Supporting Information for

Synthesis, Reduction and C–H Activation Chemistry of Azaborinines with Redox-Active Organoboryl Substituents

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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. Solvents were stored under argon over activated 4 Å molecular sieves. Liquid-phase NMR spectra were acquired on a Bruker Avance 400 spectrometer (^{1}H: 400.6, ^{13}C: 100.7, ^{11}B: 128.5, ^{31}P: 162.2 MHz), a Bruker Avance 500 spectrometer (^{1}H: 500.1, ^{13}C: 125.8, ^{11}B: 160.5, ^{31}P: 202.5 MHz) or a Bruker Avance Neo I 600 spectrometer (^{1}H: 600.2 MHz). Chemical shifts (δ) are provided 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: $BF_3{\cdot}OEt_2$, ^{31}P: 85% H_3PO_4,). High-resolution mass-spectroscopic (HRMS) data was acquired on a MRMS device Exactive Plus with Orbitrap detector from Thermo-Scientific with a LIFDI 700 ion source from Linden CMS. UV-vis spectra were acquired on a METTLER TOLEDO UV-vis-Excellence UV5 spectrophotometer inside a glovebox. Solid-state IR spectra were recorded on a Bruker FT-IR spectrometer ALPHA II inside a glovebox. EPR measurements at X-band (9.39 GHz) were carried out using a Bruker ELEXSYS E580 CW EPR spectrometer. 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 counterelectrode, and a silver wire, separated by a Vycor tip, serving as the reference electrode. Formal redox potentials are referenced to the ferrocene/ferrocenium ($[Cp_2Fe]^{+/0}$) redox couple by using decamethylferrocene ($[Cp^*_2Fe]$; $E_{1/2}$ = −0.427 V in THF) as an internal standard. Tetra(*n*-butyl)ammonium hexafluorophosphate ($[nBu_4N][PF_6]$) was employed as the supporting electrolyte. Compensation for resistive losses (iR drop) was employed for all measurements.

Solvents and reagents were purchased from Sigma-Aldrich or Alfa Aesar.

Compounds **1**,[1] **9**,[1] 9,10-dibromo-9,10-diboraanthracene (DBA^{Br2}),[2] 5-bromodibenzo[*b*,*d*]borole (DBB^{Br}),[3] 1-chlorotetraphenylborole (TPB^{Cl})[4] and KC_8[5] were synthesised following literature procedures.

Synthetic procedures

Synthesis of 2

To a suspension of **1** (20.0 mg, 37.3 µmol, 1.00 equiv.) in benzene (1 mL), DBA^{Br2} (12.4 mg, 37.3 µmol, 1.00 equiv.) was added and the mixture stirred for an hour, yielding an orange solution with a colourless precipitate. The suspension was filtered, and the filtrate dried *in vacuo*. The resulting solid was washed with pentane (3 x 2 mL) and dried again, yielding **2** (21.2 mg, 29.8 µmol, 80%) as an orange solid. Single crystals suitable for X-ray diffraction analysis were obtained by slow vapour diffusion of pentane into a saturated benzene solution of **2**. ^{1}H NMR (500.1 MHz, C_6D_6): δ = 8.24–8.19 (m, 2H, C*H*, *o*-DBA-*H*), 7.92–7.87 (m, 2H, C*H*, *o*-DBA-*H*), 7.35–7.29 (m, 4H, C*H*, Ph-C*H*), 7.24–7.20 (m, 2H, C*H*, Ph-C*H*), 7.17–7.15 (m, 2H, C*H*, Ph-C*H*)*, 7.08–6.99 (m, 4H, C*H*, *m*-DBA-*H*), 6.99–6.93 (m, 4H, C*H*, Ph-C*H*), 6.89–6.75 (m, 6H, C*H*, Ph-C*H*), 6.75–6.60 (m, 5H, C*H*, Ph-C*H*), 6.38–6.32 (m, 2H, C*H*, Ph-C*H*) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 155.5 (C_q), 146.2 (C_q), 144.9 (br, C_q-DBA_B), 144.0 (C_q), 143.4 (br, C_q-DBA_B), 142.9 (br, C_{qB}), 142.0 (C_q), 141.8 (br, C_{qB}), 140.1 (C_q), 140.1 (C_q), 138.5 (*C*H-*o*-DBA), 136.6 (*C*H-*o*-DBA), 134.3 (*C*H), 133.4 (*C*H-*m*-DBA), 133.0 (*C*H), 132.7 (*C*H-*m*-DBA), 131.9 (*C*H), 131.7 (*C*H), 131.3 (*C*H), 128.1 (*C*H), 127.7 (*C*H), 127.7 (*C*H), 127.5 (*C*H), 127.5 (*C*H), 127.5 (*C*H), 127.5 (*C*H), 126.6 (*C*H), 126.0 (C_q), 125.8 (*C*H), 125.0 (*C*H) ppm. ^{11}B NMR (160.5 MHz, C_6D_6): δ = 61.8 (br, *B*-DBA), 35.2 (br, *B*-Aza) ppm. HRMS-LIFDI [*m/z*] calcd. for [$C_{46}H_{34}B_3NO$] = [M –Br + OH]: 649.2914; found: 649.1906. *Note: in the solid state **2** turns from orange to an insoluble yellow solid over time. X-ray diffraction identified the latter as the hydrolysis product **3**. Due to the high sensitivity of **2** no UV-Vis data could be obtained as in such a high dilution only **3** was observed.* HRMS-LIFDI [*m/z*] calcd. for [$C_{92}H_{66}B_6N_2O$] = [M]: 1280.5798; found: 1280.5728.

Synthesis of 4

To a suspension of **1** (40.0 mg, 74.6 µmol, 2.00 equiv.) in benzene (1 mL) DBA^{Br2} (12.4 mg, 37.3 µmol, 1.00 equiv.) was added and the mixture stirred at 80 °C for 20 h, yielding a yellow solution with an orange precipitate. The suspension was filtered. The solid residue was washed with benzene (3 x 1 mL) and pentane (1 x 1 mL) and dried *in vacuo*. Suspension of the solid residue in dichloromethane, followed by filtration and drying of the filtrate *in vacuo* yielded **4** as an orange solid (23.4 mg, 21.5 µmol, 58%). Single crystals suitable for X-ray diffraction analysis were obtained by storing of a saturated solution of **4** in dichloromethane at –30 °C. The ^{1}H NMR spectra shows two isomers, *syn*-**4** and *anti*-**4**

(isomers **A** and **B**), present in various ratios in different crystallisation fractions. *Note: the assignment of **A** and **B** to either the syn or anti isomer was not possible. The ^{13}C NMR data is presented as the mixture of **A** and **B**, as only a limited number of resonances could be definitively assigned to one or the other.* ^{1}H NMR (500.1 MHz, CD_2Cl_2) for isomer **A**: δ = 7.84–7.80 (m, 4H, C*H*, *o*-DBA-*H*), 7.46–7.41 (m, 4H, C*H*, *m*-DBA-*H*), 6.87–6.60 (m, 41H, C*H*, Ar-*H*), 6.60–6.51 (m, 5H, C*H*, Ar-*H*), 6.31–6.25 (m, 4H, C*H*, Ar-*H*) ppm. ^{1}H NMR (500.1 MHz, CD_2Cl_2) for isomer **B**: δ = 7.80–7.76 (m, 4H, C*H*, *o*-DBA-*H*), 7.40–7.34 (m, 4H, C*H*, *m*-DBA-*H*), 6.87–6.60 (m, 41H, C*H*, Ar-*H*), 6.60–6.51 (m, 5H, C*H*, Ar-*H*), 6.51–6.44 (m, 4H, C*H*, Ar-*H*) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 154.7 (C_q), 154.5 (C_q), 145.6 (br, C_qB-DBA, **A**), 145.4 (br, C_qB-DBA, **B**), 145.3 (C_q), 145.2 (C_q), 144.6 (C_q), 144.4 (C_q), 142.7 (C_q), 142.3 (C_q), 141.4 (C_q), 141.2 (C_q), 140.4 (C_q), 140.4 (C_q), 139.1 (C_q), 138.8 (C_q), 137.3 (*C*H-DBA, **A**), 137.3 (*C*H-DBA, **B**), 133.8 (*C*H), 133.7 (*C*H), 132.9 (*C*H), 132.9 (*C*H), 132.5 (*C*H-DBA, **A**), 132.4 (*C*H-DBA, **B**), 131.8 (*C*H), 131.4 (*C*H), 131.2 (*C*H), 131.1 (*C*H), 130.9 (*C*H), 130.9 (*C*H), 128.7 (C_6D_6) , 127.7 (*C*H), 127.6 (*C*H), 127.5 (*C*H), 127.3 (*C*H), 127.0 (*C*H), 126.8 (*C*H), 126.8 (*C*H), 126.8 (*C*H), 126.7 (*C*H), 126.6 (*C*H), 126.6 (*C*H), 126.5 (*C*H), 126.5 (*C*H), 126.3 (*C*H), 125.4 (*C*H), 125.4 (*C*H), 125.1 (*C*H), 124.1 (*C*H), 124.0 (CH) ppm. ^{11}B NMR (160.5 MHz, C_6D_6): δ = n.d. *(due to excessive broadening caused by the low symmetry and the quadrupole moment of the boron nucleus)*. HRMS-LIFDI [*m/z*] calcd. for $[C_{80}H_{58}B_4N_2]$ = [M]: 1090.4967; found: 1090.4960.

One-electron reduction of 4 to 4$^{\bullet-}$

To a suspension of **4** (20.0 mg, 18.3 µmol, 1.00 equiv.) in benzene (1 mL) KC_8 was added (2.20 mg, 16.2 µmol, 0.90 equiv.) and the mixture stirred overnight at room temperature, whereupon a colour change from orange to purple was observed. The suspension was filtered to yield a purple benzene solution of the radical anion **[4]$^{\bullet-}$**. EPR (CW, X-band, benzene, room temperature): g_{iso} = 2.0026.

Two-electron reduction of 4 to 4^{2-}

To a suspension of **4** (20.0 mg, 18.3 µmol, 1.00 equiv.) in benzene (0.7 mL) an excess of KC_8 was added (12.4 mg, 91.7 µmol, 5.00 equiv.) and the mixture stirred for 2 h at room temperature, whereupon a colour change from orange to dark red/brown was observed. The suspension was filtered and the filtrate left undisturbed at room temperature overnight, yielding a crop of dark red crystals of **[4]K$_2$** (16.1 mg, 13.8 µmol, 75%). *Note: For NMR-spectroscopic measurements, 18-crown-6 (3.00 mg) was added to the solution of **6**, as this*

*improved its solution stability. As crystals of the dianion of anti-**4** were isolated in 75% yield, anti-**4** is likely the major rotamer obtained.* ^{1}H NMR (500.1 MHz, C_6D_6): δ = 8.34–8.29 (m, 4H, C*H*, *o*-DBA-*H*), 7.47–7.36 (m, 8H, Ph-C*H*), 7.31–7.27 (m, 4H, Ph-C*H*), 7.23–7.19 (m, 4H, Ph-C*H*), 7.14–7.07 (m, 8H, C*H*, *m*-DBA-*H* + Ph-C*H*), 6.90–6.82 (m, 8H, Ph-C*H*), 6.79–6.73 (m, 4H, Ph-C*H*), 6.73–6.65 (m, 4H, Ph-C*H*), 6.65–6.57 (m, 2H, Ph-C*H*), 6.29–6.19 (m, 4H, Ph-C*H*), 6.12–5.97 (m, 6H, Ph-C*H*), 5.92–5.83 (m, 2H, Ph-C*H*) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 153.9 (C_q), 150.3 (C_q), 148.5 (C_{qB}), 146.0 (C_q), 146.0 (C_q), 143.8 (C_q), 143.1 (C_q), 142.6 (C_q), 142.5 (C_q), 133.6 (C_{qB}-DBA), 133.3 (*C*H), 133.2(*C*H), 132.9 (*C*H), 132.6 (*C*H-DBA) 131.5 (*C*H), 131.5 (*C*H), 131.4 (*C*H), 131.2 (*C*H), 131.0 (*C*H), 128.5 (*C*H), 127.1 (*C*H), 127.0 (*C*H), 126.9 (*C*H), 126.7 (*C*H), 126.6 (*C*H), 126.5 (*C*H), 126.0 (*C*H), 125.7 (*C*H), 125.6 (*C*H), 125.5 (*C*H), 125.2 (*C*H), 124.9 (*C*H), 124.8 (*C*H), 124.0 (*C*H), 117.8 (*C*H-DBA) 117.8 (*C*H-DBA) ppm. ^{11}B NMR (160.5 MHz, C_6D_6): n.d. *(due to excessive broadening caused by the low symmetry and the quadrupole moment of the boron nucleus)*. HRMS ESI-neg for $[C_{80}H_{58}B_4N_2]^{2-}$ = $[M - 2K]^{2-}$; *m*/*z*: calcd. 545.2512; found 545.2497; for $[C_{80}H_{58}B_4N_2]^{-}$ = $[M - 2K]^{-}$; *m*/*z*: calcd. 1091.5096; found 1091.5082; $[C_{80}H_{58}B_4N_2K]^{-}$ = $[M - K]^{-}$; *m*/*z*: calcd. 1129.4656; found 1129.4630.

Synthesis of 5

To a suspension of **1** (30.0 mg, 56.0 µmol, 1.00 equiv.) in benzene (1 mL) DBB^{Br} (13.6 mg, 56.0 µmol, 1.00 equiv.) was added and the mixture stirred for 10 minutes at room temperature, yielding a yellow solution with a colourless precipitate. The suspension was filtered and the filtrate dried *in vacuo*. The resulting solid was washed with benzene (1 x 1 mL) and dried again, yielding **5** as a yellow solid (17.8 mg, 20.6 µmol, 51%). Suitable single crystals for X-ray diffraction analysis were obtained by storing of a saturated solution of **5** in benzene. ^{1}H NMR (500.1 MHz, C_6D_6): δ = 7.49–7.44 (m, 2H, C*H*, Ar-*H*), 7.35–7.29 (m, 2H, C*H*, Ar-*H*), 7.27–7.20 (m, 2H, C*H*, Ar-*H*), 7.16–7.11 (m, 4H, C*H*, Ar-*H*), 6.98–6.91 (m, 6H, C*H*, Ar-*H*), 6.88–6.75 (m, 12H, C*H*, Ar-*H*), 6.68–6.62 (dt, 2H, ^{3}J = 14.7 Hz, ^{4}J = 1.0 Hz, Ar-*H*), 6.61–6.53 (m, 2H, C*H*, Ar-*H*), 6.51–6.44 (m, 1H, C*H*, Ar-*H*) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 155.5 (C_q), 152.2 (C_q-DBB), 145.3 (C_q), 143.9 (C_q), 143.1 (br, C_{qB}), 142.3 (br, C_{qB}), 142.0 (C_q), 141.4 (C_q), 140.8 (br, C_q-DBB_B), 140.3 (C_q), 133.7 (*C*H), 133.4 (*C*H), 133.1 (*C*H), 133.0 (*C*H), 131.6 (*C*H), 131.2 (*C*H), 130.0 (*C*H), 128.4 (*C*H), 128.4 (*C*H), 128.3 (*C*H), 127.6 (*C*H), 127.5 (*C*H), 127.5 (*C*H), 127.5 (*C*H), 127.4 (*C*H), 126.5 (C_q) 126.0 (*C*H), 125.8 (*C*H), 125.0 (*C*H), 119.5 (*C*H) ppm. ^{11}B NMR (128.5 MHz, C_6D_6): δ = 54.0 (br,

B-DBB), 38.1 (br, *B*-Aza) ppm. HRMS-LIFDI [*m/z*] calcd. for [$C_{46}H_{33}B_2N$] = [M]: 621.2794; found 621.2789.

One-electron reduction of 5 to 5$^{\bullet}$

To a suspension of **5** (45.0 mg, 52.1 µmol, 1.00 equiv.) in benzene (1 mL), KC_8 (21.1 mg, 156 µmol, 3.00 equiv.) was added and an immediate colour change from yellow to dark red/brown was observed. The mixture was filtered after 1 min and an EPR spectrum was recorded. EPR (CW, X-band, benzene, 298 K): g_{iso} = 2.0028.

Reduction of 5 to 6

To a suspension of **5** (45.0 mg, 52.1 µmol, 1.00 equiv.) in benzene (1 mL), KC_8 (21.1 mg, 156 µmol, 3.00 equiv.) was added and an immediate colour change from yellow to dark red/brown was observed. The reaction mixture was filtered after one minute at room temperature, the filtrate left undisturbed at room temperature overnight, yielding a dark purple precipitate (10.8 mg, 16.4 µmol, 32%) and a colourless supernatant. The precipitate was not soluble in common solvents and the colourless supernatant was transferred to another vial, in which slow evaporation of the solvent at room temperature yielded (2.4 mg, 3.65 µmol, 7%) of colourless single crystals of **6** suitable for X-ray structural analysis. ^{11}B NMR (160.5 MHz, C_6D_6): δ = –1.6 ppm. HRMS ESI-neg for $[C_{46}H_{32}B_4N]^-$ = $[M - K]^-$; *m/z*: calcd. 620.2741; found 620.2732. ***Note:*** *The reduction was also carried out with elemental potassium and elemental lithium. In each case, the reaction results in, among other things, overreduction. If one equivalent of reducing agent is used, complete conversion does not occur. The formation of* ***6*** *can be followed by NMR spectroscopy.* H_2 *is released during the reaction. A characterisation via* ^{13}C *and 2D NMR spectroscopy was not possible, because* ***6*** *crystallises over time in low yields and cannot be redissolved.*

Synthesis of 8

To a suspension of **1** (30.0 mg, 56.0 µmol, 1.00 equiv.) in benzene (1 mL) TPB^{Cl} (22.5 mg, 58.8 µmol, 1.10 equiv.) was added and the mixture stirred for two days at room temperature, yielding a red solution with a colourless precipitate. The suspension was filtered and the filtrate dried *in vacuo*. The resulting solid was washed with pentane (3 x 2 mL) and dried again, yielding **8** as a pale yellow solid (24.8 mg, 30.0 µmol, 54%). Suitable single crystals for X-ray diffraction analysis were obtained by slow vapour diffusion of pentane into a saturated benzene solution. Two diastereomers (**8A** and **8B**) are formed in a 74:26 ratio,

corresponding to the formal *syn*- and *anti*- additions of the Ph–H bond across the borolyl moiety. NMR data is given for the mixture of **8A** and **8B** ^{1}H NMR (500.1 MHz, C_6D_6): δ = 7.81–7.76 (m, 1H, C*H*, Ph-C*H*), 7.72–7.62 (m, 2H, C*H*, Ph-C*H*), 7.40–7.27 (m, 4H, C*H*, Ph-C*H*), 7.09–7.02 (m, 2H, C*H*, Ph-C*H*), 7.02–6.56 (m, 34H, C*H*, Ph-C*H*), 6.45–6.39 (m, 0.8H, C*H*, Ph-C*H*), 6.19–6.12 (m, 0.2H, C*H*, Ph-C*H*), 3.51 (s, 1H, BC*H*Ph) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 157.8 (C_q), 157.2 (C_q), 151.7 (C_q), 149.7 (C_q), 148.2 (C_q), 147.9 (C_q), 146.8 (C_q), 146.1 (br, C_{qB}), 145.0 (C_q), 143.8 (C_q), 143.8 (C_q), 143.5 (C_q), 142.2 (C_q), 141.9 (br, C_{qB}), 141.7 (C_q), 141.2 (C_q), 141.1 (C_q), 140.9 (C_q), 140.6 (C_q), 140.4 (C_q), 140.2 (C_q), 139.7 (C_q), 139.1 (C_q), 138.4 (C_q), 137.6 (C_q), 137.4 (C_q), 135.2 (*C*H), 133.8 (*C*H), 133.3 (*C*H), 132.9 (*C*H), 132.9 (*C*H), 132.4 (*C*H), 132.1 (*C*H), 131.9 (*C*H), 131.8 (*C*H), 131.6 (*C*H), 131.5 (*C*H), 131.3 (*C*H), 131.2 (*C*H), 131.0 (*C*H), 131.0 (*C*H), 130.5 (*C*H), 130.5 (*C*H), 130.4 (*C*H), 130.2 (*C*H), 130.1 (*C*H), 130.0 (*C*H), 129.9 (*C*H), 129.5 (*C*H), 129.4 (*C*H), 129.0 (*C*H), 129.0 (*C*H), 128.7 (*C*H), 128.6 (*C*H), 127.8 (*C*H), 127.1 (*C*H), 127.1 (*C*H), 127.0 (*C*H), 127.0 (*C*H), 126.9 (*C*H), 126.9 (*C*H), 126.8 (*C*H), 126.6 (*C*H), 126.4 (*C*H), 126.2 (*C*H), 126.1 (*C*H), 125.9 (*C*H), 125.9 (*C*H), 124.8 (*C*H), 53.2 (*C*H) ppm. ^{11}B NMR (128.5 MHz, C_6D_6): δ = 38.3 (br) ppm. HRMS-LIFDI [*m/z*] calcd. for [$C_{62}H_{45}B_2N$] = [M]: 825.3733; found 825.3724.

Reduction of 9 to 11

To a suspension of **9** (30.0 mg, 47.9 µmol, 1.00 equiv.) in C_6D_6 (0.7 mL) KC_8 (20.0 mg, 148 µmol, 3.00 equiv.) was added and a colour change from colourless to purple was observed. For a complete conversion the reaction mixture was stirred at room temperature for 72 h. The suspension was filtered, and all volatiles were removed *in vacuo* and the remaining solid was washed with pentane to yield **11** as colourless solid (24.3 mg, 41.7 µmol, 94%). Suitable colourless single crystals for X-ray structural analysis were obtained by adding THF (two drops) to a reaction solution and slowly evaporating the solvent at room temperature. ^{1}H NMR (500.1 MHz, C_6D_6): δ = 7.74–7.58 (m, 4H, Ph-C*H*), 7.58–7.45 (m, 4H, Ph-C*H*), 7.28–7.17 (m, 3H, Ph-C*H*), 7.13–6.94 (m, 6H, Ph-C*H*), 6.94–6.77 (m, 7H, Ph-C*H*), 6.77–6.70 (m, 2H, Ph-C*H*), 6.70–6.63 (m, 1H, Ph-C*H*), 6.63–6.53 (m, 1H, Ph-C*H*), 6.53–6.41 (m, 1H, Ph-C*H*), 4.20 (br, s, 1H, B*H*) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 164.5 (br, C_{qB}), 158.5 (br, C_{qB}), 154.9 (C_q), 151.3 (C_q), 149.0 (br, C_{qB}), 146.6 (C_q), 143.7 (C_q), 142.8 (C_q), 142.4 (C_q), 141.0 (br, C_{qB}), 134.8 (*C*H), 133.0 (*C*H), 132.4 (*C*H), 131.8 (*C*H), 131.6 (*C*H), 131.4 (*C*H), 131.3 (*C*H), 128.6 (*C*H), 128.6 (*C*H), 127.5 (*C*H), 127.2 (*C*H), 127.2 (*C*H), 127.2 (*C*H), 126.9 (*C*H), 126.7 (*C*H), 125.6 (*C*H), 125.5 (*C*H), 125.4 (*C*H), 125.0 (*C*H), 124.9 (*C*H), 124.0 (*C*H), 123.1 (C_q) ppm. ^{11}B NMR (160.5 MHz, C_6D_6): δ = –4.1 ppm. HRMS-LIFDI [*m/z*]

calcd. for [$C_{40}H_{29}B_2NK$] = [M]: 584.2096; found: 584.2096. FT-IR (solid-state): $\tilde{\nu}$(B-H) = 2278 cm^{-1}.

NMR spectra of isolated compounds

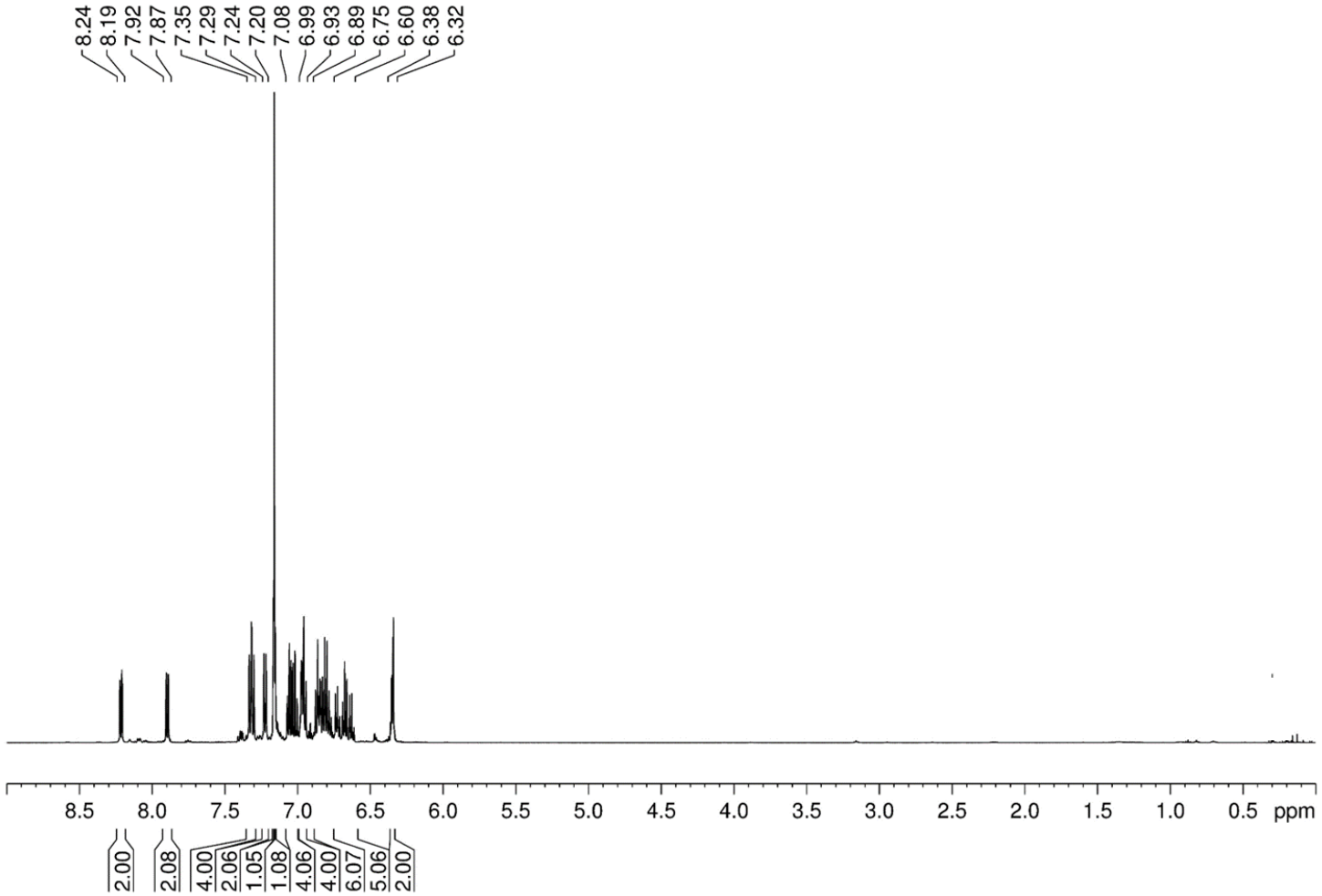


Figure S1. $^{1}H\{^{11}B\}$ NMR spectrum of **2** in C_6D_6.

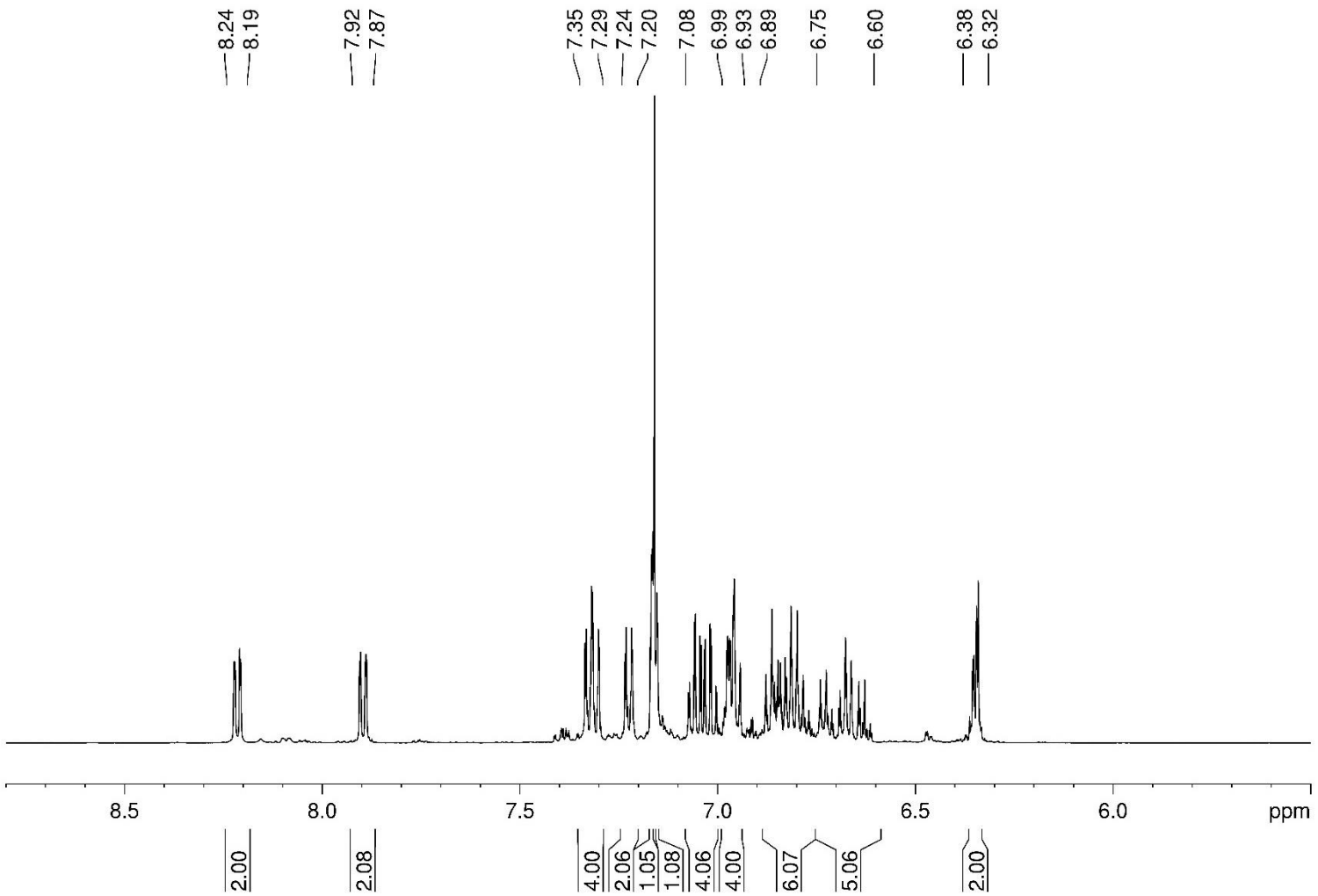


Figure S2. $^{1}H\{^{11}B\}$ NMR spectrum of **2** in C_6D_6 with close-up of the aromatic region.

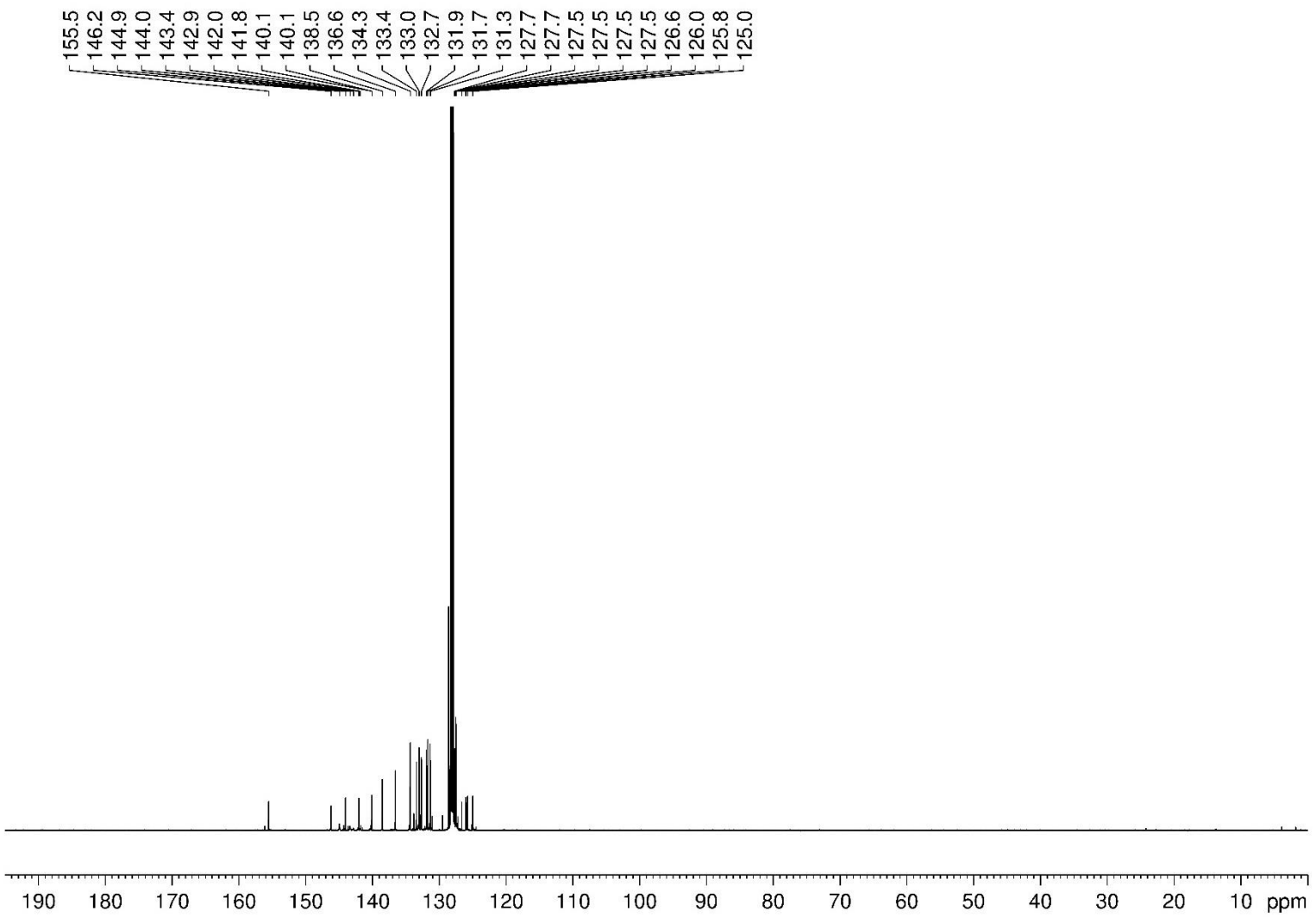


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6.

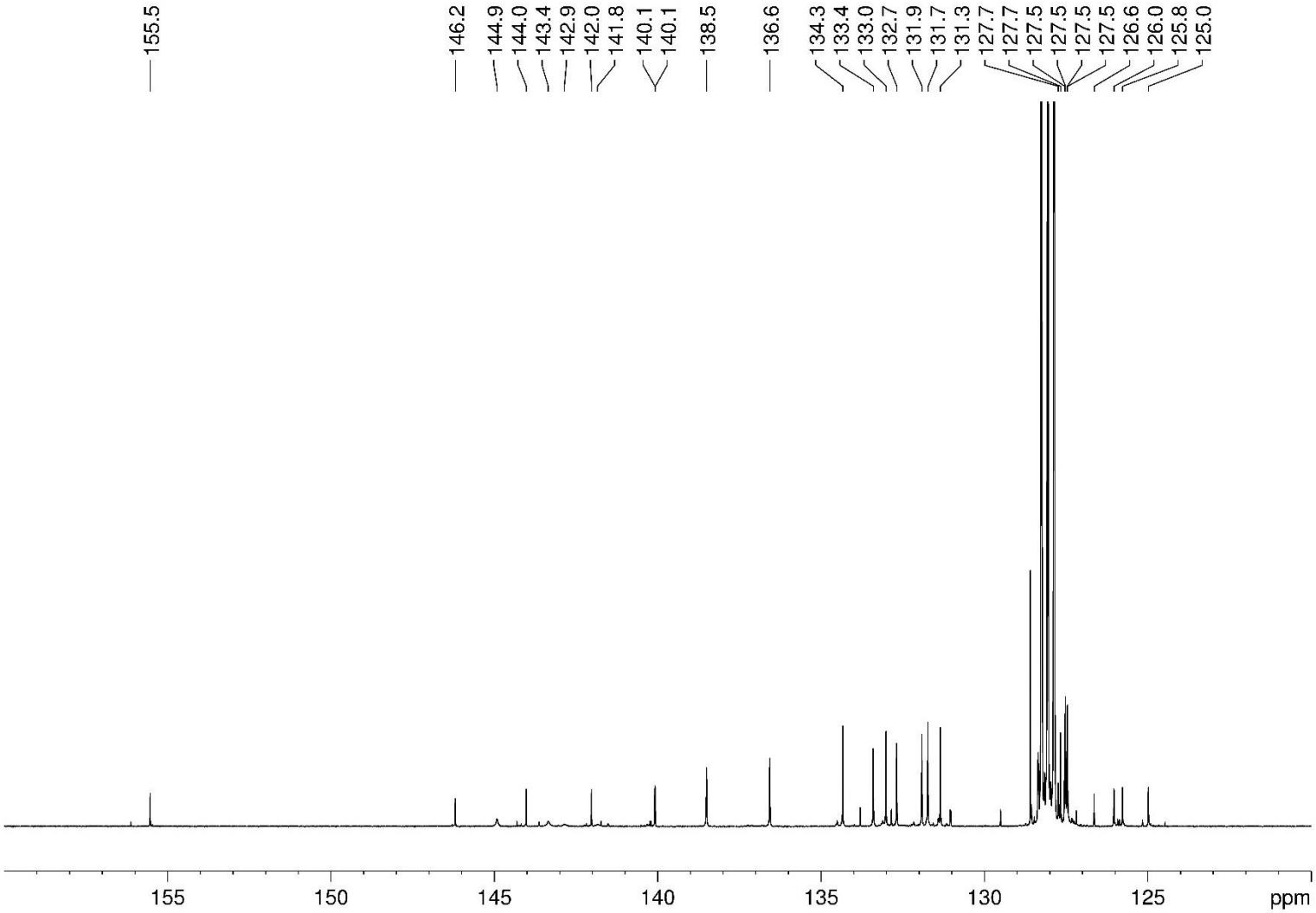


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 with close-up of the aromatic region.

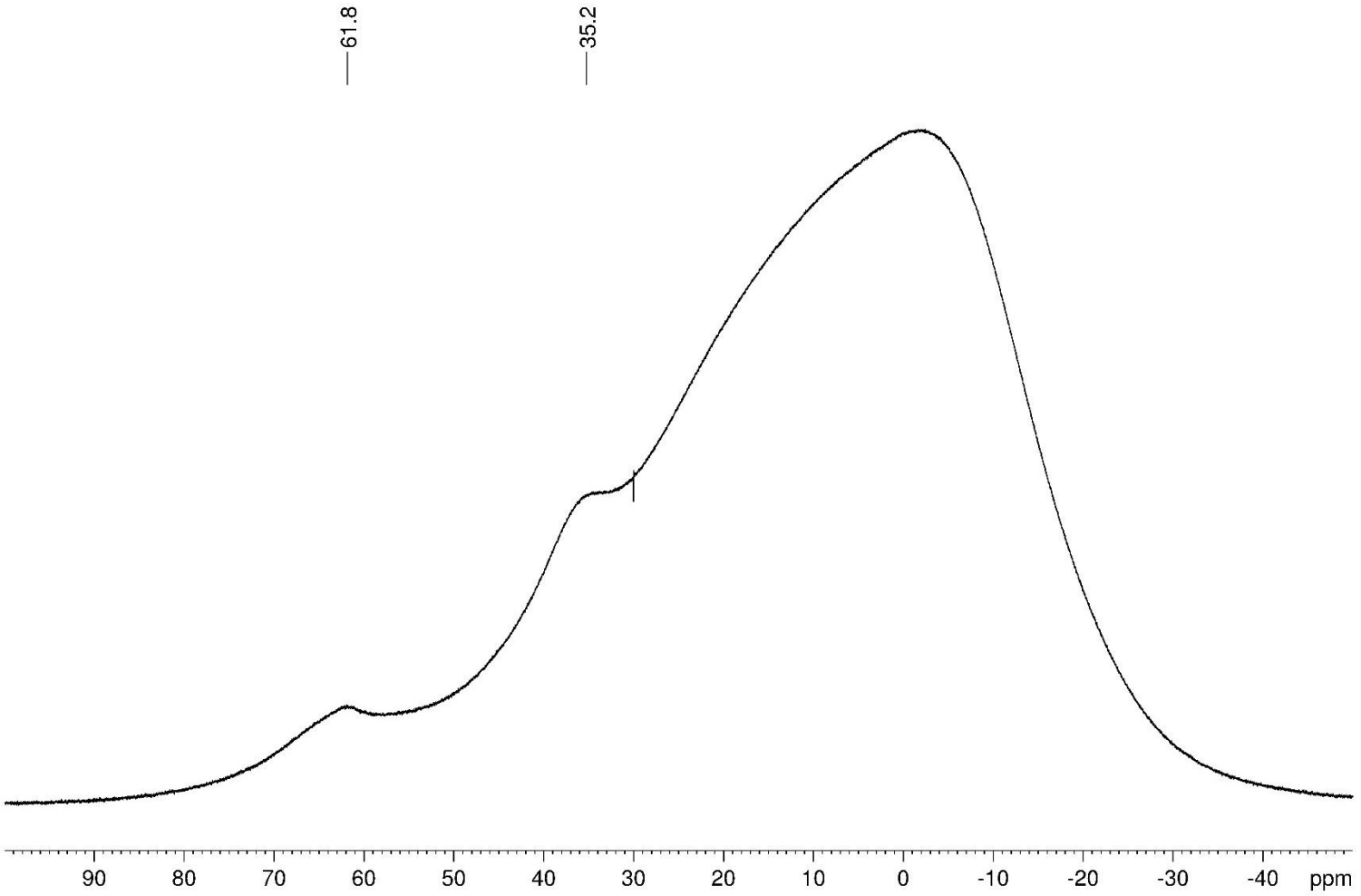


Figure S5. $^{11}B\{^{1}H\}$ NMR spectrum of **2** in C_6D_6.

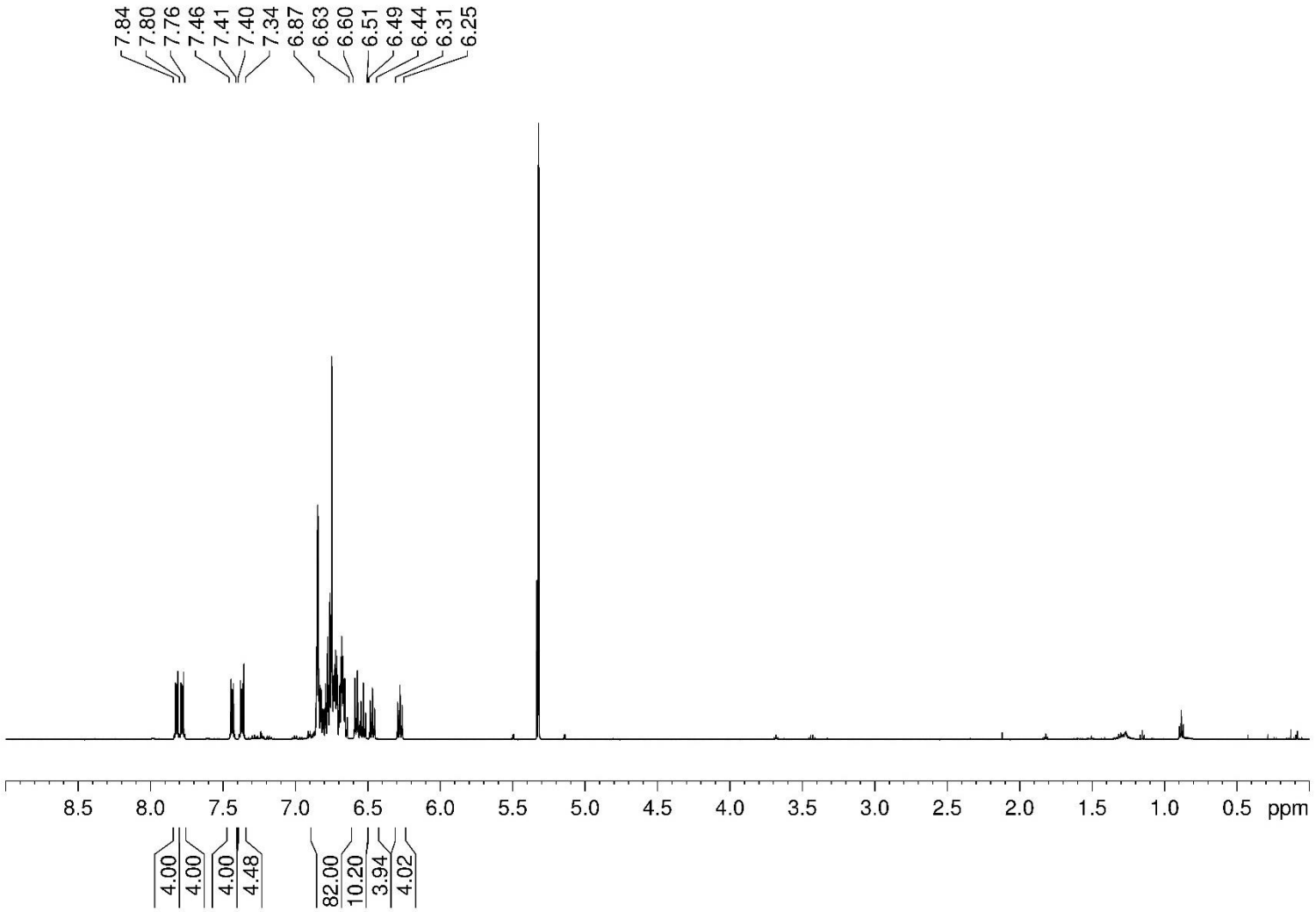


Figure S6. $^{1}H\{^{11}B\}$ NMR spectrum of **4** in CD_2Cl_2.

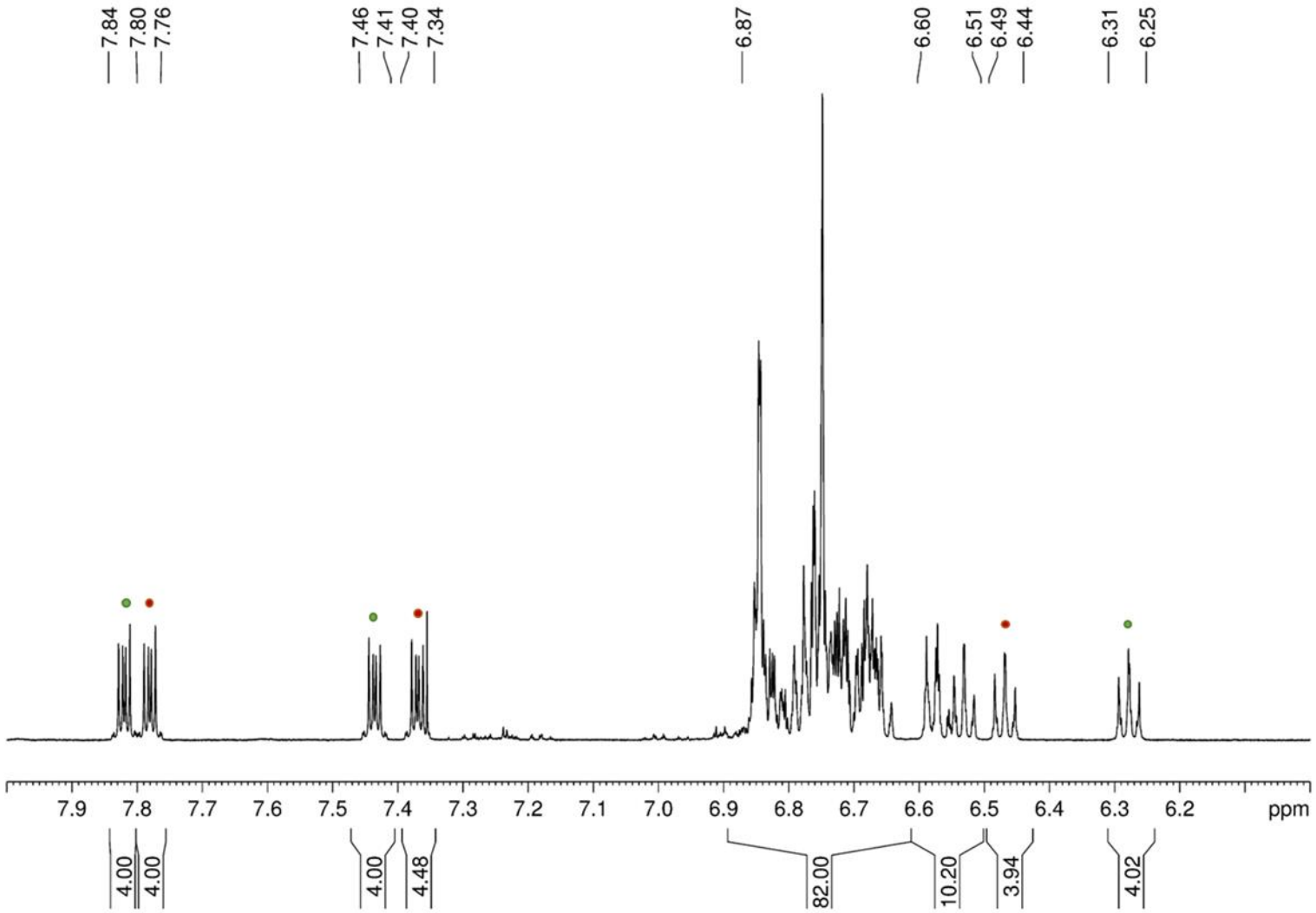


Figure S7. $^{1}H\{^{11}B\}$ NMR spectrum of **4** in CD_2Cl_2 with close-up of the aromatic region, showing the *anti* and *syn* rotamers in a ca. 1:1 ratio. (Rotamer **A**: ●, **B**: ●).

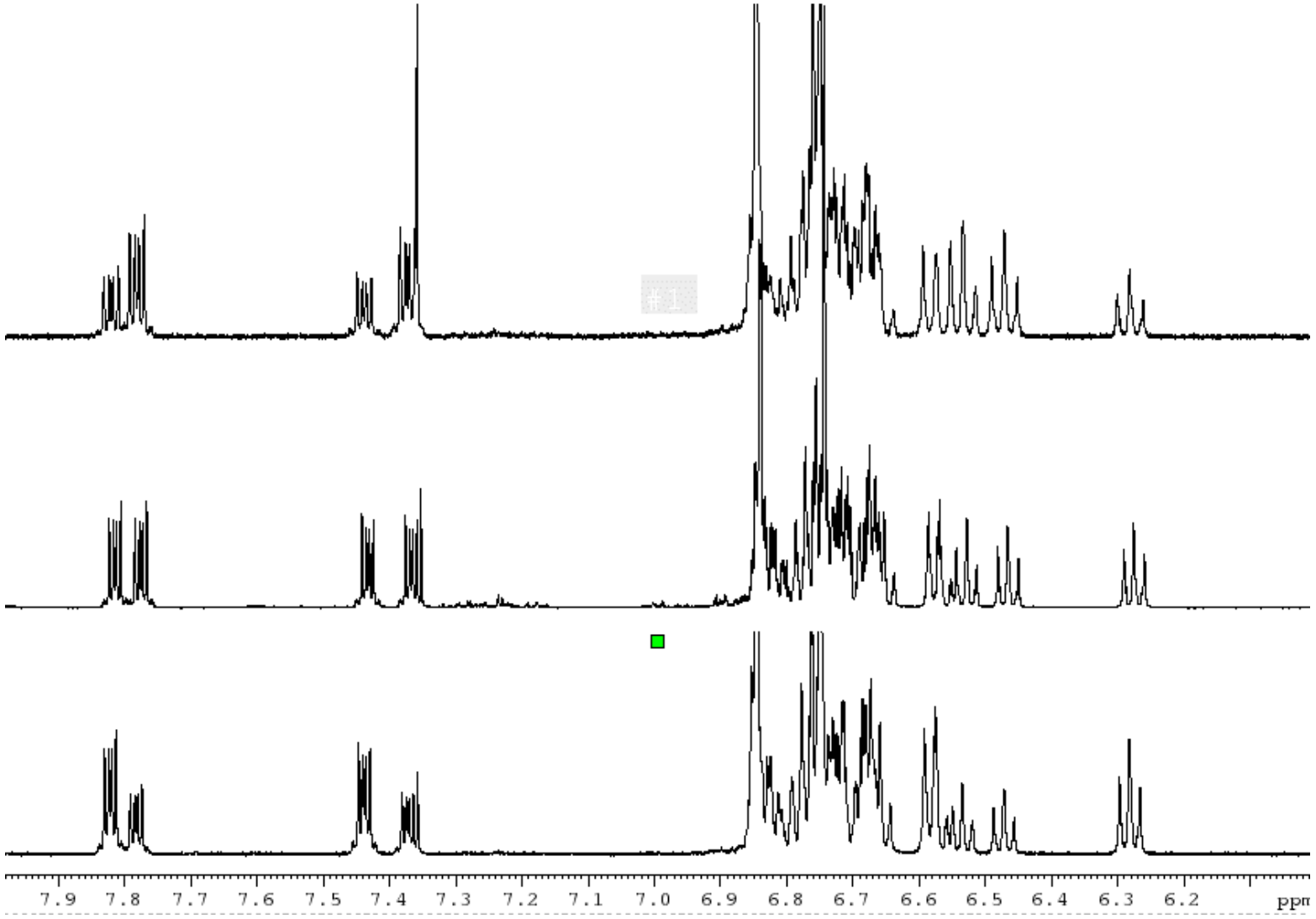


Figure S8. $^{1}H\{^{11}B\}$ NMR spectrum of **4** in CD_2Cl_2 with close-up of the aromatic region showing the *anti* and *syn* rotamers in three different ratios.

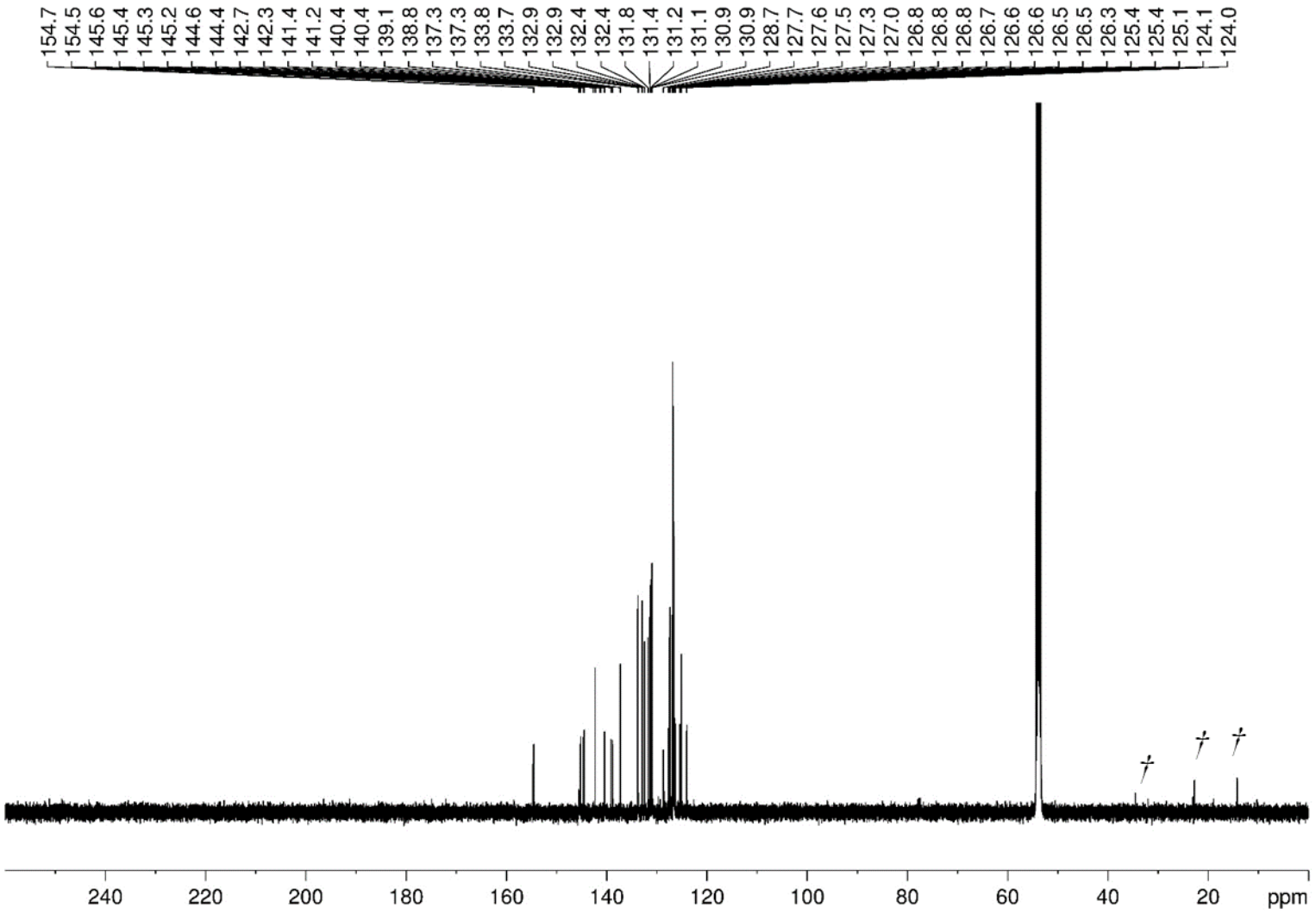


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2 (*† pentane).*

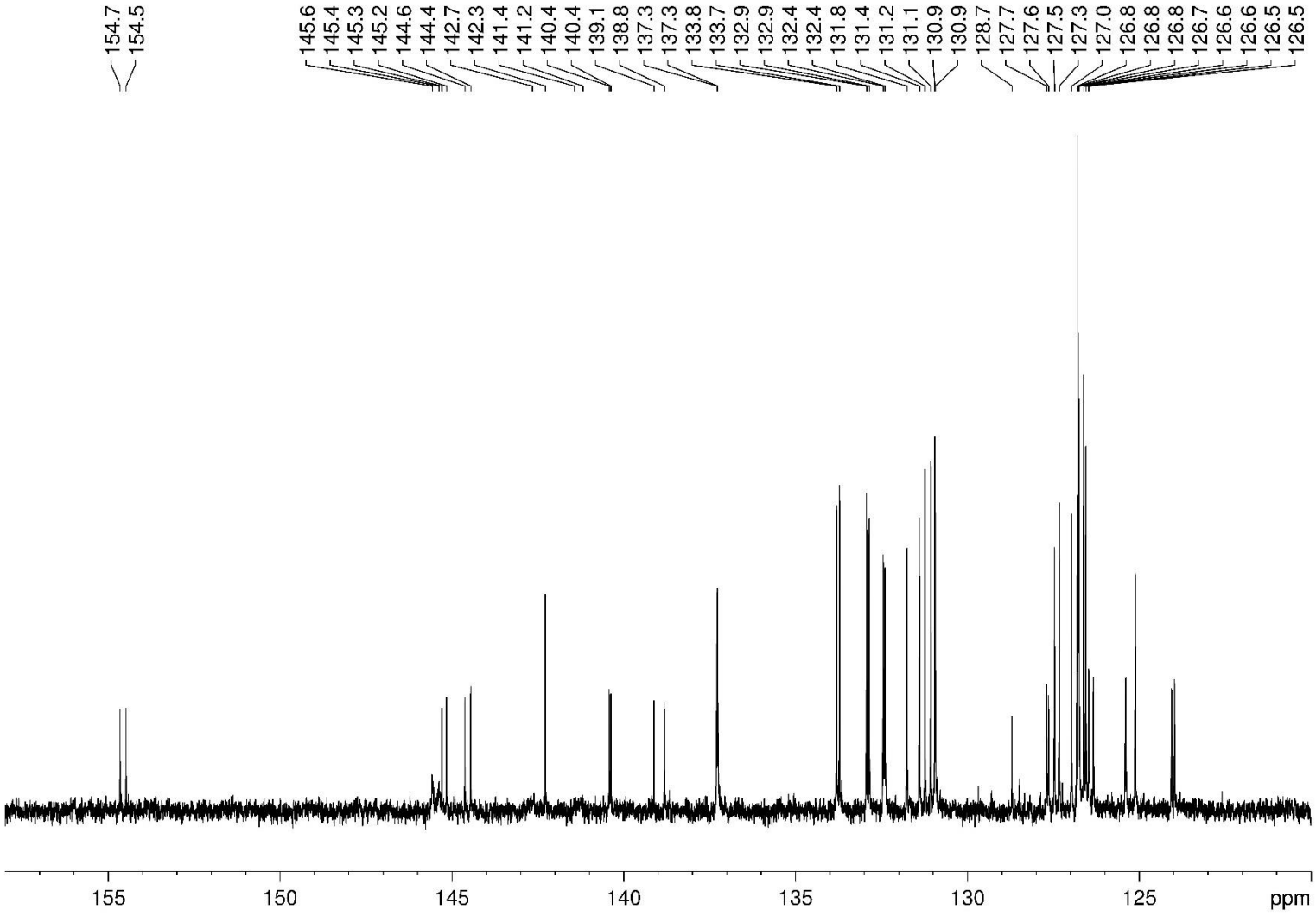


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2 with close-up of the aromatic region.

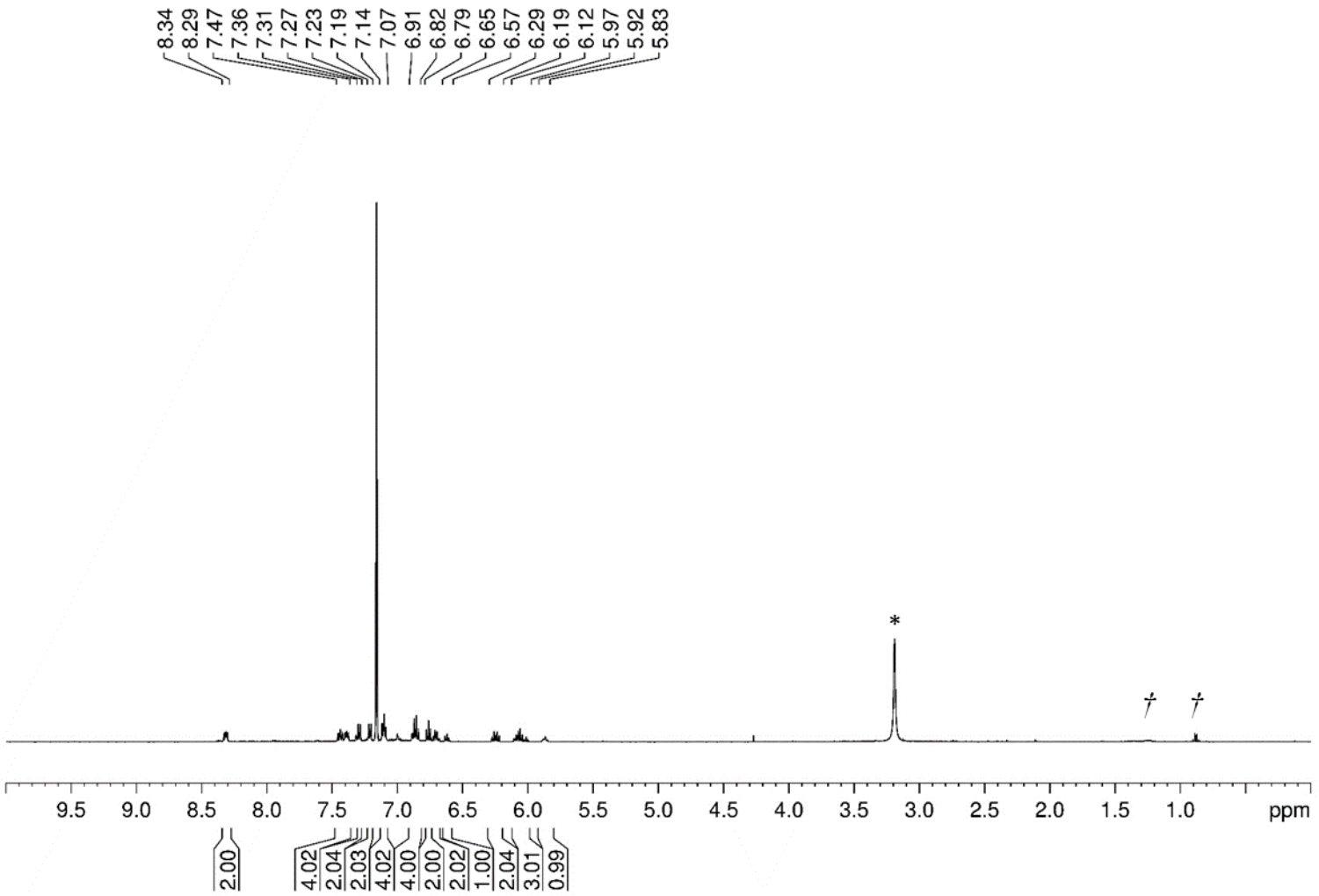


Figure S11. $^{1}H\{^{11}B\}$ NMR spectrum of **[4]K$_2$** in C_6D_6 (*† pentane, * 18-crown-6).*

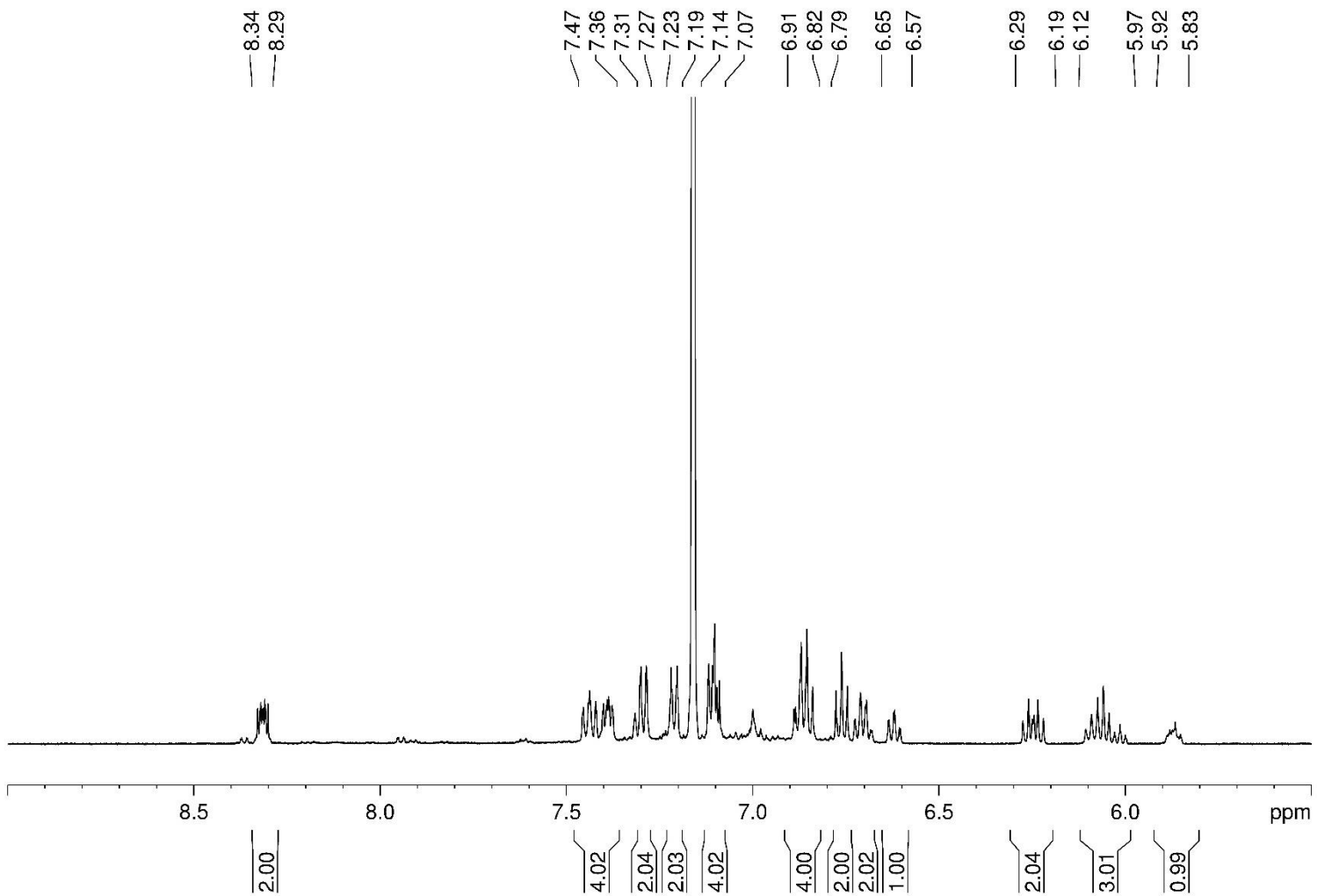


Figure S12. $^{1}H\{^{11}B\}$ NMR spectrum of **[4]K$_2$** in C_6D_6 with close-up of the aromatic region. Small impurities are present, arising from the slow decomposition of **[4]K$_2$** in solution.

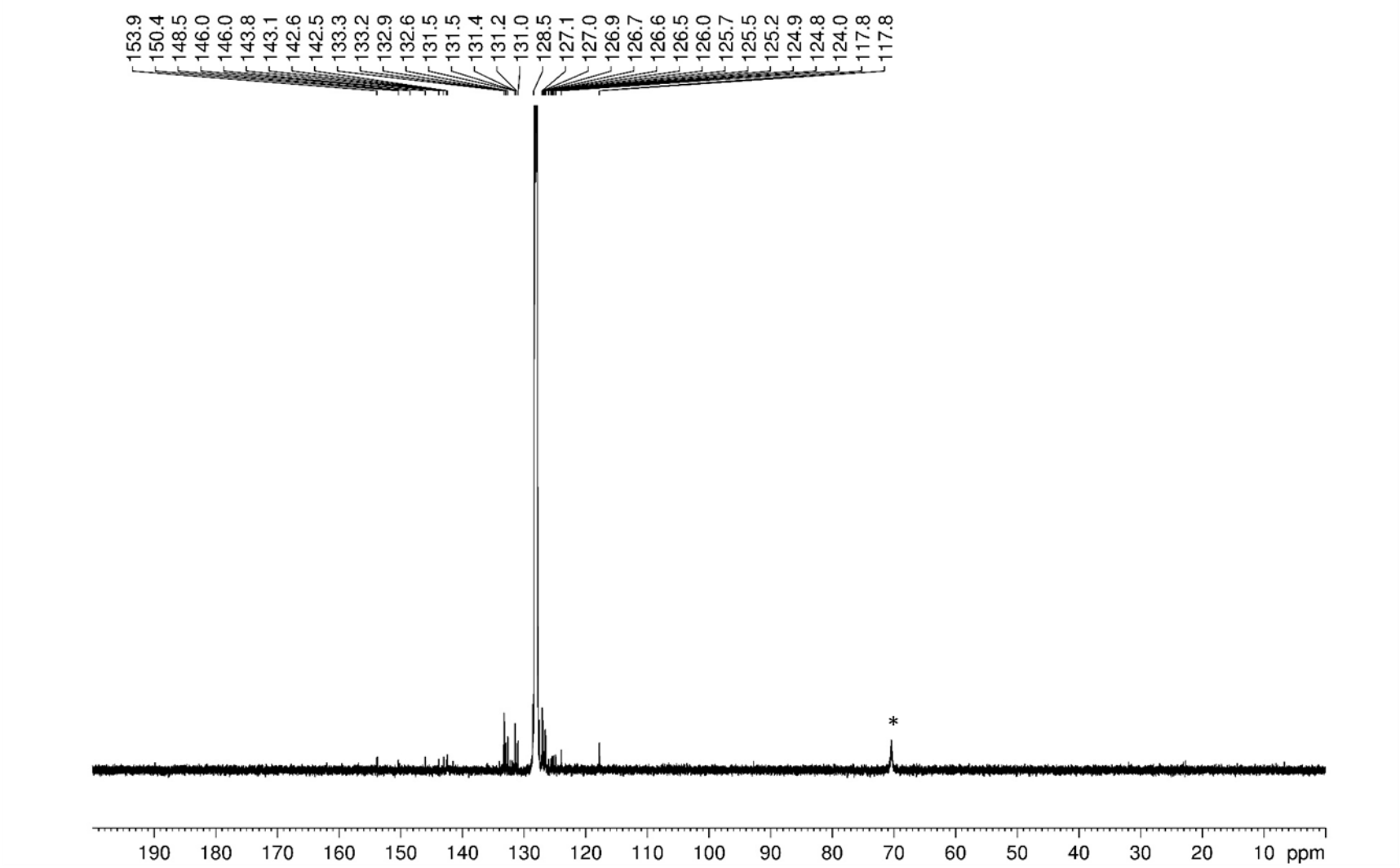


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **[4]K2** in C_6D_6 (** 18-crown-6).*

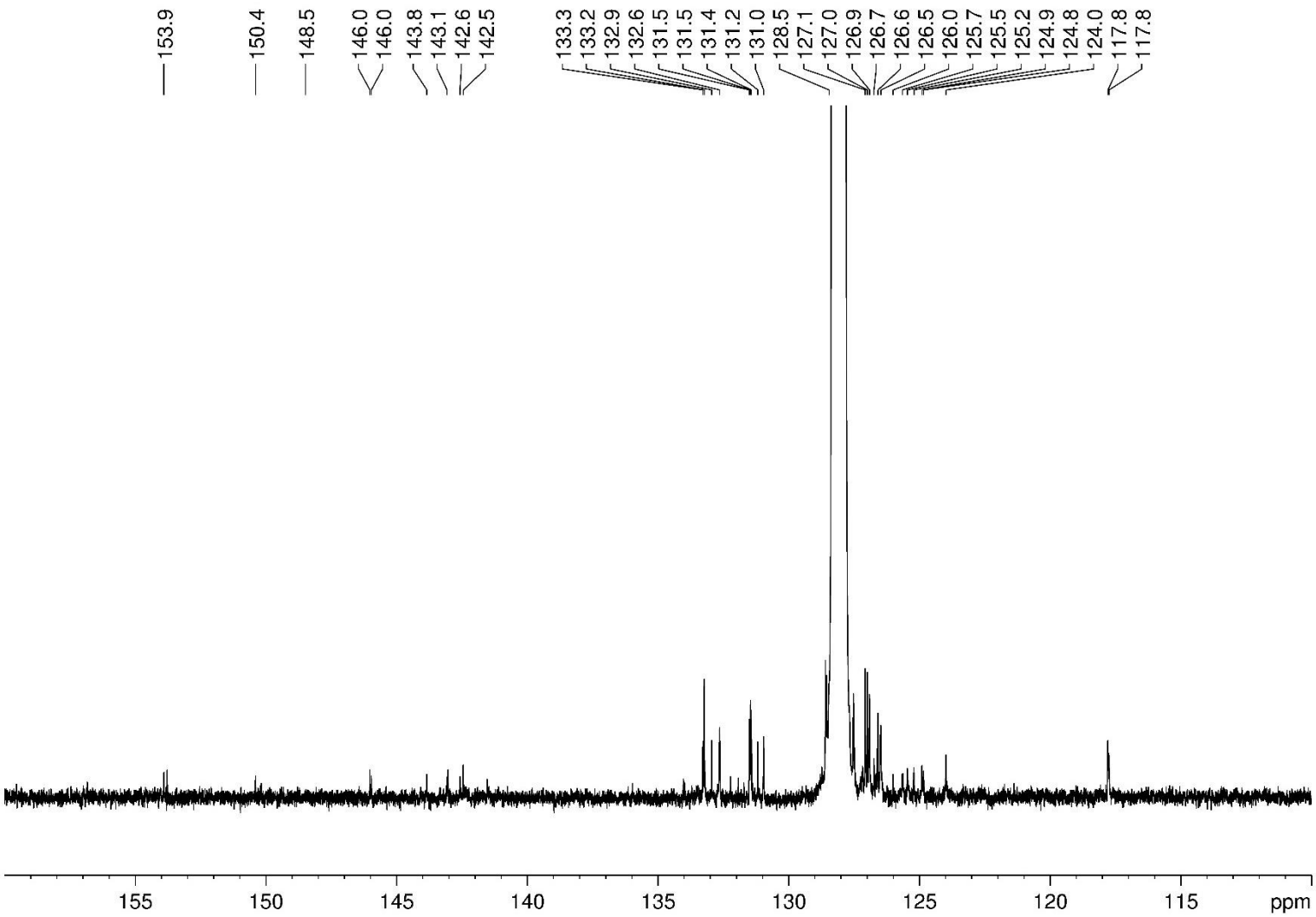


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **[4]K$_2$** in C_6D_6 with close-up of the aromatic region.

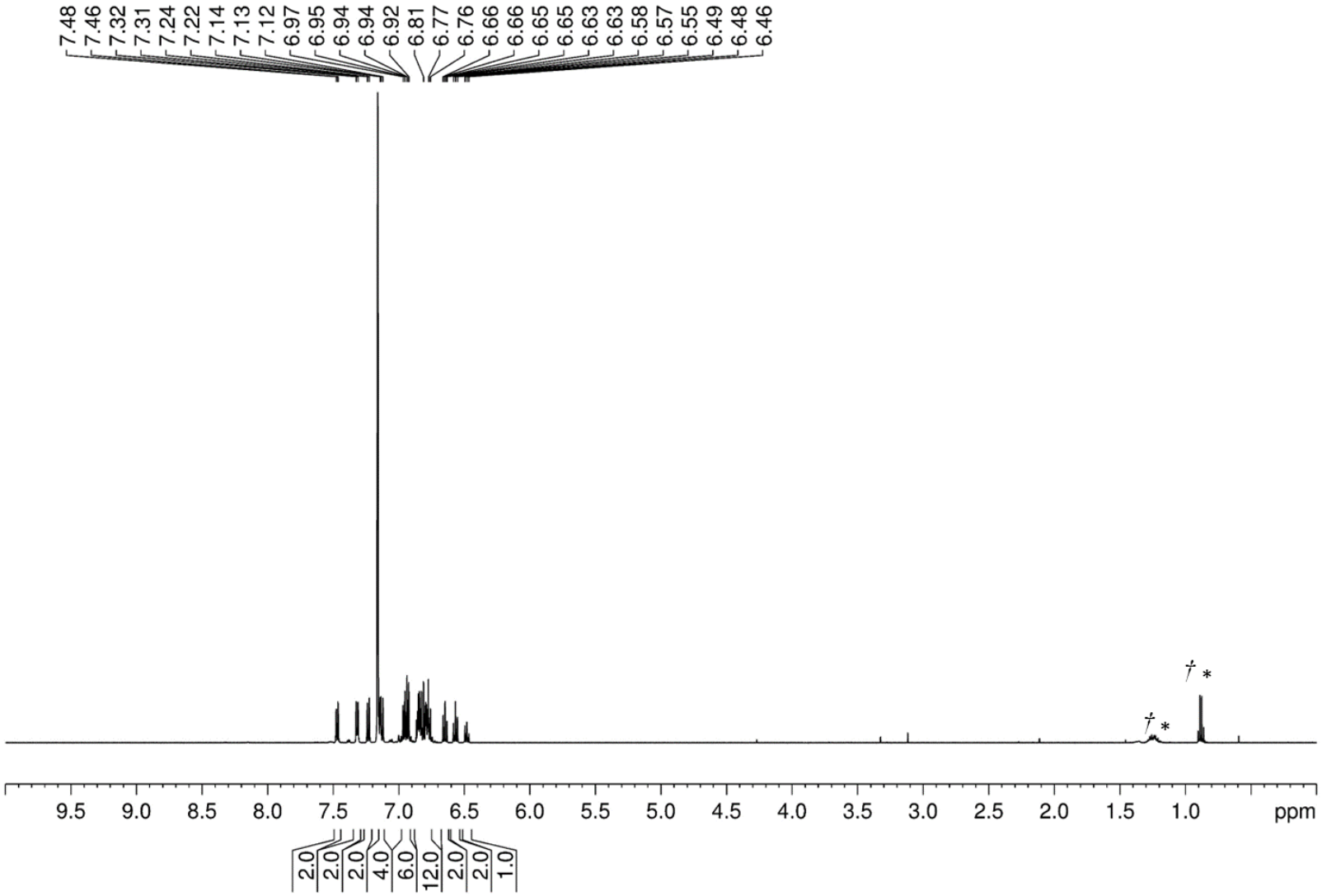


Figure S15. $^{1}H\{^{11}B\}$ NMR spectrum of **5** in C_6D_6 (*† pentane, * hexane).*

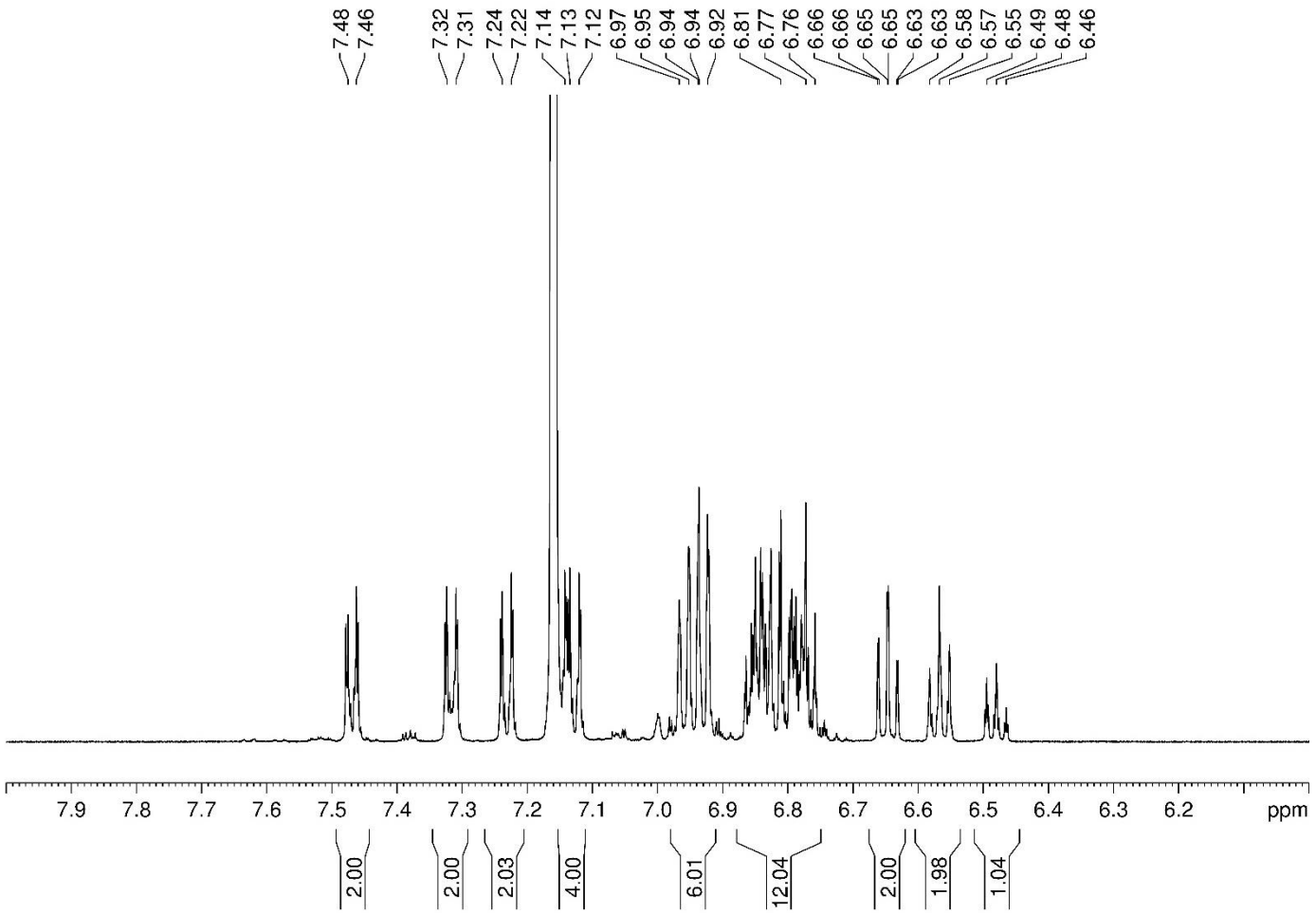


Figure S16. $^{1}H\{^{11}B\}$ NMR spectrum of **5** in C_6D_6 with close-up of the aromatic region.

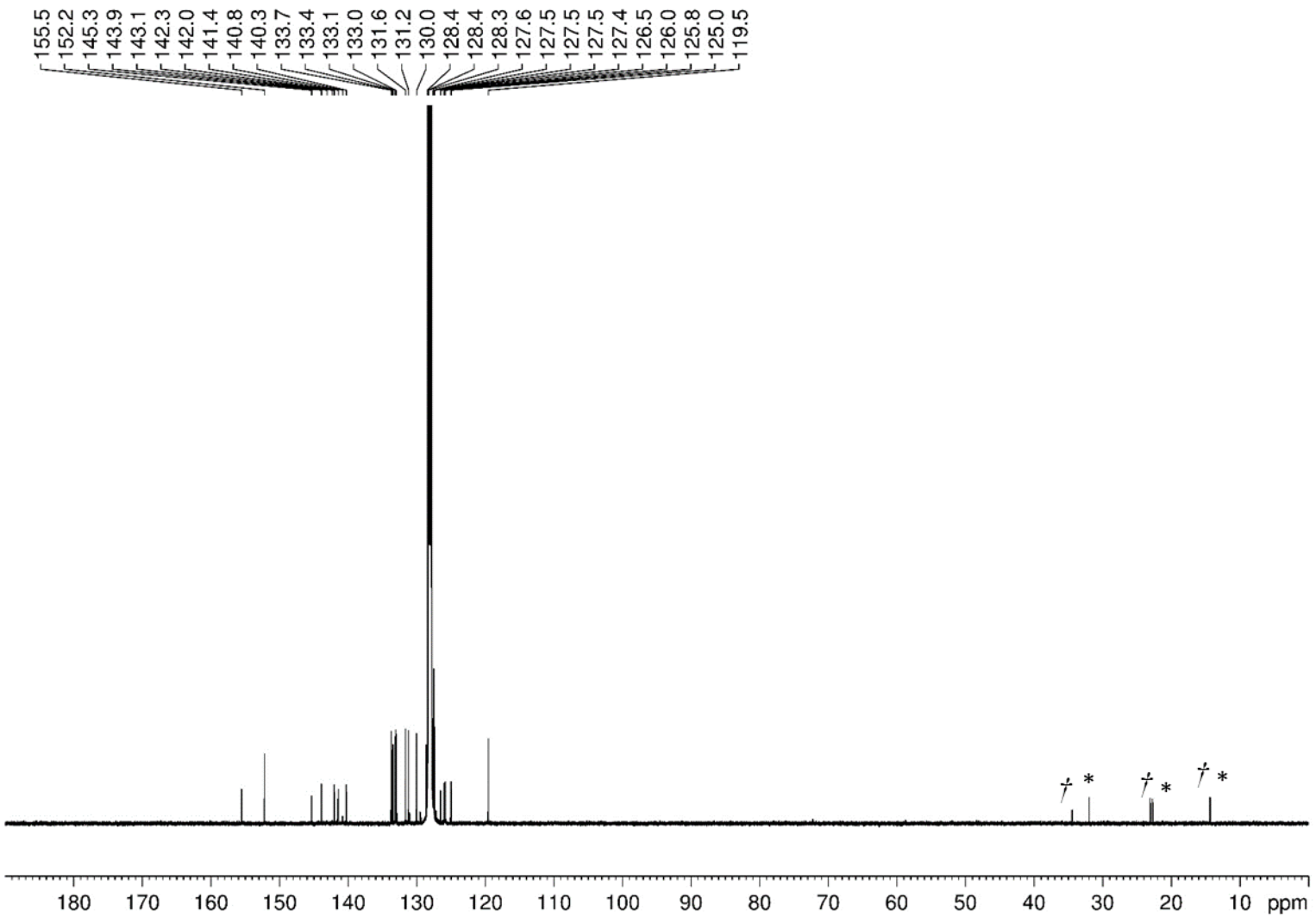


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 (*† pentane, * hexane).*

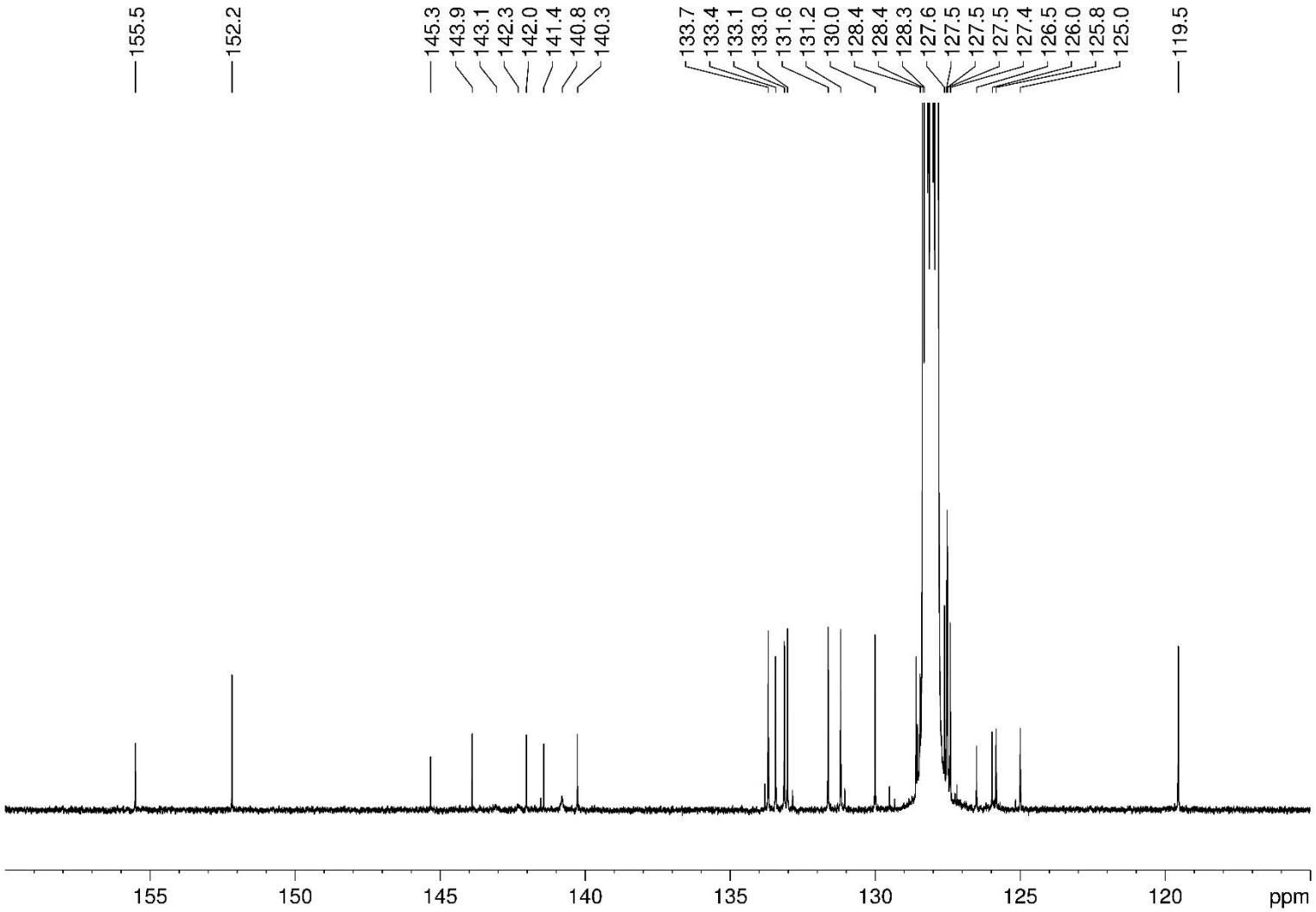


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 with close-up of the aromatic region.

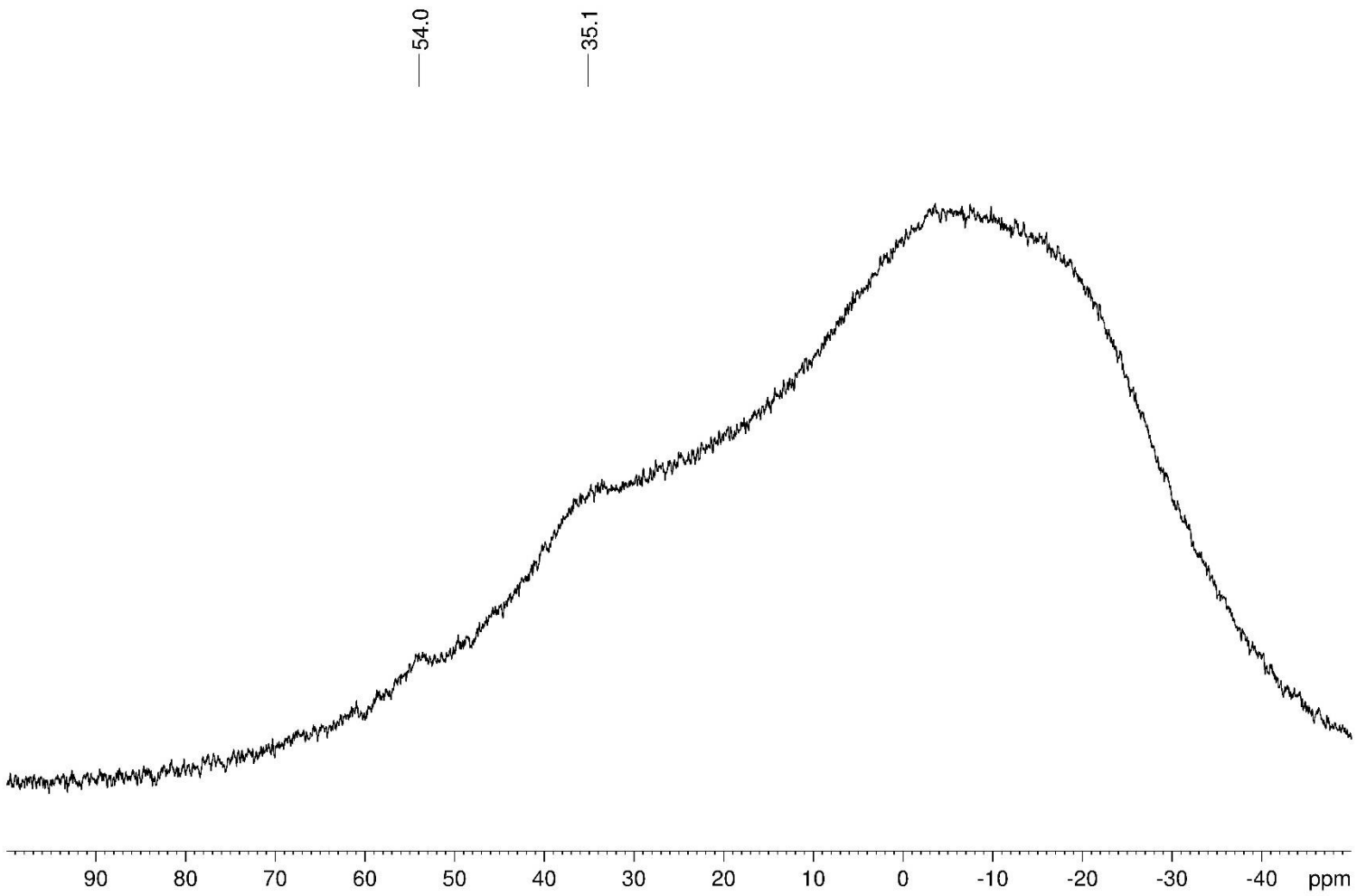


Figure S19. $^{11}B\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

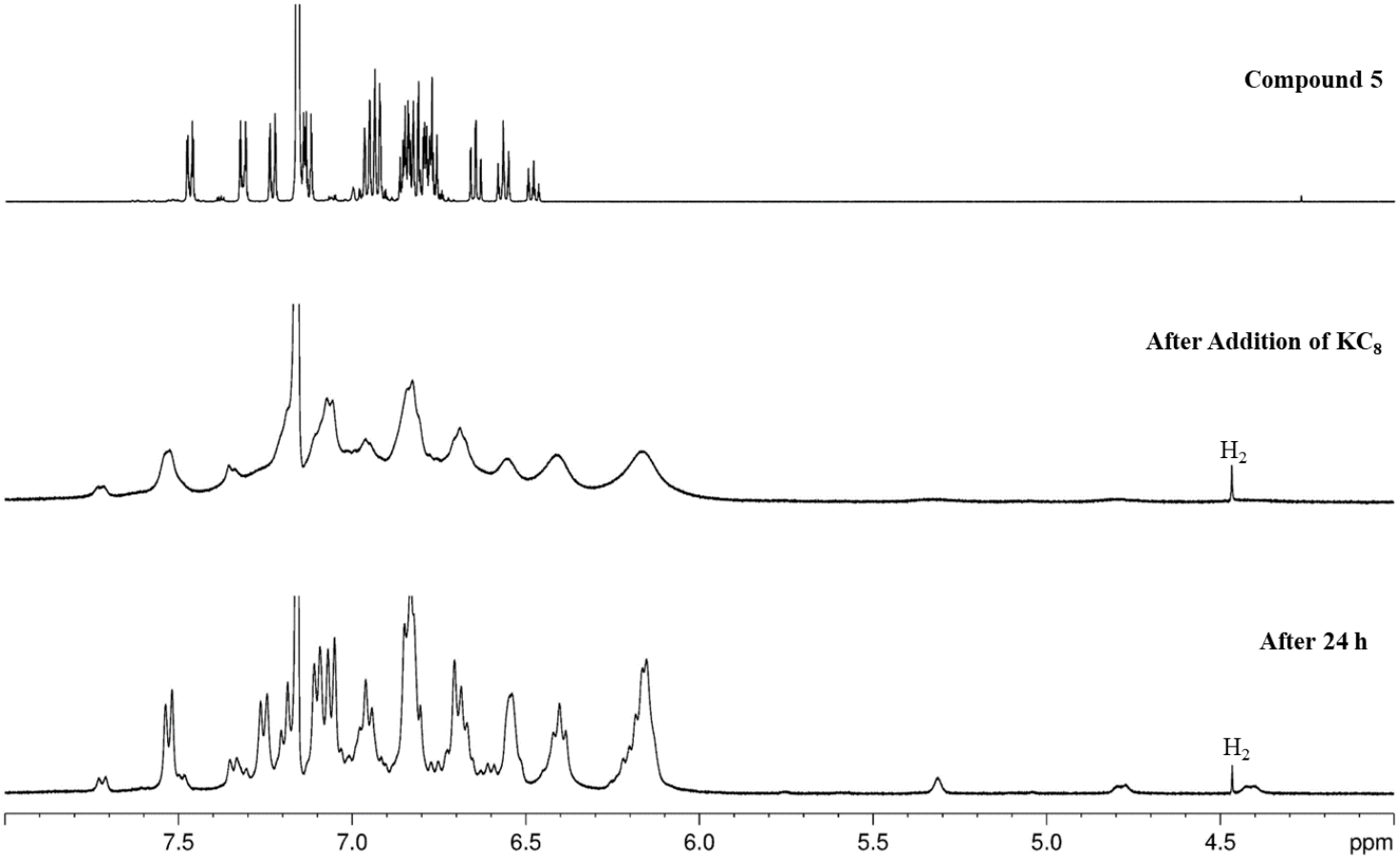


Figure S20. Stacked $^{1}H\{^{11}B\}$ NMR spectra of the reduction of **5** with KC_8 in C_6D_6 with close-up of the aromatic region.

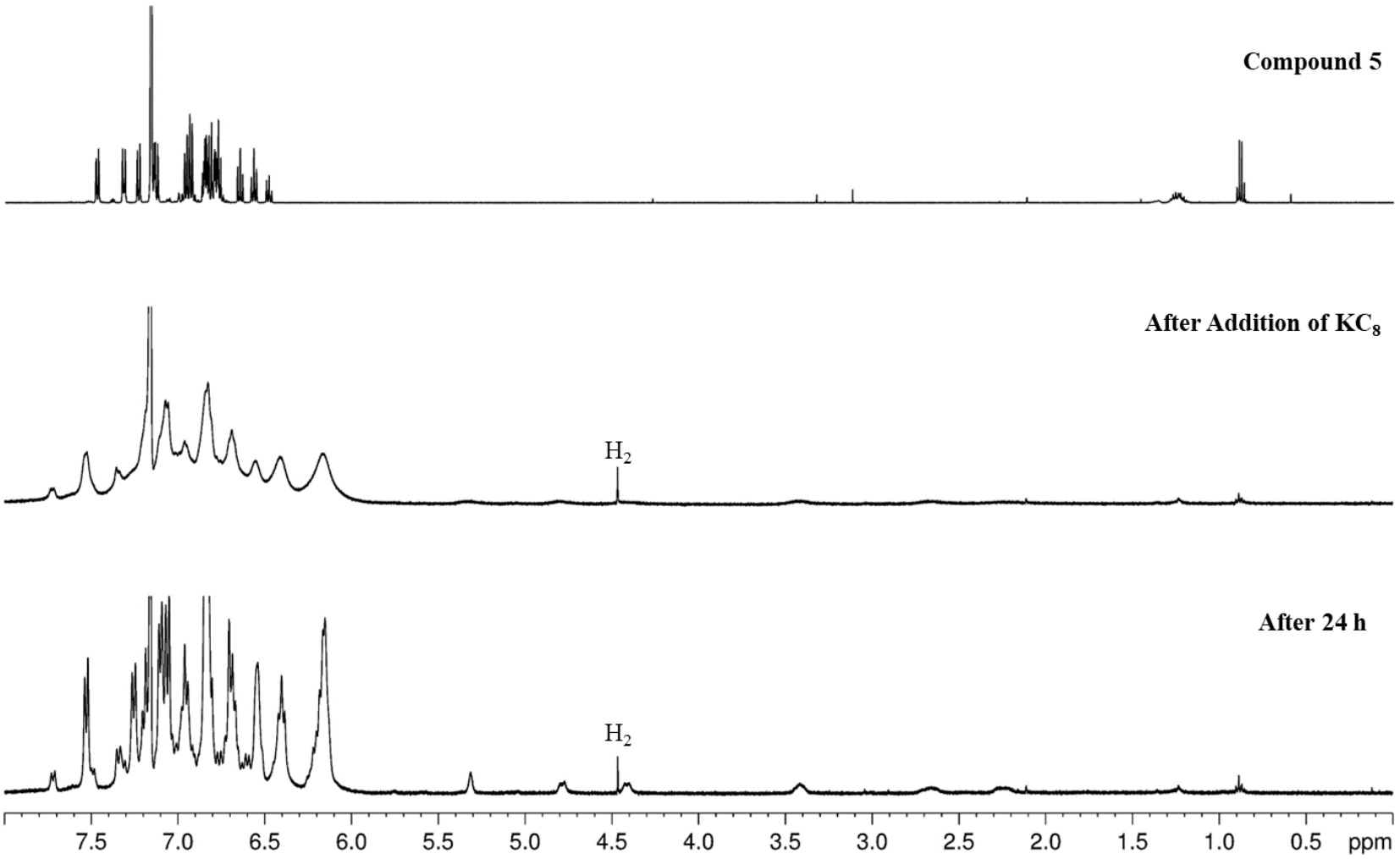


Figure S21. Stacked $^{1}H\{^{11}B\}$ NMR spectra of the reduction of **5** with KC_8 in C_6D_6.

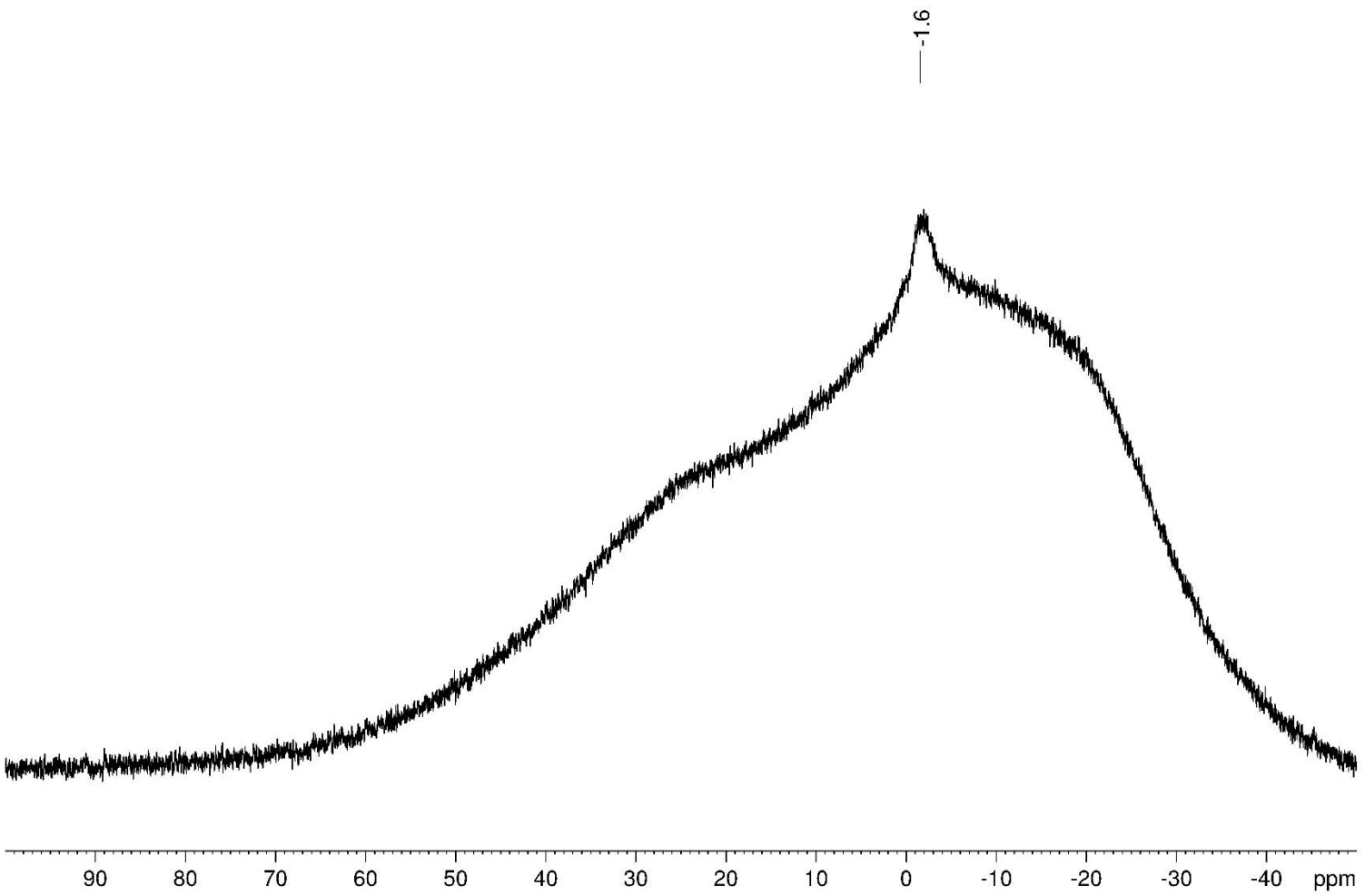


Figure S22. $^{11}B\{^{1}H\}$ NMR spectrum of **6** in C_6D_6.

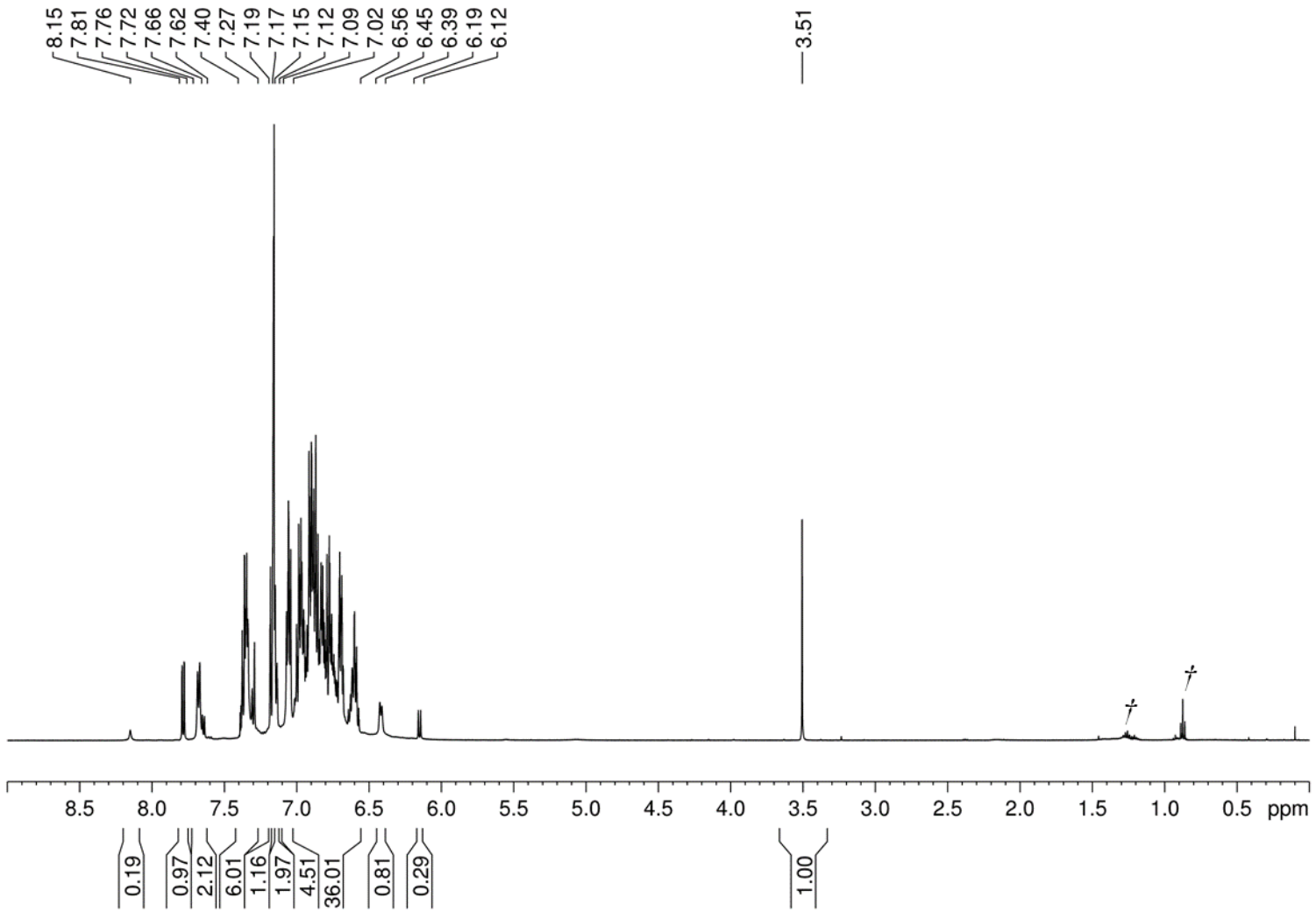


Figure S23. $^{1}H\{^{11}B\}$ NMR spectrum of **8** in C_6D_6 (*† pentane)*.

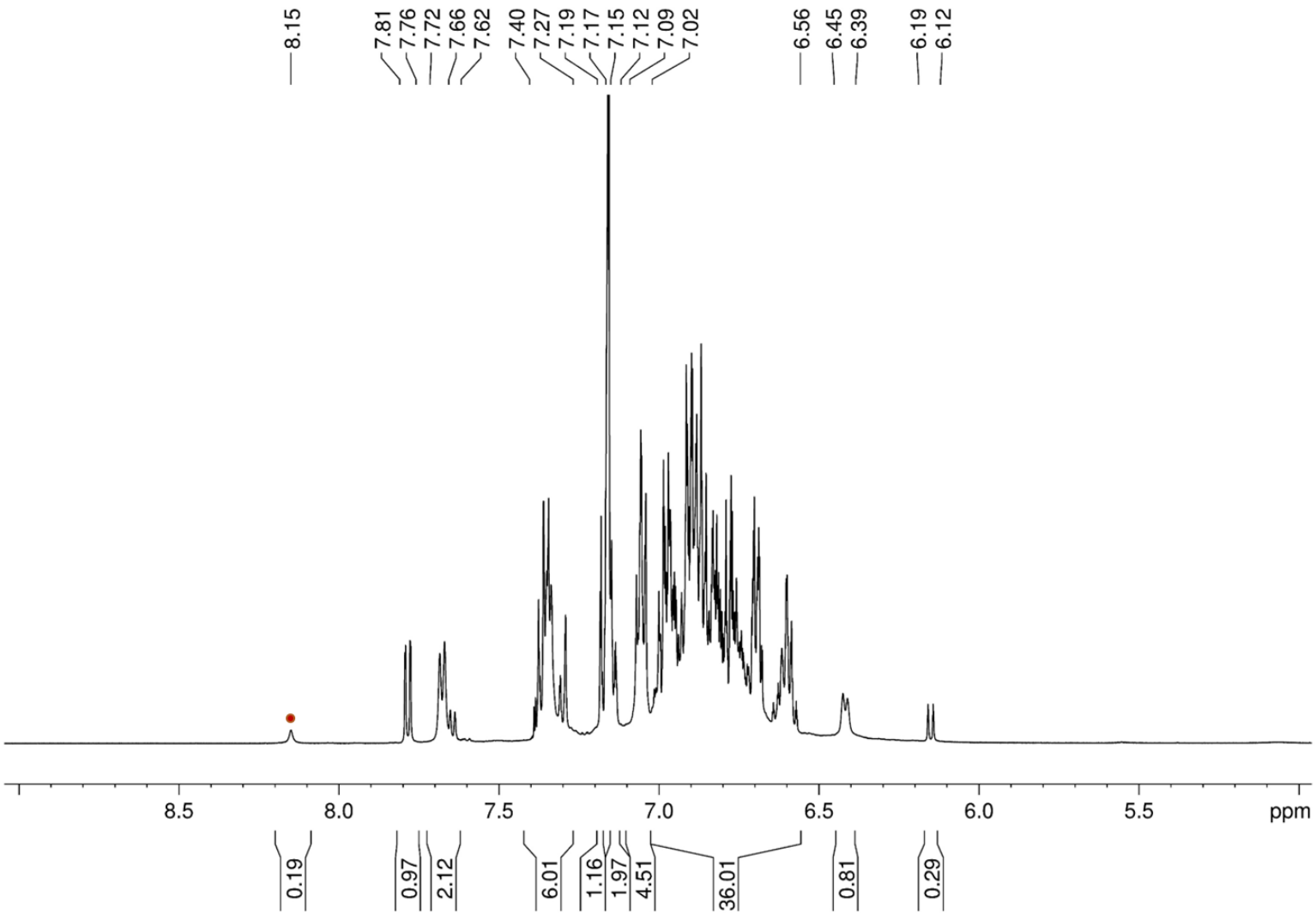


Figure S24. $^{1}H\{^{11}B\}$ NMR spectrum of **8** in C_6D_6 with close-up of the aromatic region (● **C** as impurity 14%, exactly assigned signals in the $^{13}C\{^{1}H\}$ NMR).

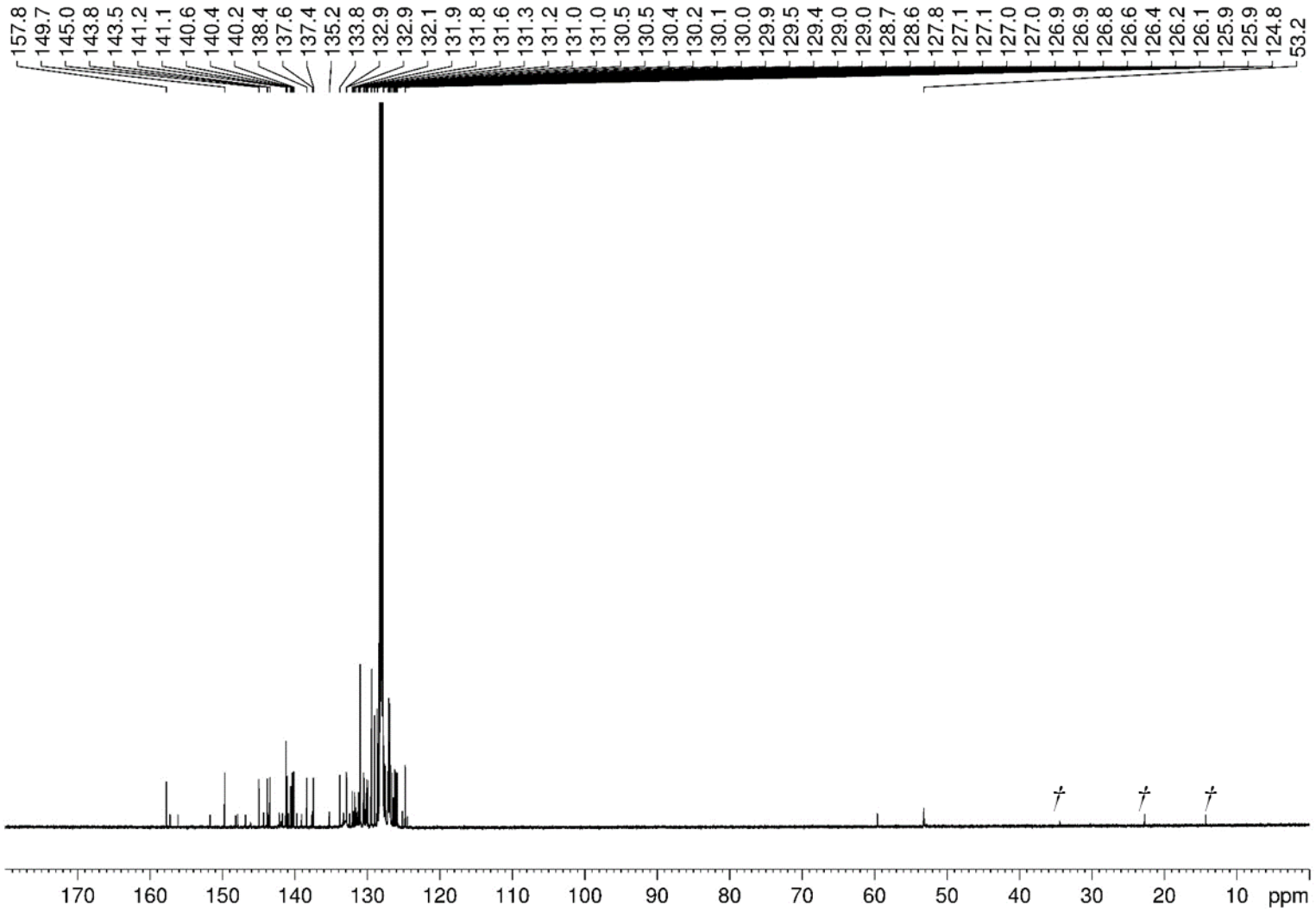


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of **8** in C_6D_6 (*† pentane).*

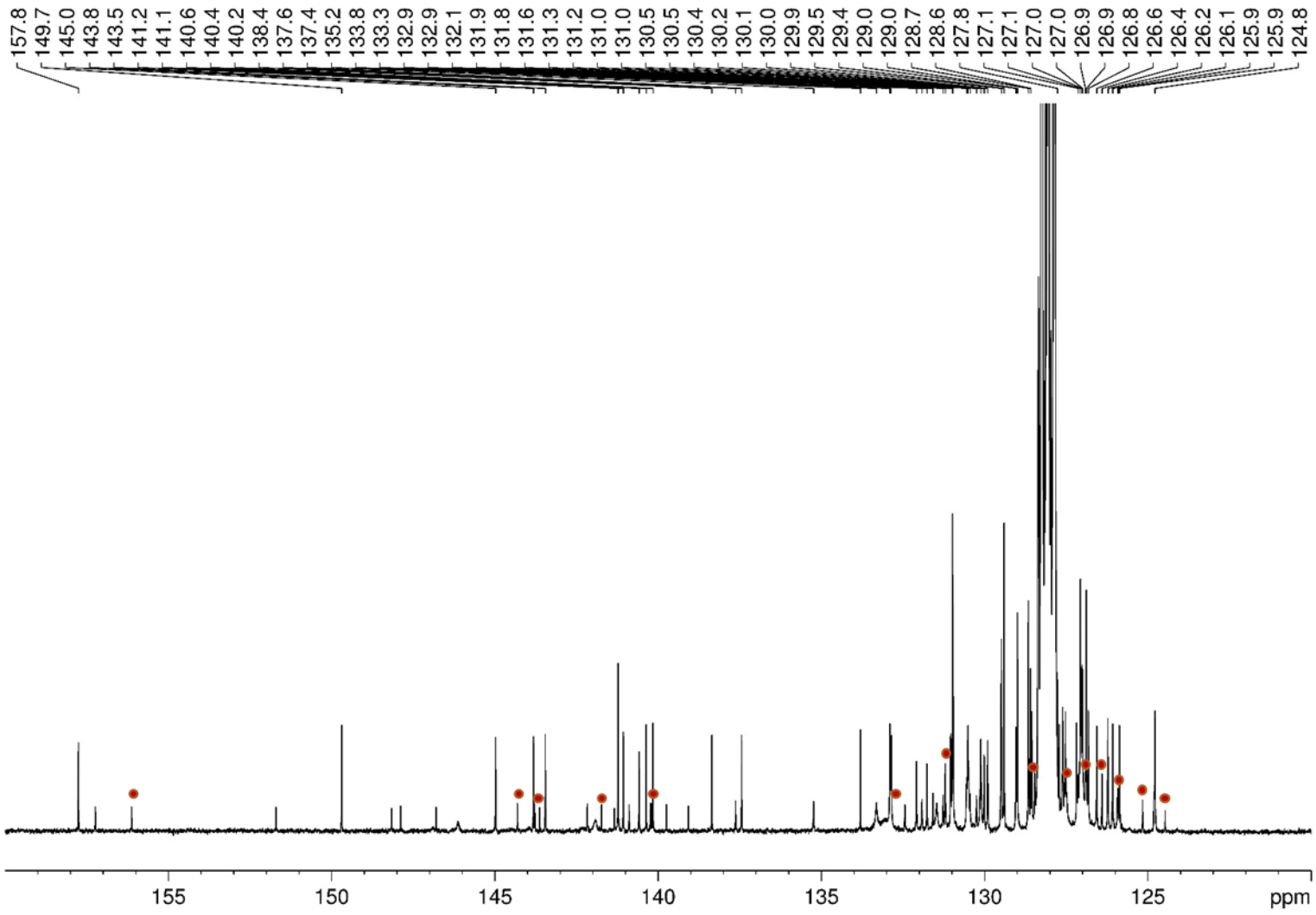


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of **(Ph)(Cl-Borol)** in C_6D_6 with close-up of the aromatic region (● C as impurity).

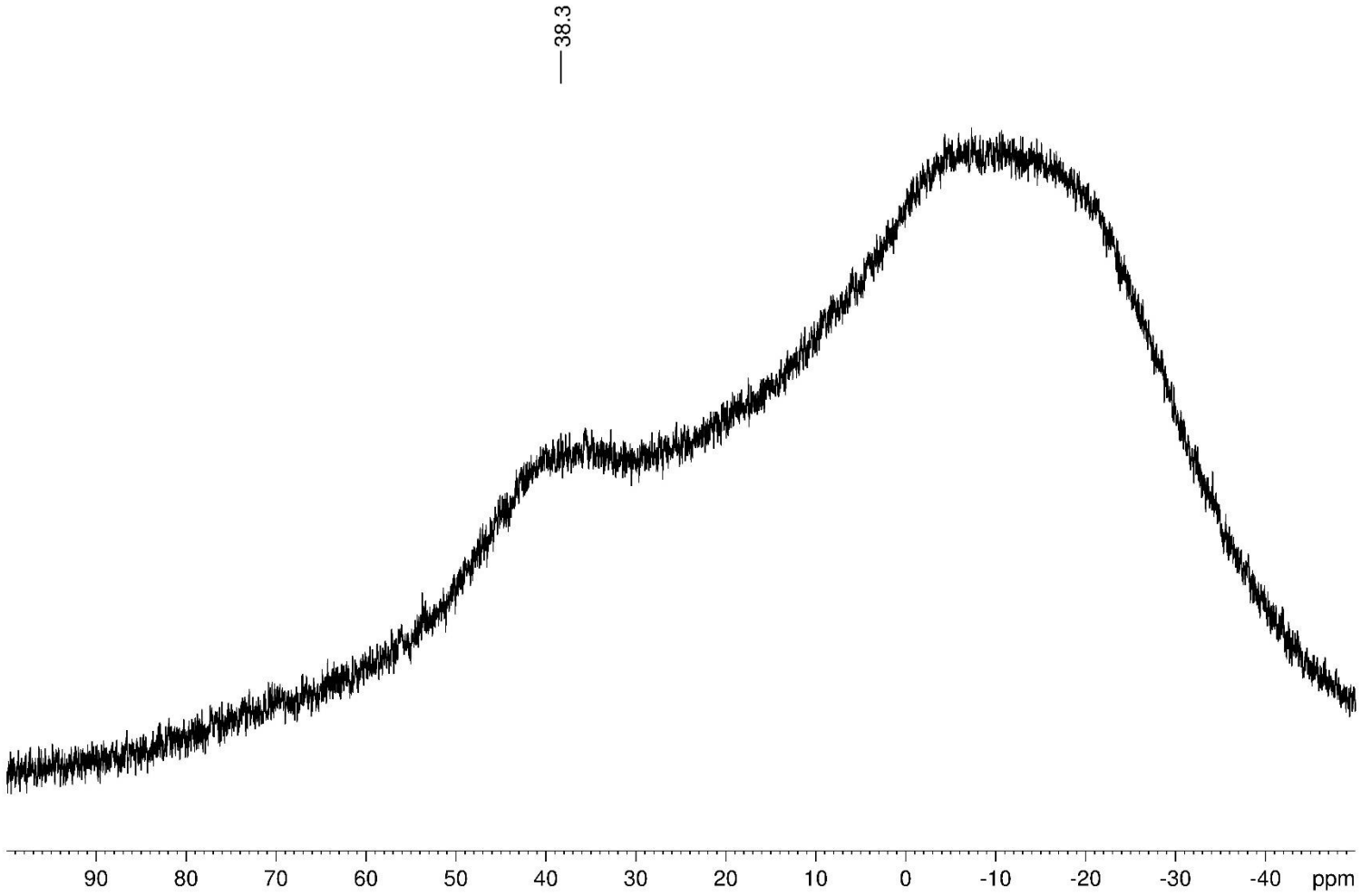


Figure S27. $^{11}B\{^{1}H\}$ NMR spectrum of **8** in C_6D_6.

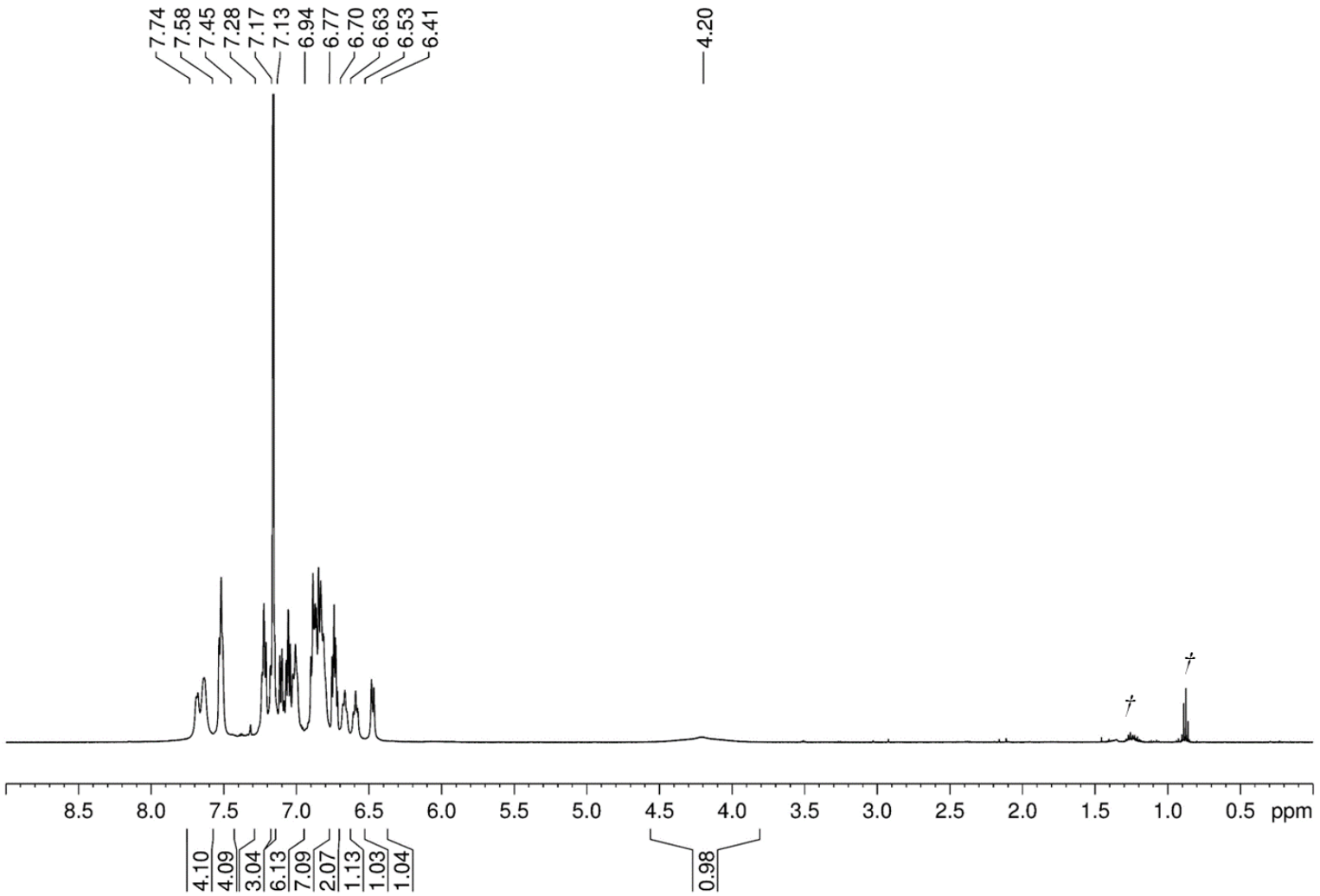


Figure S28. $^{1}H\{^{11}B\}$ NMR spectrum of **[11]K** in C_6D_6 (*† pentane).*

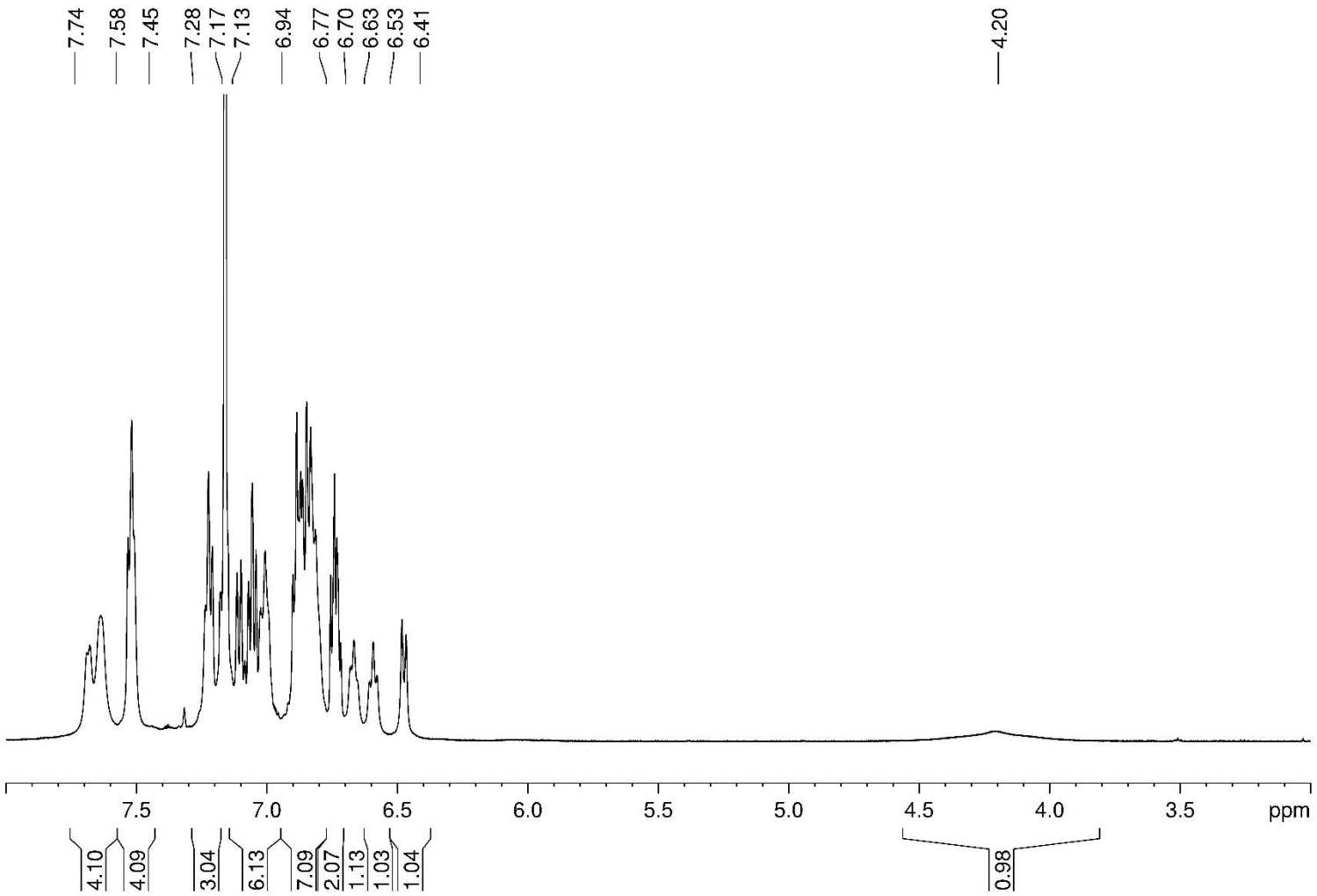


Figure S29. $^{1}H\{^{11}B\}$ NMR spectrum of **[11]K** in C_6D_6 with close-up of the aromatic region.

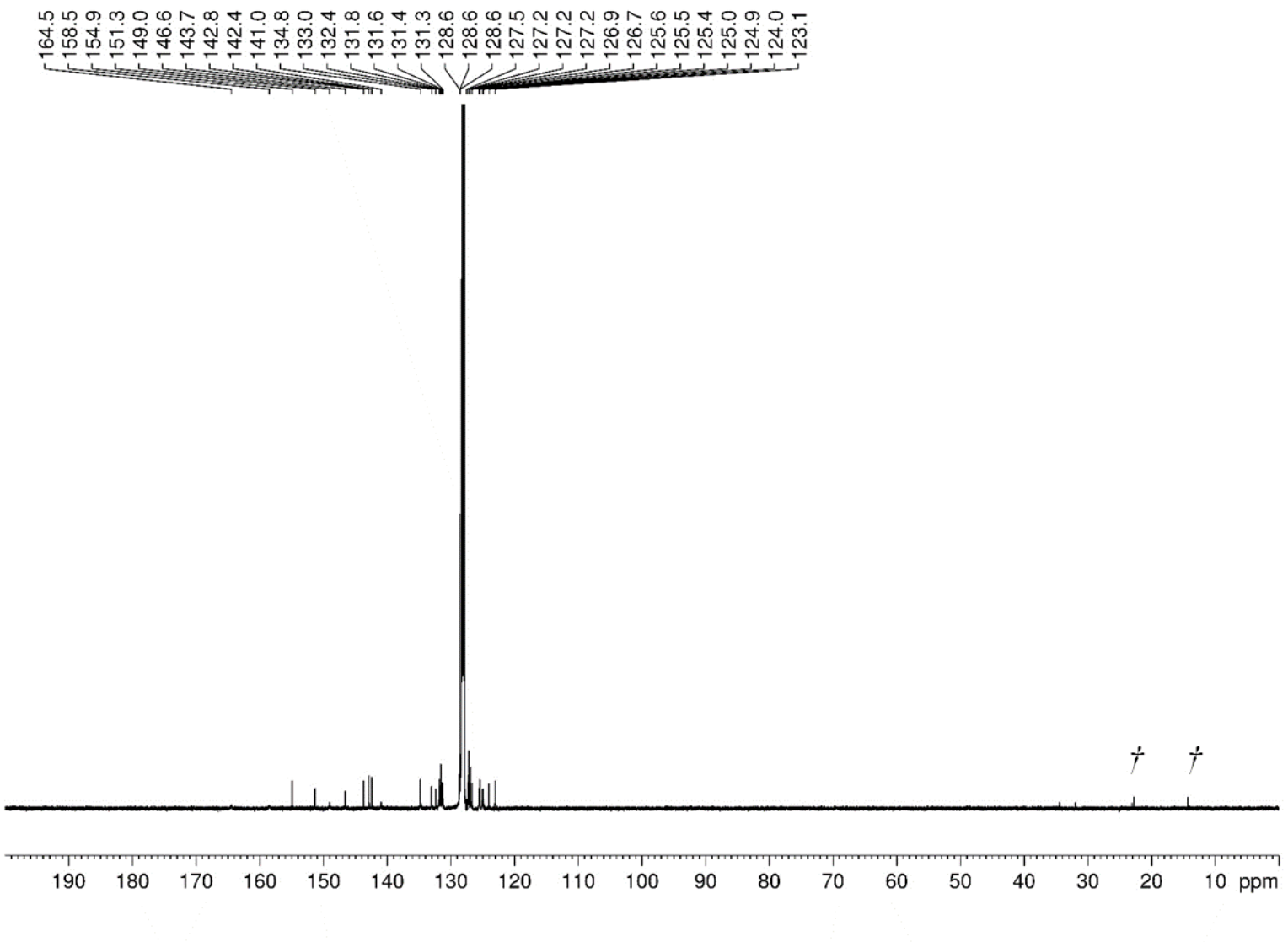


Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of **[11]K** in C_6D_6 (*† pentane).*

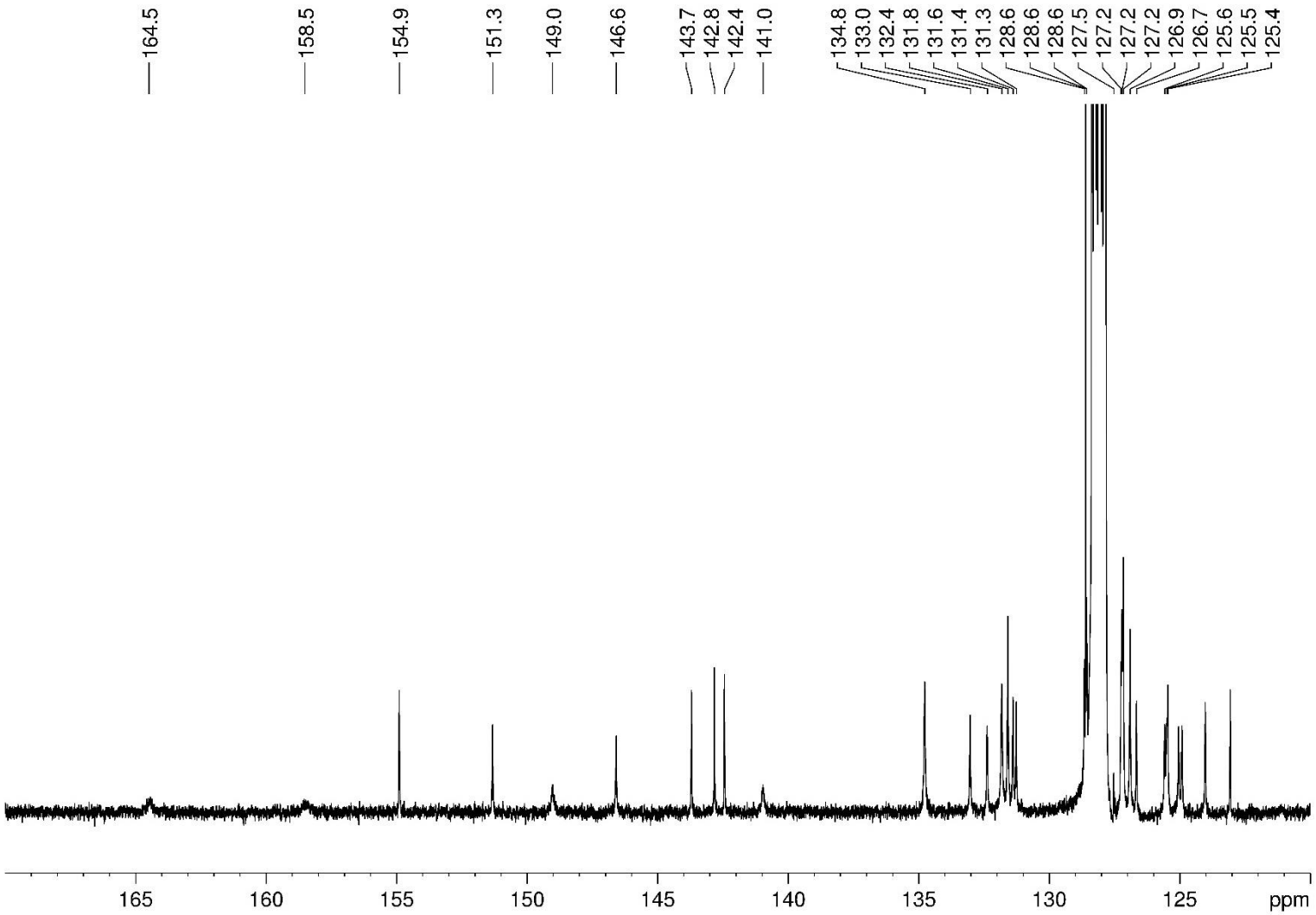


Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum of **[11]K** in C_6D_6 with close-up of the aromatic region.

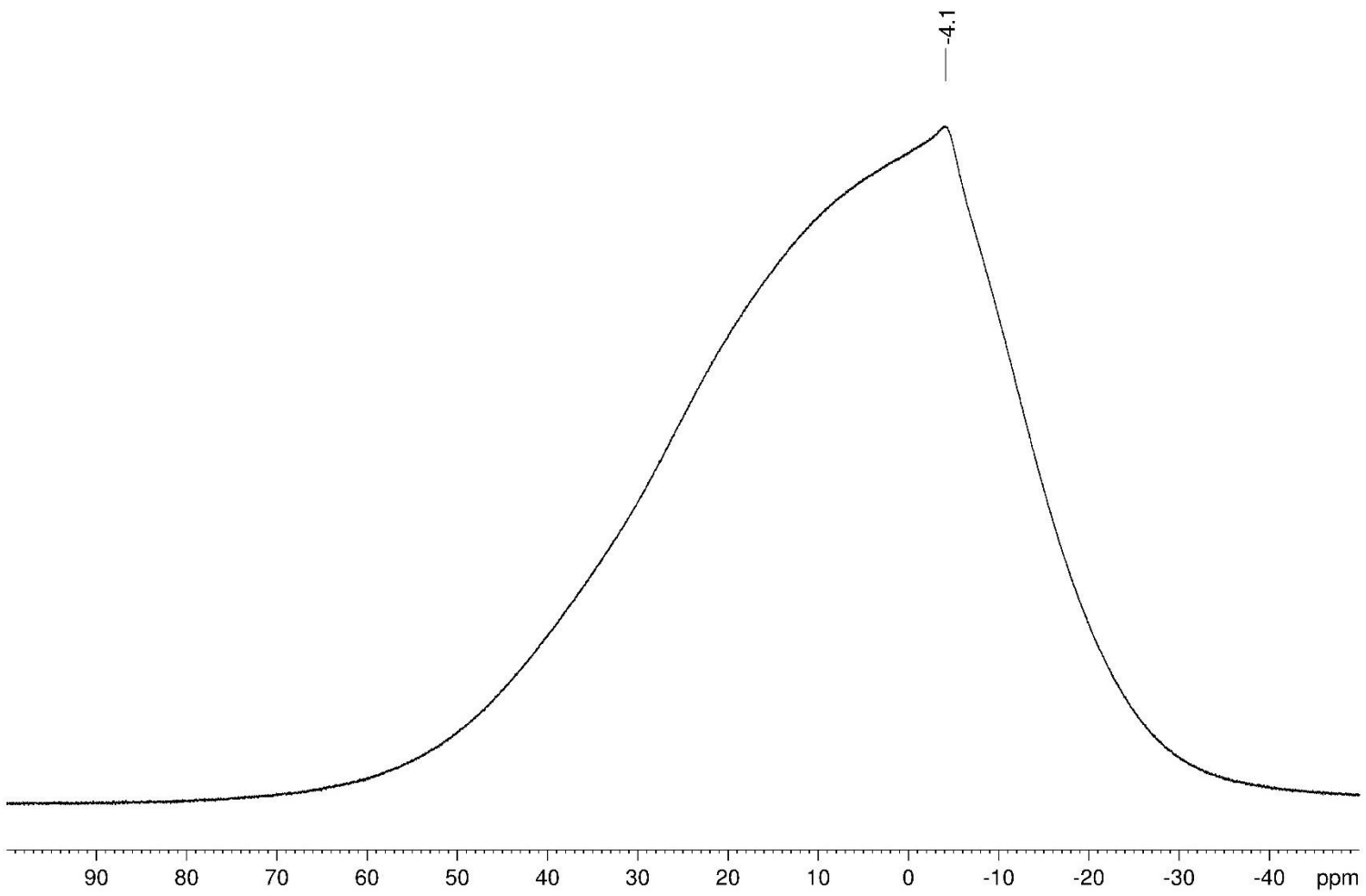


Figure S32. $^{11}B\{^{1}H\}$ NMR spectrum of **11** in C_6D_6.

Cyclic voltammetry

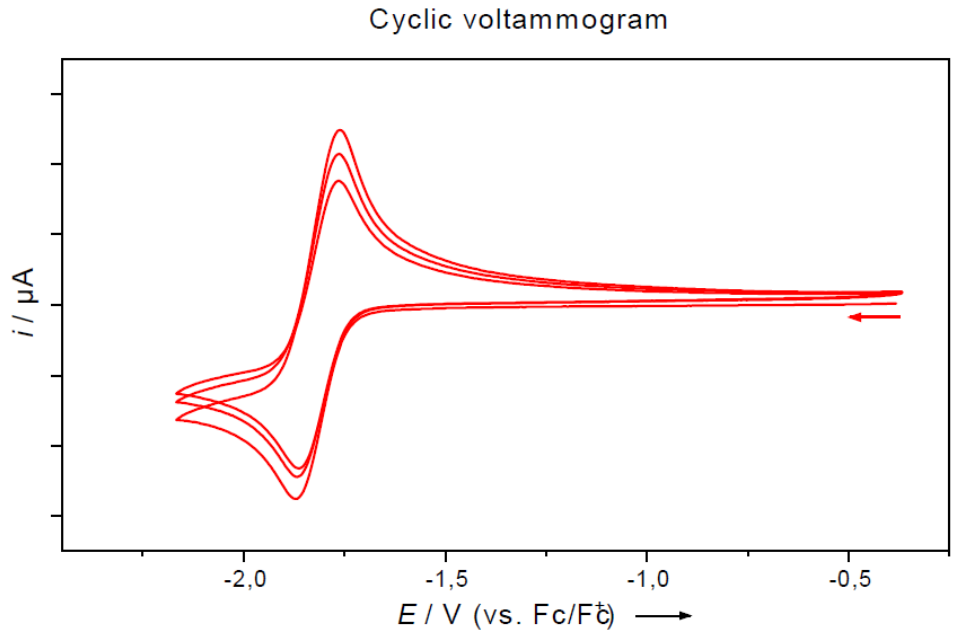


Figure S33. Cyclic voltammogram of **4** in DCM/0.1 M [*n*Bu$_4$N][PF$_6$] measured at 250 mV s^{-1} with voltammetric response in three cycles. Formal potential: $E_{1/2}$ = −1.81 V.

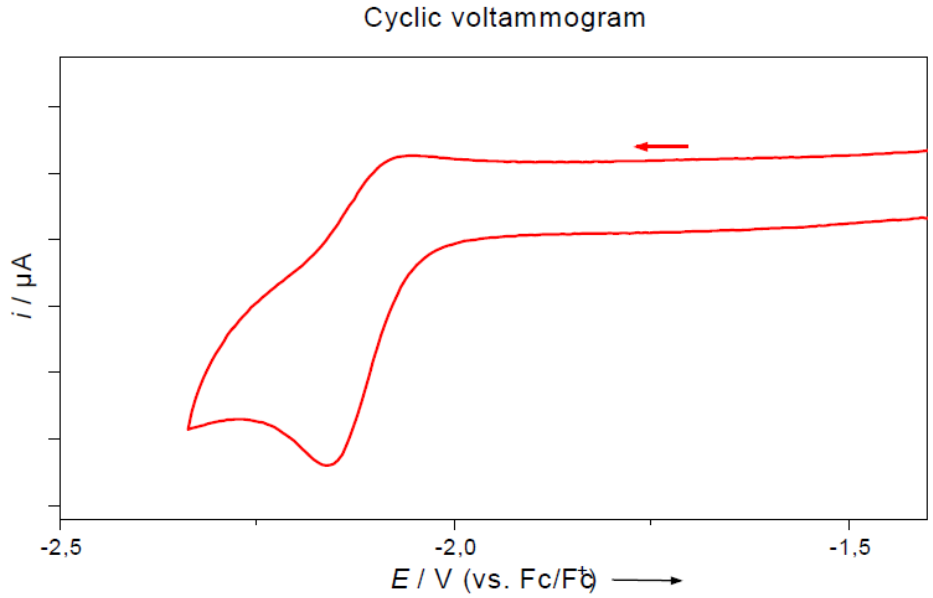


Figure S34. Cyclic voltammogram of **5** in THF/0.1 M [*n*Bu$_4$N][PF$_6$] measured at 250 mV s^{-1} with voltammetric response. Formal potential: E_{pc} = −2.17 V.

EPR spectra

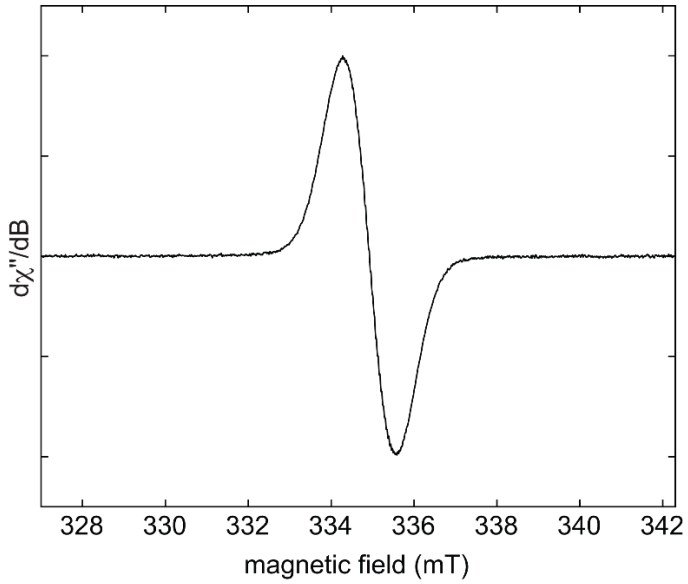


Figure S35. Experimental continuous-wave (CW) X-band EPR spectrum of **4**$^{\bullet-}$ with 18-crown-6 in benzene at room temperature. The signal is centred around a *g* value of 2.0026. Experimental parameters: microwave frequency = 9.39 GHz; microwave power = 0.2 mW; modulation amplitude = 0.5 G; conversion time = 20 ms; modulation frequency = 100 kHz.

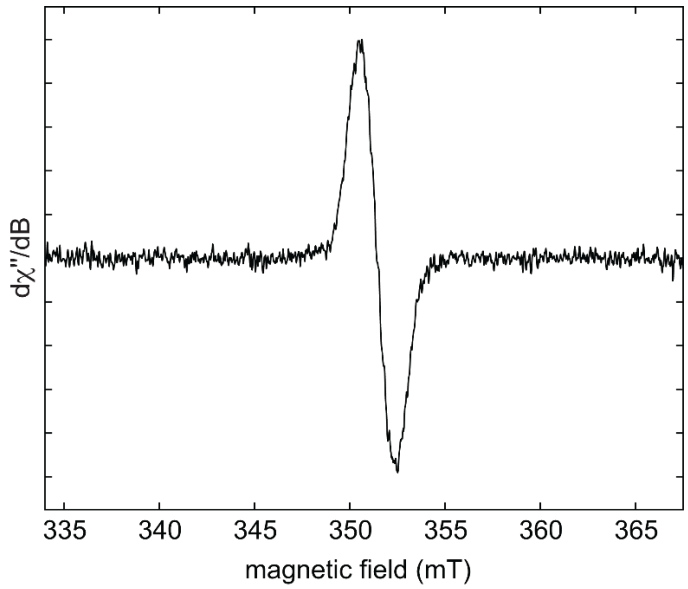


Figure S36. Experimental continuous-wave (CW) X-band EPR spectrum of **5**$^{\bullet-}$ in benzene at room temperature. The signal is centered around a g_{iso} factor of 2.0028 with a peak-to-peak linewidth of 1.9 mT. Experimental parameters: microwave frequency = 9.85 GHz; microwave power = 1 mW; modulation amplitude = 0.5 G; conversion time = 60 ms; modulation frequency = 100 kHz.

UV-vis spectra

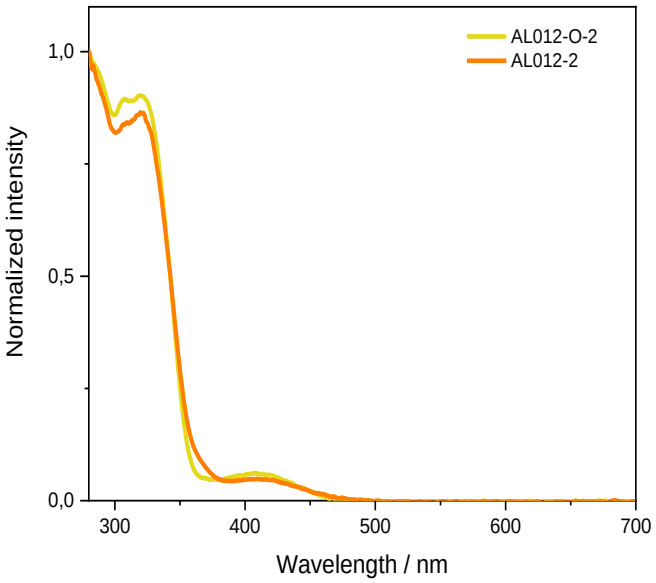


Figure S37. UV-vis absorption spectra of **2** (orange) and its decomposition product **3** (yellow) in benzene at 23 °C. Absorption maxima for **2**: λ_{max} = 320 nm, λ_2 = 417 nm; for **3**: λ_{max} = 320 nm, λ_2 = 414 nm.

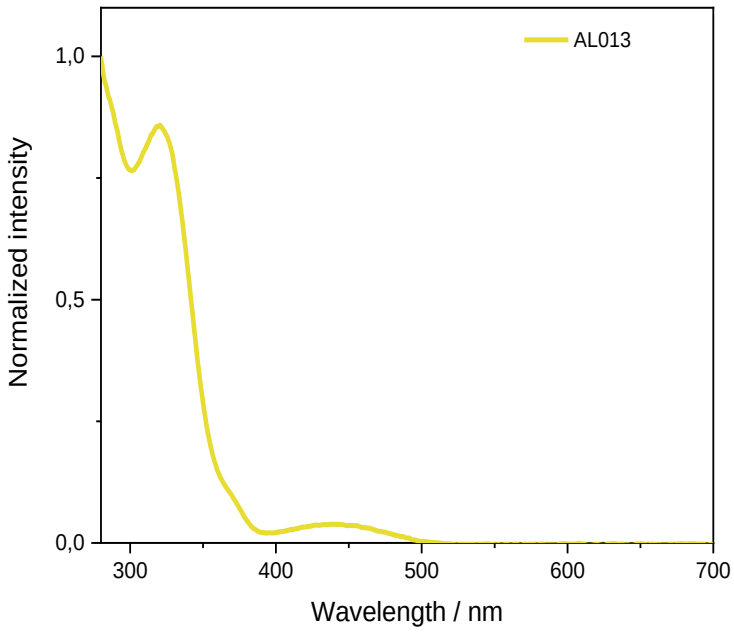


Figure S38. UV-vis absorption spectrum of **4** (yellow) in benzene at 23 °C. λ_{max} = 320 nm, λ_2 = 366 (shoulder) nm, λ_3 = 444 nm.

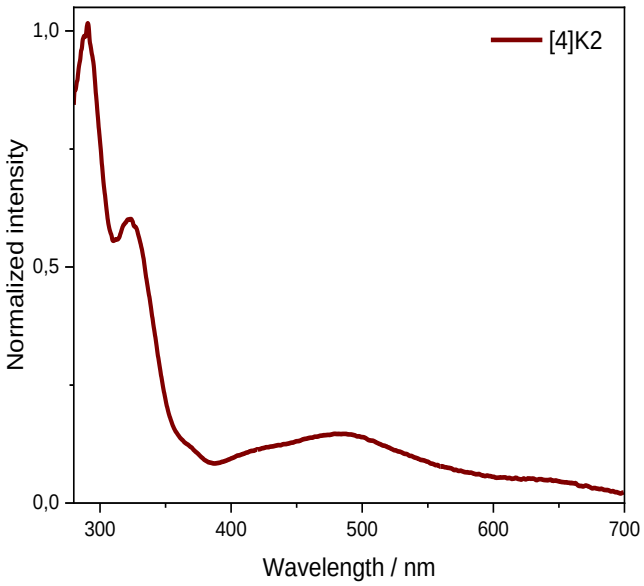


Figure S39. UV-vis absorption spectrum of **[4]K$_2$** (dark red) in benzene at 23 °C. (λ_{max} = 289 nm, λ_2 = 322 nm, λ_{max1} = 430, λ_{max2} = 480, λ_3 = 640). *Note: the spectrum had to be recorded in the presence of excess KC_8, left to settle at the bottom of the cuvette, due to the rapid oxidation of **[4]K$_2$** back to **[4]K** at such low concentrations and in the absence of excess reducing agent.*

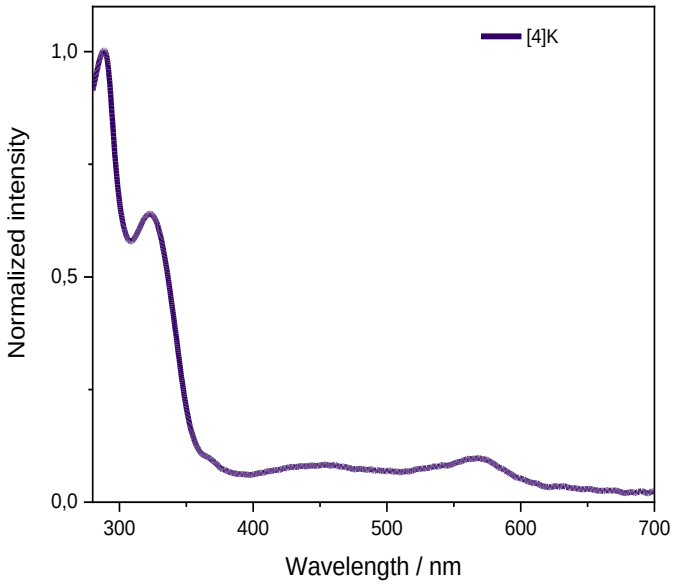


Figure S40. UV-vis absorption spectrum of **4**$^{\bullet-}$ (purple) in benzene at 23 °C. Absorption maxima: λ_{max} = 289 nm, λ_2 = 323 nm, λ_3 = 569 (broad) nm, λ_4 = 454 (very broad) nm, λ_5 = 368 (shoulder) nm.

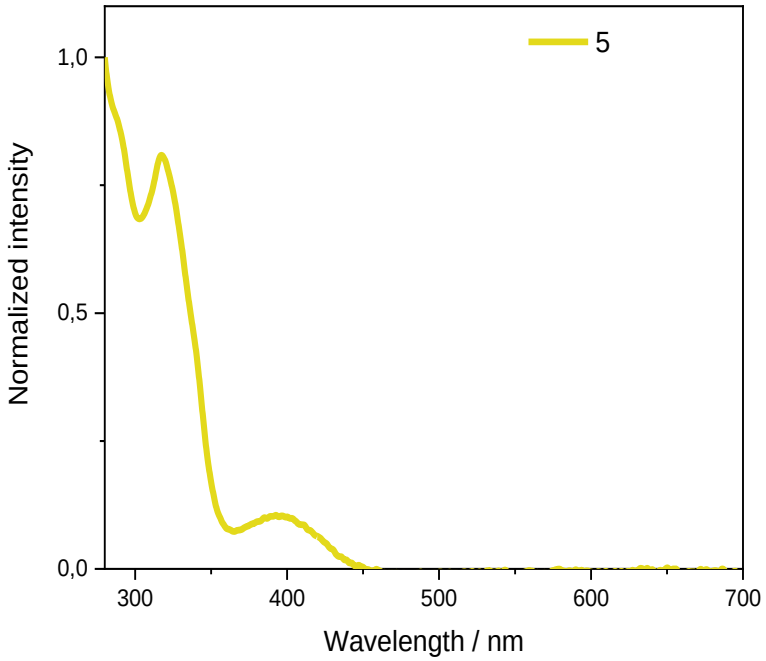


Figure S41. UV-vis absorption spectrum of **5** (yellow) in benzene at 23 °C. Absorption maxima: λ_{max} = 319 nm, λ_2 = 398 nm.

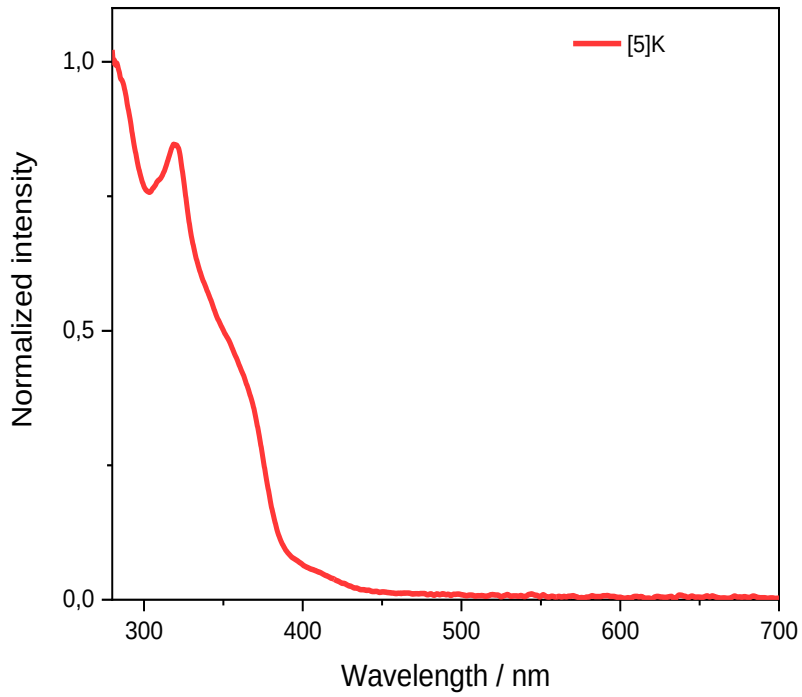


Figure S42. UV-vis absorption spectrum of **5** (yellow) in benzene at 23 °C. Absorption maxima: λ_{max} = 319 nm, λ_2 = 360 (shoulder) nm, λ_3 = 412 (shoulder) nm.

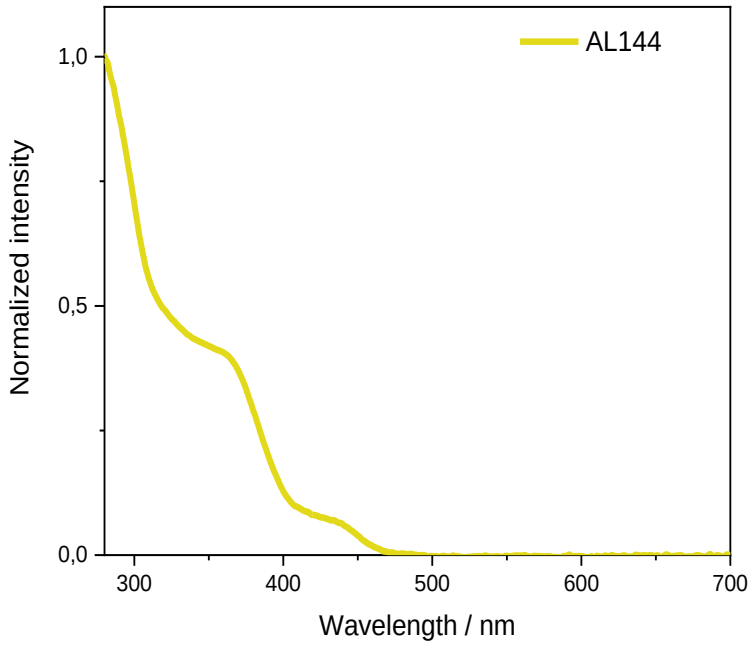


Figure S43. UV-vis absorption spectrum of **8** (light yellow) in benzene at 23 °C. Absorption maxima: λ_{max} = 364 nm, λ_2 = 440 nm.

IR spectra

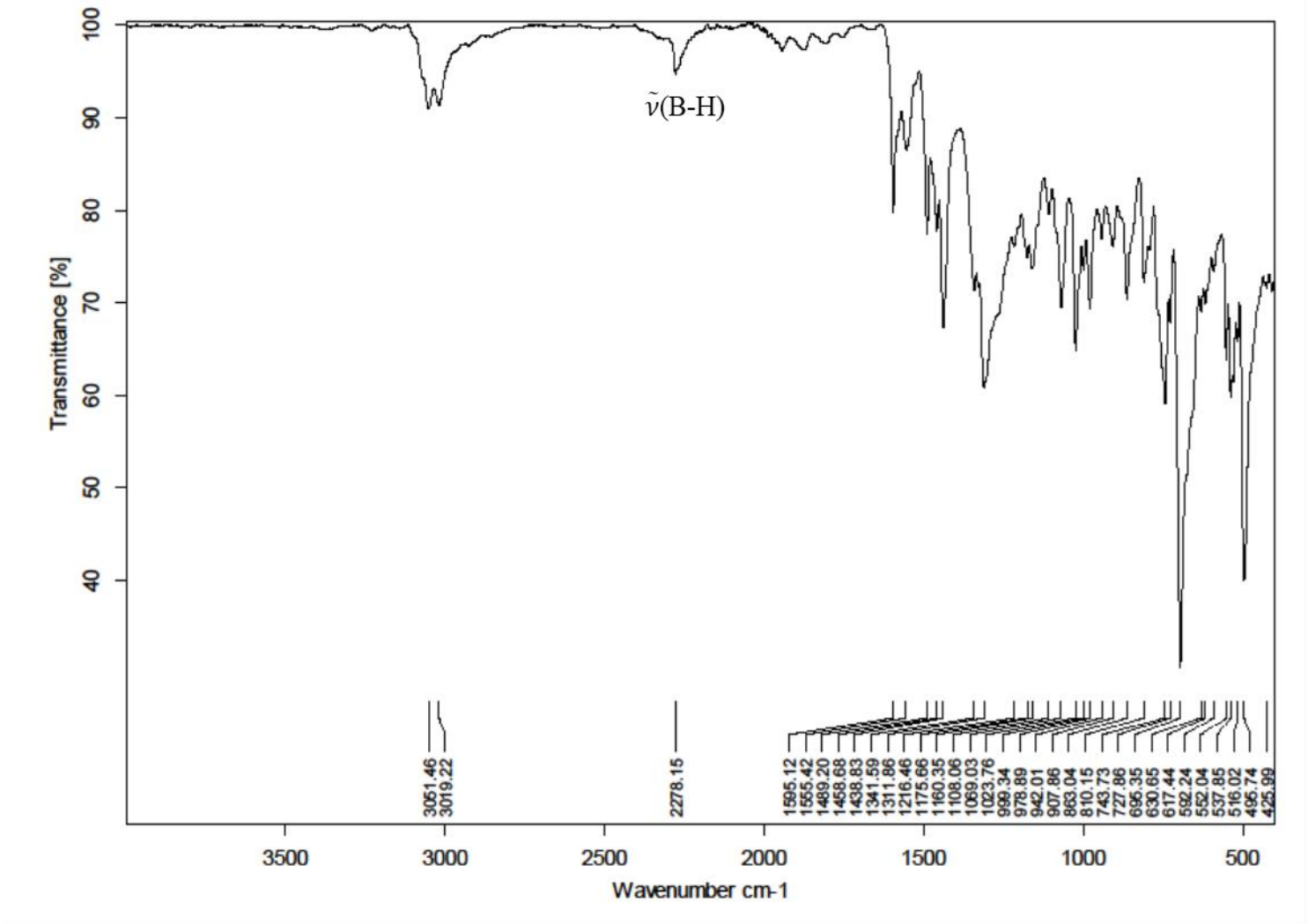


Figure S44. Solid-state IR spectrum of **11**.

X-ray crystallographic data

The crystal data of **2**, **4**, **[4]K$_2$**, **[6]K**, **8**, and **[11]K-thf** were collected on a *XtaLAB Synergy Dualflex HyPix* diffractometer with a Hybrid Pixel array detector and multi-layer mirror monochromated $Cu_{K\alpha}$ radiation. The crystal data of **3** and **5** were collected on a *Bruker D8 Quest* diffractometer with a CMOS area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structures were solved using the intrinsic phasing method,[6] refined with the ShelXL program[7] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication nos. CCDC 2301167-2301174. 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 crystallographically-characterised compounds.

Compound	CCDC number
2	2301171
3	2301169
4	2301168
[4]K$_2$	2301173
5	2301167
6	2301172
8	2301170
[11]K-thf	2301174

Refinement details for 2: One outlying reflection (2 1 1) was omitted. The asymmetric unit contains half a benzene molecule positioned on an inversion center and was modelled as twofold disordered in a 72:28 ratio using PART -1 20.5 and PART -2 -20.5. The benzene rings within this disorder were idealised using AFIX 66. ADPs within the disorder were restrained with SIMU and ISOR 0.01.

Crystal data for 2: $C_{46}H_{33}B_3BrN\cdot(C_6H_6)_{1.5}$, M_r = 829.23, yellow block, 0.464×0.365×0.253 mm^3, triclinic space group $P\ \bar{1}$, a = 12.42275(16) Å, b = 12.5117(2) Å, c = 15.82000(18) Å, α = 99.0555(12)°, β = 95.7000(10)°, γ = 117.2083(15)°, V = 2118.10(5) Å^3, Z = 2.00, ρ_{calcd} = 1.300 g·cm^{-3}, μ = 1.612 mm^{-1}, F(000) = 858.000, T = 99.99(10) K, R_1 = 0.0469, wR_2 = 0.1297, 8037 independent reflections [$2\theta \leq 140.126°$] and 599 parameters.

Refinement details for 3: The asymmetric unit contains one threefold-disordered dichloromethane molecule (RESI 8, 81 and 82 DCM), modelled with 3 FVAR summed up to 1 (SUMP) in an 80:14:6 ratio. ADPs within the disorder were restrained with SIMU 0.005. 1,2- and 1,3-distances of all three CH_2Cl_2 molecules were restrained to similarity with SAME.

Crystal data for 3: $C_{92}H_{66}B_6N_2O\cdot(CH_2Cl_2)_4$, M_r = 1620.03, yellow block, 0.539×0.213×0.13 mm^3, orthorhombic space group *Pnna*, a = 14.931(7) Å, b = 49.55(3) Å, c = 11.093(8) Å, V = 8208(9) Å^3, Z = 4, ρ_{calcd} = 1.311 g·cm^{-3}, μ = 0.326 mm^{-1}, F(000) = 3352, T = 100 K, R_1 = 0.0810, wR_2 = 0.1379, 8087 independent reflections [$2\theta \leq 52.044°$] and 568 parameters.

Refinement details for 4: The azaborinine ring was modelled as flip-disordered in the BNCPh unit in a 68:32 ratio. The disordered phenyl ring (RESI 6 and 61 PH) was idealised using AFIX 66. ADPs within this disorder were restrained with SIMU 0.005.

Crystal data for 4: $C_{80}H_{58}B_4N_2$, M_r = 1090.52, yellow block, 0.190×0.130×0.050 mm^3, monoclinic space group $P2_1/n$, a = 12.76130(10) Å, b = 12.1923(2) Å, c = 18.9650(2) Å, β = 91.8480(10)°, V = 2949.22(6) Å^3, Z = 2, ρ_{calcd} = 1.228 g·cm^{-3}, μ = 0.525 mm^{-1},

$F(000) = 1144$, $T = 100(2)$ K, $R_1 = 0.0513$, $wR_2 = 0.1016$, 6032 independent reflections [$2\theta \leq 150.254°$] and 437 parameters.

Refinement details for [4]K$_2$: The asymmetric unit contains 3.5 benzene molecules, of which one was modelled as twofold rotationally disordered (RESI 11 and 111) in a 72:28 ratio. The benzene rings within the disorder were idealised with AFIX 66 and the ADPs restrained to similarity with SIMU 0.005.

Crystal data for [4]K$_2$: $C_{110}H_{88}B_4K_2N_2 \cdot (C_6H_6)_7$, $M_r = 1715.48$, red plate, 0.090×0.060×0.020 mm^3, triclinic space group $P\bar{1}$, $a = 10.0169(2)$ Å, $b = 14.8735(3)$ Å, $c = 16.2360(3)$ Å, $\alpha = 86.734(2)°$, $\beta = 84.599(2)°$, $\gamma = 82.053(2)°$, $V = 2382.70(8)$ Å^3, $Z = 1$, $\rho_{calcd} = 1.196$ g·cm^{-3}, $\mu = 1.274$ mm^{-1}, $F(000) = 904$, $T = 100(2)$ K, $R_1 = 0.0596$, $wR_2 = 0.1371$, 9623 independent reflections [$2\theta \leq 151.578°$] and 533 parameters.

Refinement details for 5: Eight reflections affected by the beamstop were omitted and an extinction coefficient was applied.

Crystal data for 5: $C_{46}H_{33}B_2N$, $M_r = 621.35$, yellow block, 0.243×0.177×0.129 mm^3, monoclinic space group $P2_1/c$, $a = 11.907(5)$ Å, $b = 11.428(3)$ Å, $c = 25.172(7)$ Å, $\beta = 103.401(16)°$, $V = 3332(2)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.239$ g·cm^{-3}, $\mu = 0.070$ mm^{-1}, $F(000) = 1304$, $T = 100(2)$ K, $R_1 = 0.0651$, $wR_2 = 0.1898$, 6290 independent reflections [$2\theta \leq 51.36°$] and 443 parameters.

Refinement details for 6: Two of the benzene solvent molecules in the lattice showed rotational disorder in a 51:49 and 22:78 ratio, respectively. The benzene rings within the disorders were idealised with AFIX 66 and their ADPs restrained using SIMU and RIGU.

Crystal data for 6: $C_{46}H_{32}B_2KN \cdot (C_6H_6)_4$, $M_r = 971.87$, light purple block, 0.200×0.080×0.050 mm^3, monoclinic space group $P2_1/c$, $a = 18.8567(2)$ Å, $b = 18.5384(2)$ Å, $c = 16.4824(2)$ Å, $\beta = 105.8370(10)°$, $V = 5543.09(11)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.165$ g·cm^{-3},

μ = 1.154 mm^{-1}, F(000) = 2048, T = 100(2) K, R_1 = 0.0677, wR_2 = 0.1595, 11140 independent reflections [2θ≤150.836°] and 729 parameters.

Crystal data for 8: $C_{62}H_{45}B_2N\cdot(C_6H_6)$, M_r = 903.71, clear colourless block, 0.209×0.190×0.076 mm^3, monoclinic space group $P2_1/c$, a = 13.6357(2) Å, b = 15.1081(2) Å, c = 25.2435(3) Å, β = 103.8450(10)°, V = 5049.31(12) Å^3, Z = 4, ρ_{calcd} = 1.189 g·cm^{-3}, μ = 0.507 mm^{-1}, F(000) = 1904, T = 100.00(10) K, R_1 = 0.0557, wR_2 = 0.1065, 10170 independent reflections [2θ≤154.854°] and 640 parameters.

Refinement details for [11]K-thf: The crystals were heavily twinned needles and twinning could not be resolved. The structure was solved using only the data from the first twinning component hence the very high R values. The structure is solely used as proof of connectivity and not discussed**.**

Crystal data for [11]K-thf: $C_{40}H_{31}B_2NK\cdot(OC_4H_8)$, M_r = 658.48, colourless needle, 0.10×0.05×0.02 mm^3, monoclinic space group $P2_1/c$, a = 12.8131(15) Å, b = 27.705(3) Å, c = 11.8914(11) Å, β = 103.878(11)°, V = 4098.0(7) Å^3, Z = 4, ρ_{calcd} = 1.067 g·cm^{-3}, μ = 1.361 mm^{-1}, F(000) = 1388, T = 100(2) K, R_1 = 0.2416, wR_2 = 0.6100, 7501 independent reflections [2θ≤136.50°] and 201 parameters.

Computational details

All density functional theory (DFT) calculations were carried out at the B3LYP[8]-D3(BJ)[9]-def2-SVP[10] level of theory using the Turbomole[11] user interface TmoleX2022.[12] The defpp-ecp[13] basis set was applied to Br atoms to account for relativistic effects. True minima were confirmed by frequency calculations, which provided no imaginary frequencies. ^{11}B NMR shifts were calculated at the B3LYP-D3(BJ)-def2-SVP level of theory using using hexaphenyl-1,2-azaborinine ($\delta(^{11}B)_{exp}$ = ppm) 34.6 ppm). Molecular orbital (MO) and spin density representations were created using the graphics interface of TmoleX2022.

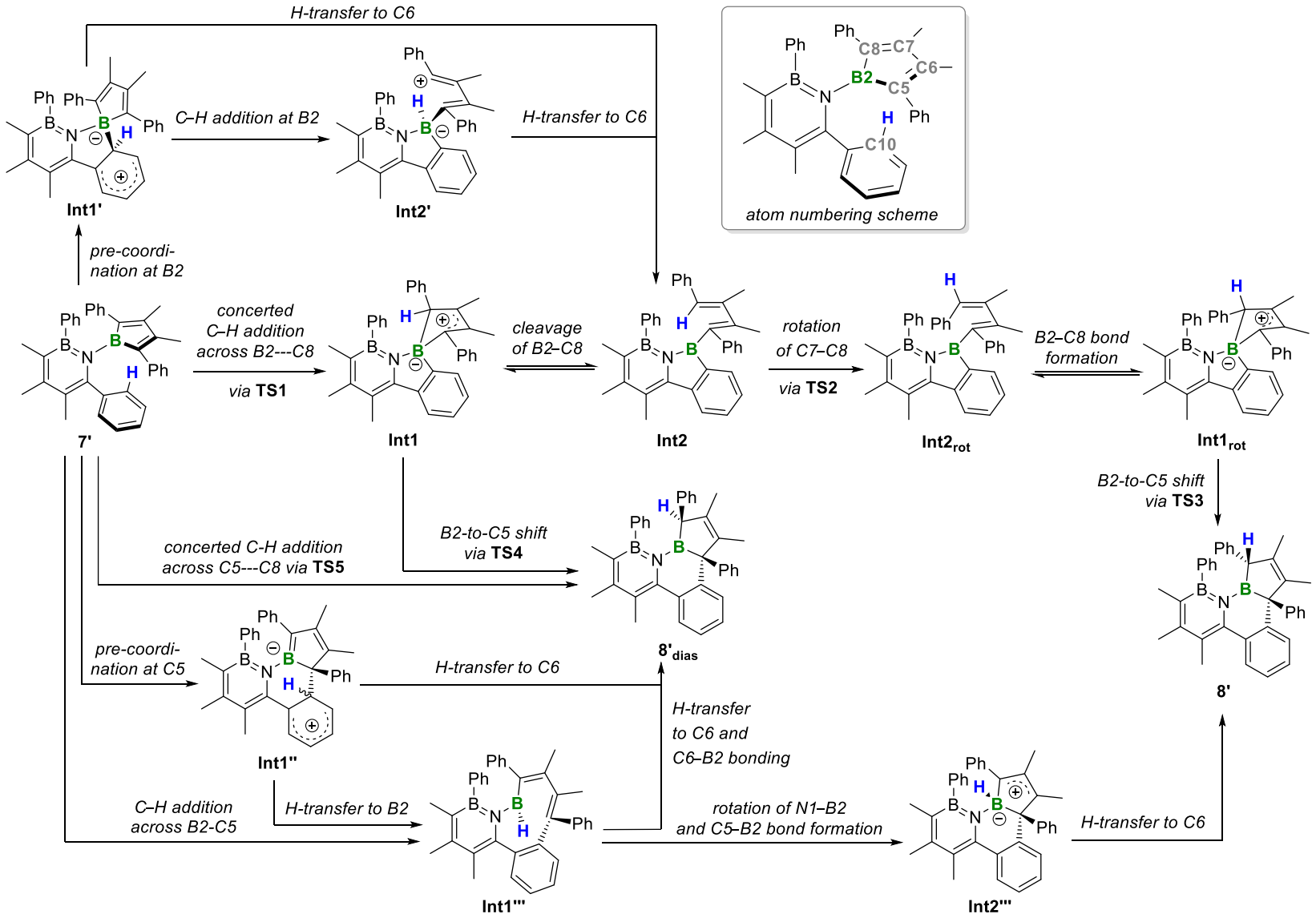
Table S2. Calculated ^{11}B NMR shieldings (ppm) at the B3LYP-D3(BJ)-def2-SVP level of theory and corresponding ^{11}B NMR shifts (ppm) using the known shift of hexaphenyl-1,2-azaborinine (**C_4BNPh_6**) as a reference.

Compound	calcd. ^{11}B NMR shieldings		calcd. ^{11}B NMR shifts	
	$B_{azaborinine}$	$B_{substituent}$	$B_{azaborinine}$	$B_{substituent}$
C_4BNPh_6	72.7	–	34.6	–
2	73.8	57.6 (*B*N), 41.4 (*B*Br)	33.5	49.7 (*B*N), 66.2 (*B*Br)
anti-**4**	73.0	57.0	34.3	50.3
[4]K_2	73.3	80.6 (avg. B2/B2')	34.0	26.7
5	73.2	53.1	34.1	54.2
6^-	72.0	107.9	35.3	–0.6
7	73.7	52.0	33.6	55.3
8	71.7	44.9	35.6	62.4
11^-	72.5	111.1	34.8	–3.8

The mechanism of formation of **8** from **7** was assessed using a model system, in which all remote phenyl substituents (i.e. which are not in direct contact with the reaction centres) were replaced with methyl groups. Calculations were carried out at the B3LYP-D3(BJ)-def2-SVP level of theory. Intermediates or transition states were confirmed by full frequency calculations, which provided no or a single negative frequency, respectively. Gibbs free energies were calculated as follows:

$$G(298\ K) = E_{SCF} + ZPVE + CP_{298K}$$

where E_{SCF} is the SCF energy, *ZPVE* the zero-point vibrational energy, and CP_{298K} the chemical potential at 298 K.



Scheme S1. Possible mechanisms of formation of **8'** from **7'** explored computationally.

Given the use of a simplified system single-point calculations at a higher level of theory and/or involving solvent correction were not carried out. The results thus simply provide a qualitative comparison of the various reaction pathways explored (Scheme S1).

Starting from the nucleophilic attack of C10 at B2 attempts to optimise the potential intermediates **Int1'** and **Int2'** systematically yielded **Int2**. Starting from the nucleophilic attack of C10 at C5 the resulting intermediate **Int1''** lies ca. 35 kcal mol^{-1} higher in energy than **7'**, making this pathway unviable at room temperature. The direct addition of C10–H10 across C5–B2 would yield the intermediate **Int1'''**, which lies 22 kcal mol^{-1} higher in energy than **7'**, again making this pathway highly unlikely.

The remaining viable pathways are:

a) The addition of C10–H10 across B2–C8 via the transition state **TS1** and the metastable intermediate **Int1**, yielding **Int2**, which then converts by C7=C8 bond rotation to the more stable rotamer $\mathbf{Int2_{rot}}$ via **TS2**, followed by nucleophilic attack of C8 at B2 to yield the metastable intermediate $\mathbf{Int1_{rot}}$ and a B2-to-C5 shift of C10 via **TS3**.

b) From **Int1** a B2-to-C5 shift of C10 via **TS4** yields the diastereomer $\mathbf{8'_{dias}}$.

c) The concerted addition of C10–H10 across C5···C8 via **TS5**, which yields the diastereomer $\mathbf{8'_{dias}}$, which may then isomerise to **8'** by B2–C8 cleavage and rotation of the C8 moiety. All attempts to locate **TS5**, however, systematically converged to **TS1**, making this pathway highly unlikely.

The results of the calculations are summarised in Table S3.

Table S3. SCF energies (E_{SCF}, Ha), relative SCF energies ($\Delta E_{SCF,}$ kcal mol^{-1}), ZPVE-corrected energies (E_{SCF} + ZPVE, Ha), chemical potential at 298 K (CP_{298}, Ha), relative Gibbs free energy (ΔG, kcal mol^{-1}) and minimum IR frequency (ν_{min}, cm^{-1}) of the various starting materials, products, (postulated) intermediates and transition states for the rearrangement of **7'** to **8'** optimised at the B3LYP-D3(BJ)-def2-SVP level of theory.

Compound	E_{SCF} (Ha)	ΔE_{SCF} (kcal mol^{-1})	E_{SCF} + ZPVE (Ha)	CP_{298} (Ha)	ΔG (kcal mol^{-1})	ν_{min} (cm^{-1})
7'	–1533.655190	0.00	–1533.034828	0.552982	0.00	18.95
TS1	–1533.610907	27.79	–1532.994543	0.549691	23.21	–1468.01
Int1	–1533.645821	5.88	–1533.025135	0.553202	6.22	12.11
Int2	–1533.662251	–4.43	–1533.041161	0.554756	–2.86	21.05
TS2	–1533.607104	28.58	–1532.987965	0.544982	24.15	–171.39
Int2$_{rot}$	–1533.666940	–7.37	–1533.045815	0.553633	–6.49	18.15
Int1$_{rot}$	–1533.64485	6.49	–1533.023977	0.553038	6.84	13.07
TS3	–1533.634307	13.10	–1533.014641	0.552213	12.18	–294.96
8'	–1533.671710	–10.37	–1533.049656	0.554425	–8.40	15.43
TS4	–1533.629194	16.31	–1533.00933	0.554329	16.85	–307.66
8'$_{dias}$	–1533.661993	–4.27	–1533.040265	0.555662	–1.73	17.46
TS5	*systematically converges toward TS1*					
Int1''	–1533.590973	40.30	–1532.972227	0.553157	39.39	21.34
Int1'''	–1533.614067	25.8	–1336.8146703	0.424951	21.55	34.18

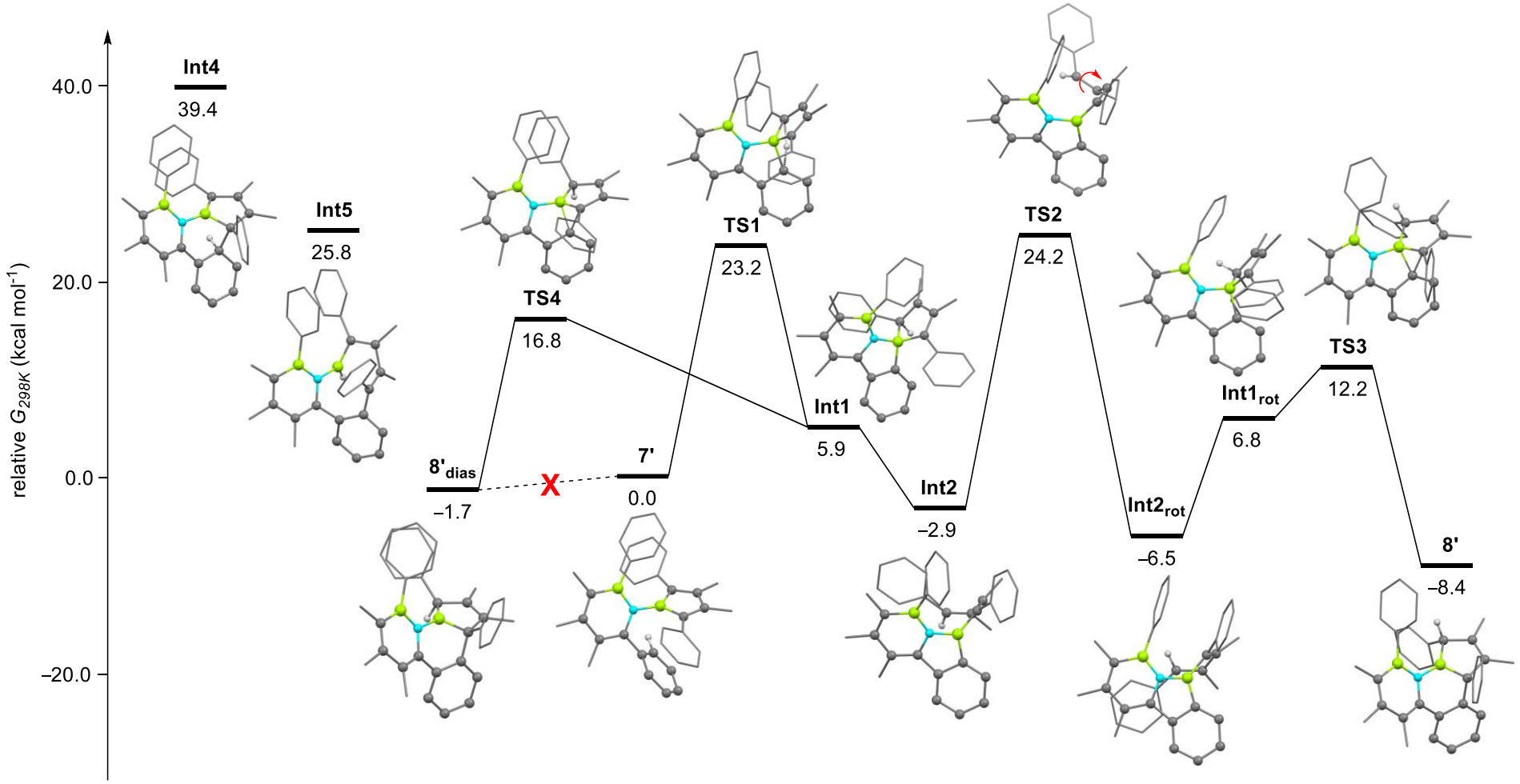


Figure S45. Computed mechanism for the rearrangement of **7'** to **8'** optimised at the B3LYP-D3(BJ)-def2-SVP level of theory. Relative Gibbs free energies at 298 K (kcal mol^{-1}) in parentheses. Optimised structures in ball-and-stick representations with peripheral substituents in capped-stick representation. Breaking/forming bonds in TS are dashed. Colour code: carbon = grey, boron = green, nitrogen = blue, hydrogen = white.

Cartesian coordinates

Hexaphenyl-1,2-azaborinine

E = –1619.99745164576 Ha

ν_{min} = 19.66 cm^{-1}

N	3.96684	3.587595	-0.019056
C	3.640723	2.24114	-0.044667
B	2.958011	4.628865	-0.008133
C	2.317149	1.83201	-0.066867
C	1.242661	2.795175	-0.055187
C	1.506422	4.159535	-0.017405
C	4.752603	1.244624	-0.039663
C	5.614253	1.136298	1.06257
H	5.475167	1.79582	1.921144
C	6.642274	0.192795	1.068889
H	7.303486	0.11789	1.935778
C	6.824894	-0.654097	-0.028459
H	7.630548	-1.392529	-0.023777
C	5.970618	-0.553382	-1.130153
H	6.104368	-1.21378	-1.990542
C	4.940739	0.388478	-1.134297
H	4.266892	0.460025	-1.990039
C	2.00574	0.369913	-0.109261
C	2.368755	-0.477994	0.948066
H	2.890095	-0.059818	1.811541
C	2.074758	-1.842202	0.904953
H	2.366673	-2.48631	1.738469
C	1.408385	-2.381953	-0.198709
H	1.176423	-3.449469	-0.233499
C	1.038358	-1.546438	-1.256963
H	0.514734	-1.958346	-2.123509
C	1.334157	-0.183291	-1.210858
H	1.036491	0.467072	-2.035935
C	-0.164005	2.288421	-0.091128
C	-0.663991	1.463323	0.927831
H	-0.011792	1.177772	1.755248
C	-1.981884	1.005394	0.890876
H	-2.356224	0.366924	1.695187
C	-2.818349	1.357105	-0.172697
H	-3.849144	0.995034	-0.204366
C	-2.328644	2.17556	-1.194601
H	-2.975696	2.45772	-2.029091
C	-1.01354	2.641319	-1.150482
H	-0.63643	3.291634	-1.942192
C	0.399496	5.154466	0.037106

C	-0.55927	5.126395	1.065074
H	-0.502612	4.345295	1.825589
C	-1.576525	6.080223	1.125323
H	-2.30928	6.039298	1.935675
C	-1.660471	7.082415	0.15404
H	-2.458163	7.828356	0.199097
C	-0.712799	7.124492	-0.872725
H	-0.765127	7.905665	-1.635681
C	0.309143	6.175141	-0.924867
H	1.054376	6.222624	-1.721551
C	3.376383	6.147409	0.028545
C	2.864027	6.988736	1.034906
H	2.177933	6.577798	1.780093
C	3.203147	8.342148	1.097784
H	2.795723	8.9694	1.895345
C	4.051108	8.89641	0.13434
H	4.312285	9.957353	0.175261
C	4.558563	8.085164	-0.885021
H	5.219008	8.510052	-1.645915
C	4.229209	6.728532	-0.928805
H	4.649568	6.109583	-1.725265
C	5.359591	3.957014	-0.051308
C	5.935047	4.584687	1.05594
C	7.275852	4.971021	1.01908
C	8.046155	4.72886	-0.121859
C	7.46676	4.102104	-1.229144
C	6.124462	3.720537	-1.197107
H	5.321965	4.777459	1.937731
H	7.719293	5.466123	1.886314
H	9.095999	5.030353	-0.149349
H	8.061009	3.912282	-2.12626
H	5.663137	3.23519	-2.05854

Compound 2

E_{SFC} = –2313.6639264 Ha

ν_{min} = 8.95 cm^{-1}

Br	9.048697	5.90073	7.923413
B	7.303152	5.932992	8.812636
C	6.152632	5.061353	8.233904
C	6.292165	4.29998	7.058708
H	7.254801	4.289799	6.542651
C	5.222948	3.568084	6.538936
H	5.352679	2.986285	5.622547
C	3.985078	3.586765	7.189003
H	3.142244	3.022072	6.781637
C	3.831063	4.327374	8.362524

H	2.861421	4.336064	8.866522
C	4.897375	5.061658	8.906276
N	3.428176	5.796264	10.967234
B	2.480224	6.882524	10.887854
C	3.135787	4.624397	11.628508
C	1.151676	6.685868	11.607509
C	0.919636	5.475376	12.255595
B	4.715869	5.897925	10.211348
C	1.918796	4.433934	12.264213
C	5.852076	6.834041	10.725025
C	5.67899	7.631381	11.867362
H	4.721116	7.615738	12.391366
C	6.70582	8.449215	12.34314
H	6.545993	9.070864	13.228034
C	7.937925	8.470365	11.68265
H	8.746695	9.107743	12.04966
C	8.135489	7.670865	10.555343
H	9.103301	7.68229	10.049112
C	7.110258	6.846356	10.055664
C	2.895161	8.179508	10.094979
C	3.345849	8.134333	8.761934
H	3.347392	7.186392	8.219745
C	3.783159	9.286173	8.098764
H	4.12888	9.220114	7.063688
C	3.778532	10.515538	8.759983
H	4.125657	11.417338	8.248714
C	3.316793	10.587945	10.079813
H	3.3	11.549224	10.600543
C	2.873528	9.436378	10.730343
H	2.505815	9.510987	11.757215
C	0.151767	7.787583	11.637107
C	-0.307698	8.364628	10.44029
H	0.063821	7.980461	9.488105
C	-1.228638	9.413755	10.454003
H	-1.576173	9.84113	9.509711
C	-1.699459	9.920754	11.668503
H	-2.417045	10.74517	11.680856
C	-1.241144	9.366582	12.867802
H	-1.598431	9.757748	13.824166
C	-0.327931	8.311374	12.85111
H	0.021892	7.882281	13.791921
C	-0.375132	5.221456	12.959219
C	-0.409892	4.940748	14.333802
H	0.524939	4.895976	14.895711
C	-1.624212	4.718288	14.984923
H	-1.632978	4.505289	16.056948
C	-2.823922	4.762172	14.268474

H	-3.774792	4.583361	14.77691
C	-2.799869	5.036895	12.898047
H	-3.732852	5.075364	12.329929
C	-1.585344	5.269807	12.250732
H	-1.569149	5.498079	11.183236
C	1.65388	3.135541	12.953243
C	2.453126	2.711902	14.026348
H	3.275967	3.347184	14.360754
C	2.207947	1.494657	14.665072
H	2.841504	1.182878	15.499474
C	1.155078	0.679204	14.241031
H	0.960677	-0.273064	14.740986
C	0.3503	1.091253	13.174311
H	-0.476922	0.461656	12.836571
C	0.597969	2.30823	12.537762
H	-0.037735	2.629415	11.710182
C	4.210389	3.589293	11.612163
C	3.998205	2.335458	11.017547
H	3.011916	2.093301	10.619428
C	5.039453	1.415321	10.917218
H	4.863183	0.448728	10.439007
C	6.309938	1.729802	11.414781
H	7.126938	1.009442	11.327336
C	6.525873	2.964737	12.028175
H	7.509619	3.21466	12.432768
C	5.481072	3.888034	12.130643
H	5.652004	4.843333	12.627585

Compound *anti*-4

E_{SFC} = –3288.5685438 Ha

ν_{min} = 5.50 cm^{-1}

N	8.777079	6.399622	8.130894
B	9.58698	5.246647	7.811397
C	9.16876	7.670184	7.758904
C	10.825484	5.479931	6.955773
C	11.137319	6.783704	6.583719
B	7.492026	6.179814	8.871492
C	10.313016	7.888979	7.006461
C	6.320523	5.439257	8.14167
C	6.453944	4.966541	6.825837
H	7.395438	5.117162	6.293049
C	5.40845	4.298864	6.1839
H	5.539975	3.930584	5.163074
C	4.195597	4.098375	6.850812
H	3.376947	3.570397	6.354709
C	4.032903	4.589426	8.147703

H	3.075801	4.454549	8.657855
C	5.073527	5.266387	8.806065
C	9.191512	3.83457	8.384118
C	9.148513	3.610069	9.772341
H	9.32569	4.439487	10.462259
C	8.917693	2.333795	10.294574
H	8.916295	2.18289	11.375235
C	8.690312	1.257669	9.436126
H	8.501686	0.260078	9.841319
C	8.709999	1.461729	8.051541
H	8.536264	0.622731	7.372421
C	8.973282	2.730654	7.537793
H	9.022796	2.867356	6.454495
C	11.641102	4.32444	6.491498
C	12.204332	3.427976	7.416339
H	12.050908	3.598825	8.483639
C	12.951798	2.32896	6.989411
H	13.384376	1.649147	7.728238
C	13.140594	2.093397	5.624588
H	13.721724	1.230564	5.288997
C	12.57635	2.969447	4.692151
H	12.714041	2.793901	3.621833
C	11.837094	4.072528	5.121962
H	11.403457	4.754571	4.387945
C	12.338362	7.071927	5.741156
C	12.211354	7.69796	4.491586
H	11.221217	7.990359	4.13696
C	13.335407	7.950497	3.703745
H	13.2174	8.43516	2.731172
C	14.607453	7.590603	4.158576
H	15.488577	7.792483	3.544167
C	14.74522	6.970479	5.403781
H	15.735394	6.683793	5.767235
C	13.618822	6.708862	6.185487
H	13.726913	6.212567	7.151826
C	10.683523	9.286947	6.632099
C	9.823592	10.077361	5.853799
H	8.871197	9.659079	5.521465
C	10.170723	11.383999	5.505337
H	9.486826	11.983056	4.898472
C	11.388435	11.923619	5.929144
H	11.662237	12.945914	5.65612
C	12.254969	11.145529	6.702971
H	13.210479	11.557381	7.037889
C	11.90502	9.839699	7.049517
H	12.588072	9.233572	7.647972
C	8.303457	8.784874	8.232033

C	8.820946	9.77785	9.077955
H	9.886369	9.777706	9.312992
C	7.979984	10.738356	9.637423
H	8.39404	11.494728	10.309021
C	6.609475	10.72267	9.355061
H	5.941933	11.46163	9.804584
C	6.091313	9.755669	8.493547
H	5.029113	9.741487	8.262973
C	6.934528	8.796996	7.928416
H	6.519527	8.053992	7.244765
N	3.524032	5.774282	10.88622
B	2.572711	6.847831	10.759383
C	3.233542	4.636776	11.600863
C	1.26311	6.701094	11.528469
C	1.038301	5.527413	12.241771
B	4.857111	5.894674	10.210512
C	2.025387	4.478664	12.26323
C	6.011105	6.64603	10.932808
C	5.827479	7.202785	12.209763
H	4.832134	7.186703	12.661784
C	6.896605	7.759006	12.916171
H	6.736769	8.187788	13.908976
C	8.175951	7.754335	12.351687
H	9.020422	8.17347	12.905112
C	8.369722	7.230295	11.070849
H	9.369073	7.251617	10.629529
C	7.30267	6.691394	10.335671
C	2.820316	8.100126	9.825694
C	2.776199	7.976702	8.423368
H	2.777763	6.983989	7.967965
C	2.676898	9.099525	7.594569
H	2.620239	8.972332	6.510143
C	2.644794	10.380681	8.152587
H	2.560278	11.259854	7.508646
C	2.736424	10.529967	9.540946
H	2.719152	11.528193	9.986258
C	2.817518	9.403219	10.360617
H	2.833551	9.536349	11.445501
C	0.268256	7.809633	11.5456
C	-0.292614	8.294501	10.351536
H	-0.003136	7.838235	9.403169
C	-1.207373	9.348748	10.362512
H	-1.631976	9.705785	9.42051
C	-1.573923	9.950406	11.569898
H	-2.286886	10.778909	11.579274
C	-1.018324	9.484497	12.765336
H	-1.295645	9.947813	13.71602

C	-0.109213	8.425393	12.751743
H	0.317786	8.063916	13.689528
C	-0.236299	5.3179	12.994622
C	-0.228566	5.091927	14.379613
H	0.723885	5.060713	14.912023
C	-1.422553	4.906308	15.078167
H	-1.397862	4.735338	16.15747
C	-2.644685	4.933268	14.399904
H	-3.579779	4.78312	14.945544
C	-2.663231	5.153862	13.019657
H	-3.613921	5.17824	12.480854
C	-1.468778	5.349578	12.324567
H	-1.486023	5.534236	11.248806
C	1.742056	3.193426	12.972099
C	2.504436	2.784924	14.076936
H	3.318934	3.421513	14.427627
C	2.233931	1.579526	14.727613
H	2.840751	1.278755	15.585631
C	1.190007	0.762072	14.285778
H	0.976158	-0.181132	14.794951
C	0.419346	1.160681	13.189473
H	-0.401379	0.530118	12.837856
C	0.694005	2.365132	12.540187
H	0.085787	2.67631	11.688185
C	4.259805	3.550719	11.63299
C	4.035132	2.353312	10.937347
H	3.13416	2.250351	10.329945
C	4.934832	1.293305	11.04206
H	4.747178	0.365219	10.496994
C	6.06763	1.414669	11.851337
H	6.765729	0.579755	11.94293
C	6.307748	2.607654	12.535713
H	7.191852	2.710639	13.169367
C	5.413769	3.673586	12.422229
H	5.593753	4.595638	12.975737

Compound *syn*-4

E_{SFC} = –3288.5692270 Ha

ν_{min} = 9.18 cm^{-1}

N	8.897643	6.632838	8.431928
B	9.174632	7.921181	7.82492
C	9.707905	5.541011	8.186793
C	10.359281	7.989077	6.863096
C	11.107242	6.839013	6.63987
B	7.597282	6.403819	9.139391
C	10.792606	5.609066	7.326891

C	6.527499	5.491514	8.447079
C	6.728478	4.963591	7.16047
H	7.638757	5.213889	6.610665
C	5.789935	4.115211	6.569248
H	5.970211	3.711907	5.569223
C	4.622365	3.776985	7.261623
H	3.891176	3.10247	6.808357
C	4.383073	4.330195	8.520817
H	3.446053	4.10529	9.036487
C	5.309547	5.20082	9.120581
C	8.311028	9.167359	8.239499
C	6.905185	9.175488	8.264013
H	6.341568	8.335441	7.846929
C	6.191245	10.233999	8.831748
H	5.103944	10.197228	8.86281
C	6.874903	11.325239	9.371484
H	6.31787	12.149017	9.825983
C	8.272597	11.361438	9.320798
H	8.815115	12.219065	9.728339
C	8.976132	10.297856	8.754301
H	10.068235	10.33488	8.727919
C	10.706988	9.276847	6.203339
C	9.739047	9.980976	5.466043
H	8.735253	9.561726	5.371126
C	10.042756	11.200673	4.858936
H	9.274444	11.726148	4.285618
C	11.320325	11.75258	4.989594
H	11.558047	12.710296	4.519439
C	12.290095	11.071033	5.731332
H	13.291259	11.495263	5.845412
C	11.986684	9.846743	6.328625
H	12.750702	9.320895	6.904095
C	12.257743	6.846795	5.684467
C	13.562735	6.560967	6.113956
H	13.741018	6.317185	7.162897
C	14.629595	6.584694	5.214414
H	15.640322	6.363824	5.567059
C	14.406493	6.884641	3.867238
H	15.241094	6.898997	3.16163
C	13.109718	7.167511	3.428722
H	12.925724	7.406053	2.378019
C	12.045515	7.153681	4.33196
H	11.035182	7.389308	3.991546
C	11.641936	4.397093	7.120798
C	12.360271	3.832383	8.18592
H	12.291884	4.28936	9.175451
C	13.151277	2.697981	7.994158

H	13.702741	2.272676	8.836697
C	13.238947	2.109065	6.72959
H	13.858794	1.221808	6.577416
C	12.530559	2.66468	5.659663
H	12.594905	2.213356	4.666213
C	11.740627	3.798613	5.854625
H	11.195311	4.233871	5.014716
C	9.374929	4.303321	8.94633
C	9.121559	3.083785	8.298717
H	9.188017	3.031002	7.211966
C	8.773447	1.952676	9.0327
H	8.565928	1.01379	8.513529
C	8.68179	2.018106	10.427703
H	8.400675	1.132876	11.001589
C	8.945771	3.221401	11.082067
H	8.88134	3.281317	12.168766
C	9.287329	4.358618	10.347067
H	9.507022	5.292264	10.866847
N	3.584595	5.815016	11.002402
B	2.54292	6.726584	10.59636
C	3.323659	4.731542	11.80487
C	1.143036	6.451699	11.140214
C	0.948954	5.336108	11.949016
B	4.951242	5.988373	10.413805
C	2.04774	4.46605	12.281536
C	5.956132	6.989631	11.041209
C	5.620642	7.735216	12.184449
H	4.609732	7.658864	12.593792
C	6.555252	8.566739	12.803791
H	6.275266	9.150042	13.684901
C	7.856442	8.644748	12.29503
H	8.596684	9.286438	12.779694
C	8.202102	7.920473	11.152836
H	9.211536	8.012336	10.746987
C	7.26345	7.112575	10.491761
C	2.814114	7.930824	9.607676
C	3.190182	7.741307	8.263562
H	3.449298	6.742946	7.907542
C	3.195689	8.800996	7.349859
H	3.479796	8.619661	6.309899
C	2.831045	10.084218	7.762577
H	2.829899	10.912668	7.049678
C	2.481671	10.303785	9.0999
H	2.199962	11.305549	9.434688
C	2.473521	9.240556	10.003019
H	2.156628	9.423125	11.033081
C	0.016607	7.374739	10.828939

C	-0.345179	7.64085	9.49704
H	0.202056	7.151487	8.68899
C	-1.385617	8.521303	9.196295
H	-1.650434	8.709214	8.152425
C	-2.08076	9.166349	10.223378
H	-2.892445	9.859935	9.989042
C	-1.7263	8.918988	11.553043
H	-2.260724	9.419372	12.365042
C	-0.690772	8.031682	11.850853
H	-0.421899	7.840781	12.891719
C	-0.406605	5.003816	12.486137
C	-0.642321	4.941851	13.868029
H	0.179841	5.130381	14.560927
C	-1.912938	4.641448	14.361423
H	-2.079456	4.601676	15.440979
C	-2.967219	4.387519	13.479157
H	-3.961435	4.147948	13.864898
C	-2.742064	4.443046	12.100663
H	-3.560538	4.248191	11.402893
C	-1.473071	4.75371	11.609283
H	-1.302257	4.809854	10.532438
C	1.817214	3.253804	13.125613
C	2.415803	3.121556	14.3879
H	3.058792	3.921774	14.759624
C	2.201688	1.982528	15.166489
H	2.678936	1.898234	16.146289
C	1.378484	0.955483	14.696457
H	1.208661	0.063799	15.30528
C	0.771175	1.078173	13.443027
H	0.122668	0.282282	13.067749
C	0.989249	2.217198	12.666544
H	0.508096	2.312248	11.690825
C	4.463513	3.838477	12.1755
C	4.499472	2.509304	11.726052
H	3.733745	2.160457	11.031286
C	5.475602	1.629471	12.191341
H	5.483484	0.594327	11.841645
C	6.428829	2.065772	13.116341
H	7.182089	1.370935	13.496522
C	6.421659	3.394649	13.545407
H	7.16702	3.745193	14.263835
C	5.450046	4.279088	13.071981
H	5.429891	5.3079	13.432921

Compound [4]K

E_{SFC} = –3888.42257969913 Ha

ν_{min} = 24.29 cm^{-1}

B	2.035513	7.586059	13.349737
C	0.023448	6.201962	13.237775
N	1.09675	6.782091	12.610041
C	-0.237521	6.388752	14.591242
C	0.616362	7.228447	15.3897
C	1.736963	7.830698	14.829757
C	2.226475	5.491981	9.025347
K	0.12449	3.50808	9.449656
B	1.264935	6.686241	11.100124
C	3.013689	4.442258	8.477939
H	3.170177	4.412312	7.39546
C	3.578531	3.449371	9.270367
H	4.176915	2.654577	8.816267
C	3.383795	3.475733	10.675555
H	3.827257	2.698147	11.303917
C	2.649655	4.508718	11.246845
H	2.518858	4.535257	12.333132
C	2.061227	5.540392	10.465935
C	3.348432	8.19085	12.708572
C	4.453583	7.374973	12.400955
H	4.340728	6.288445	12.406388
C	5.712332	7.921127	12.131773
H	6.557974	7.261239	11.918836
C	5.890254	9.308026	12.139059
H	6.874425	9.738767	11.936427
C	4.795398	10.139915	12.394013
H	4.921502	11.225992	12.395177
C	3.546937	9.584189	12.67961
H	2.714573	10.248661	12.92596
C	2.598177	8.73859	15.637483
C	3.971784	8.482931	15.789701
H	4.404462	7.599423	15.317123
C	4.786576	9.344207	16.526036
H	5.85195	9.122428	16.630737
C	4.246848	10.489598	17.118615
H	4.885291	11.167859	17.690712
C	2.883843	10.762075	16.968867
H	2.450107	11.656399	17.42442
C	2.07016	9.894656	16.238164
H	1.006058	10.112863	16.126919
C	0.27522	7.422731	16.83278
C	-0.94774	7.993831	17.216768
H	-1.662568	8.294773	16.448518
C	-1.25605	8.180158	18.565297

H	-2.211669	8.630948	18.845439
C	-0.348418	7.788878	19.553922
H	-0.590607	7.930969	20.610278
C	0.871711	7.216576	19.18247
H	1.589369	6.910195	19.947958
C	1.181815	7.039873	17.833061
H	2.140876	6.605484	17.544374
C	-1.399424	5.694513	15.226831
C	-2.719014	5.982183	14.844597
H	-2.897439	6.734475	14.073378
C	-3.798464	5.324672	15.438308
H	-4.818151	5.56448	15.125499
C	-1.191392	4.737102	16.232994
H	-0.170915	4.514248	16.55174
C	-2.267497	4.079596	16.830855
H	-2.083239	3.338913	17.61343
C	-3.576685	4.368877	16.433689
H	-4.42032	3.855521	16.902116
C	-0.885206	5.298535	12.457421
C	-0.915432	3.924581	12.764143
H	-0.221941	3.533368	13.510889
C	-1.849323	3.073072	12.160964
H	-1.875335	2.014896	12.435381
C	-2.768183	3.583616	11.233129
H	-3.511561	2.926507	10.774394
C	-2.734277	4.946654	10.908437
H	-3.449292	5.357726	10.19211
C	-1.801194	5.796572	11.512523
H	-1.798193	6.858759	11.268578
B	1.099841	5.535728	5.807841
C	2.608361	7.436703	6.077233
N	1.755762	6.512397	6.633306
C	2.921101	7.433992	4.72148
C	2.356615	6.445848	3.845579
C	1.451652	5.501284	4.32857
C	0.581095	7.73907	10.211592
B	1.539491	6.547711	8.142329
C	-0.171446	8.802835	10.768941
H	-0.208539	8.912512	11.857054
C	-0.867889	9.702134	9.972544
H	-1.441574	10.513731	10.428926
C	-0.832119	9.567106	8.569956
H	-1.383732	10.269615	7.938946
C	-0.076921	8.553862	7.995605
H	-0.033213	8.473723	6.905572
C	0.652045	7.628172	8.780969
C	0.008151	4.546907	6.400817

C	-1.188059	5.027666	6.975069
H	-1.3175	6.102453	7.122814
C	-2.225142	4.16036	7.343507
H	-3.148564	4.566075	7.763398
C	-2.084063	2.777177	7.168218
H	-2.896345	2.099852	7.444852
C	-0.89689	2.272845	6.618426
H	-0.779274	1.196981	6.461992
C	0.125952	3.149582	6.235534
H	1.026383	2.742584	5.769465
C	0.881269	4.458729	3.430776
C	-0.508728	4.345431	3.253556
H	-1.167368	5.051327	3.764583
C	-1.053862	3.353769	2.435468
H	-2.138072	3.291784	2.308302
C	-0.218361	2.443376	1.781853
H	-0.643023	1.66534	1.142209
C	1.166417	2.538957	1.952343
H	1.830622	1.833922	1.445157
C	1.708097	3.535716	2.765761
H	2.790679	3.608339	2.888912
C	2.755535	6.452959	2.404635
C	4.097884	6.288279	2.029553
H	4.858891	6.170325	2.803322
C	4.465829	6.279016	0.683246
H	5.515712	6.146296	0.409524
C	3.497179	6.445535	-0.311072
H	3.785333	6.443688	-1.365435
C	2.158012	6.615373	0.051948
H	1.393378	6.746379	-0.718122
C	1.790692	6.613703	1.398648
H	0.742923	6.736054	1.679445
C	3.839092	8.481685	4.181413
C	5.160682	8.592875	4.641012
H	5.516843	7.90393	5.409431
C	6.016071	9.572027	4.132615
H	7.041228	9.642464	4.505461
C	3.397701	9.37812	3.194934
H	2.373824	9.300445	2.823474
C	4.250374	10.357763	2.683989
H	3.886728	11.046149	1.916635
C	5.564173	10.458763	3.151166
H	6.233024	11.225525	2.75185
C	3.149272	8.482466	6.993587
C	2.757071	9.819396	6.834998
H	2.105857	10.089982	6.002011
C	3.176787	10.792171	7.742356

H	2.850359	11.827549	7.615969
C	3.997475	10.438809	8.817198
H	4.313794	11.1905	9.543894
C	4.4121	9.113919	8.967809
H	5.049021	8.833657	9.804736
C	3.993932	8.141526	8.05927
H	4.322024	7.10914	8.184054

Compound [4]K_2

E_{SFC} = –4488.2772565 Ha

ν_{min} = 6.07 cm^{-1}

B	1.885355	7.698403	13.489849
C	-0.078525	6.292207	13.279581
N	0.980135	6.92197	12.68211
C	-0.343245	6.377703	14.645333
C	0.494754	7.165968	15.502567
C	1.598797	7.832804	14.98124
C	2.383051	5.735126	9.111644
K	-0.314301	4.73947	9.457722
B	1.190406	6.820859	11.150122
C	3.25807	4.706273	8.627087
H	3.418628	4.629985	7.54607
C	3.880985	3.802625	9.46121
H	4.534942	3.028325	9.049373
C	3.660992	3.868876	10.869102
H	4.150267	3.147358	11.53005
C	2.825723	4.83561	11.38659
H	2.653591	4.867572	12.467872
C	2.153493	5.801129	10.565829
C	3.155922	8.447329	12.899673
C	4.341463	7.773441	12.539986
H	4.360234	6.68166	12.539582
C	5.501245	8.470934	12.179886
H	6.405925	7.917504	11.913438
C	5.505772	9.872291	12.16391
H	6.411845	10.418668	11.889043
C	4.34005	10.565253	12.513674
H	4.332505	11.658692	12.518023
C	3.188194	9.857447	12.881054
H	2.297686	10.414167	13.185066
C	2.443729	8.699864	15.848907
C	3.820634	8.457187	15.993133
H	4.266358	7.604519	15.477044
C	4.619844	9.282986	16.786058
H	5.687495	9.0692	16.885789
C	4.059633	10.37927	17.44827

H	4.684373	11.028399	18.067313
C	2.692366	10.637505	17.310848
H	2.241882	11.491887	17.823322
C	1.895613	9.806305	16.521689
H	0.827749	10.011883	16.422173
C	0.166009	7.237538	16.959282
C	-1.061857	7.753785	17.40098
H	-1.791124	8.101685	16.667041
C	-1.356632	7.826544	18.763378
H	-2.316648	8.235512	19.089019
C	-0.43015	7.374806	19.707773
H	-0.662099	7.427331	20.774637
C	0.795023	6.856332	19.278666
H	1.526876	6.502362	20.00942
C	1.091262	6.793053	17.9161
H	2.053203	6.398529	17.583148
C	-1.471026	5.593238	15.23892
C	-2.811398	5.907524	14.968417
H	-3.038488	6.748386	14.309993
C	-3.851356	5.167449	15.535223
H	-4.88868	5.429624	15.310717
C	-1.200581	4.522267	16.105752
H	-0.16177	4.276275	16.336915
C	-2.236552	3.781804	16.677287
H	-2.003479	2.95277	17.350622
C	-3.567675	4.100102	16.391735
H	-4.380323	3.52152	16.83843
C	-0.990715	5.423158	12.464027
C	-0.869941	4.025653	12.551706
H	-0.041406	3.600134	13.12114
C	-1.811392	3.184449	11.946289
H	-1.708654	2.100314	12.03931
C	-2.890445	3.730706	11.241644
H	-3.632592	3.077504	10.776693
C	-3.011131	5.123365	11.136199
H	-3.845994	5.560099	10.582915
C	-2.071131	5.961121	11.743223
H	-2.174234	7.043695	11.662028
B	0.967158	5.811289	5.831774
C	2.931886	7.216311	6.042219
N	1.87252	6.587529	6.639519
C	3.197364	7.129637	4.676698
C	2.359329	6.341299	3.819525
C	1.254339	5.67586	4.340598
C	0.469665	7.77434	10.209965
B	1.66228	6.68866	8.171497
C	-0.405421	8.803147	10.694539

H	-0.56598	8.879402	11.775556
C	-1.028334	9.706805	9.860437
H	-1.682349	10.481053	10.272279
C	-0.808298	9.640602	8.452543
H	-1.297635	10.362075	7.791591
C	0.027045	8.673934	7.935065
H	0.199328	8.642079	6.853804
C	0.699246	7.708376	8.755828
C	-0.303782	5.062787	6.421726
C	-1.489267	5.736765	6.781425
H	-1.507879	6.82855	6.782036
C	-2.649178	5.03937	7.14131
H	-3.55381	5.592879	7.407759
C	-2.653893	3.638014	7.157062
H	-3.560058	3.091709	7.431769
C	-1.488246	2.944948	6.807255
H	-1.480855	1.851508	6.802714
C	-0.336274	3.652654	6.440069
H	0.554169	3.095866	6.135995
C	0.409269	4.808717	3.473152
C	-0.967407	5.05217	3.328102
H	-1.412754	5.905719	3.843073
C	-1.766883	4.225983	2.535846
H	-2.834408	4.440199	2.435692
C	-1.207138	3.128642	1.874998
H	-1.832049	2.479325	1.256326
C	0.159899	2.869631	2.013249
H	0.60997	2.014231	1.502114
C	0.956914	3.701189	2.801764
H	2.024577	3.494922	2.901978
C	2.689168	6.267844	2.363143
C	3.916568	5.749314	1.922874
H	4.64484	5.401228	2.657715
C	4.212145	5.674575	0.560756
H	5.171809	5.263904	0.236223
C	3.286952	6.126561	-0.384777
H	3.519422	6.072183	-1.451435
C	2.062309	6.647461	0.04291
H	1.331503	7.001744	-0.688739
C	1.765231	6.712672	1.405199
H	0.803647	7.108962	1.737096
C	4.326239	7.912411	4.082969
C	5.666165	7.597038	4.354428
H	5.892012	6.757336	5.014752
C	6.707166	8.334425	3.786046
H	7.744132	8.071055	4.010814
C	4.057316	8.982197	3.214191

H	3.018869	9.2293	2.982602
C	5.094335	9.719984	2.641095
H	4.862428	10.54779	1.965851
C	6.425004	9.400334	2.927244
H	7.238476	9.976669	2.479144
C	3.844012	8.085563	6.857645
C	3.723471	9.48306	6.769638
H	2.89513	9.908635	6.199951
C	4.664977	10.324206	7.375104
H	4.562435	11.408341	7.281834
C	5.743779	9.777961	8.080138
H	6.485879	10.431185	8.545132
C	5.864264	8.385297	8.185837
H	6.698931	7.948513	8.739373
C	4.92426	7.547636	7.578735
H	5.027157	6.465062	7.660173
K	3.166959	8.770067	9.863644

Compound 5

E_{SFC} = –1875.04061554499 Ha

ν_{min} = 15.28 cm^{-1}

B	4.117713	9.640684	17.90167
C	4.686819	9.243476	19.257873
C	5.240483	7.974749	19.398269
C	5.260656	7.044678	18.293248
C	4.724741	7.398614	17.065519
N	4.160099	8.640448	16.856601
B	3.66829	9.004641	15.508237
C	4.48932	9.11098	14.177161
C	5.839054	8.950231	13.867918
H	6.552163	8.6701	14.647598
C	6.283304	9.142689	12.550677
H	7.340253	9.014836	12.303863
C	5.372905	9.495056	11.550243
H	5.72487	9.64047	10.525337
C	4.010618	9.669145	11.845061
H	3.311898	9.952312	11.053509
C	3.574861	9.481274	13.154005
C	2.202651	9.625586	13.707362
C	1.02477	9.957677	13.043187
H	1.018717	10.150879	11.967246
C	-0.168514	10.04346	13.779078
H	-1.098515	10.306759	13.268004
C	-0.181198	9.798343	15.155577
H	-1.118245	9.874917	15.712711
C	1.007729	9.462473	15.820518

H	0.999462	9.284381	16.899117
C	2.201416	9.37689	15.105838
C	3.50261	11.044699	17.549062
C	3.938118	11.776378	16.427373
H	4.775035	11.40675	15.828125
C	3.326911	12.978208	16.056719
H	3.681358	13.521375	15.176754
C	2.260567	13.476329	16.807609
H	1.772562	14.410684	16.517774
C	1.82509	12.777396	17.940029
H	0.996883	13.168084	18.537485
C	2.44764	11.584659	18.309216
H	2.102926	11.053857	19.200511
C	4.61346	10.190997	20.403049
C	5.15667	11.483132	20.294117
H	5.648812	11.776109	19.364493
C	5.07769	12.388584	21.353817
H	5.514169	13.385256	21.247672
C	4.438087	12.026231	22.542684
H	4.371597	12.735772	23.371477
C	3.880462	10.749336	22.661037
H	3.37357	10.455991	23.584234
C	3.969381	9.842562	21.60383
H	3.534898	8.84634	21.705803
C	5.831352	7.540753	20.701673
C	6.906637	8.249286	21.25887
H	7.302077	9.119417	20.731151
C	7.464729	7.855958	22.476384
H	8.304222	8.41753	22.894232
C	6.948235	6.75259	23.161794
H	7.382183	6.446015	24.116957
C	5.872462	6.044041	22.61842
H	5.460935	5.18072	23.147598
C	5.32258	6.432327	21.395797
H	4.488795	5.870148	20.971173
C	5.849442	5.68298	18.468466
C	7.206715	5.526485	18.792294
H	7.829773	6.413472	18.923412
C	7.760653	4.25582	18.955122
H	8.819287	4.154614	19.20771
C	6.964986	3.116696	18.798509
H	7.397734	2.121386	18.927621
C	5.611914	3.259708	18.478618
H	4.980737	2.37566	18.35642
C	5.060618	4.532161	18.316198
H	4.003053	4.640774	18.066412
C	4.680455	6.471153	15.900849

C	5.851531	5.915624	15.363481
H	6.808716	6.112293	15.848604
C	5.797933	5.137568	14.208401
H	6.719611	4.7241	13.791569
C	4.572852	4.89404	13.576449
H	4.535805	4.28999	12.666603
C	3.399172	5.422886	14.11606
H	2.436348	5.230504	13.636765
C	3.451591	6.202988	15.273976
H	2.527862	6.601368	15.698142

Radical anion 5$^{\bullet-}$

E_{SFC} = –1875.08201625805 Ha

ν_{min} = 13.37 cm^{-1}

B	4.046721	9.644732	17.885814
C	4.64123	9.254467	19.233828
C	5.221805	7.987821	19.362111
C	5.234611	7.069699	18.260494
C	4.674568	7.432766	17.031393
N	4.114688	8.665302	16.823974
B	3.656535	9.029981	15.436224
C	4.519843	9.105176	14.160666
C	5.886593	8.92479	13.877852
H	6.576967	8.649211	14.681766
C	6.375	9.090551	12.579665
H	7.440066	8.942373	12.37291
C	5.505682	9.443845	11.530704
H	5.896935	9.569637	10.516291
C	4.140385	9.638595	11.783239
H	3.469331	9.919218	10.964381
C	3.645095	9.476486	13.078663
C	2.272031	9.64104	13.574368
C	1.11303	9.973829	12.869104
H	1.15268	10.151998	11.789149
C	-0.1078	10.078653	13.549308
H	-1.017586	10.342037	13.000735
C	-0.166611	9.84915	14.93684
H	-1.123947	9.941243	15.46015
C	0.988034	9.514768	15.648458
H	0.929103	9.353393	16.729867
C	2.227446	9.404551	14.992683
C	3.398611	11.057849	17.606779
C	3.830779	11.880668	16.548555
H	4.623942	11.529053	15.883909
C	3.254093	13.131219	16.315242
H	3.606678	13.744699	15.481115

C	2.215895	13.589269	17.133559
H	1.753363	14.562693	16.944375
C	1.771264	12.791556	18.191042
H	0.959306	13.139237	18.836956
C	2.364147	11.547335	18.424698
H	2.014607	10.940149	19.264448
C	4.592798	10.192797	20.386231
C	5.112303	11.496357	20.272918
H	5.558364	11.804322	19.325441
C	5.059723	12.392898	21.341115
H	5.473759	13.398407	21.222604
C	4.475547	12.013863	22.553951
H	4.430624	12.71685	23.390588
C	3.944491	10.726473	22.68161
H	3.478998	10.416111	23.621803
C	4.003318	9.830857	21.612702
H	3.584334	8.828781	21.722474
C	5.848638	7.567065	20.653568
C	6.917972	8.298729	21.195056
H	7.279905	9.179025	20.660289
C	7.510485	7.918705	22.400298
H	8.343702	8.502367	22.801724
C	7.038931	6.800284	23.094573
H	7.500929	6.502382	24.039954
C	5.970481	6.067033	22.569619
H	5.591893	5.190737	23.10336
C	5.384446	6.446053	21.360761
H	4.555756	5.865524	20.951331
C	5.83779	5.713242	18.425763
C	7.196905	5.563052	18.748417
H	7.813017	6.4559	18.871469
C	7.762489	4.297919	18.916241
H	8.823078	4.207975	19.167701
C	6.978342	3.150683	18.762782
H	7.419871	2.158636	18.892569
C	5.624313	3.284171	18.440493
H	5.000004	2.395046	18.314915
C	5.062454	4.55124	18.275998
H	4.006247	4.650428	18.018442
C	4.616736	6.469297	15.892305
C	5.776365	5.895301	15.353784
H	6.748762	6.169236	15.765456
C	5.69506	4.983772	14.296981
H	6.611068	4.553455	13.882994
C	4.453685	4.633627	13.765413
H	4.390483	3.926476	12.933588
C	3.287535	5.198776	14.299434

H	2.309745	4.935226	13.887903
C	3.369193	6.110287	15.350895
H	2.460157	6.557127	15.757203

Anion 6^{-}

E_{SFC} = –1874.53549674187 Ha

ν_{min} = 14.69 cm^{-1}

B	0.229617	1.96489	0.532287
N	0.323666	0.701171	-0.129662
C	-0.035655	-1.309384	-1.44473
B	-0.797942	0.040936	-1.030113
C	-0.451502	-2.405249	-2.205859
H	-1.43732	-2.387969	-2.681867
C	0.37572	-3.523738	-2.346378
H	0.047384	-4.380988	-2.943187
C	1.622026	-3.557665	-1.705559
H	2.259613	-4.442402	-1.795241
C	2.060317	-2.470804	-0.944451
H	3.023692	-2.530688	-0.443031
C	1.238881	-1.334566	-0.831702
C	1.457037	-0.063716	-0.092002
C	2.608342	0.369891	0.57651
C	2.59668	1.617579	1.282261
C	1.463177	2.435756	1.300657
C	-1.305937	1.000805	-2.241445
C	-0.608107	1.66771	-3.248493
H	0.480863	1.565797	-3.314461
C	-1.285765	2.485	-4.165377
H	-0.729556	3.01426	-4.946051
C	-2.676082	2.632394	-4.082673
H	-3.200237	3.276391	-4.795814
C	-3.396678	1.964021	-3.086154
H	-4.481066	2.092822	-3.015374
C	-2.713243	1.155462	-2.172031
C	-3.263046	0.414224	-1.018466
C	-4.593006	0.338035	-0.592789
H	-5.387376	0.842487	-1.151498
C	-4.900247	-0.371291	0.574675
H	-5.936828	-0.427547	0.921854
C	-3.885177	-1.008358	1.299787
H	-4.134146	-1.561133	2.211575
C	-2.554753	-0.938544	0.858437
H	-1.766254	-1.44005	1.430588
C	-2.225505	-0.222678	-0.292753
C	-1.085237	2.836759	0.393301
C	-1.138962	3.88891	-0.538456

H	-0.264639	4.095572	-1.161546
C	-2.292751	4.655722	-0.711364
H	-2.310968	5.450385	-1.462835
C	-3.42809	4.394736	0.062137
H	-4.338218	4.986248	-0.076785
C	-2.235463	2.599562	1.164932
H	-2.240263	1.777757	1.884954
C	-3.393408	3.365617	1.006583
H	-4.278916	3.13969	1.607441
C	0.476842	4.087765	2.919551
H	-0.301147	3.355995	3.142118
C	0.465105	5.328503	3.559424
H	-0.324222	5.555116	4.282196
C	1.449942	6.279408	3.275813
H	1.440253	7.252929	3.774384
C	2.442561	5.972846	2.339656
H	3.21543	6.708954	2.098832
C	2.452327	4.730339	1.704358
H	3.22854	4.505531	0.970804
C	1.475849	3.754723	1.985035
C	3.827497	2.01219	2.03961
C	3.776189	2.153291	3.435288
H	2.827877	1.977701	3.947386
C	4.90959	2.521942	4.16235
H	4.846295	2.625764	5.249272
C	6.119319	2.762922	3.504434
H	7.00789	3.053462	4.071968
C	6.182491	2.631116	2.11394
H	7.1225	2.818852	1.587324
C	5.048171	2.257316	1.391156
H	5.104171	2.152898	0.306327
C	3.864453	-0.434727	0.549061
C	4.627021	-0.52417	-0.62782
H	4.26156	-0.023547	-1.527704
C	5.821431	-1.245688	-0.65947
H	6.397085	-1.304122	-1.58766
C	6.281962	-1.891649	0.492709
H	7.218682	-2.455676	0.471507
C	5.535949	-1.808217	1.672103
H	5.888005	-2.307562	2.579246
C	4.340054	-1.086804	1.69737
H	3.760683	-1.016953	2.620448

Compound 7

E_{SFC} = –2491.1960807 Ha

ν_{min} = 10.70 cm^{-1}

B	3.115854	3.093005	19.849548
N	2.191364	3.586803	18.813876
B	0.76852	3.438789	19.038923
C	-1.030197	2.987046	22.450693
H	-1.772913	3.519586	23.049932
C	0.298781	2.827611	20.408403
C	3.265332	3.645163	21.320225
C	6.261766	4.927783	18.59257
H	6.775853	5.451064	19.402398
C	8.0629	0.435525	22.187438
H	9.007798	0.803558	22.595178
C	-0.428057	4.732459	15.564864
C	0.878902	1.6534	20.925907
H	1.61143	1.098037	20.332718
C	2.273245	4.279038	14.105538
H	1.689453	3.356454	14.095372
C	4.779784	1.84216	20.919078
C	-1.28177	3.796986	14.961165
H	-1.313396	2.776749	15.348564
C	2.428167	4.667953	21.961208
C	4.894801	1.937657	24.11289
H	4.573365	0.954541	23.765144
C	4.801029	3.043251	23.24801
C	4.182037	4.189292	17.560054
C	5.798758	3.34567	25.864478
H	6.18642	3.462879	26.879621
C	4.865741	4.864069	18.587255
H	4.30611	5.361371	19.381046
C	1.861984	4.435618	16.583852
C	2.453284	4.963246	15.317985
C	-0.677786	3.471984	21.193151
H	-1.149473	4.38309	20.81977
C	-0.423674	1.829293	22.954722
H	-0.697989	1.451836	23.943452
C	6.31635	3.674814	16.526175
H	6.880119	3.192934	15.724313
C	-2.42746	4.944308	17.929267
H	-1.957357	5.894769	17.669923
C	7.059037	1.342082	21.842661
H	7.220634	2.412514	21.98098
C	5.222616	4.301416	23.715526
H	5.153354	5.163907	23.049674

C	2.699336	4.062919	17.622958
C	4.263764	2.900487	21.880564
C	3.199923	6.15131	15.313266
H	3.346503	6.691552	16.251155
C	5.839789	0.890444	21.306193
C	5.720514	4.450496	25.009615
H	6.047817	5.434576	25.354802
C	-0.405882	6.044346	15.067362
H	0.256919	6.780664	15.525663
C	4.405287	1.110285	18.502392
C	4.143724	1.902923	19.711343
C	7.858706	-0.937363	22.02059
H	8.641998	-1.646978	22.298838
C	5.646394	-0.493178	21.141677
H	4.701265	-0.850877	20.728385
C	0.529014	1.158415	22.186893
H	1.002218	0.248949	22.566466
C	5.38113	2.090582	25.412338
H	5.438761	1.222539	26.073944
C	4.926095	3.602344	16.524177
C	2.827957	4.766926	12.921511
H	2.67772	4.220093	11.987094
C	6.990822	4.331717	17.562393
H	8.082699	4.377701	17.56422
C	3.343747	0.783218	17.634034
H	2.326252	1.077472	17.895585
C	1.128066	5.473242	23.860932
H	0.785669	5.336575	24.890052
C	0.42832	4.328511	16.722422
C	6.644817	-1.398713	21.49975
H	6.476189	-2.470847	21.370434
C	-0.148455	3.861121	17.899105
C	-1.625531	3.797406	18.065874
C	5.934955	0.038549	16.933156
H	6.955887	-0.239144	16.657654
C	5.707117	0.723605	18.124706
H	6.55001	0.997607	18.759109
C	-2.061657	5.471393	13.395716
H	-2.695571	5.758419	12.552872
C	-2.252811	2.587095	18.408947
H	-1.643762	1.689126	18.53226
C	1.983679	4.532759	23.291584
H	2.287823	3.659748	23.868734
C	4.869707	-0.279744	16.082693
H	5.051472	-0.813212	15.146272
C	3.572062	5.950834	12.929367
H	4.005698	6.334038	12.002174

C	3.755838	6.641984	14.130271
H	4.334494	7.569204	14.146549
C	-3.635268	2.520065	18.591329
H	-4.101336	1.566013	18.851492
C	1.971878	5.779946	21.224505
H	2.281967	5.902201	20.18592
C	-2.088648	4.161126	13.88187
H	-2.745546	3.418595	13.421615
C	-3.80853	4.881982	18.120618
H	-4.41144	5.787371	18.01099
C	-1.219544	6.412877	13.994929
H	-1.192622	7.440227	13.622724
C	3.571933	0.09484	16.441198
H	2.729966	-0.146109	15.787005
C	1.118847	6.724694	21.796788
H	0.780384	7.577696	21.20284
C	0.691274	6.575833	23.11873
H	0.015938	7.309665	23.565876
C	-4.419955	3.668106	18.449376
H	-5.501839	3.618149	18.596945
H	4.40922	3.056963	15.735569

Compound 8

E_{SFC} = –2491.2121642 Ha

ν_{min} = 8.01 cm^{-1}

B	3.016406	3.472832	20.080931
N	2.100347	3.977257	19.076515
B	0.685995	3.679188	19.146987
C	-1.145192	3.193015	22.558455
H	-1.629568	3.809391	23.320949
C	0.057972	3.033987	20.439587
C	2.968263	3.450946	21.661698
H	2.130147	2.88379	22.089345
C	5.914415	6.471596	17.576937
H	6.25319	7.396944	17.10508
C	8.691648	2.078793	22.024948
H	9.364903	2.49164	22.780707
C	-0.183312	4.335611	15.412046
C	0.081344	1.636165	20.601407
H	0.549461	1.014387	19.833117
C	3.606028	4.328524	14.870358
H	3.933891	3.400878	15.340519
C	5.101909	2.562014	20.910338
C	0.204899	3.537019	14.325386
H	1.054886	2.860683	14.434043
C	2.88816	4.883596	22.173912

C	4.980538	1.003422	23.614171
H	5.077577	0.319083	22.769009
C	4.591587	2.334903	23.373045
C	4.118001	4.889119	18.033562
C	5.117217	1.42979	25.993381
H	5.322278	1.080389	27.008551
C	4.587336	6.069406	17.433808
H	3.90111	6.689376	16.86003
C	1.950354	4.599202	16.74576
C	2.584028	5.072243	15.478067
C	-0.577065	3.796526	21.432588
H	-0.615685	4.88468	21.336093
C	-1.090467	1.804974	22.713153
H	-1.529795	1.331528	23.594991
C	6.340635	4.532839	18.955752
H	7.02762	3.942243	19.559425
C	-2.502524	4.126891	18.636678
H	-2.174793	4.955909	19.267051
C	7.378055	2.53861	21.946952
H	7.031744	3.312867	22.633188
C	4.46132	3.202153	24.473288
H	4.168023	4.239349	24.312037
C	2.690196	4.473697	17.906335
C	4.299651	2.772847	21.987686
C	2.150175	6.252735	14.854139
H	1.346061	6.834194	15.309657
C	6.484951	2.03151	20.981586
C	4.727156	2.752749	25.769217
H	4.629803	3.444895	26.60978
C	-1.277424	5.199849	15.259027
H	-1.593116	5.815886	16.103249
C	4.147425	1.716025	18.706365
C	4.427982	2.935875	19.585281
C	9.148637	1.098691	21.137428
H	10.178293	0.737097	21.197383
C	6.961749	1.053267	20.088876
H	6.297519	0.642455	19.330019
C	-0.478258	1.025469	21.72667
H	-0.440795	-0.062062	21.83338
C	5.240105	0.555134	24.908814
H	5.539227	-0.483433	25.072695
C	5.007112	4.122462	18.830515
C	4.191678	4.759165	13.678441
H	4.986828	4.165948	13.219439
C	6.797641	5.694098	18.328174
H	7.841643	5.996459	18.442464
C	3.423614	0.637735	19.24578

H	3.120932	0.666484	20.295334
C	1.824271	6.590322	23.546467
H	1.045226	6.871924	24.260094
C	0.539423	4.254002	16.717901
C	8.277653	0.591003	20.170357
H	8.622612	-0.174265	19.470087
C	-0.125677	3.855316	17.864367
C	-1.560966	3.462265	17.834098
C	4.240939	0.526441	16.584886
H	4.574249	0.48643	15.544358
C	4.554915	1.641449	17.368035
H	5.13836	2.459493	16.943812
C	-1.56912	4.471838	12.968345
H	-2.107057	4.525384	12.018426
C	-2.005372	2.395747	17.033694
H	-1.285935	1.864055	16.407823
C	1.89395	5.273857	23.082755
H	1.177774	4.531121	23.436176
C	3.509343	-0.533464	17.126761
H	3.26075	-1.403066	16.513631
C	3.760157	5.942012	13.071897
H	4.216566	6.280102	12.138171
C	2.734943	6.686674	13.663771
H	2.386439	7.60984	13.193787
C	-3.347199	2.012612	17.029498
H	-3.669932	1.178908	16.40024
C	3.820091	5.845997	21.747761
H	4.618683	5.562342	21.058861
C	-0.485661	3.600241	13.114437
H	-0.173661	2.968069	12.279173
C	-3.8475	3.751283	18.62818
H	-4.563729	4.287924	19.256016
C	-1.961821	5.27256	14.044627
H	-2.809709	5.954356	13.940424
C	3.104878	-0.474126	18.464832
H	2.538927	-1.299818	18.903953
C	3.749687	7.162638	22.206966
H	4.483038	7.894868	21.859425
C	2.749404	7.541973	23.107569
H	2.6951	8.571802	23.469541
C	-4.275818	2.691147	17.824696
H	-5.327351	2.392888	17.820428

Anion 11^{-}

E_{SFC} = –1644.93622700141 Ha

ν_{min} = 19.26 cm^{-1}

C	5.392928	20.317923	3.537571
C	6.018524	21.135225	2.579583
H	6.275598	20.711158	1.604934
C	4.593336	14.570542	2.311117
C	8.065969	18.872162	4.504593
C	5.654354	13.882033	1.698309
H	6.587121	14.41922	1.51052
C	8.735205	18.473409	3.331574
H	8.426819	17.545899	2.836708
C	3.402535	13.868367	2.554539
H	2.567798	14.394447	3.022618
C	5.074226	20.903499	4.775442
H	4.601402	20.291686	5.547857
C	3.071381	16.48012	0.812833
C	3.430077	19.355983	1.264268
C	6.337151	22.467913	2.849056
H	6.8442	23.071784	2.090535
C	2.675006	20.383708	1.862535
H	2.609533	20.421097	2.951309
C	8.49467	20.071056	5.098635
H	7.979921	20.423256	5.997081
C	9.526728	20.841645	4.55219
H	9.820563	21.780644	5.032805
C	9.766684	19.231582	2.771859
H	10.259575	18.894856	1.853454
C	5.371936	22.241092	5.04994
H	5.114871	22.668843	6.024236
C	6.012844	23.028213	4.088248
H	6.261139	24.071851	4.304536
C	3.274398	12.523048	2.200672
H	2.336344	11.996609	2.39884
C	10.167725	20.426322	3.381628
H	10.968647	21.030244	2.943275
C	5.532709	12.537374	1.344502
H	6.3728	12.021719	0.870419
C	2.019883	21.347182	1.094023
H	1.439647	22.130497	1.590673
C	2.108606	21.31879	-0.301212
H	1.598903	22.075354	-0.904759
C	3.529973	15.755361	-0.298678
H	4.596797	15.546072	-0.392894
C	1.695475	16.739234	0.91489
H	1.330374	17.312903	1.769319
C	2.865423	20.315136	-0.914044

H	2.953669	20.283395	-2.004222
C	4.339603	11.850916	1.594089
H	4.240404	10.797992	1.315486
C	3.5161	19.351469	-0.142062
H	4.110083	18.578831	-0.632953
C	1.27403	15.565101	-1.161408
H	0.577792	15.210538	-1.926701
C	0.804168	16.28543	-0.059229
H	-0.263733	16.499447	0.041232
C	2.642681	15.303747	-1.27731
H	3.023165	14.74225	-2.135335
B	5.083405	18.798868	3.217009
N	5.744408	17.771228	3.95655
C	7.158818	16.473839	5.4403
B	6.829295	18.005058	5.094574
C	8.01571	15.901289	6.386497
H	8.648555	16.548953	7.002761
C	8.06332	14.514401	6.558086
H	8.736017	14.073384	7.301358
C	7.235874	13.684403	5.788904
H	7.25487	12.600588	5.938879
C	6.381318	14.230192	4.827592
H	5.738787	13.565981	4.253666
C	6.361713	15.623445	4.635434
C	5.563941	16.445928	3.688759
C	4.726421	16.017923	2.647335
C	4.007598	16.981668	1.869521
C	4.138275	18.355738	2.103513
H	6.326724	18.575719	6.065766

Compound 7'

E_{SFC} = –1533.6551899 Ha

ν_{min} = 18.95 cm^{-1}

B	3.108679	3.103118	19.8428
N	2.186333	3.602283	18.812508
B	0.762939	3.442356	19.021998
C	-0.99809	3.055069	22.471835
H	-1.696021	3.624703	23.090706
C	0.287831	2.845258	20.401905
C	3.243768	3.622495	21.327994
C	6.22309	5.092471	18.607003
H	6.70925	5.675911	19.392714
C	-0.395148	4.621342	15.477327
C	0.809568	1.635424	20.899568
H	1.509004	1.05308	20.292662
C	4.783761	1.854913	20.89114

C	2.44227	4.661809	21.983081
C	4.892507	3.046031	23.213694
C	4.180355	4.244377	17.583943
C	4.830051	4.993975	18.581736
H	4.242744	5.515139	19.339054
C	1.866986	4.439237	16.57558
C	2.424558	5.069339	15.319996
C	-0.633727	3.534769	21.214212
H	-1.043801	4.48714	20.86902
C	-0.454256	1.857251	22.950667
H	-0.736137	1.481789	23.938099
C	6.350562	3.718097	16.62274
H	6.9414	3.200024	15.863746
C	2.699346	4.081491	17.619487
C	4.26757	2.896407	21.860924
C	5.817437	0.864202	21.329928
C	4.388805	1.111574	18.488099
C	4.161838	1.936305	19.679831
C	0.448834	1.145258	22.159142
H	0.87533	0.2056	22.520497
C	4.960962	3.611172	16.602871
C	6.987643	4.454007	17.6278
H	8.077903	4.528788	17.646414
C	3.308644	0.771804	17.645574
H	2.300271	1.091809	17.911553
C	1.208574	5.499114	23.919149
H	0.886631	5.367114	24.955608
C	0.436687	4.259568	16.68708
C	-0.149853	3.79338	17.856085
C	-1.64938	3.610219	17.953428
C	5.876643	-0.036239	16.92463
H	6.889057	-0.335442	16.639761
C	5.677719	0.695181	18.095692
H	6.540362	0.998725	18.689788
C	2.023284	4.536485	23.323159
H	2.295263	3.642443	23.885086
C	4.792649	-0.368889	16.10593
H	4.949155	-0.937918	15.186026
C	1.99224	5.787678	21.261247
H	2.273657	5.901612	20.213898
C	3.506971	0.040433	16.474321
H	2.650022	-0.209476	15.843228
C	1.180524	6.752247	21.85752
H	0.849133	7.61507	21.273627
C	0.784282	6.61462	23.191585
H	0.141974	7.36643	23.657162
H	4.471884	2.991819	15.849566

H	5.861666	-0.001482	20.655615
H	6.824585	1.318936	21.357324
H	5.611981	0.503153	22.350754
H	4.620326	4.002043	23.680957
H	5.991539	2.985603	23.152125
H	4.573579	2.238314	23.897726
H	1.864022	5.978508	15.050532
H	2.355997	4.390631	14.451936
H	3.477364	5.352259	15.433227
H	-0.002563	4.151873	14.561351
H	-1.443475	4.3224	15.587316
H	-0.379216	5.710597	15.298473
H	-1.934807	3.155949	18.911318
H	-2.19214	4.568846	17.870459
H	-2.041179	2.956247	17.155053

Transition state TS1

E_{SFC} = –1533.6109071 Ha

v_{min} = –1468.01 cm^{-1}

B	3.785804	3.15055	19.30298
N	2.58058	3.401127	18.42868
B	1.262758	2.942057	18.751083
C	0.199028	1.777606	22.312209
H	-0.367837	2.182606	23.155533
C	1.065028	2.043759	20.037175
C	3.645399	3.777974	20.883458
C	6.359829	4.172603	18.526368
H	6.859187	3.828897	19.436368
C	-0.601639	4.655539	15.765586
C	1.633073	0.76142	20.150866
H	2.192764	0.341851	19.312674
C	4.78586	1.687702	20.94485
C	2.817358	4.93236	21.25453
C	4.316066	2.867356	23.189616
C	4.282367	4.503153	17.259237
C	4.971777	4.081581	18.420536
H	4.453888	4.244408	19.746601
C	1.812091	4.670635	16.521369
C	2.078352	5.67971	15.427517
C	0.32736	2.522285	21.136976
H	-0.136281	3.510325	21.079757
C	0.796742	0.51627	22.410602
H	0.698132	-0.070305	23.328329
C	6.432323	5.090667	16.293675
H	7.008818	5.468053	15.445275
C	2.835672	4.219436	17.342068

C	4.238762	2.830064	21.691104
C	5.430381	0.539079	21.66813
C	5.04783	0.913291	18.529088
C	4.545416	1.785366	19.598114
C	1.505366	0.004871	21.319576
H	1.963513	-0.986383	21.378738
C	5.042862	4.990436	16.181207
C	7.096085	4.694386	17.461051
H	8.183733	4.772268	17.528749
C	4.274043	0.721735	17.364088
H	3.298593	1.203503	17.289842
C	1.20606	6.038764	22.723975
H	0.604437	6.021331	23.636747
C	0.465157	4.201098	16.739693
C	0.146047	3.365012	17.805067
C	-1.273556	2.888716	18.021543
C	6.784717	-0.482136	17.523934
H	7.778065	-0.934884	17.583434
C	6.320844	0.307643	18.576808
H	6.967642	0.486001	19.43704
C	2.030772	4.953859	22.426514
H	2.025102	4.089415	23.08727
C	5.990415	-0.683609	16.391047
H	6.353535	-1.302881	15.566887
C	2.713597	6.040732	20.384962
H	3.293034	6.061572	19.460449
C	4.734335	-0.073678	16.315117
H	4.110115	-0.213331	15.428768
C	1.885198	7.122196	20.68029
H	1.829165	7.963047	19.984191
C	1.128377	7.131585	21.855623
H	0.477014	7.977802	22.08762
H	4.571029	5.258128	15.238748
H	-0.869731	5.714402	15.930239
H	-0.264344	4.572882	14.720737
H	-1.523029	4.070372	15.865245
H	6.429777	0.795694	22.062941
H	5.541847	-0.335033	21.014083
H	4.81475	0.237284	22.53116
H	4.188477	3.884569	23.581704
H	5.282194	2.475438	23.543274
H	3.531452	2.230249	23.634914
H	-1.341011	2.234661	18.90142
H	-1.975636	3.726576	18.180395
H	-1.658226	2.315737	17.158862
H	2.341652	5.208697	14.462463
H	2.895987	6.361232	15.696348

H	1.195486	6.304896	15.241411

Metastable intermediate Int1

E_{SFC} = –1533.6458205 Ha

v_{min} = 12.11 cm^{-1}

B	3.345325	2.637169	19.791910
N	1.966500	3.043578	19.190856
B	0.731925	2.324966	19.222986
C	0.219347	-1.180839	20.937722
H	-0.207561	-1.586560	21.859804
C	0.729822	0.767106	19.536289
C	3.298461	2.553672	21.448193
C	5.660621	3.967652	19.198923
H	6.311392	3.206415	19.643984
C	1.274013	-0.125955	18.591915
H	1.686751	0.268630	17.660901
C	3.797732	0.345653	20.694576
H	4.352448	2.839336	21.632273
C	3.439609	4.786155	18.639337
C	4.275279	3.807904	19.223110
C	0.874657	5.077237	18.453280
C	0.183723	0.198724	20.699969
H	-0.290847	0.845644	21.442436
C	0.790671	-2.039887	19.995657
H	0.823936	-3.117413	20.177779
C	5.405236	6.034350	17.967397
H	5.848750	6.892290	17.454507
C	2.023793	4.355639	18.747365
C	3.277075	1.119264	21.751794
C	4.585903	0.735381	18.304746
C	3.917935	1.132321	19.534899
C	1.308317	-1.505351	18.811278
H	1.744274	-2.166144	18.056540
C	4.012714	5.896400	17.994297
C	6.232309	5.082853	18.573848
H	7.319039	5.201590	18.539071
C	4.212539	1.376652	17.099252
H	3.424521	2.129078	17.128210
C	-0.409732	4.429482	18.508721
C	-0.532509	3.087059	18.855735
C	6.267956	-0.517027	17.051454
H	7.089033	-1.238122	17.036085
C	5.635302	-0.211471	18.255286
H	5.986411	-0.681846	19.172656
C	5.854754	0.099927	15.865893
H	6.344961	-0.148607	14.920940

C	4.823883	1.047221	15.893773
H	4.509414	1.541084	14.971474
H	3.404906	6.639886	17.483555
C	-1.886700	2.410851	18.883577
C	-1.628554	5.255832	18.156566
C	2.876029	0.547722	23.066927
C	0.961614	6.545988	18.105910
C	4.104747	-1.119148	20.851131
C	2.441783	3.570934	22.118784
C	2.962003	4.869079	22.280095
C	2.172620	5.905896	22.774776
C	0.838992	5.666853	23.121785
C	0.308462	4.383551	22.966525
C	1.100654	3.348250	22.464586
H	3.996173	5.066145	21.985374
H	2.598807	6.906871	22.882457
H	0.215897	6.478939	23.504483
H	-0.735545	4.188085	23.223799
H	0.667537	2.358870	22.323413
H	-2.565780	2.863770	19.628740
H	-2.406689	2.466478	17.910660
H	-1.793033	1.345830	19.136901
H	2.531434	1.321622	23.763435
H	2.083018	-0.205981	22.937494
H	3.737604	0.020529	23.514149
H	3.385791	-1.597826	21.529772
H	4.046817	-1.644779	19.890034
H	5.113870	-1.282567	21.270599
H	-1.819894	6.028433	18.921712
H	-1.498409	5.785822	17.199283
H	-2.534033	4.643774	18.077824
H	0.036264	7.075136	18.365915
H	1.773675	7.038820	18.656607
H	1.137073	6.723181	17.028350

Intermediate Int2

E_{SFC} = –1533.66225139212 Ha

v_{min} = 21.05 cm^{-1}

B	3.508568	3.370164	19.720432
N	2.256235	3.549413	18.983271
B	0.985701	2.885453	19.152857
C	0.027334	-0.320819	21.204565
H	-0.625999	-0.609998	22.032600
C	0.943079	1.433140	19.763399
C	2.642044	5.735673	21.538403
C	5.956717	4.278911	18.999138

H	6.507428	3.678638	19.729605
C	-1.175166	5.403998	17.064795
C	1.698875	0.435680	19.115013
H	2.364238	0.718240	18.294617
C	3.734227	3.519591	22.184677
C	1.210006	5.426142	21.465248
C	5.051439	5.671687	22.082903
C	3.840469	4.965715	17.988583
C	4.565483	4.200302	18.938360
C	1.304103	5.258992	17.555096
C	1.451779	6.547967	16.781366
C	0.105060	1.018453	20.814856
H	-0.500461	1.758762	21.337553
C	0.776165	-1.291288	20.532982
H	0.715626	-2.340457	20.833763
C	5.929275	5.859568	17.166264
H	6.468761	6.497552	16.461069
C	2.400008	4.642949	18.110273
C	3.708538	4.995523	21.922287
C	3.971768	3.108975	23.619081
C	3.942651	1.218136	21.212318
C	3.686808	2.675047	21.118862
C	1.613289	-0.908403	19.483191
H	2.216521	-1.655350	18.962032
C	4.530926	5.791099	17.091114
C	6.644493	5.115651	18.111126
H	7.734981	5.180155	18.143974
C	4.835674	0.626064	20.297115
H	5.299884	1.247510	19.526722
C	-0.788922	4.197964	22.123283
H	-1.245010	3.371661	22.673788
C	-0.025557	4.691888	17.739704
C	-0.230759	3.545549	18.483377
C	-1.612151	2.945323	18.608809
C	3.648239	-0.967836	22.245768
H	3.157333	-1.592926	22.995903
C	3.344516	0.392614	22.179281
H	2.600729	0.812253	22.856739
C	0.599164	4.340988	22.123833
H	1.214504	3.620781	22.661970
C	4.554996	-1.535784	21.347525
H	4.790110	-2.601744	21.401453
C	0.376382	6.329932	20.776604
H	0.833445	7.174517	20.254576
C	5.145005	-0.731891	20.367344
H	5.848574	-1.165677	19.651823
C	-1.007634	6.169946	20.752718

H	-1.628355	6.884776	20.206591
C	-1.600598	5.108290	21.440598
H	-2.686816	4.990934	21.447775
H	4.017131	6.356610	16.315746
H	2.864586	6.777092	21.279163
H	-2.067309	2.739721	17.624496
H	-1.588997	1.996021	19.157993
H	-2.300892	3.618608	19.147223
H	2.325725	7.119734	17.115145
H	0.575352	7.195219	16.919275
H	1.554710	6.380223	15.693880
H	4.460482	2.128291	23.697538
H	3.018349	3.051808	24.174446
H	4.589375	3.852766	24.145050
H	-0.955634	5.633426	16.010197
H	-2.099513	4.817257	17.096216
H	-1.383834	6.367260	17.562483
H	5.815999	5.185170	21.458241
H	5.403299	5.607750	23.126680
H	5.002944	6.735124	21.807579

Transition state TS2

E_{SFC} = –1533.60710377602 Ha

v_{min} = –171.39 cm^{-1}

B	0.779046	-0.395384	-1.029639
N	-0.610558	0.000553	-1.296464
B	-1.808105	-0.391096	-0.598436
C	-1.801369	-2.347150	2.792016
H	-1.664614	-2.138270	3.856814
C	-1.823371	-1.544228	0.481445
C	0.766103	1.611825	1.526001
C	2.985245	0.290971	-2.416297
H	3.658938	-0.335773	-1.824539
C	-4.303450	2.000499	-2.450445
C	-2.147227	-2.852945	0.077204
H	-2.281734	-3.069517	-0.986438
C	1.930769	-0.588128	1.097073
C	0.515300	2.294413	2.789775
C	3.281049	1.594189	1.008316
C	0.731475	1.136524	-2.856870
C	1.628577	0.344000	-2.095217
C	-1.794956	1.646877	-2.632286
C	-1.770670	2.776489	-3.636568
C	-1.655450	-1.315997	1.858755
H	-1.411934	-0.314416	2.220363
C	-2.129750	-3.637019	2.366368

H	-2.245255	-4.445007	3.093704
C	2.582309	1.799616	-4.263525
H	2.957258	2.361829	-5.123015
C	-0.636358	0.978278	-2.307503
C	1.945265	0.905550	1.036683
C	2.552035	-1.138769	2.359798
C	1.146489	-2.770126	0.048892
C	1.306788	-1.305208	0.124228
C	-2.299477	-3.887886	1.002335
H	-2.540467	-4.895895	0.655905
C	1.215159	1.857052	-3.958241
C	3.469399	1.030936	-3.501301
H	4.529518	0.999689	-3.765266
C	1.050681	-3.359151	-1.230474
H	1.110641	-2.719489	-2.115839
C	1.218401	3.236790	4.930039
H	2.023229	3.520456	5.613418
C	-3.051692	1.286853	-1.989787
C	-3.106674	0.324100	-0.998171
C	-4.414961	-0.027050	-0.322939
C	0.899473	-4.999896	1.006621
H	0.814593	-5.634999	1.892242
C	1.058609	-3.622877	1.165211
H	1.051845	-3.205553	2.169017
C	1.533547	2.691740	3.687634
H	2.579500	2.545725	3.415965
C	0.819154	-5.565485	-0.268029
H	0.691442	-6.644446	-0.386996
C	-0.827098	2.499756	3.184882
H	-1.629392	2.207232	2.502413
C	0.891202	-4.734224	-1.390501
H	0.823099	-5.159833	-2.395144
C	-1.137245	3.046792	4.428226
H	-2.183964	3.182692	4.712440
C	-0.117026	3.419467	5.309674
H	-0.359431	3.844775	6.286526
H	0.561740	2.444128	-4.599236
H	-0.137167	1.053857	1.247776
H	-5.140893	-0.469246	-1.028874
H	-4.261057	-0.758633	0.481158
H	-4.905427	0.856396	0.121341
H	-0.872763	3.397021	-3.515333
H	-2.634690	3.440985	-3.521754
H	-1.782305	2.410468	-4.678790
H	3.027544	-2.113721	2.178525
H	1.776714	-1.276196	3.133434
H	3.302204	-0.456353	2.782096

H	-4.377691	2.020390	-3.549006
H	-5.211204	1.524295	-2.063717
H	-4.314514	3.051772	-2.112485
H	3.696330	1.506478	-0.012033
H	4.026623	1.139871	1.683484
H	3.195280	2.666331	1.233545

Intermediate Int2$_{rot}$

E_{SFC} = –1533.6669399 Ha

ν_{min} = 18.15 cm^{-1}

B	3.514317	3.50783	19.711477
N	2.361868	3.604128	18.788913
B	1.089179	2.942247	18.872617
C	0.042183	0.752228	21.938412
H	-0.382713	0.894844	22.936007
C	0.863265	1.717982	19.845021
C	2.438994	5.051026	21.397094
C	5.920961	4.704043	19.428919
H	6.38238	4.171355	20.265675
C	-0.822327	5.11191	16.231383
C	1.122478	0.410173	19.394648
H	1.554899	0.259832	18.401602
C	3.948238	3.312167	22.13846
C	1.964705	6.282832	20.768348
C	4.594839	5.78816	22.508386
C	3.974952	5.126983	18.014174
C	4.585804	4.462711	19.10585
C	1.552639	5.169912	17.11691
C	1.769426	6.412124	16.283854
C	0.312435	1.861542	21.130547
H	0.073501	2.859309	21.510856
C	0.302441	-0.536475	21.465458
H	0.089163	-1.406688	22.091958
C	6.064653	6.262161	17.582658
H	6.65161	6.958397	16.977513
C	2.573019	4.664804	17.892692
C	3.611435	4.752374	22.037509
C	4.485404	2.756855	23.432073
C	3.989359	1.1568	20.815848
C	3.764547	2.605528	20.97598
C	0.843178	-0.704497	20.187657
H	1.062652	-1.707199	19.813099
C	4.727736	6.021474	17.239606
C	6.664194	5.617342	18.670923
H	7.711639	5.815107	18.912826

C	4.539511	0.679081	19.608125
H	4.805063	1.393675	18.824324
C	2.31583	8.380319	19.575213
H	3.000153	9.15037	19.210154
C	0.244766	4.540385	17.13786
C	-0.027212	3.462202	17.964022
C	-1.39848	2.821953	17.986885
C	3.863372	-1.14991	21.595057
H	3.571365	-1.865058	22.36835
C	3.646564	0.212578	21.801184
H	3.153156	0.543727	22.714178
C	2.821553	7.301317	20.300508
H	3.896147	7.223726	20.45652
C	4.42383	-1.604406	20.398578
H	4.589916	-2.672778	20.238417
C	0.591291	6.380585	20.459969
H	-0.080258	5.579094	20.777345
C	4.758238	-0.681841	19.401576
H	5.190412	-1.025613	18.458196
C	0.087663	7.457272	19.734202
H	-0.979234	7.504588	19.501947
C	0.949465	8.465994	19.290527
H	0.560048	9.307883	18.712556
H	4.3121	6.519556	16.366854
H	1.733431	4.22587	21.3191
H	-1.675578	2.394585	17.0065
H	-1.441118	2.005055	18.719743
H	-2.192116	3.543116	18.25087
H	2.412619	7.128904	16.809367
H	0.824828	6.929744	16.081256
H	2.234406	6.190595	15.306273
H	5.07718	1.84471	23.274685
H	3.666011	2.507772	24.129713
H	5.12008	3.492608	23.948528
H	-0.443945	5.283913	15.211866
H	-1.694774	4.453049	16.157837
H	-1.17724	6.087976	16.607646
H	5.38279	5.943892	21.74994
H	5.102074	5.463476	23.428406
H	4.112721	6.755856	22.703452

Metastable intermediate Int1$_{rot}$

E_{SFC} = –1533.6448495 Ha

ν_{min} = 13.07 cm^{-1}

B	3.345325	2.637169	19.791910
N	2.054510	3.171314	19.132202

B	0.780811	2.533568	19.142011
C	0.487114	-0.556465	21.535972
H	0.250559	-0.754747	22.585676
C	0.717474	1.046076	19.697602
C	3.298461	2.553672	21.448193
C	5.806198	3.763064	19.313559
H	6.364519	2.951604	19.788449
C	1.067729	-0.036928	18.867200
H	1.301180	0.148282	17.815790
C	3.962141	0.355545	20.618845
H	2.263789	2.714774	21.799194
C	3.697389	4.756835	18.615795
C	4.415136	3.714476	19.249111
C	1.174350	5.190724	18.150798
C	0.409875	0.748176	21.036818
H	0.116942	1.557252	21.712738
C	0.860541	-1.610619	20.695096
H	0.925596	-2.630798	21.083325
C	5.795013	5.878782	18.142535
H	6.336092	6.722884	17.706396
C	2.248067	4.435383	18.609904
C	3.645506	1.126195	21.736094
C	4.291681	0.728381	18.114991
C	3.839984	1.131788	19.437204
C	1.139106	-1.347333	19.351896
H	1.421594	-2.162736	18.679853
C	4.399070	5.839946	18.056202
C	6.501980	4.847140	18.767328
H	7.593689	4.885276	18.822305
C	3.768702	1.386210	16.975321
H	2.980849	2.125574	17.111556
C	-0.144447	4.611659	18.123553
C	-0.388968	3.315961	18.580127
C	5.838238	-0.464598	16.644956
H	6.667530	-1.165339	16.520252
C	5.342270	-0.199327	17.920244
H	5.813348	-0.678170	18.776228
C	5.280876	0.169451	15.530889
H	5.666304	-0.044103	14.530575
C	4.241732	1.093411	15.701330
H	3.816486	1.604107	14.834464
H	3.888005	6.646878	17.537208
C	-1.774025	2.707590	18.532233
C	-1.272070	5.454449	17.565000
C	3.694600	0.585353	23.126287
C	1.389098	6.618876	17.702608
C	4.335348	-1.100236	20.729604

C	4.191284	3.504869	22.212919
C	3.719870	4.770526	22.593803
C	4.550824	5.679731	23.251516
C	5.873643	5.340472	23.553310
C	6.357176	4.084085	23.181778
C	5.525220	3.181689	22.516364
H	2.688619	5.046264	22.358241
H	4.161808	6.661489	23.533845
H	6.522514	6.050041	24.072786
H	7.390349	3.804327	23.405958
H	5.929437	2.211269	22.216695
H	-2.512327	3.287082	19.114969
H	-2.170211	2.638918	17.502872
H	-1.765811	1.687463	18.943099
H	3.519296	1.366587	23.876115
H	2.920809	-0.195078	23.229894
H	4.659796	0.097386	23.341029
H	3.790708	-1.579419	21.554501
H	4.088156	-1.648464	19.812124
H	5.413733	-1.234213	20.927933
H	-1.503906	6.304990	18.229763
H	-1.012368	5.882695	16.583715
H	-2.194795	4.876264	17.441930
H	0.455332	7.193388	17.709268
H	2.089063	7.142840	18.369041
H	1.801306	6.687659	16.679352

Transition state TS3

E_{SFC} = –1533.6343068 Ha

ν_{min} = –294.96 cm^{-1}

B	3.059512	2.878196	19.647674
N	1.864653	3.415844	18.901384
B	0.526334	2.919172	18.99378
C	-0.843019	0.890447	22.039481
H	-1.491673	1.060417	22.903388
C	0.214779	1.740574	20.000912
C	3.199382	2.600829	21.230458
C	5.687696	4.094102	19.334564
H	6.237014	3.367632	19.935568
C	-1.05892	5.190325	16.225027
C	0.805508	0.473939	19.833399
H	1.45058	0.29985	18.969624
C	4.876819	1.334486	20.058682
C	3.119884	3.788792	22.152743
C	5.021794	1.348153	22.613138
C	3.634254	4.756577	18.173389

C	4.354124	3.846487	19.00003
C	1.302385	4.917519	17.087749
C	1.737509	5.846584	15.97761
C	-0.628383	1.916835	21.114074
H	-1.115572	2.884383	21.268384
C	-0.226764	-0.352332	21.862276
H	-0.391035	-1.156344	22.584666
C	5.606068	6.181547	18.128879
H	6.085837	7.108255	17.803702
C	2.215779	4.395739	17.996047
C	4.431923	1.724785	21.292139
C	6.068063	0.472243	19.751385
C	4.083387	1.388096	17.605951
C	4.056524	1.925817	18.984013
C	0.592001	-0.561177	20.747851
H	1.066873	-1.534326	20.592969
C	4.274853	5.942075	17.777216
C	6.319896	5.26101	18.90166
H	7.361347	5.453457	19.169608
C	4.408393	2.11889	16.451703
H	4.730853	3.154952	16.540893
C	4.098329	5.769919	23.188511
H	4.968307	6.412599	23.349092
C	-0.08066	4.52506	17.170783
C	-0.510758	3.564735	18.081368
C	-1.96307	3.143662	18.128968
C	3.640888	-0.552341	16.190147
H	3.338322	-1.598733	16.099566
C	3.709547	0.036251	17.452415
H	3.459176	-0.551608	18.338094
C	4.217226	4.637057	22.380224
H	5.177613	4.41441	21.913316
C	3.95437	0.191078	15.048082
H	3.90154	-0.268595	14.058252
C	1.898728	4.115445	22.765868
H	1.036385	3.465389	22.603014
C	4.34141	1.524898	15.188357
H	4.600073	2.115954	14.306013
C	1.77437	5.250973	23.56972
H	0.811411	5.482788	24.032923
C	2.87465	6.085202	23.786251
H	2.780458	6.972532	24.417458
H	3.730549	6.707167	17.228692
H	2.343684	1.940045	21.459406
H	-2.337633	2.823897	17.140937
H	-2.111544	2.304112	18.821455
H	-2.624347	3.963621	18.464524

H	1.630613	6.915557	16.239275
H	1.134078	5.683718	15.074101
H	2.783642	5.676664	15.692685
H	6.766307	1.004797	19.082448
H	5.781007	-0.448366	19.218648
H	6.61625	0.179742	20.6571
H	-0.983775	4.768983	15.206269
H	-2.096814	5.059043	16.552936
H	-0.87284	6.271367	16.136083
H	5.31542	2.244781	23.182811
H	5.894328	0.686855	22.526092
H	4.258381	0.838218	23.226459

Compound 8'

E_{SFC} = –1533.6717098 Ha

ν_{min} = 15.43 cm^{-1}

B	3.014091	3.424975	20.081868
N	2.096527	3.93091	19.081178
B	0.676253	3.667597	19.148658
C	-1.256112	2.982928	22.471061
H	-1.877757	3.535387	23.18118
C	0.074284	2.953525	20.420271
C	2.992023	3.466109	21.664967
H	2.17559	2.88407	22.117962
C	5.908821	6.44425	17.651592
H	6.245968	7.384197	17.207972
C	-0.224423	4.631597	15.47193
C	0.328702	1.588029	20.652942
H	0.949285	1.029208	19.946387
C	5.092324	2.51489	20.919327
C	2.862553	4.906612	22.135363
C	4.706285	2.626196	23.431691
C	4.118769	4.834386	18.05219
C	4.586038	6.033356	17.487269
H	3.891488	6.672026	16.941079
C	1.950462	4.591519	16.761269
C	2.608645	4.928066	15.441865
C	-0.742196	3.630304	21.343126
H	-0.96386	4.69015	21.188954
C	-0.972448	1.631894	22.694447
H	-1.37181	1.124488	23.576582
C	6.328498	4.484903	19.000979
H	7.012183	3.893686	19.607938
C	2.689949	4.433559	17.915569
C	4.339095	2.833184	21.994919
C	6.424595	1.809622	20.963654

C	4.179386	1.64044	18.71372
C	4.42266	2.867166	19.591114
C	-0.183178	0.932364	21.775909
H	0.034784	-0.127187	21.936178
C	5.001763	4.062482	18.849285
C	6.787847	5.65938	18.400257
H	7.826989	5.969398	18.536129
C	3.678018	0.468995	19.310176
H	3.527642	0.447181	20.39214
C	1.657371	6.649725	23.335876
H	0.812035	6.947262	23.962463
C	0.512856	4.384812	16.768572
C	-0.157468	3.986281	17.911246
C	-1.658119	3.792275	17.913119
C	4.087143	0.5106	16.557719
H	4.256986	0.534492	15.477945
C	4.383381	1.640469	17.326034
H	4.781522	2.531855	16.839663
C	1.786539	5.316507	22.935981
H	1.043037	4.579307	23.244422
C	3.580315	-0.643045	17.1605
H	3.347586	-1.524722	16.558202
C	3.815593	5.867485	21.754346
H	4.669684	5.567491	21.14271
C	3.379937	-0.659392	18.544432
H	2.989836	-1.556954	19.031794
C	3.68714	7.200002	22.150816
H	4.437592	7.931044	21.838411
C	2.604884	7.598513	22.941824
H	2.503531	8.641437	23.252879
H	-2.197373	4.723887	17.666855
H	-2.014805	3.457552	18.896244
H	-1.980313	3.035609	17.176265
H	4.735998	3.594046	23.961985
H	5.682638	2.137687	23.559177
H	3.941694	2.015962	23.944902
H	0.038648	3.871789	14.715804
H	0.038917	5.608171	15.035487
H	-1.311812	4.604088	15.601801
H	2.385016	5.953161	15.098822
H	3.698127	4.819894	15.483602
H	2.242403	4.250401	14.655277
H	6.687112	1.404228	19.975351
H	7.242632	2.481558	21.276604
H	6.418115	0.967311	21.673646

Transition state TS4

E_{SFC} = –1533.6291943 Ha

ν_{min} = –307.66 cm^{-1}

B	3.177467	2.642471	19.823211
N	1.994639	3.382370	19.258960
B	0.630232	2.958175	19.386099
C	-1.207004	0.512586	21.809665
H	-1.993324	0.567144	22.567205
C	0.245661	1.657822	20.202651
C	3.596606	2.345695	21.356611
C	5.907867	3.609852	19.320643
H	6.419915	2.786494	19.824043
C	0.826476	0.406491	19.916044
H	1.627733	0.335326	19.179423
C	4.812582	0.867867	19.888549
H	4.203148	3.216869	21.676276
C	3.839547	4.569184	18.422090
C	4.537923	3.521802	19.074040
C	1.457678	5.039166	17.575993
C	-0.776818	1.676681	21.171245
H	-1.239093	2.629034	21.442875
C	-0.628901	-0.719192	21.489143
H	-0.969304	-1.633664	21.982555
C	5.938337	5.795785	18.298734
H	6.481740	6.697882	18.006266
C	2.376965	4.376506	18.377667
C	4.583094	1.210812	21.191478
C	3.915302	1.435081	17.497781
C	3.988350	1.675518	18.962336
C	0.395512	-0.766881	20.541555
H	0.863259	-1.721840	20.285693
C	4.563179	5.720152	18.064746
C	6.617089	4.745498	18.926299
H	7.691023	4.816943	19.114951
C	2.670789	1.436717	16.841053
H	1.758867	1.604724	17.410878
C	0.053210	4.767776	17.740662
C	-0.400441	3.759515	18.584972
C	4.993714	1.051360	15.342802
H	5.907823	0.917648	14.758688
C	5.075042	1.248218	16.720067
H	6.054574	1.296763	17.196484
C	3.746411	1.034572	14.708244
H	3.681583	0.878987	13.628283
C	2.587578	1.229183	15.462275
H	1.608407	1.228979	14.977214
H	4.053015	6.584763	17.645473

C	-1.879038	3.442837	18.642346
C	-0.926987	5.602192	16.940842
C	5.343287	0.658355	22.364626
C	1.900535	5.982955	16.480910
C	5.799731	-0.176622	19.448753
C	2.528880	2.209304	22.415456
C	1.898694	3.369303	22.896228
C	0.925625	3.300037	23.893612
C	0.567703	2.063982	24.439804
C	1.178568	0.902999	23.961624
C	2.144610	0.974556	22.955678
H	2.180280	4.339489	22.477341
H	0.448408	4.216711	24.250775
H	-0.190830	2.005547	25.224472
H	0.890720	-0.072058	24.361823
H	2.590397	0.055676	22.572004
H	-2.442360	4.199678	19.220039
H	-2.338054	3.408217	17.640275
H	-2.063503	2.473379	19.122150
H	4.904621	0.987645	23.316203
H	5.356523	-0.444109	22.361627
H	6.397687	0.987228	22.346109
H	6.016234	-0.886312	20.259913
H	5.425510	-0.748004	18.586224
H	6.764312	0.267251	19.141188
H	-0.580933	6.637991	16.816021
H	-1.079700	5.189144	15.926828
H	-1.911405	5.639789	17.423684
H	1.223275	5.920453	15.617811
H	1.911948	7.042142	16.797379
H	2.903805	5.733382	16.113618

Compound 8'$_{rot}$

E_{SFC} = –1533.66199272533 Ha

ν_{min} = 17.46 cm^{-1}

B	2.931214	3.246063	20.130033
N	2.279506	3.654318	18.893730
B	0.897734	3.350374	18.600823
C	-1.912406	1.877562	20.890958
H	-2.870374	2.180760	21.320608
C	0.077037	2.438826	19.588785
C	2.701810	3.686081	21.633030
H	3.008080	4.754947	21.542339
C	6.467103	5.960900	18.352366
H	6.958261	6.859312	17.970740
C	0.873817	4.555971	14.883710

C	0.547852	1.132633	19.826543
H	1.495343	0.812526	19.388327
C	4.707626	2.346731	21.511435
C	1.357983	3.696405	22.316295
C	3.985590	3.051500	23.835912
C	4.518716	4.486152	18.389579
C	5.184720	5.633125	17.917566
H	4.672893	6.296973	17.221532
C	2.700398	4.363650	16.623906
C	3.657741	4.680701	15.495389
C	-1.169031	2.789548	20.142035
H	-1.559930	3.799570	19.995014
C	-1.430548	0.580702	21.103725
H	-2.017567	-0.134156	21.686601
C	6.441464	4.035008	19.806743
H	6.934928	3.424646	20.560953
C	3.143966	4.156784	17.917219
C	3.837171	2.953776	22.347374
C	5.927361	1.567824	21.939984
C	4.336443	1.262245	19.223894
C	4.361873	2.549207	20.036507
C	-0.193464	0.211575	20.574445
H	0.195816	-0.798253	20.732234
C	5.149133	3.693108	19.383879
C	7.107376	5.146133	19.288620
H	8.115300	5.387127	19.635519
C	3.886541	0.077549	19.834288
H	3.600337	0.099723	20.888255
C	-0.359772	2.571894	23.621849
H	-0.731145	1.662002	24.099152
C	1.297053	4.211111	16.295212
C	0.376880	3.751779	17.222226
C	-1.073958	3.563714	16.836500
C	4.595294	0.018265	17.144781
H	4.879083	0.004853	16.089122
C	4.696527	1.209860	17.868903
H	5.063319	2.108282	17.372026
C	0.857812	2.545045	22.942550
H	1.427674	1.615261	22.886469
C	4.140713	-1.149497	17.761789
H	4.063447	-2.080434	17.194710
C	0.590614	4.869018	22.371506
H	0.965958	5.775980	21.888611
C	3.790363	-1.114660	19.114978
H	3.436812	-2.020832	19.614059
C	-0.636368	4.896474	23.039414
H	-1.216852	5.822459	23.070080

C	-1.112017	3.748964	23.677487
H	-2.066835	3.768264	24.208920
H	-1.571855	4.526547	16.621592
H	-1.642875	3.074067	17.636711
H	-1.185495	2.942151	15.931530
H	4.087760	4.109942	24.137638
H	4.866624	2.507742	24.204299
H	3.097120	2.671067	24.363866
H	1.148476	3.751814	14.177689
H	1.362321	5.472770	14.521531
H	-0.209613	4.701930	14.805018
H	3.602422	5.730882	15.159278
H	4.699327	4.473608	15.766481
H	3.419298	4.060694	14.617643
H	6.416726	1.092293	21.078213
H	6.674398	2.206555	22.442068
H	5.669477	0.765020	22.650046

Intermediate Int4

E_{SFC} = –1533.5909873 Ha

ν_{min} = 21.34 cm^{-1}

B	3.275870	2.267970	17.931789
N	2.276648	3.313385	17.772603
B	0.910124	2.993964	17.423732
C	3.380508	0.970484	18.735563
C	5.831434	6.128562	19.432212
H	6.172455	7.098744	19.800090
C	-0.239385	6.591018	16.426933
C	5.422366	1.244470	17.605747
C	5.181290	-0.871595	19.035662
C	4.081198	4.806884	18.342287
C	4.579197	6.025561	18.833408
H	3.963029	6.918839	18.778912
C	1.971797	5.653857	17.202897
C	2.564074	6.993868	16.826482
C	6.230653	3.767384	19.124660
H	6.861188	2.882942	19.224689
C	2.766744	4.631698	17.736739
C	4.657857	0.408585	18.442284
C	6.786748	0.966112	17.070690
C	4.967818	3.140986	15.987294
C	4.742207	2.515977	17.333333
C	4.884253	3.582046	18.577256
C	6.666747	4.992996	19.558619
H	7.663024	5.095614	19.996748
C	4.377826	2.533309	14.865128

H	3.785774	1.625630	15.005854
C	0.588312	5.416566	16.907386
C	0.010112	4.153884	17.036932
C	-1.444658	3.937598	16.686769
C	5.888822	4.843674	14.508445
H	6.488738	5.748052	14.376468
C	5.734810	4.298541	15.787406
H	6.223529	4.778365	16.636062
C	5.286623	4.236196	13.404695
H	5.406274	4.663796	12.406022
C	4.532460	3.071883	13.587664
H	4.056768	2.585510	12.732062
H	-2.121164	4.466682	17.383008
H	-1.709730	2.872928	16.723022
H	-1.690137	4.303250	15.674324
H	4.777097	-1.032550	20.045746
H	6.278802	-0.876107	19.098639
H	4.885832	-1.745189	18.429463
H	-0.077957	6.779643	15.350084
H	0.016565	7.521113	16.954908
H	-1.312568	6.414869	16.565833
H	2.388578	7.787487	17.575835
H	3.645953	6.921716	16.658804
H	2.118626	7.350875	15.886828
H	6.778098	0.933492	15.967199
H	7.481388	1.788348	17.331432
H	7.209917	0.019698	17.434152
H	4.281343	2.939468	19.332682
C	0.465211	1.479529	17.350169
C	-0.543514	0.962858	18.183437
C	-0.934228	-0.376441	18.115722
C	-0.327176	-1.237426	17.197171
C	0.670146	-0.747088	16.349800
C	1.055757	0.593817	16.429575
H	-1.019378	1.617453	18.918187
H	-1.706760	-0.752597	18.791105
H	-0.628728	-2.286998	17.143700
H	1.147522	-1.410224	15.622839
H	1.830838	0.962591	15.751933
C	2.414066	0.454978	19.707885
C	2.094917	-0.914455	19.802602
C	1.140847	-1.369292	20.713496
C	0.487000	-0.472387	21.561751
C	0.787592	0.891702	21.479390
C	1.729485	1.348119	20.560569
H	2.560848	-1.623129	19.117865
H	0.897578	-2.434357	20.751504

H	-0.256997	-0.831499	22.277244
H	0.279561	1.605541	22.133236
H	1.950605	2.415558	20.495609

Intermediate Int5

E_{SFC} = –1533.6140670 Ha

ν_{min} = 28.44 cm^{-1}

B	2.985215	1.939155	18.520314
N	2.238253	3.121748	18.066548
B	0.865515	3.027643	17.603324
C	2.867878	0.437840	18.017420
C	6.285675	5.636422	19.248854
H	6.693420	6.360154	19.958833
C	-0.077647	6.802516	17.967645
C	4.977299	1.250224	17.467567
C	4.481377	-1.263655	16.941398
C	4.345028	4.432145	18.360253
C	4.919668	5.354330	19.253353
H	4.268469	5.864549	19.964331
C	2.127079	5.542354	18.082749
C	2.781628	6.906578	17.974782
C	6.584919	4.030910	17.478567
H	7.237805	3.479124	16.797666
C	2.854028	4.369637	18.227104
C	4.023560	0.100132	17.377301
C	6.039117	1.044633	18.521553
C	4.019479	2.557743	15.546571
C	4.735994	2.451262	16.838359
C	5.226416	3.695110	17.517831
C	7.119606	5.005420	18.324257
H	8.185756	5.241516	18.284414
C	4.040616	1.488156	14.628180
H	4.587441	0.579995	14.877603
C	0.690183	5.499376	17.901949
C	0.040091	4.315929	17.613990
C	-1.437224	4.323685	17.289460
C	2.725024	3.838764	13.922415
H	2.213098	4.765960	13.654014
C	3.373997	3.746183	15.154525
H	3.366805	4.605019	15.823061
C	2.726444	2.756815	13.038578
H	2.217885	2.830727	12.074338
C	3.399482	1.583127	13.394371
H	3.431675	0.737729	12.702460
H	-2.053653	4.531075	18.183855
H	-1.766170	3.356804	16.888620

H	-1.694468	5.097590	16.546413
H	4.045707	-2.061027	17.562159
H	5.578970	-1.343126	16.985302
H	4.189034	-1.471133	15.896747
H	-0.124517	7.294533	16.978850
H	0.378154	7.520701	18.662942
H	-1.113942	6.636405	18.289809
H	2.732359	7.486092	18.912733
H	3.837861	6.840263	17.691191
H	2.273530	7.509834	17.207601
H	6.817181	0.372533	18.117969
H	6.528766	1.974142	18.830961
H	5.614804	0.550185	19.409063
H	3.671462	2.132471	19.496843
C	0.224496	1.694099	17.057717
C	-0.854669	1.050124	17.690786
C	-1.506266	-0.033815	17.099764
C	-1.100338	-0.493826	15.843121
C	-0.032193	0.130514	15.194884
C	0.620623	1.208509	15.799275
H	-1.190718	1.399561	18.670946
H	-2.329848	-0.525876	17.623105
H	-1.610966	-1.340805	15.376831
H	0.297226	-0.219174	14.212271
H	1.446482	1.686881	15.276533
C	1.848411	-0.522225	18.477558
C	1.441307	-1.637366	17.724575
C	0.505456	-2.540637	18.231484
C	-0.042898	-2.354260	19.502258
C	0.344005	-1.244601	20.261457
C	1.271689	-0.339063	19.751283
H	1.820902	-1.769239	16.712155
H	0.189582	-3.389088	17.618943
H	-0.775734	-3.063138	19.895998
H	-0.083787	-1.082691	21.254358
H	1.566388	0.527920	20.348838

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