

Supporting Information for

***Boroles from alumoles: accessing boroles with alkyl-substituted backbones via
transtrielation***

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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 (^1H : 500.1 MHz, ^{11}B : 160.5 MHz, ^{13}C : 1265.8 MHz) at room temperature if not stated otherwise. Chemical shifts (δ) are reported in ppm and internally referenced to the carbon nuclei ($^{13}\text{C}\{^1\text{H}\}$) or residual protons (^1H) of the solvent. Heteronuclei NMR spectra are referenced to external standards (^{11}B : $\text{BF}_3\cdot\text{OEt}_2$). Resonances are given as singlet (s), doublet (d), triplet (t), septet (sept) or multiplet (m). High-resolution mass spectrometry (HRMS) data were obtained from a Thermo Scientific Exactive Plus spectrometer. UV-vis spectra were measured on a METTLER TOLEDO UV-vis-Excellence UV5 spectrophotometer at room temperature. Cyclic voltammetry experiments were performed using a *Gamry Instruments* Reference 600 potentiostat. A standard three-electrode cell configuration was employed using a platinum disk working electrode, a platinum wire counter electrode, and a silver wire, separated by a *Vycor* tip, serving as the reference electrode. Formal redox potentials are referenced to the ferrocene/ferrocenium ($[\text{Cp}_2\text{Fe}]^{+/0}$) redox couple by using decamethylferrocene ($[\text{Cp}^*_2\text{Fe}]$; $E_{1/2} = -0.427$ V in THF)¹ as an internal standard. Tetra-*n*-butylammonium hexafluorophosphate ($[\text{nBu}_4\text{N}][\text{PF}_6]$) was employed as the supporting electrolyte. Compensation for resistive losses (*iR* drop) was employed for all measurements. Unless stated otherwise, solvents and reagents were purchased from Sigma-Aldrich or Alfa Aesar. 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (**1**),² DurBBr₂,³ DurBCl₂,³ MesBBr₂,⁴ MesBCl₂,⁵ (*o*-tolyl)BBr₂,⁶ (*o*-tolyl)BCl₂,⁵ [$(\eta^5$ -C₅H₅)Fe(η^5 -C₅H₄BBr₂)] (FcBBr₂),⁷ PhBCl₂,⁴ PhBBr₂⁴ and C₄Et₄Li₂⁸ were synthesized using literature procedures.

Numbering of the carbon atoms for the assignment of NMR shifts was done in accordance with Figure S1.

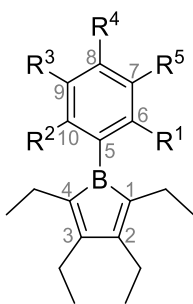


Figure S1. NMR numbering scheme for the borole compounds.

Synthetic procedures

Synthesis of Me₂SnC₄Et₄

To a solution of C₄Et₄Li₂ (250.0 mg, 1.40 mmol) in benzene (5 mL) was added dropwise a solution of Me₂SnCl₂ (308.2 mg, 1.40 mmol) in benzene (5 mL), leading to the immediate formation of a colorless solid (LiCl). The reaction mixture was stirred for 30 min at room temperature and then filtered. Evaporation of the solution at a pressure of 1.2 mbar afforded the product as a colorless oil (404.9 mg, 1.29 mmol, 92%). The spectral data match those reported in the literature.⁹

Synthesis of MesBC₄Et₄ (2)

A) To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (40.0 mg, 0.0944 mmol) in benzene (0.25 mL) was added dropwise a solution of dibromo(mesityl)borane (27.4 mg, 0.0944 mmol) in benzene (0.25 mL). The resulting reaction mixture was heated to 80 °C for 1 d and subsequently evaporated *in vacuo*. The residue was redissolved in pentane to remove the side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) and subsequent filtration. Evaporation of the remaining solution *in vacuo* afforded the product as a dark red oil (25.3 mg, 0.860 mmol, 91%).

B) To a solution of 2,3,4,5-tetraethyl-1,1-dimethyl-1*H*-stannole (250 mg, 0.799 mmol) in benzene (3 mL) was added dropwise a solution of dichloro(mesityl)borane (176 mg, 0.878 mmol) in benzene (2 mL). The resulting reaction mixture was heated to 100 °C for 7 d before all volatile components were removed *in vacuo*. Extraction of the residue with pentane and removal of the solvent *in vacuo* afforded a dark red oil (225 mg, 0.764 mmol, 96%).

¹H NMR (500 MHz, benzene-*d*₆): δ (ppm) = 6.77 (s, 2H, *m*-ArH), 2.26 (s, 6H, (Ar-*o*-CH₃)₂), 2.19 (s, 3H, Ar-*p*-CH₃), 2.06 (q, 4H, C2(CH₂CH₃), C3(CH₂CH₃)), 2.04 (q, 4H, C1(CH₂CH₃), C4(CH₂CH₃)), 0.99 (t, ³*J* = 7.58 Hz, 6H, C2(CH₂CH₃), C3(CH₂CH₃)), 0.88 (t, ³*J* = 7.53 Hz, 6H, C1(CH₂CH₃), C4(CH₂CH₃)). **¹¹B NMR** (160 MHz, benzene-*d*₆): δ (ppm) = 77.58 (br s). **¹³C NMR** (126 MHz, benzene-*d*₆): δ (ppm) = 164.1 (C2(CH₂CH₃), C3(CH₂CH₃)), 140.1 (*C*-*I*-Ar), 137.0 (*C*-*p*-Ar), 136.9 (br, C1(CH₂CH₃), C4(CH₂CH₃)), 135.8 (*C*-*o*-Ar), 127.4 (CH-Ar), 21.6 (CH₃-*o*-Ar), 21.3 (CH₃-*p*-Ar), 21.0 (C1(CH₂CH₃), C4(CH₂CH₃)), 20.2 (C2(CH₂CH₃), C3(CH₂CH₃)), 15.2 (C1(CH₂CH₃), C4(CH₂CH₃)), 14.2 ((C2(CH₂CH₃), C3(CH₂CH₃)). **HRMS LIFDI** for [C₂₁H₃₁BH]⁺ = [M+H⁺]: calcd. 295.2592; found 295.2579.

Synthesis of DurBC₄Et₄ (3)

A) To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (40 mg, 0.0944 mmol) in benzene (0.25 mL) was added dropwise a solution of dibromo(duryl)borane (28.7 mg, 0.0944 mmol) in benzene (0.25 mL). The resulting reaction mixture was heated to 80 °C for 3 d and evaporated *in vacuo*. The residue was redissolved in pentane to remove the side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) and subsequent filtration. Evaporation of the remaining solution *in vacuo* afforded a dark red oil (27.4 mg, 0.0856 mmol, 94%). Single crystals of **3** suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated hexane solution at -30 °C.

¹H NMR (500 MHz, benzene-*d*₆): δ (ppm) = 6.86 (s, 1H, *p*-ArH), 2.17 (s, 6H, (Ar-*o*-CH₃)₂), 2.10 (s, 6H, (Ar-*m*-CH₃)₂), 2.09 (m, 8H, C1(CH₂CH₃), C2(CH₂CH₃), C3(CH₂CH₃), C4(CH₂CH₃)), 1.01 (t, 6H, ³*J* = 7.58 Hz, C1(CH₂CH₃), C4(CH₂CH₃)), 0.89 (t, 6H, ³*J* = 7.53 Hz, C2(CH₂CH₃), C3(CH₂CH₃)). **¹¹B NMR** (160 MHz, benzene-*d*₆): δ (ppm) = 76.46 (br s). **¹³C NMR** (126 MHz, benzene-*d*₆): δ (ppm) = 163.7 (C2(CH₂CH₃), C3(CH₂CH₃)), 143.4 (*C*-i-Ar), 137.1 ((C1(CH₂CH₃), C4(CH₂CH₃)), 133.3 (*C*-*o*-Ar), 131.3 (*C*-*m*-Ar), 131.1 (CH-Ar), 21.0 (C1(CH₂CH₃), (C4(CH₂CH₃)), 20.1 (C2(CH₂CH₃), (C3(CH₂CH₃)), 19.2 ((Ar-*o*-CH₃)₂), 19.0 ((Ar-*m*-CH₃)₂), 15.1 (C2(CH₂CH₃), C3(CH₂CH₃)), 14.2 (C1(CH₂CH₃), C4(CH₂CH₃)). **HRMS LIFDI** for [C₂₂H₃₃B] = [M]: calcd. 308.2675; found 308.2662.

Synthesis of FcBC₄Et₄ (4)

A) To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (20.0 mg, 0.0472 mmol) in pentane (0.25 mL) was added dropwise a solution of dibromo(ferrocenyl)borane (16.8 mg, 0.0472 mmol) in pentane (0.25 mL), upon which the reaction solution immediately turned dark orange. The side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide was removed by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) and subsequent filtration. Evaporation of the remaining solution *in vacuo* afforded a dark red oil (12.4 mg, 0.0344 mmol, 73%).

B) To a solution of 2,3,4,5-tetraethyl-1,1-dimethyl-1*H*-stannole (40.0 mg, 0.128 mmol) in benzene (0.25 mL) was added dropwise a solution of dibromo(ferrocenyl)borane (45.4 mg, 0.878 mmol) in benzene (0.25 mL). All volatile components were removed *in vacuo*. Extraction

of the residue with pentane and removal of the solvent *in vacuo* afforded a dark orange oil (44.0 mg, 0.122 mmol, 96%).

¹H NMR (500 MHz, benzene-*d*₆): δ (ppm) = 4.54 (t, $^3J = 1.83$ Hz, 2H, C7H, C8H), 4.51 (t, $^3J = 1.85$ Hz, 2H, C6H, C9H), 3.98 (s, 5H, (Cp-CH)), 2.33 (q, $^3J = 7.43$ Hz, 4H, C1(CH₂CH₃), C4(CH₂CH₃)), 2.26 (q, $^3J = 7.56$ Hz, 4H, C2(CH₂CH₃), C3(CH₂CH₃)), 1.18 (t, $^3J = 7.52$ Hz, 6H, C1(CH₂CH₃), C4(CH₂CH₃)), 1.10 (t, $^3J = 7.56$ Hz, 6H, C2(CH₂CH₃), C3(CH₂CH₃)). **¹¹B NMR** (160 MHz, benzene-*d*₆): δ (ppm) = 54.65 (br s). **¹³C NMR** (126 MHz, benzene-*d*₆): δ (ppm) = 160.2 (C2(CH₂CH₃), C3(CH₂CH₃)), 138.0 (C1(CH₂CH₃), C4(CH₂CH₃)), 78.0 (C6, C9), 77.0 (C7, C8), 75.6 (C5), 70.7 (CH-Cp), 21.8 (C1(CH₂CH₃), C4(CH₂CH₃)), 20.0 (C2(CH₂CH₃), C3(CH₂CH₃)), 16.6 (C1(CH₂CH₃), C4(CH₂CH₃)), 15.2 (C2(CH₂CH₃), C3(CH₂CH₃)). **HRMS LIFDI** for [C₂₂H₂₉BFe]⁺ = [M+H⁺]: calcd. 360.1706; found 360.1688.

Synthesis of PhBC₄Et₄ (5)

To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (20.0 mg, 0.047 mmol) in benzene (0.25 mL) was added dropwise a solution of dibromo(phenyl)borane (11.7 mg, 0.047 mmol) in benzene (0.25 mL), upon which the reaction solution quickly turned red with almost immediate discoloration. Removal of all volatile components *in vacuo* afforded a colorless oil. The oil was redissolved in pentane. The side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide could not be removed by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) without partial formation of the respective adduct **5a**.

Synthesis of (CAAC^{Me})PhBC₄Et₄ (5a)

To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (20.0 mg, 0.047 mmol) in benzene (0.25 mL) was added dropwise a solution of dibromo(phenyl)borane (11.7 mg, 0.047 mmol) in benzene (0.25 mL), upon which the reaction solution quickly turned red with almost immediate discoloration. All volatile components were removed *in vacuo*. The residue was redissolved in pentane to remove the side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) and subsequent filtration. The addition of another equivalent of CAAC^{Me} led to a change in color from colorless to intensively orange alongside with the formation of an orange solid. The removal of all volatiles *in vacuo* and subsequent washing with pentane resulted in the isolation of a crystalline

orange solid (11.2 mg, 0.0472 mmol, 44%). Single crystals of **5a** suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated pentane solution at 20 °C.

¹H NMR (500 MHz, benzene-*d*₆): δ (ppm) = 7.13 (t, ³*J* = 7.77 Hz, 1H, dip-*p*-CH), 6.96–6.91 (m, 5H, dip-*m*-CH, ph-*o*-CH, ph-*p*-CH), 6.85–6.81 (m, 2H, ph-*m*-CH), 3.04 (sept, ³*J* = 6.63 Hz, 2H, C(CH(CH₃)₂), 2.72–2.64 (m, 2H, C1(CH₂CH₃) and C4(CH₂CH₃); one hydrogen atom of CH₂, respectively), 2.61–2.48 (m, 6H, C1(CH₂CH₃) and C4(CH₂CH₃); one hydrogen atom of CH₂, respectively and C2(CH₂CH₃), C3(CH₂CH₃)), 1.62 (s, 6H, C_{carbene}C(CH₃)₂), 1.46 (s, 2H, CH₂), 1.35 (t, ³*J* = 7.53 Hz, 6H, C2(CH₂CH₃), C3(CH₂CH₃)), 1.12 (d, ³*J* = 6.70 Hz, 6H, C(CH(CH₃)₂)), 1.08–1.06 (m, 12H, C(CH(CH₃)₂) and C1(CH₂CH₃), C4(CH₂CH₃)), 0.98–0.95 (m, 12H, NC(CH₃)₂). **¹¹B NMR** (160 MHz, benzene-*d*₆): δ (ppm) = –3.90. **¹³C NMR** (126 MHz, benzene-*d*₆): δ (ppm) = 241.5 (C_{carbene}), 160.2 (C1, C4), 150.4 (C5), 150.1 (C2, C3), 146.0 (C-*o*-dip), 138.2 (C-*i*-dip), 134.8 (C-*o*-ph), 129.9 (C-*p*-dip), 125.9 (C-*m*-ph), 125.6 (C-*m*-dip), 122.9 (C-*p*-ph), 76.9 (NC(CH₃)₂), 57.1 (C_{carbene}C(CH₃)₂), 53.5 (CH₂), 34.8 (C_{carbene}C(CH₃)₂), 29.4 (NC(CH₃)₂), 29.0 (C(CH(CH₃)₂), 25.9 (C1(CH₂CH₃), C4(CH₂CH₃)), 25.8 (C(CH(CH₃)₂), 25.3 (C(CH(CH₃)₂), 21.2 (C2(CH₂CH₃), C3(CH₂CH₃)), 16.3 (C1(CH₂CH₃), C4(CH₂CH₃)), 15.2 (C2(CH₂CH₃), C3(CH₂CH₃)). **HRMS LIFDI** for [C₃₈H₅₆BN] = [M]: calcd. 537.4500; found 538.4490. **Elemental analysis** calcd. for C₃₈H₅₆BN [537.68 g/mol]: C 84.89, H 10.50, N 2.61%; found: C 82.57, H 10.32, N 2.62%.

Synthesis of *o*-TolBC₄Et₄ (**6**)

A) To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (22.0 mg, 0.0519 mmol) in benzene (0.25 mL) was added dropwise a solution of dichloro(*o*-tolyl)borane (13.6 mg, 0.0519 mmol) in benzene (0.25 mL), upon which the reaction solution immediately turned intensively purple. Removal of all volatile components *in vacuo* afforded a dark purple oil. The residue was redissolved in pentane. The side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide could not be removed by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) and subsequent filtration without partial formation of the respective adduct **6a**.

B) To a solution of 2,3,4,5-tetraethyl-1,1-dimethyl-1*H*-stannole (40.0 mg, 0.128 mmol) in benzene (0.25 mL) a solution of dichloro(*o*-tolyl)borane (23.0 mg, 0.133 mmol) was added dropwise, upon which the reaction solution immediately turned intensively purple. All volatile components were removed *in vacuo*. Extraction of the residue with pentane and removal of the solvent *in vacuo* afforded a dark purple oil (31.0 mg, 0.116 mmol, 91%).

¹H NMR (500 MHz, benzene-*d*₆, 343 K): δ (ppm)= 7.21–7.19 (m, 1H, *o*-ArH), 7.14–7.11 (m, 2H, C8H, C9H), 7.10–7.05 (m, 1H, C7H), 2.30 (s, 3H, Ar-*o*-CH₃), 2.09 (q, ³*J* = 7.62 Hz, 4H, C2(CH₂CH₃), C3(CH₂CH₃)), 2.05 (q, ³*J* = 7.77 Hz, 4H, C1(CH₂CH₃), C4(CH₂CH₃)), 1.01 (t, ³*J* = 7.57 Hz, 6H, C2(CH₂CH₃), C3(CH₂CH₃)), 0.83 (t, ³*J* = 7.50 Hz, 6H, C1(CH₂CH₃), C4(CH₂CH₃)). **¹¹B NMR** (160 MHz, benzene-*d*₆, 343 K): δ (ppm)= 74.57 (br s). **¹³C NMR** (126 MHz, benzene-*d*₆, 343 K): δ (ppm)= 164.6 (C2(CH₂CH₃), C3(CH₂CH₃)), 143.6 (C5), 137.8 (C6), 137.8 (br.; (C1(CH₂CH₃), C4(CH₂CH₃))), 129.3 (C7), 128.4 (C8), 127.4 (C10), 125.1 (C9), 22.5 (CH₃-*o*-Ar), 20.6 (C2(CH₂CH₃), C3(CH₂CH₃)), 20.2 (C1(CH₂CH₃), C4(CH₂CH₃)), 15.0 (C1(CH₂CH₃, C4(CH₂CH₃))), 13.9 (C2(CH₂CH₃, C3(CH₂CH₃))).

HRMS LIFDI for [C₁₉H₂₇B]⁺ = [M⁺]: calcd. 266.2200; found 266.2195.

Synthesis of (CAAC^{Me})*o*-TolBC₄Et₄ (**6a**)

To a solution of 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (50.0 mg, 0.118 mmol) in benzene (0.25 mL) was added dropwise a solution of dibromo(*o*-tolyl)borane (20.4 mg, 0.118 mmol) in benzene (0.25 mL), upon which the reaction solution immediately turned intensively purple. All volatile components were removed *in vacuo*. The residue was redissolved in pentane to remove the side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide by addition of 1-(2,6-diisopropylphenyl)-3,3,5,5-tetramethylpyrrolidin-2-ylidene (CAAC^{Me}) and subsequent filtration. The addition of another equivalent of CAAC^{Me} led to the formation of a red solid. The removal of all volatiles *in vacuo* and subsequent washing with pentane resulted in the isolation of a crystalline orange-red solid (20.50 mg, 0.0372 mmol, 33%). Single crystals of **6a** suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated hexane solution at –30 °C.

¹H NMR (500 MHz, benzene-*d*₆): δ (ppm) = 7.06 (t, ³*J* = 7.75 Hz, 1H, dip-*p*-CH), 6.94 (d, ³*J* = 7.30 Hz, 1H, C7H), 6.89 (d, ³*J* = 7.75 Hz 2H, dip-*m*-CH), 6.82 (apparent dt, ³*J* = 7.30 Hz, 1H, C8H), 6.80 (d, ³*J* = 7.55 Hz, 1H, C10H), 6.28–6.25 (m, 1H, C19H), 3.08 (sept, ³*J* = 6.60 Hz, 2H, C(CH(CH₃)₂), 2.71–2.64 (m, 2H, C1(CH₂CH₃) and C4(CH₂CH₃); one hydrogen atom of CH₂, respectively), 2.59–2.49 (m, 6H, C1(CH₂CH₃) and C4(CH₂CH₃); one hydrogen atom of CH₂, respectively and C2(CH₂CH₃), C3(CH₂CH₃)), 2.39 (s, 3H, CH₃-*o*-Ar), 1.62 (s, 6H, C_{carbene}C(CH₃)₂), 1.47 (s, 2H, CH₂), 1.35 (t, ³*J* = 7.50 Hz, 6H, C2(CH₂CH₃), C3(CH₂CH₃)), 1.17 (d, ³*J* = 6.55 Hz, 6H, C(CH(CH₃)₂)), 1.08 (d, ³*J* = 6.60 Hz, 6H, C(CH(CH₃)₂)), 0.98–0.95 (m, 12H, NC(CH₃)₂ and C1(CH₂CH₃), C4(CH₂CH₃)). **¹¹B NMR** (160 MHz, benzene-*d*₆): δ (ppm) = –2.67. **¹³C NMR** (126 MHz, benzene-*d*₆): δ (ppm) = 242.2

(C_{carbene}), 157.2 (C1, C4), 156.8 (C1, C4), 151.5 (C2, C3), 146.3 (C5), 145.4 (C-*o*-dip), 141.6 (C6), 139.0 (C10), 138.8 (C-*i*-dip), 130.0 (C7), 129.7 (C-*p*-dip), 125.6 (C-*m*-dip), 122.3 (C8), 121.2 (C9), 77.6 (NC(CH₃)₂), 58.3 (C_{carbene}C(CH₃)₂), 53.0 (CH₂), 34.8 (C_{carbene}C(CH₃)₂), 29.7 (NC(CH₃)₂), 28.7 (C(CH(CH₃)₂), 26.3 (C1(CH₂CH₃), C4(CH₂CH₃)), 26.1 (C(CH(CH₃)₂), 24.9 (C(CH(CH₃)₂), 23.7 (CH₃-*o*-Ar), 21.3 (C2(CH₂CH₃), C3(CH₂CH₃)), 16.2 (C1(CH₂CH₃), C4(CH₂CH₃)), 14.7 (C2(CH₂CH₃), C3(CH₂CH₃)). **HRMS LIFDI** for [C₃₉H₅₈BN] = [M]: calcd. 551.4657; found 551.4648. **Elemental analysis** calcd. for C₃₉H₅₈BN [551.71 g/mol]: C 84.90, H 10.60, N 2.54%; found: C 83.90, H 10.57, N 2.47%.

NMR spectra of isolated compounds

Note: Additional small signals are observed in the NMR spectra of the boroles, indicating the presence of residual side products that were not completely removed during the workup of the reactions. These signals correspond to either aluminum dibromide or dimethyltin dihalide species. The captions of the NMR spectra also indicate the route (Al or Sn) by which the products were obtained.

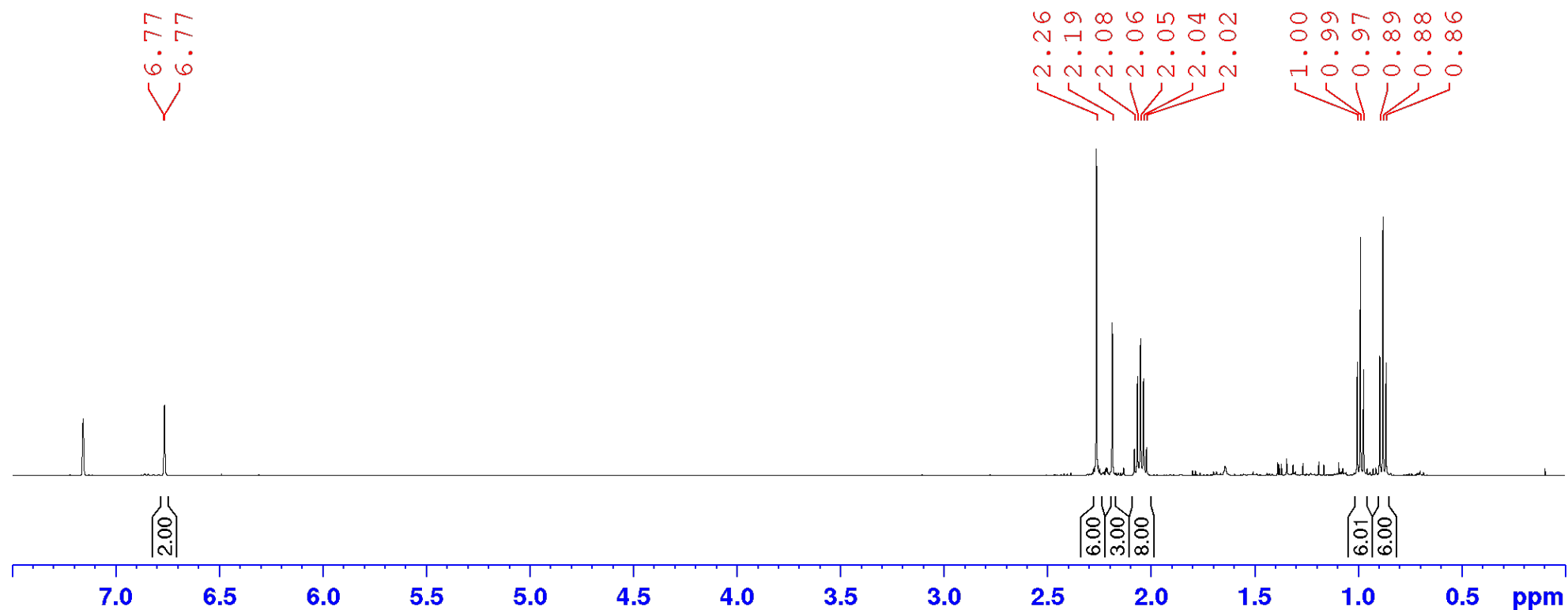


Figure S2. $^1\text{H}\{^{11}\text{B}\}$ NMR spectrum of **2** in C_6D_6 (Al route).

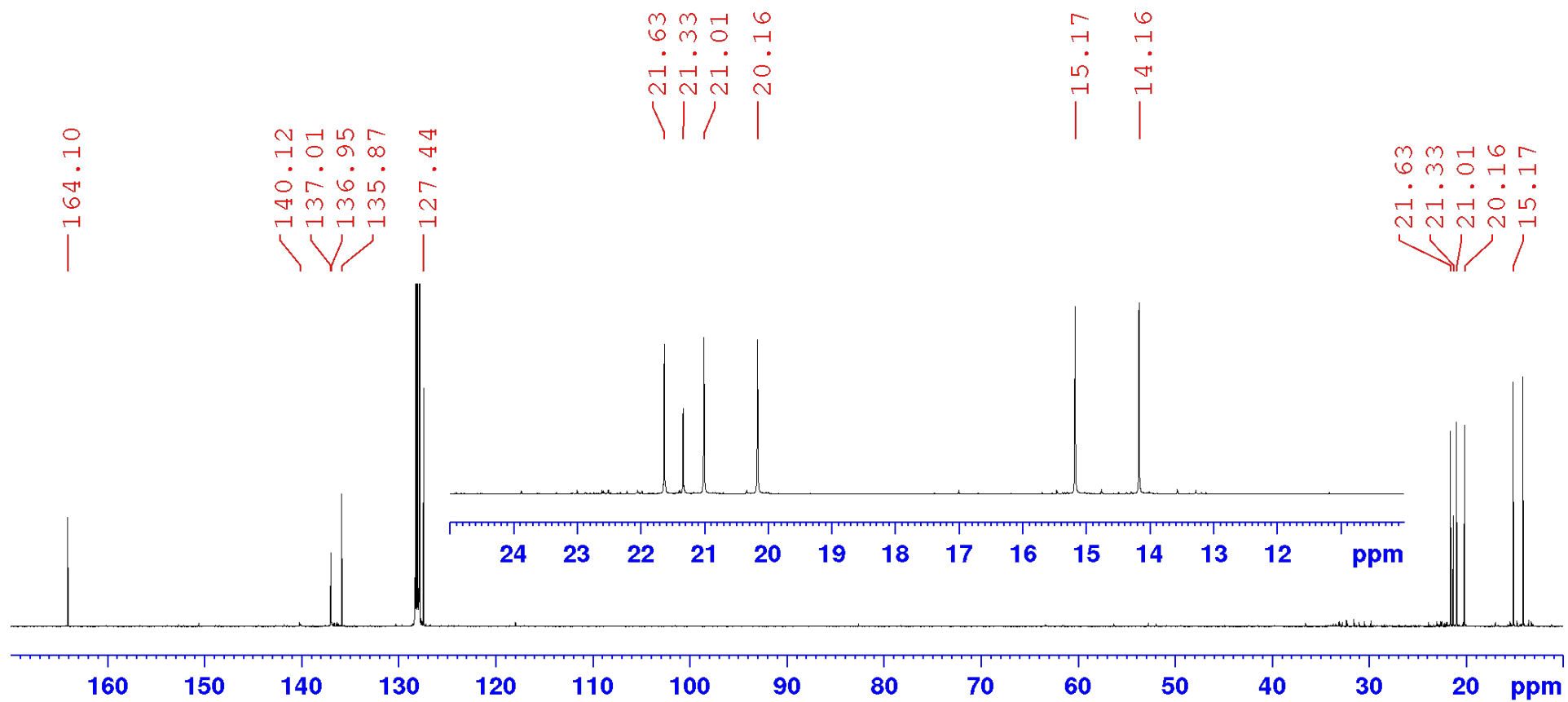


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 (Al route).

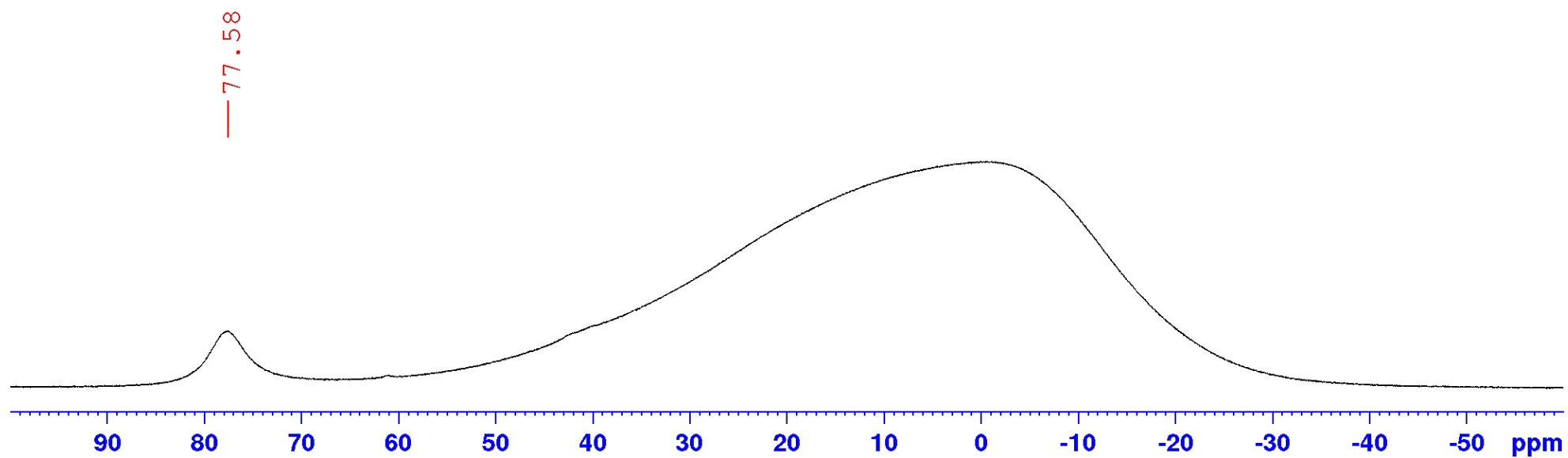


Figure S4. ^{11}B NMR spectrum of **2** in C_6D_6 (Al route).

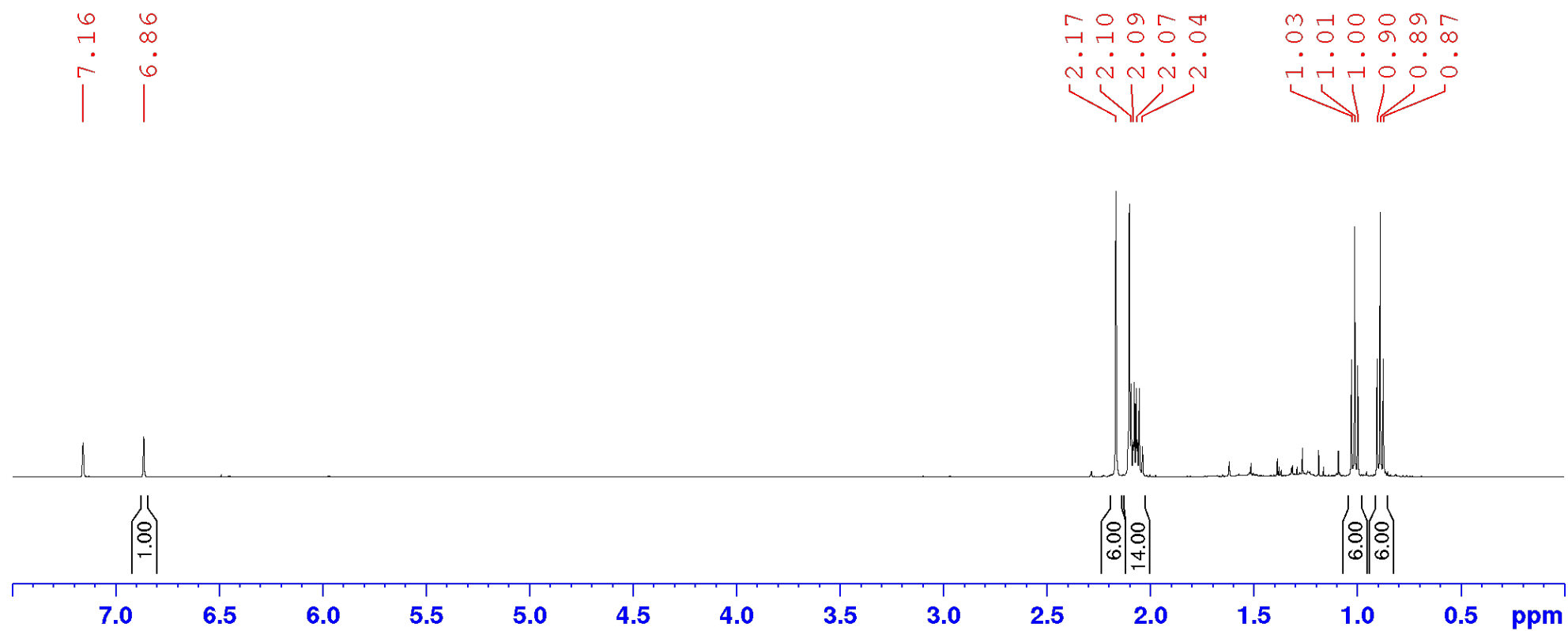


Figure S5. $^1\text{H}\{^{11}\text{B}\}$ NMR spectrum of **3** in C_6D_6 (Al route).

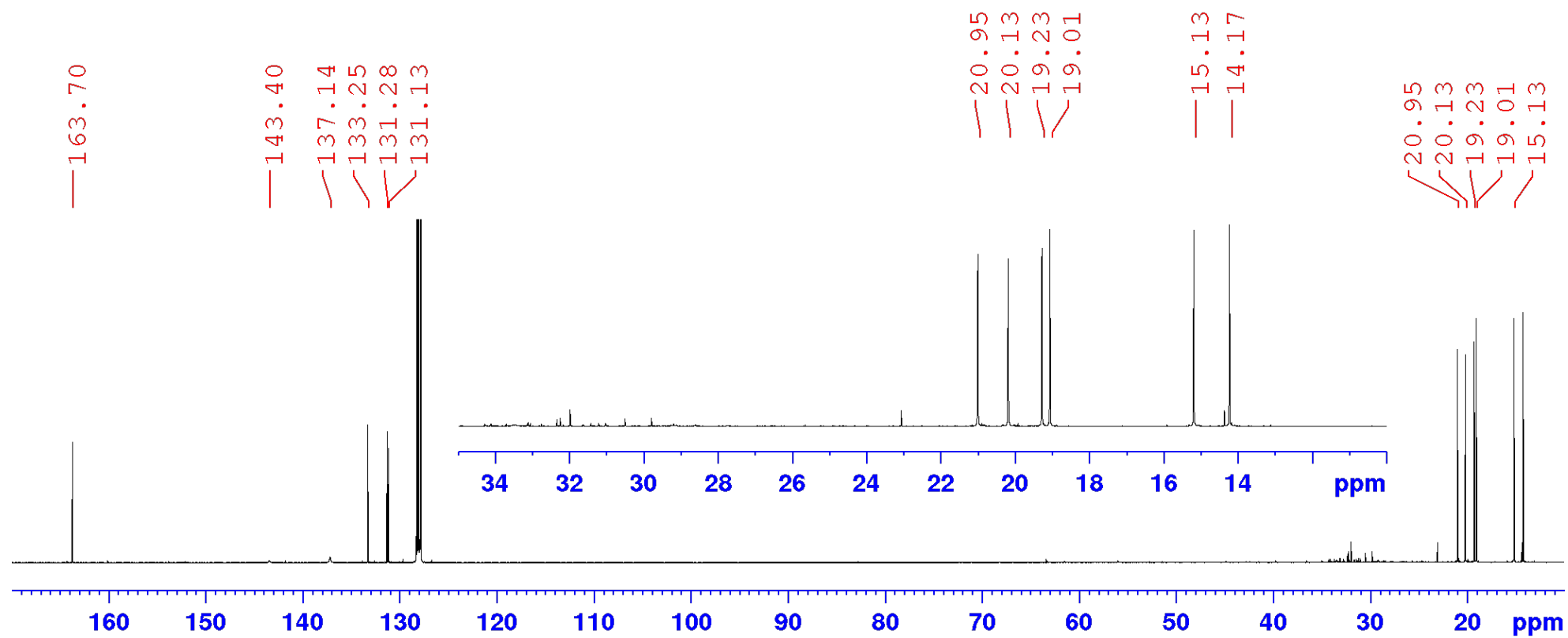


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6 (Al route).

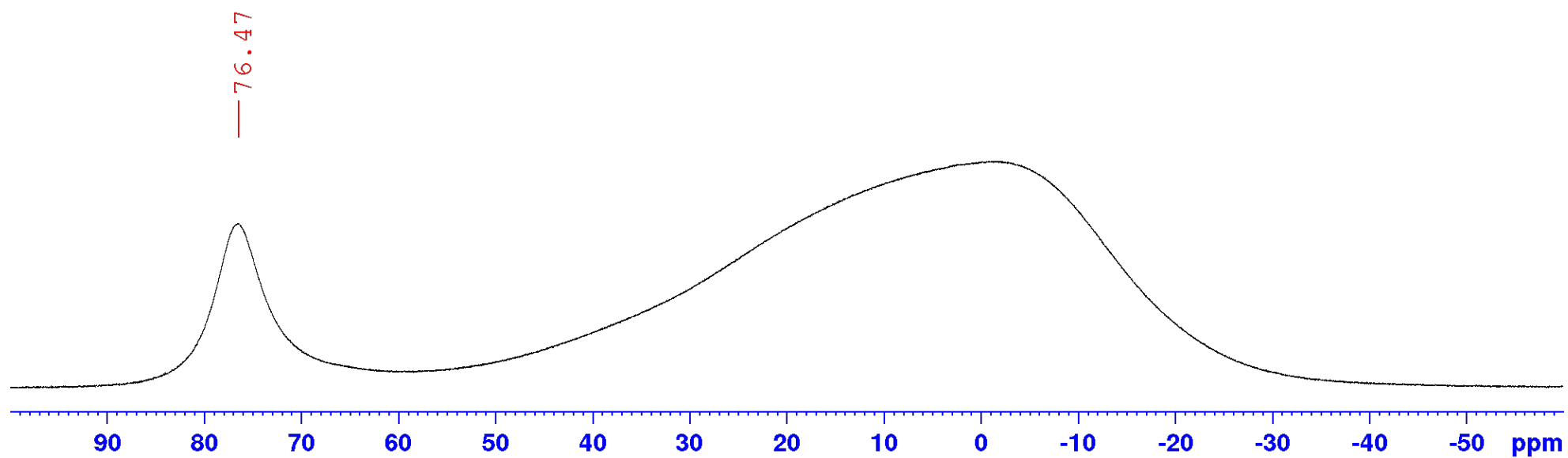


Figure S7. ^{11}B NMR spectrum of **3** in C_6D_6 (Al route).

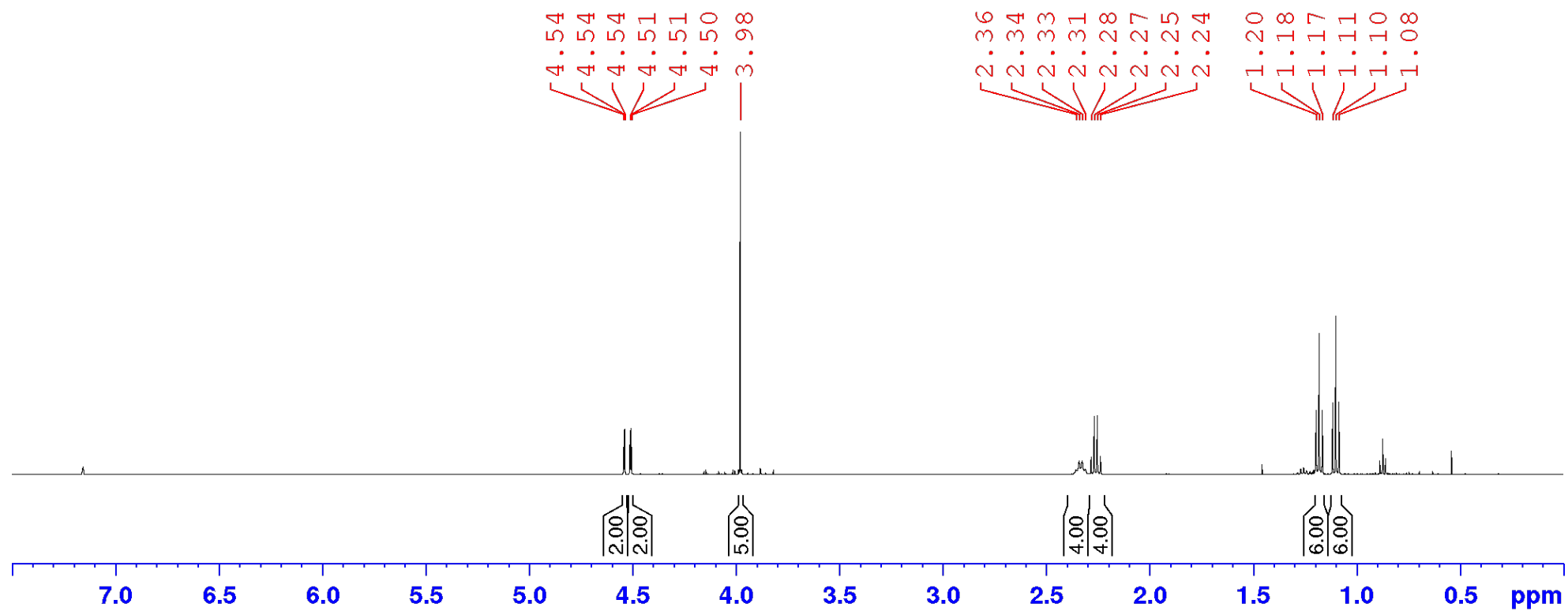


Figure S8. $^1\text{H}\{^{11}\text{B}\}$ NMR spectrum of **4** in C_6D_6 (Sn route).

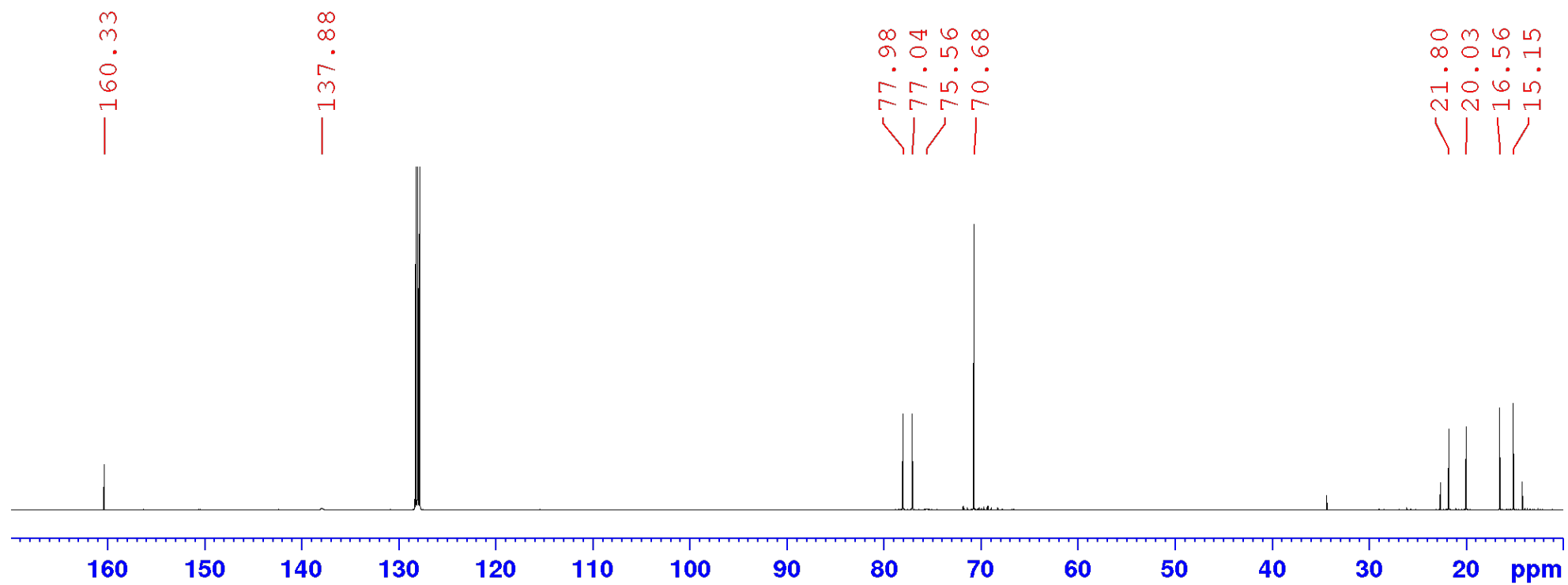


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4 in C_6D_6 (Sn route).

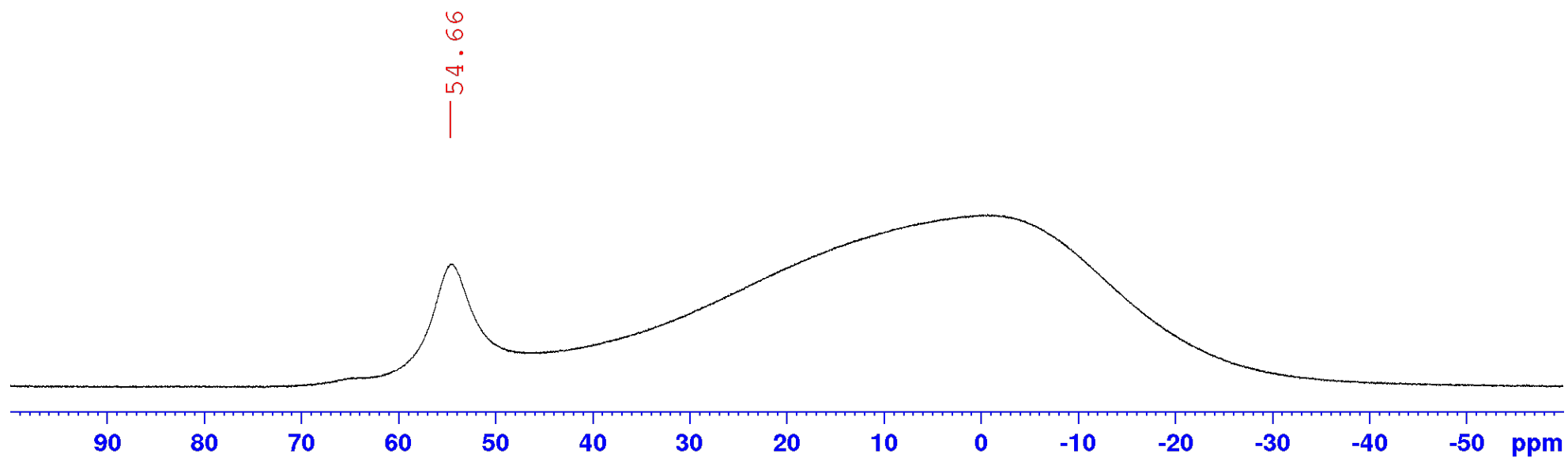


Figure S10. ^{11}B NMR spectrum of **4** in C_6D_6 (Sn route).

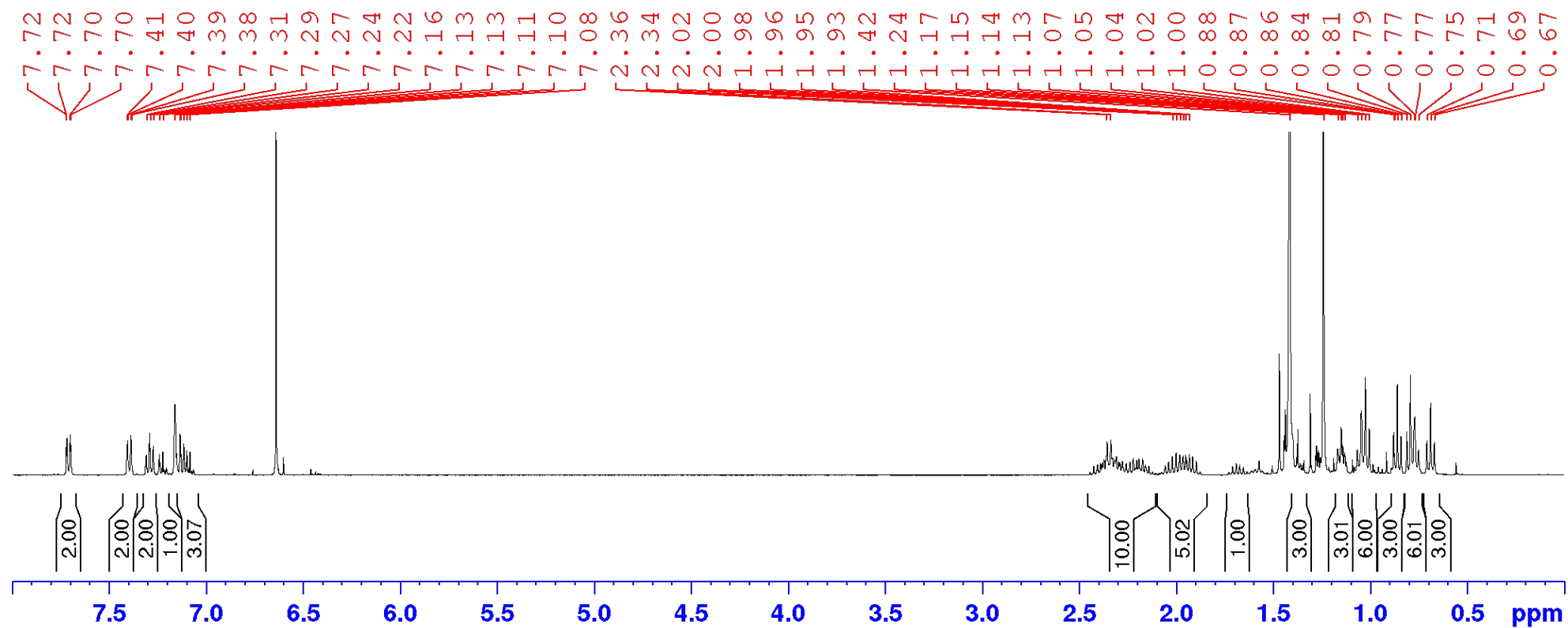


Figure S11. ^1H NMR spectrum of **5** in C_6D_6 . The peaks at $\delta(\text{ppm}) = 6.64$ (s, 2H, ArH), 1.42 (s, 18 H, $\text{C}(\text{CH}_3)_2(\text{CH}_3)$), and 1.24 (s, 9H, $\text{C}(\text{CH}_3)_2(\text{CH}_3)$) are due to the side product 1-(η^5 -1,2,4-tris(*tert*-butyl)cyclopentadienyl)aluminum dibromide (Al route).

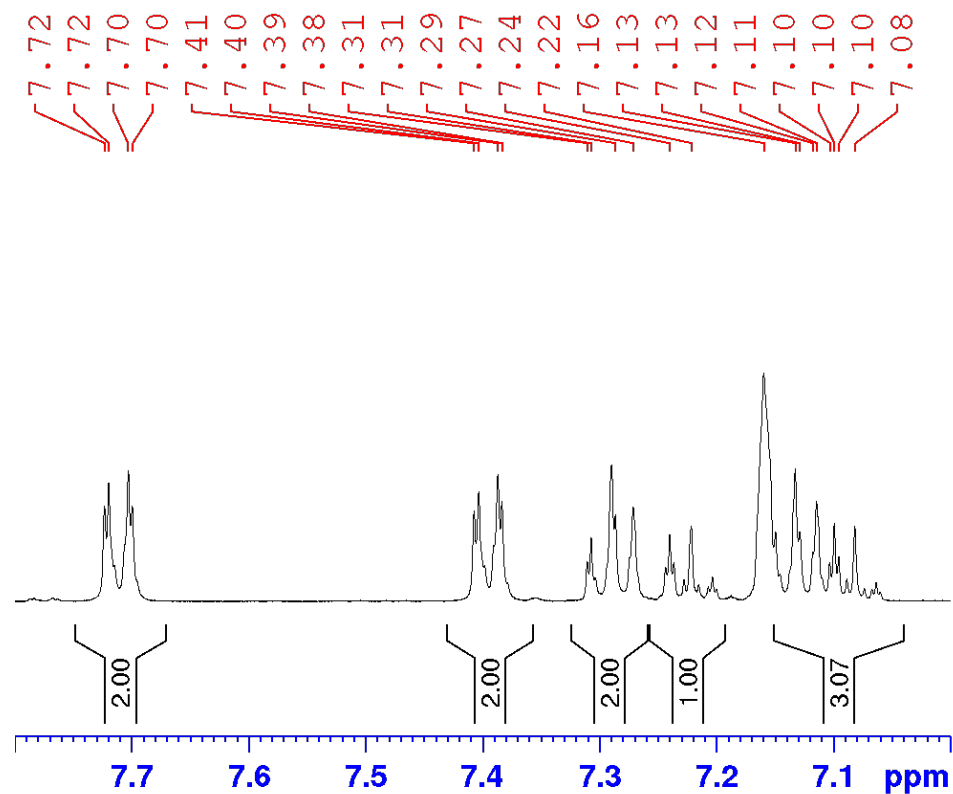


Figure S12. ^1H NMR spectrum of **5** in C_6D_6 with expansion of the aryl region (A1 route).

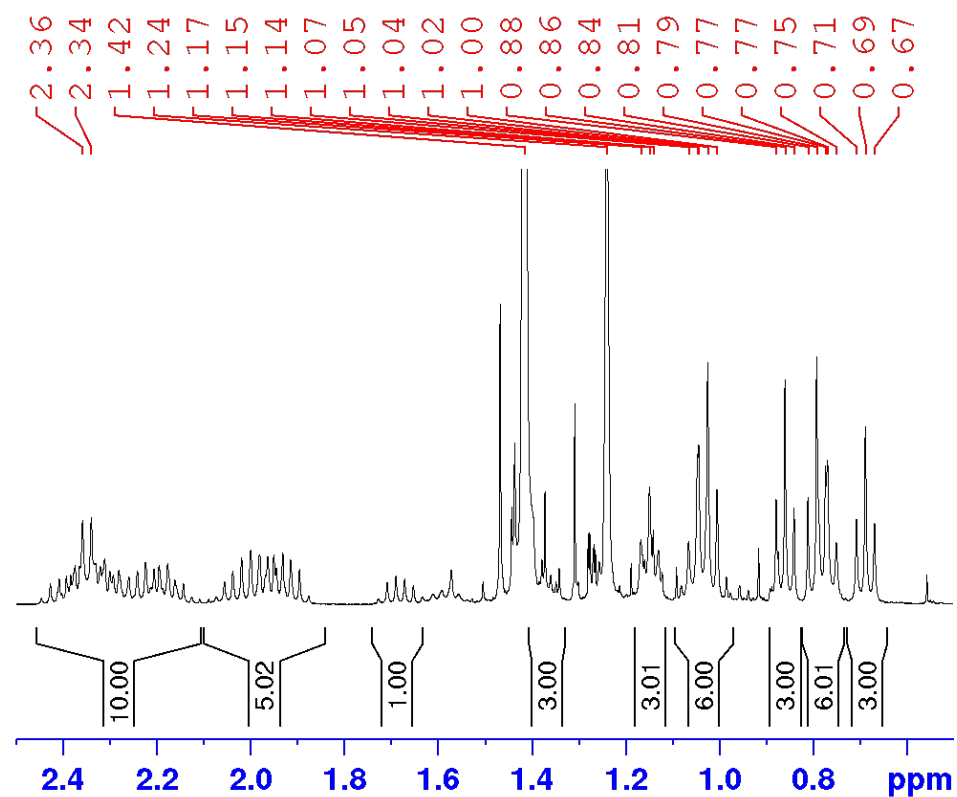


Figure S13. ^1H NMR spectrum of **5** in C_6D_6 with expansion of the aliphatic region (A1 route).

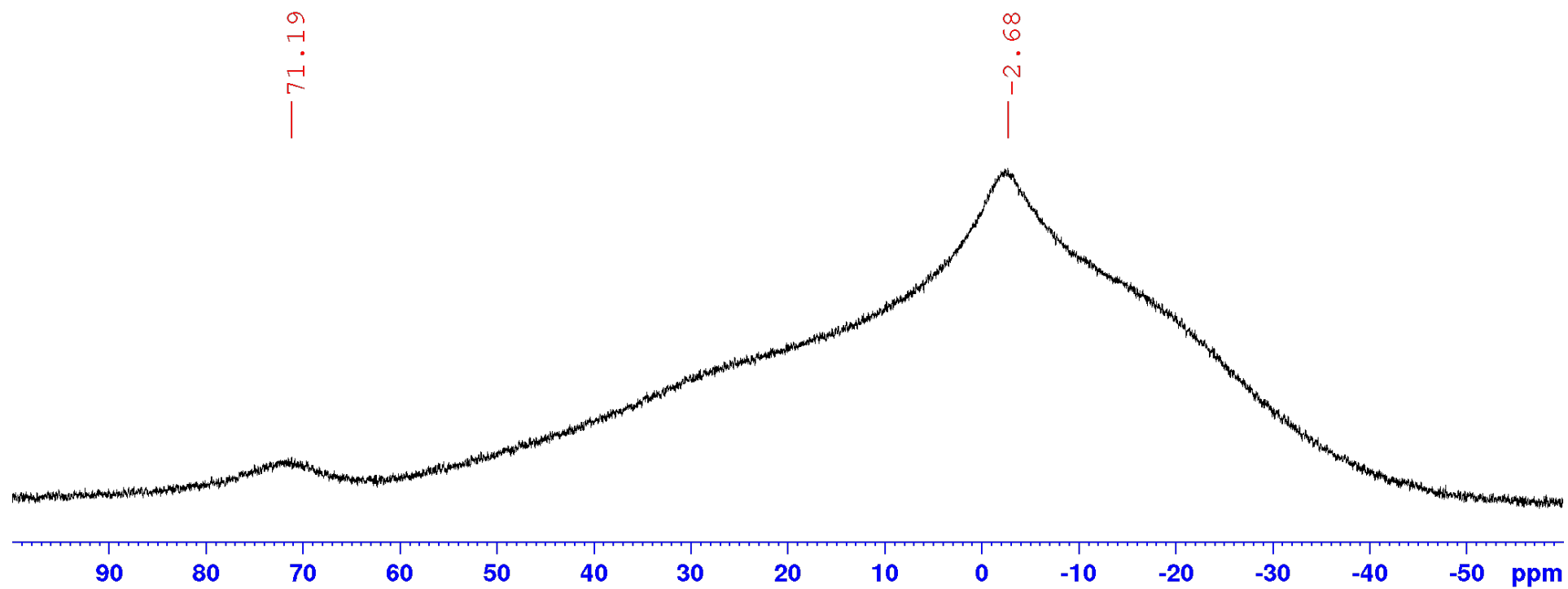


Figure S14. ^{11}B NMR spectrum of **5** in C_6D_6 (Al route).

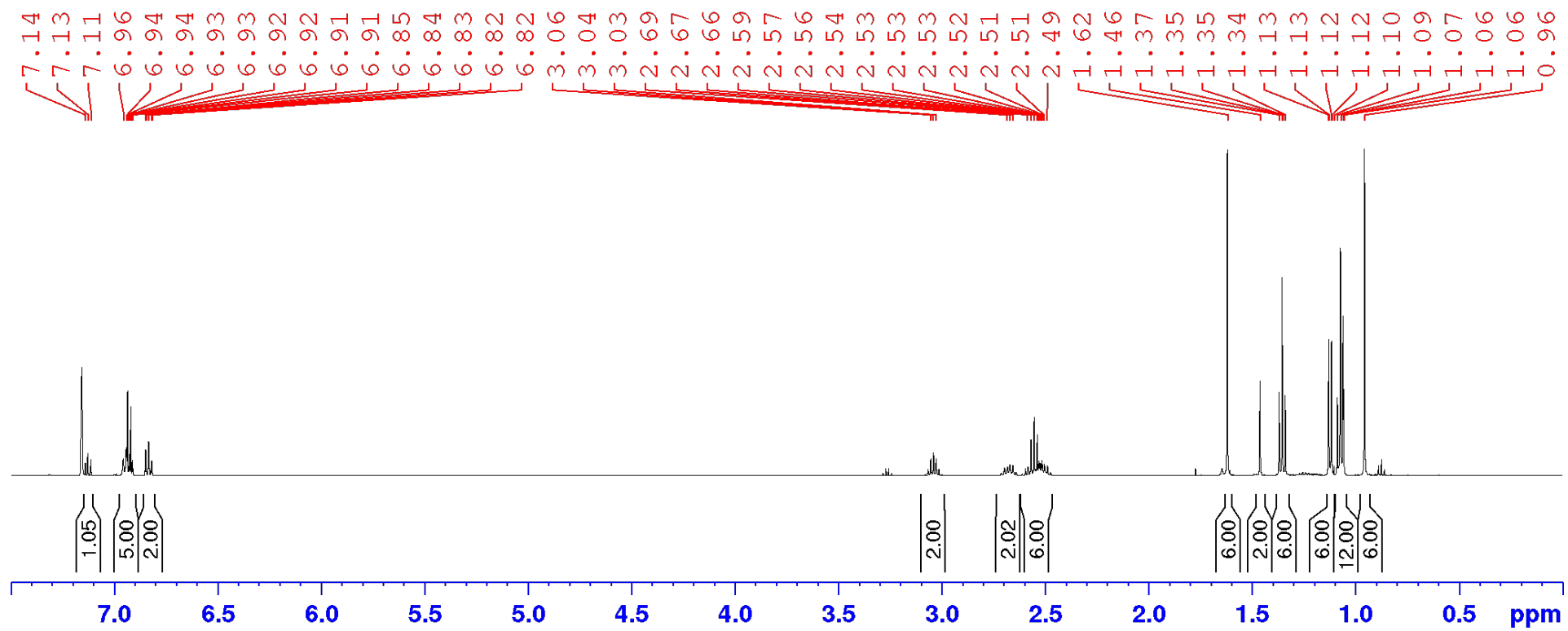


Figure S15. ^1H NMR spectrum of **5a** in C_6D_6 .

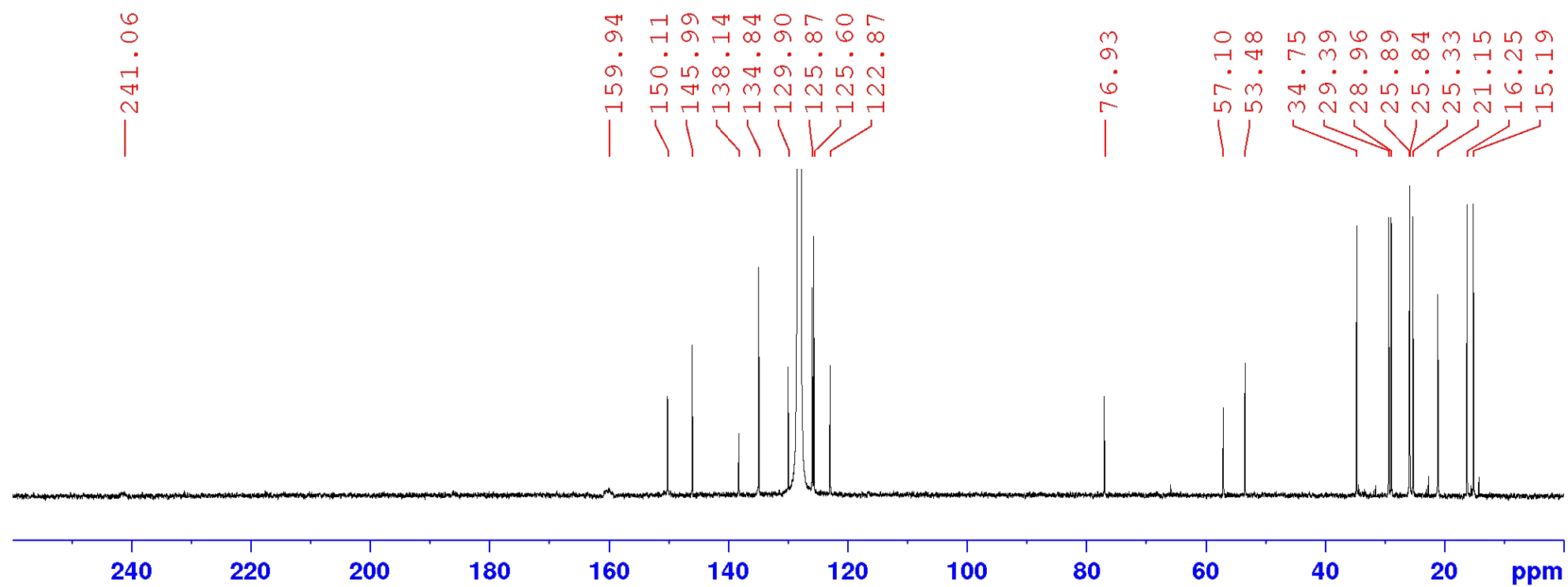


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5a** in C_6D_6 .

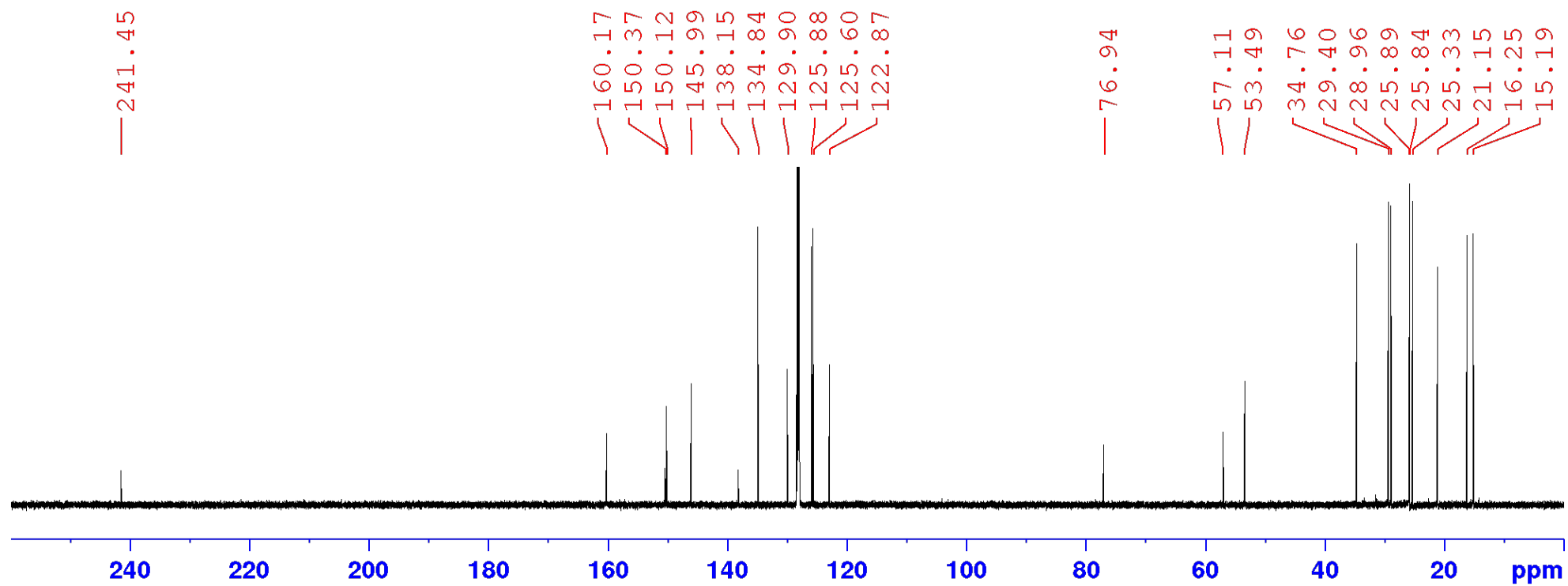


Figure S17. $^{13}\text{C}\{^1\text{H},^{11}\text{B}\}$ NMR spectrum of **5a** in C_6D_6 .

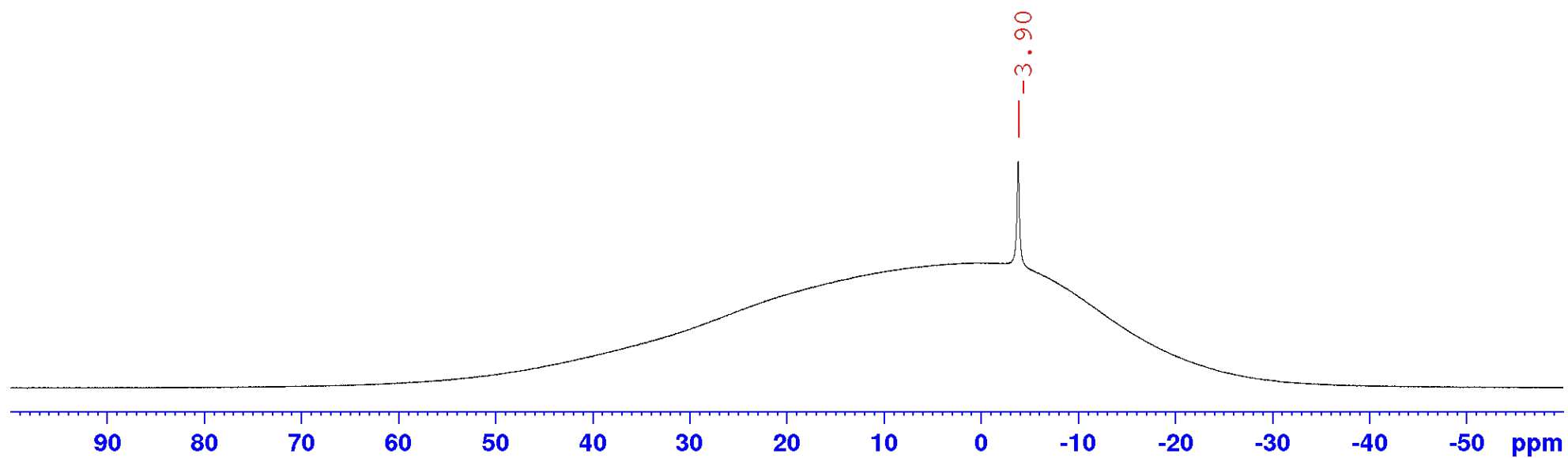


Figure S18. ^{11}B NMR spectrum of **5a** in C_6D_6 .

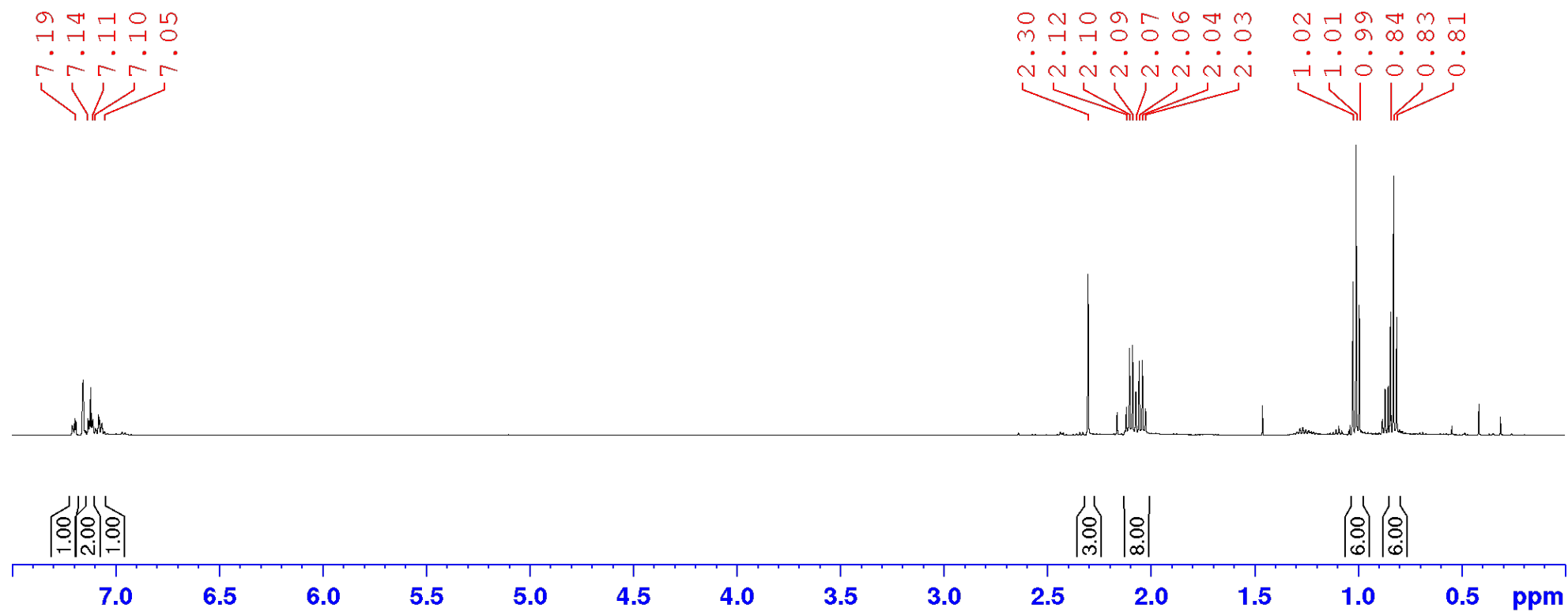


Figure S19. ^1H NMR spectrum of **6** in C_6D_6 at $70\text{ }^\circ\text{C}$ (Sn route).

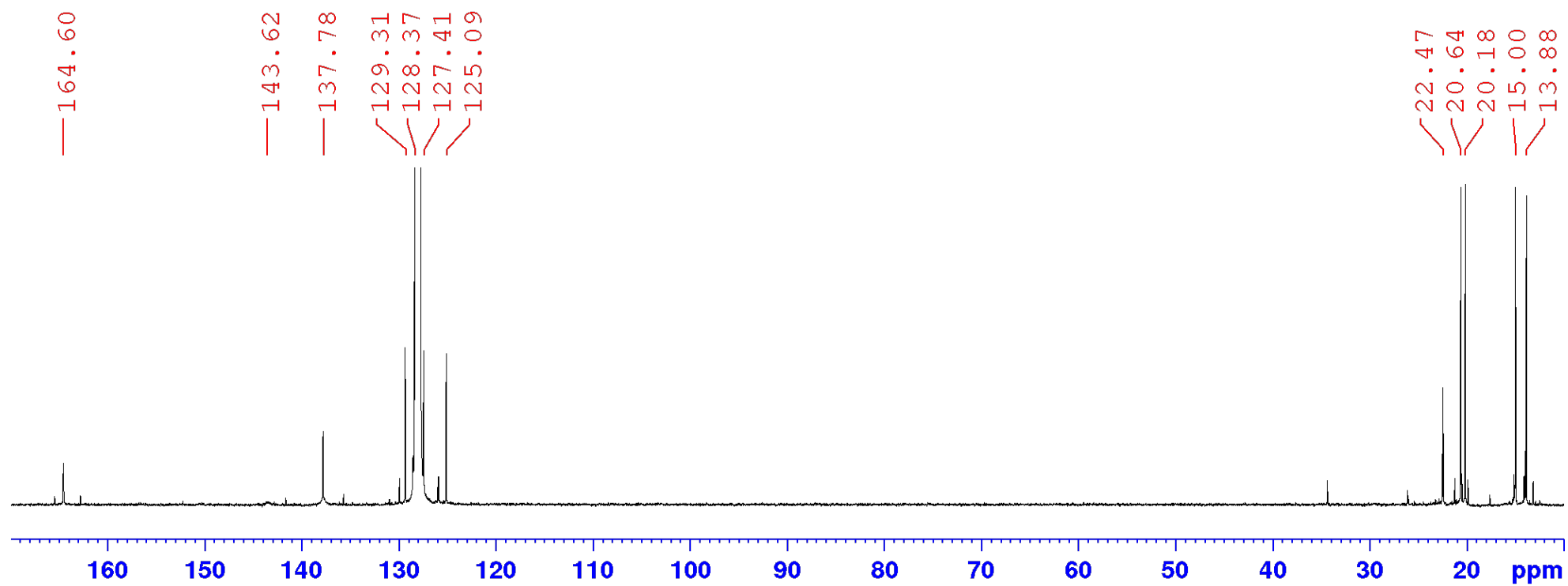


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** in C_6D_6 at $70\text{ }^\circ\text{C}$ (Sn route).

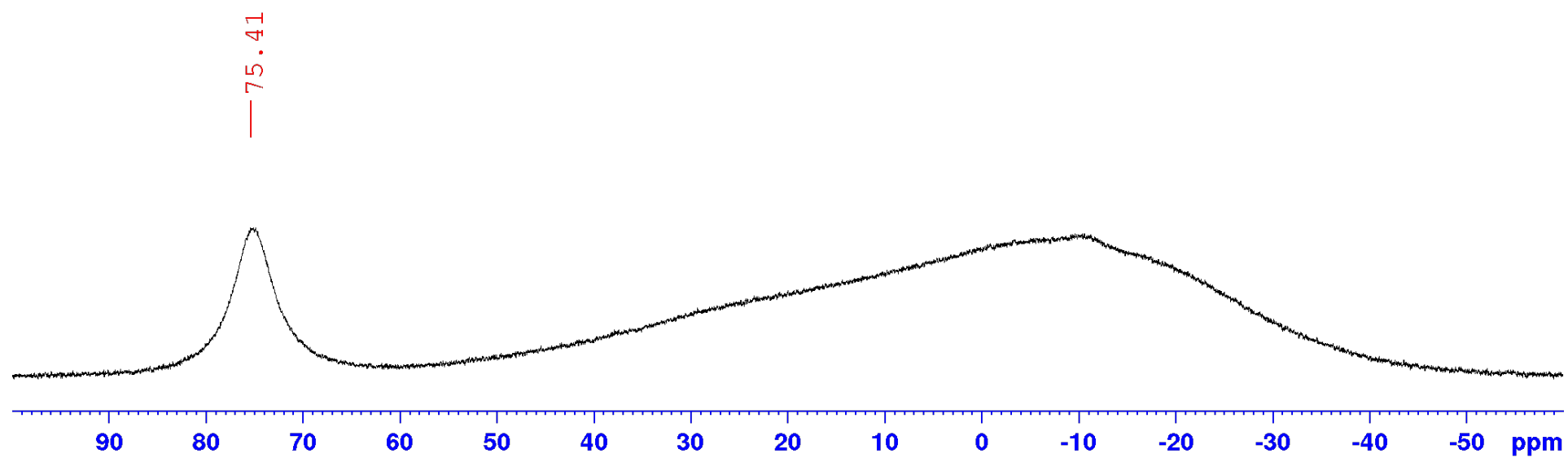


Figure S21. ^{11}B NMR spectrum of **6** in C_6D_6 at $70\text{ }^\circ\text{C}$ (Sn route).

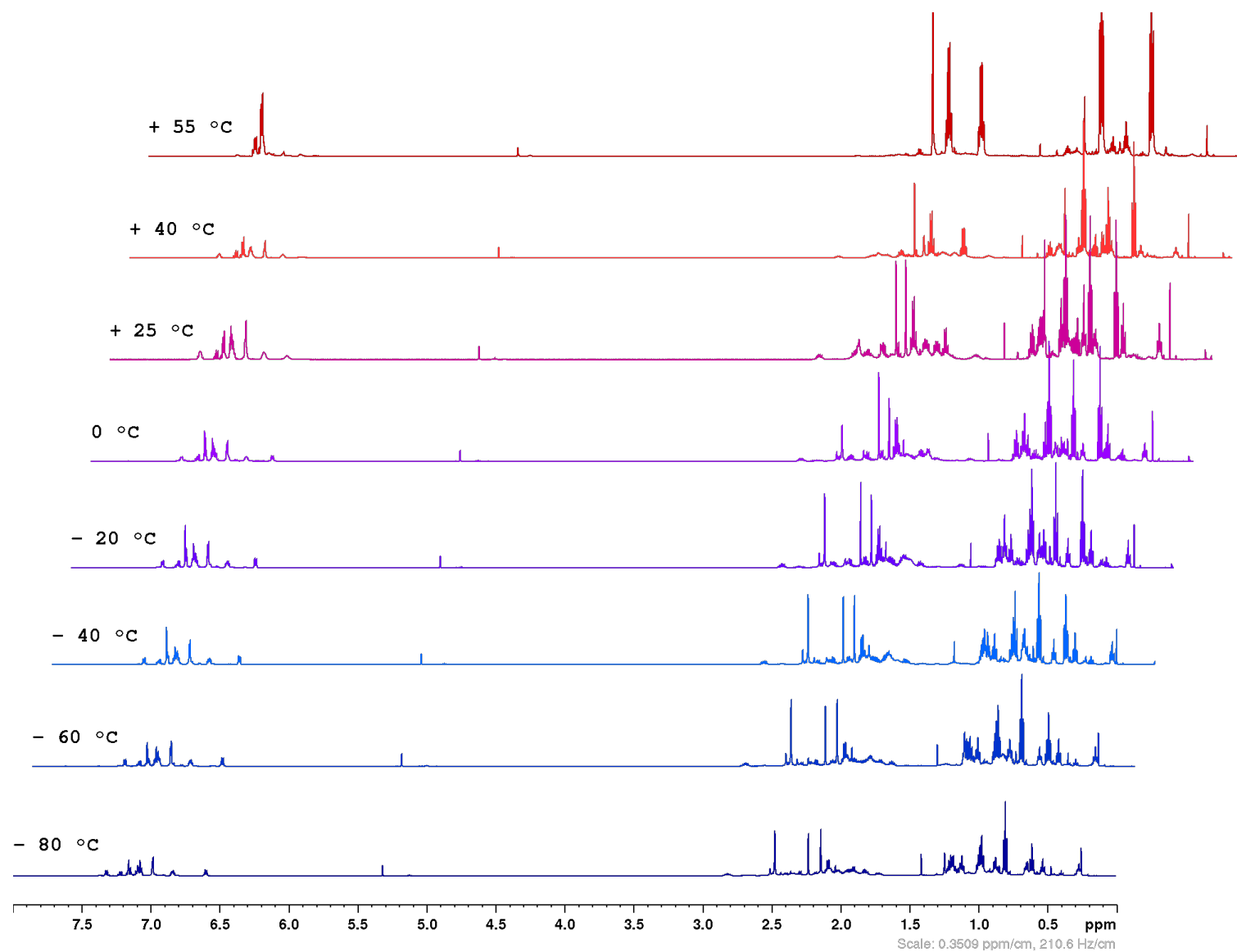


Figure S22. VT ¹H NMR of **6** in CD₂Cl₂ (Sn route).

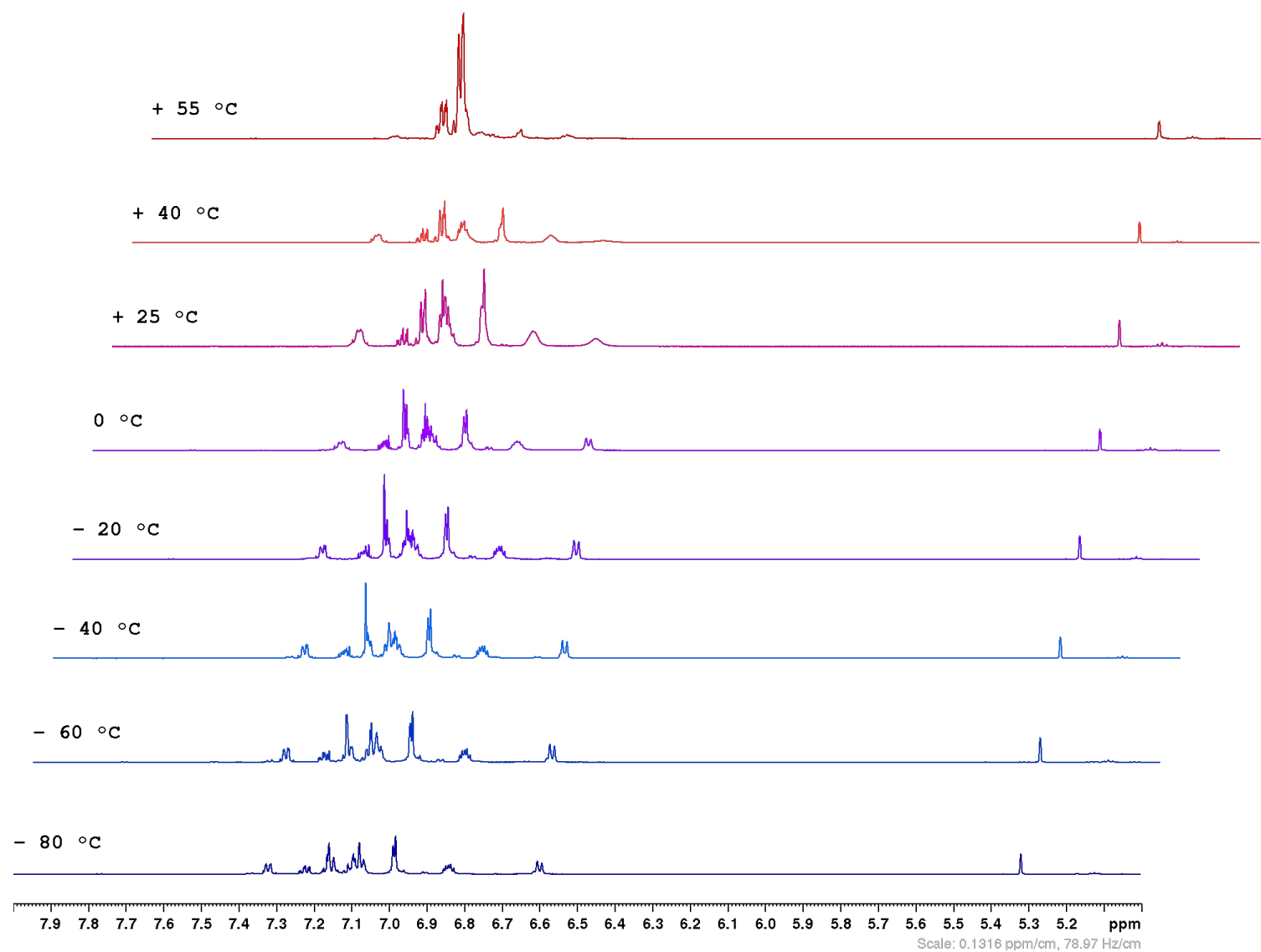


Figure S23. VT ¹H NMR of **6** in CD₂Cl₂ with expansion of the aryl region (Sn route).

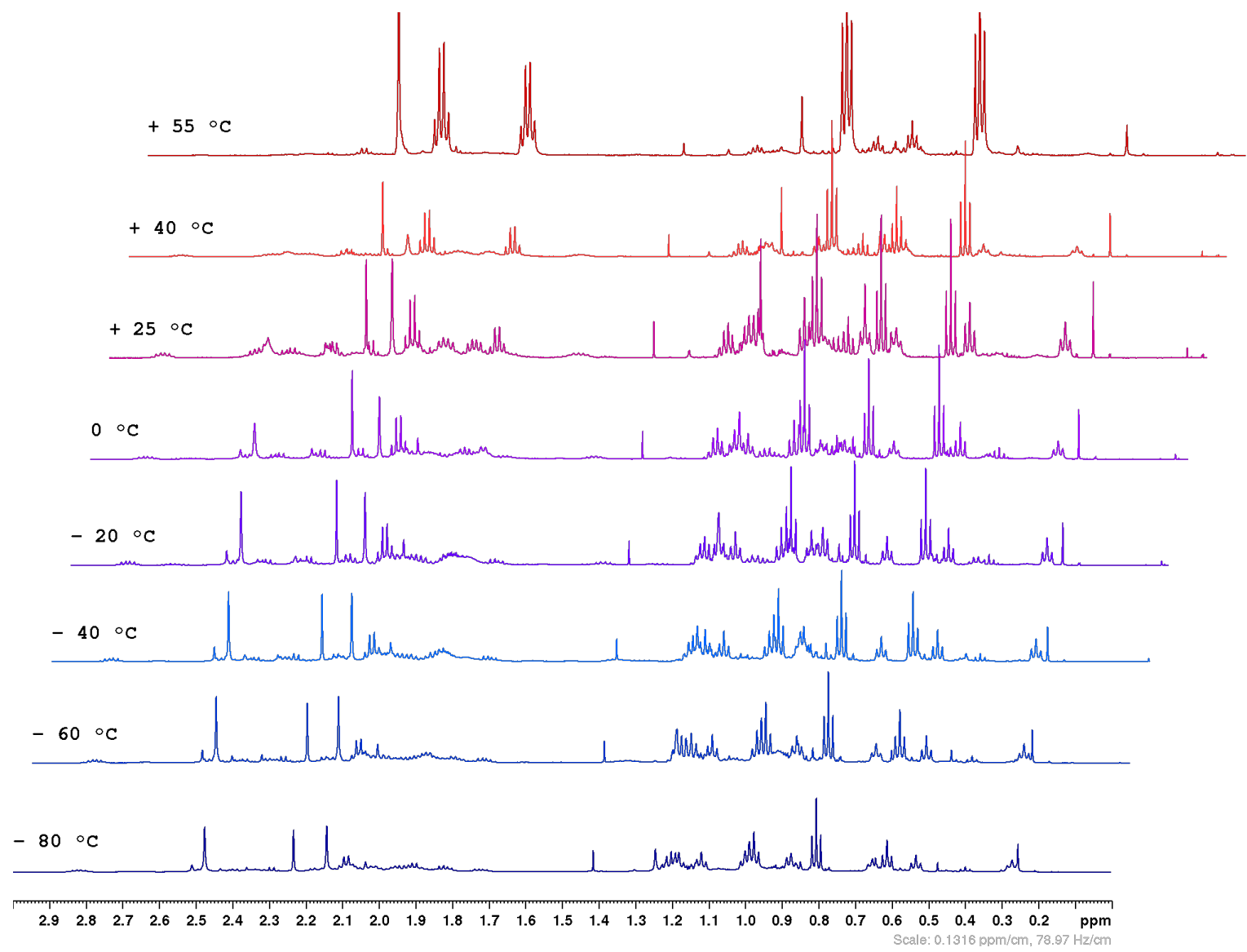


Figure S24. VT ¹H NMR of **6** in CD₂Cl₂ with expansion of the aliphatic region (Sn route)

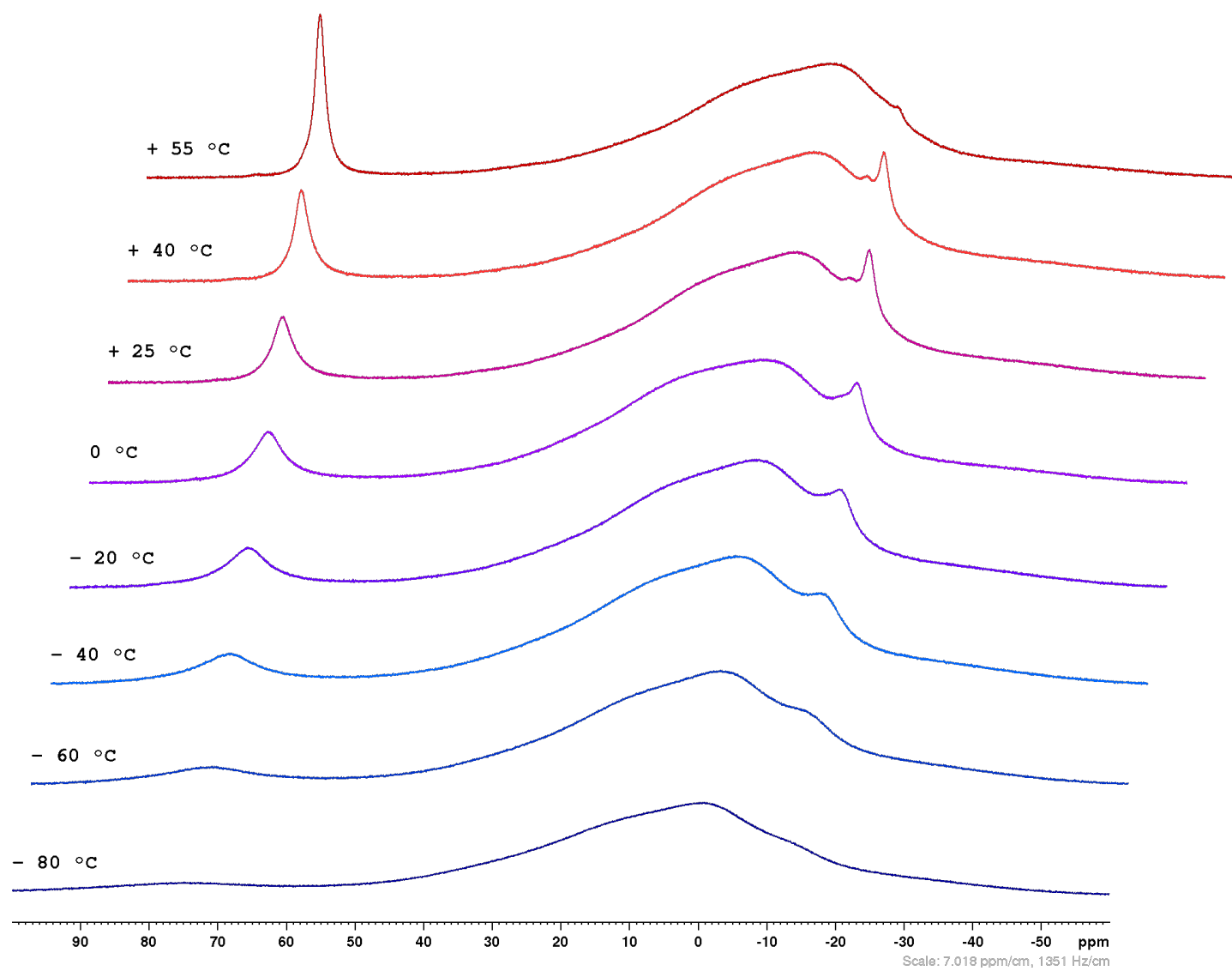


Figure S25. VT ^{11}B NMR of **6** in CD_2Cl_2 (Sn route).

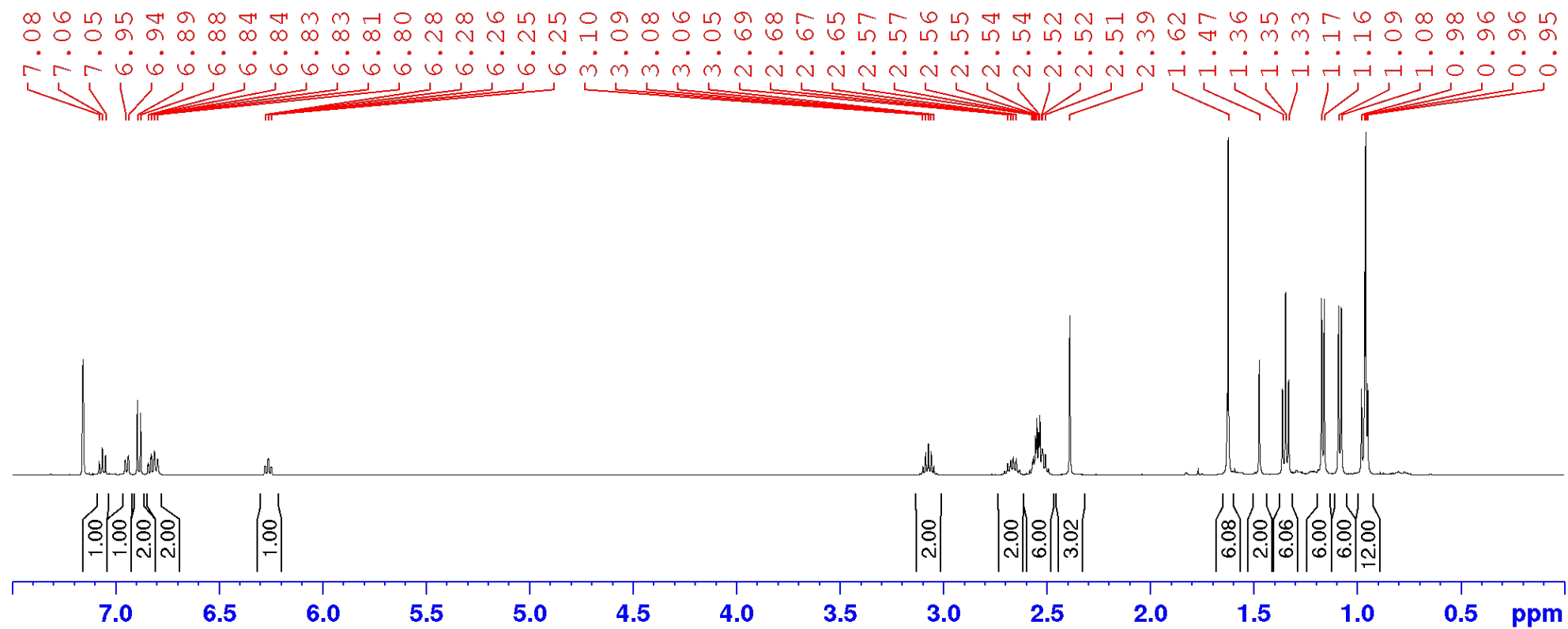


Figure S26. ^1H NMR spectrum of **6a** in C_6D_6 .

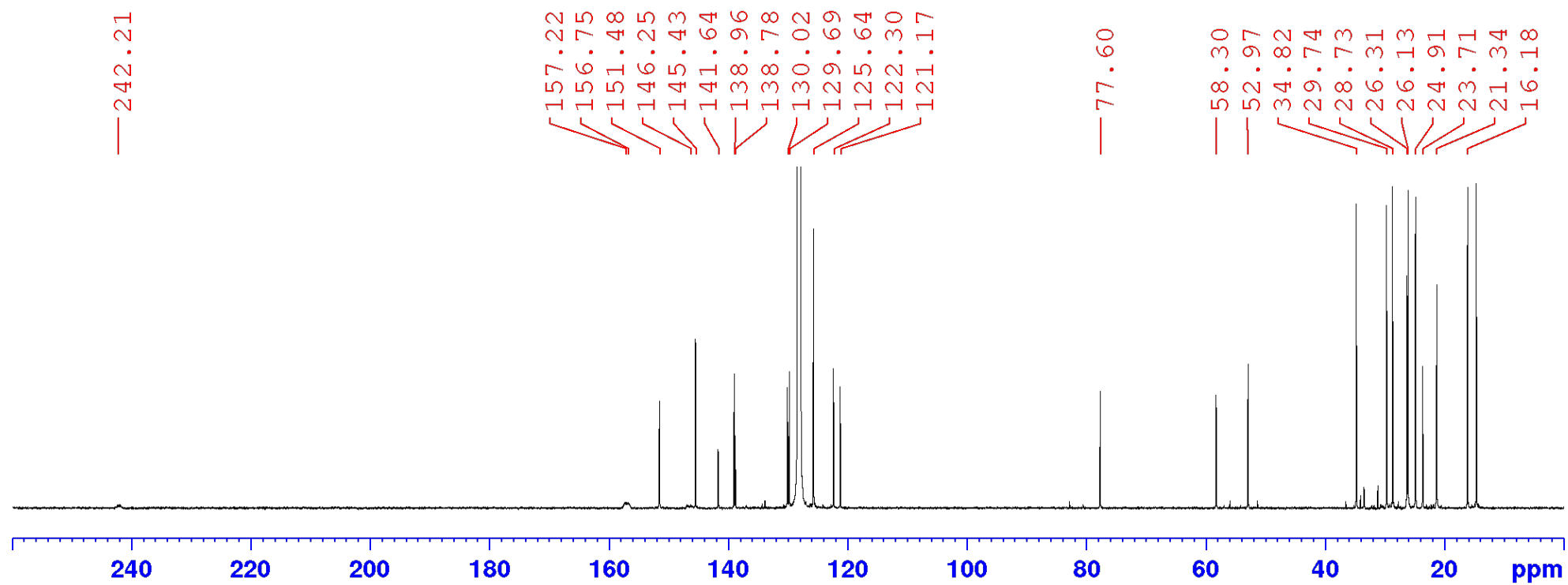


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6a** in C_6D_6 .

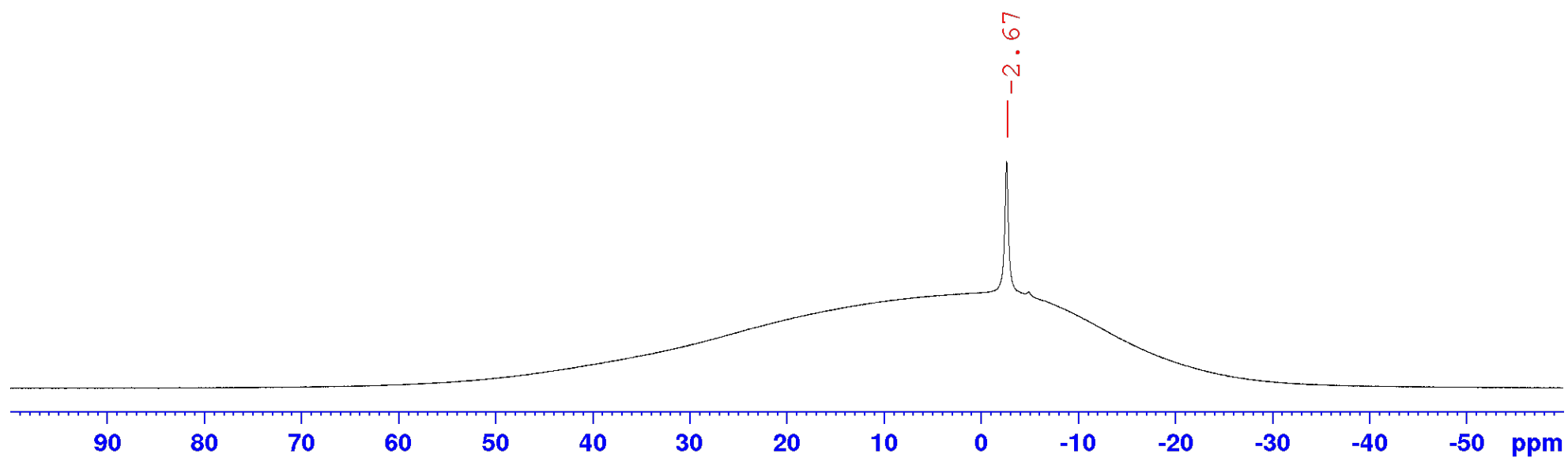


Figure S28. ^{11}B NMR spectrum of **6a** in C_6D_6 .

UV-vis spectra

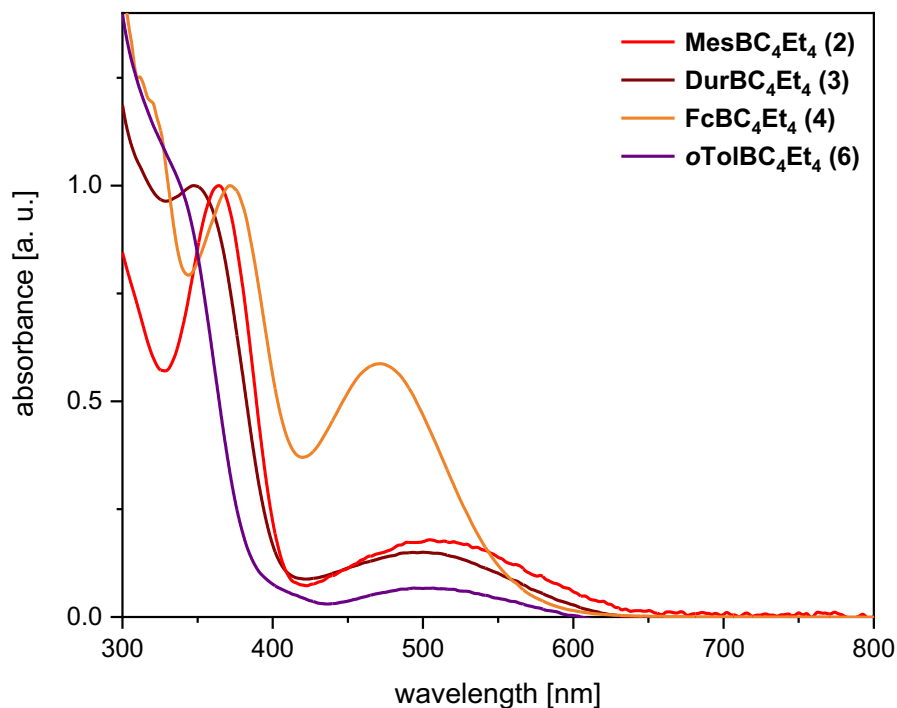


Figure S29. UV-vis absorption spectra of **2** (red), **3** (brown), **4** (orange), and **6** (purple) in DCM at 23 °C.

Table S1. Observed absorption wavelengths [nm] of **2**, **3**, **4** and **6**.

| compound | solvent | $\lambda_{\max(1)}$ | shoulder | $\lambda_{\max(2)}$ |
|----------|---------|---------------------|----------|---------------------|
| 2 | DCM | 505 | -- | 364 |
| 3 | | 500 | -- | 347 |
| 4 | | 472 | -- | 372 |
| 6 | | 507 | 337 | -- |

Cyclic voltammetry

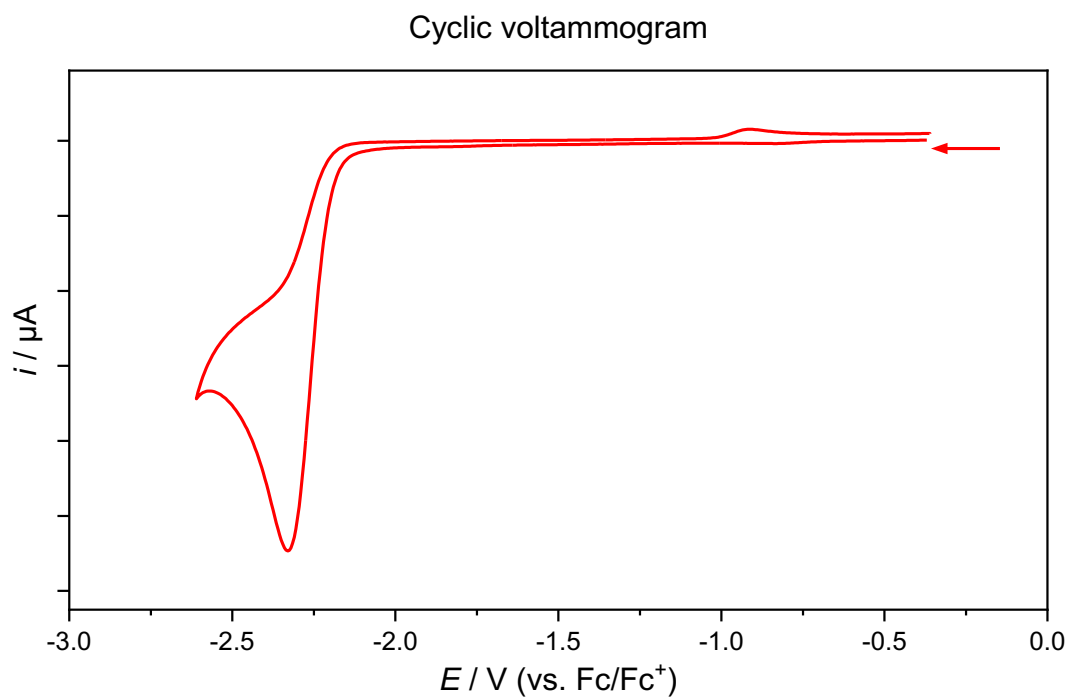


Figure S30. Cyclic voltammogram of **2** in DCM/0.1 M [*n*Bu₄N][PF₆] measured at 250 mV s⁻¹. Formal reduction potential: $E_{\text{pc}} = -2.33$ V.

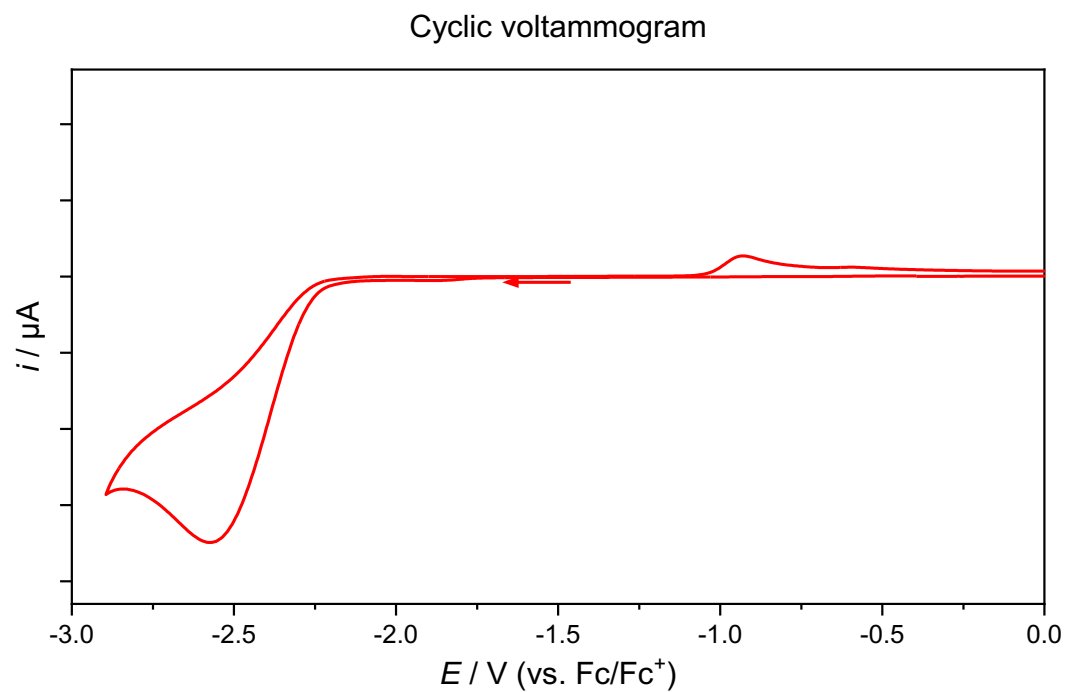


Figure S31. Cyclic voltammogram of **3** in DCM/0.1 M [*n*Bu₄N][PF₆] measured at 250 mV s⁻¹. Formal reduction potential: $E_{\text{pc}} = -2.57$ V.

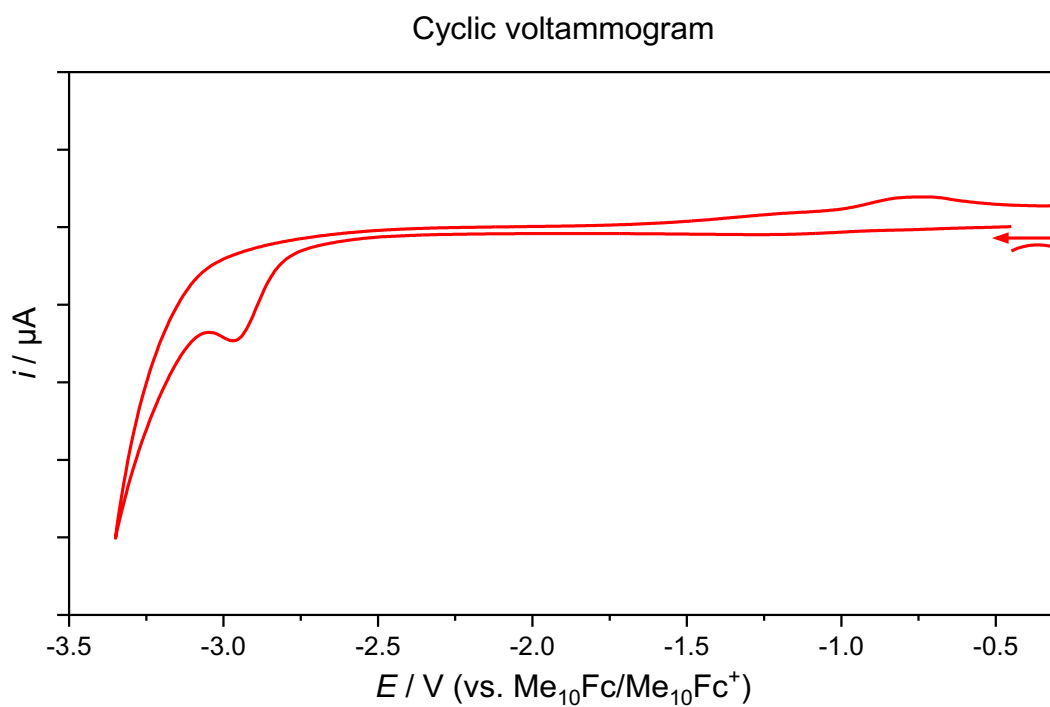


Figure S32. Cyclic voltammogram of **4** in THF/0.1 M [*n*Bu₄N][PF₆] measured at 250 mV s⁻¹. Formal reduction potential: $E_{pc} = -2.97$ V.

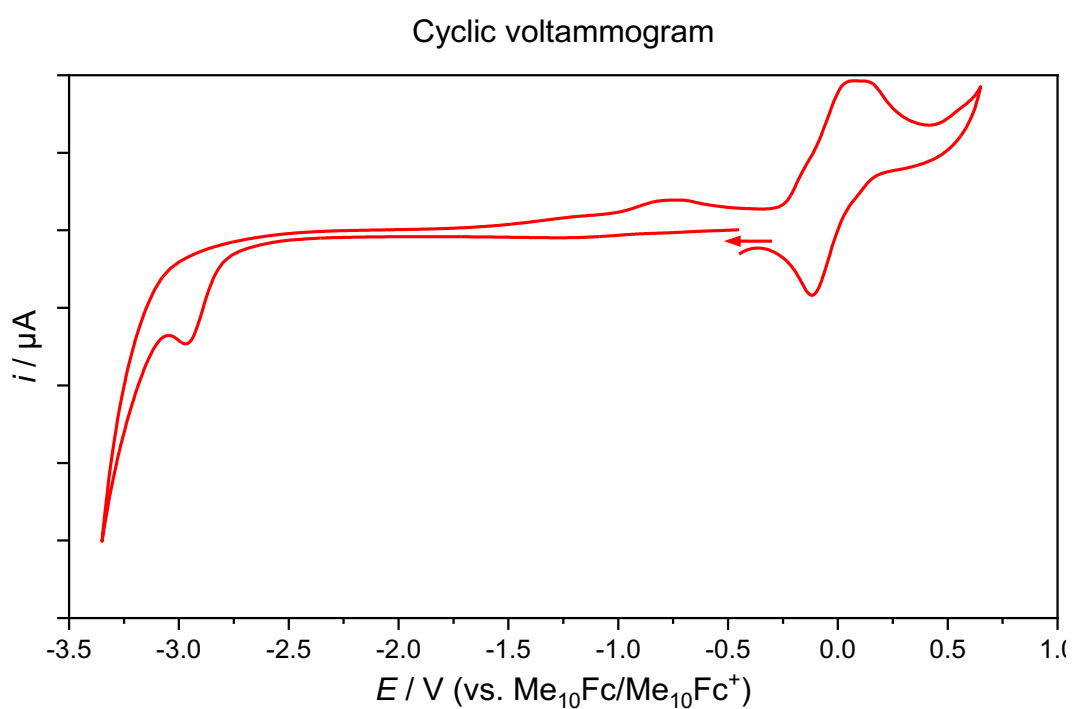


Figure S33. Cyclic voltammogram of **4** in THF/0.1 M [*n*Bu₄N][PF₆] measured at 250 mV s⁻¹ including the oxidation of the ferrocene unit ($E_{1/2} = \text{ca. } -0.02$ V).

X-ray crystallographic data

The crystal data of **3**, **5a** and **6a** were collected on a RIGAKU XTALAB SYNERGY-R diffractometer with a HPA area detector and multi-layer mirror monochromated $\text{Cu}_{K\alpha}$ radiation. The structure was solved using the intrinsic phasing method,¹⁰ refined with the SHELXL program¹¹ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically.

Refinement details for 3: The molecule was refined as disordered over the mirror plane with local symmetry switched off. The atomic displacement parameters of the atoms were restrained with the RIGU keyword in the ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list). The U_{ii} displacement parameters of all atoms positioned close to the symmetry plane were restrained with the ISOR keyword to approximate isotropic behavior. The atomic displacement parameters of atoms whose symmetry equivalents overlapped were constrained to the same volumes. The distances in the ethyl groups were restrained during refinement to the same value. To keep the axial position of the Br atom in the minor component of the disorder (duryl bromide is a 3% impurity) the 1--3 distances B-C(Dur) were restrained. ADPs of this atom were based on C4 of the duryl group and were kept constrained during refinement. Data were refined as a two-component twin. Twin-law was computed with CrystalsPro during indexing. Less than 1.5% of reflections were overlapping between both twin domains. The BASF parameter was refined to only 0.3%. However, using twin refinement improved the K statistic for weak reflections ($K = \text{mean}[F_o^2]/\text{mean}[F_c^2]$).

Crystal data for 3: $\text{C}_{22}\text{H}_{32.97}\text{BBr}_{0.03}$, $M_r = 310.66$, clear light red block, $0.070 \times 0.040 \times 0.020 \text{ mm}^3$, monoclinic space group $P2_1/m$, $a = 9.7239(7) \text{ \AA}$, $b = 9.0900(5) \text{ \AA}$, $c = 11.1927(8) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 97.359(7)^\circ$, $\gamma = 90^\circ$, $V = 981.18(12) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{calcd}} = 1.052 \text{ g}\cdot\text{cm}^{-3}$, $\mu = 0.488 \text{ mm}^{-1}$, $F(000) = 342$, $T = 100(2) \text{ K}$, $R_I = 0.1138$, $wR_2 = 0.2398$, 2030 independent reflections [$2\theta \leq 147.174^\circ$] and 197 parameters.

Crystal data for 5a: $\text{C}_{38}\text{H}_{56}\text{BN}$, $M_r = 537.64$, clear light orange block, $0.220 \times 0.120 \times 0.090 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 16.9907(2) \text{ \AA}$, $b = 10.55440(10) \text{ \AA}$, $c = 18.3576(2) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 96.4760(10)^\circ$, $\gamma = 90^\circ$, $V = 3271.00(6) \text{ \AA}^3$,

$Z = 4$, $\rho_{\text{calcd}} = 1.092 \text{ g}\cdot\text{cm}^{-3}$, $\mu = 0.448 \text{ mm}^{-1}$, $F(000) = 1184$, $T = 100(2) \text{ K}$, $R_I = 0.0507$, $wR_2 = 0.1110$, 6637 independent reflections [$2\theta \leq 150.716^\circ$] and 373 parameters.

Crystal data for 6a: $\text{C}_{39}\text{H}_{58}\text{BN}$, $M_r = 551.67$, clear orange block, $0.170 \times 0.080 \times 0.060 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 17.1660(2) \text{ \AA}$, $b = 10.52710(10) \text{ \AA}$, $c = 18.3364(2) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 96.4030(10)^\circ$, $\gamma = 90^\circ$, $V = 3292.87(6) \text{ \AA}^3$, $Z = 4$, $\rho_{\text{calcd}} = 1.113 \text{ g}\cdot\text{cm}^{-3}$, $\mu = 0.457 \text{ mm}^{-1}$, $F(000) = 1216$, $T = 100(2) \text{ K}$, $R_I = 0.0440$, $wR_2 = 0.1016$, 6242 independent reflections [$2\theta \leq 140.14^\circ$] and 383 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-2263083 (**3**), CCDC-2263084 (**5a**), and CCDC-2263085 (**6a**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Computational details

All calculations were done using the Gaussian 16, Revision C.01¹² quantum chemistry program package. Geometry optimizations for the closed-shell singlet and the triplet states of MesBC₄Et₄ (**2**) and MesBC₄Ph₄ were performed at the (U)PBE0-D3(BJ)¹³⁻¹⁶/6-31+G(d,p)¹⁷⁻²⁴ 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. The vertical and adiabatic singlet-triplet energy gaps were obtained at the (U)PBE0-D3(BJ)/6-311+G(d,p)²⁵⁻²⁶ level of theory (see Table S2).

To assess the aromaticity character of the systems, calculations of the nucleus-independent chemical shift (NICS)²⁷⁻²⁹ at the PBE0-D3(BJ)/6-311+G(d,p) level of theory were performed. These were accomplished by using the gauge-independent atomic orbital (GIAO)³⁰⁻³² method. The corresponding values were obtained by placing dummy atoms in the centers of BC₄ rings and at distances of 0.1 Å along the axis perpendicular to the ring centers (see Table S3). For the NICS_{zz} scan, the zz component of the magnetic shielding tensor was used (see Figure S34).³³ Furthermore, the anisotropy of the induced current density (ACID)³⁴⁻³⁵ method at the PBE0-D3(BJ)/6-311+G(d,p) level of theory was used to further confirm and support the results (see Figure S35). For this only the relevant π -orbitals were considered.

To analyze the bonding situations in the different systems, the Wiberg bond indices (WBIs)³⁶ and the Mayer bond order (MBOs)³⁷ as well as natural bond orbital (NBO)³⁸ charges were obtained at the PBE0-D3(BJ)/6-311G(d,p) level of theory (see Table S4). For the former two the Multiwfn 3.8³⁹ tool was used and for the last the NBO 7³⁸ program package.

The frontier orbitals are plotted in Figure S36 and their energetic level is given at the PBE0-D3(BJ)/6-311+G(d,p)/SMD(benzene) level of theory. For graphic representation GaussView 6.0.16⁴⁰ was used.

Table S2. Vertical and adiabatic singlet-triplet energy gaps of MesBC₄Et₄ and MesBC₄Ph₄ at the (U)PBE0-D3(BJ)/6-311+G(d,p) level of theory.

| | MesBC ₄ Et ₄ | MesBC ₄ Ph ₄ |
|-------------------------------|------------------------------------|------------------------------------|
| Vertical singlet-triplet gap | 32.5 kcal mol ⁻¹ | 25.8 kcal mol ⁻¹ |
| Adiabatic singlet-triplet gap | 16.3 kcal mol ⁻¹ | 13.0 kcal mol ⁻¹ |

Table S3. NICS and NICS_{zz} values of MesBC₄Et₄ and MesBC₄Ph₄ at the (U)PBE0-D3(BJ)/6-311+G(d,p) level of theory.

| | MesBC ₄ Et ₄ | MesBC ₄ Ph ₄ |
|----------------------------|------------------------------------|------------------------------------|
| NICS(0) | 16.38 ppm | 14.75 ppm |
| NICS(-1/+1) | 8.66 / 9.01 ppm | 8.00 / 8.00 ppm |
| NICS _{zz} (0) | 59.10 ppm | 52.50 ppm |
| NICS _{zz} (-1/+1) | 32.76 / 33.20 ppm | 27.74 / 27.76 ppm |

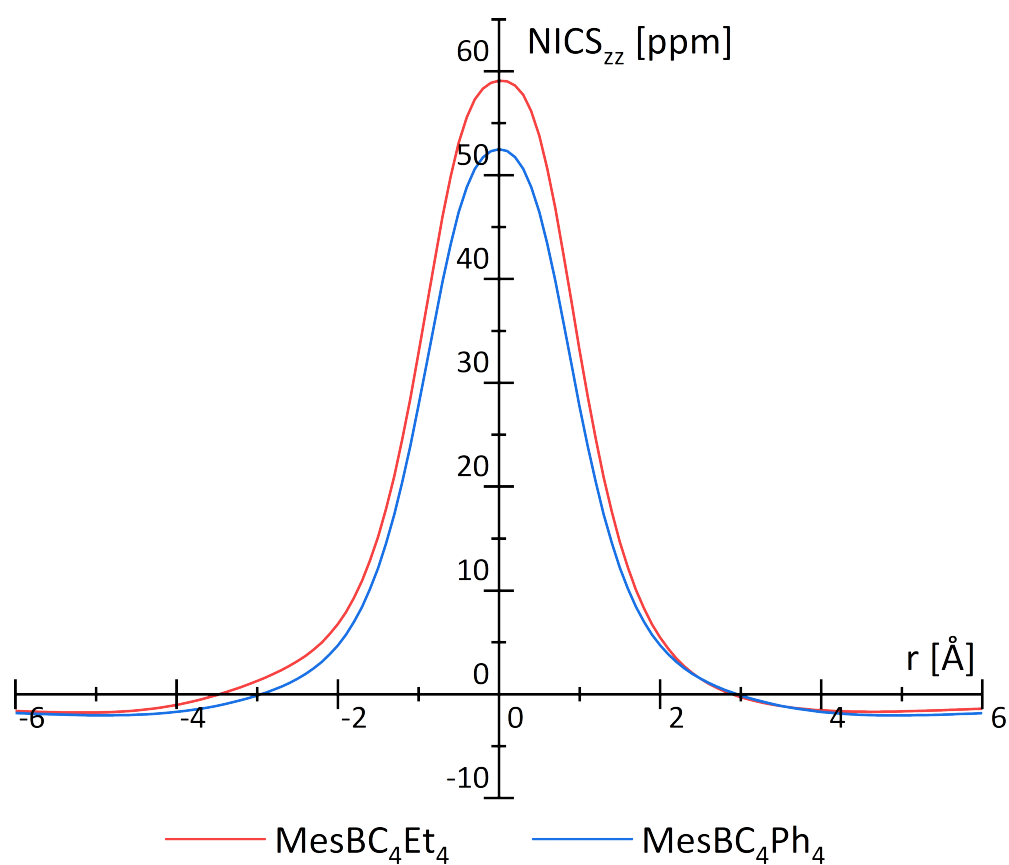


Figure S34. NICS_{zz} scans of MesBC₄Et₄ and MesBC₄Ph₄.

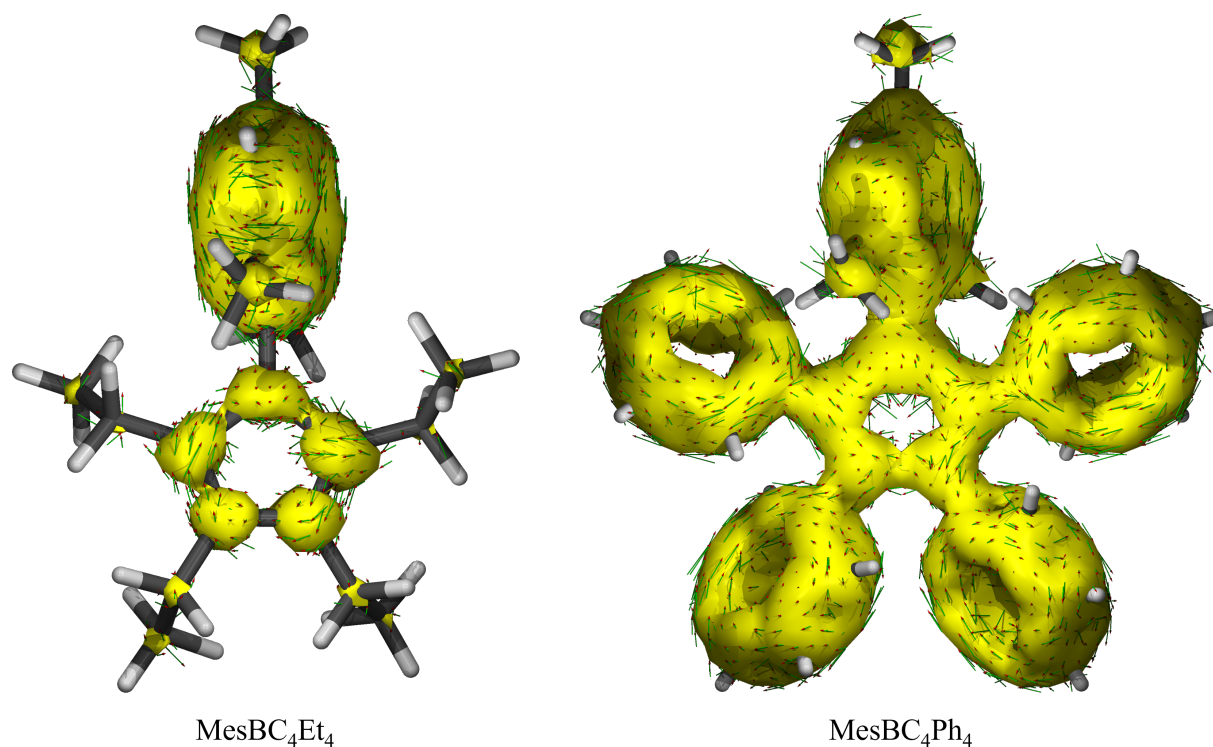
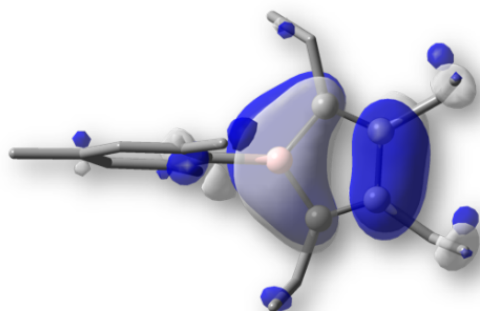


Figure S35. ACID plots of MesBC₄Et₄ and MesBC₄Ph₄. Only the relevant π -orbitals were considered.

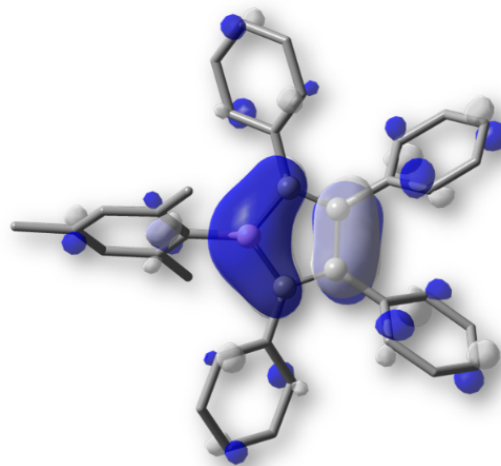
Table S4. WBIs, MBOs and NBOs of MesBC₄Et₄ and MesBC₄Ph₄ at the PBE0-D3(BJ)/6-311G(d,p) level of theory.

| | MesBC ₄ Et ₄ | | MesBC ₄ Ph ₄ | |
|-------|------------------------------------|-------|------------------------------------|-------|
| | WBI | MBO | WBI | MBO |
| B1–C1 | 0.980 | 0.900 | 0.969 | 0.877 |
| B1–C4 | 0.985 | 0.901 | 0.969 | 0.877 |
| B1–C5 | 1.001 | 0.899 | 1.020 | 0.940 |
| C1–C2 | 1.717 | 1.875 | 1.638 | 1.799 |
| C2–C3 | 0.966 | 0.972 | 0.965 | 0.959 |
| C3–C4 | 1.717 | 1.866 | 1.638 | 1.799 |
| | NBO charges | | NBO charges | |
| B1 | 1.007 | | 1.026 | |
| C1 | –0.406 | | –0.400 | |
| C2 | 0.057 | | 0.054 | |

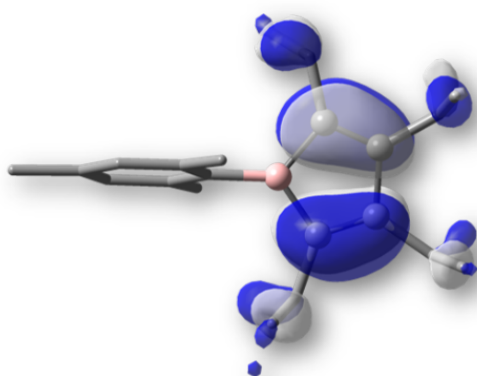
| | | |
|----|--------|--------|
| C3 | 0.057 | 0.054 |
| C4 | -0.410 | -0.400 |



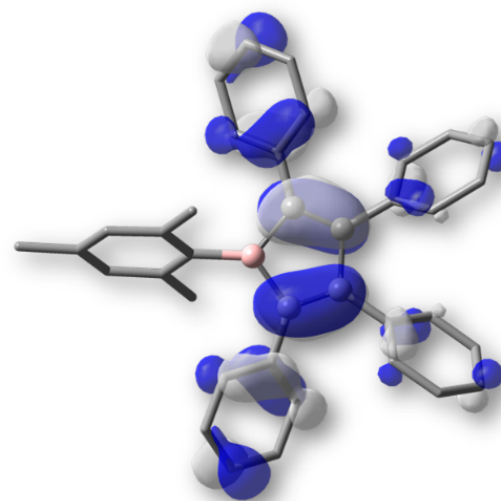
LUMO (E = -2.087 eV)



LUMO (E = -2.904 eV)



HOMO (E = -5.572 eV)



HOMO (E = -5.701 eV)

Figure S36. Frontier orbitals of MesBC₄Et₄ (**2**) and MesBC₄Ph₄ with their corresponding energetic level at the PBE0-D3(BJ)/6-311+G(d,p)/SMD(benzene) level of theory.

Cartesian Coordinates

Compound 2, PBE0-D3(BJ)/6-31+G(d,p)

Geometry of the lowest singlet state

Energy + Zero-point correction = -842.373701 E_h

| | | | |
|---|--------------|--------------|--------------|
| C | -1.051364000 | 1.242111000 | -0.501462000 |
| C | -2.319687000 | 0.771843000 | -0.501175000 |
| C | -1.105778000 | -1.251515000 | -0.155232000 |
| C | -2.352097000 | -0.744808000 | -0.293777000 |
| B | -0.130459000 | -0.013287000 | -0.232467000 |
| C | 1.415180000 | -0.005554000 | -0.038124000 |
| C | 1.977375000 | -0.193341000 | 1.239259000 |
| C | 2.270200000 | 0.191402000 | -1.139244000 |
| C | 3.363384000 | -0.178528000 | 1.395338000 |
| C | 3.652603000 | 0.197854000 | -0.951820000 |
| C | 4.219708000 | 0.018548000 | 0.310690000 |
| H | 3.786538000 | -0.321829000 | 2.388625000 |
| H | 4.303703000 | 0.339829000 | -1.813244000 |
| C | -3.572643000 | 1.571409000 | -0.670733000 |
| C | -4.315381000 | 1.825189000 | 0.645332000 |
| H | -4.637044000 | 0.891866000 | 1.115689000 |
| C | -3.632807000 | -1.526353000 | -0.233559000 |
| C | -3.995721000 | -1.952961000 | 1.193869000 |
| H | -3.224185000 | -2.605986000 | 1.611675000 |
| C | -0.730300000 | -2.694186000 | -0.014257000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.159110000 | -3.175514000 | -1.163703000 |
| H | 1.085039000 | -2.593313000 | -1.206759000 |
| C | -0.606783000 | 2.667534000 | -0.602104000 |
| C | -0.149119000 | 3.223087000 | 0.750299000 |
| H | -0.966798000 | 3.197535000 | 1.478571000 |
| C | 1.697952000 | 0.313288000 | -2.526264000 |
| H | 2.361662000 | 0.876927000 | -3.188626000 |
| H | 1.547781000 | -0.676924000 | -2.974546000 |
| H | 0.720860000 | 0.809521000 | -2.518991000 |
| C | 1.086067000 | -0.343108000 | 2.443106000 |
| H | 1.586396000 | -0.887670000 | 3.249311000 |
| H | 0.795852000 | 0.638222000 | 2.839244000 |
| H | 0.158719000 | -0.871874000 | 2.196303000 |
| C | 5.709759000 | 0.064645000 | 0.502457000 |
| H | 6.045742000 | 1.085632000 | 0.720903000 |
| H | 6.024202000 | -0.568399000 | 1.337644000 |
| H | 6.238633000 | -0.268608000 | -0.395381000 |
| H | 0.236255000 | 2.740862000 | -1.302799000 |
| H | -1.401617000 | 3.306341000 | -1.007030000 |
| H | 0.195258000 | 4.258778000 | 0.657298000 |
| H | 0.678488000 | 2.628440000 | 1.150707000 |
| H | -3.323934000 | 2.533484000 | -1.129942000 |
| H | -4.246012000 | 1.061644000 | -1.372937000 |
| H | -5.206294000 | 2.438322000 | 0.475605000 |
| H | -3.668659000 | 2.349911000 | 1.355364000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.458494000 | -0.947696000 | -0.660969000 |
| H | -3.535623000 | -2.424467000 | -0.856488000 |
| H | -4.948207000 | -2.492898000 | 1.210795000 |
| H | -4.083477000 | -1.087851000 | 1.858092000 |
| H | -1.621905000 | -3.330361000 | 0.047168000 |
| H | 0.429730000 | -4.229561000 | -1.039867000 |
| H | -0.354875000 | -3.066077000 | -2.124757000 |
| H | -0.183383000 | -2.843616000 | 0.928302000 |

Compound MesBC₄Ph₄, PBE0-D3(BJ)/6-31+G(d,p)

Geometry of the lowest singlet state

Energy + Zero-point correction = -1451.348924 E_h

| | | | |
|---|--------------|--------------|--------------|
| C | 0.046435000 | 1.255670000 | -0.058388000 |
| C | 1.313676000 | 0.761662000 | -0.042684000 |
| C | 0.048784000 | -1.255636000 | 0.054757000 |
| C | 1.315093000 | -0.759182000 | 0.040238000 |
| B | -0.911446000 | -0.000887000 | -0.002053000 |
| C | -2.463609000 | -0.002100000 | -0.000787000 |
| C | -3.177772000 | -0.533213000 | -1.093899000 |
| C | -3.174725000 | 0.522752000 | 1.097236000 |
| C | -4.571804000 | -0.518509000 | -1.078532000 |
| C | -4.568772000 | 0.497457000 | 1.090804000 |
| C | -5.287158000 | -0.010500000 | 0.007169000 |
| H | -5.114116000 | -0.919982000 | -1.933012000 |
| H | -5.108416000 | 0.887089000 | 1.952383000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.560882000 | 1.539366000 | -0.102762000 |
| C | 3.586526000 | 1.343128000 | 0.832633000 |
| C | 2.738112000 | 2.502815000 | -1.105914000 |
| C | 4.749730000 | 2.104835000 | 0.776585000 |
| H | 3.466676000 | 0.595622000 | 1.610995000 |
| C | 3.907887000 | 3.250729000 | -1.170747000 |
| H | 1.946350000 | 2.658863000 | -1.832611000 |
| C | 4.916479000 | 3.057274000 | -0.226803000 |
| H | 5.531175000 | 1.947017000 | 1.514329000 |
| H | 4.031834000 | 3.989130000 | -1.957718000 |
| H | 5.828976000 | 3.644515000 | -0.275269000 |
| C | 2.563774000 | -1.534399000 | 0.101949000 |
| C | 2.741846000 | -2.497191000 | 1.105581000 |
| C | 3.590052000 | -1.336357000 | -0.832366000 |
| C | 3.913046000 | -3.242740000 | 1.171902000 |
| H | 1.949595000 | -2.654656000 | 1.831438000 |
| C | 4.754736000 | -2.095688000 | -0.774812000 |
| H | 3.469549000 | -0.589315000 | -1.611075000 |
| C | 4.922293000 | -3.047510000 | 0.229026000 |
| H | 4.037597000 | -3.980684000 | 1.959206000 |
| H | 5.536679000 | -1.936498000 | -1.511734000 |
| H | 5.835913000 | -3.632904000 | 0.278663000 |
| C | -0.361734000 | -2.663443000 | 0.044618000 |
| C | 0.307204000 | -3.633387000 | -0.721448000 |
| C | -1.495287000 | -3.062406000 | 0.771058000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.131025000 | -4.951991000 | -0.743943000 |
| H | 1.170803000 | -3.342404000 | -1.311391000 |
| C | -1.929235000 | -4.384806000 | 0.753397000 |
| H | -2.041313000 | -2.323292000 | 1.349674000 |
| C | -1.249054000 | -5.336604000 | -0.002851000 |
| H | 0.399277000 | -5.683081000 | -1.348036000 |
| H | -2.806718000 | -4.669143000 | 1.327456000 |
| H | -1.590673000 | -6.367532000 | -0.022620000 |
| C | -0.366912000 | 2.662624000 | -0.047722000 |
| C | -1.500759000 | 3.059672000 | -0.774742000 |
| C | 0.299492000 | 3.633558000 | 0.719313000 |
| C | -1.937245000 | 4.381235000 | -0.756963000 |
| H | -2.044707000 | 2.319633000 | -1.354131000 |
| C | -0.141320000 | 4.951299000 | 0.741995000 |
| H | 1.163247000 | 3.344043000 | 1.309752000 |
| C | -1.259497000 | 5.334059000 | 0.000174000 |
| H | -2.814712000 | 4.664217000 | -1.331734000 |
| H | 0.387092000 | 5.683176000 | 1.346790000 |
| H | -1.603069000 | 6.364336000 | 0.020016000 |
| C | -2.436859000 | 1.080400000 | 2.284930000 |
| H | -3.124230000 | 1.323317000 | 3.099849000 |
| H | -1.698471000 | 0.369033000 | 2.674019000 |
| H | -1.896506000 | 1.995432000 | 2.017208000 |
| C | -2.443309000 | -1.093794000 | -2.282257000 |
| H | -3.133160000 | -1.340761000 | -3.093857000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.708022000 | -0.381996000 | -2.676329000 |
| H | -1.899916000 | -2.006742000 | -2.013609000 |
| C | -6.789401000 | 0.014956000 | -0.002926000 |
| H | -7.161646000 | 0.948268000 | -0.442718000 |
| H | -7.198711000 | -0.810604000 | -0.592716000 |
| H | -7.196556000 | -0.053892000 | 1.010122000 |

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