Supporting Information for

Synthesis and Reactivity of a Benzo-Fused 1,2-Diborete Biradicaloid

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Contents

Methods and materials

All manipulations were performed either under an atmosphere of dry argon or *in vacuo* using standard Schlenk line or glovebox techniques. Deuterated solvents were dried over molecular sieves and degassed by three freeze-pump-thaw cycles prior to use. All other solvents were distilled and degassed from appropriate drying agents. Both deuterated and non-deuterated solvents were stored under argon over activated 4 Å molecular sieves. Liquid-phase NMR spectra were acquired on a Bruker Avance 500 spectrometer or on a Bruker Avance Neo I 500 (^{1}H: 500.1 MHz, ^{11}B: 129.9 or 160.5 MHz). Chemical shifts (δ) are reported in ppm and internally referenced to the carbon nuclei (^{13}C{^{1}H}) or residual protons (^{1}H) of the solvent. Heteronuclei NMR spectra are referenced to external standards (^{11}B: $BF_3{\cdot}OEt_2$). Resonances are given as singlet (s), doublet (d), triplet (t), septet (sept) or multiplet (m). ^{13}C{^{1}H,^{11}B} and ^{13}C{^{1}H,^{11}B} HMBC NMR spectra were recorded using a Bruker Avance Neo I 600 (^{1}H: 600.2 MHz, ^{11}B: 192.6). The solid-state ^{11}B RSHE/MAS (RSHE = rotor-synchronized Hahn-Echo) NMR spectra of **2** were recorded using a Bruker Avance Neo 400 spectrometer operating at 128.4 MHz for ^{11}B, using a 4 mm (o. d.) ZrO_2 rotor. The solid-state ^{11}B magic-angle spinning (MAS) spectra were acquired by a rotor-synchronized Hahn-Echo (RSHE) at a spinning speed of 14.8 kHz. The ^{11}B second-order quadrupolar powder pattern of **2** (Figure S5) were simulated with the software package SOLA[1] within Topspin™ by Bruker. EPR measurements at X-band (9.85 GHz) were carried out at room temperature using a Bruker ELEXSYS E580 CW EPR spectrometer. CW EPR spectra were measured at 298 K, with a microwave frequency of 9.38 GHz, microwave power of 0.2 mW, modulation amplitude of 0.5 G, conversion time of 60 ms and modulation frequency of 100 kHz. The spectral simulations were performed using MATLAB 9.11.0 (R2021b) and the EasySpin 5.2.33 toolbox.[2] High-resolution mass spectrometry (HRMS) data were obtained from a Thermo Scientific Exactive Plus spectrometer. UV-vis data could not be acquired for any of the low-valent compounds as these decomposed too rapidly under dilute conditions in the cuvette.

Solvents and reagents were purchased from Sigma-Aldrich or Alfa Aesar. 2,3-bis(trimethylsilyl) naphthalene,[3] 1-(2,6-di*iso*propylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC),[4] KC_8[5] and [Fc][PF_6] (Fc = $(C_5H_5)_2Fe$)[6] were synthesized using literature procedures. CO was used as purchased.

Synthetic procedures

Synthesis of 1

The literature-known synthetic route was optimized in the following manner and hitherto missing ^{13}C NMR data obtained. In a thick-walled Schlenk flask a solution of (2-dichlorborylphenyl)trimethylsilane (21.8 g, 94.2 mmol, 1.00 equiv.) in DCM (40 mL) was cooled to −78 °C and a solution of BCl_3 in CH_2Cl_2 (2.00 M, 141 mL, 282 mmol, 3.00 equiv.) was added via syringe. The reaction mixture was then frozen with liquid N_2, the Schlenk flask subjected to high vacuum, the tap closed, and the flask slowly heated to 95 °C. The reaction mixture was stirred at this temperature for two days prior to removal of the solvent *in vacuo* and distillation (BP = 52 °C at $8.5 \cdot 10^{-2}$ mbar) yielded **1** as a colorless viscous liquid (20.5 g, 85.8 mmol, 91%). NMR data showed that the 1,3 isomer of **1**, compound **2**, was always formed in small amounts (< 5%), independent of the reaction conditions or stoichiometry, and could not be separated either by distillation or chromatography. NMR data for **1**: ^1H NMR (500 MHz, C_6D_6): δ = 7.87–7.85 (dd, ^3J = 5.6 Hz, ^4J = 3.3 Hz, 2H, 3,6-H_{Bn}), 7.64–7.63 (dd, ^3J = 5.6 Hz, ^4J = 3.3 Hz, 2H, 4,5-H_{Bn}) ppm. $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ = 142.6 (1,2-C_qB), 134.0 (3,6-CH$_{Bn}$), 132.2 (4,5-CH$_{Bn}$) ppm. ^{11}B NMR (160 MHz, C_6D_6): δ = 56.7 (s) ppm. NMR data for **2**: ^1H NMR (500 MHz, C_6D_6): δ = 8.91 (s, 1H, 2- H_{Bn}), 8.44 (dd, ^3J = 7.6 Hz, ^4J = 1.5 Hz, 2H, 4,6-H_{Bn}), 7.71 (tm, ^3J = 7.6 Hz, 1H, 5-H_{Bn}) ppm. HRMS-ASAP neg. calcd. for $[C_6H_4B_2Cl_5]^-$ = [**1** + Cl]$^-$: 274.8918; found 274.8919.

Synthesis of 3-I*i*Pr

To a solution of **1** (1.46 g, 6.11 mmol, 1.00 equiv.) in toluene (50 mL) a solution of I*i*Pr (1.91 g, 12.5 mmol, 2.05 equiv.) in toluene (100 mL) was added dropwise at −78 °C. The mixture was stirred and allowed to warm to room temperature overnight. To the resulting suspension hexane was added to cause the product to precipitate further. After filtration the resulting solid was washed with hexane (3 × 10 mL) and benzene (3 × 10 mL). The solid residue was dried *in vacuo*, yielding **3-I*i*Pr** as an off-white solid (1.44 g, 2.64 mmol, 43%). Single crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of a saturated benzene solution. *Note: **3-IiPr** always crystallized together with ca. 6% of its 1,3 isomer, **4-IiPr**, resulting from the impurity **2** present in the starting material **1**.* NMR data for **3-I*i*Pr**: ^1H NMR (500.1 MHz, CD_2Cl_2): δ = 8.98 (dd, ^3J = 5.8 Hz, ^4J = 3.5 Hz, 2H, H_{Bn}), 7.41 (dd, ^3J = 5.8 Hz, ^4J = 3.5 Hz, 2H, H_{Bn}), 6.21 (s, 4H, NCH), 5.13-5.87 (v. br, 4H, C$H_{i\text{Pr}}$), 1.06 (br s, 12H, C$H_{3\text{-}i\text{Pr}}$), 1.05 (br s, 12H, C$H_{3\text{-}i\text{Pr}}$) ppm. $^{13}C\{^1H\}$ NMR (125.8 MHz, CD_2Cl_2): δ = 159.2 (C_q), 149.7

(C_q), 136.3 (CH_{Bn}), 126.7 (CH_{Bn}), 116.4 (NC*H*), 49.7 (CH_{iPr}), 23.7 ($CH_{3\text{-}iPr}$), 22.8 ($CH_{3\text{-}iPr}$) ppm. ^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 3.7 ppm. ^{1}H NMR data for **4-I*i*Pr** (500.1 MHz, CD_2Cl_2): δ = 7.69 (dd, ^3J = 5.4 Hz, ^4J = 3.1 Hz, 1H, H_{Bn}), 7.32 (dd, ^3J = 5.4 Hz, ^4J = 3.1 Hz, 1H, H_{Bn}), 7.11-7.15 (m, 1H, H_{Bn}), 7.00-7.03 (m, 1H, H_{Bn}), 6.29 (s, 4H, NC*H*), 5.95 (sept, ^3J = 6.6 Hz, 4H, CH_{iPr}), 1.06 (overlapping with **3-I*i*Pr**, 12H, C$H_{3\text{-}iPr}$), 0.95 (d, ^3J = 6.6 Hz, 12H, C$H_{3\text{-}iPr}$) ppm. HRMS-LIFDI calcd. for $[C_{24}H_{36}B_2Cl_3N_4]^+$ = [**3-I*i*Pr** – Cl]$^+$: 507.2181; found 507.2186.

Synthesis of 3-CAAC

To a solution of freshly distilled **1** (1.82 g, 7.59 mmol, 1.00 equiv.) in toluene (50 mL) a solution of CAAC (4.44 g, 15.6 mmol, 2.05 equiv.) in toluene (250 mL) was added dropwise at −78 °C. The yellow suspension was stirred and allowed to warm to room temperature overnight prior to filtration. The resulting colorless solid was washed with hexane (3 × 10 mL) and benzene (3 × 10 mL) and dried *in vacuo*, yielding **3-CAAC** as a colorless solid (4.28 g, 5.27 mmol, 70%). **3-CAAC** is only soluble in chlorinated solvents, in which it reacts to yield the ionic species **5**. Therefore, only solid-state NMR data of **3-CAAC** was acquired. Single crystals of **3-CAAC** suitable for X-ray crystallographic analysis were nevertheless obtained from an attempted reduction with 2.2 equiv. sodium in diethyl ether. ^{11}B NMR (RSHE/MAS, 14.8 kHz): δ_{iso} = 4.0 (C_Q = 1.6 MHz, η_Q = 0.5) ppm. ^{15}N NMR (CP/MAS, 10.0 kHz): δ = –164.1 ppm. HRMS-LIFDI calcd. for $[C_{46}H_{66}B_2Cl_3N_2]^+$ = [**3-CAAC** – Cl]$^+$: 773.4472; found: 773.4464.

Isolation of 4-CAAC

During the workup of **3-CAAC** a small amount of the 1,3 isomer **4-CAAC**, resulting from the impurity **2** present in the starting material **1**, was isolated as a colorless solid from the benzene washing fractions (112 mg, 138 µmol, 8%). Considering that the compound **2** was present as ca. 9% of the starting material, this corresponds to ca. 88% of the maximum theoretical yield. Single crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of a saturated toluene solution. Given that **4-CAAC** is an unwanted byproduct, no ^{13}C NMR data was acquired. ^{1}H NMR (400.6 MHz, C_6D_6): δ = 8.57 (br s, 1H, H_{Bn}), 8.11 (br d, ^3J = 7.4 Hz, 2H, H_{Bn}), 7.53 (br t, ^3J = 7.4 Hz, 1H, H_{Bn}), 7.09 (br m, 6H, H_{Dip}), 3.07 (br m, 4H, CH_{iPr}), 1.80 (br s, 12H, CH_3), 1.33 (br s, 4H, CH_2), 1.25 (br s, 12H, CH_3), 1.22 (br s, 6H, CH_3), 1.20 (br s, 6H, CH_3), 0.84 (br s, 12H, CH_3) ppm. ^{11}B NMR (128.5 MHz, C_6D_6): δ = 4.7 (br) ppm. HRMS-LIFDI calcd. for $[C_{46}H_{66}B_2Cl_3N_2]^+$ = [**4-CAAC** – Cl]$^+$: 775.4443; found: 775.4423.

Synthesis of 5

Recrystallization of **3-CAAC** (3.39 g, 4.18 mmol) from dichloromethane yielded **5** (2.30 g, 2.72 mmol, 65%). In solution **5** decomposed slowly to [CAACH]Cl, identifiable by its characteristic ^{1}H NMR singlet at 11.35 ppm.**Error! Reference source not found.** NMR data for **5**: ^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 14.26 (s, [*H*Cl_2]$^-$), 7.53 (t, ^{3}J = 7.8 Hz, 2H, H_{Bn}), 7.38 (d, ^{3}J = 7.8 Hz, 2H, H_{Bn}), 7.06-7.36 (m, 6H, H_{Dip}), 2.72 (br sept, ^{3}J = 6.5 Hz, 2H, C*H*$_{i Pr}$), 2.66 (br, 2H, C*H*$_{i Pr}$), 2.17 (two d, AB system, ^{2}J = 13.8 Hz, 2H, C*H*$_2$), 1.54 (br, 6H, C*H*$_{3\text{-}i Pr}$), 1.49 (s, 6H, C*H*$_3$), 1.36-1.42 (m, 30H, C*H*$_3$), 1.08 (br, 6H, C*H*$_{3\text{-}i Pr}$) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 211.8 ($C_{carbene}$), 148.2 (C_q), 144.9, 144.6 (C_q), 144.4, 138.3 (Cq), 133.5 (Cq), 132.0, 131.7 (CHAr), 126.3 (CHDip), 125.6, 125.6, 83.3 (Cq), 55.6 (Cq), 53.2 (CH2), 49.6 (CH2), 48.7 (Cq), 32.0 (Cq), 31.2, 30.3, 30.0, 29.9, 28.6, 28.4, 26.9, 26.8, 26.6, 25.8 (Cq), 25.4, 25.1, 25.0 (Cq), 22.1 ppm. ^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 14.0 (br) ppm. HRMS-LIFDI calc. for $[C_{46}H_{66}B_2Cl_3N_2]^+$ = [**5** – HCl_2]$^+$: 773.4472; found: 773.4464.

Synthesis of 6

THF (0.6 mL) was added to a mixture of **3-I*i*Pr** (200 mg, 368 µmol) and lithium sand (21.7 mg, 3.12 mmol, 8.5 equiv.) and the mixture was stirred vigorously at rt. Color changes to green then to deep red were observed over the course of 1 h. After filtration and solvent removal from the filtrate, **6** was isolated as a green solid (126 mg, 313 µmol, 85%). ^{1}H NMR (500 MHz, C_6D_6): δ = 7.88 (dm, ^{3}J = 6.8 Hz, 1H, H_{Bn}), 7.38 (ddd, ^{3}J = 7.1, 7.6 Hz, ^{4}J = 1.2 Hz, 1H, H_{Bn}), 7.12 (ddd, ^{3}J = 6.8, 7.6Hz, ^{4}J = 1.1 Hz, 1H, H_{Bn}), 6.69 (dm, ^{3}J = 7.1 Hz, 1H, H_{Bn}), 6.18 (s, 2H, NC*H*$_{IiPr}$), 6.01 (d, ^{3}J = 6.3 Hz, 1H, NC*H*$_{C3N2B}$), 5.80 (d, ^{3}J = 6.3 Hz, 1H, NC*H*$_{C3N2B}$), 5.00 (sept, ^{3}J = 6.6 Hz, 1H, C*H*$_{i Pr}$), 4.90 (sept, ^{3}J = 6.8 Hz, 2H, C*H*$_{i Pr}$), 3.19 (sept, ^{3}J = 6.6 Hz, 1H, C*H*$_{i Pr}$), 1.35 (d, ^{3}J = 6.6 Hz, 6H, C*H*$_{3\text{-}i Pr}$) 1.15 (d, ^{3}J = 6.6 Hz, 6H, C*H*$_{3\text{-}i Pr}$), 0.90 (d, ^{3}J = 6.8 Hz, 6H, C*H*$_{3\text{-}i Pr}$), 0.86 (d, ^{3}J = 6.8 Hz, 6H, C*H*$_{3\text{-}i Pr}$) ppm. ^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ = 167.9 (br, $C_{q\text{-}Bn}$), 164.0 ($C_{carbene}$, detected by HMBC), 143.9 (br, *C*=B, detected by HMBC), 142.5 ($C_{q\text{-}Bn}$), 129.2 (*C*H$_{Bn}$), 129.0 (*C*H$_{Bn}$), 121.5 (*C*H$_{Bn}$), 119.6 (*C*H$_{Bn}$), 115.9 (N*C*H$_{IiPr}$), 114.6 (N*C*H$_{C3N2B}$), 104.1 (N*C*H$_{C3N2B}$), 53.0 (*C*H$_{i Pr\text{-}\ C3N2B}$), 50.9 (*C*H$_{i Pr\text{-}NHC}$), 48.6 (*C*H$_{i Pr\text{-}C3N2B}$), 23.6 (*C*H$_{3\text{-}i Pr}$), 23.0 (*C*H$_{3\text{-}i Pr}$), 22.4 (*C*H$_{3\text{-}i Pr}$), 21.3 (*C*H$_{3\text{-}i Pr}$) ppm. 11B NMR (160.5 MHz, C_6D_6): δ = 39.9 (br, *B*N), 12.9 (*B*C$_{NHC}$) ppm. HRMS LIFDI calcd. (*m*/*z*) for $[C_{24}H_{37}B_2N_4]^+$ = [**6** + H]$^+$: 403.3199; found: 403.3194.

One-electron reduction of 3-CAAC

THF (0.6 mL) was added to a mixture of **3-CAAC** (100 mg, 123 µmol) and KC_8 (15.0 mg, 111 µmol, 0.90 equiv.) and the mixture stirred vigorously at rt. After 2 h the suspension was filtered through celite and the resulting yellow filtrate left to slowly evaporate under ambient conditions in the glovebox, yielding **8** as an off-white solid (68.0 mg, 87.7 µmol, 71%). ^{11}B NMR (160.5 MHz, THF): silent. HRMS-LIFDI calcd. (*m*/*z*) for $[C_{46}H_{66}B_2Cl_3N_2]^+$ = [**8**]$^+$: 773.4472; found: 773.4458. *Note: attempts to recrysatllise **8** systematically led to the isolation of the hydrogen-abstraction product **8-H**, which was confirmed by X-ray crystallographic analysis.*

Two-electron reduction of 3-CAAC

Diethyl ether (0.6 mL) was added to a mixture of **3-CAAC** (0.10 g, 0.12 mmol) and sodium metal (6.0 mg, 0.27 mmol, 2.2 equiv.) and the mixture stirred vigorously at rt. After 2 h the suspension was filtered over celite and the resulting brown filtrate left to slowly evaporate under ambient conditions in the glovebox. An isolated yield could not be determined as **9** decomposed rapidly upon complete removal of the solvent. ^{11}B NMR (160.5 MHz, Et_2O): silent. HRMS-LIFDI calcd. (*m*/*z*) for $[C_{46}H_{66}B_2ClN_2]^+$ = [**9** – Cl]$^+$: 703.5095; found: 703.5074.

Synthesis of 10

Diethyl ether (0.6 mL) was added to a mixture of **3-CAAC** (100 mg, 123 µmol) or **5** (104 mg, 123 µmol) and sodium metal (14.2 mg, 617 µmol, 5.00 equiv.) and the mixture stirred energetically at rt. Successive color changes from colorless to gray to green (2 h) to red (2.5 h) were observed. After filtration the filtrate was rapidly evaporated under ambient conditions in the glovebox, yielding **10** as a red solid (49.1 mg, 73.4 µmol, 59%). Solvent removal *in vacuo* led to decomposition. **10** is easily reduced at rt by excess sodium to **11-Na**, which cannot be separated from **10** due to its very similar solubility. However, at temperatures below –40 °C no reduction of **10** was observed. Single crystals of **10** suitable for X-ray crystallographic analysis were obtained by rapid evaporation from a saturated diethyl ether solution. ^{11}B NMR (128.5 MHz, Et_2O): silent. HRMS-LIFDI calcd. (*m*/*z*) for $[C_{46}H_{67}B_2N_2]^+$ = [**10** + H]$^+$: 669.5485; found: 669.5479.

Synthesis of 11-Li

THF (1 mL) was rapidly added to a mixture of **3-CAAC** (0.10 g, 0.12 mmol) and lithium sand (7.3 mg, 1.1 mmol, 8.5 equiv.) and the mixture stirred vigorously at rt. The reaction mixture instantly turned green, then rapidly to brown. After 30 min the suspension was filtered and the

solvent of the filtrate evaporated. The residual solid was washed with cold hexane (3 x 1 mL), extracted with THF (2 mL), then slowly concentrated *in vacuo*, yielding **11-Li** as brown-red crystals suitable for X-ray crystallographic analysis. These decomposed rapidly upon complete removal of the solvent, which is why no yield was determined and no NMR data acquired beyond ^{11}B NMR. ^{11}B NMR (160.5 MHz, THF): δ = 26.0 (br) ppm. HRMS-LIFDI calcd. (*m*/*z*) for $[C_{46}H_{67}B_2N_2]^+$ = [**11-Li** – 2 Li + H]$^+$: 669.5485; found: 669.5472.

Synthesis of 11-Na

1 mL diethyl ether was rapidly added to a mixture of **3-CAAC** (100 mg, 123 µmol) or **5** (104 mg, 123 µmol) and sodium metal (14.2 mg, 617 µmol, 5.00 equiv.) and the mixture stirred vigorously at rt. Successive color changes from colorless to gray to green (2 h) to red (2.5 h) were observed. After 3 h the suspension was filtered and the filtrate was slowly concentrated in vacuo, yielding deep red crystals of **11-Na** suitable for X-ray crystallographic analysis (93.0 mg, 108 µmol, 87%). ^{1}H NMR (600 MHz, C_6D_6): δ = 7.23–7.16 (m, 6H, H_{Bn} + H_{Dip}), 6.34 (m, 2H, H_{Bn}), 5.00 (m, 2H, *p*-H_{Dip}), 3.66 (sept, ^3J = 6.8 Hz, 4H, C$H_{i\text{Pr}}$), 3.09 (q, ^3J = 6.7 Hz, 8H, C$H_{2\text{-Et2O}}$), 2.16 (s, 4H, C$H_{2\text{-CAAC}}$), 2.02 (s, 12H, C$H_{3\text{-CAAC}}$), 1.39 (d, ^3J = 6.8 Hz, 12H, C$H_{3\text{-}i\text{Pr}}$), 1.26 (d, ^3J = 6.8 Hz, 12H, C$H_{3\text{-}i\text{Pr}}$), 1.21 (br s, 12H, C$H_{3\text{-CAAC}}$), 0.93 (t, ^3J =6.7 Hz, 12H, C$H_{3\text{-Et2O}}$) ppm. ^{13}C{^{1}H} NMR (151 MHz, C_6D_6): δ = 167.8 (C_qB), 164.2 ($C_{carbene}$, detected by HMBC), 149.5 (*o*-C_{Dip}), 149.0 (*i*-C_{Dip}), 148.9 (*o*-C_{Dip}), 128.3 (CH_{Dip}), 125.7 (CH_{Bn}), 124.4 (CH_{Dip}), 124.4 (CH_{Bn}), 122.4 (CH_{Bn}), 65.8 ($CH_{2\text{-Et2O}}$), 63.0 (CH_2), 62.3 (NC_q), 43.1 (NC_q(CH$_3$)$_2$), 37.1 (C(CH$_3$)$_2$), 30.6 (NC(CH$_3$)$_2$), 28.3 ($CH_{i\text{Pr}}$), 25.6 ($CH_{3\text{-}i\text{Pr}}$), 24.9 ($CH_{3\text{-}i\text{Pr}}$), 15.2 ($CH_{3\text{-Et2O}}$) ppm. ^{11}B NMR (192.6 MHz, C_6D_6): δ = 22.2 (br) ppm. HRMS-LIFDI calcd. for $[C_{46}H_{67}B_2N_2]^+$ = [**11-Na** – 2 Na + H]$^+$: 669.5485; found: 669.5475.

Synthesis of 11-K

1 mL THF was rapidly added to a mixture of **3-CAAC** (0.10 g, 0.12 mmol) and KC_8 (142 mg, 1.05 mmol, 8.50 equiv.) and the mixture stirred vigorously at rt. The reaction mixture instantly turned green, then rapidly to brown. After 3 h the suspension was filtered and the solvent of the filtrate evaporated under ambient conditions. Dark brown single crystals of **11-K** suitable for X-ray crystallographic analysis were obtained by slow diffusion of pentane into a saturated toluene solution. Both the ^{1}H and ^{13}C{^{1}H} NMR spectra showed no distinct resonances, only some extremely broad signals, indicating strongly hindered rotation in solution. ^{11}B NMR (128.5 MHz, Tol): δ = 24.5 (br) ppm. HRMS-LIFDI calcd. (*m*/*z*) for $[C_{46}H_{67}B_2N_2]^+$ = [**11-K** –

2 K + H]$^+$: 669.5485; found: 669.5468. Elemental analysis (C, H, N) calcd. (%) for $C_{46}H_{66}B_2K_2N_2$: C 73.94; H 8.91; N 3.75; found: C 73.58; H 9.28; N 3.38.

Reduction of 5 under CO

5 (23 mg, 29 µmol, 1.0 equiv.) was combined with lithium sand (1.0 mg, 0.14 mmol, 5.0 equiv.) and carefully layered with 0.5 mL THF without stirring. The mixture was immediately frozen with liquid N_2 and the argon atmosphere exchanged against 1 bar CO through three freeze-pump-thaw cycles. In the meantime, the frozen mixture had already started turning deep red. Upon thawing and stirring the reaction mixture turned orange, then brown. After 1 h at rt all volatiles were removed *in vacuo*. The solid residue was dissolved in pentane and filtered. Removal of volatiles from the filtrate yielded an orange solid consisting of a mixture of **12** and **13**. Slow evaporation of a saturated pentane solution yielded red cocrystals of **12** and **13** suitable for X-ray crystallographic analysis. The ^{1}H and ^{13}C NMR spectra were too complex and broadened by hindered rotation to deconvolute. ^{11}B NMR (128.5 MHz, d_8-THF): δ = –2.4 (**12**), –10.1 (**13**) ppm. HRMS-LIFDI calcd. for $[C_{47}H_{66}B_2N_2O]^+$ = [**12** + H]$^+$: 696.5356; found: 696.5338. Through direct reaction of 20 mg of **10** under an atmosphere of CO complex **13** was obtained selectively. Both the ^{1}H and ^{13}C{^{1}H} NMR spectra show no distinct resonances, only some extremely broad signals, indicating strongly hindered rotation in solution. The ^{11}B NMR spectrum indicates the presence of two rotational isomers. ^{11}B NMR (128.5 MHz, C_6D_6): δ = –11.2 (br), –12.2 (br) ppm. HRMS-LIFDI calcd. for $[C_{48}H_{66}B_2N_2O_2]^+$ = [**13**]$^+$: 724.5305; found: 724.5281. IR (solid-state): $\tilde{\nu}$(C=O) = 1978, 1969 cm^{-1}. Compound **12** could not be prepared selectively, due to the difficulty in obtaining the biradical **9** selectively.

NMR spectra of isolated compounds

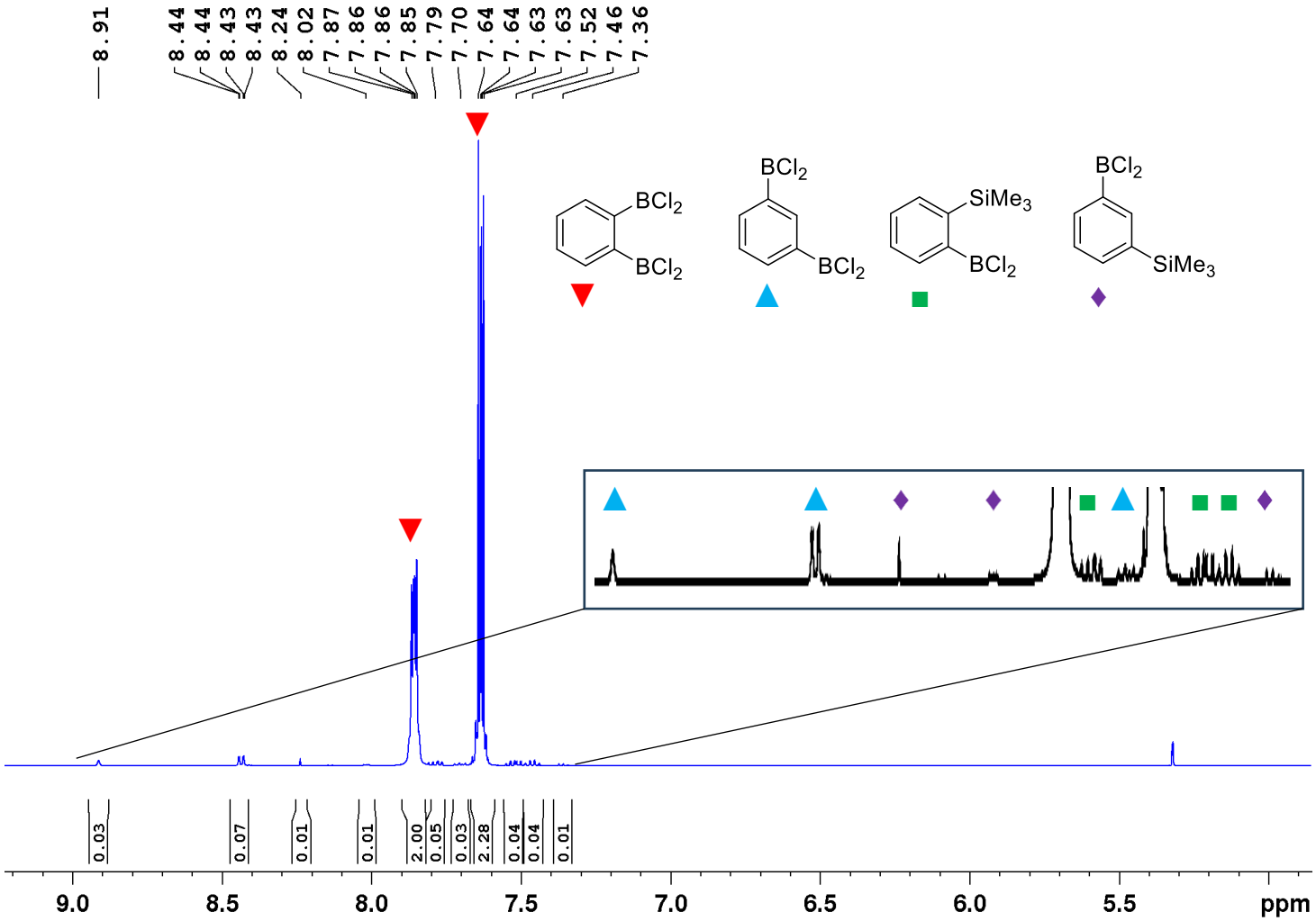

Figure S1. ^{1}H NMR spectrum of **1** in C_6D_6 with expansion of the side-product resonances. These correspond to the 1,3 isomer of **1**, 1,3-$(BCl_2)C_6H_4$ (▲ ca. 3%), leftover 1-BCl_2-2-$(SiMe_3)C_6H_4$ (■ ca. 4%), and the 1,3 isomer of the latter, 1-BCl_2-3-$(SiMe_3)C_6H_4$ (♦ ca. 1%).

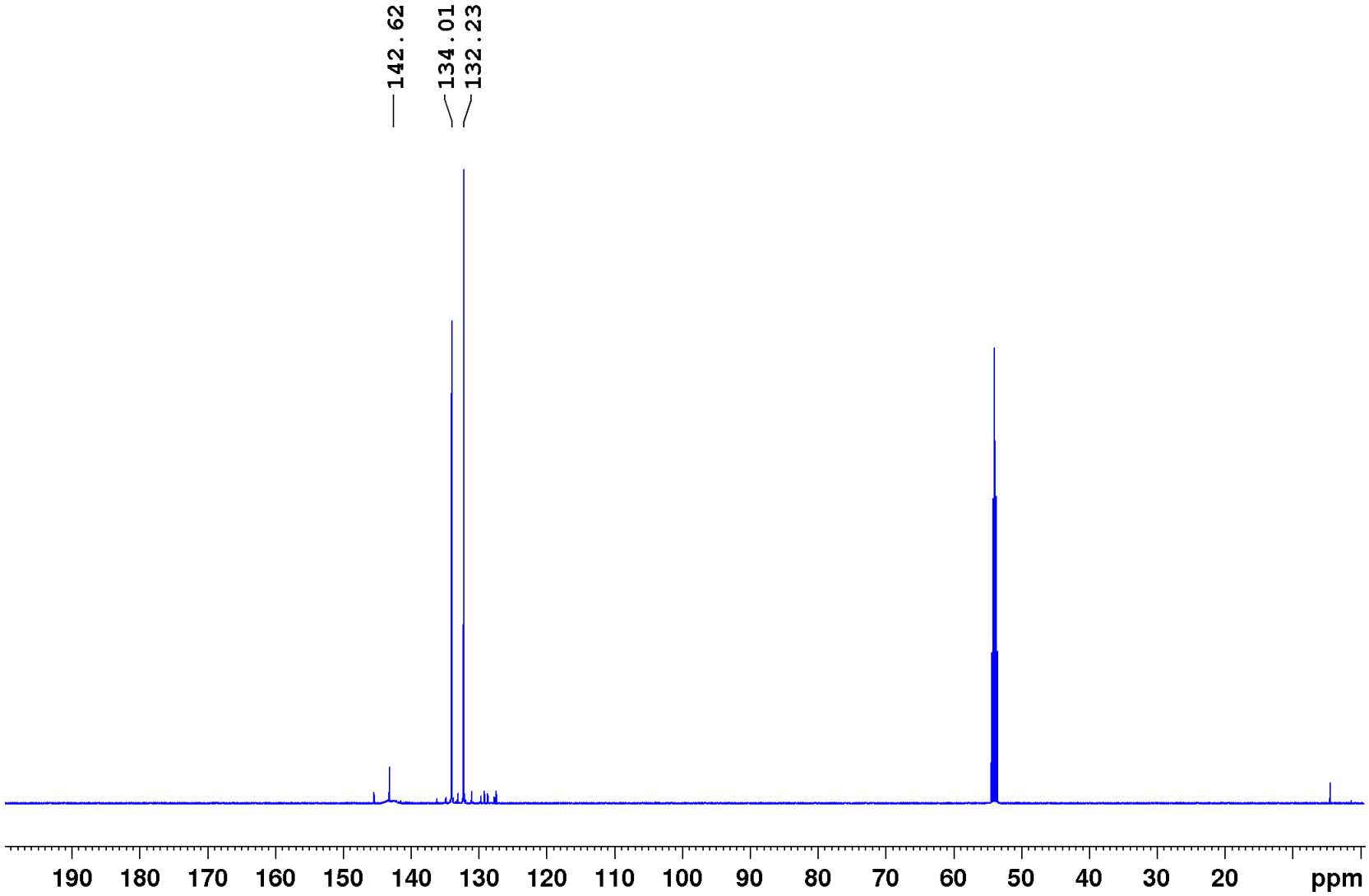

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6. The impurities in the aromatic region correspond to the 1,3-isomer of **1**, 1,3-$(BCl_2)C_6H_4$ (ca. 3%), residual 1-BCl_2-2-$(SiMe_3)C_6H_4$ (ca. 4%), and the 1,3 isomer of the latter, 1-BCl_2-3-$(SiMe_3)C_6H_4$ (ca. 1%).

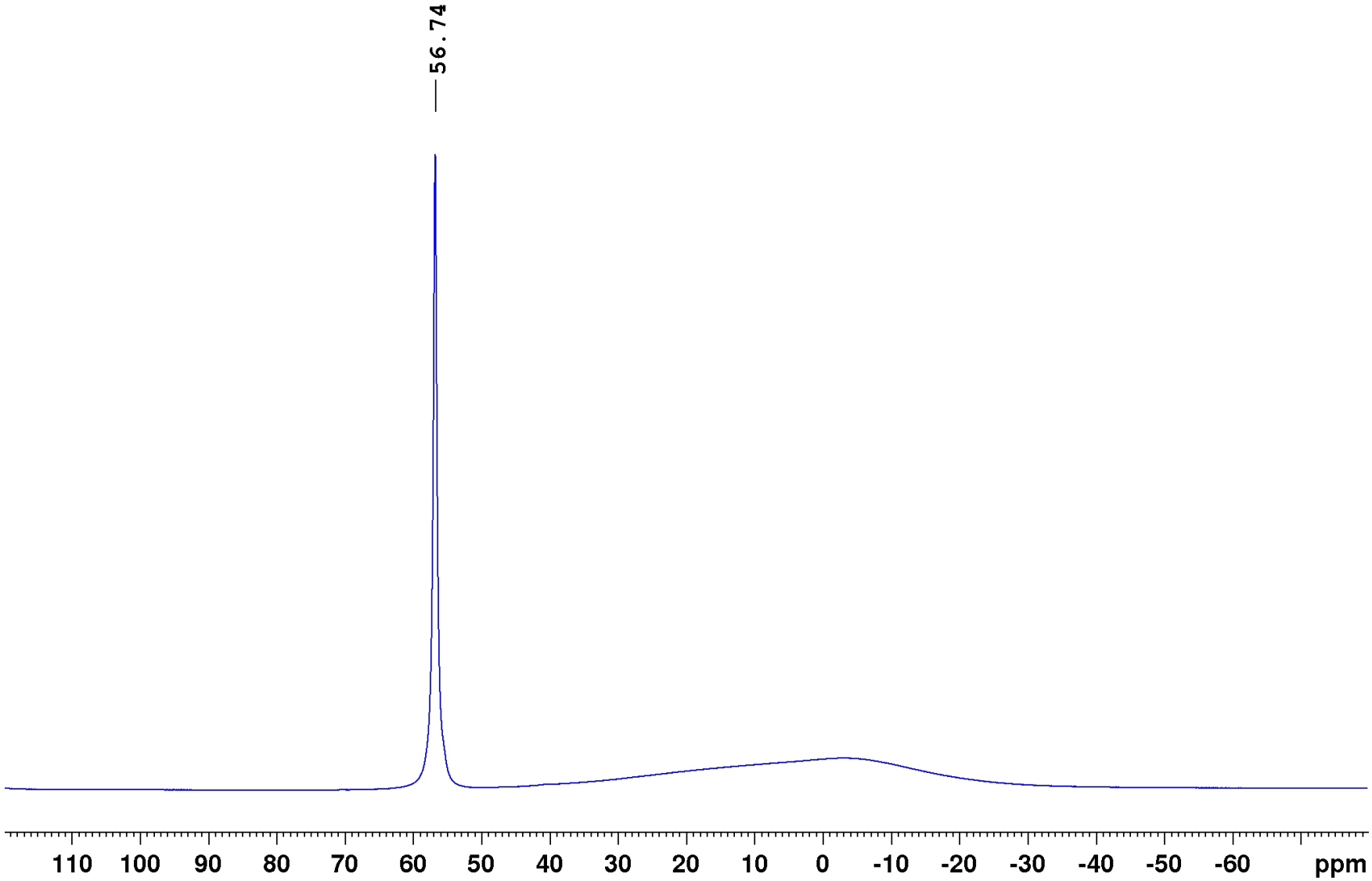

Figure S3. ^{11}B NMR spectrum of **1** in C_6D_6.

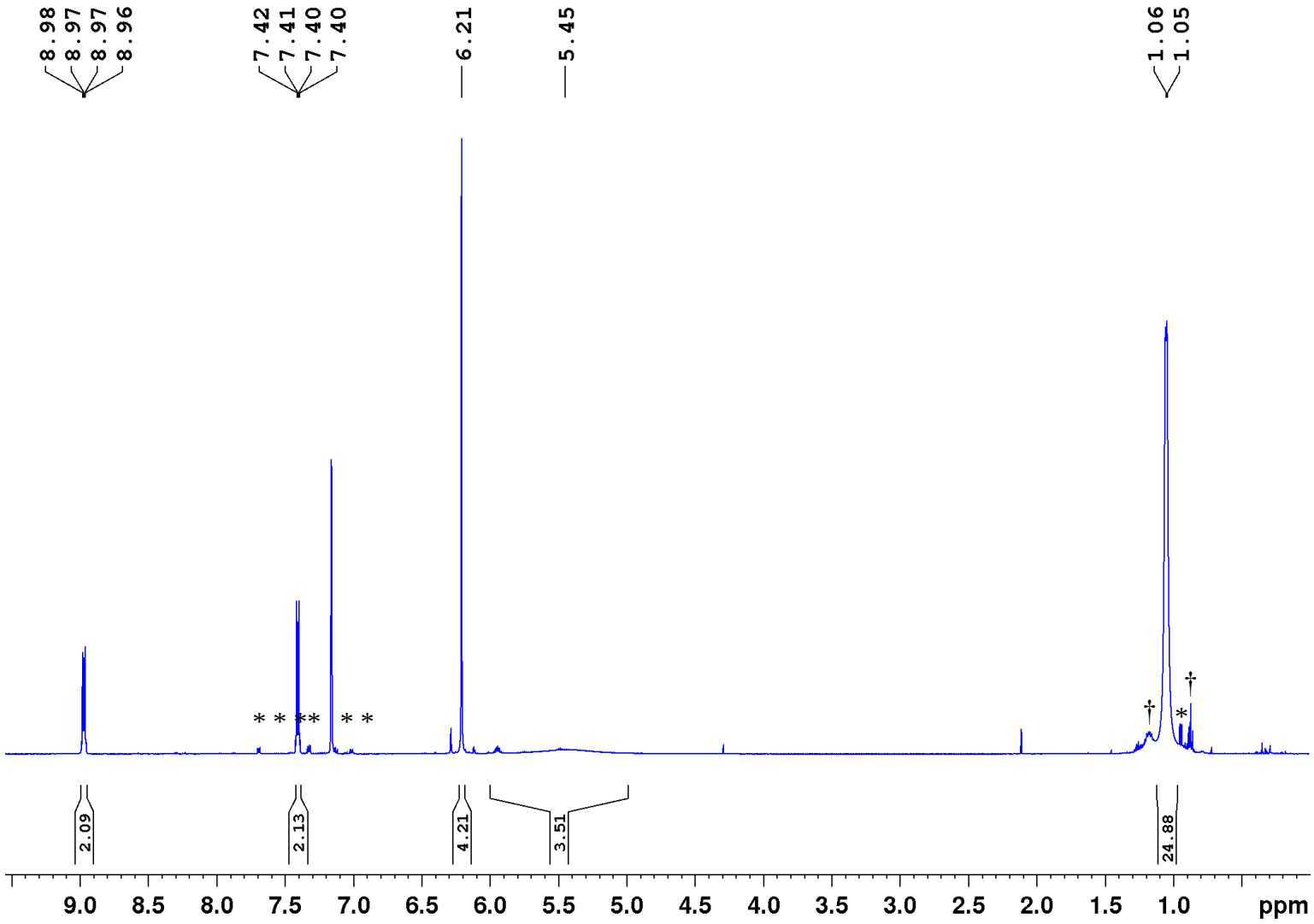

Figure S4. ^{1}H NMR spectrum of **3-I*i*Pr** in CD_2Cl_2. The additional resonances marked with * correspond to the 1,3 isomer **4-I*i*Pr** (ca. 6%), those with † to residual pentane from washing.

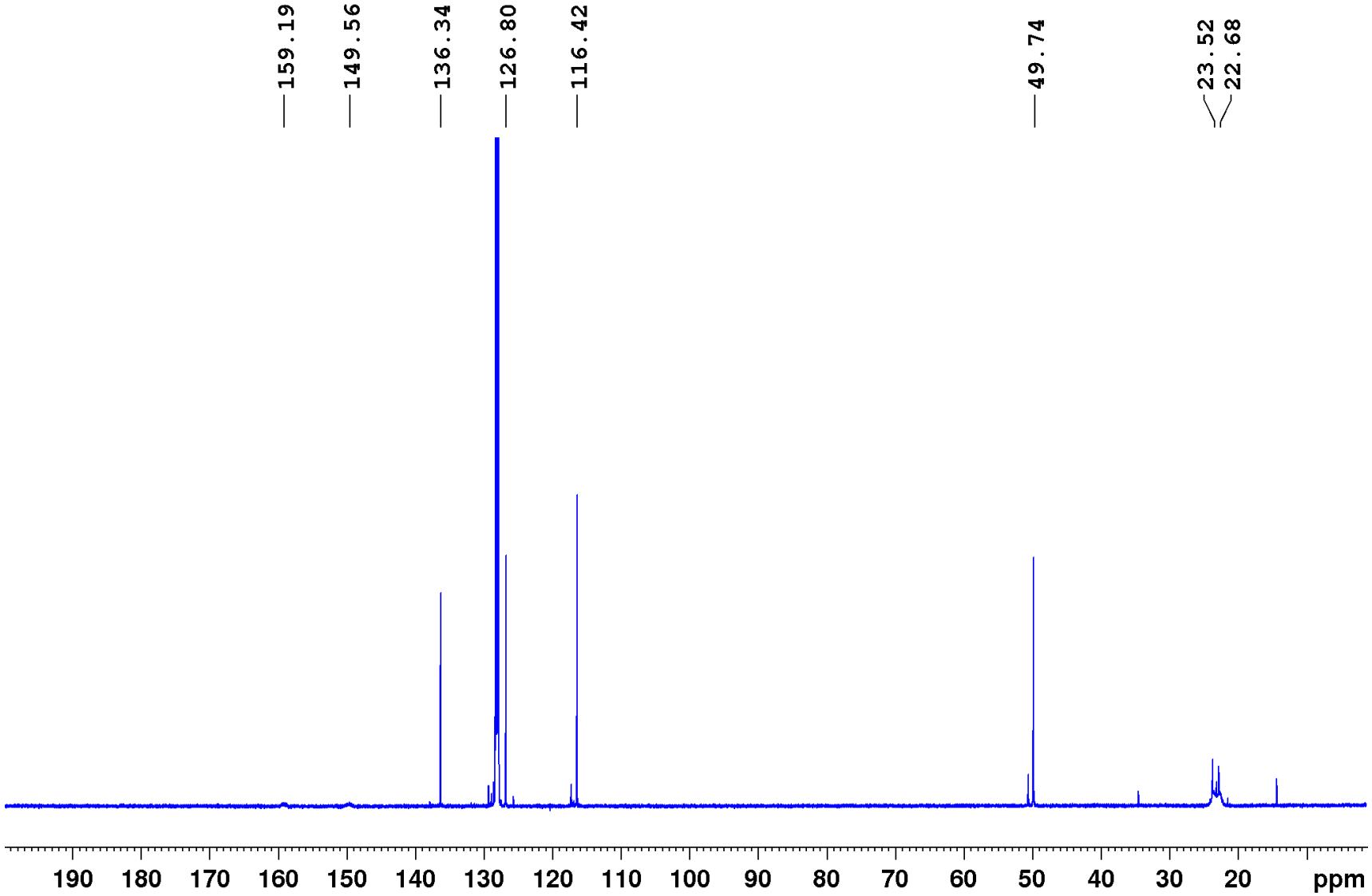

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **3-I*i*Pr** in CD_2Cl_2. The impurities correspond to **4-I*i*Pr** (ca. 6%).

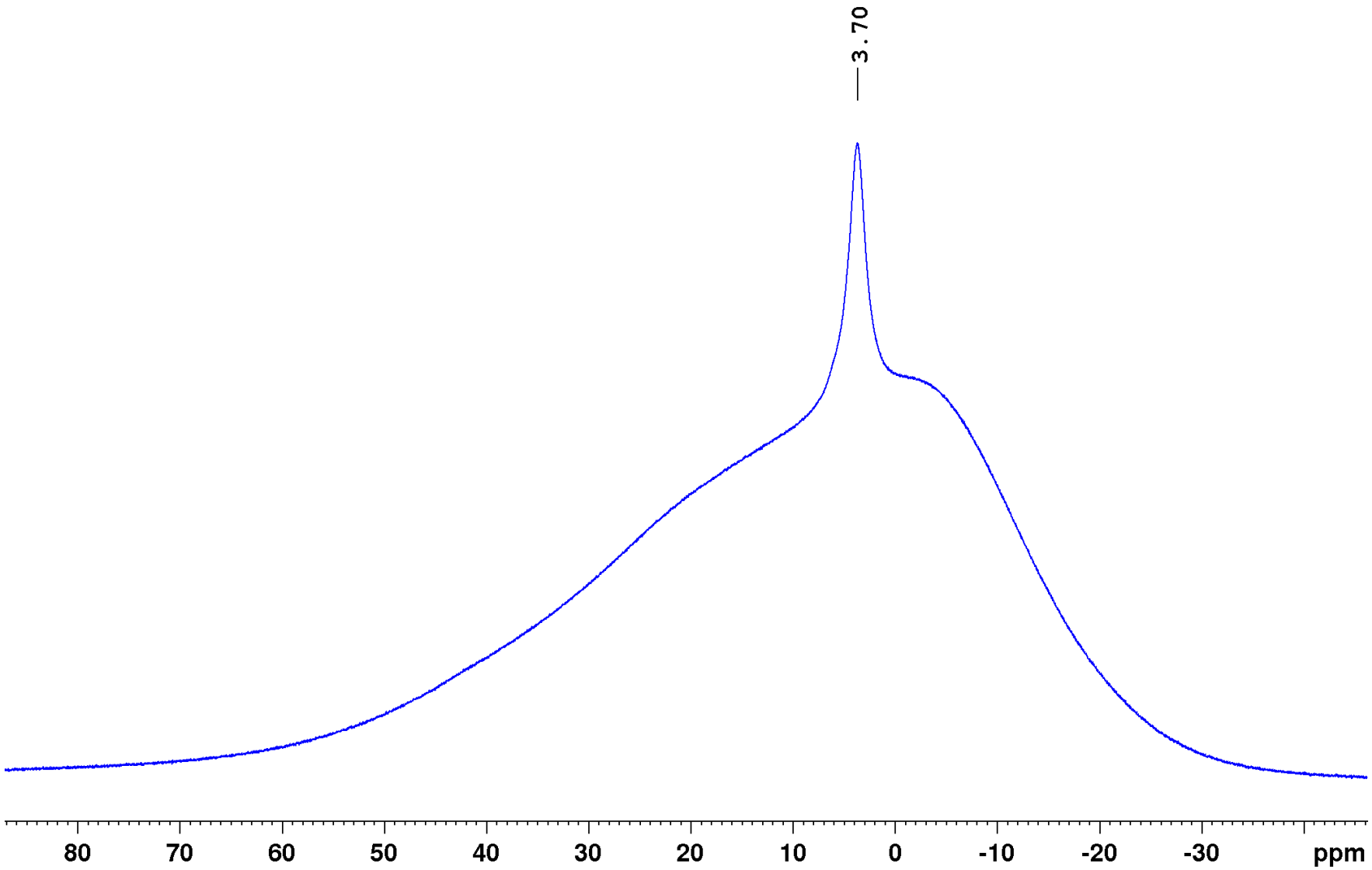

Figure S6. ^{11}B NMR spectrum of **3-I*i*Pr** in CD_2Cl_2.

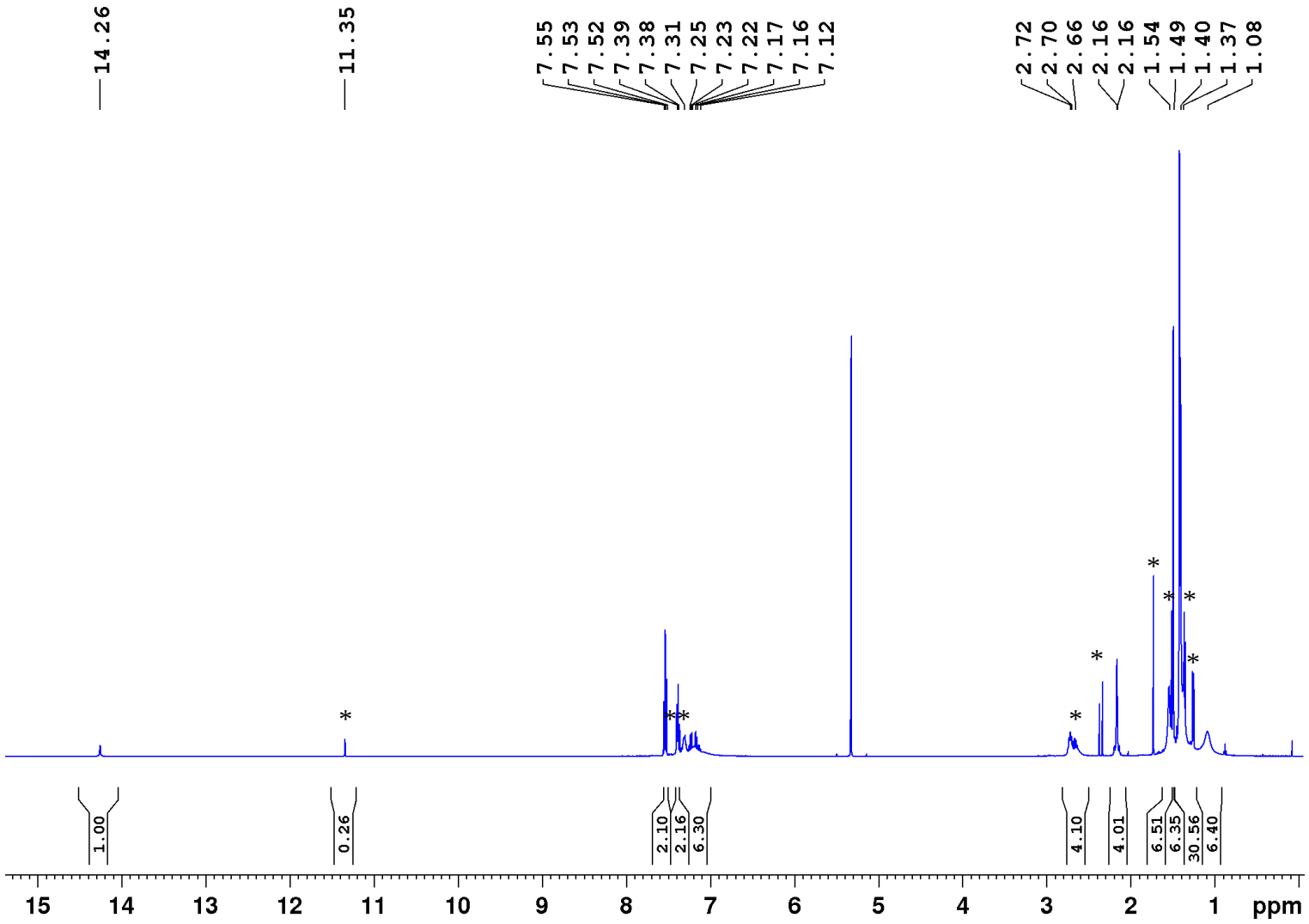

Figure S7. ^{1}H NMR spectrum of **5** in CD_2Cl_2, contaminated with the decomposition product [CAACH]Cl (*, ca. 20%).

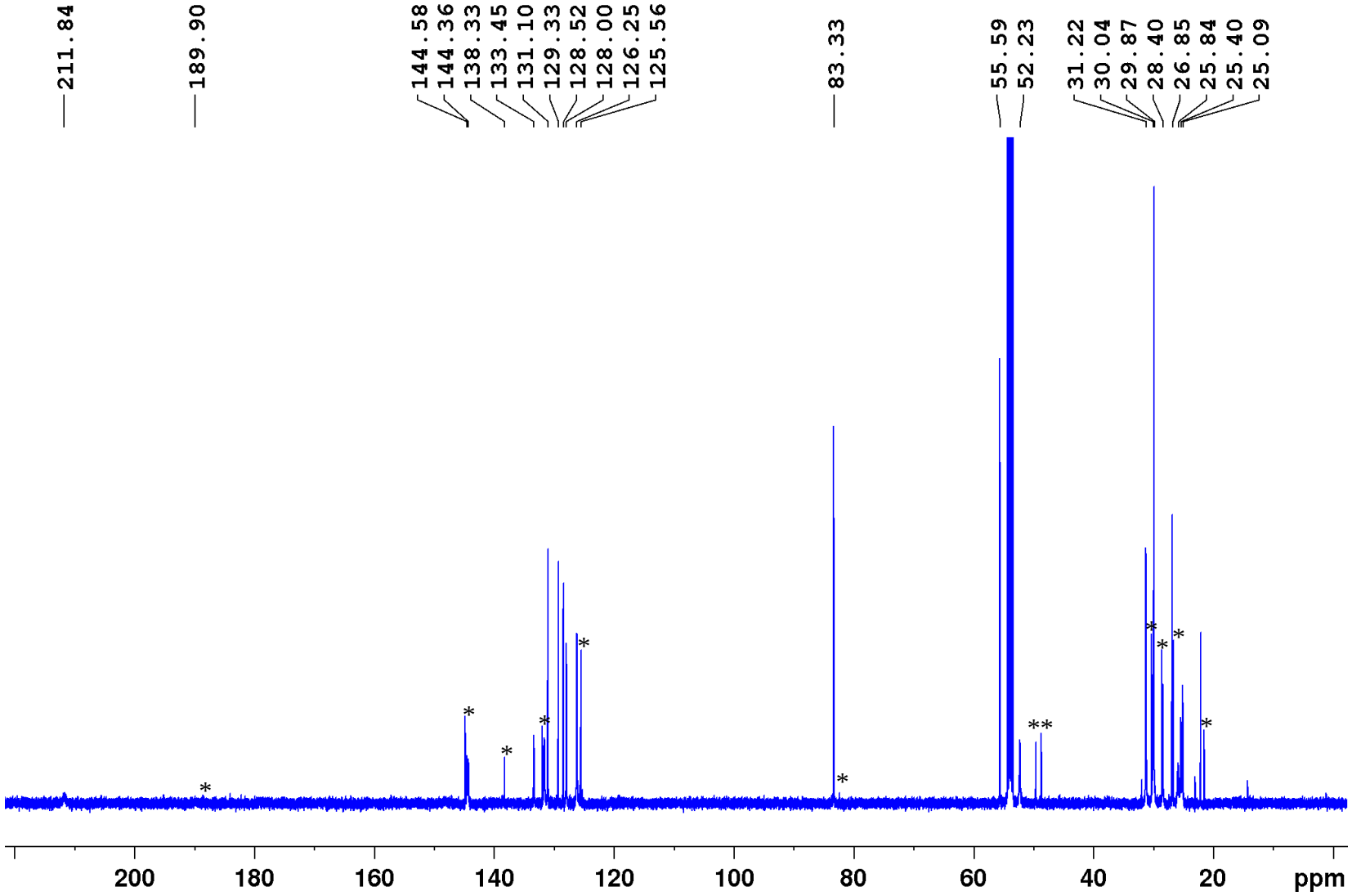

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in CD_2Cl_2, contaminated with the decomposition product [CAACH]Cl (*, ca. 20%).

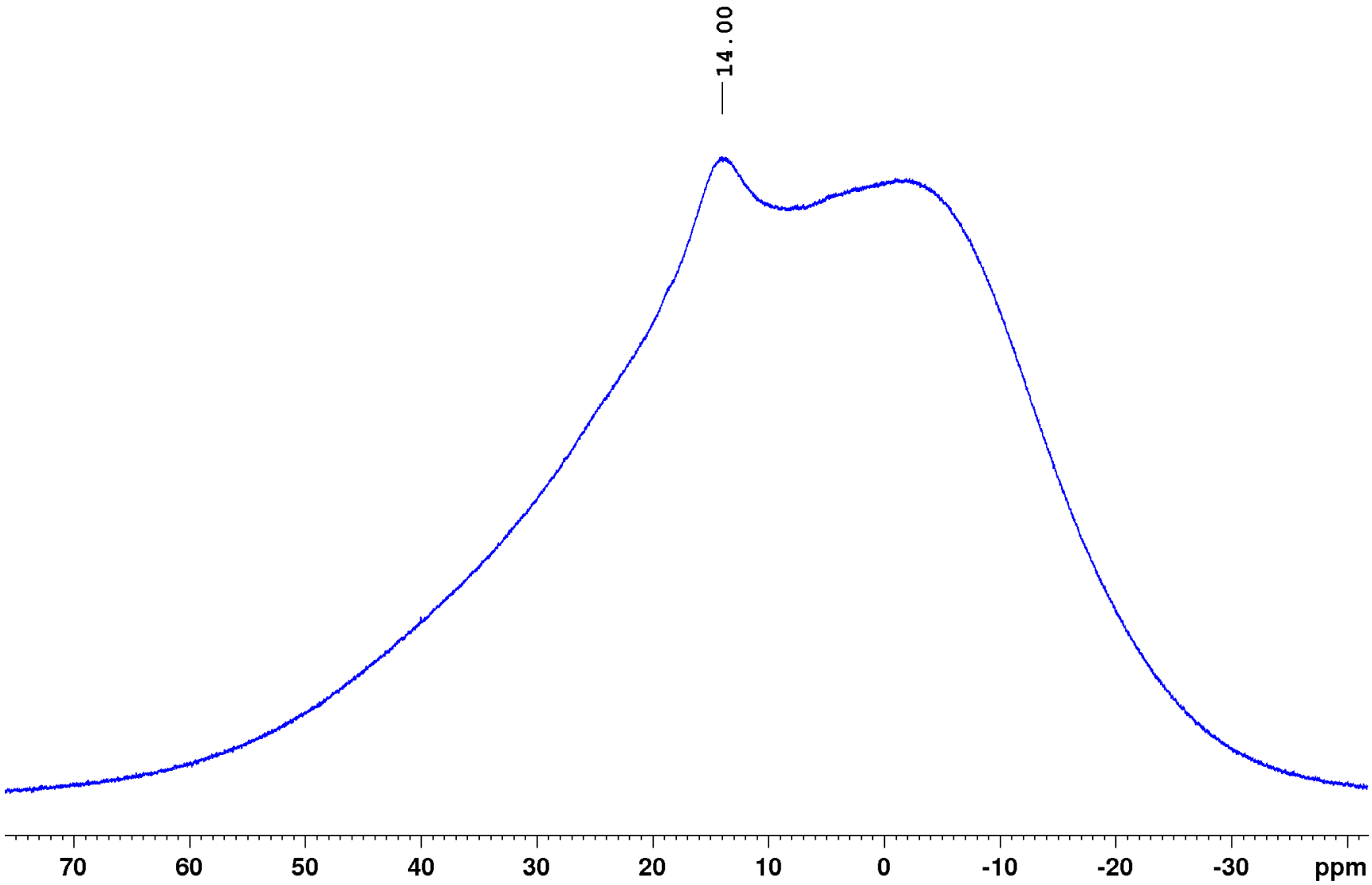

Figure S9. ^{11}B NMR spectrum of **5** in CD_2Cl_2.

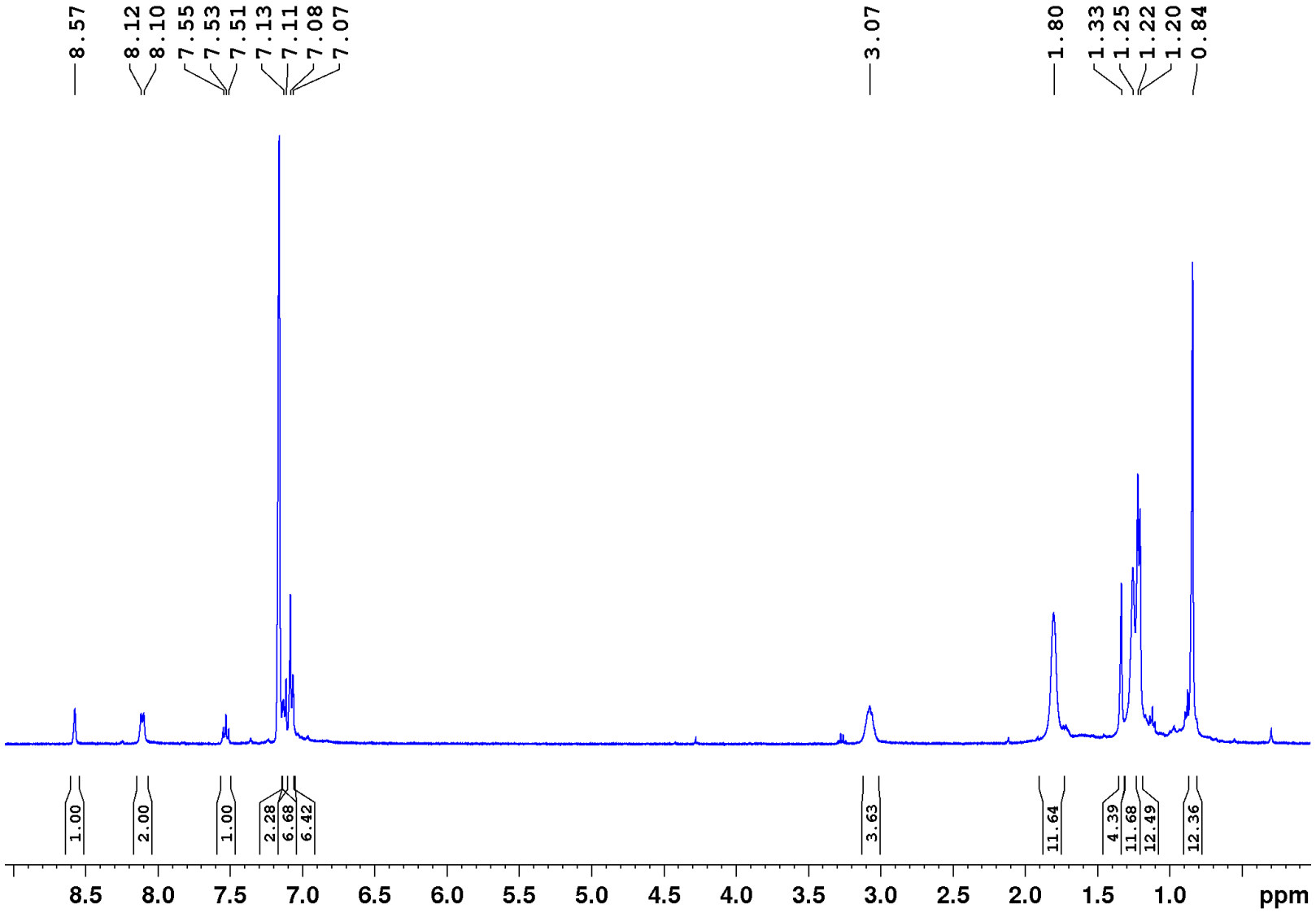

Figure S10. ^{1}H NMR spectrum of **4-CAAC** in C_6D_6.

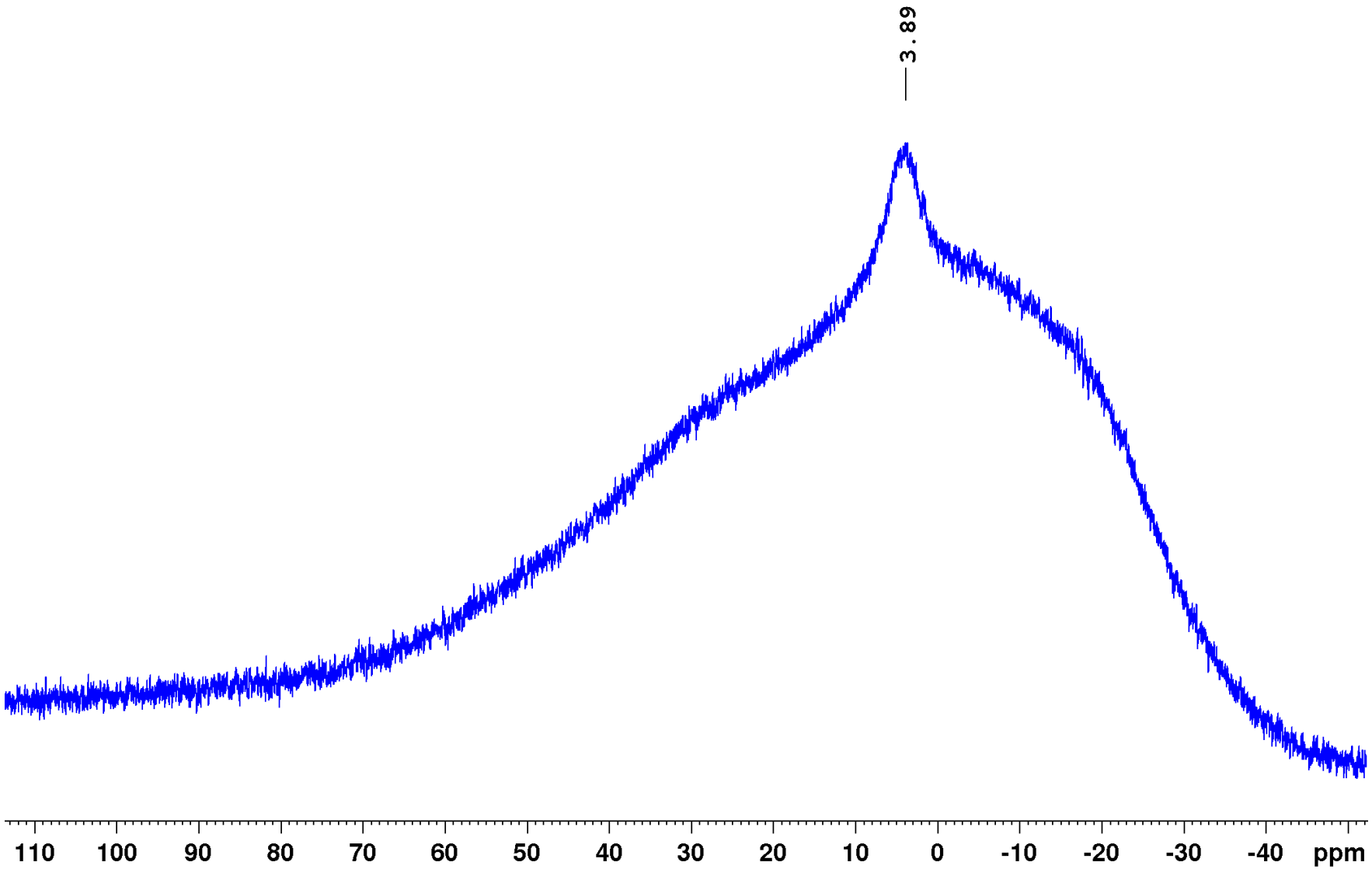

Figure S11. ^{11}B NMR spectrum of **4-CAAC** in C_6D_6.

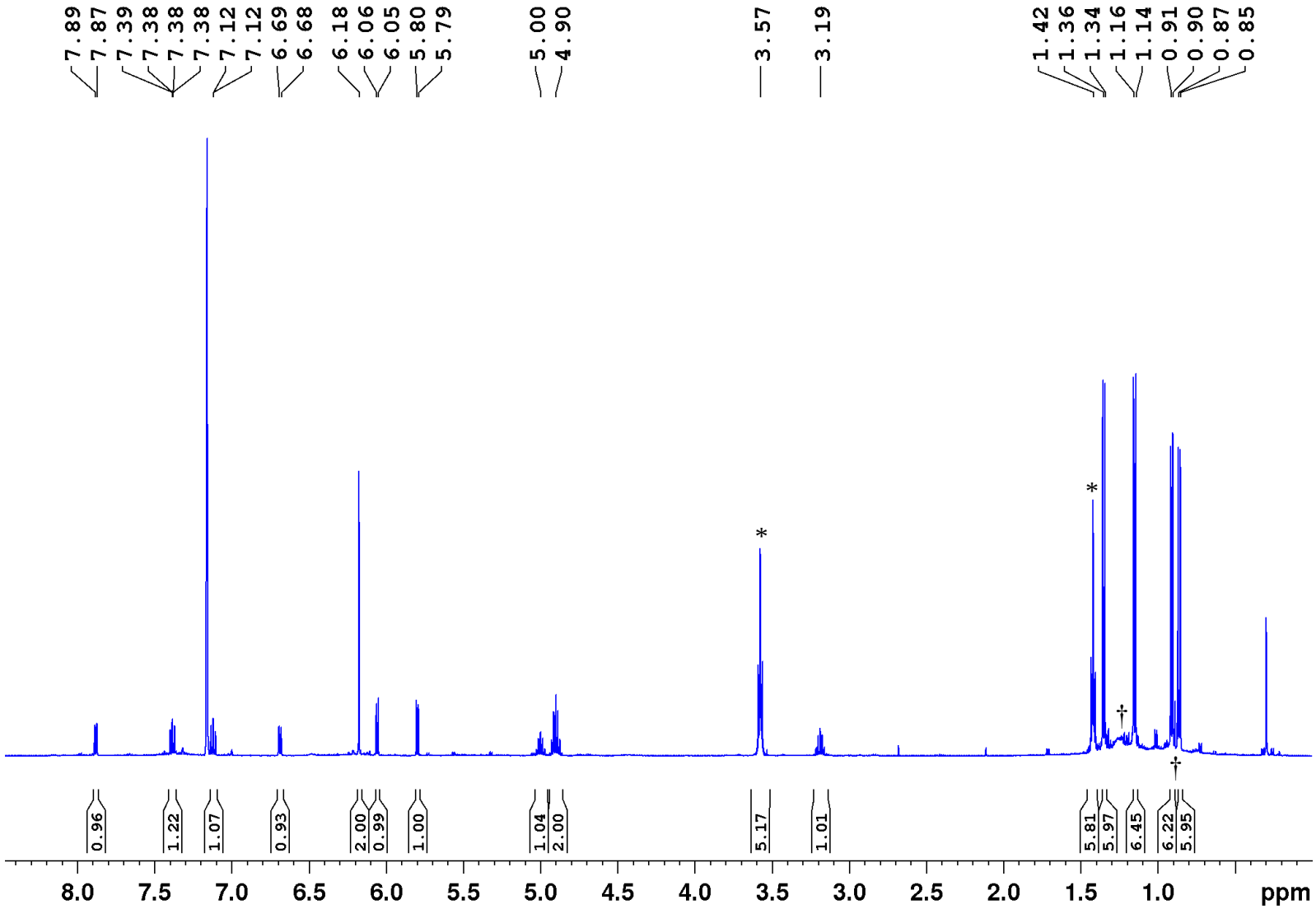

Figure S12. ^{1}H NMR spectrum of **6** in C_6D_6. Residual THF from crystallization marked with * and †, respectively.

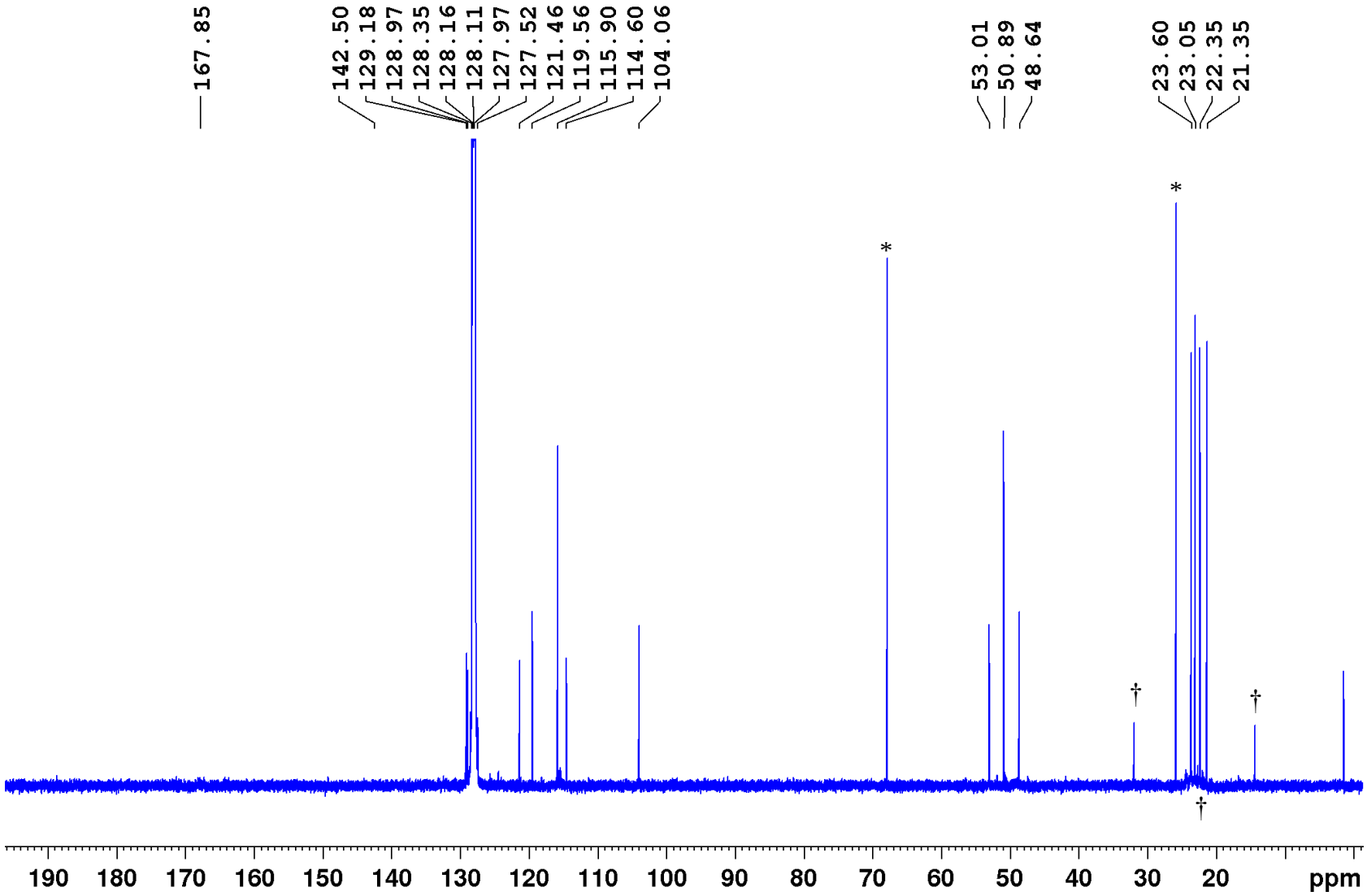

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in C_6D_6. Residual THF and hexane from crystallization marked with * and †, respectively.

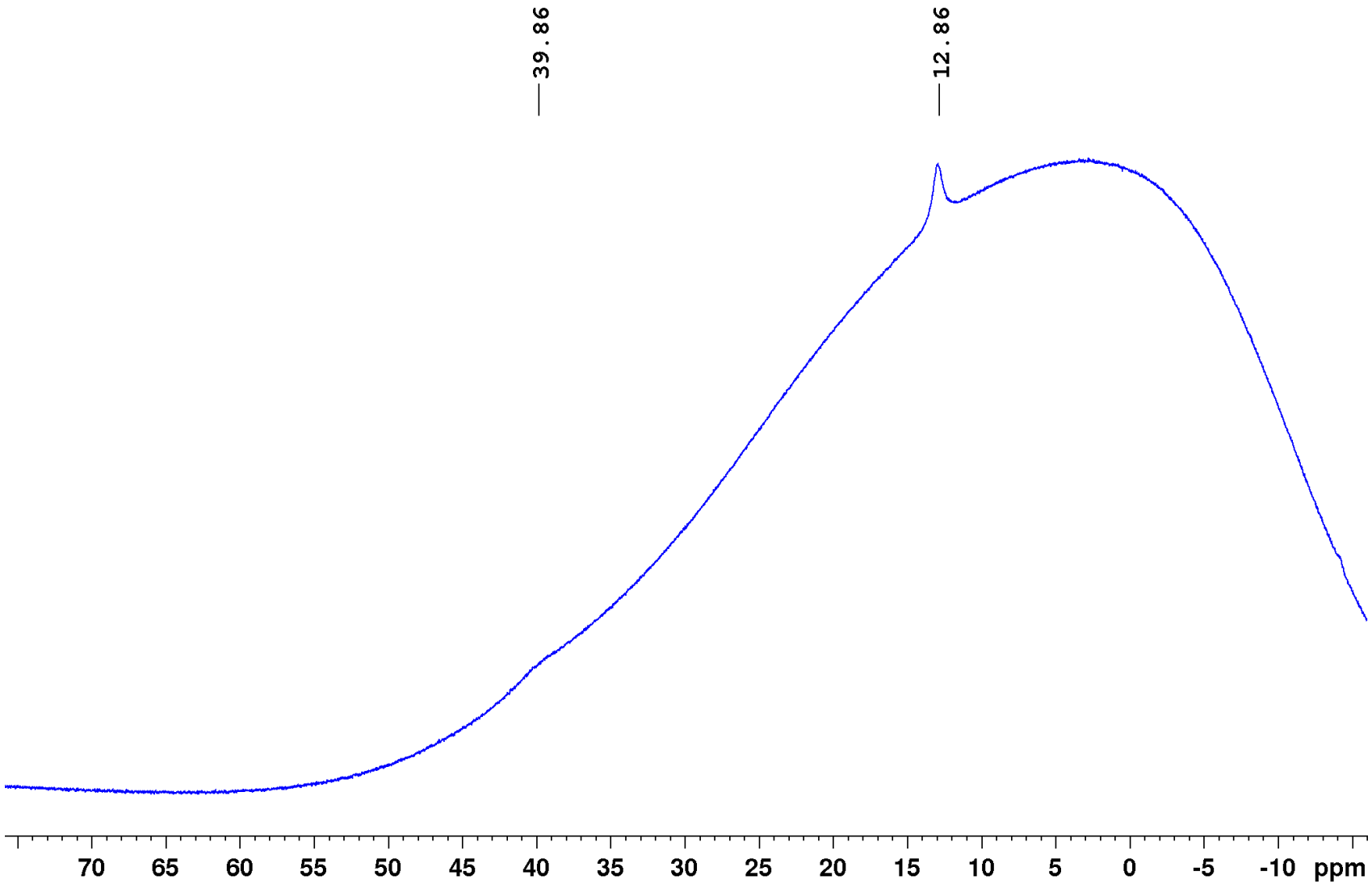

Figure S14. ^{11}B NMR spectrum of **6** in C_6D_6.

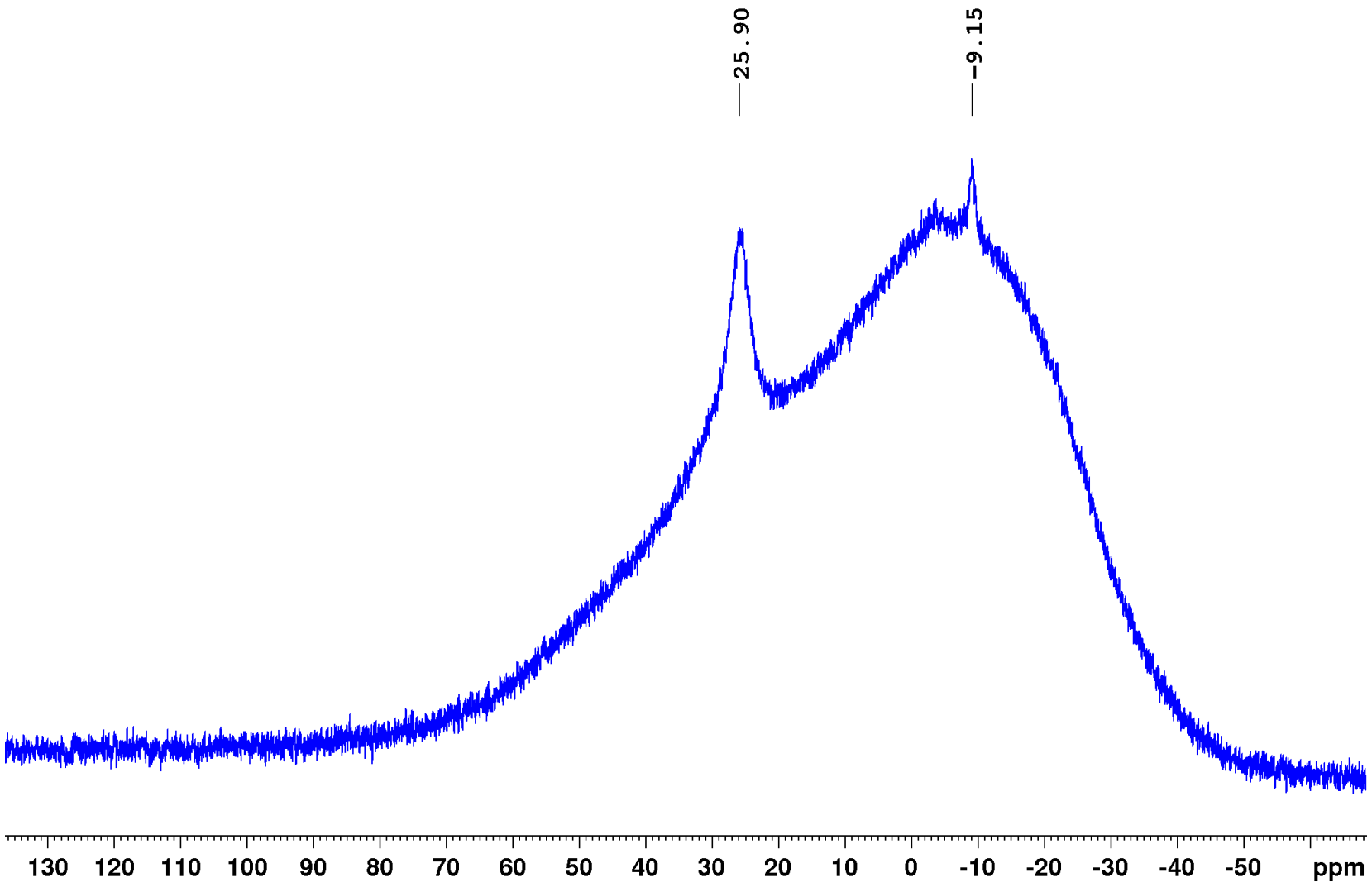

Figure S15. ^{11}B NMR spectrum of isolated **11-Li** in C_6D_6, showing already signs of decomposition at –9.2 ppm.

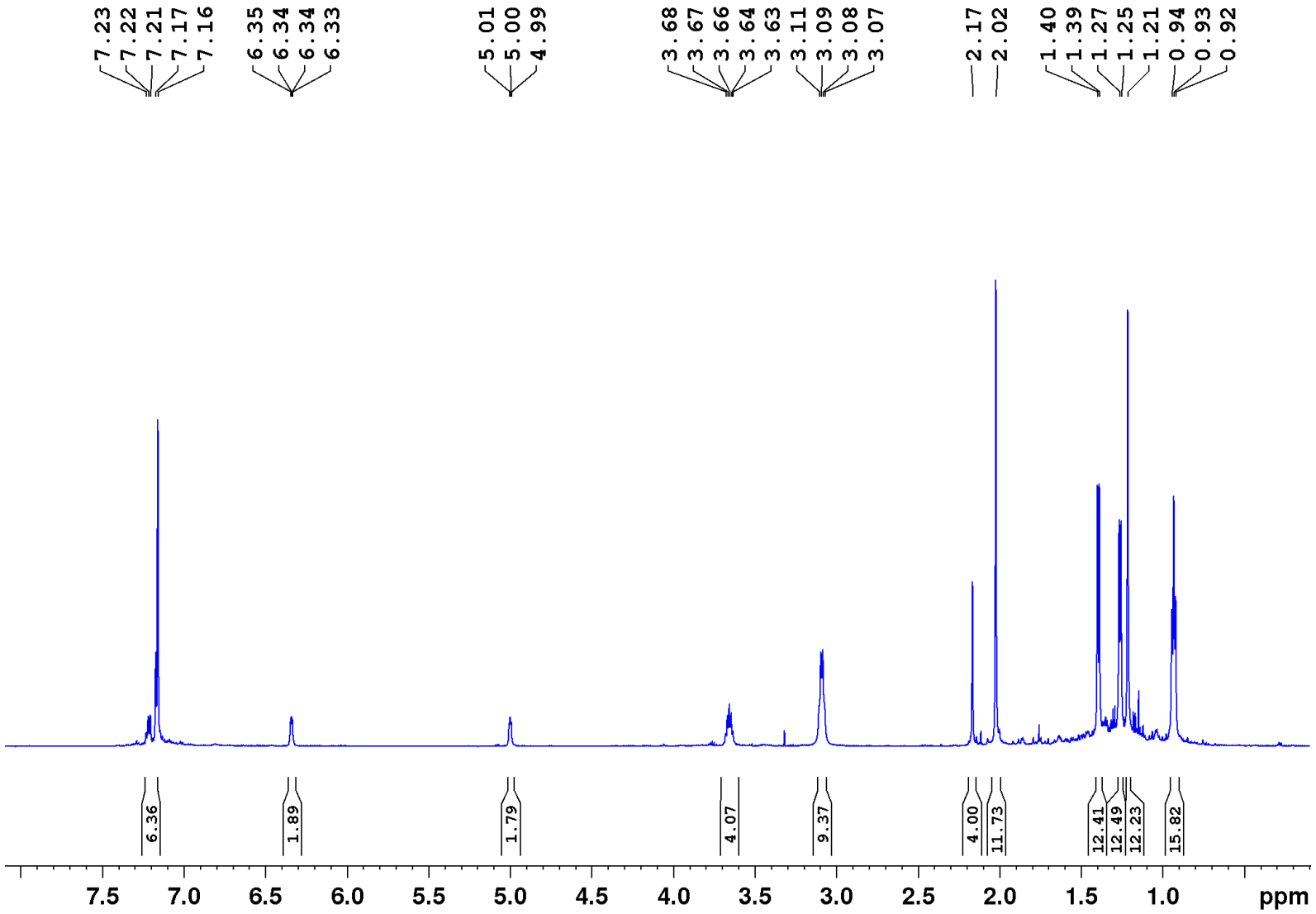

Figure S16. ^{1}H NMR spectrum of **11-Na** in C_6D_6.

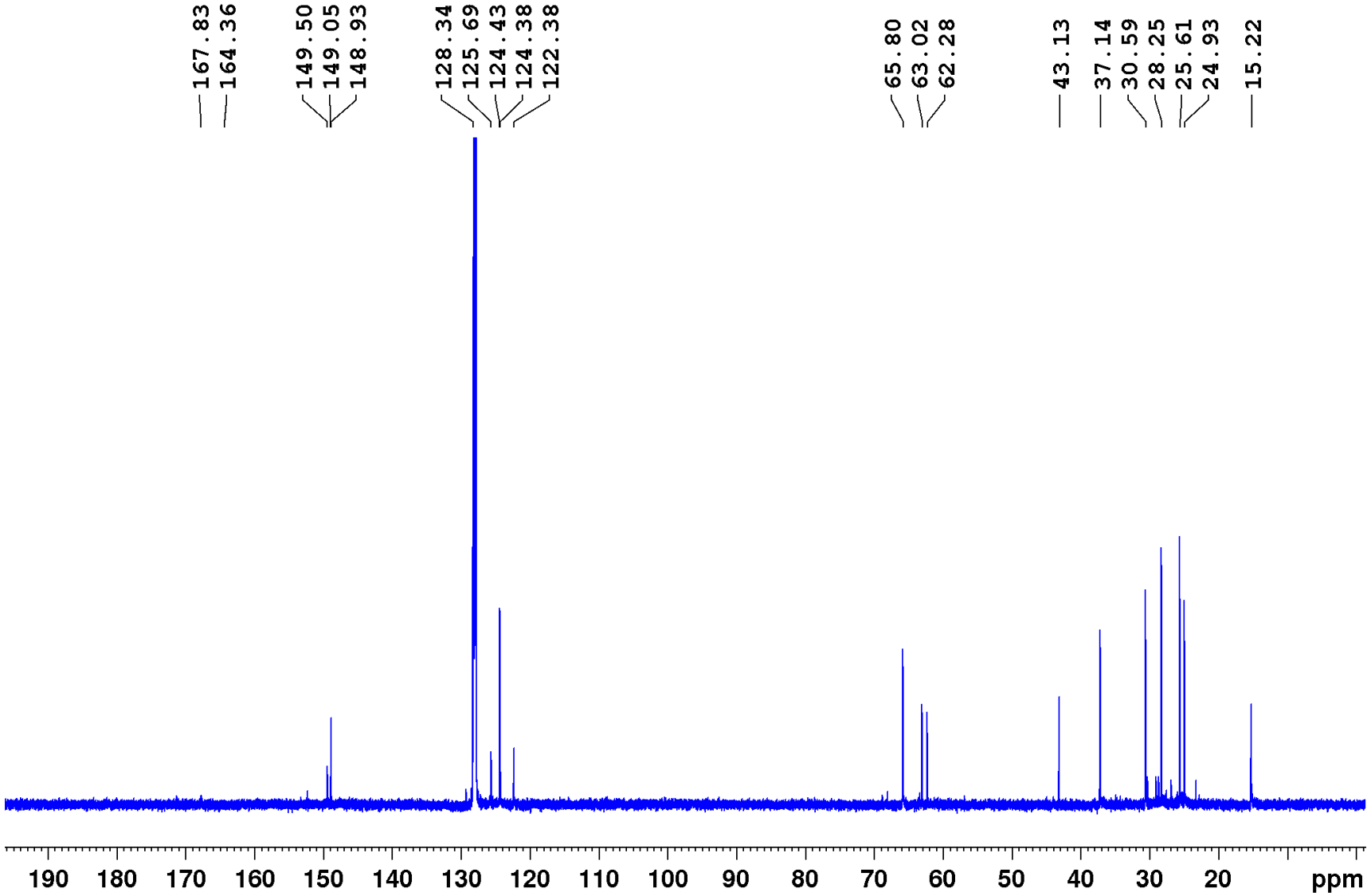

Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of **11-Na** in C_6D_6.

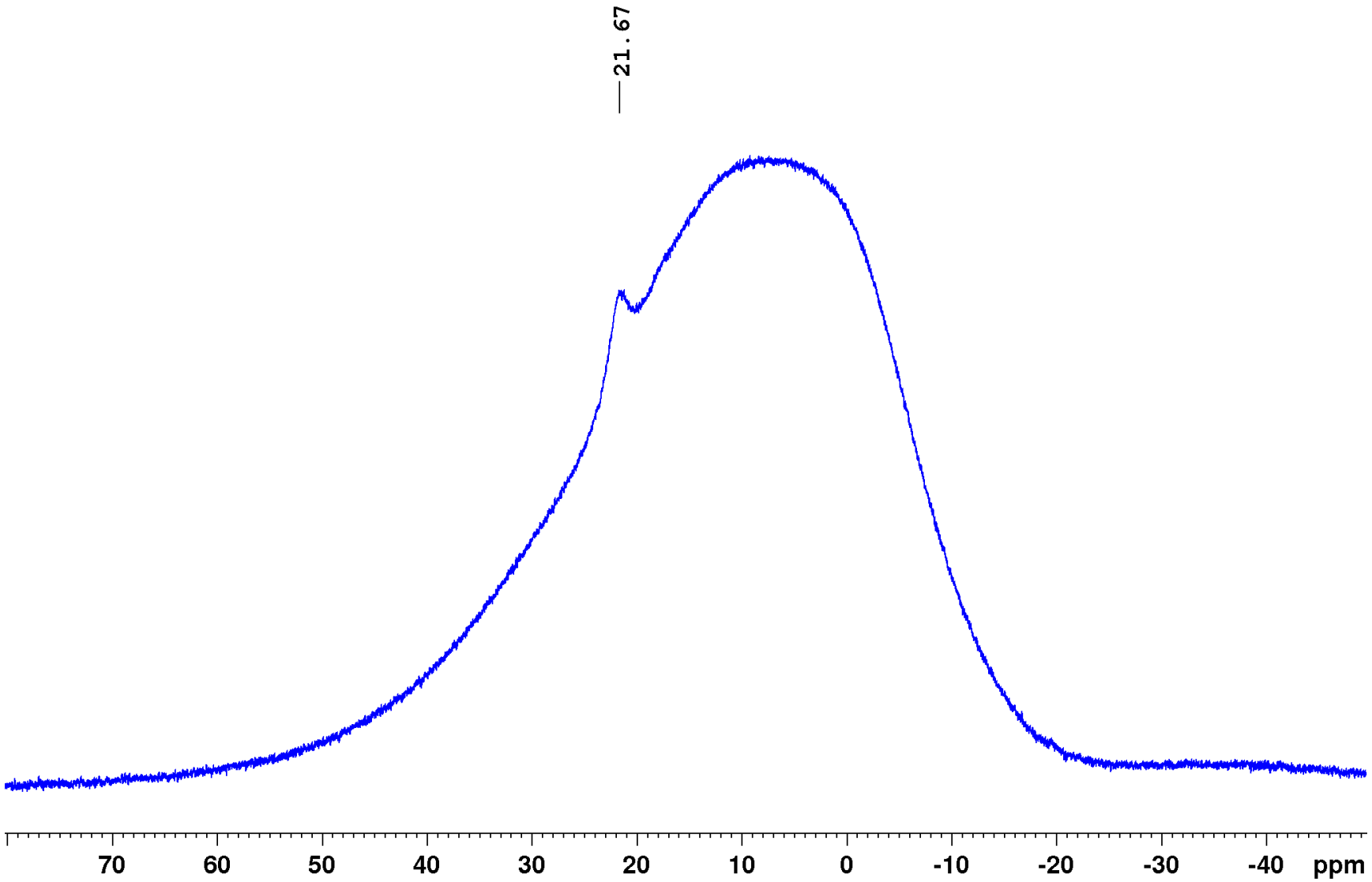

Figure S18. ^{11}B NMR spectrum of **11-Na** in C_6D_6.

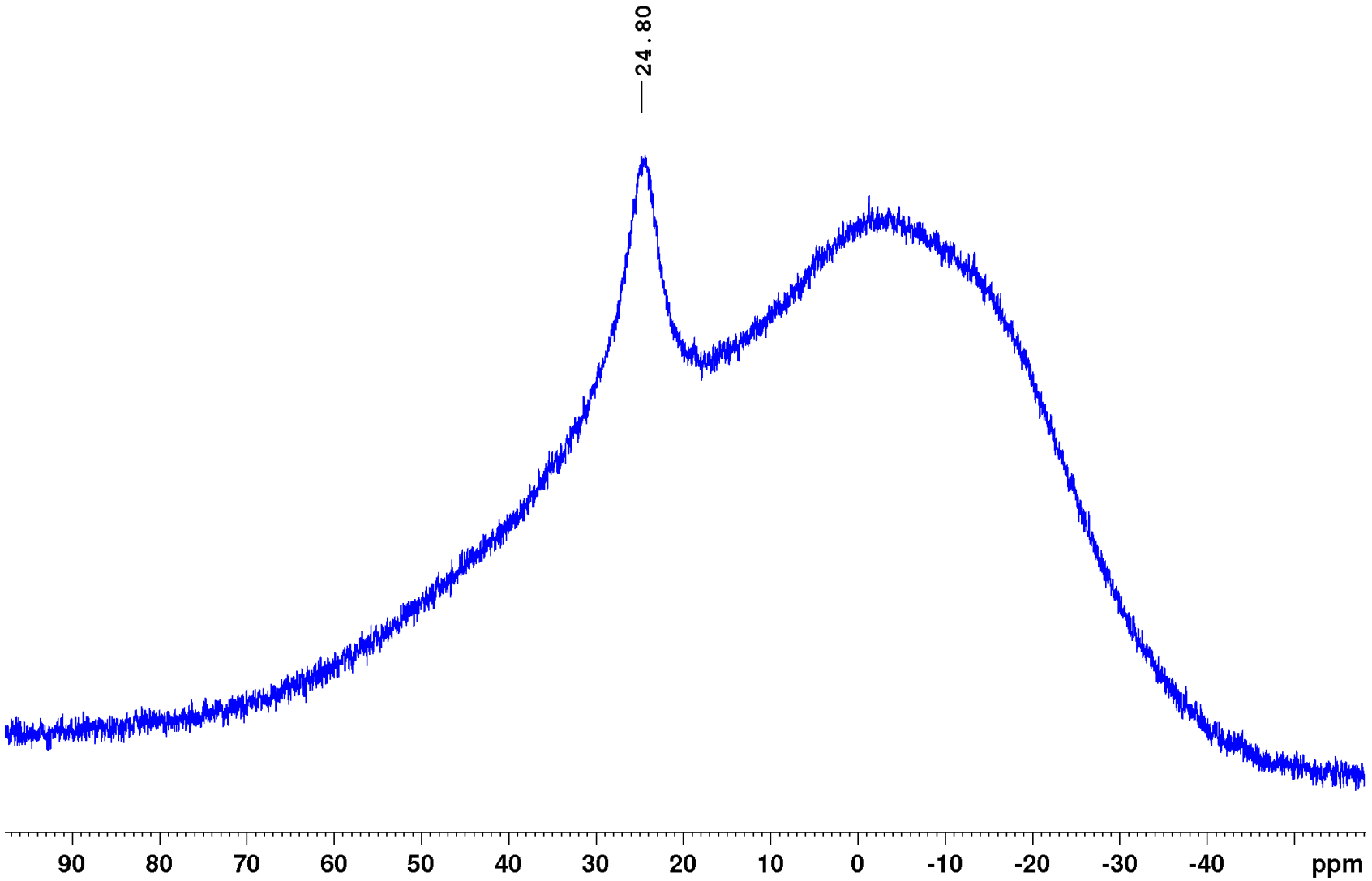

Figure S19. ^{11}B NMR spectrum of **11-K** in toluene.

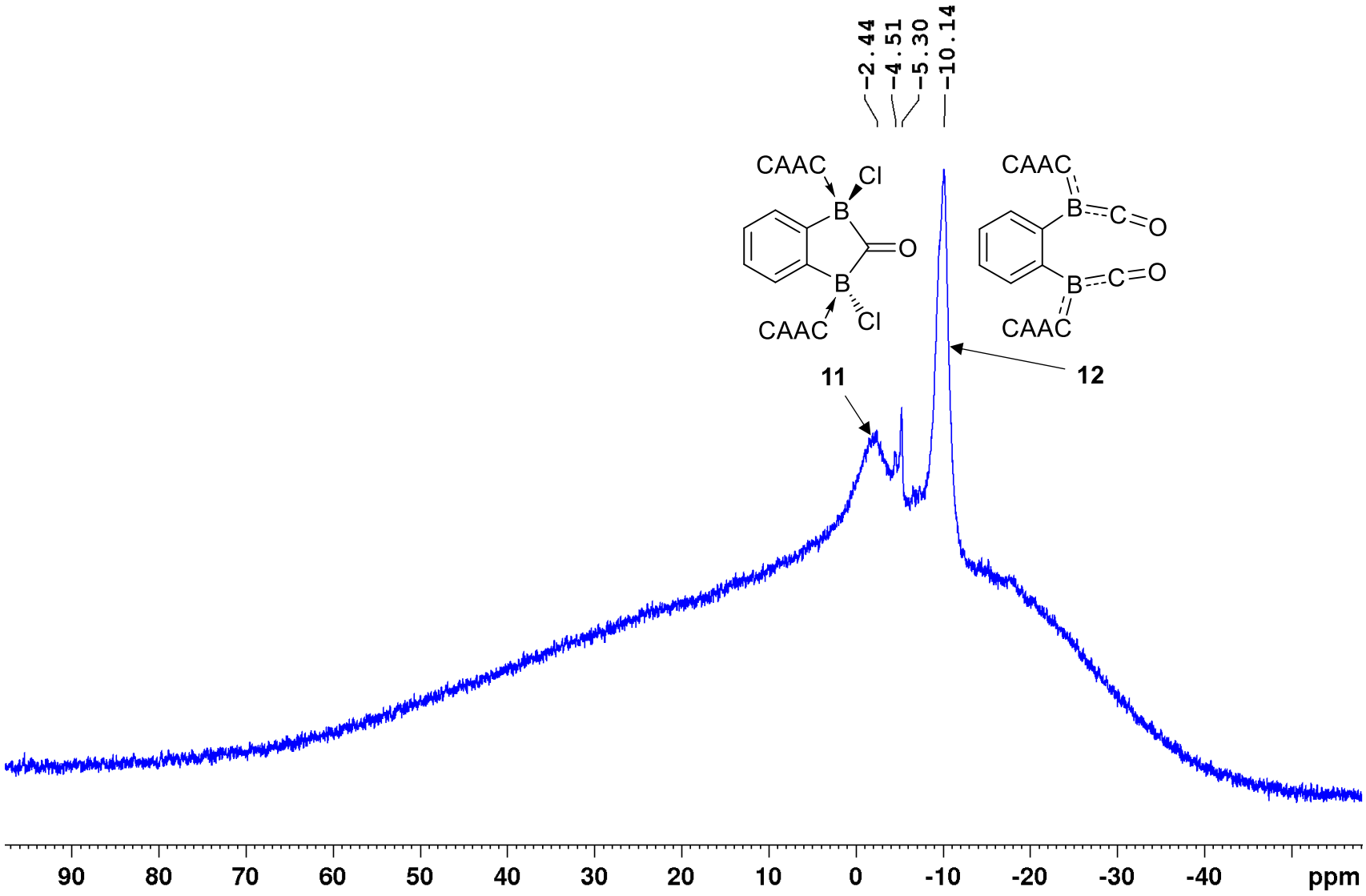

Figure S20. ^{11}B NMR spectrum of *in-situ*-generated **12** and **13** in THF.

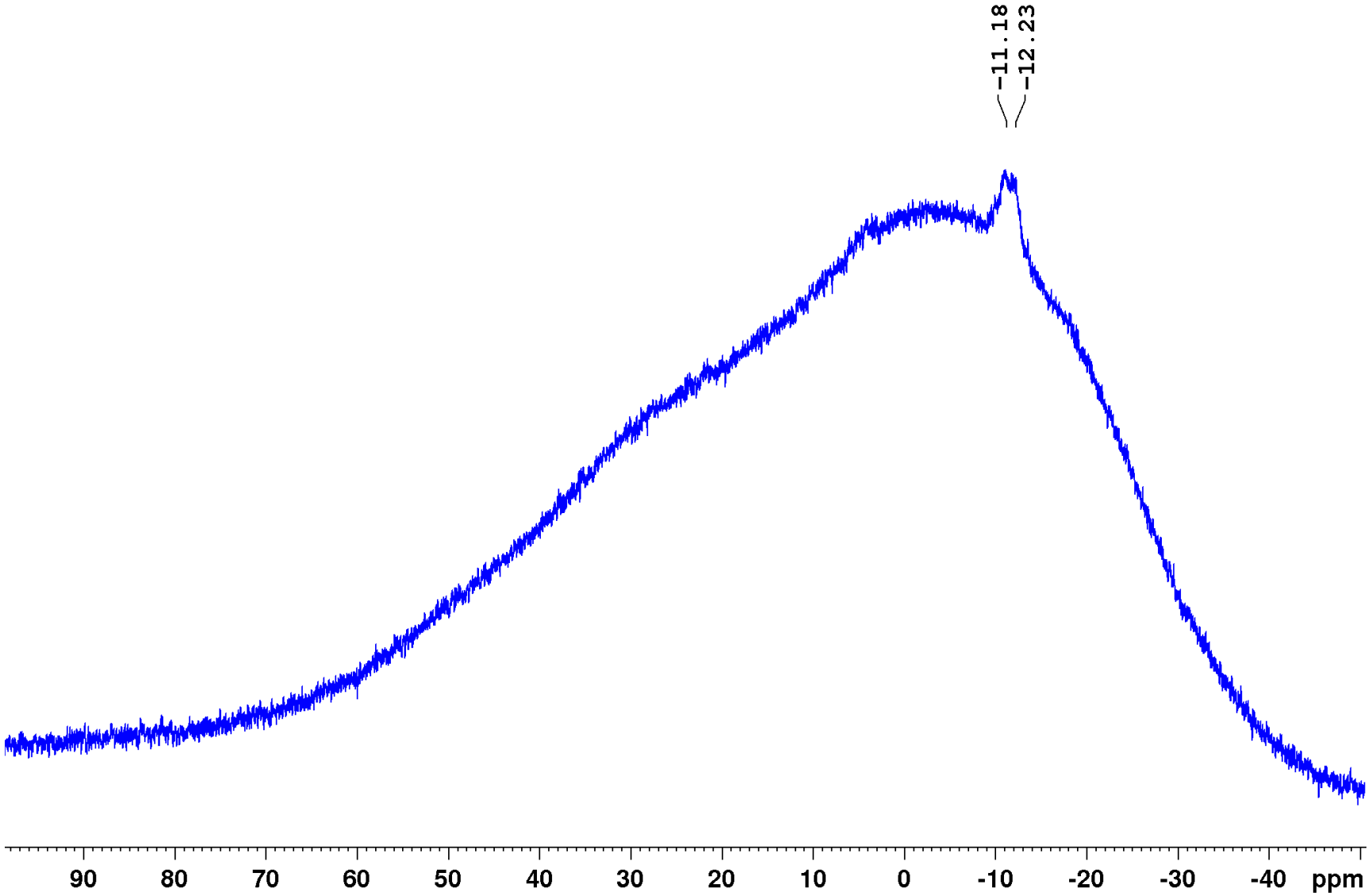

Figure S21. ^{11}B NMR spectrum of **13** in C_6D_6.

EPR spectroscopy

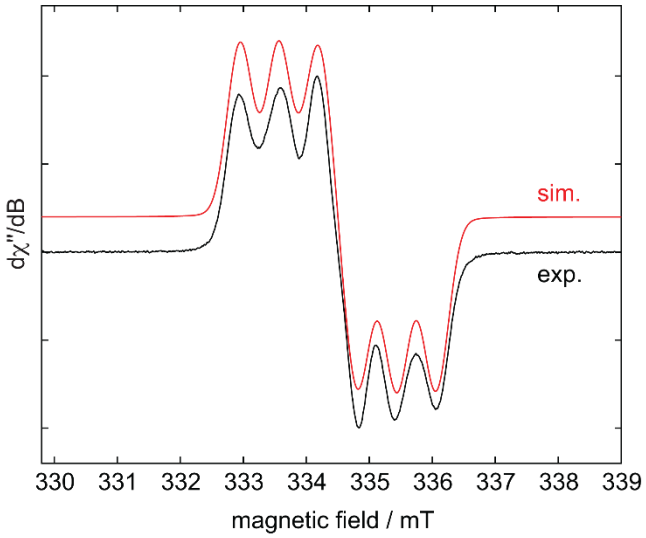

Figure S22. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of **8** in THF at room temperature. Best-fit simulation parameters: g_{iso} = 2.0038, $a(^{10,11}B, 2B)$ = 2.4 MHz, $a(^{14}N, 2N)$ = 17.5 MHz, and $a(^{35,37}Cl, 1Cl)$ = 4.6 MHz.

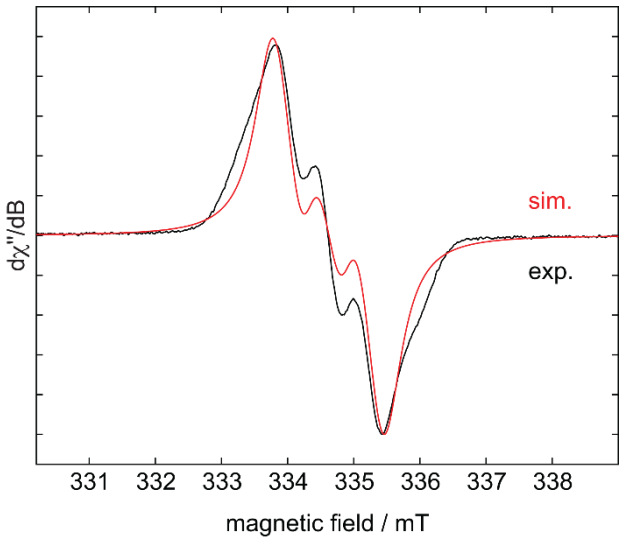

Figure S23. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of **9** in THF at room temperature. The additional broadening of the experimental spectrum indicates the presence of another radical species. Best-fit simulation parameters: g_{iso} = 2.0028, $a(^{14}N, 1N)$ = 16.4 MHz, and $a(^{10,11}B, 1B)$ = 3.7 MHz.

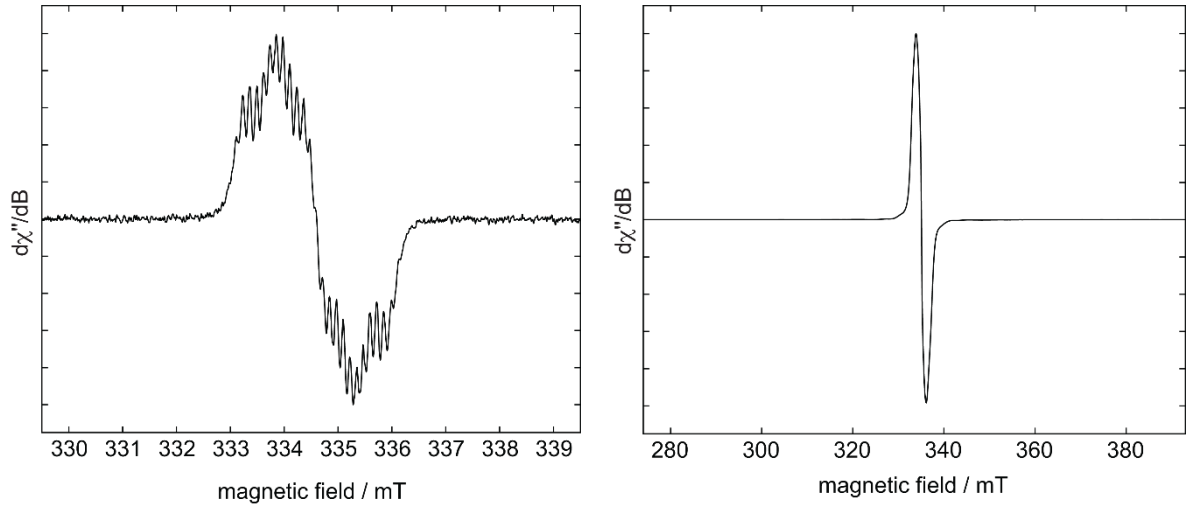

Figure S24. Room-temperature X-band EPR spectrum of **10** in diethyl ether (left) and in powder form (right). The isotropic *g* factor is 2.0030.

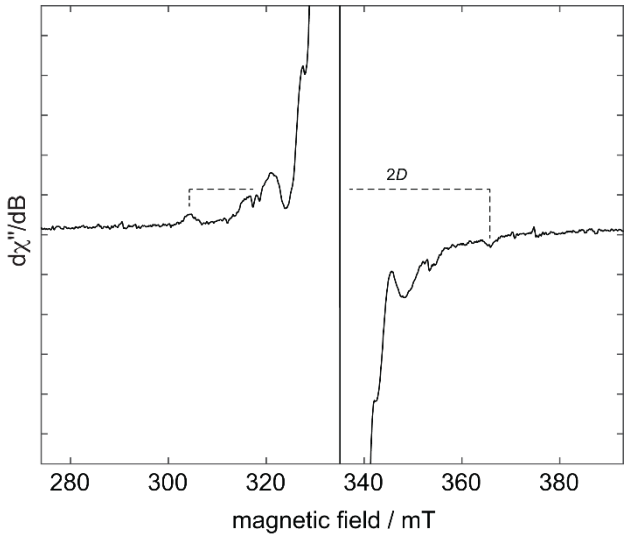

Figure S25. Expanded view of the solid-state X-band EPR spectrum of **10** at room temperature showing the weak zero-field splitting. The separation of the outermost peaks indicates a *D* value of ca. 31 mT (ca. 840 MHz). According to the point-dipole approximation, this corresponds to a spin-spin distance of about 4.5 Å.

Cyclic voltammetry

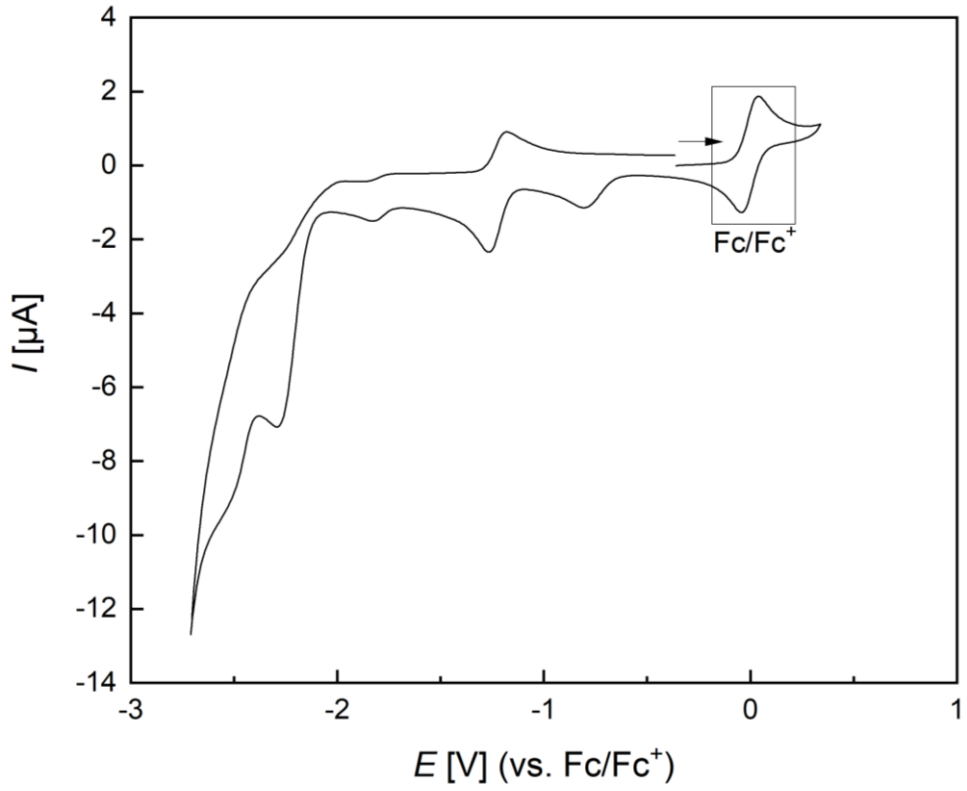

Figure S26. Cyclovoltammogramm of **5** in CH_2Cl_2 at rt calibrated versus the ferrocene/ferrocenium couple (Fc/Fc^+). Scan Rate: 250 mV s^{-1}. Partially reversible reduction at $E_{1/2}$ = –1.22 V. Irreversible reduction events at E_{pc} = –0.81, –1.83 V and –2.29 V. Start of another reduction at E_{pc} = –2.52 V.

IR spectroscopy

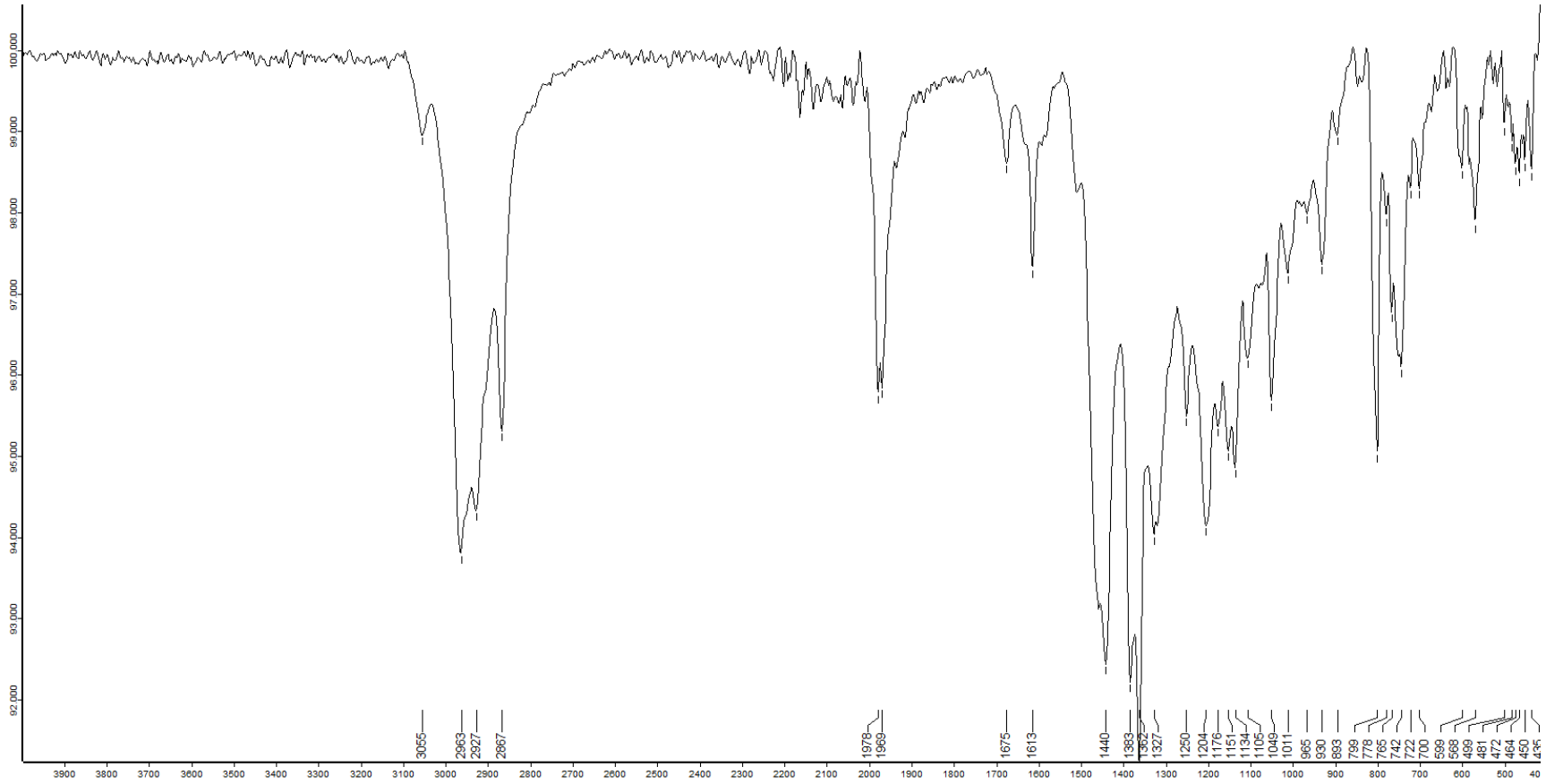

Figure S27. Solid-state IR spectrum of **13**.

X-ray crystallographic data

The crystal data of **3-I*i*Pr**, **5** were collected on a BRUKER X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The crystal data of **3-CAAC**, **4-CAAC**, **8-H**, **10**, **11-Li**, **11-Na**, and the cocrystal of {**12**+**13**} were collected on a Rigaku XtaLAB Synergy-R diffractometer with a HPA area detector and multi-layer mirror monochromated $Cu_{K\alpha}$ radiation. The structures were solved using the intrinsic phasing method,[7] refined with the SHELXL program,[8] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center under the deposition numbers CCDC 2411656-2411665. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. CCDC numbers of the X-ray crystallographic data presented herein.

Structure	CCDC number
3-CAAC	2411656
3-IiPr	2411660
4-CAAC	2411661
5	2411659
8-H	2411663
10	2411665
11-Li	2411662
11-Na	2411658
11-K	2411664
12+**13**	2411661

Refinement details for 3-I*i*Pr: The asymmetric unit contains a toluene molecule modelled as twofold rotationally disordered in a 79:21 ratio. The benzene rings within this disorder were idealized with AFIX 66 and ADPs restrained to similarity with SIMU 0.005.

Crystal data for 3-I*i*Pr: $C_{24}H_{36}B_2Cl_4N_4 \cdot C_7H_8$, M_r = 636.12, colourless block, 0.294×0.152×0.105 mm^3, orthorhombic space group $P2_12_12_1$, a = 9.698(7) Å, b = 14.501(11) Å, c = 23.777(17) Å, V = 3344(4) Å^3, Z = 4, ρ_{calcd} = 1.264 g·cm^{-3}, μ = 0.381 mm^{-1}, F(000) = 1344, T = 100(2) K, R_1 = 0.0792, wR_2 = 0.1223, Flack parameter = –0.05(5), 6355 independent reflections [$2\theta \leq 51.362°$] and 420 parameters.

Refinement details for 3-CAAC: Two reflections, (0 2 0) and (1, 1, 11), were removed from refinement as outliers.

Crystal data for 3-CAAC: $C_{46}H_{66}B_2Cl_4N_2$, M_r = 810.42, colourless block, 0.073×0.067×0.032 mm^3, monoclinic space group $C2/c$, a = 15.6161(4) Å, b = 9.7783(3) Å, c = 27.3476(7) Å, α = 90°, β = 91.064(2)°, γ = 90°, V = 4175.2(2) Å^3, Z = 4, ρ_{calcd} = 1.289 g·cm^{-3}, μ = 2.833 mm^{-1}, F(000) = 1736, T = 100(2) K, R_1 = 0.0920, wR_2 = 0.2158, 3921 independent reflections [$2\theta \leq 149.84°$] and 252 parameters.

Refinement details for 4-CAAC: Two outlying reflections were omitted (0 -1 2, 1 2 2). The asymmetric unit contains two half-toluene molecules positioned on inversion centers and modelled as rotationally twofold disordered in 76:34 and 59:41 ratios, respectively. The benzene rings within these disorders were idealized using AFIX 66 and their ADPs were restrained to similarity with SIMU 0.005.

Crystal data for 4-CAAC: $C_{46}H_{66}B_2Cl_4N_2 \cdot (C_7H_8)$, M_r = 902.56, colorless block, 0.167×0.136×0.067 mm^3, triclinic space group $P\bar{1}$, a = 10.58090(10) Å, b = 15.0567(2) Å, c = 16.8473(2) Å, α = 103.9340(10)°, β = 90.5890(10)°, γ = 101.8350(10)°, V = 2544.61(5) Å^3, Z = 2, ρ_{calcd} = 1.178 g·cm^{-3}, μ = 2.374 mm^{-1}, F(000) = 968,

T = 99.99(10) K, R_1 = 0.0424, wR_2 = 0.1031, 10517 independent reflections [$2\theta \leq 135{,}368°$] and 713 parameters.

Crystal data for 5: $C_{46}H_{67}B_2Cl_5N_2$, M_r = 846.88, colourless block, 0.289×0.198×0.129 mm^3, triclinic space group $P\bar{1}$, a = 9.316(3) Å, b = 16.088(5) Å, c = 16.888(6) Å, α = 65.233(11)°, β = 78.069(18)°, γ = 78.392(13)°, V = 2230.0(12) Å^3, Z = 2, ρ_{calcd} = 1.261 g·cm^{-3}, μ = 0.360 mm^{-1}, F(000) = 904, T = 100(2) K, R_1 = 0.0832, wR_2 = 0.1063, 9554 independent reflections [$2\theta \leq 53.72°$] and 517 parameters.

Crystal data for 8-H: $C_{46}H_{67}B_2Cl_3N_2 \cdot (C_6H_{14})_{0.5}$, M_r = 819.07, colourless block, 0.154×0.126×0.079 mm^3, triclinic space group $P\bar{1}$, a = 12.1063(2) Å, b = 12.2167(2) Å, c = 16.7570(3) Å, α = 69.520(2)°, β = 82.6670(10)°, γ = 85.9860(10)°, V = 2301.85(7) Å^3, Z = 2, ρ_{calcd} = 1.182 g·cm^{-3}, μ = 2.051 mm^{-1}, F(000) = 886, T = 100(2) K, R_1 = 0.0476, wR_2 = 0.0991, 9136 independent reflections [$2\theta \leq 150.018°$] and 522 parameters.

Crystal data for 10: $C_{46}H_{66}B_2N_2$, M_r = 668.62, red plate, 0.110×0.064×0.050 mm^3, monoclinic space group $P2_1/c$, a = 13.8578(3) Å, b = 17.4398(4) Å, c = 17.2654(6) Å, β = 102.684(3)°, V = 4070.8(2) Å^3, Z = 4, ρ_{calcd} = 1.091 g·cm^{-3}, μ = 0.453 mm^{-1}, F(000) = 1464, T = 100.00(11) K, R_1 = 0.0975, wR_2 = 0.1326, 7430 independent reflections [$2\theta \leq 136.488°$] and 467 parameters.

Refinement details for 11-Li: The reflection (2 1 9) was omitted as an outlier. The asymmetric unit contains two THF solvent molecules. The first was modelled as twofold disordered (RESI 61 and 62 THF) in a 90:10 ratio. The second was modelled as threefold disordered (RESI 71, 72 and 73) in a 69:13:18 ratio using three FVAR summed up to 1.0 with SUMP. 1,2- and 1,3-distances within these disorders were restrained to similarity with SAME. ADPs were restrained to similarity with SIMU 0.005. One of the Li-bound THF ligands was also modelled as twofold disordered in its carbon atoms (RESI 21 and 22) in a 69:31 ratio. ADPs within this disorder were restrained to similarity with SIMU 0.005.

Crystal data for 11-Li: $C_{54}H_{82}B_2Li_2N_2O_4 \cdot (C_4H_8O)_2$, M_r = 970.92, colourless block, 0.190×0.150×0.100 mm^3, orthorhombic space group *Pbcn*, a = 29.0869(3) Å, b = 14.7935(2) Å, c = 26.7494(3) Å, V = 11510.2(2) Å^3, Z = 8, ρ_{calcd} = 1.121 g·cm^{-3}, μ = 0.507 mm^{-1}, F(000) = 4256, T = 100(2) K, R_1 = 0.0602, wR_2 = 0.1214, 10519 independent reflections [$2\theta \leq 136.486°$] and 841 parameters.

Crystal data for 11-Na: $C_{54}H_{86}B_2N_2Na_2O_2$, M_r = 862.84, colourless block, 0.222×0.136×0.079 mm^3, space group $P\bar{1}$, a = 11.3160(2) Å, b = 12.6875(2) Å, c = 20.2610(2) Å, α = 105.4830(10)°, β = 97.1240(10)°, γ = 109.0190(10)°, V = 2578.25(7) Å^3, Z = 2, ρ_{calcd} = 1.111 g·cm^{-3}, μ = 0.638 mm^{-1}, F(000) = 944, T = 100.01(10) K, R_1 = 0.0615, wR_2 = 0.1047, 10432 independent reflections [$2\theta \leq 149.992°$] and 579 parameters.

Refinement details for 11-K: The unit cell contains a highly disordered half-toluene molecule positioned on an inversion center, which was treated as a diffuse contribution to the overall scattering without specific positions by the Platon program Squeeze.[9] 407 electrons were thus removed from the unit cell, which correspond to eight toluene molecules. The toluene molecule π-coordinated to the potassium cation K2 was modelled as twofold rotationally disordered in a 69:31 ratio. The benzene rings within the disorder were idealized with AFIX 66. ADPs were restrained to similarity with SIMU 0.005 and ISOR 0.01. 1,2 and 1,3 distances within the disorder were restrained to similarity with SAME.

Crystal data for 11-K: $C_{46}H_{68}B_2K_2N_2 \cdot C_7H_8 \cdot [(C_7H_8)_{0.5}]_{(squeezed)}$, M_r = 885.06, colourless block, 0.182×0.081×0.069 mm^3, orthorhombic space group $I4_1/a$, a = 42.8936(2) Å, b = 42.8936(2) Å, c = 11.12220(10) Å, V = 20463.3(3) Å^3, Z = 16, ρ_{calcd} = 1.149g·cm^{-3}, μ = 1.905 mm^{-1}, F(000) = 7264, T = 100.00(10) K, R_1 = 0.0616, wR_2 = 0.1379, 9375 independent reflections [$2\theta \leq 136.494°$] and 614 parameters.

Refinement details for {12+13} cocrystal: The asymmetric unit contains 2.5 highly disordered THF molecules, which have been treated as a diffuse contribution to the overall scattering

without specific atom positions by the Platon program Squeeze.[9] 400 electrons were thus removed from the unit cell, corresponding to ten molecules of THF overall.

Crystal data for {12+13} cocrystal: $C_{47}H_{166}B_2Cl_2N_2O \cdot C_{48}H_{166}B_2N_2O_2 \cdot [(C_4H_8O)_{2.5}]_{(squeezed)}$, M_r = 1852.76, dark grey needle, 0.490×0.280×0.070 mm^3, monoclinic space group $P2/c$, a = 20.4539(5) Å, b = 15.8908(3) Å, c = 17.0278(4) Å, β = 107.486(2)°, V = 5278.8(2) Å^3, Z = 2, ρ_{calcd} = 1.166 g·cm^{-3}, μ = 0.993 mm^{-1}, $F(000)$ = 1616, T = 100(2) K, R_1 = 0.0826, wR_2 = 0.2013, 10044 independent reflections [$2\theta \leq 140.136°$] and 504 parameters.

Computational details

All calculations were carried out using the Gaussian 16, Revision C.01,[10] and the ORCA 5.0.4[11] quantum chemistry program packages. Geometry optimizations of the systems **8**, **9**, **10** and **11** were performed at the (U)ωB97X-D[12]/Def2-SVP[13] level of theory. All optimized geometries were characterized as minima on the corresponding potential energy surface by vibrational frequency calculations, which revealed that all eigenvalues of the Hessian matrices are positive. To analyse the diradical character as well as the ground state multiplicity[14] of **9** and **10**, single-point calculations using the *complete-active-space self-consistent field* (CASSCF)[15] and the *domain-based local pair natural orbital* (DLPNO)[16] approximation of *the N-electron valence state 2nd order perturbation theory* (NEVPT2)[17-19] were performed. An active space of two electrons in two molecular orbitals was constructed. The Def2-TZVP[13] basis set was chosen for these calculations, which were carried out in combination with the *resolution of identity* approximation for coulomb integrals (RI-J)[20-21] and the numerical *chain-of-spheres* integration for the Hartree-Fock exchange integrals (COSX).[22-23] The biradical character y_0[24-26] was obtained from the *natural orbital occupation numbers* (NOON)[27] of the CASSCF(2,2) calculations:

$$y_0 = 1 - \frac{ON_{HONO} - ON_{LUNO}}{1 + \left(\frac{ON_{HONO} - ON_{LUNO}}{2}\right)^2} \qquad \text{(S1)}$$

ON_{HONO} and ON_{LUNO} are the occupation numbers of the *highest occupied natural orbital* (HONO) and the *lowest unoccupied natural orbital* (LUNO).

To investigate the aromaticity of **10**, calculations of the *nucleus-independent chemical shift* (NICS)[28-30] were performed at the ωB97X-D/Def2-TZVP level of theory, using the *gauge-independent atomic orbital* (GIAO)[31-33] method. The corresponding values were obtained by placing a dummy atom in the centre of the C_2B_2 ring and at distances of 0.1 Å along the axis perpendicular to the ring centre. For the $NICS_{zz}$ scan, the zz component of the magnetic shielding tensor was used.[34]

Mayer bond orders (MBOs)[35] for systems **5**, **8**, **8'**, and **8-H** were calculated to analyse the B–Cl bonding situations in the compounds, computed at the ωB97X-D/Def2-SVP level of theory. For this, the Multiwfn 3.8[36] tool was used. For graphical representation GaussView 6.0.16[37] was used.

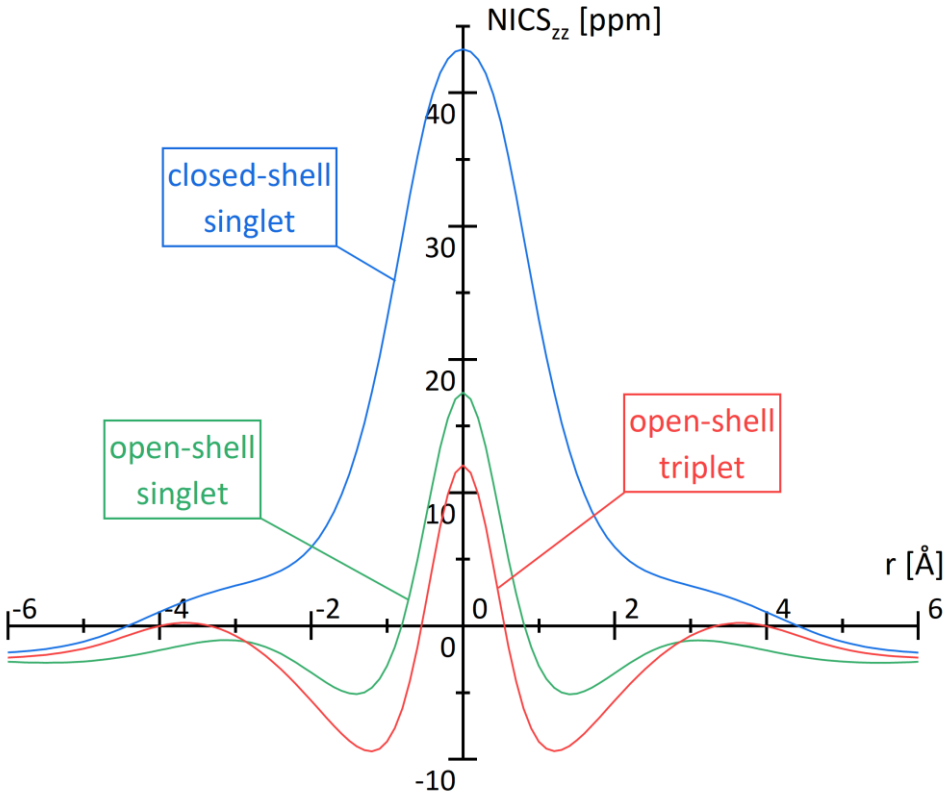

Figure S28. NICS$_{zz}$ curves of the electronic states of compound **10** at the (U)ωB97X-D/Def2-TZVP//(U)ωB97X-D/Def2-SVP level of theory.

Cartesian Coordinates

Compound 5, ωB97X-D/Def2-SVP

Geometry of the lowest singlet ground state

Energy = –3330.11509967 E_h

B	-1.5090750	0.9803390	0.2639150
N	-3.5231530	-0.3404420	-0.8645320
C	-1.3608820	3.5745680	0.2620340
H	-2.4323450	3.5868400	0.4834200
C	-0.6965620	2.3483870	0.1128550
C	-2.5305580	0.5012050	-0.9546620
C	-0.6832310	4.7844040	0.1397850
H	-1.2203860	5.7278700	0.2569100
C	-4.1460820	-0.8690230	0.3448660
C	-5.6401850	1.2627860	0.4734300
H	-5.0986250	1.5146860	-0.4460380
C	-3.7152090	-2.0996330	0.8823450
C	-2.4068430	0.9956060	-2.3954280
C	-5.2110040	-0.1343250	0.9145300
C	-2.4635040	-2.8539420	0.4452590
H	-2.0126190	-2.3185040	-0.4041670
C	-5.8758330	-0.7014850	2.0037880
H	-6.6987470	-0.1542780	2.4672060
C	-4.1298460	-0.7514340	-2.2079000
C	-0.9934890	1.1521560	-2.9482460
H	-1.0663310	1.3864950	-4.0208040
H	-0.4113700	0.2283780	-2.8449660
H	-0.4413220	1.9658230	-2.4659090
C	-5.2650130	2.3282970	1.5135960
H	-5.5690130	3.3237490	1.1554220
H	-4.1883460	2.3421520	1.7198270

H	-5.7826460	2.1467900	2.4680710
C	-3.1626480	-0.0829850	-3.1829880
H	-2.4415880	-0.8252550	-3.5562550
H	-3.6832970	0.3339780	-4.0554450
C	-4.4312760	-2.6158660	1.9660020
H	-4.1229100	-3.5685600	2.4007600
C	-3.1201530	2.3654550	-2.4682300
H	-3.1585590	2.6769820	-3.5222060
H	-2.5666790	3.1312130	-1.9110170
H	-4.1500640	2.3348830	-2.0879080
C	-5.5075210	-1.9368250	2.5175110
H	-6.0488980	-2.3622300	3.3644760
C	-7.1430160	1.3542190	0.1749500
H	-7.3775450	2.3252880	-0.2862190
H	-7.7365300	1.2860640	1.0989620
H	-7.4938250	0.5633210	-0.5009400
C	-1.4284580	-2.8705520	1.5827150
H	-0.4667300	-3.2633860	1.2160910
H	-1.7626580	-3.5240030	2.4029190
H	-1.2621970	-1.8695700	1.9998220
C	-2.7455680	-4.2973620	0.0075890
H	-1.8232200	-4.7628180	-0.3723970
H	-3.5085600	-4.3672240	-0.7773680
H	-3.0901070	-4.9066230	0.8566250
C	-5.5699520	-0.2698580	-2.3629070
H	-5.9377040	-0.6180820	-3.3378560
H	-5.6654020	0.8217580	-2.3439310
H	-6.2171630	-0.7021420	-1.5895770
C	-4.1089820	-2.2680350	-2.3567430
H	-4.4706870	-2.5147130	-3.3651200
H	-4.7706200	-2.7596600	-1.6308880

H	-3.0938770	-2.6725060	-2.2586240
B	1.5093310	0.9804960	-0.2640250
N	3.5231930	-0.3404450	0.8645480
C	1.3609580	3.5746580	-0.2621440
H	2.4324290	3.5869980	-0.4835060
C	0.6967010	2.3484380	-0.1129910
C	2.5306580	0.5012720	0.9546130
C	0.6832300	4.7844510	-0.1398990
H	1.2203320	5.7279490	-0.2570020
C	4.1460850	-0.8691150	-0.3448190
C	5.6404190	1.2625100	-0.4733010
H	5.0989040	1.5144220	0.4461940
C	3.7150520	-2.0996570	-0.8823030
C	2.4068820	0.9957440	2.3953450
C	5.2111120	-0.1345550	-0.9144350
C	2.4631670	-2.8537060	-0.4452920
H	2.0121850	-2.3180270	0.4039350
C	5.8758800	-0.7017900	-2.0036940
H	6.6988540	-0.1546790	-2.4671130
C	4.1297860	-0.7514670	2.2079470
C	0.9935030	1.1523120	2.9481020
H	1.0663020	1.3866960	4.0206520
H	0.4113980	0.2285240	2.8448390
H	0.4413430	1.9659540	2.4657130
C	5.2652510	2.3280900	-1.5133970
H	5.5693560	3.3234980	-1.1551860
H	4.1885650	2.3420570	-1.7195280
H	5.7828070	2.1466050	-2.4679180
C	3.1626810	-0.0827980	3.1829950
H	2.4415820	-0.8249610	3.5563970
H	3.6833930	0.3342480	4.0553750

C	4.4310800	-2.6159960	-1.9659330
H	4.1225720	-3.5686280	-2.4007260
C	3.1201640	2.3656070	2.4680770
H	3.1584250	2.6772700	3.5220180
H	2.5667580	3.1312990	1.9107010
H	4.1501250	2.3349880	2.0879050
C	5.5074230	-1.9370860	-2.5174240
H	6.0487520	-2.3625490	-3.3643910
C	7.1432650	1.3538560	-0.1748890
H	7.3778620	2.3249280	0.2862340
H	7.7367210	1.2856390	-1.0989310
H	7.4940640	0.5629620	0.5010090
C	1.4283360	-2.8704120	-1.5829380
H	0.4664830	-3.2630190	-1.2164000
H	1.7625820	-3.5240910	-2.4029420
H	1.2622990	-1.8694980	-2.0002900
C	2.7449640	-4.2970660	-0.0072570
H	1.8224950	-4.7623010	0.3727010
H	3.5078330	-4.3668520	0.7778280
H	3.0895440	-4.9065700	-0.8561020
C	5.5699860	-0.2701300	2.3629160
H	5.9376890	-0.6183020	3.3379020
H	5.6656320	0.8214640	2.3438120
H	6.2171290	-0.7026070	1.5896360
C	4.1086690	-2.2680570	2.3568620
H	4.4702840	-2.5147310	3.3652690
H	4.7702780	-2.7598150	1.6310700
H	3.0935080	-2.6723850	2.2587030
Cl	-2.1631060	0.7397830	1.9583990
Cl	2.1633170	0.7397980	-1.9584550
Cl	0.0000190	-0.3640710	-0.0000660

Compound 8, ωB97X-D/Def2-SVP

Geometry of the lowest doublet ground state

Energy = –3330.28513733 E_h

B	-1.4595910	0.5582860	0.1828410
N	-3.7511160	-0.3599630	-0.8576080
C	-1.4178260	3.1070560	0.0434790
H	-2.4981700	3.0131220	0.1830670
C	-0.6374030	1.9379960	-0.0103040
C	-2.5952660	0.2442270	-0.9875360
C	-0.8787340	4.3839110	-0.0635330
H	-1.5276340	5.2618260	-0.0151530
C	-4.5001130	-0.6341120	0.3627080
C	-5.4271250	1.7996930	0.3517180
H	-4.7510900	1.8900980	-0.5088270
C	-4.3929070	-1.8946520	0.9872520
C	-2.3520830	0.5438950	-2.4709460
C	-5.3875200	0.3556710	0.8431170
C	-3.3310250	-2.9379620	0.6591860
H	-2.7508790	-2.5852010	-0.2052520
C	-6.2242380	0.0192630	1.9099060
H	-6.9155330	0.7693680	2.2993870
C	-4.4145700	-0.7510680	-2.1722380
C	-0.9235530	0.3705940	-2.9787940
H	-0.9199280	0.5351640	-4.0675980
H	-0.5349910	-0.6343200	-2.7736800
H	-0.2363200	1.0932270	-2.5268170
C	-4.9070760	2.7548480	1.4370550
H	-4.8358590	3.7787800	1.0380110
H	-3.9207370	2.4484920	1.8057710
H	-5.5954290	2.7801990	2.2963400
C	-3.2927980	-0.4501540	-3.1624900

H	-2.7354000	-1.3743950	-3.3770290
H	-3.6773770	-0.0665650	-4.1176120
C	-5.2584490	-2.1691630	2.0500340
H	-5.1915510	-3.1375630	2.5497100
C	-2.7762770	2.0076480	-2.7383860
H	-2.8257870	2.1583380	-3.8271170
H	-2.0409680	2.7089090	-2.3272750
H	-3.7585270	2.2615360	-2.3168720
C	-6.1798190	-1.2355220	2.4999960
H	-6.8461560	-1.4763790	3.3307910
C	-6.8246230	2.2545890	-0.0894920
H	-6.7705310	3.2622080	-0.5294350
H	-7.5103390	2.3143090	0.7695560
H	-7.2813490	1.5854910	-0.8298500
C	-2.3440750	-3.0746210	1.8286790
H	-1.5101160	-3.7327200	1.5409480
H	-2.8393970	-3.5186920	2.7070770
H	-1.9296780	-2.1023320	2.1188720
C	-3.9200130	-4.3173450	0.3335730
H	-3.1202530	-4.9964540	0.0009050
H	-4.6872290	-4.2854910	-0.4510420
H	-4.3796150	-4.7724910	1.2245800
C	-5.6822460	0.0613390	-2.4282220
H	-6.0981310	-0.2435170	-3.3987850
H	-5.4984570	1.1410120	-2.4667840
H	-6.4385910	-0.1451850	-1.6598170
C	-4.7819480	-2.2300460	-2.1932320
H	-5.1829300	-2.4667000	-3.1896240
H	-5.5535190	-2.4726570	-1.4498300
H	-3.9048310	-2.8661500	-2.0251370
B	1.8897370	0.9588490	-0.2404630

N	3.8464500	-0.3351980	0.8898770
C	1.2923060	3.3853260	-0.2714390
H	2.3724890	3.5064980	-0.4008740
C	0.7647950	2.0837780	-0.1495240
C	2.7481330	0.4905630	0.9252660
C	0.4964450	4.5251640	-0.2322420
H	0.9483190	5.5155030	-0.3264830
C	4.5472810	-0.7495230	-0.2938450
C	5.7446360	1.5412690	-0.3891610
H	5.1455730	1.6928790	0.5159260
C	4.2684810	-2.0062150	-0.8763660
C	2.5272720	0.9156530	2.3830940
C	5.5159180	0.1104280	-0.8616550
C	3.1114070	-2.8978820	-0.4411360
H	2.6303310	-2.4235460	0.4258130
C	6.2476060	-0.3447180	-1.9612680
H	6.9986580	0.3090080	-2.4109710
C	4.4063030	-0.6833160	2.2318890
C	1.0718500	0.9050180	2.8491030
H	1.0363870	1.0281430	3.9438180
H	0.5777800	-0.0415750	2.5931050
H	0.4860460	1.7178230	2.4048830
C	5.2448200	2.5563100	-1.4263000
H	5.3449020	3.5807680	-1.0338120
H	4.1940560	2.3809120	-1.6886610
H	5.8338780	2.4955610	-2.3555470
C	3.3111860	-0.1548680	3.1604930
H	2.6256460	-0.9785570	3.4125030
H	3.7215710	0.2299680	4.1058420
C	5.0358450	-2.4149530	-1.9707410
H	4.8351230	-3.3858500	-2.4298460

C	3.1052490	2.3258810	2.6123320
H	3.0626370	2.5801920	3.6837630
H	2.5177990	3.0749670	2.0636310
H	4.1509140	2.4124140	2.2848160
C	6.0274440	-1.6033580	-2.5043670
H	6.6138080	-1.9426430	-3.3612020
C	7.2108480	1.8296890	-0.0463820
H	7.3077080	2.8331420	0.3966550
H	7.8440940	1.8098710	-0.9472490
H	7.6246900	1.1030450	0.6658780
C	2.0492050	-2.9948070	-1.5456230
H	1.1824270	-3.5715280	-1.1865690
H	2.4503200	-3.5076090	-2.4348380
H	1.6987550	-2.0017450	-1.8512490
C	3.5633570	-4.3105150	-0.0486290
H	2.7155520	-4.8800700	0.3629360
H	4.3661910	-4.3067650	0.7001440
H	3.9323820	-4.8650290	-0.9259670
C	5.7669380	-0.0241490	2.4891020
H	6.1247500	-0.3177800	3.4867430
H	5.7218020	1.0707750	2.4596760
H	6.5084200	-0.3656490	1.7534110
C	4.5894720	-2.1905140	2.4088740
H	4.9489340	-2.3885130	3.4296770
H	5.3334980	-2.5910690	1.7052330
H	3.6441100	-2.7307350	2.2748510
Cl	-2.1772310	0.5364400	1.9235480
Cl	2.3199250	0.5462740	-1.9627150
Cl	-0.3916930	-0.9962260	-0.0416170

8', ωB97X-D/Def2-SVP

Energy = –3330.25032052 E_h

B	-1.537900000	1.022539000	0.207557000
N	-3.505867000	-0.415459000	-0.833810000
C	-1.400238000	3.604843000	0.110452000
H	-2.482247000	3.592034000	0.276118000
C	-0.704818000	2.387818000	0.039355000
C	-2.505962000	0.489062000	-0.940593000
C	-0.750689000	4.828873000	-0.020451000
H	-1.317692000	5.761236000	0.035849000
C	-4.140293000	-0.869055000	0.381458000
C	-5.642555000	1.243507000	0.374686000
H	-5.077004000	1.433794000	-0.543922000
C	-3.707476000	-2.056708000	1.012058000
C	-2.399885000	0.913581000	-2.407918000
C	-5.220549000	-0.121490000	0.906361000
C	-2.436093000	-2.808772000	0.634046000
H	-1.992617000	-2.307352000	-0.238129000
C	-5.897419000	-0.626084000	2.018923000
H	-6.731714000	-0.059088000	2.437811000
C	-4.044521000	-0.906376000	-2.149839000
C	-0.989599000	1.114846000	-2.958820000
H	-1.053036000	1.290802000	-4.044371000
H	-0.361574000	0.231405000	-2.792873000
H	-0.483325000	1.976467000	-2.508783000
C	-5.280589000	2.365574000	1.357260000
H	-5.541030000	3.344662000	0.924985000
H	-4.211036000	2.359406000	1.600296000
H	-5.837849000	2.258319000	2.301642000
C	-3.071438000	-0.259164000	-3.137633000
H	-2.296425000	-0.989202000	-3.416801000

H	-3.573498000	0.056341000	-4.063742000
C	-4.429804000	-2.519253000	2.116054000
H	-4.110704000	-3.438141000	2.613054000
C	-3.182005000	2.230941000	-2.601310000
H	-3.217481000	2.480325000	-3.673711000
H	-2.681285000	3.056168000	-2.077805000
H	-4.215635000	2.171100000	-2.234184000
C	-5.522962000	-1.823863000	2.612084000
H	-6.069918000	-2.203750000	3.477675000
C	-7.136789000	1.316228000	0.036847000
H	-7.366045000	2.269403000	-0.464344000
H	-7.754897000	1.272696000	0.947084000
H	-7.460137000	0.499439000	-0.622567000
C	-1.407953000	-2.734503000	1.774204000
H	-0.441059000	-3.142758000	1.438888000
H	-1.741165000	-3.327628000	2.640794000
H	-1.250971000	-1.701784000	2.108433000
C	-2.683334000	-4.281202000	0.280962000
H	-1.749034000	-4.746491000	-0.070510000
H	-3.442179000	-4.411969000	-0.500841000
H	-3.016869000	-4.848705000	1.163812000
C	-5.495949000	-0.480120000	-2.386802000
H	-5.828210000	-0.882991000	-3.354414000
H	-5.619812000	0.608658000	-2.419164000
H	-6.155784000	-0.888971000	-1.609484000
C	-3.984659000	-2.429344000	-2.248252000
H	-4.314995000	-2.732291000	-3.252936000
H	-4.649338000	-2.907400000	-1.514888000
H	-2.962389000	-2.801329000	-2.104076000
B	1.586939000	1.074535000	-0.243536000
N	3.491565000	-0.399870000	0.849884000

C	1.334235000	3.655319000	-0.283082000
H	2.414295000	3.685384000	-0.457041000
C	0.699040000	2.413022000	-0.127091000
C	2.542019000	0.556946000	0.924888000
C	0.627547000	4.853387000	-0.231567000
H	1.150688000	5.804831000	-0.353927000
C	4.142234000	-0.881729000	-0.347502000
C	5.743401000	1.140639000	-0.185769000
H	5.206356000	1.267941000	0.760672000
C	3.695835000	-2.039851000	-1.020148000
C	2.467719000	1.070566000	2.363483000
C	5.272504000	-0.166715000	-0.809057000
C	2.396285000	-2.772867000	-0.708658000
H	1.929501000	-2.282971000	0.155770000
C	5.963819000	-0.653620000	-1.918890000
H	6.832260000	-0.105594000	-2.290466000
C	3.939509000	-0.931669000	2.182011000
C	1.055697000	1.183654000	2.938337000
H	1.118987000	1.473925000	3.998862000
H	0.518612000	0.228269000	2.874248000
H	0.456335000	1.940056000	2.419186000
C	5.384089000	2.343987000	-1.065516000
H	5.677264000	3.281918000	-0.567844000
H	4.308148000	2.376416000	-1.279176000
H	5.910862000	2.295559000	-2.032001000
C	3.292489000	0.047660000	3.172941000
H	2.642807000	-0.497406000	3.871257000
H	4.057272000	0.551679000	3.780902000
C	4.440085000	-2.492971000	-2.115070000
H	4.109866000	-3.388447000	-2.646173000
C	3.139482000	2.458740000	2.427073000

H	3.186075000	2.788935000	3.477176000
H	2.566873000	3.205745000	1.863516000
H	4.166999000	2.436992000	2.034205000
C	5.565051000	-1.817448000	-2.562635000
H	6.122621000	-2.188297000	-3.425346000
C	7.243564000	1.138209000	0.129662000
H	7.509484000	2.030557000	0.717271000
H	7.850430000	1.163667000	-0.788598000
H	7.543934000	0.248552000	0.701706000
C	1.413319000	-2.657136000	-1.884631000
H	0.426399000	-3.050019000	-1.592541000
H	1.765567000	-3.241290000	-2.749675000
H	1.289596000	-1.615596000	-2.204839000
C	2.602779000	-4.257027000	-0.378696000
H	1.651895000	-4.707786000	-0.054087000
H	3.342961000	-4.422652000	0.415147000
H	2.942919000	-4.815713000	-1.264642000
C	5.461069000	-0.968764000	2.325784000
H	5.709279000	-1.423165000	3.295966000
H	5.898695000	0.037065000	2.310410000
H	5.932860000	-1.572843000	1.537568000
C	3.391908000	-2.343501000	2.397154000
H	3.631794000	-2.671772000	3.419429000
H	3.848585000	-3.056204000	1.700405000
H	2.299278000	-2.369897000	2.276609000
Cl	-2.143716000	0.832823000	1.950497000
Cl	2.237639000	0.884291000	-1.967755000
Cl	0.033947000	-0.317546000	-0.009355000

Compound 8-H, ωB97X-D/Def2-SVP

Geometry of the lowest singlet ground state

Energy = –3330.89203022 E_h

B	-1.8156680	0.8346710	0.2351850
N	-3.9866360	-0.2493760	-0.8904180
C	-1.2882830	3.2489500	0.2592050
H	-2.3636840	3.3396310	0.4415540
C	-0.7150360	1.9684170	0.1225790
C	-2.5753630	0.1408090	-0.9820350
C	-0.5359250	4.4131130	0.1566760
H	-1.0173320	5.3878920	0.2619540
C	-4.6489870	-0.6934010	0.2935540
C	-5.8002840	1.6070530	0.4778020
H	-5.2269580	1.7319420	-0.4468390
C	-4.4000340	-1.9710080	0.8579730
C	-2.4972820	0.8056360	-2.3903750
C	-5.5792960	0.1702960	0.9288620
C	-3.3384250	-2.9292270	0.3298070
H	-2.9182630	-2.4928250	-0.5846290
C	-6.2700940	-0.2726490	2.0598630
H	-6.9851020	0.3954070	2.5470350
C	-4.5522920	-0.5722090	-2.2247510
C	-1.0992810	0.7920720	-3.0037450
H	-1.1549390	1.0823420	-4.0653900
H	-0.6394920	-0.2062460	-2.9497140
H	-0.4203750	1.4951950	-2.5050750
C	-5.2470740	2.6093000	1.4994170
H	-5.3439860	3.6387350	1.1182690
H	-4.1892250	2.4188460	1.7226980
H	-5.7982210	2.5536820	2.4521860
C	-3.4190540	-0.1419460	-3.1723510

H	-2.8338820	-1.0278710	-3.4671230
H	-3.8020150	0.3144730	-4.0980170
C	-5.1101590	-2.3664860	1.9954150
H	-4.9161930	-3.3496820	2.4316500
C	-3.0403240	2.2416390	-2.4075520
H	-3.2969580	2.5396980	-3.4362380
H	-2.2910650	2.9533250	-2.0370080
H	-3.9428620	2.3488350	-1.7910840
C	-6.0489780	-1.5356150	2.5909690
H	-6.5956470	-1.8663620	3.4771470
C	-7.2701840	1.9249510	0.1838670
H	-7.3652230	2.9321470	-0.2517530
H	-7.8769270	1.9087520	1.1034160
H	-7.7159250	1.2086530	-0.5197800
C	-2.1844670	-3.0913680	1.3280550
H	-1.3935700	-3.7275380	0.8999250
H	-2.5323700	-3.5677800	2.2588580
H	-1.7393300	-2.1242520	1.5921520
C	-3.9115150	-4.3074620	-0.0234110
H	-3.1434730	-4.9271290	-0.5125680
H	-4.7743650	-4.2372150	-0.6990910
H	-4.2391820	-4.8462290	0.8796270
C	-5.8510870	0.1985320	-2.5036350
H	-6.2349120	-0.0614810	-3.5018280
H	-5.7074020	1.2858670	-2.4709150
H	-6.6227300	-0.0742180	-1.7698860
C	-4.8696140	-2.0600750	-2.4319200
H	-5.2688600	-2.2155010	-3.4460800
H	-5.6273990	-2.4083830	-1.7140540
H	-3.9746680	-2.6873530	-2.3304030
B	1.5318500	0.5004310	-0.1999610

N	3.8460930	-0.2950320	0.8778020
C	1.4138720	3.0596990	-0.1969920
H	2.4896960	2.9992420	-0.3810700
C	0.6803890	1.8666250	-0.0727500
C	2.6792400	0.2905740	0.9798970
C	0.8314770	4.3172560	-0.0920000
H	1.4421910	5.2173300	-0.1947290
C	4.5814020	-0.6368820	-0.3336390
C	5.4500120	1.8115720	-0.5066170
H	4.7872930	1.9447600	0.3587560
C	4.4897370	-1.9391890	-0.8683680
C	2.4399110	0.6814670	2.4441500
C	5.4347570	0.3373180	-0.8991970
C	3.4610980	-2.9816020	-0.4450230
H	2.8911710	-2.5832350	0.4064860
C	6.2567410	-0.0527010	-1.9591290
H	6.9225100	0.6838530	-2.4134650
C	4.5335800	-0.5777490	2.2077660
C	1.0214590	0.5077490	2.9844200
H	1.0305760	0.7484080	4.0588490
H	0.6573230	-0.5190590	2.8586920
H	0.3087520	1.1809980	2.4959760
C	4.8885730	2.6801470	-1.6428390
H	4.8015490	3.7269340	-1.3120400
H	3.9032070	2.3284410	-1.9718330
H	5.5599230	2.6628510	-2.5155400
C	3.4109440	-0.2450100	3.1868130
H	2.8792310	-1.1685900	3.4612310
H	3.7917530	0.2050980	4.1139320
C	5.3387980	-2.2662050	-1.9295160
H	5.2839050	-3.2675870	-2.3609130

C	2.8323730	2.1687370	2.6141120
H	2.9108470	2.3841140	3.6901170
H	2.0669110	2.8269810	2.1875530
H	3.7938140	2.4229980	2.1475080
C	6.2285600	-1.3453690	-2.4620080
H	6.8824790	-1.6276420	-3.2895640
C	6.8445510	2.3240820	-0.1235440
H	6.7770030	3.3585220	0.2466880
H	7.5141540	2.3371160	-0.9971220
H	7.3274100	1.7169540	0.6528390
C	2.4535210	-3.2253570	-1.5790110
H	1.6454530	-3.8848400	-1.2277660
H	2.9422070	-3.7156100	-2.4361100
H	2.0047580	-2.2879730	-1.9270510
C	4.0927650	-4.3196030	-0.0367520
H	3.3187540	-4.9926420	0.3622830
H	4.8766340	-4.2130870	0.7244790
H	4.5437140	-4.8255620	-0.9043660
C	5.7774690	0.2889490	2.3933740
H	6.2109360	0.0650280	3.3781380
H	5.5617430	1.3628170	2.3586460
H	6.5332250	0.0518310	1.6333570
C	4.9481100	-2.0396770	2.3231270
H	5.3688970	-2.1952700	3.3272220
H	5.7181210	-2.3077130	1.5868580
H	4.0904600	-2.7134250	2.2113800
Cl	-2.3074140	0.4995860	1.9265020
Cl	2.2010470	0.3653480	-1.9454610
Cl	0.4836970	-1.0441390	0.1645680
H	-1.9135730	-0.7605090	-1.0648310

Compound 9, ωB97X-D/Def2-SVP

Geometry of the lowest triplet ground state

Energy = –2870.16892129 E_h

B	-0.0603690	1.6047550	0.8856790
N	0.8283750	3.7691340	-0.2418160
C	-0.1834320	1.3648290	3.4213540
H	-0.3395370	2.4461280	3.4306800
C	-0.0520190	0.7078000	2.1881140
C	0.9462140	2.7240500	0.6411960
C	-0.1153830	0.6855630	4.6374560
H	-0.2196270	1.2316520	5.5780930
C	-0.3914320	4.1458360	-0.8996350
C	-1.3970120	4.9369510	1.3548580
H	-0.4151680	4.6075300	1.7160690
C	-0.5442590	3.8914800	-2.2815270
C	2.3241790	2.8206390	1.3243480
C	-1.4279520	4.7589300	-0.1587290
C	0.4607510	3.0944660	-3.1036210
H	1.3277780	2.8907610	-2.4615930
C	-2.5783850	5.1667810	-0.8397710
H	-3.3886620	5.6415010	-0.2815370
C	1.9931160	4.7072420	-0.2284360
C	3.0776260	1.4855750	1.3510220
H	4.1010960	1.6472390	1.7271110
H	3.1400980	1.0416420	0.3477860
H	2.5858490	0.7539980	2.0066110
C	-2.4456420	4.0448630	2.0336380
H	-2.3634070	4.1219640	3.1292570
H	-2.3280280	2.9902720	1.7516510
H	-3.4661280	4.3510970	1.7540600
C	3.0586920	3.8129590	0.4023060

H	3.5621960	3.2494890	-0.3989340
H	3.8286430	4.3936080	0.9306900
C	-1.7127760	4.3254020	-2.9122580
H	-1.8448700	4.1353050	-3.9798800
C	2.2564030	3.3603830	2.7696010
H	3.2500550	3.7247190	3.0748830
H	1.9651420	2.5677370	3.4685740
H	1.5423110	4.1871140	2.8881810
C	-2.7200350	4.9687700	-2.2060980
H	-3.6268450	5.2980380	-2.7180700
C	-1.5911430	6.3962150	1.7826150
H	-1.4670240	6.4935710	2.8723910
H	-2.6021260	6.7562940	1.5358220
H	-0.8712100	7.0695600	1.2974910
C	-0.1087470	1.7320300	-3.5141950
H	0.6450750	1.1625470	-4.0794810
H	-0.9949380	1.8476660	-4.1590240
H	-0.4009850	1.1412320	-2.6386780
C	0.9339710	3.8498570	-4.3521450
H	1.7569580	3.3036020	-4.8386100
H	1.2856880	4.8652990	-4.1255170
H	0.1227250	3.9386030	-5.0917690
C	1.6888820	5.9651600	0.5977770
H	2.5806670	6.6078970	0.6275600
H	1.4023600	5.7395390	1.6306060
H	0.8759750	6.5386800	0.1300210
C	2.4182800	5.1787460	-1.6174980
H	3.2736220	5.8615540	-1.5084470
H	1.6107080	5.7308830	-2.1188940
H	2.7359360	4.3489390	-2.2595880
B	0.0603690	-1.6047550	0.8856790

N	-0.8283750	-3.7691340	-0.2418160
C	0.1834320	-1.3648290	3.4213540
H	0.3395370	-2.4461280	3.4306800
C	0.0520190	-0.7078000	2.1881140
C	-0.9462140	-2.7240500	0.6411960
C	0.1153830	-0.6855630	4.6374560
H	0.2196270	-1.2316520	5.5780930
C	0.3914320	-4.1458360	-0.8996350
C	1.3970120	-4.9369510	1.3548580
H	0.4151680	-4.6075300	1.7160690
C	0.5442590	-3.8914800	-2.2815270
C	-2.3241790	-2.8206390	1.3243480
C	1.4279520	-4.7589300	-0.1587290
C	-0.4607510	-3.0944660	-3.1036210
H	-1.3277780	-2.8907610	-2.4615930
C	2.5783850	-5.1667810	-0.8397710
H	3.3886620	-5.6415010	-0.2815370
C	-1.9931160	-4.7072420	-0.2284360
C	-3.0776260	-1.4855750	1.3510220
H	-4.1010960	-1.6472390	1.7271110
H	-3.1400980	-1.0416420	0.3477860
H	-2.5858490	-0.7539980	2.0066110
C	2.4456420	-4.0448630	2.0336380
H	2.3634070	-4.1219640	3.1292570
H	2.3280280	-2.9902720	1.7516510
H	3.4661280	-4.3510970	1.7540600
C	-3.0586920	-3.8129590	0.4023060
H	-3.5621960	-3.2494890	-0.3989340
H	-3.8286430	-4.3936080	0.9306900
C	1.7127760	-4.3254020	-2.9122580
H	1.8448700	-4.1353050	-3.9798800

C	-2.2564030	-3.3603830	2.7696010
H	-3.2500550	-3.7247190	3.0748830
H	-1.9651420	-2.5677370	3.4685740
H	-1.5423110	-4.1871140	2.8881810
C	2.7200350	-4.9687700	-2.2060980
H	3.6268450	-5.2980380	-2.7180700
C	1.5911430	-6.3962150	1.7826150
H	1.4670240	-6.4935710	2.8723910
H	2.6021260	-6.7562940	1.5358220
H	0.8712100	-7.0695600	1.2974910
C	0.1087470	-1.7320300	-3.5141950
H	-0.6450750	-1.1625470	-4.0794810
H	0.9949380	-1.8476660	-4.1590240
H	0.4009850	-1.1412320	-2.6386780
C	-0.9339710	-3.8498570	-4.3521450
H	-1.7569580	-3.3036020	-4.8386100
H	-1.2856880	-4.8652990	-4.1255170
H	-0.1227250	-3.9386030	-5.0917690
C	-1.6888820	-5.9651600	0.5977770
H	-2.5806670	-6.6078970	0.6275600
H	-1.4023600	-5.7395390	1.6306060
H	-0.8759750	-6.5386800	0.1300210
C	-2.4182800	-5.1787460	-1.6174980
H	-3.2736220	-5.8615540	-1.5084470
H	-1.6107080	-5.7308830	-2.1188940
H	-2.7359360	-4.3489390	-2.2595880
Cl	-1.4279520	1.2665060	-0.2538490
Cl	1.4279520	-1.2665060	-0.2538490

Compound 10, ωB97X-D/Def2-SVP

Geometry of the lowest singlet ground state

Energy = –1949.92424648 E_h

N	3.3953810	0.7664790	0.3875830
C	2.0947810	1.2107160	0.4222100
B	0.8593610	0.4594410	-0.0643900
N	-3.3953360	0.7664960	-0.3875890
C	2.0860830	2.5735010	1.1177140
B	-0.8593420	0.4594360	0.0646020
C	3.5058900	2.6765250	1.7118410
H	3.8848660	3.7092630	1.7261040
H	3.4927030	2.3196210	2.7534830
C	5.1100140	2.4621820	-0.2752270
H	5.7084670	1.7465020	-0.8567400
H	5.7931380	3.2263500	0.1239500
H	4.4102600	2.9575620	-0.9583280
C	4.4021400	1.7454360	0.8850460
C	5.4926350	1.1093230	1.7494150
H	6.0467880	0.3358190	1.1973240
H	5.0884210	0.6653210	2.6665820
H	6.2089540	1.8894130	2.0463500
C	1.0353570	2.6176470	2.2341560
H	1.0705940	3.5831410	2.7653600
H	1.2131000	1.8128840	2.9640620
H	0.0227330	2.4729960	1.8346010
C	1.8384340	3.7108110	0.1132840
H	2.6193270	3.7516890	-0.6578450
H	1.8202650	4.6848690	0.6289470
H	0.8819700	3.5808110	-0.4023310
C	3.8049810	-0.4699020	-0.1978830
C	4.4950160	-2.7662090	0.0649330

H	4.6557450	-3.6434900	0.6954030
C	4.0058190	-1.5897420	0.6389000
C	4.7657970	-2.8458700	-1.2956980
H	5.1556140	-3.7720360	-1.7237530
C	4.5057580	-1.7544410	-2.1156060
H	4.6750500	-1.8395810	-3.1915410
C	4.7477570	0.9555680	-3.5008140
H	4.9863950	0.1468890	-4.2093280
H	5.6707750	1.2045370	-2.9576810
H	4.4562650	1.8342370	-4.0966230
C	3.6634440	-1.5770730	2.1231750
H	3.4476050	-0.5370320	2.4004030
C	4.8237970	-2.0777200	2.9914420
H	4.9807760	-3.1606120	2.8665160
H	4.6052910	-1.9040690	4.0564860
H	5.7708370	-1.5743490	2.7493590
C	4.0056880	-0.5572990	-1.5924640
C	2.3571050	0.1707490	-3.3461320
H	2.0546040	0.9973480	-4.0080630
H	1.5152070	-0.0560900	-2.6776580
H	2.5398560	-0.7155340	-3.9749770
C	3.6125840	0.5573030	-2.5525030
H	3.3451410	1.4354780	-1.9528800
C	2.3909590	-2.3784380	2.4217060
H	1.5159810	-1.9507200	1.9170880
H	2.1943380	-2.3803110	3.5053750
H	2.4886700	-3.4249950	2.0928390
C	-3.5057060	2.6766020	-1.7117800
H	-3.8846730	3.7093440	-1.7260250
H	-3.4924290	2.3197520	-2.7534380
C	-4.4020410	1.7454760	-0.8851200

C	-5.1100500	2.4621690	0.2751050
H	-5.7931450	3.2263430	-0.1241100
H	-4.4103770	2.9575270	0.9583020
H	-5.7085510	1.7464530	0.8565250
C	-5.4924460	1.1094100	-1.7496370
H	-6.2087290	1.8895150	-2.0466230
H	-6.0466660	0.3358920	-1.1976340
H	-5.0881330	0.6654390	-2.6667760
C	-1.8383880	3.7107950	-0.1130200
H	-1.8200920	4.6848740	-0.6286370
H	-0.8820060	3.5807170	0.4027310
H	-2.6193910	3.7516830	0.6579970
C	-1.0351270	2.6177190	-2.2338700
H	-1.2128000	1.8129760	-2.9638160
H	-0.0225390	2.4730620	-1.8342270
H	-1.0703210	3.5832280	-2.7650480
C	-3.8050010	-0.4698980	0.1978060
C	-4.0058540	-0.5573430	1.5923660
C	-4.5059870	-1.7545030	2.1154100
H	-4.6753880	-1.8396820	3.1913240
C	-4.7659500	-2.8459000	1.2954340
H	-5.1558260	-3.7720760	1.7234150
C	-4.4950420	-2.7661860	-0.0651680
H	-4.6557370	-3.6434340	-0.6956950
C	-4.0057780	-1.5897020	-0.6390410
C	-3.6633000	-1.5769580	-2.1232930
H	-3.4475180	-0.5368920	-2.4004720
C	-2.3907320	-2.3782130	-2.4217570
H	-2.1940320	-2.3800330	-3.5054120
H	-2.4883820	-3.4247880	-2.0929310
H	-1.5158270	-1.9504370	-1.9170610

C	-4.8235470	-2.0776670	-2.9916630
H	-5.7706420	-1.5743690	-2.7496440
H	-4.9804590	-3.1605730	-2.8667720
H	-4.6049700	-1.9039780	-4.0566860
C	-3.6128630	0.5572220	2.5524970
H	-3.3453510	1.4354240	1.9529490
C	-2.3574810	0.1706400	3.3462590
H	-1.5155080	-0.0561820	2.6778720
H	-2.5403080	-0.7156610	3.9750580
H	-2.0550540	0.9972190	4.0082500
C	-4.7481490	0.9554420	3.5006930
H	-4.4567280	1.8340800	4.0965830
H	-4.9868690	0.1467240	4.2091340
H	-5.6711010	1.2044390	2.9574630
C	0.6200940	-1.0727730	-0.3480390
C	-0.6201000	-1.0727710	0.3482920
C	-1.1561830	-2.2822590	0.8221550
H	-2.0515850	-2.3062290	1.4440040
C	-0.5547350	-3.4727640	0.4319430
H	-0.9756140	-4.4251210	0.7651800
C	0.5547380	-3.4727660	-0.4316670
H	0.9756220	-4.4251250	-0.7648940
C	1.1561750	-2.2822630	-0.8219010
H	2.0515750	-2.3062360	-1.4437540
C	-2.0859550	2.5735340	-1.1175280
C	-2.0947280	1.2107250	-0.4220750

Compound 11, ωB97X-D/Def2-SVP

Geometry of the lowest singlet ground state

Energy = –1949.86207578 E_h

N	3.4673420	0.7223740	0.4289270
C	2.0781700	1.2120560	0.3428080
B	0.8809730	0.4663470	-0.0812160
N	-3.4674120	0.7221190	-0.4295370
C	2.1103210	2.5940540	1.0179920
B	-0.8808490	0.4663240	0.0792730
C	3.5245850	2.6860850	1.6345320
H	3.9202060	3.7170450	1.6615450
H	3.4885380	2.3231370	2.6751620
C	5.1210580	2.4571830	-0.3490560
H	5.7628960	1.7478350	-0.8947950
H	5.7574440	3.2843570	0.0104790
H	4.3927230	2.8696030	-1.0570630
C	4.4297550	1.7378740	0.8338700
C	5.5611940	1.1923750	1.7199710
H	6.1333320	0.4089460	1.1971950
H	5.1712060	0.7678840	2.6546150
H	6.2594120	2.0052320	1.9820570
C	1.0555670	2.6941250	2.1309900
H	1.0455360	3.6955150	2.6069360
H	1.2547230	1.9353710	2.9042370
H	0.0594300	2.4673010	1.7252770
C	1.8941830	3.7581170	0.0312560
H	2.6396910	3.7475920	-0.7771870
H	1.9524980	4.7423740	0.5381730
H	0.9102810	3.6735200	-0.4428170
C	3.8903820	-0.4613770	-0.2023700
C	4.7082560	-2.7459440	0.0027340

H	4.9308540	-3.6195080	0.6231630
C	4.1828580	-1.5959990	0.5988790
C	4.9153140	-2.8125060	-1.3702050
H	5.3259410	-3.7192420	-1.8243990
C	4.5476670	-1.7326690	-2.1667240
H	4.6544790	-1.8067320	-3.2534440
C	4.6029360	1.0262840	-3.5129860
H	4.8879730	0.2447960	-4.2384920
H	5.5161570	1.3412860	-2.9864800
H	4.2307680	1.8878960	-4.0921280
C	3.8490700	-1.6092340	2.0835590
H	3.5898140	-0.5740770	2.3416520
C	5.0273190	-2.0622130	2.9526090
H	5.2551880	-3.1312260	2.7997730
H	4.7894600	-1.9324470	4.0218790
H	5.9430050	-1.4914010	2.7343190
C	4.0156800	-0.5639780	-1.6119810
C	2.2792140	0.0718710	-3.3165410
H	1.9042290	0.8890560	-3.9551080
H	1.4777340	-0.2031260	-2.6164480
H	2.5025800	-0.7944260	-3.9638910
C	3.5217250	0.5323660	-2.5453600
H	3.1865380	1.3629500	-1.9111300
C	2.6047120	-2.4565940	2.3733980
H	1.7274020	-2.0598840	1.8455480
H	2.3907760	-2.4555260	3.4560190
H	2.7415240	-3.5026660	2.0510780
C	-3.5253890	2.6860440	-1.6349080
H	-3.9212960	3.7169040	-1.6615880
H	-3.4894980	2.3233500	-2.6756300
C	-4.4301590	1.7374020	-0.8343090

C	-5.1216700	2.4561920	0.3488080
H	-5.7584510	3.2831500	-0.0105160
H	-4.3934840	2.8687810	1.0568560
H	-5.7631450	1.7464390	0.8944630
C	-5.5614890	1.1917020	-1.7204270
H	-6.2599510	2.0044000	-1.9823540
H	-6.1333730	0.4080550	-1.1977030
H	-5.1714480	0.7674420	-2.6551580
C	-1.8946740	3.7581100	-0.0318900
H	-1.9535150	4.7424750	-0.5385380
H	-0.9105170	3.6736990	0.4416950
H	-2.6397820	3.7472010	0.7769100
C	-1.0565500	2.6947830	-2.1321320
H	-1.2559380	1.9363450	-2.9056250
H	-0.0602700	2.4678090	-1.7268640
H	-1.0467130	3.6963760	-2.6076550
C	-3.8900960	-0.4611890	0.2028330
C	-4.0139390	-0.5631690	1.6126430
C	-4.5454530	-1.7315710	2.1684280
H	-4.6511190	-1.8051310	3.2552930
C	-4.9141880	-2.8116870	1.3727800
H	-5.3244910	-3.7181500	1.8278090
C	-4.7087010	-2.7456940	-0.0004200
H	-4.9321820	-3.6194520	-0.6202610
C	-4.1837230	-1.5960980	-0.5976100
C	-3.8514080	-1.6101180	-2.0826230
H	-3.5923280	-0.5751290	-2.3415290
C	-2.6073570	-2.4576870	-2.3731940
H	-2.3944490	-2.4572230	-3.4560200
H	-2.7438980	-3.5035780	-2.0501700
H	-1.7295450	-2.0607200	-1.8463710

C	-5.0304940	-2.0634730	-2.9503330
H	-5.9459200	-1.4924380	-2.7315380
H	-5.2583360	-3.1323750	-2.7966870
H	-4.7936030	-1.9343380	-4.0198950
C	-3.5192770	0.5336170	2.5451420
H	-3.1843120	1.3638100	1.9102740
C	-2.2764280	0.0733750	3.3159250
H	-1.4753630	-0.2021660	2.6155740
H	-2.4995880	-0.7925000	3.9639140
H	-1.9009530	0.8908760	3.9537940
C	-4.5999060	1.0281980	3.5130800
H	-4.2272600	1.8900010	4.0916320
H	-4.8847440	0.2471030	4.2390910
H	-5.5133180	1.3431470	2.9868770
C	0.6487950	-1.1147840	-0.3067280
C	-0.6485890	-1.1147640	0.3047970
C	-1.1952000	-2.3280280	0.7404640
H	-2.1337030	-2.3620230	1.2993710
C	-0.5738880	-3.5402520	0.3948740
H	-1.0238500	-4.4898320	0.7084110
C	0.5743620	-3.5403120	-0.3959890
H	1.0244570	-4.4899430	-0.7091800
C	1.1955310	-2.3281340	-0.7419930
H	2.1340580	-2.3622240	-1.3008470
C	-2.1109180	2.5942110	-1.0188220
C	-2.0782640	1.2120560	-0.3440320

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