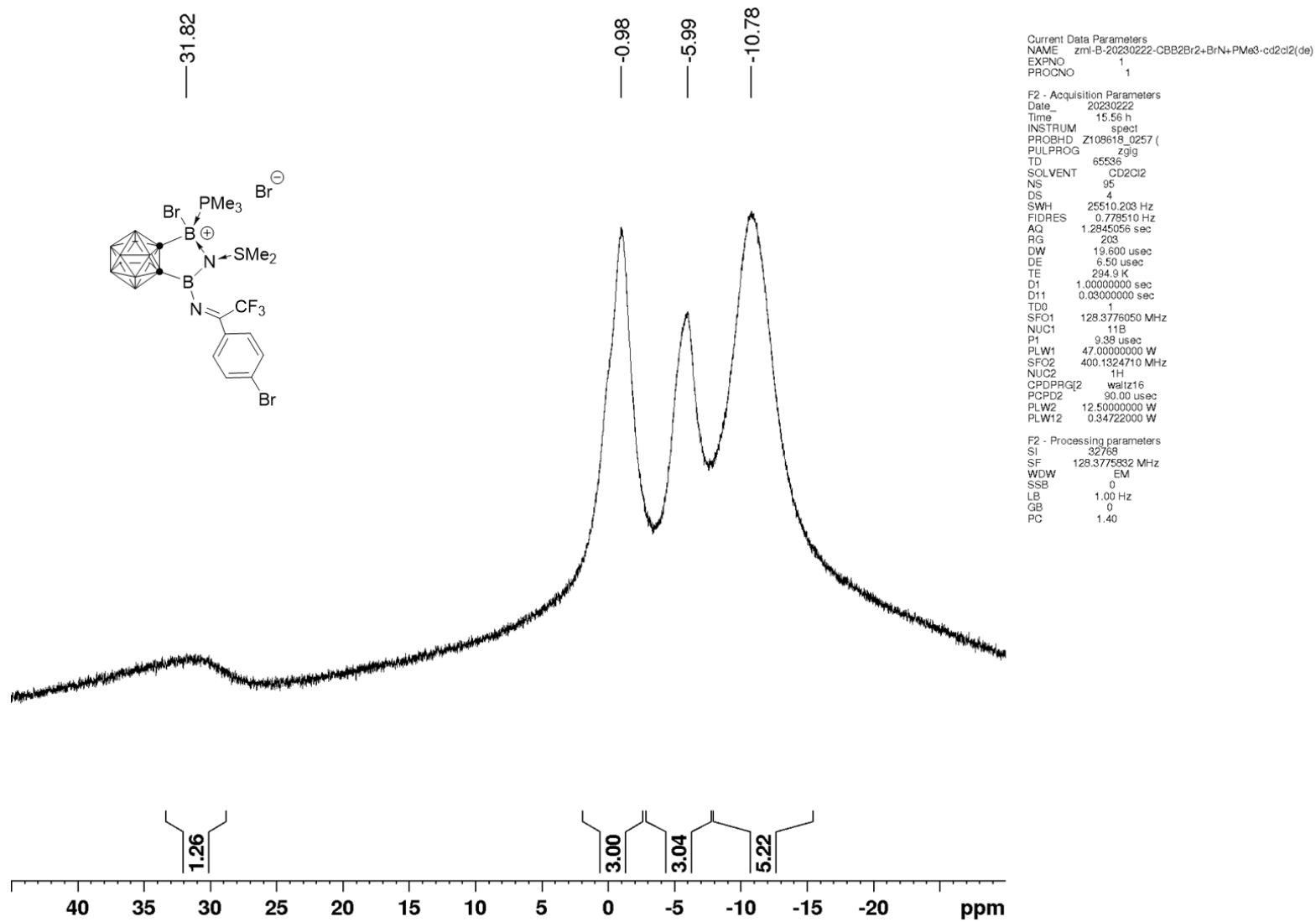


Figure S15. ¹¹B{¹H} NMR spectrum of compound 4 in CD₂Cl₂.

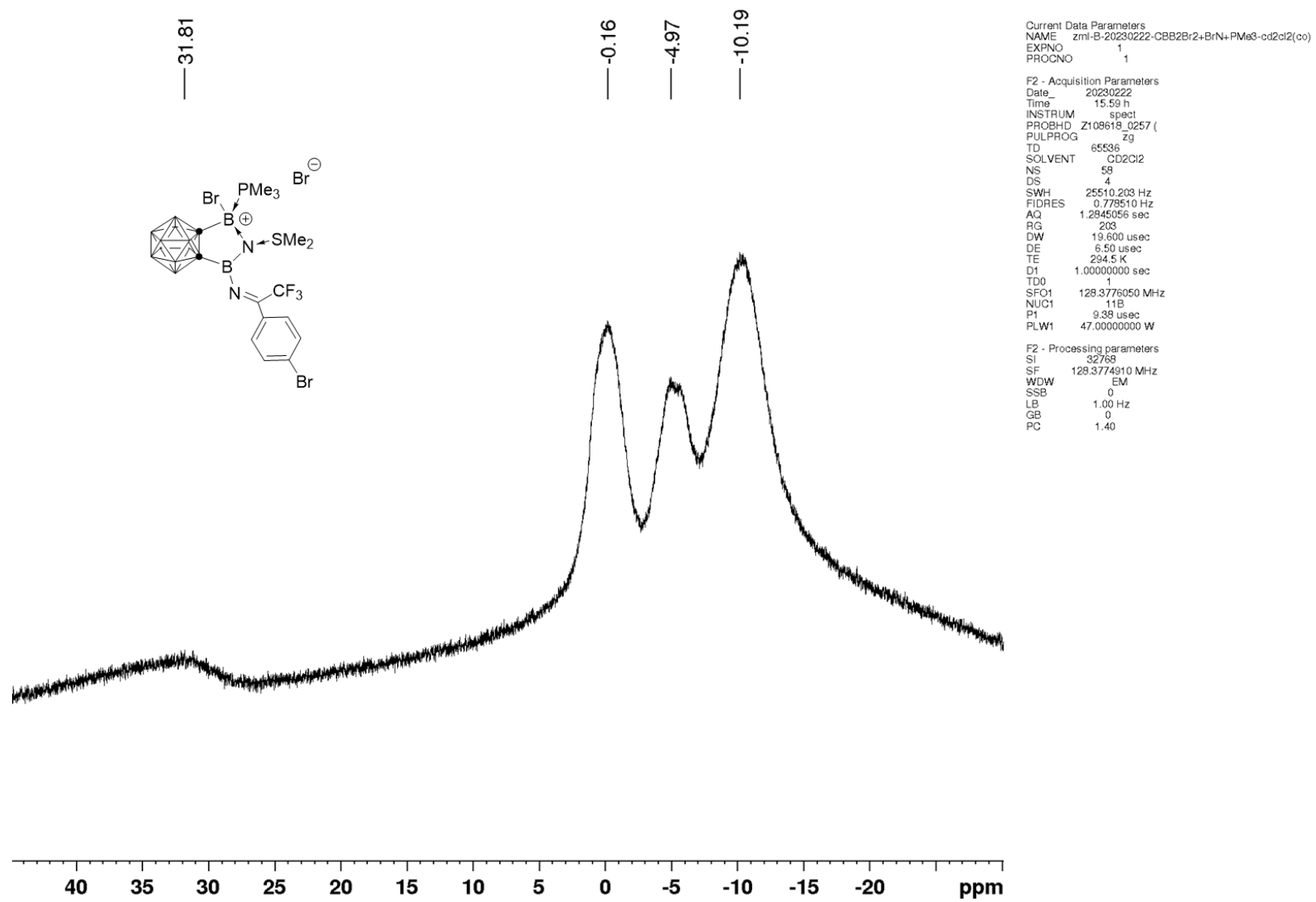
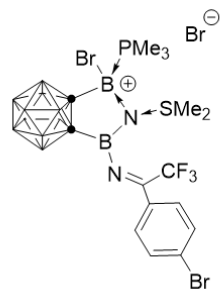
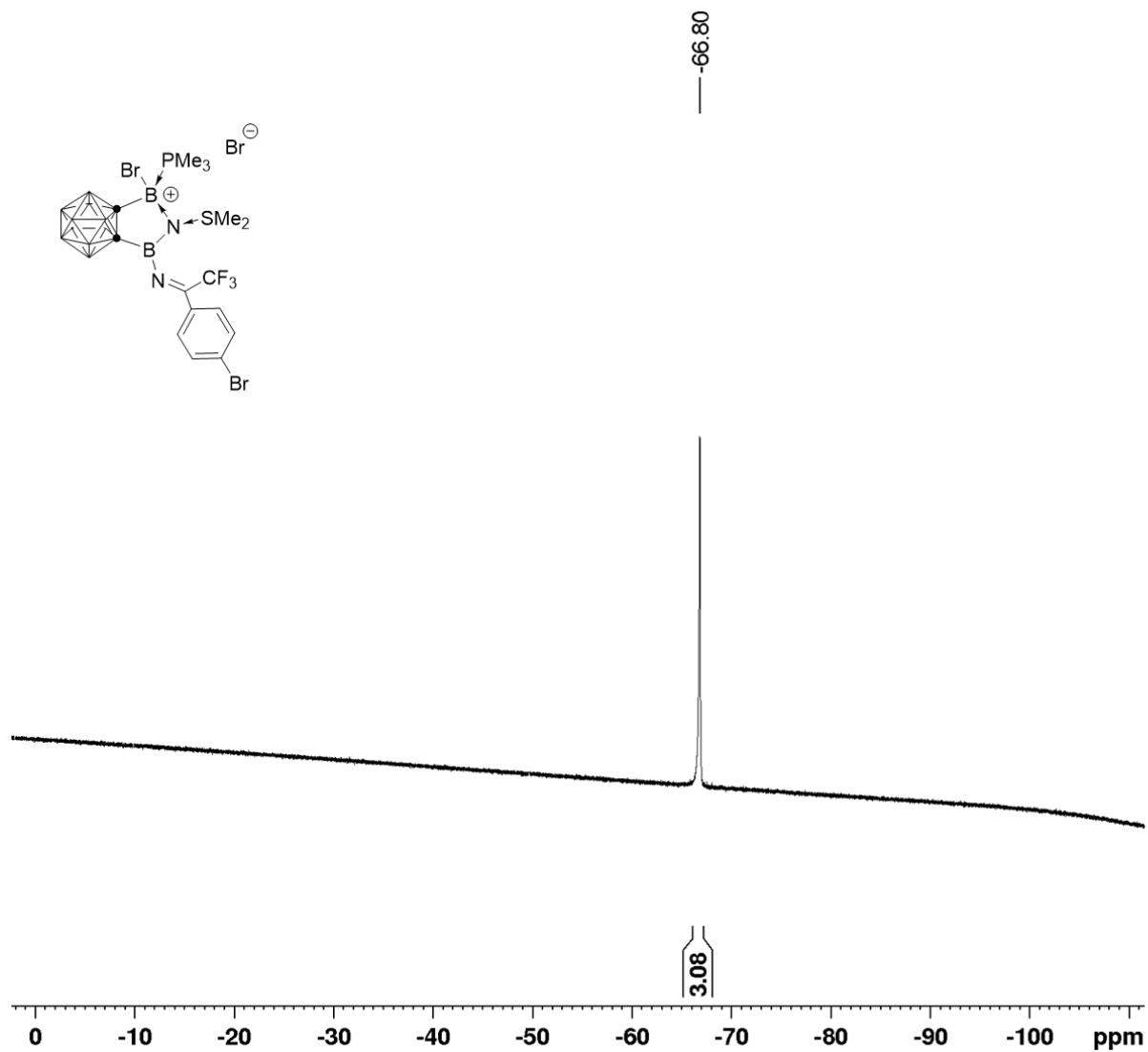


Figure S16. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **4** in CD_2Cl_2 .

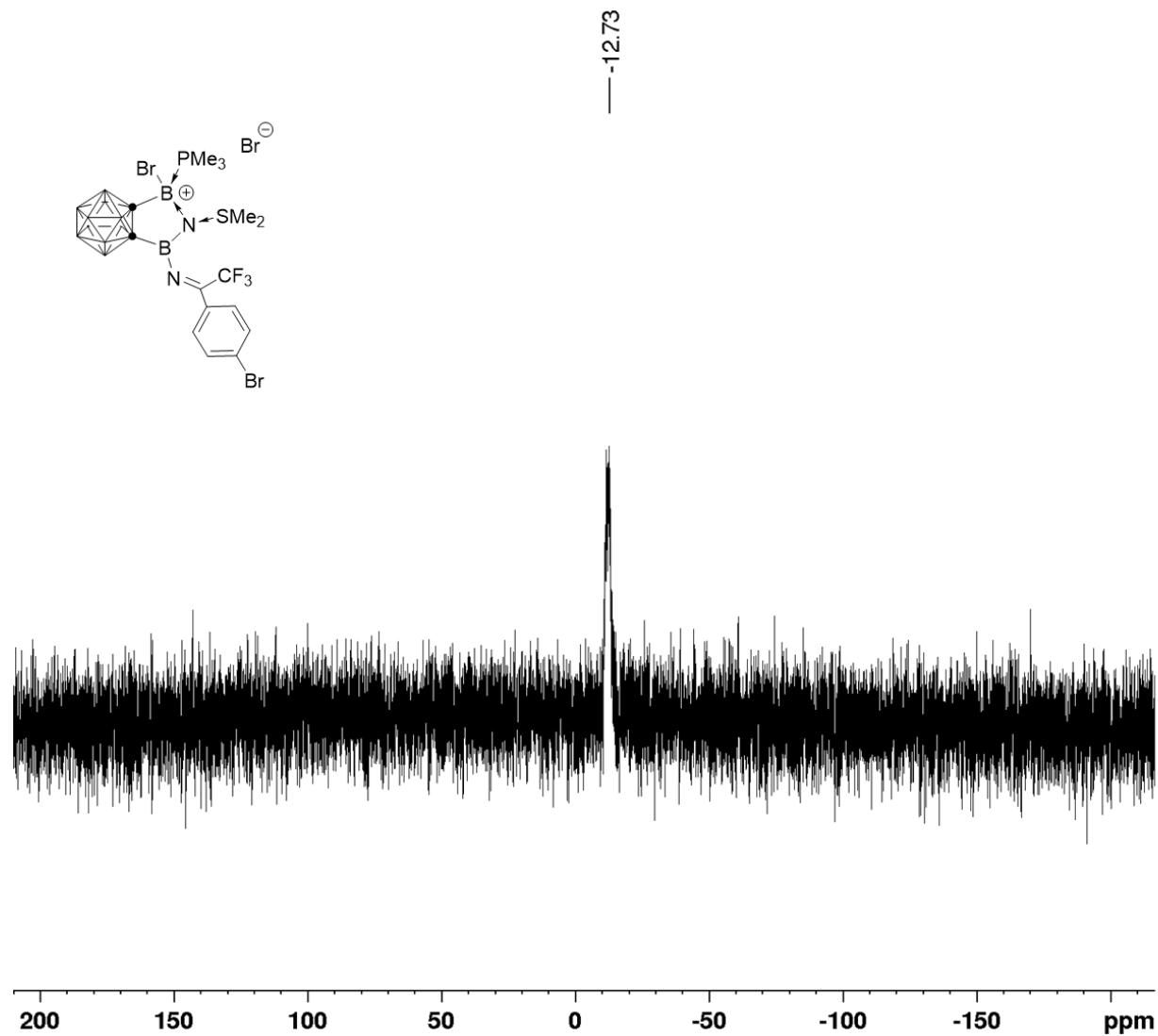


Current Data Parameters
 NAME zml-F-20230321-BrN+PMe3-cd2cl2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230321
 Time 10.31 h
 INSTRUM spect
 PROBHD Z149001_0010 ()
 PULPROG zgpg30
 TD 131072
 SOLVENT None
 NS 16
 DS 4
 SWH 113636.367 Hz
 FIDRES 1.733953 Hz
 AQ 0.5767168 sec
 RG 8.25
 DW 4.400 usec
 DE 18.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 470.5453180 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 14.82900047 W

F2 - Processing parameters
 SI 65536
 SF 470.5923772 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S17. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of compound 4 in CD_2Cl_2 .



Current Data Parameters
 NAME zml-P-20230320-BrN+PMe3-cd2cl2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230320
 Time_ 11.13 h
 INSTRUM spect
 PROBHD Z108618_0257 ()
 PULPROG zg30
 TD 65536
 SOLVENT CD2Cl2
 NS 210
 DS 4
 SWH 163043.484 Hz
 FIDRES 4.975692 Hz
 AQ 0.2009771 sec
 RG 203
 DW 3.067 usec
 DE 6.50 usec
 TE 295.7 K
 D1 2.00000000 sec
 TD0 1
 SFO1 161.9674942 MHz
 NUC1 31P
 P1 15.00 usec
 PLW1 12.00000000 W

F2 - Processing parameters
 SI 32768
 SF 161.9754949 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S18. ^{31}P NMR spectrum of compound **4** in CD_2Cl_2 .

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