Supporting Information

C-C bond-forming reactions of 2-isocyanobiphenyl•BX_3 adducts: spontaneous construction of polycyclic heteroaromatics

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1. Materials and methods

General considerations. Where indicated, glovebox synthetic manipulations were carried out in an atmosphere of dry, O_2-free N_2 in an MBraun glovebox using oven-dried glassware. 2-Isocyanobiphenyl was prepared according to a literature report[1] and thoroughly dried *in vacuo*. Dichloromethane, n-hexane, 1,1,2,2-tetrachloroethane, toluene and chloroform were obtained were obtained from commercial sources, dried over 4 Å molecular sieves, and degassed before use. Deuterated solvents were obtained from commercial sources and dried over 4 Å molecular sieves before use. All other reagents were obtained from commercial sources and used without further purification.

NMR spectra were recorded on Bruker AVIIIHD 400MHz FT-NMR, Bruker AVIIIHD 500MHz FT-NMR spectrometer or Bruker AVIIIHD 800MHz FT-NMR spectrometer. Chemical shifts are listed in parts per million and are given relative to $SiMe_4$ and referenced to a residual solvent signal (^1H, ^{13}C) or relative to an external standard (^{11}B: 15% $(Et_2O)BF_3$; ^{19}F: 15% $(Et_2O)BF_3$. Coupling constants (*J*) are quoted in Hertz (Hz). In some cases ^{11}B signals for boron-containing compounds could not be observed due to broadening and/or poor solubility.

EPR spectra were recorded on Bruker ELEXSYS-E580 EPR spectrometer.

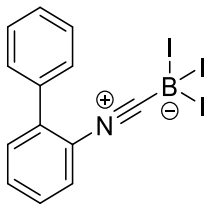
High resolution mass spectrometry experiments were performed on a Bruker ultrafleXtreme or Bruker micrOTOF-QII instrument.

Single crystal X-ray diffraction data were recorded at 100K on a Bruker D8 Venture SC-XRD with a Photon III C28 detector and multi-layered mirror monochromated CuKα radiation. The structures were solved using Shelxt methods, expanded with Fourier techniques and refined with the Shelxt software package.[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the structure factor calculation on geometrically idealized positions. Crystallographic data have been deposited with the

Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2418957-2418963. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.ac.uk/data.request/cif.

2. Synthetic procedures

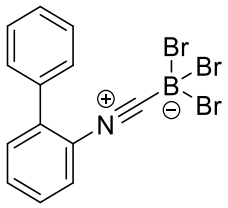
2.1 Synthesis of 1



In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.1198 g, 0.6685 mmol, 1 equiv.) was dissolved in 2 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. BI_3 (0.2225 g, 0.5683 mmol, 0.85 equiv.) was dissolved in 4 mL dichloromethane and this solution was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred at room temperature for 2 h in a sealed Schlenk flask and then concentrated *in vacuo*. 150 mL n-hexane was added to the remaining residue, and the mixture was stirred for 1 h. The n-hexane layer was collected and the residue was further extracted with 2 x 150 mL n-hexane. The combined extracts were filtered through celite, concentrated *in vacuo* to ~100 mL, and cooled to -35 °C for 24 h over which time colorless crystals formed. The supernatant was decanted and the crystals were dried *in vacuo* to afford compound **1** in 40% yield (0.1300 g, 0.2278 mmol). **^{1}H NMR** (500 MHz, CD_2Cl_2, 298 K): δ 7.80-7.72 (m, 2H), 7.67 (dd, 1H, $^{3}J_{HH}$ = 6.9 Hz, $^{4}J_{HH}$ = 1.6 Hz), 7.64-7.57 (m, 3H), 7.56-7.48 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, CD_2Cl_2, 298 K): δ 141.60, 135.38, 134.19, 132.01, 130.17, 130.08, 129.49, 129.39, 128.34, 120.98 (t, $^{1}J_{NC}$ = 13.5 Hz), B-*C* not observed. **^{11}B NMR** (160 MHz,

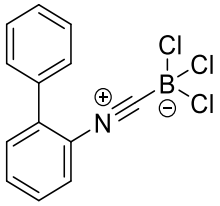
CD_2Cl_2, 298 K): δ -91.63. **HR-MS** (MALDI-TOF, Positive mode) *m/z*: $[M\text{-}BI_3+H]^+$ Calc'd $C_{13}H_{10}N$ for 180.0808; Found 180.0807.

2.2 Synthesis of 2



In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.3677 g, 2.052 mmol, 1 equiv.) was dissolved in 2 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. BBr_3 (0.1946 mL, 2.051 mmol, 1 equiv.) was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred at room temperature for 3.5 h in a sealed Schlenk flask and then concentrated *in vacuo*. 150 mL n-hexane was added to the remaining residue, and the mixture was stirred for 2 h. The n-hexane layer was collected and the residue was further extracted with 5 x 150 mL n-hexane. The combined extracts were filtered through celite, concentrated *in vacuo* to ~200 mL, and cooled to -35 °C for 24 h over which time colorless crystals formed. The supernatant was decanted and the crystals were dried *in vacuo* to afford compound **2** in 32% yield (0.2820 g, 0.6562 mmol). **^{1}H NMR** (500 MHz, CD_2Cl_2, 298 K): δ 7.82-7.76 (m, 2H), 7.67 (dd, 1H, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 1.3 Hz), 7.63-7.56 (m, 3H), 7.54 (ddd, 1H, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 1.8 Hz, $^5J_{HH}$ = 1.1 Hz), 7.53-7.49 (m, 2H). **^{13}C{^{1}H} NMR** (125 MHz, CD_2Cl_2, 298 K): δ 141.94, 135.20, 134.58, 132.04, 130.13, 130.06, 129.55, 129.25, 128.78, 120.35 (t, $^1J_{NC}$ = 14.5 Hz), B-*C* not observed. **^{11}B NMR** (160 MHz, CD_2Cl_2, 298 K): δ -25.47. **HR-MS** (MALDI-TOF, Positive mode) *m/z*: $[M\text{-}BBr_3+H]^+$ Calc'd $C_{13}H_{10}N$ for 180.0808; Found 180.0807.

2.3 Synthesis of 3

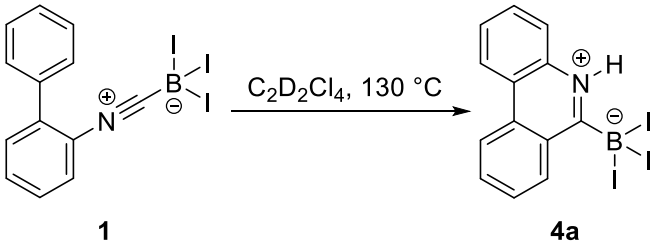


In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.7420 g, 4.140 mmol, 1 equiv.) was dissolved in 6 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. The sealed flask was moved to a Schlenk line and cooled to ~ -89 ºC under nitrogen. BCl_3 (4.140 mL, 1 M Hexanes solution, 4.140 mmol, 1 equiv.) was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred for 18 h in a sealed Schlenk flask and then concentrated *in vacuo*. In a glovebox, 150 mL n-hexane was added to the remaining residue, and the mixture was stirred for 2 h. The n-hexane layer was collected and the residue was further extracted with 5 x 150 mL n-hexane. The combined extracts were filtered through celite, concentrated *in vacuo* to ~200 mL, and cooled to -35 °C for 24 h over which time colorless crystals formed. The supernatant was decanted and the crystals were dried *in vacuo* to afford compound **3** in 36% yield (0.4420 g, 1.491 mmol). **^{1}H NMR** (500 MHz, CD_2Cl_2, 298 K): δ 7.82-7.76 (m, 2H), 7.66 (dd, 1H, $^3J_{HH}$ = 8.0 Hz, $^4J_{HH}$ = 1.3 Hz), 7.62-7.52 (m, 4H), 7.52-7.48 (m, 2H). **^{13}C{^{1}H} NMR** (125 MHz, CD_2Cl_2, 298 K): δ 142.01, 135.18, 134.60, 132.01, 130.13, 129.97, 129.54, 129.19, 128.89, 120.13(t, $^1J_{NC}$ = 14.0 Hz), B-*C* not observed. **^{11}B NMR** (160 MHz, CD_2Cl_2, 298 K): δ -3.19. **HR-MS** (MALDI-TOF, Positive mode) *m/z*: $[M\text{-}BCl_3+H]^+$ Calc'd $C_{13}H_{10}N$ for 180.0808; Found 180.0807.

2.4 NMR-scale reaction of heating compound 1 at 130 ºC

In an inert atmosphere glovebox, compound **1** (0.0272 g, 0.0477 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 ºC

for 48 h. (Figure S1 and Figure S2).



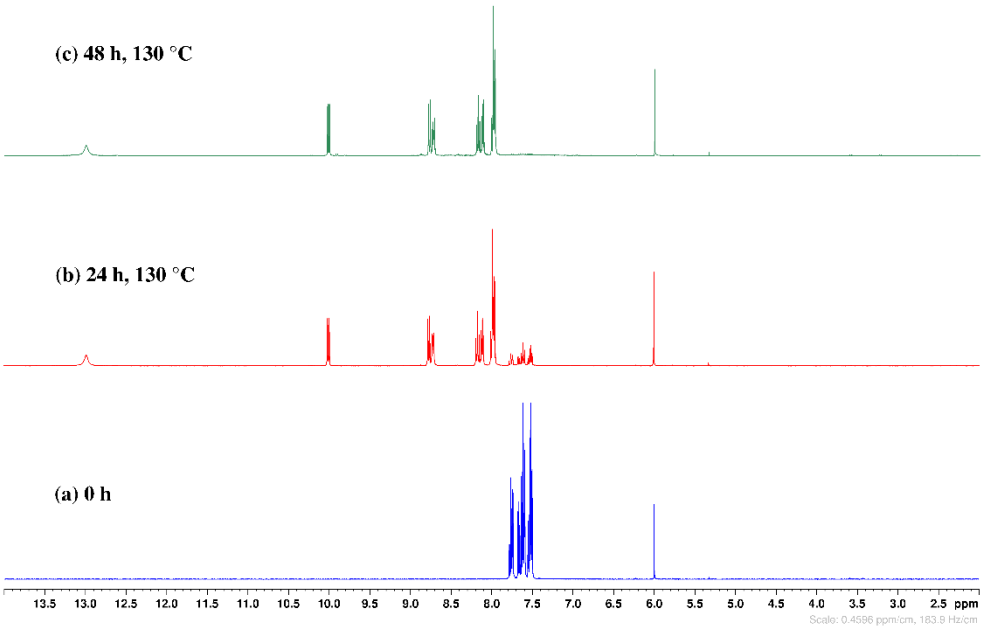


Figure S1: ^{1}H NMR spectra (400 MHz, TCE-d2, 298 K) of the reaction progress of heating compound **1** at 130 °C for (a) 0 h, (b) 24 h, and (c) 48 h.

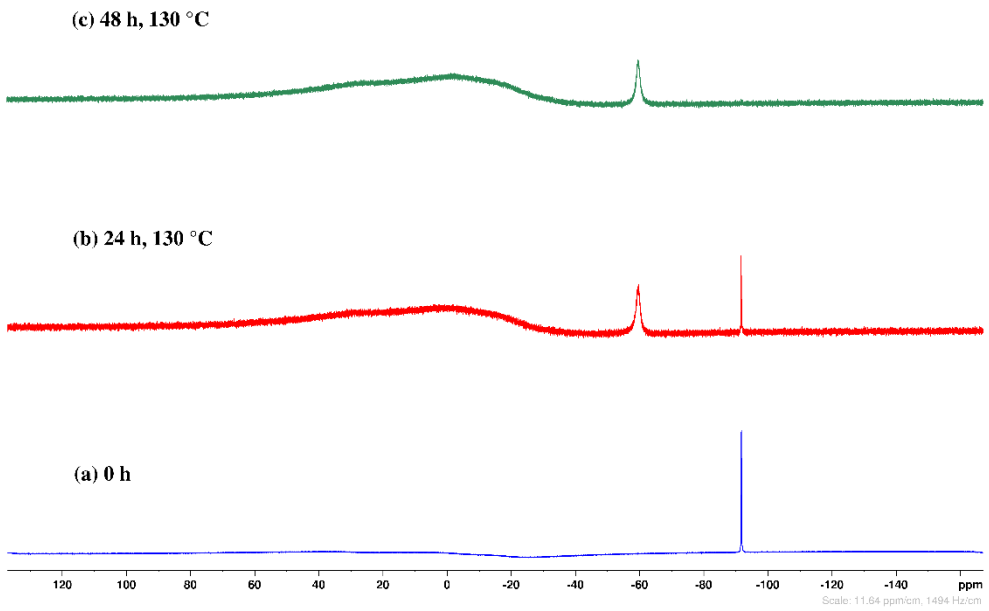
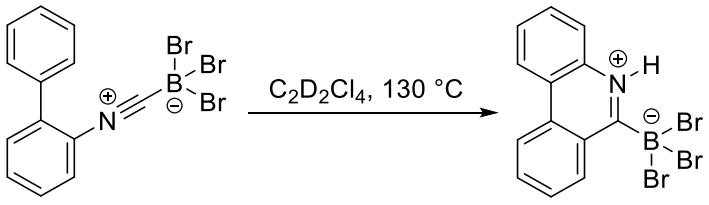


Figure S2: ^{11}B NMR spectra (128 MHz, TCE-d2, 298 K) of the reaction progress of heating compound **1** at 130 ℃ for (a) 0 h, (b) 24 h, and (c) 48 h.

2.5 NMR-scale reaction of heating compound 2 at 130 ℃

In an inert atmosphere glovebox, compound **2** (0.0128 g, 0.0298 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 ℃ for 48 h. (Figure S3 and Figure S4).



2 **5a**

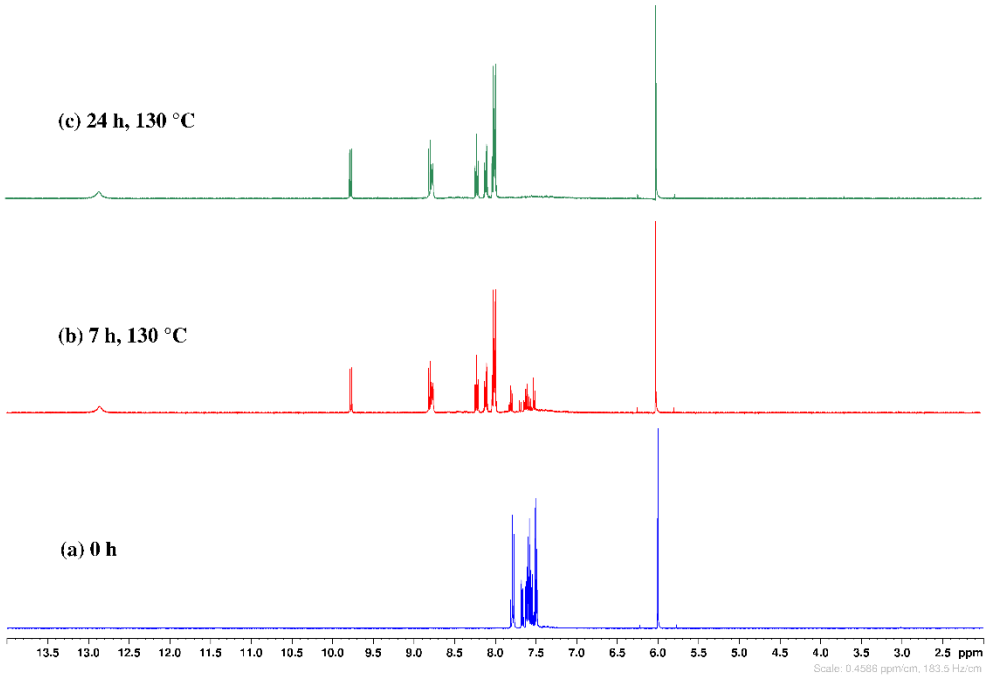


Figure S3: ^{1}H NMR spectra (400 MHz, TCE-d2, 298 K) of reaction progress of heating compound **2** at 130 °C for (a) 0 h, (b) 7 h, and (c) 24 h**.**

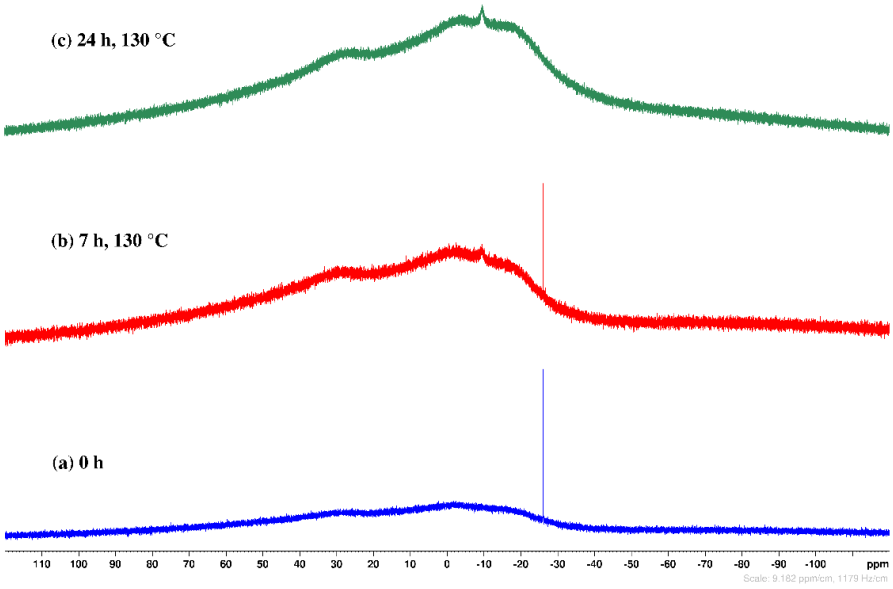
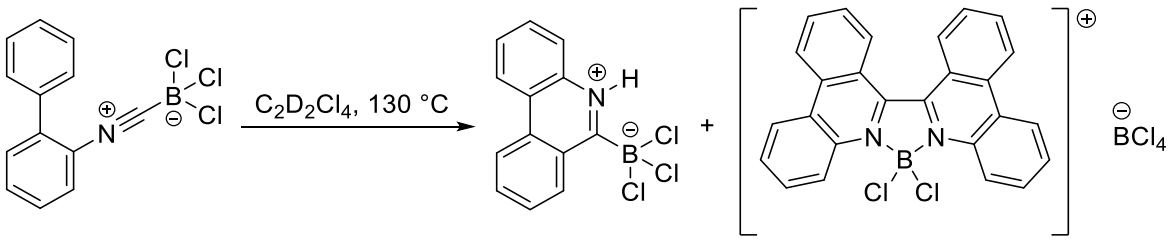


Figure S4: ^{11}B NMR spectra (128 MHz, TCE-d2, 298 K) of reaction progress of heating compound **2** at 130 °C for (a) 0 h, (b) 7 h, and (c) 24 h.

2.6 NMR-scale reaction of heating compound 3 at 130 ℃

In an inert atmosphere glovebox, compound **3** (0.0239 g, 0.0806 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 ℃ for 48 h. (Figure S5 and Figure S6).



3 **6a** **6b**

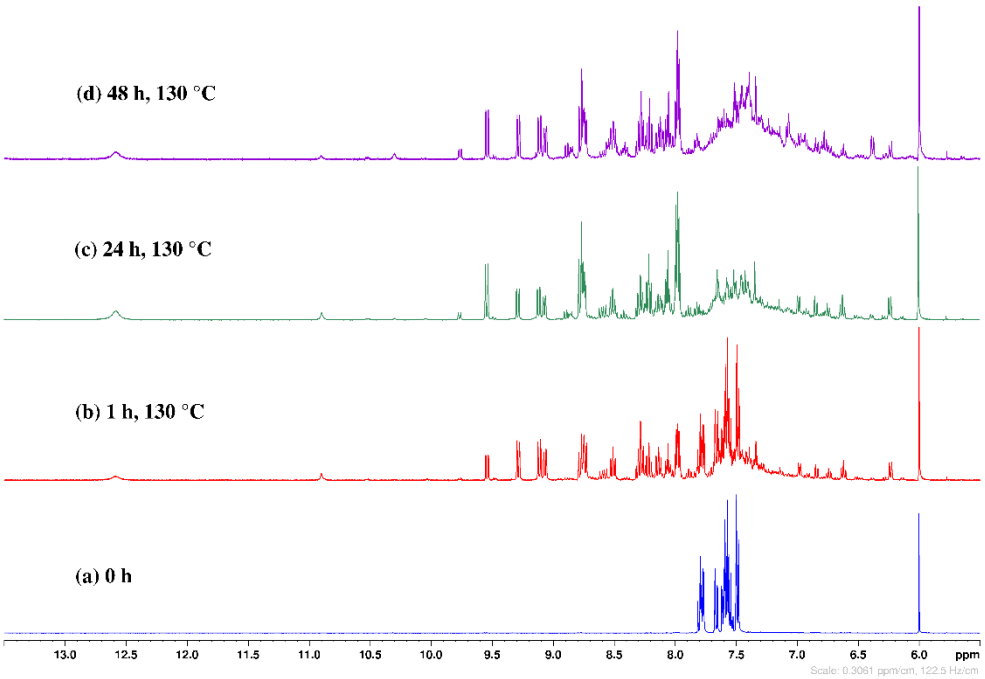


Figure S5: ^{1}H NMR spectra (400 MHz, TCE-d2, 298 K) of reaction progress of heating compound **3** at 130 ℃. (a) 0 h, (b) 1 h, (c) 24 h, and (d) 48 h**.**

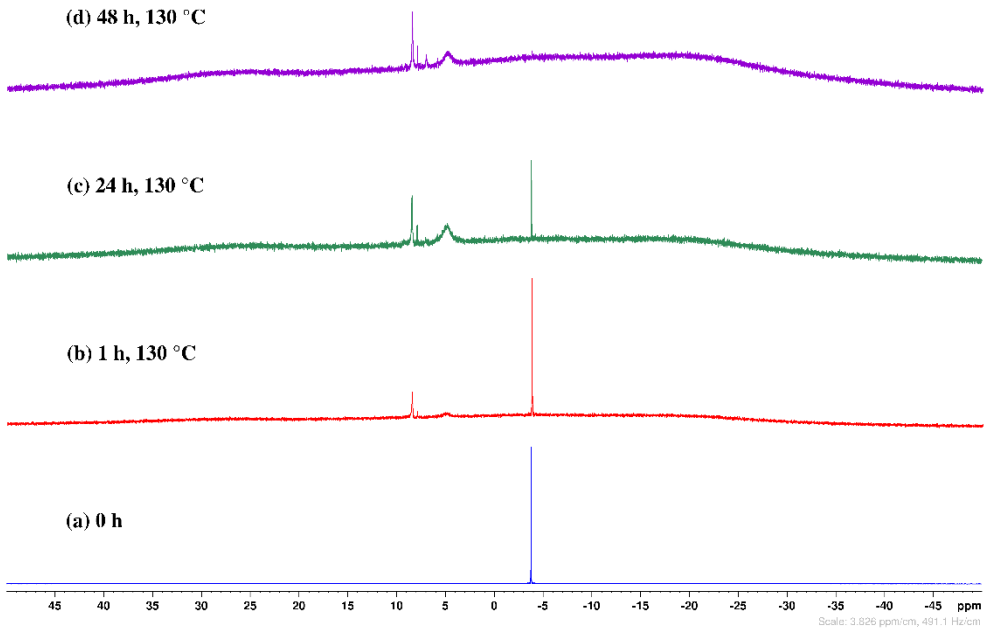
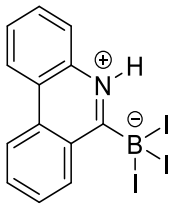


Figure S6: ^{11}B NMR spectra (128 MHz, TCE-d2, 298 K) of reaction progress of heating compound **3** at 130 °C. (a) 0 h, (b) 1 h, (c) 24 h, and (d) 48 h**.**

2.7 Synthesis of 4a



NMR-scale synthesis of **4a** from **1**:

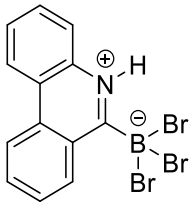
In an inert atmosphere glovebox, compound **1** (0.0272 g, 0.0477 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 °C for 48 h. Upon standing at room temperature, colorless crystals form from solution. The supernatant was decanted and the crystals were dried *in vacuo* to afford compound **4a** in 75% yield (0.0205 g, 0.0359 mmol). **^{1}H NMR** (500 MHz, TCE-d2, 298 K): δ 12.98

(br, s, 1H, N-H), 10.00 (dd, 1H, $^{3}J_{HH}$ = 8.6 Hz, $^{4}J_{HH}$ =1.0), 8.77 (d, 1H, $^{3}J_{HH}$ =8.4), 8.75-8.69 (m, 1H), 8.17 (ddd, 1H, $^{3}J_{HH}$ = 8.7 Hz, $^{3}J_{HH}$ = 7.1 Hz, $^{4}J_{HH}$ = 1.3 Hz), 8.14-8.09 (m, 1H), 8.02-7.94 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, TCE-d2, 298 K): δ 138.01, 137.29, 135.75, 133.13, 132.84, 131.91, 129.13, 126.72, 126.65, 124.98, 123.96, 122.42, B-*C* not observed. **^{11}B NMR** (160 MHz, TCE-d2, 298 K): δ -59.08. **HR-MS** (MALDI-TOF, negative mode) *m/z*: $[M-H]^-$ Calc'd for $C_{13}H_8BI_3N$ 569.7892; Found 569.7891.

Bulk-scale synthesis of **4a** from 2-isocyanobiphenyl:

In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.2630 g, 1.467 mmol, 1 equiv.) was dissolved in 3 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. BI_3 (0.4884 g, 1.247 mmol, 0.85 equiv.) was dissolved in 6 mL dichloromethane and this solution was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred at room temperature for 2 h and then concentrated *in vacuo*. 200 mL n-hexane was added to the remaining residue and stirred for 1 h. The hexane layer was filtered through celite and concentrated *in vacuo*. This residue was dissolved in 5 mL 1,1,2,2-tetrachloroethane and heated in a sealed Schlenk tube at 130 °C for 48 h. Upon cooling to room temperature, colorless crystals form. The supernatant was decanted, and the crystals were washed sequentially with 3 x 3 mL 1,1,2,2-tetrachloroethane and 3 x 3 mL n-hexane, then dried *in vacuo* to afford compound **4a** in 52% yield (0.3700 g, 0.6483 mmol). Compound **4a** prepared in this way was spectroscopically identical to that prepared on an NMR scale described above.

2.8 Synthesis of 5a



NMR-scale synthesis of **5a** from **2**:

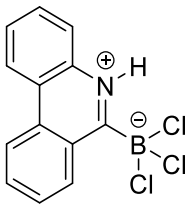
In an inert atmosphere glovebox, compound **2** (0.0128 g, 0.0298 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 °C for 24 h. Upon standing at room temperature, colorless crystals form from solution. The supernatant was decanted and the crystals were dried in vacuo to afford compound **5a** in 70% yield (0.0090 g, 0.021 mmol). **^{1}H NMR** (500 MHz, TCE-d2, 298 K): δ 12.84 (br, s, 1H, N-H), 9.75 (d, 1H, $^{3}J_{HH}$ = 8.6 Hz), 8.82-8.71 (m, 2H), 8.20 (ddd, 1H, $^{3}J_{HH}$ = 8.8 Hz, $^{3}J_{HH}$ = 7.0 Hz, $^{4}J_{HH}$ = 1.3 Hz), 8.12-8.06 (m, 1H), 8.04-7.94 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, TCE-d2, 298 K): δ 136.34, 135.45, 134.37, 131.34, 130.79, 130.37, 128.50, 125.17, 125.14, 123.27, 122.43, 121.02, B-*C* not observed. **^{11}B NMR** (160 MHz, TCE-d2, 298 K): δ -9.04. **HR-MS** (MALDI-TOF, negative mode) *m/z*: $[M-H]^-$ Calc'd for $C_{13}H_8BBr_3N$ 427.8288; Found 427.8281.

Bulk-scale synthesis of **5a** from 2-isocyanobiphenyl:

In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.4227 g, 2.359 mmol, 1 equiv.) was dissolved in 3 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. BBr_3 (0.2240 mL, 2.360 mmol, 1 equiv.) was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred at room temperature for 3.5 h in a sealed Schlenk flask and then concentrated *in vacuo*. 100 mL toluene was added to the remaining residue, and the mixture was stirred for 0.5 h. The toluene layer

was filtered through celite and concentrated *in vacuo*. This residue was dissolved in 6 mL 1,1,2,2-tetrachloroethane and heated in a sealed Schlenk tube at 130 ℃ for 24 h. Upon cooling to room temperature, colorless crystals form. The supernatant was decanted, and the crystals were washed sequentially with 3 x 3 mL 1,1,2,2-tetrachloroethane and 3 x 3 mL n-hexane, then dried *in vacuo* to afford compound **5a** in 67% yield (0.6790 g, 1.580 mmol). Compound **5a** prepared in this way was spectroscopically identical to that prepared on an NMR scale described above.

2.9 Synthesis of 6a



NMR-scale synthesis of **6a** from **3**:

In an inert atmosphere glovebox, compound **3** (0.0239 g, 0.0806 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 ℃ for 48 h. Upon cooling to room temperature, red crystals and colorless crystals form. In an inert atmosphere glovebox, the supernatant was decanted and the crystals were washed with 3 x 2 mL dichloromethane. The supernatant and wash were combined, removed from the glovebox, and washed with 5 mL water. The organic layer was collected, concentrated *in vacuo* and transferred to the glovebox. The remaining residue was dissolved in 3 mL chloroform. The chloroform solution was layered with 2 mL n-hexane and cooled to -35 °C for 24 h over which time colorless crystals formed. The supernatant was decanted, and the crystals were washed with 2 mL n-hexane then dried *in vacuo* to afford compound **6a** in 8.3% yield (0.0020 g, 0.0067 mmol). **^{1}H NMR** (500

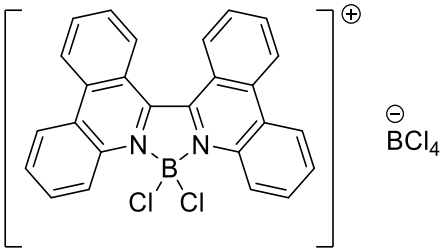
MHz, CD_2Cl_2, 298 K): δ 12.64 (br, s, 1H, N-H), 9.55 (d, 1H, $^3J_{HH}$ = 8.7 Hz), 8.84-8.75 (m, 2H), 8.21 (ddd, 1H, $^3J_{HH}$ = 8.8 Hz, $^3J_{HH}$ = 7.1 Hz, $^4J_{HH}$ = 1.3 Hz), 8.13-8.07 (m, 1H), 8.02-7.94 (m, 3H). **^{13}C{^{1}H} NMR** (200 MHz, CD_2Cl_2, 298 K): δ 136.93, 136.03, 135.15, 131.82, 131.66, 130.77, 129.51, 126.12, 126.02, 123.98, 123.19, 121.82, B-*C* not observed. **^{11}B NMR** (160 MHz, CD_2Cl_2, 298 K): δ 5.44. **HR-MS** (MALDI-TOF, negative mode) *m/z*: $[M-H]^-$ Calc'd for $C_{13}H_8BCl_3N$ 293.9823; Found 293.9827.

Bulk-scale synthesis of **6a** from 2-isocyanobiphenyl:

In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.7437 g, 4.150 mmol, 1 equiv.) was dissolved in 6 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. The sealed flask was moved to a Schlenk line and cooled to ~ -89 ºC under nitrogen. BCl_3 (4.150 mL 1M Hexanes solution, 4.150 mmol, 1 equiv.) was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred for 18 h in a sealed Schlenk flask and then concentrated *in vacuo*. In a glovebox, 100 mL toluene was added to the remaining residue, and the mixture was stirred for 0.5 h. The toluene layer was filtered through celite and concentrated *in vacuo*. This residue was dissolved in 6 mL 1,1,2,2-tetrachloroethane and heated in a sealed Schlenk tube at 130 ºC for 48 h. Upon cooling to room temperature, red crystals formed. The supernatant was collected, removed from the glovebox, and washed with 8 mL water. The organic layer was collected, concentrated *in vacuo* and transferred to the glovebox. The remaining residue was dissolved in 8 mL chloroform. The chloroform solution was layered with 6 mL n-hexane and cooled to -35 °C for 24 h over which time colorless crystals formed. The supernatant was decanted, and the crystals were washed with 2 x 2 mL n-hexane then dried *in vacuo* to afford compound **6a** in 4.6% yield (0.0574 g, 0.194 mmol). Compound **6a** prepared in this way was spectroscopically identical to that prepared on

an NMR scale described above.

2.10 Synthesis of 6b



NMR-scale synthesis of **6b** from **3**:

In an inert atmosphere glovebox, compound **3** (0.0239 g, 0.0806 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 °C for 48 h. Upon cooling to room temperature, red crystals and colorless crystals formed. In an inert atmosphere glovebox, the supernatant was decanted and the crystals were washed with 3 x 2 mL dichloromethane. While the colorless crystals were dissolved completely, the red crystals remained. The remaining red crystals were dried *in vacuo* to afford compound **6b** in 16% yield (0.0038 g, 0.0064 mmol). **^{1}H NMR** (500 MHz, CD_2Cl_2, 298 K): δ 9.31 (dd, 2H, $^{3}J_{HH}$ = 8.0 Hz, $^{4}J_{HH}$ = 1.5 Hz), 9.13 (d, 2H, $^{3}J_{HH}$ = 8.6 Hz), 9.08 (dd, 2H, $^{3}J_{HH}$ = 7.9 Hz, $^{4}J_{HH}$ = 1.8 Hz), 8.74 (d, 2H, $^{3}J_{HH}$ = 8.6 Hz), 8.50 (ddd, 2H, $^{3}J_{HH}$ = 8.7 Hz, $^{3}J_{HH}$ = 7.0 Hz, $^{4}J_{HH}$ = 1.2 Hz), 8.34-8.24 (m, 4H), 8.12 (ddd, 2H, $^{3}J_{HH}$ = 8.9 Hz, $^{3}J_{HH}$ = 7.0 Hz, $^{4}J_{HH}$ = 1.1 Hz). **^{13}C{^{1}H} NMR** (200 MHz, CD_2Cl_2, 298 K): δ 147.55, 138.53, 138.48, 133.99, 133.19, 132.83, 130.66, 130.26, 127.81, 124.28, 124.23, 123.95, 121.53. **^{11}B NMR** (160 MHz, CD_2Cl_2, 298 K): δ 9.12, 6.82. **HR-MS** (MALDI-TOF, positive mode) *m/z*: $[M+H]^+$ Calc'd for $C_{26}H_{17}BCl_2N_2$ 438.0861; Found 438.0868. **HR-MS** (ESI-TOF, positive mode) *m/z*: $[M]^+$ Calc'd for $C_{26}H_{16}BCl_2N_2$ 437.0783; Found 437.0787.

Bulk-scale synthesis of **6b** from 2-isocyanobiphenyl:

In an inert atmosphere glovebox, 2-isocyanobiphenyl (0.7437 g, 4.150 mmol, 1 equiv.) was dissolved in 6 mL dichloromethane in a 250 mL Schlenk flask equipped with a magnetic stir bar. The sealed flask was moved to a Schlenk line and cooled to ~ -89 ºC under nitrogen. BCl_3 (4.150 mL 1M Hexanes solution, 4.150 mmol, 1 equiv.) was added dropwise to the 2-isocyanobiphenyl solution. The reaction mixture was stirred for 18 h in a sealed Schlenk flask and then concentrated *in vacuo*. In a glovebox, 100 mL toluene was added to the remaining residue, and the mixture was stirred for 0.5 h. The toluene layer was filtered through celite and concentrated *in vacuo*. This residue was dissolved in 6 mL 1,1,2,2-tetrachloroethane and heated in a sealed Schlenk tube at 130 ℃ for 48 h. Upon cooling to room temperature, red crystals formed. In a glovebox, the supernatant was decanted, and the red crystals were washed with 5 x 3 mL dichloromethane then dried *in vacuo* to afford compound **6b** in 13.3% yield (0.1630 g, 0.2759 mmol). Compound **6b** prepared in this way was spectroscopically identical to that prepared on an NMR scale described above.

3. NMR spectra

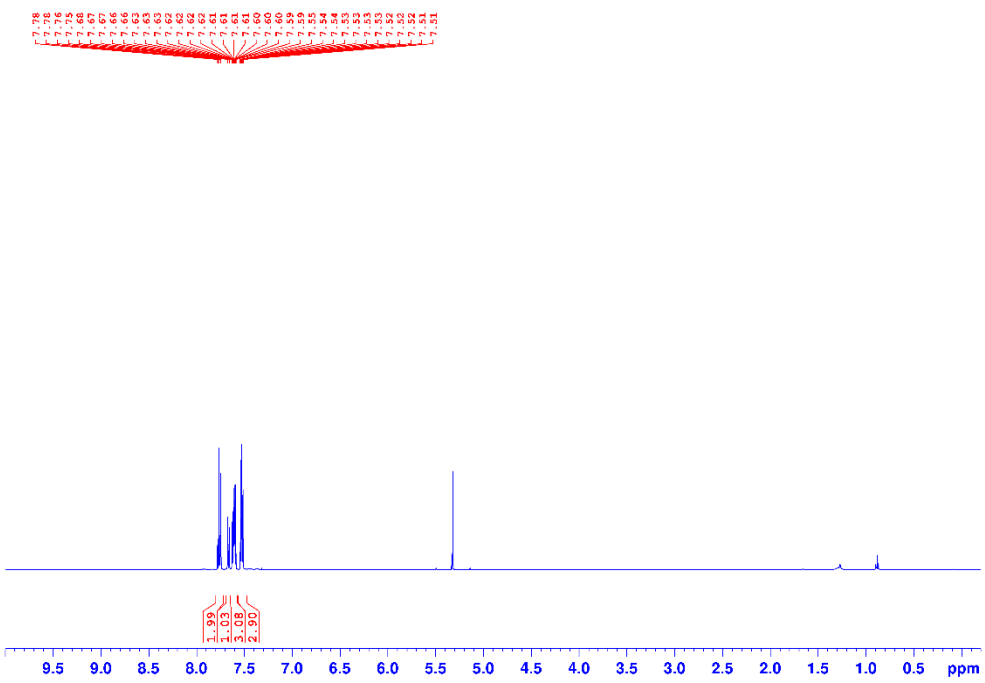


Figure S7: ^{1}H NMR spectrum of compound **1** (500 MHz, CD_2Cl_2, 298 K).

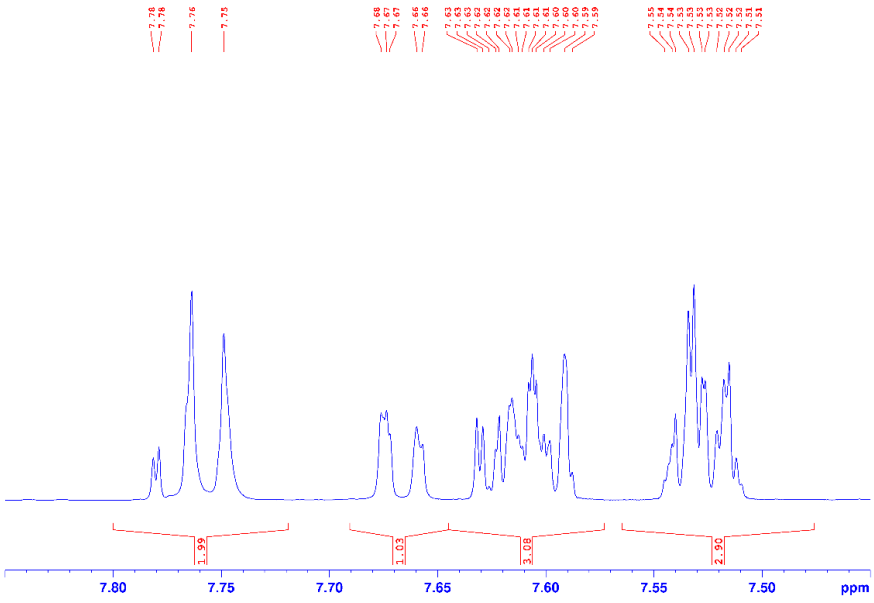


Figure S8: Magnified aromatic region of the ^{1}H NMR spectrum of compound **1** (500 MHz, CD_2Cl_2, 298 K).

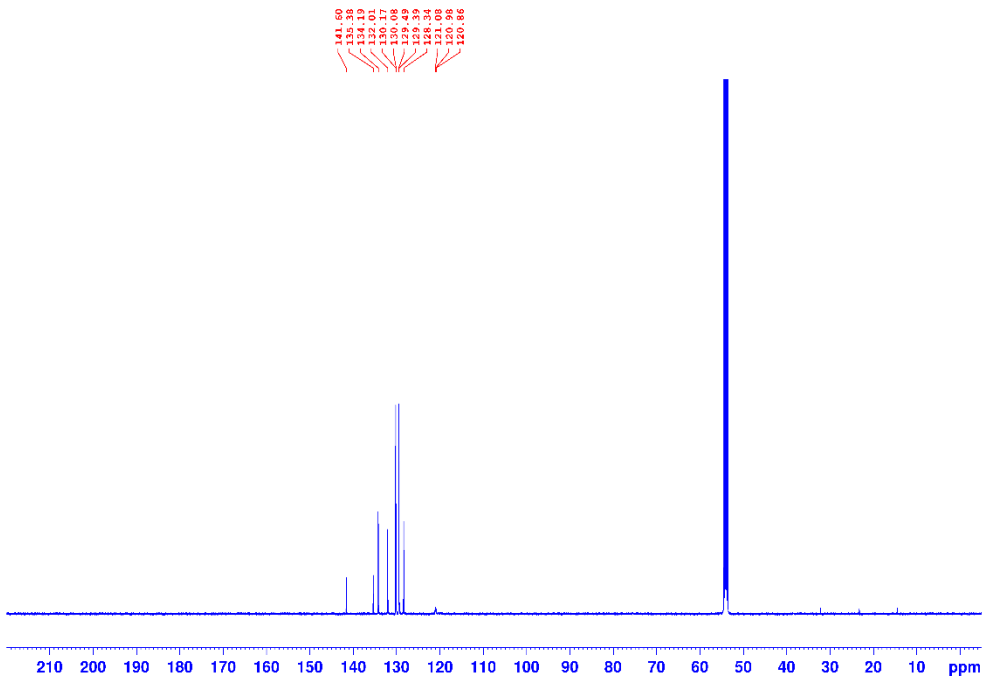


Figure S9: ^{13}C NMR spectrum of compound **1** (125 MHz, CD_2Cl_2, 298 K).

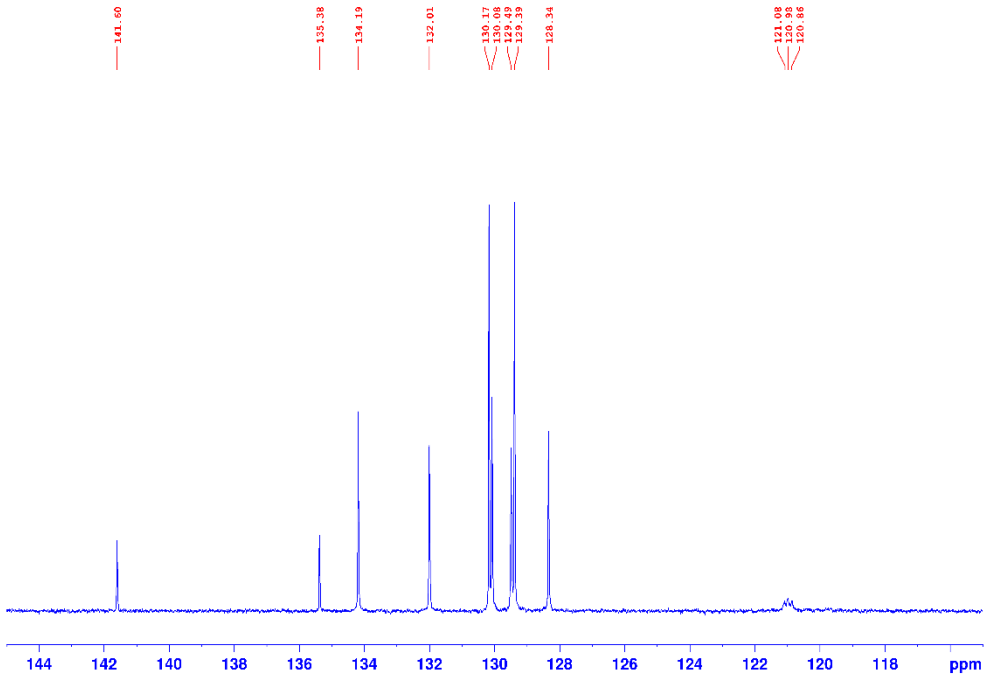


Figure S10: Magnified aromatic region of the ^{13}C NMR spectrum of compound **1** (125 MHz, CD_2Cl_2, 298 K).

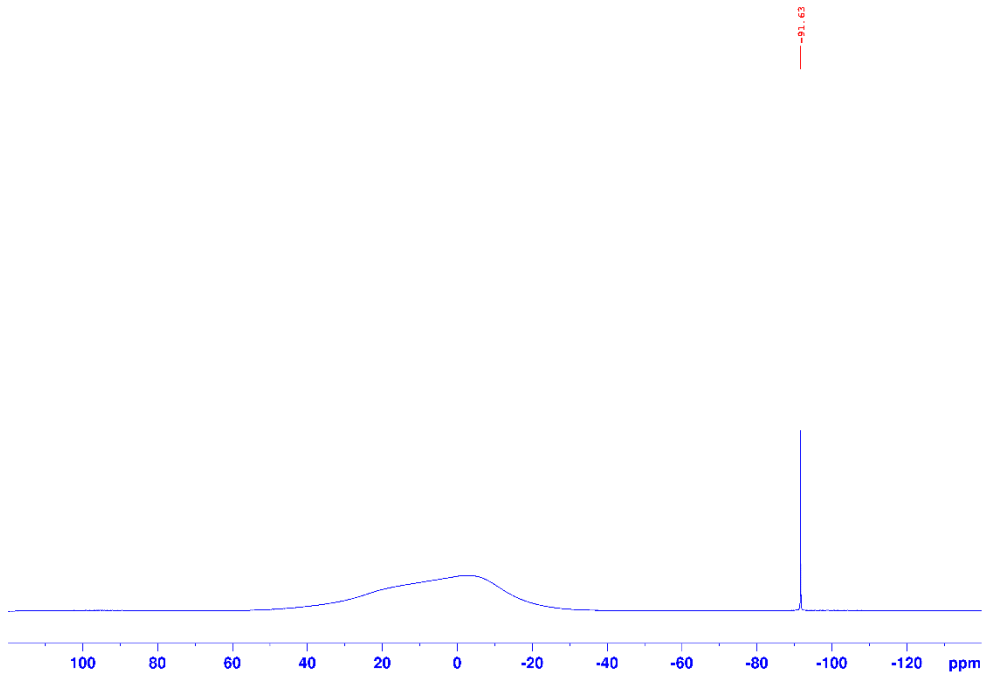


Figure S11: ^{11}B NMR spectrum of compound **1** (160 MHz, CD_2Cl_2, 298 K).

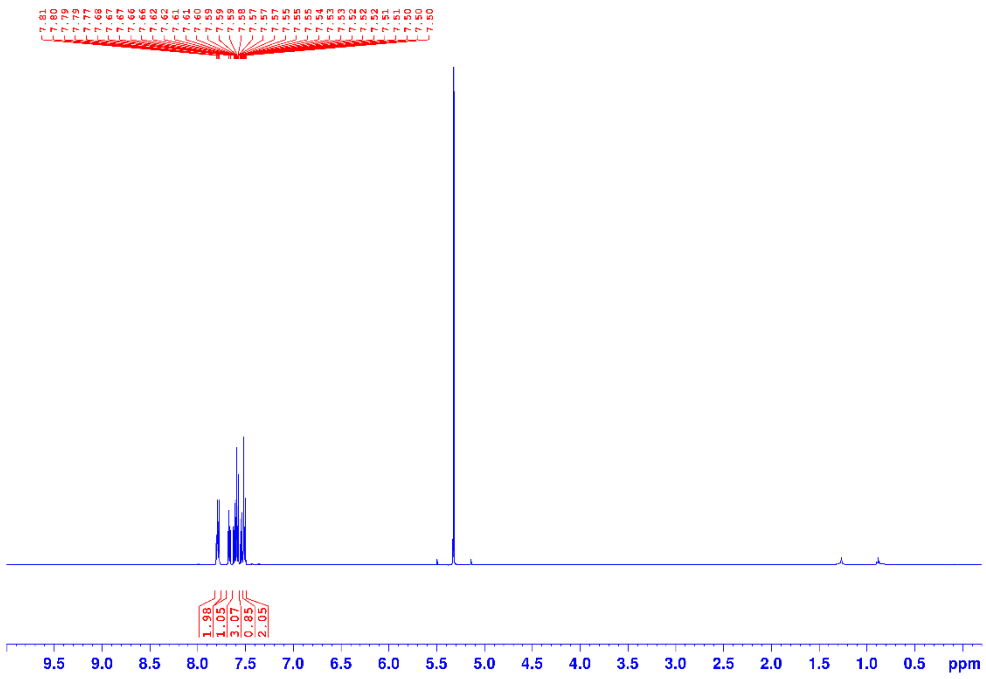


Figure S12: ^{1}H NMR spectrum of compound **2** (500 MHz, CD_2Cl_2, 298 K).

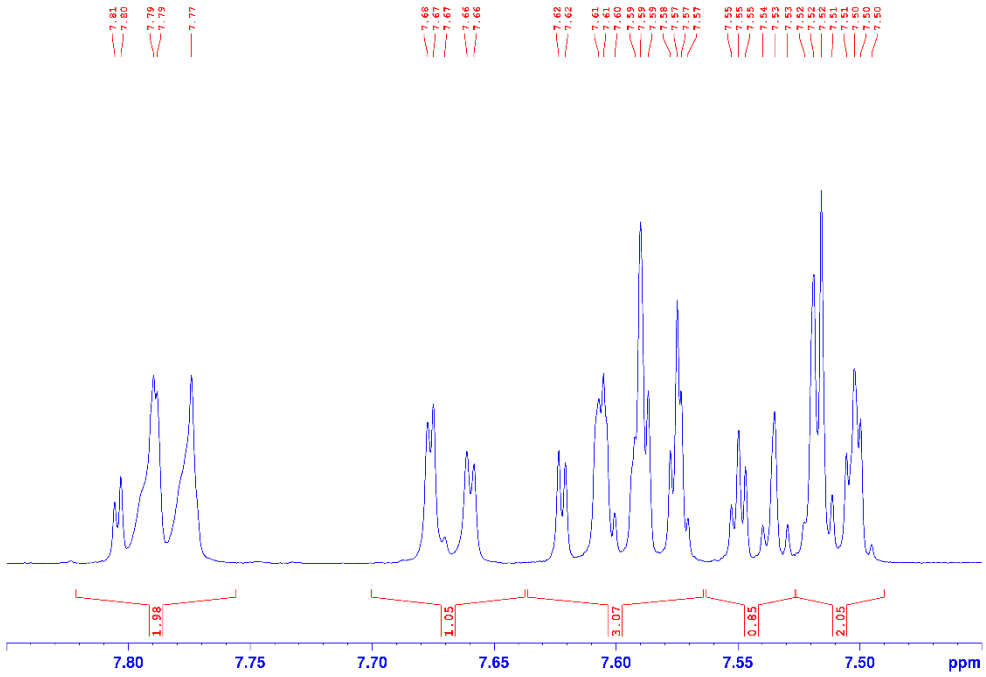


Figure S13: Magnified aromatic region of the ^{1}H NMR spectrum of compound **2** (500 MHz, CD_2Cl_2, 298 K).

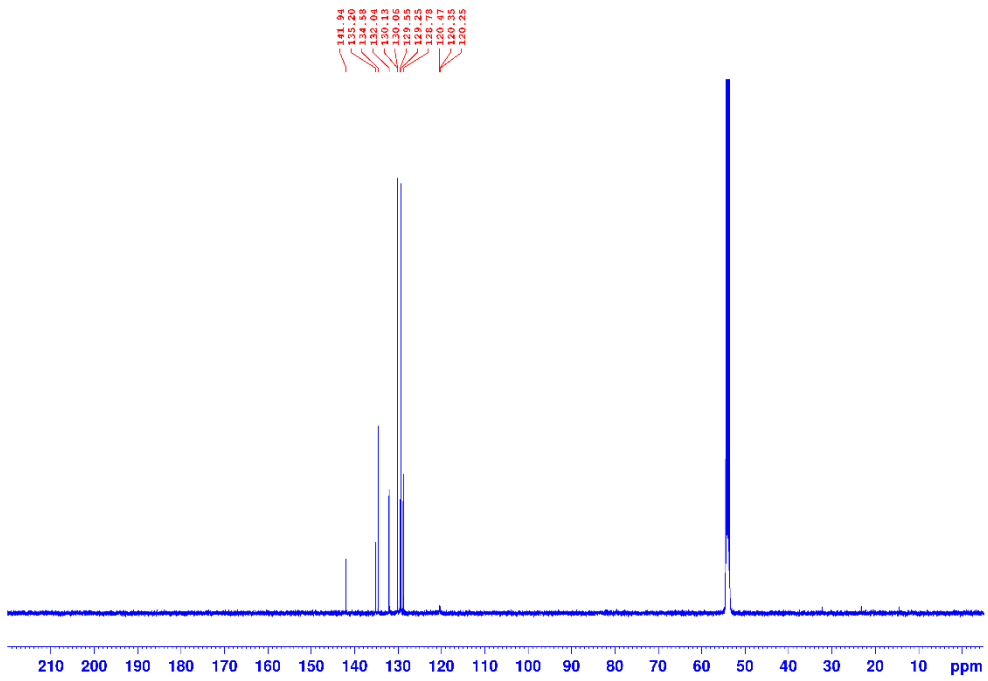


Figure S14: ^{13}C NMR spectrum of compound **2** (125 MHz, CD_2Cl_2, 298 K).

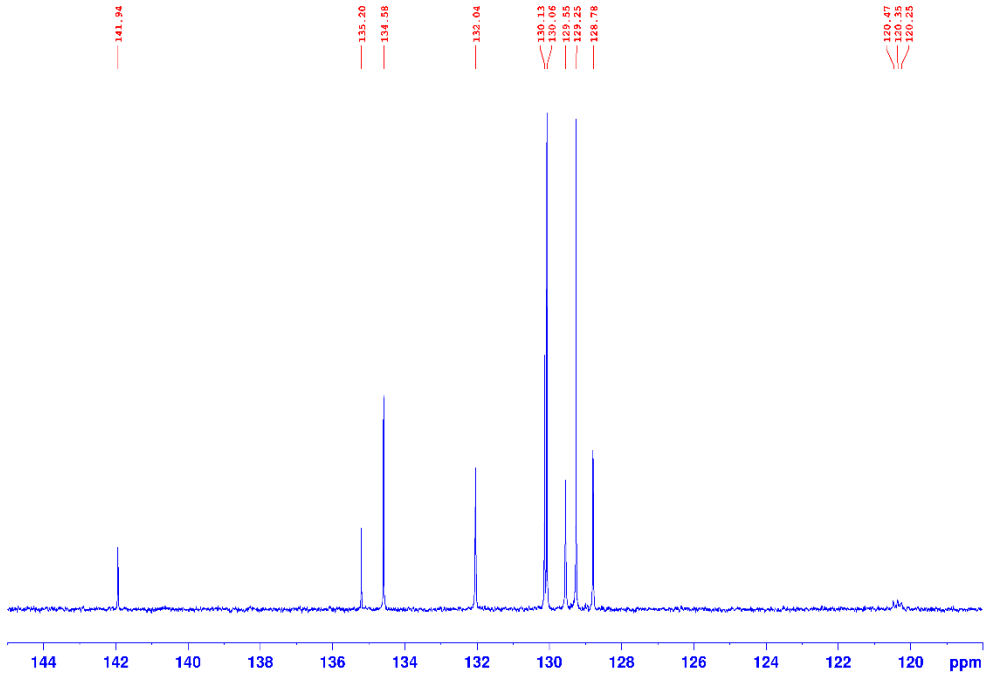


Figure S15: Magnified aromatic region of the ^{13}C NMR spectrum of compound **2** (125 MHz, CD_2Cl_2, 298 K).

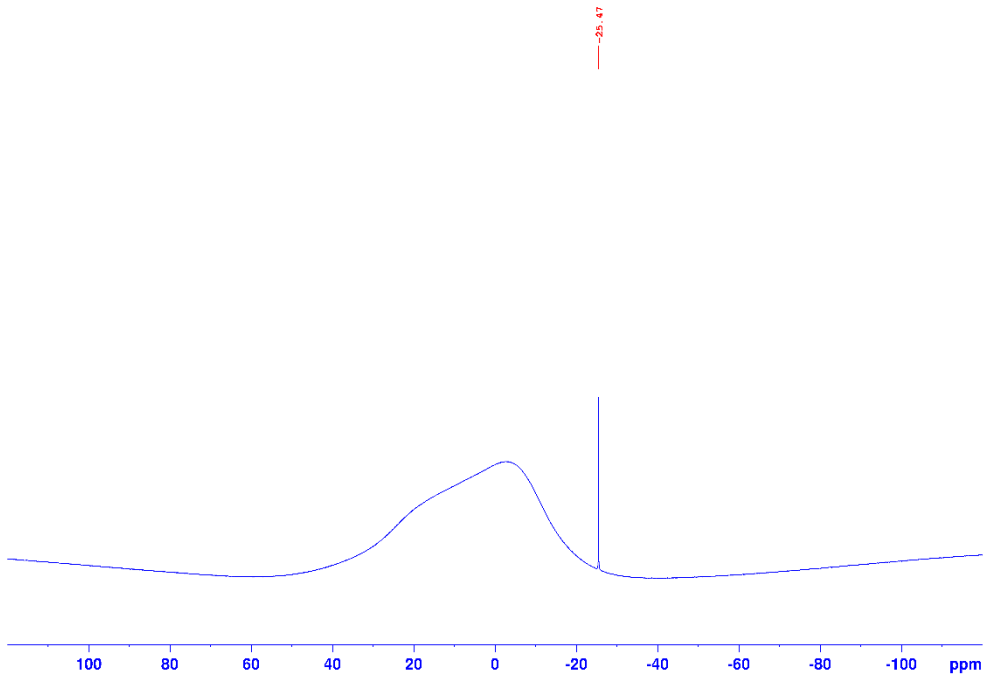


Figure S16: ^{11}B NMR spectrum of compound **2** (160 MHz, CD_2Cl_2, 298 K).

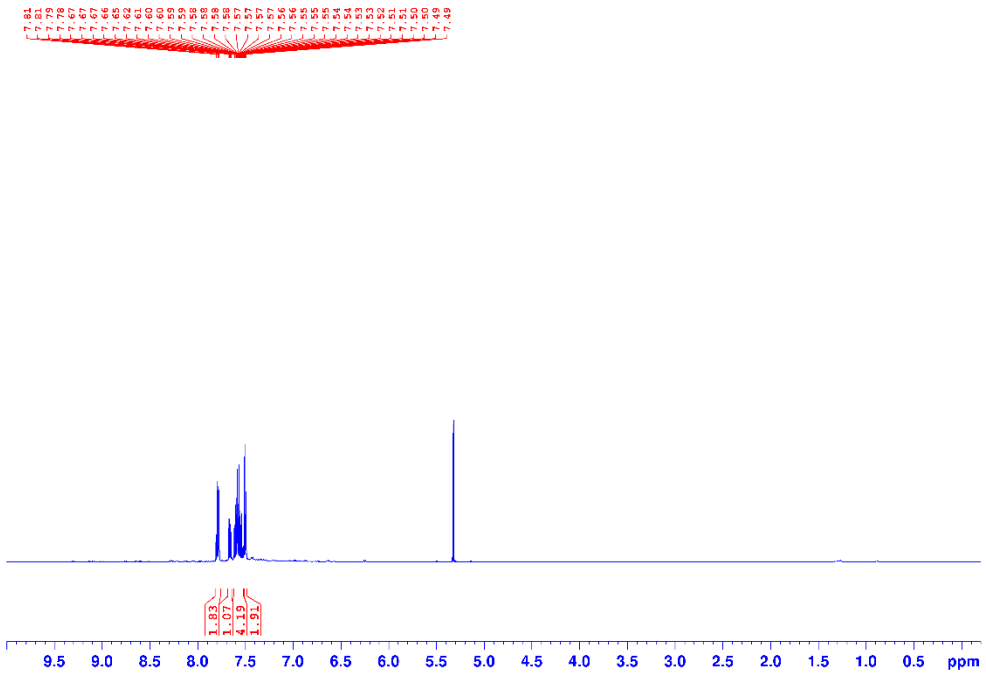


Figure S17: ^{1}H NMR spectrum of compound **3** (500 MHz, CD_2Cl_2, 298 K).

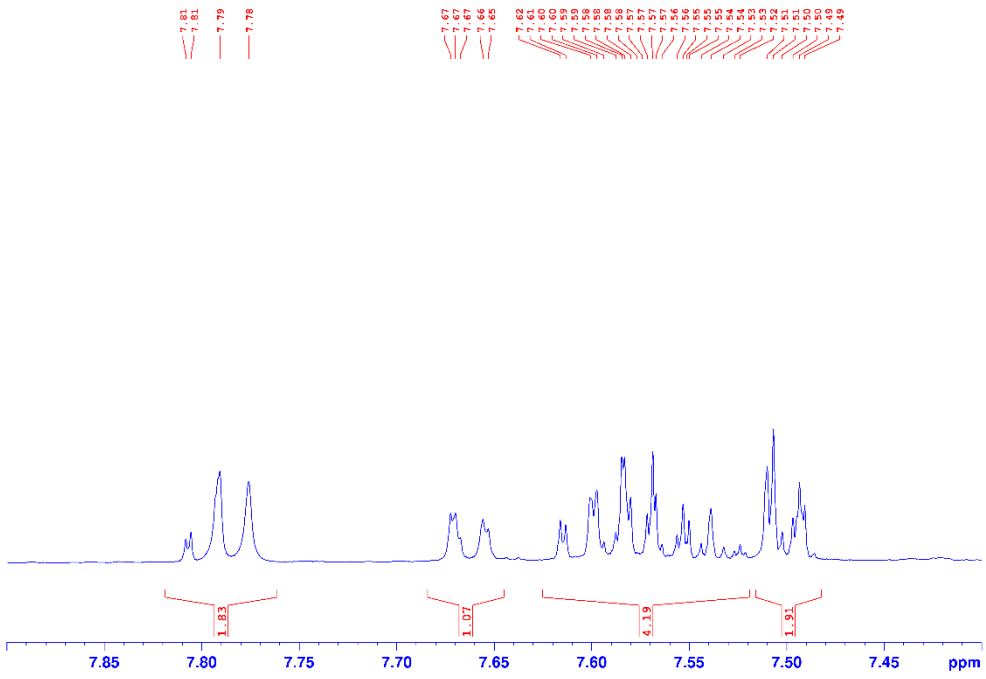


Figure S18: Magnified aromatic region of the ^{1}H NMR spectrum of compound **3** (500 MHz, CD_2Cl_2, 298 K).

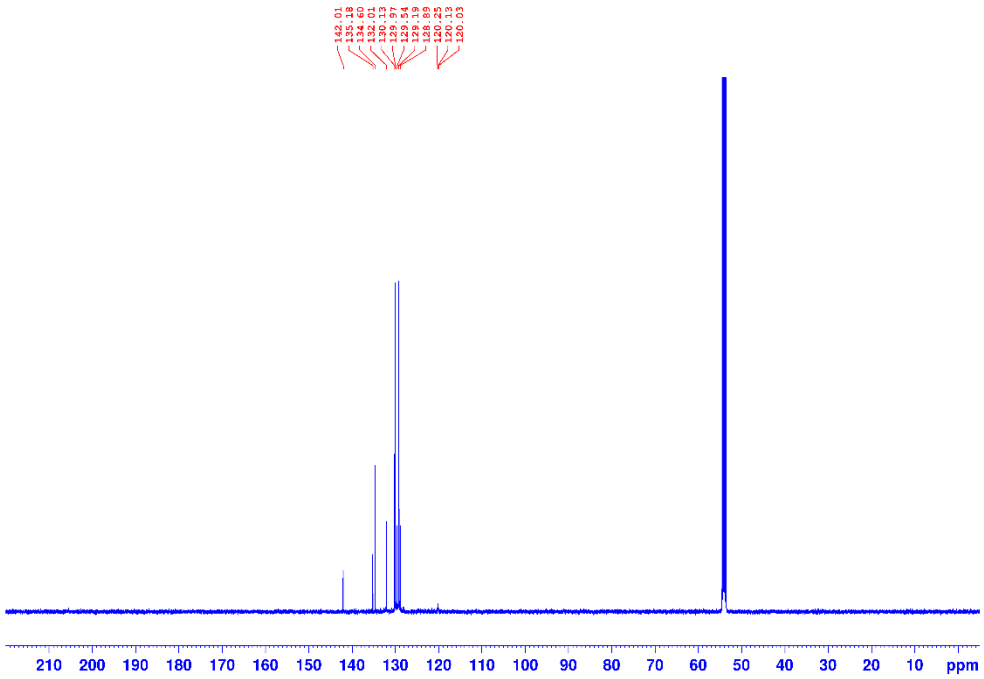


Figure S19: ^{13}C NMR spectrum of compound **3** (125 MHz, CD_2Cl_2, 298 K).

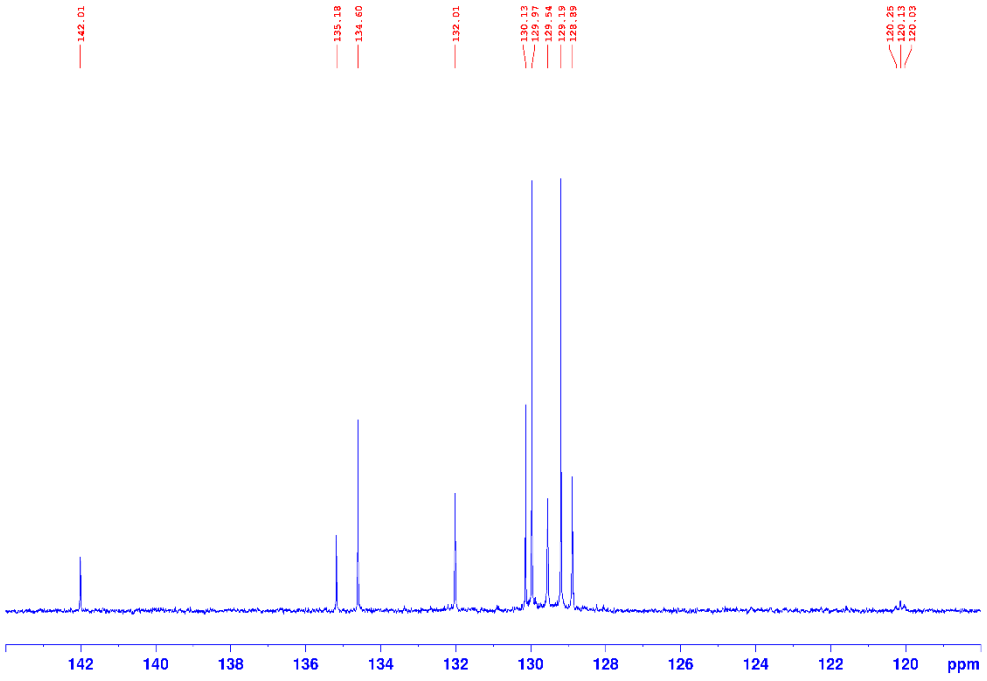


Figure S20: Magnified aromatic region of the ^{13}C NMR spectrum of compound **3** (125 MHz, CD_2Cl_2, 298 K).

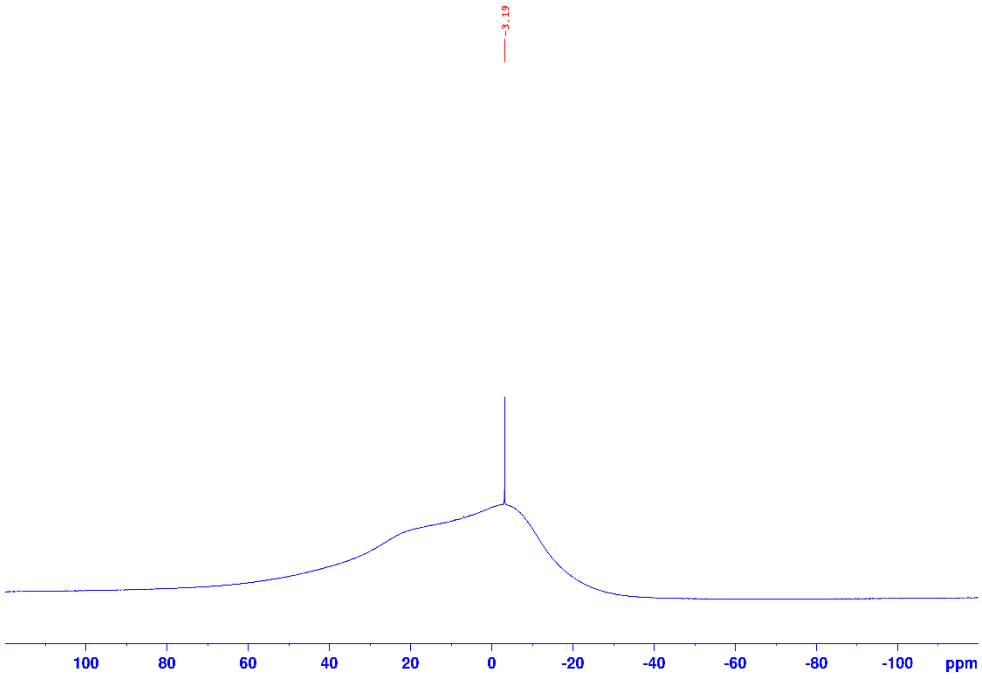


Figure S21: ^{11}B NMR spectrum of compound **3** (160 MHz, CD_2Cl_2, 298 K).

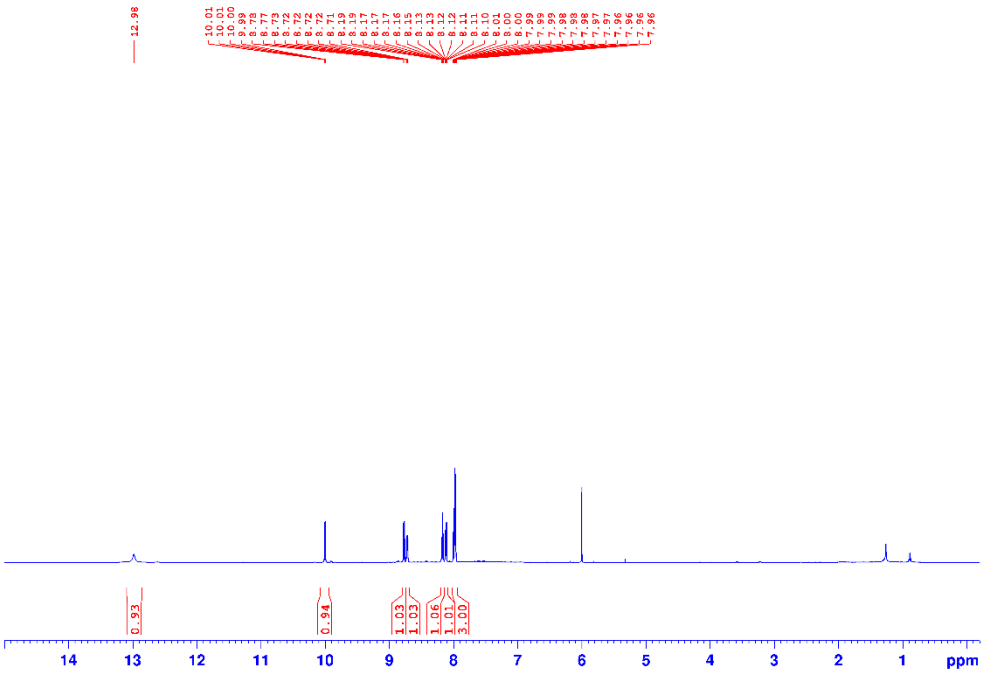


Figure S22: ^{1}H NMR spectrum of compound **4a** (500 MHz, TCE-d2, 298 K).

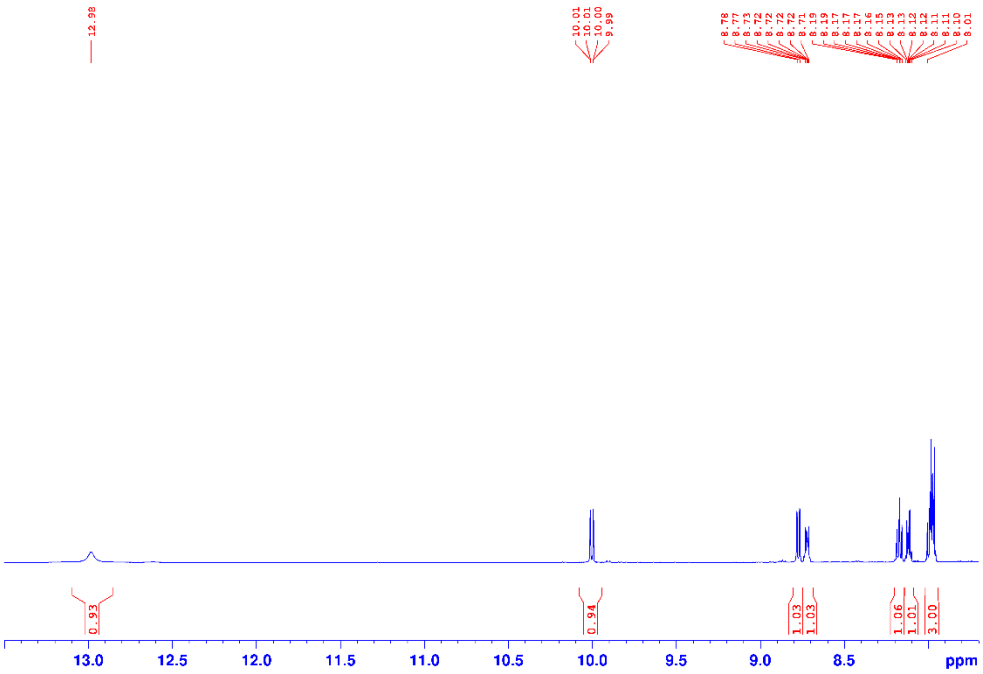


Figure S23: Magnified aromatic region of the ^{1}H NMR spectrum of compound **4a** (500 MHz, TCE-d2, 298 K).

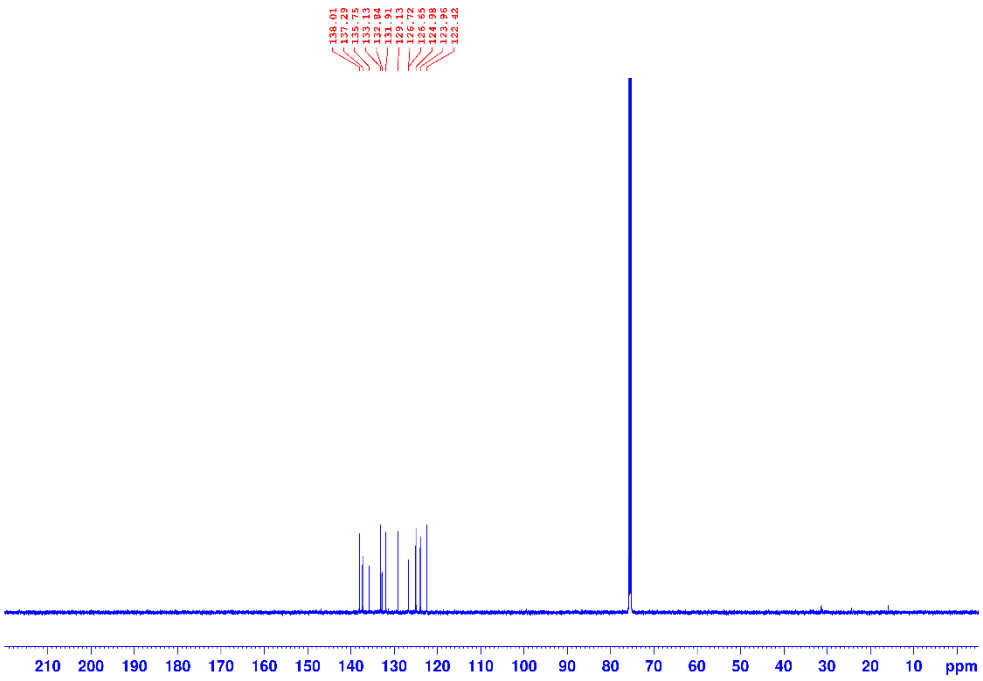


Figure S24: ^{13}C NMR spectrum of compound **4a** (125 MHz, TCE-d2, 298 K).

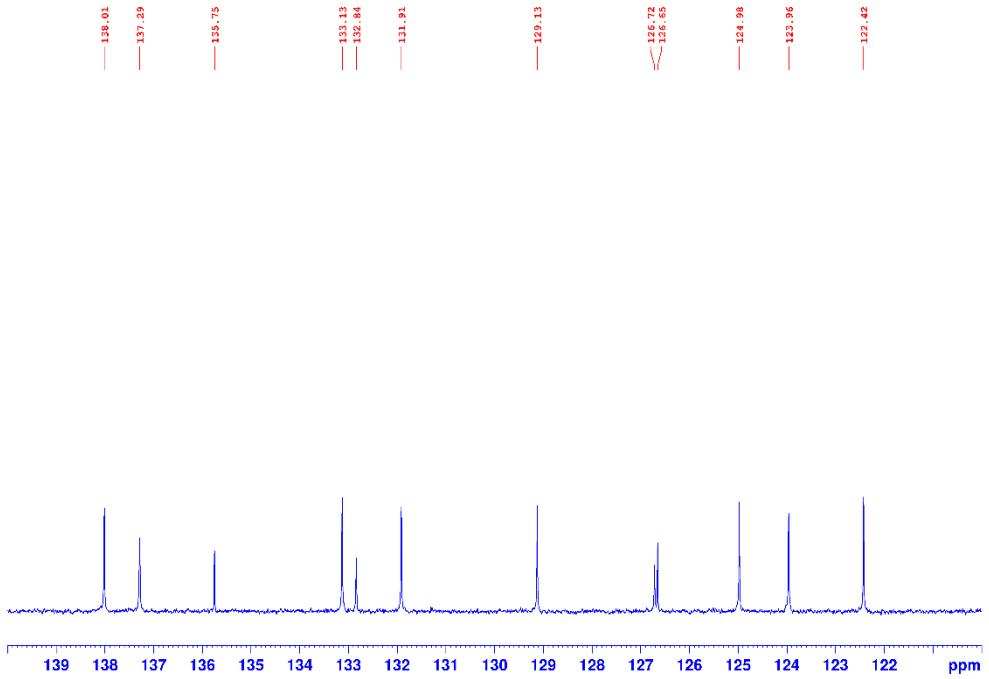


Figure S25: Magnified aromatic region of the ^{13}C NMR spectrum of compound **4a** (125 MHz, TCE-d2, 298 K).

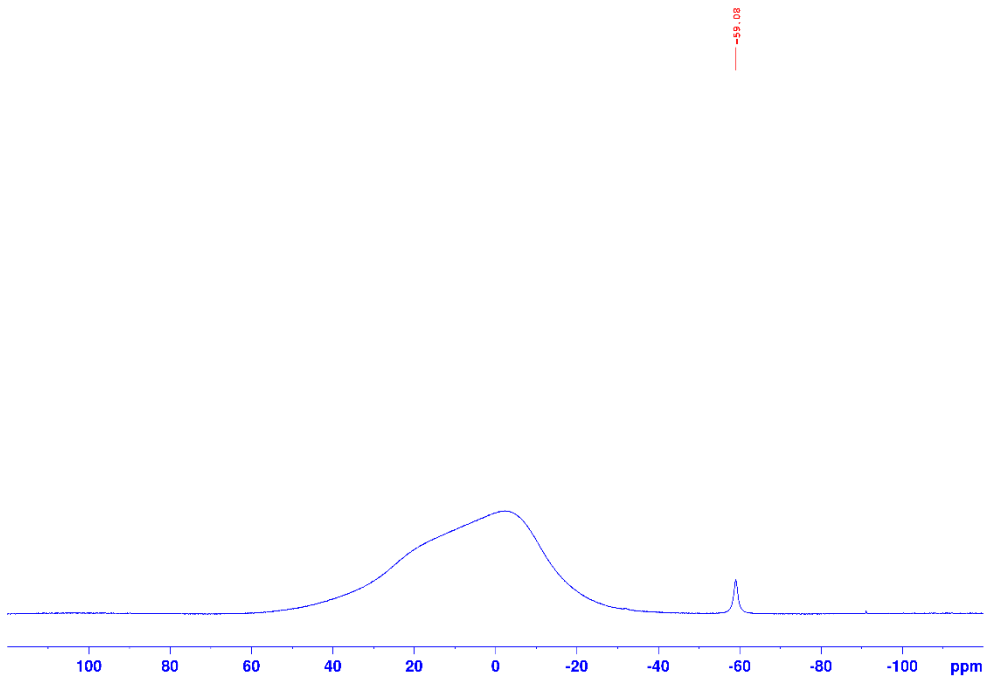


Figure S26: ^{11}B NMR spectrum of compound **4a** (160 MHz, TCE-d2, 298 K).

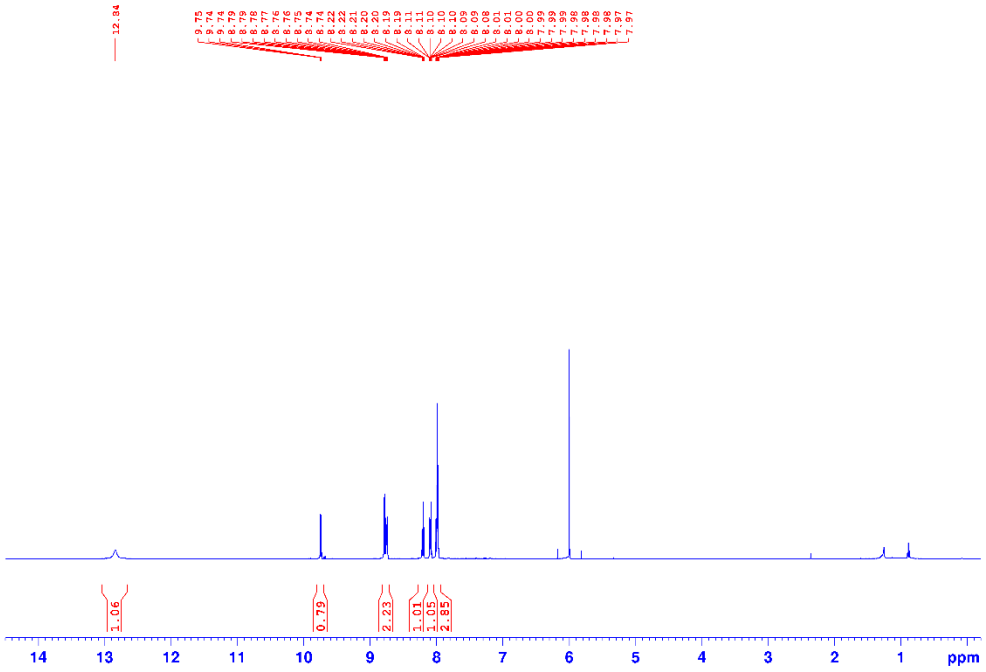


Figure S27: ^{1}H NMR spectrum of compound **5a** (500 MHz, TCE-d2, 298 K).

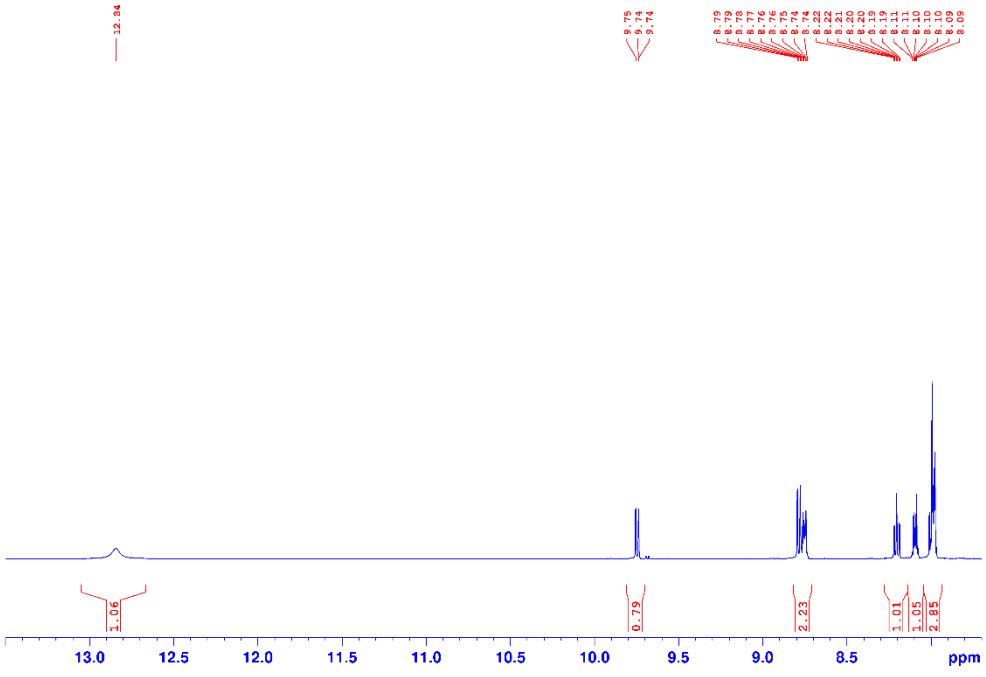


Figure S28: Magnified aromatic region of the ^{1}H NMR spectrum of compound **5a** (500 MHz, TCE-d2, 298 K).

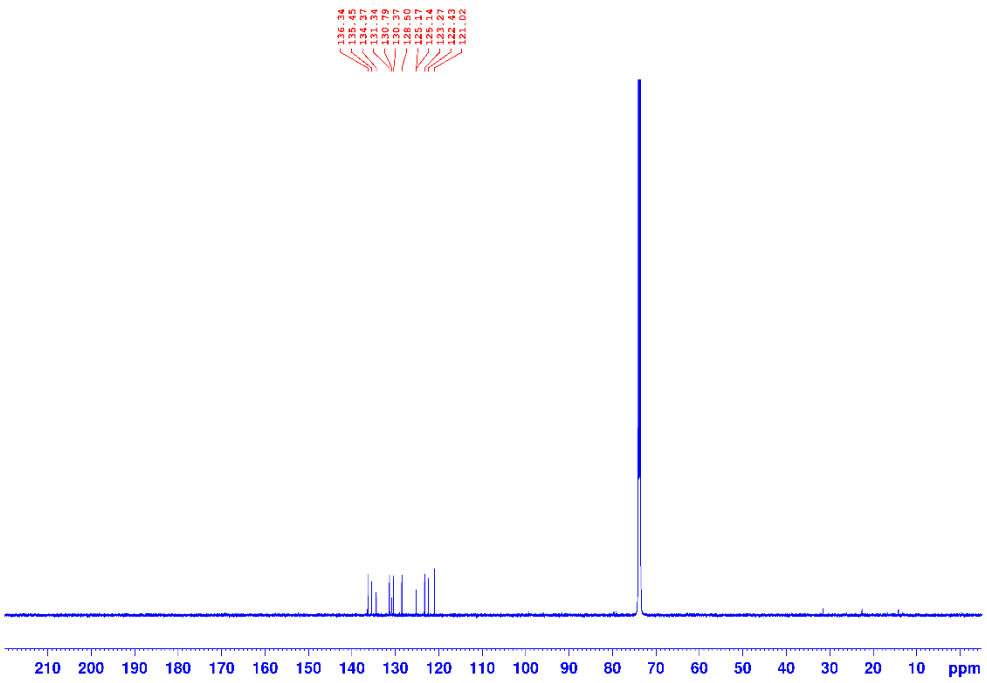


Figure S29: ^{13}C NMR spectrum of compound **5a** (125 MHz, TCE-d2, 298 K).

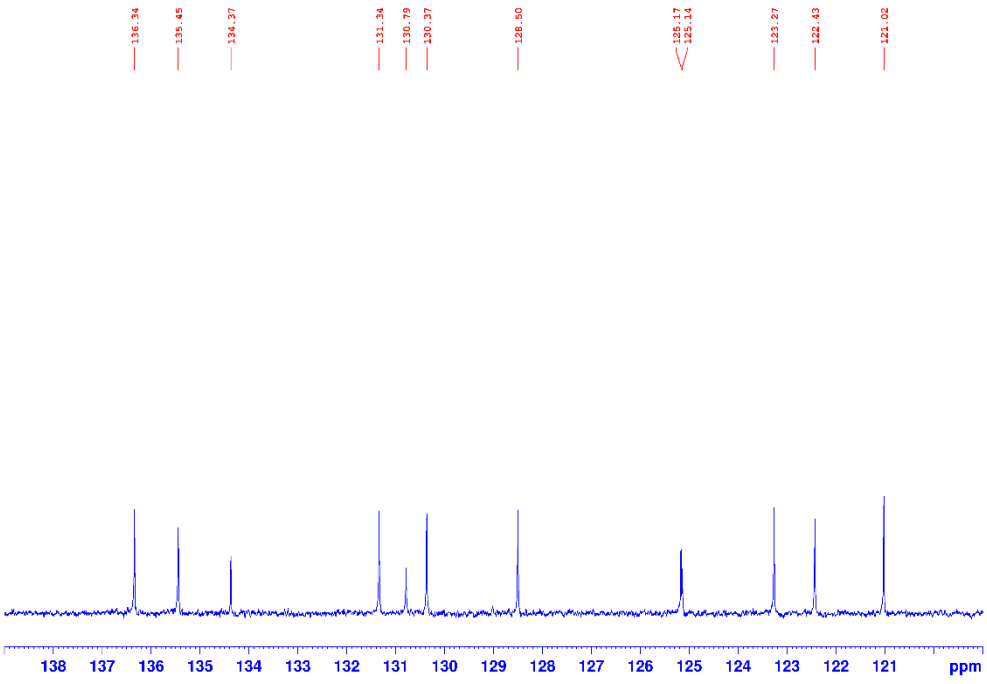


Figure S30: Magnified aromatic region of the ^{13}C NMR spectrum of compound **5a** (125 MHz, TCE-d2, 298 K).

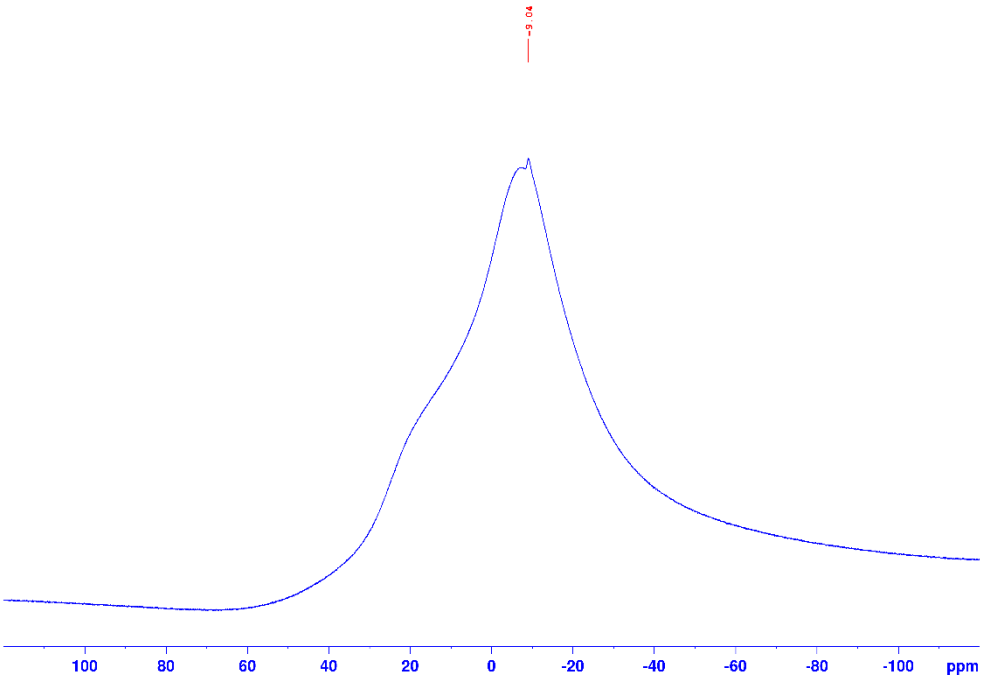


Figure S31: ^{11}B NMR spectrum of compound **5a** (160 MHz, TCE-d2, 298 K).

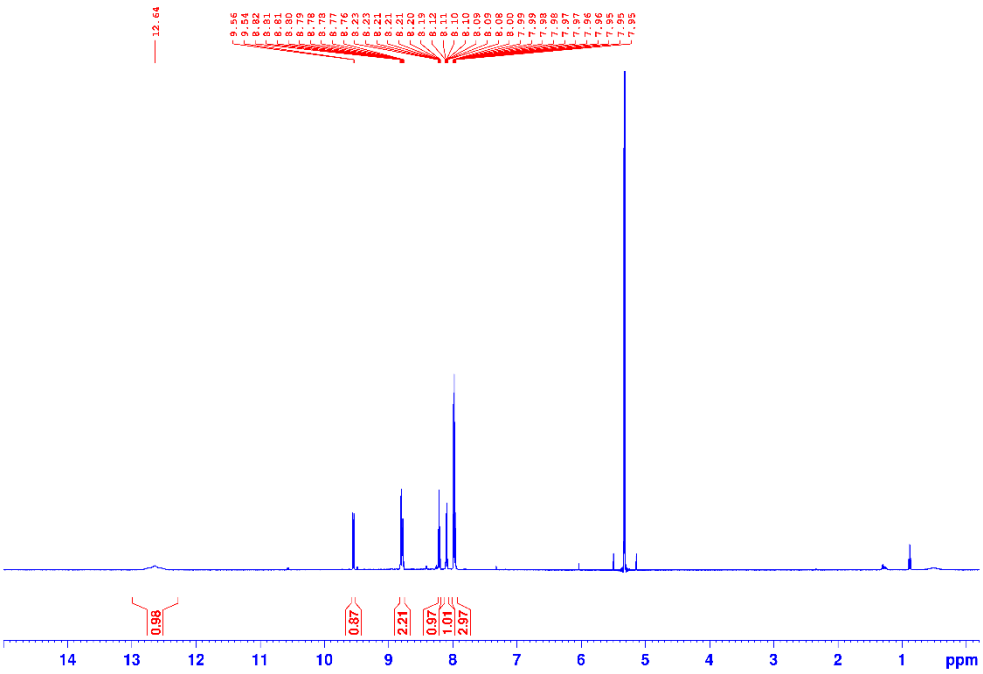


Figure S32: ^{1}H NMR spectrum of compound **6a** (500 MHz, CD_2Cl_2, 298 K).

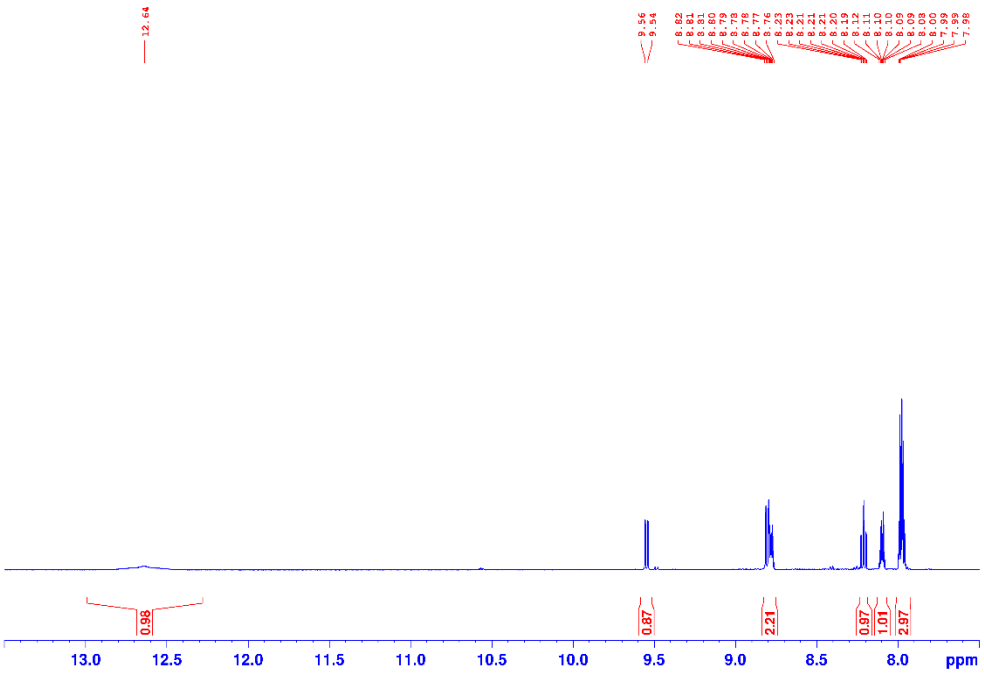


Figure S33: Magnified aromatic region of the ^{1}H NMR spectrum of compound **6a** (500 MHz, CD_2Cl_2, 298 K).

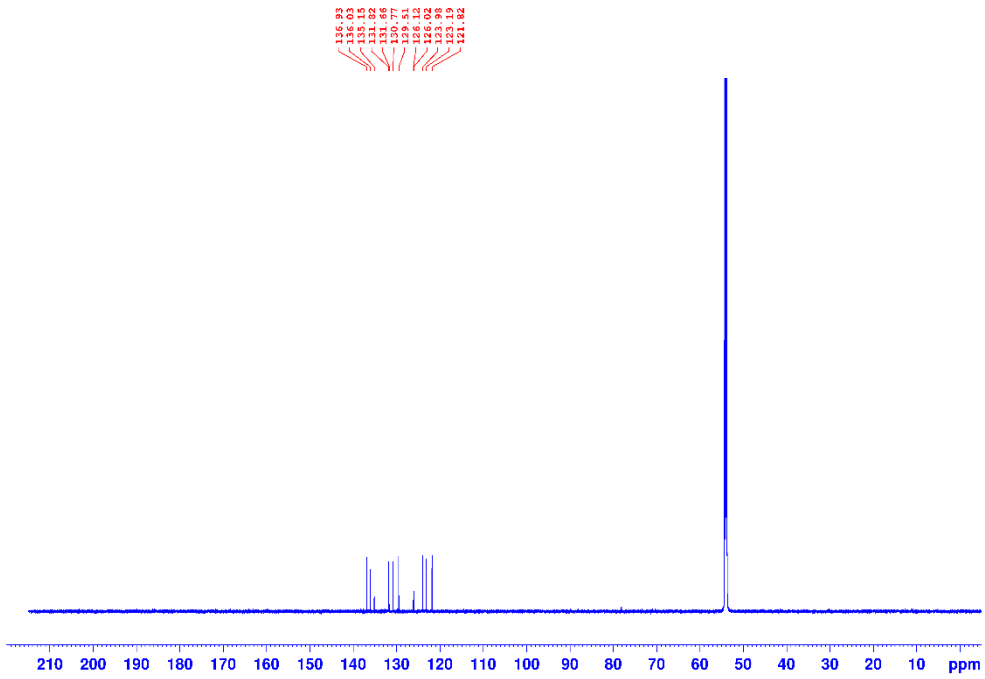


Figure S34: ^{13}C NMR spectrum of compound **6a** (200 MHz, CD_2Cl_2, 298 K).

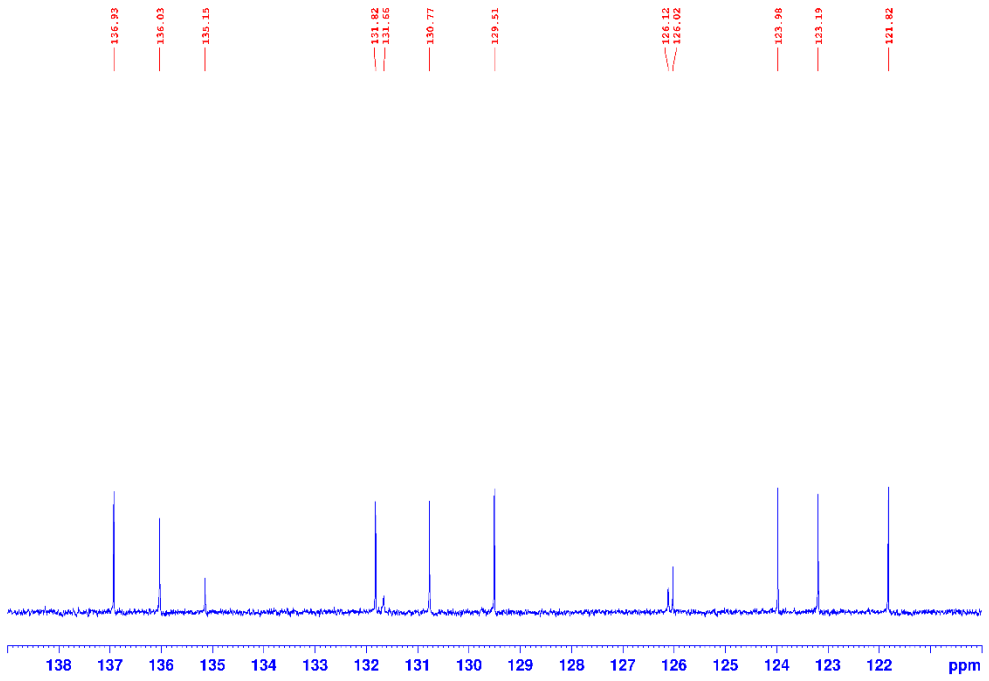


Figure S35: Magnified aromatic region of the ^{13}C NMR spectrum of compound **6a** (200 MHz, CD_2Cl_2, 298 K).

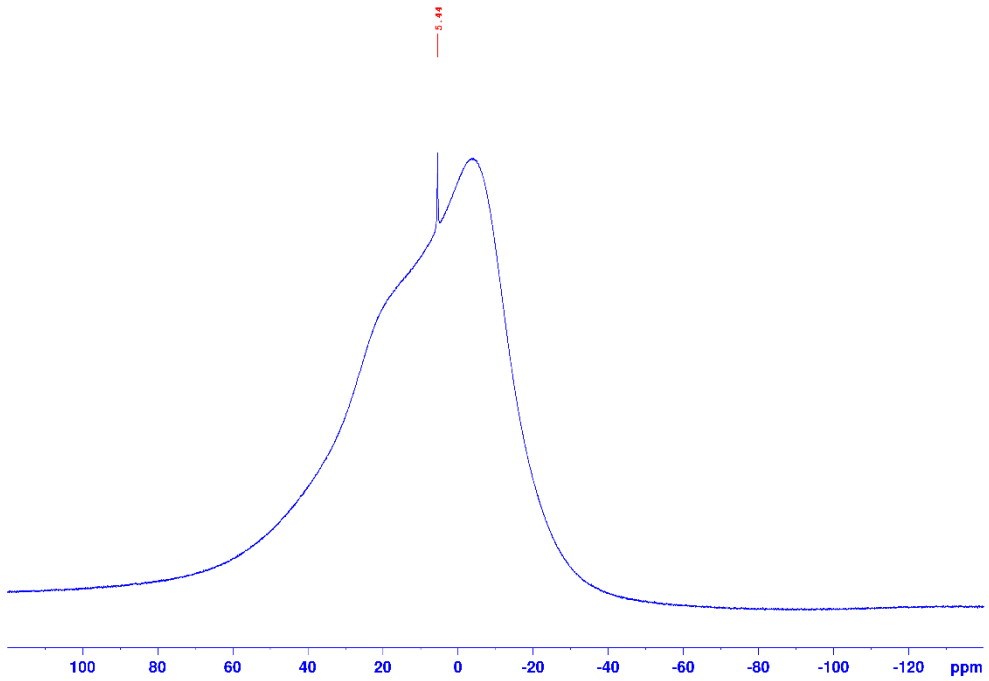


Figure S36: ^{11}B NMR spectrum of compound **6a** (160 MHz, CD_2Cl_2, 298 K).

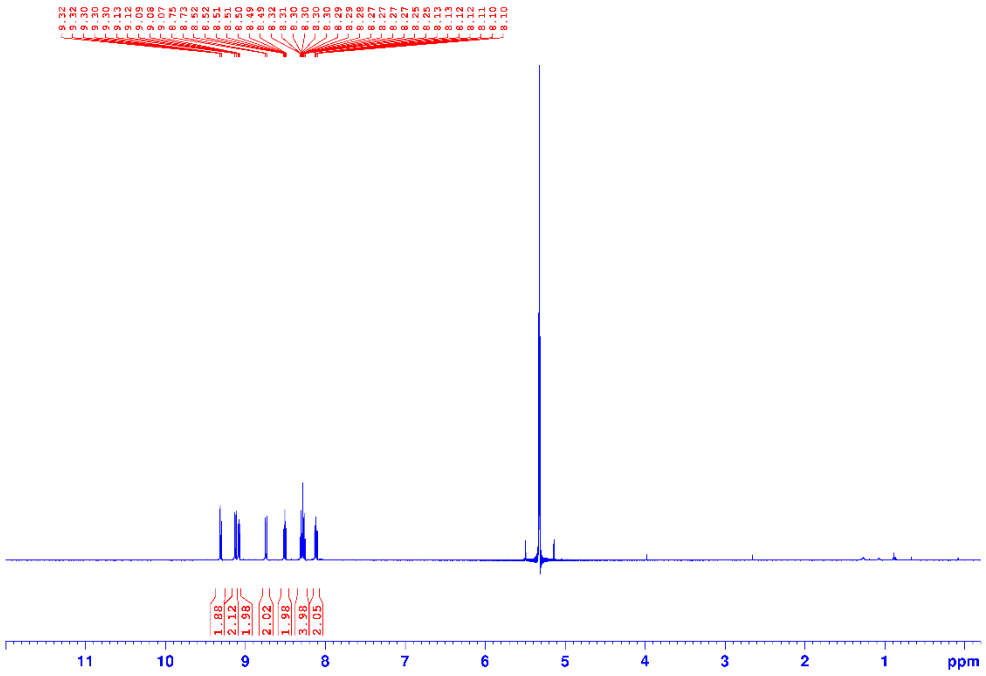


Figure S37: ^{1}H NMR spectrum of compound **6b** (500 MHz, CD_2Cl_2, 298 K).

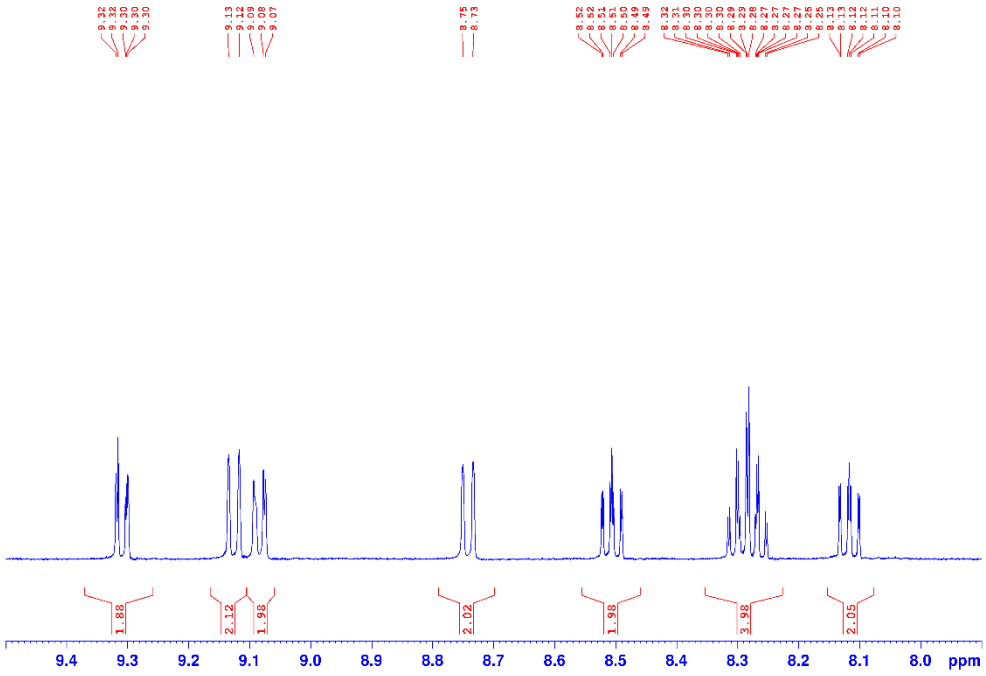


Figure S38: Magnified aromatic region of the ^{1}H NMR spectrum of compound **6b** (500 MHz, CD_2Cl_2, 298 K).

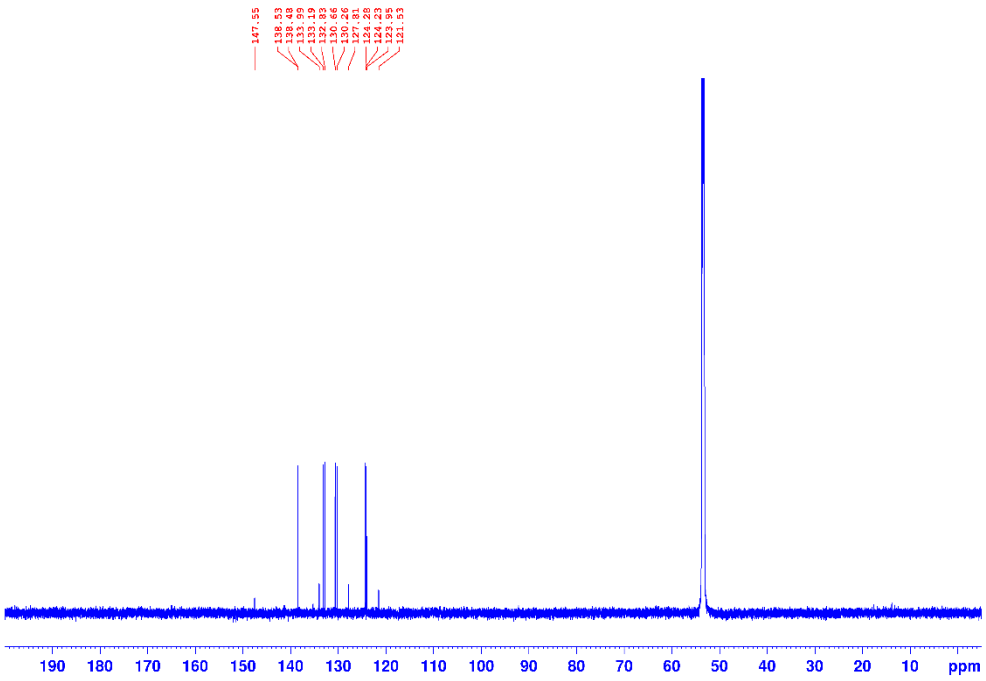


Figure S39: ^{13}C NMR spectrum of compound **6b** (200 MHz, CD_2Cl_2, 298 K).

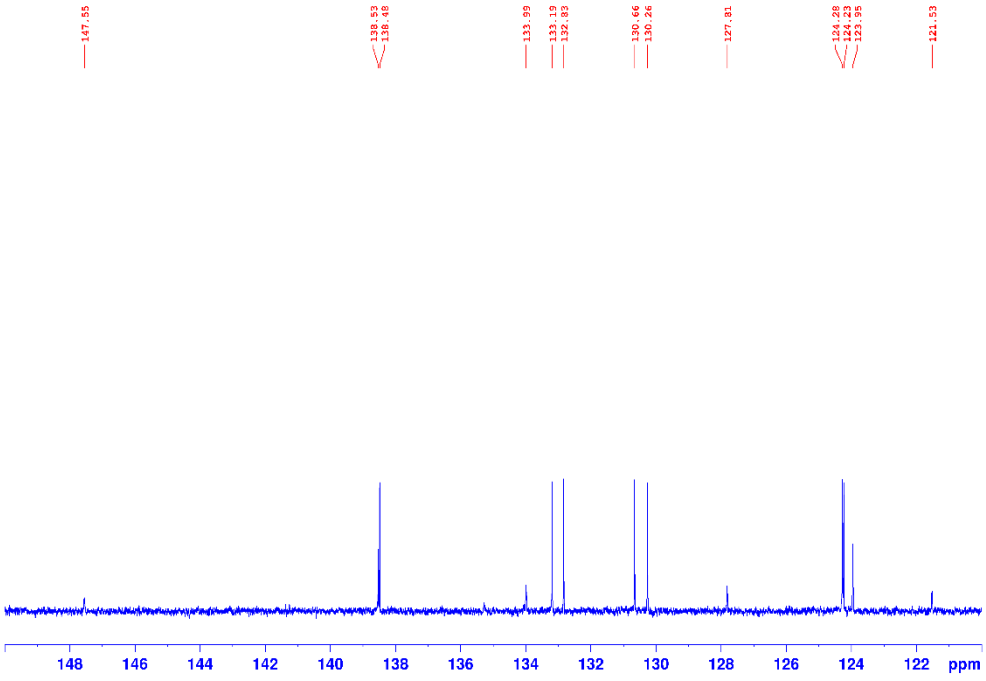


Figure S40: Magnified aromatic region of the ^{13}C NMR spectrum of compound **6b** (200 MHz, CD_2Cl_2, 298 K).

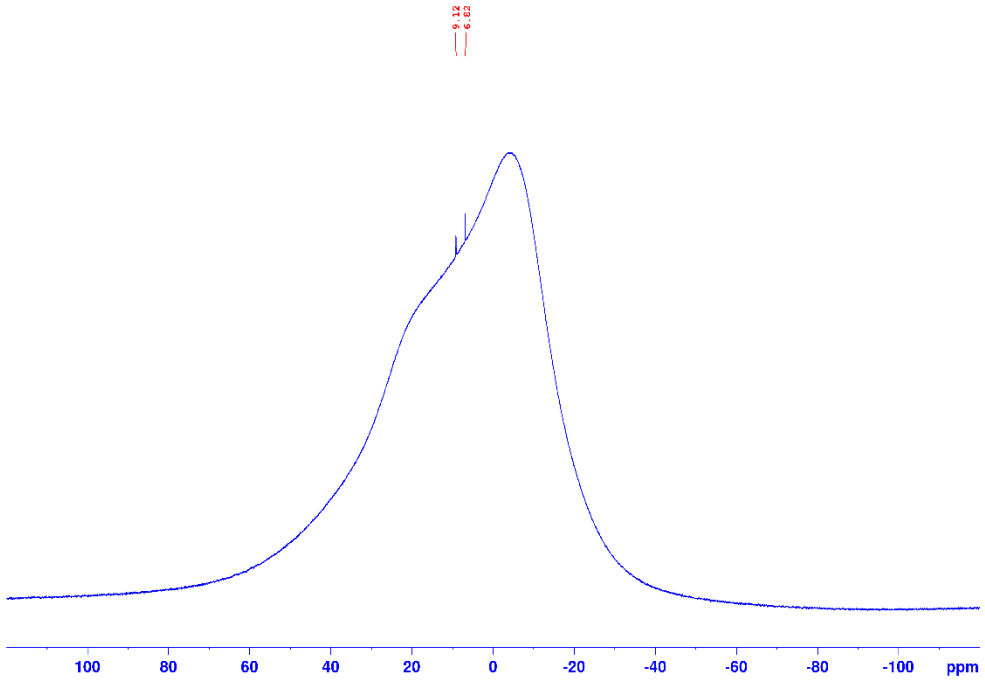


Figure S41: ^{11}B NMR spectrum of compound **6b** (160 MHz, CD_2Cl_2, 298 K).

4. Simulated and measured HR-MS spectra

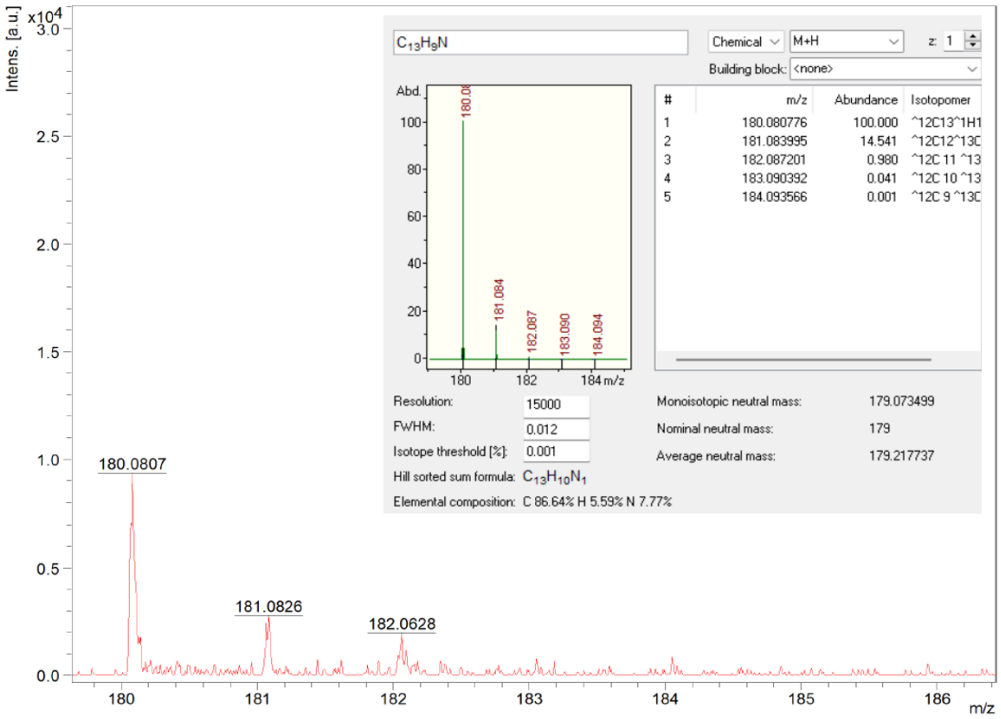


Figure S42. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **1** (MALDI-TOF, positive mode) *m/z*: $[M\text{-}BI_3+H]^+$ Calc'd $C_{13}H_{10}N$.

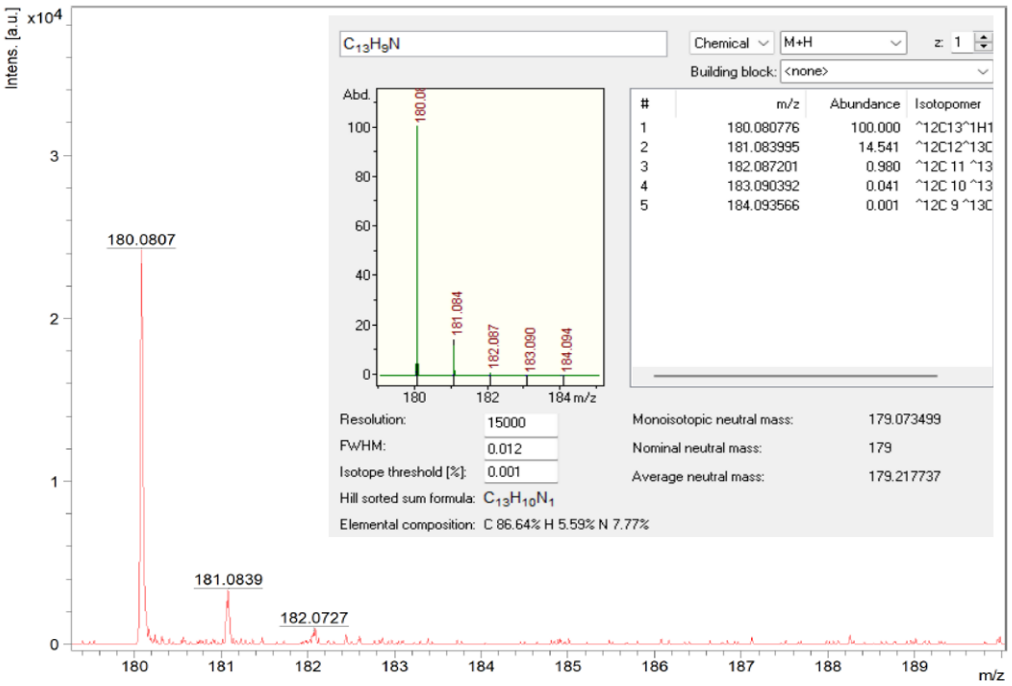


Figure S43. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **2** (MALDI-TOF, positive mode) *m/z*: $[M\text{-}BBr_3+H]^+$ Calc'd $C_{13}H_{10}N$.

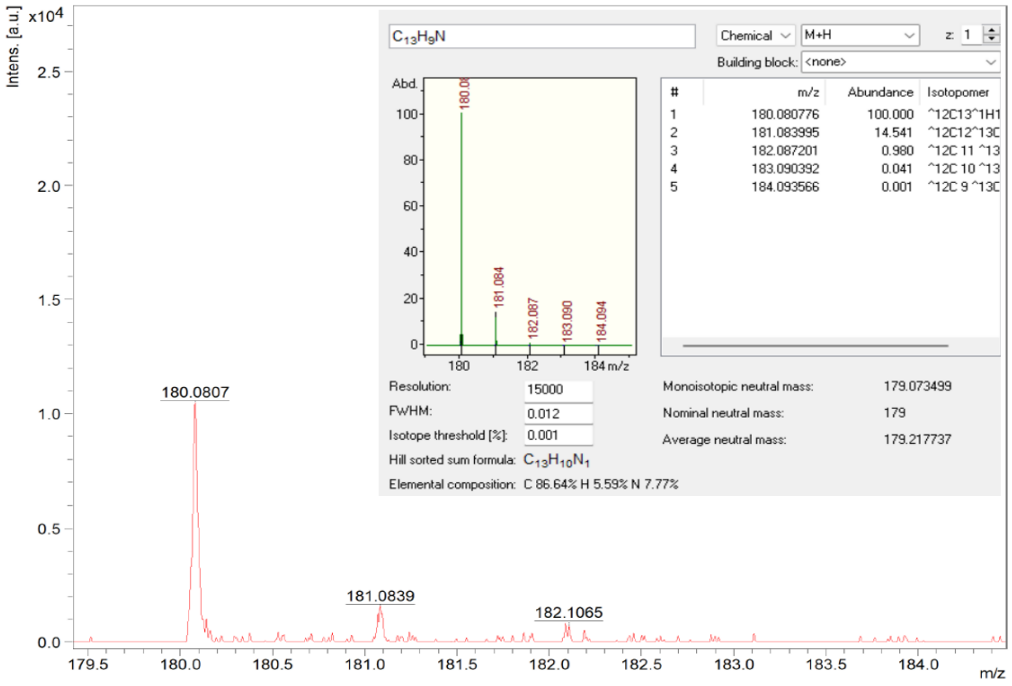


Figure S44. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **3** (MALDI-TOF, positive mode) *m/z*: $[M\text{-}BCl_3+H]^+$ Calc'd $C_{13}H_{10}N$.

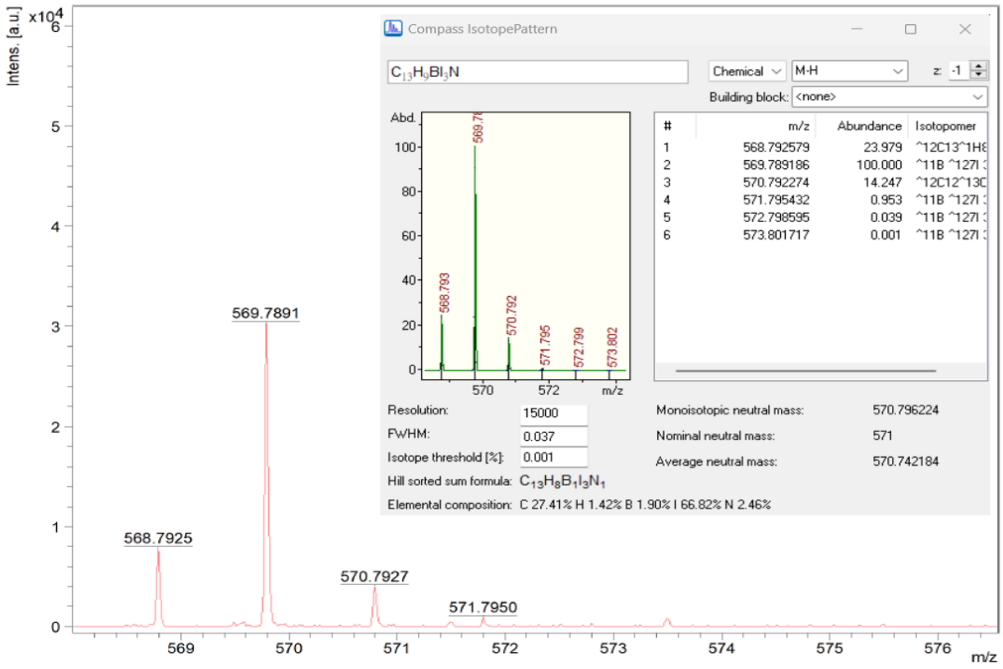


Figure S45. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **4a** (MALDI-TOF, negative mode) *m/z*: $[M-H]^-$ Calc'd for $C_{13}H_8BI_3N$.

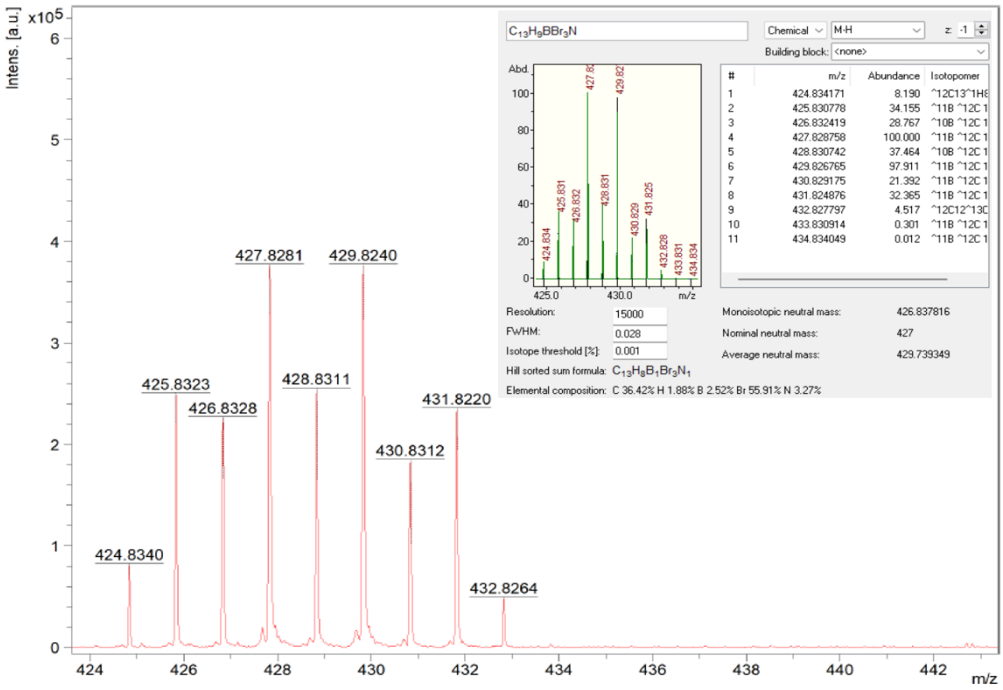


Figure S46. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **5a** (MALDI-TOF, negative mode) *m/z*: $[M-H]^-$ Calc'd for $C_{13}H_8BBr_3N$.

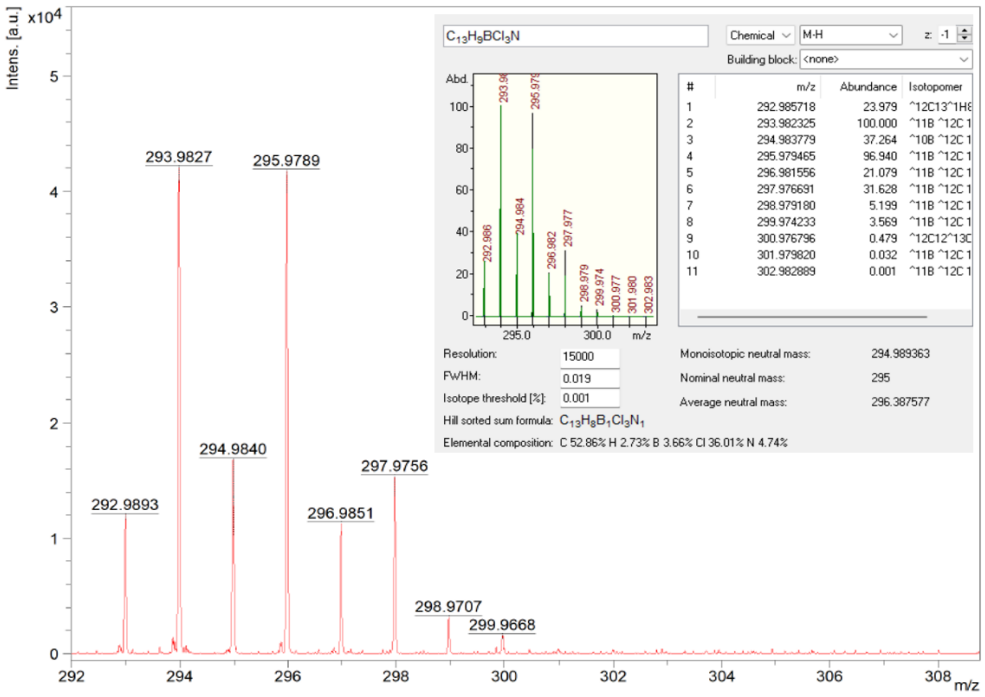


Figure S47. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **6a** (MALDI-TOF, negative mode) *m/z*: $[M-H]^-$ Calc'd for $C_{13}H_8BCl_3N$.

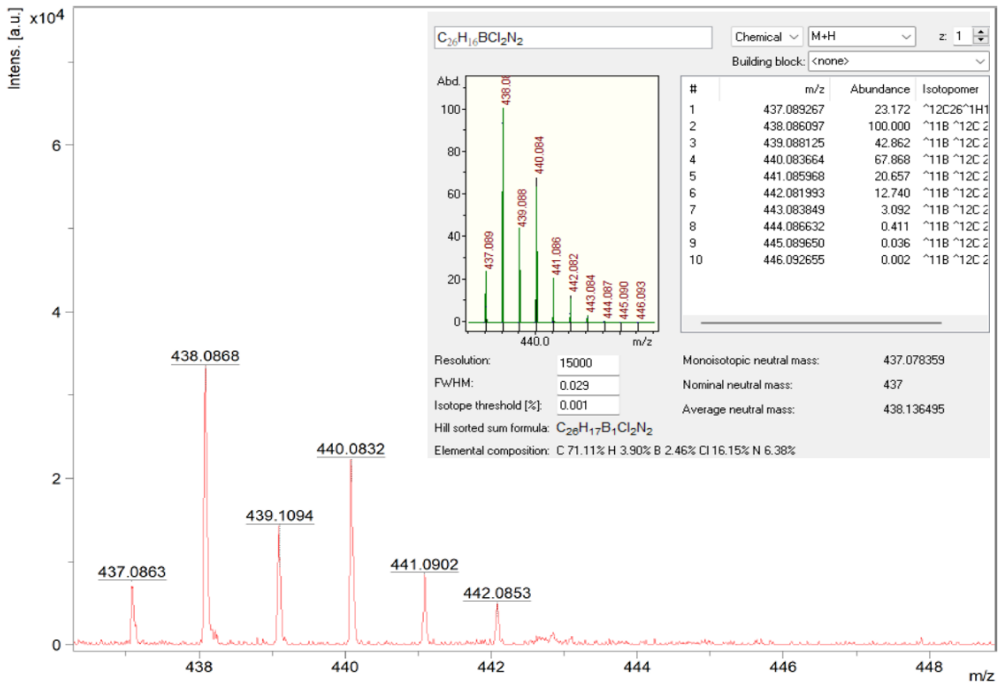


Figure S48. Simulated (right) and found (left) patterns of the high-resolution mass spectrum of **6b** (MALDI-TOF, positive mode) *m/z*: $[M+H]^+$ Calc'd for $C_{26}H_{17}BCl_2N_2$.

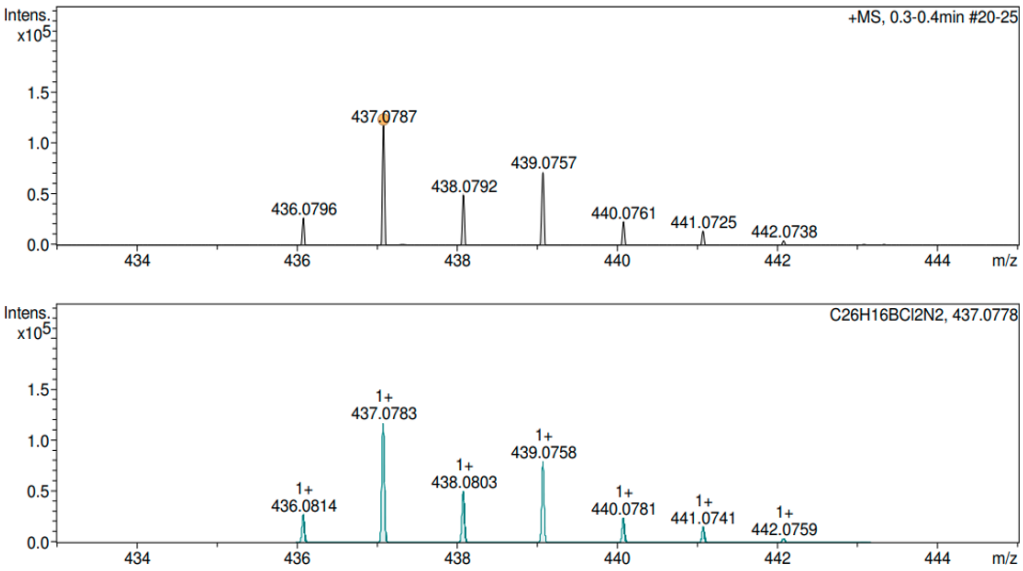


Figure S49. Simulated (bottom) and found (top) patterns of the high-resolution mass spectrum of **6b** (ESI-TOF, positive mode) *m/z*: $[M]^+$ Calc'd for $C_{26}H_{16}BCl_2N_2$.

5. Mechanistic studies

5.1

In an inert atmosphere glovebox, compound **1** (0.0088 g, 0.015 mmol) was dissolved in 2.1 mL 1,1,2,2-tetrachloroethane-d2 and the solution was divided equally into three J-Young NMR tubes. The first J-Young NMR tube was heated at 130 °C for 3 h without any additional steps. The second J-Young NMR tube was heated at 130 °C for 3 h while isolated from light using aluminum foil. The third J-Young NMR tube was degassed using five freeze-pump-thaw cycles and then heated at 130 °C for 3 h.

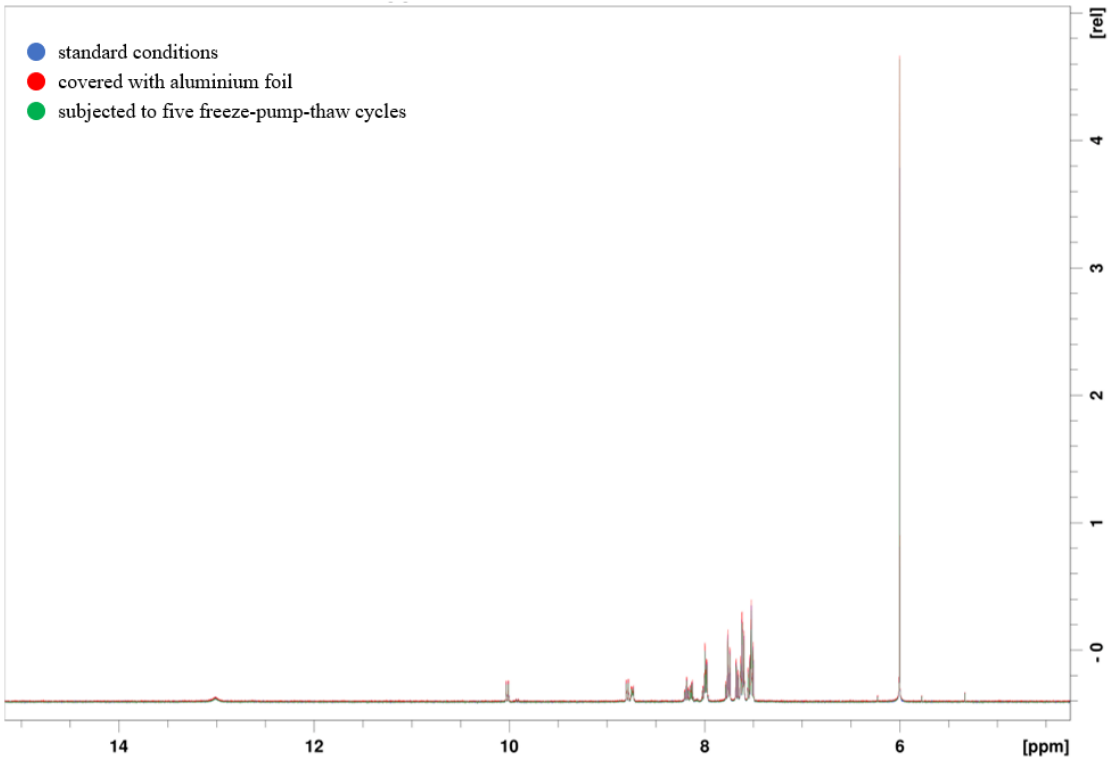
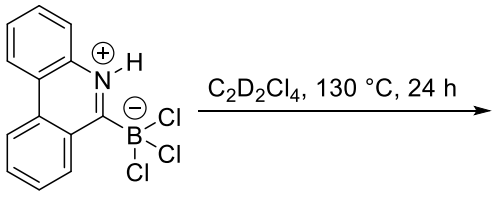


Figure S50: ^{1}H NMR spectra (400 MHz, TCE-d2, 298 K) of the reaction progress of heating compound **1** at 130°C for 3 h. Blue: standard conditions, red: covered with aluminum foil, and green: subjected to five freeze-pump-thaw cycles.

5.2



6a

In an inert atmosphere glovebox, compound **6a** (0.0015 g, 0.0051 mmol) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in a J-Young NMR tube and heated at 130 °C for 24 h, after which an ^{1}H NMR spectrum was measured.

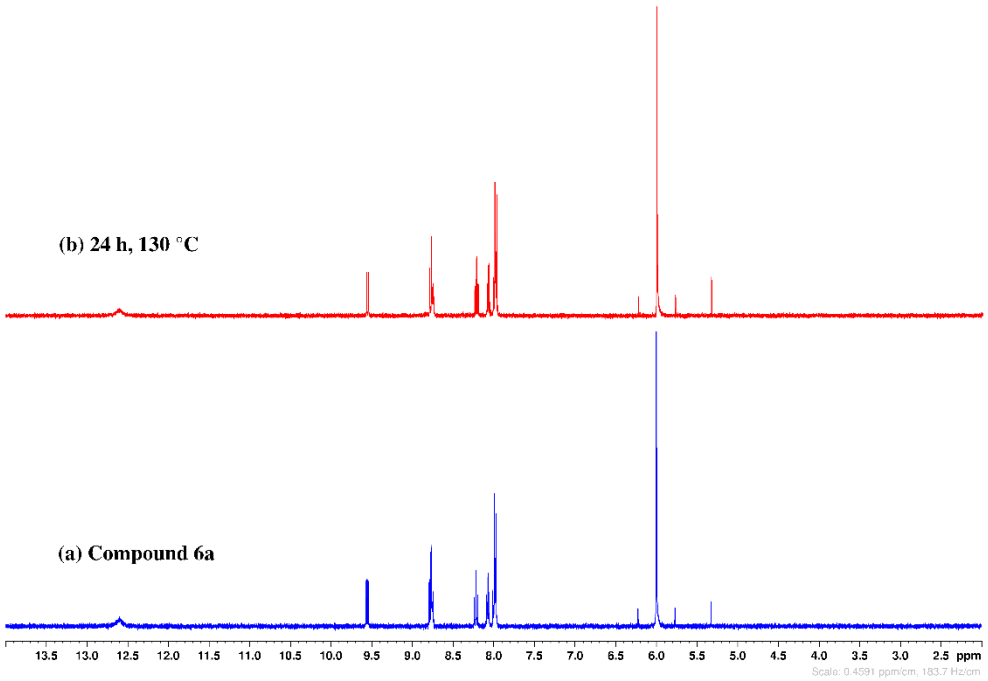
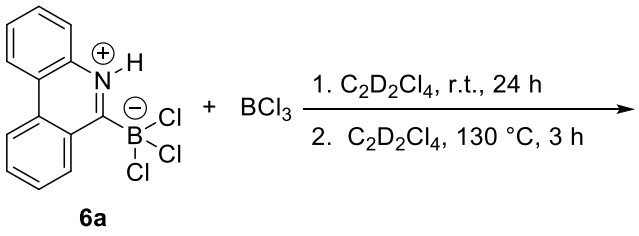


Figure S51: ^{1}H NMR spectra (400 MHz, TCE-d2, 298 K) of (a) compound **6a** and (b) compound **6a** after heating at 130 ℃ for 24 h.

5.3



6a

In an inert atmosphere glovebox, compound **6a** (0.0038 g, 0.013 mmol, 1 equiv.) was dissolved in 0.8 mL 1,1,2,2-Tetrachloroethane-d2 in an NMR tube equipped with septum. The NMR tube was removed from the glovebox and BCl_3 (0.013 mL 1M Hexanes solution, 0.013 mmol, 1 equiv.) was added dropwise to compound **6a** solution at room temperature using a nitrogen-flushed syringe. ^{1}H NMR spectra were collected after 24 h at room temperature, and after a subsequent 3 h at 130 °C.

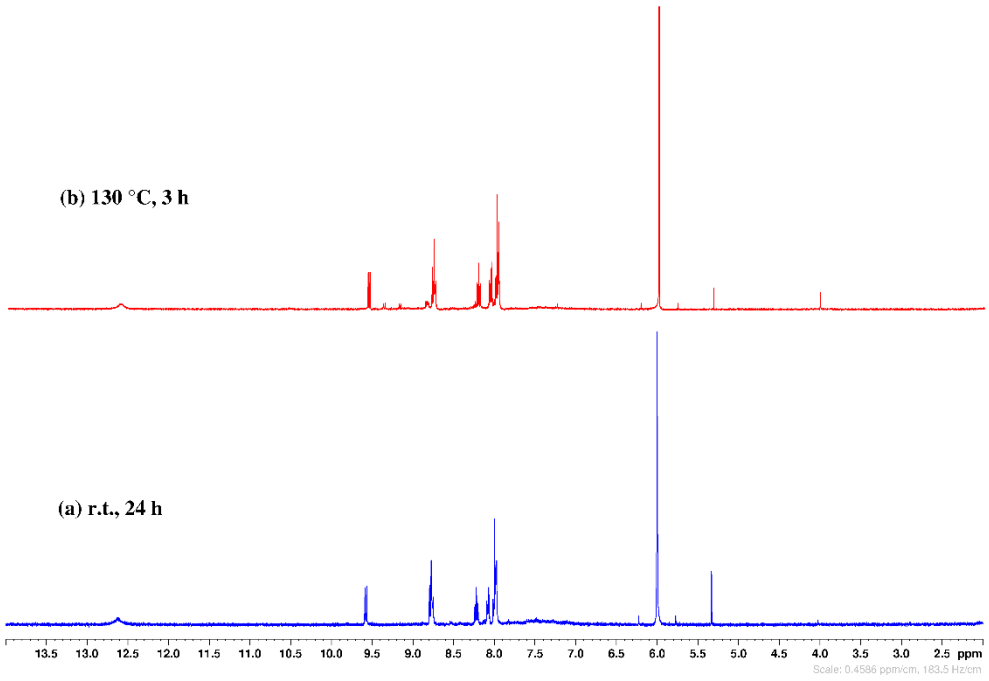
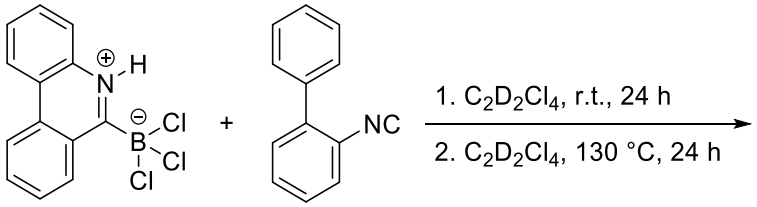


Figure S52: Reaction of compound **6a** and BCl_3 measured by ^1H NMR spectroscopy (400 MHz, TCE-d2, 298 K) after (a) 24 h at room temperature and (b) after a subsequent 3 h at 130 °C.

5.4



6a

In an inert atmosphere glovebox, compound **6a (**0.0017 g, 0.0057 mmol, 1 equiv.) was dissolved in 0.4 mL 1,1,2,2-tetrachloroethane-d2. A solution of 2-isocyanobiphenyl (0.0010 g, 0.0056 mmol, 1 equiv.) in 0.4 mL 1,1,2,2-tetrachloroethane-d2 was added dropwise to the compound **6a** solution. The reaction mixture was transferred to a J-

Young NMR tube. After 24 h at room temperature, a ^{1}H NMR spectrum was collected. The reaction mixture was then heated at 130 °C for 24h, and an additional ^{1}H NMR spectrum was collected.

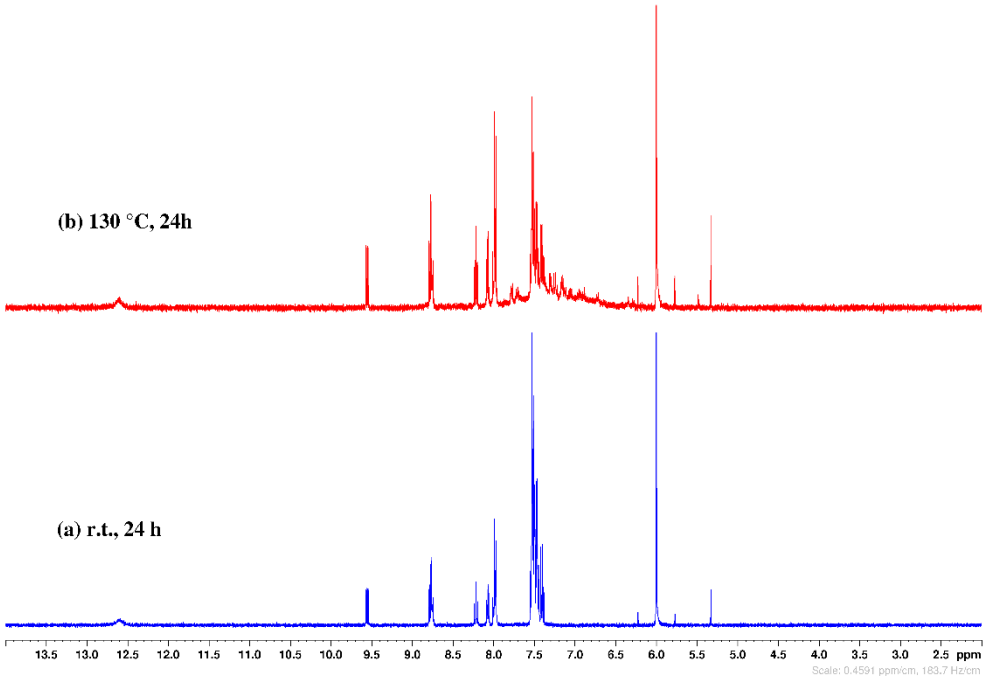


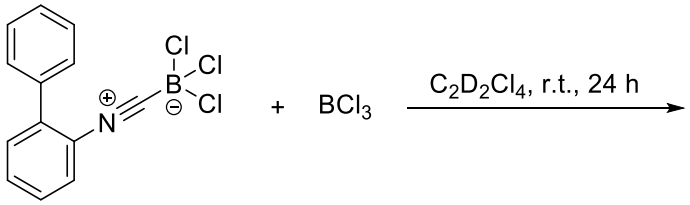
Figure S53: Reaction of compound **6a** and 2-isocyanobiphenyl measured by ^{1}H NMR spectroscopy (400 MHz, TCE-d2, 298 K) after (a) 24 h at room temperature and (b) after a subsequent 24 h at 130 °C.

5.5 - 5.6

We performed ^{1}H NMR experiments in $C_2D_2Cl_4$ between **3** and BCl_3, as well as between **3** and 2-isocyanobiphenyl, at room temperature for 24 h, followed by heating at 130 °C for 2 h (Figures S54 and S55). While the **3** was largely unreactive toward BCl_3 under these conditions, it reacted readily with 2-isocyanobiphenyl at room temperature. ^{1}H NMR spectra of the latter product mixture did not indicate formation

of **6a** or **6b**. Production of **6a** or **6b** is also not observed after further addition of BCl_3 to this mixture, either after 24 h at room temperature or after heating for an additional two hours at 130 °C. These results suggest that sequential reactions of **3** with BCl_3 then 2-isocyanobiphenyl, or with 2-isocyanobiphenyl then BCl_3, do not lead to **6b**.

5.5



3

In an inert atmosphere glovebox, compound **3** (0.0057 g, 0.019 mmol, 1 equiv.) was dissolved in 0.8 mL 1,1,2,2-tetrachloroethane-d2 in an NMR tube equipped with septum. The NMR tube was removed from the glovebox and BCl_3 (0.019 mL 1M Hexanes solution, 0.019 mmol, 1 equiv.) was added dropwise to the compound **3** solution at room temperature using a nitrogen-flushed syringe. ^1H NMR spectra were measured after 0.5 h and 24 h at room temperature.

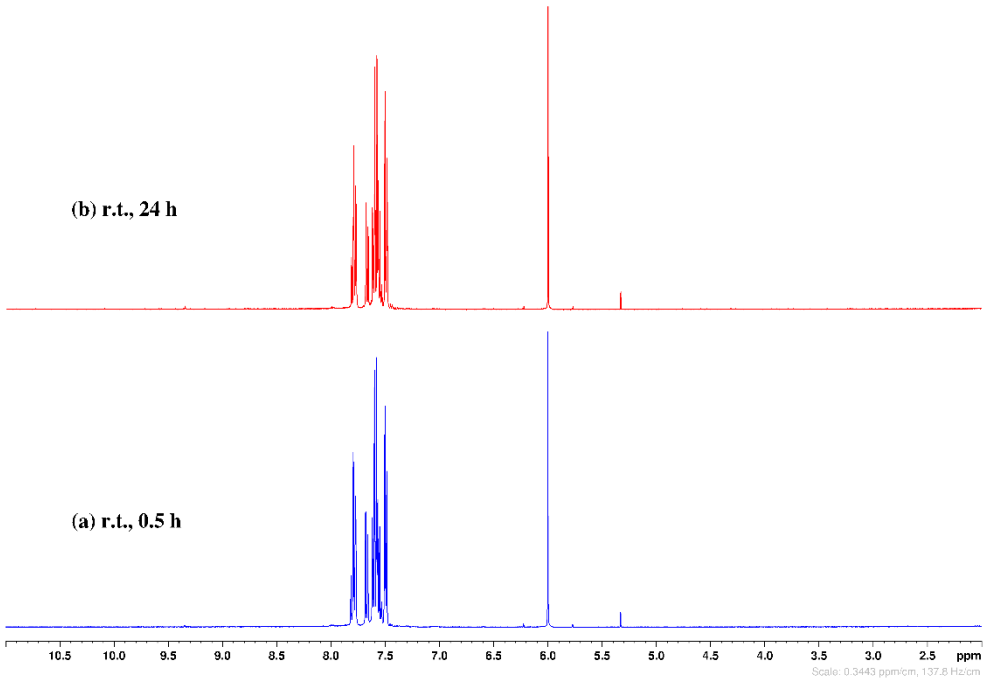
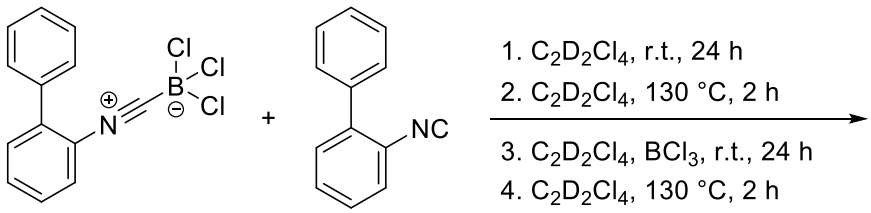


Figure S54: Reaction of compound **3** and BCl_3 measured by ^1H NMR spectroscopy (400 MHz, TCE-d2, 298 K) after (a) 0.5 h at room temperature and (b) after 24 h at room temperature.

5.6



3

In an inert atmosphere glovebox, compound **3** (0.0041 g, 0.014 mmol, 1 equiv.) was dissolved in 0.3 mL 1,1,2,2-tetrachloroethane-d2. 2-isocyanobiphenyl (0.0025 g, 0.014 mmol, 1 equiv.) was dissolved in 0.3 mL 1,1,2,2-tetrachloroethane-d2 and added

dropwise to compound **3** solution. The reaction mixture was transferred to an NMR tube. ^{1}H NMR spectra were collected after 24 h at room temperature, and after a subsequent 2 h at 130 °C. To this sample, BCl_3 (0.014 mL 1M Hexanes solution, 0.014 mmol, 1 equiv.) was added dropwise at room temperature using a nitrogen-flushed syringe. ^{1}H NMR spectra were collected after 24 h at room temperature, and after a subsequent 2 h at 130 °C.

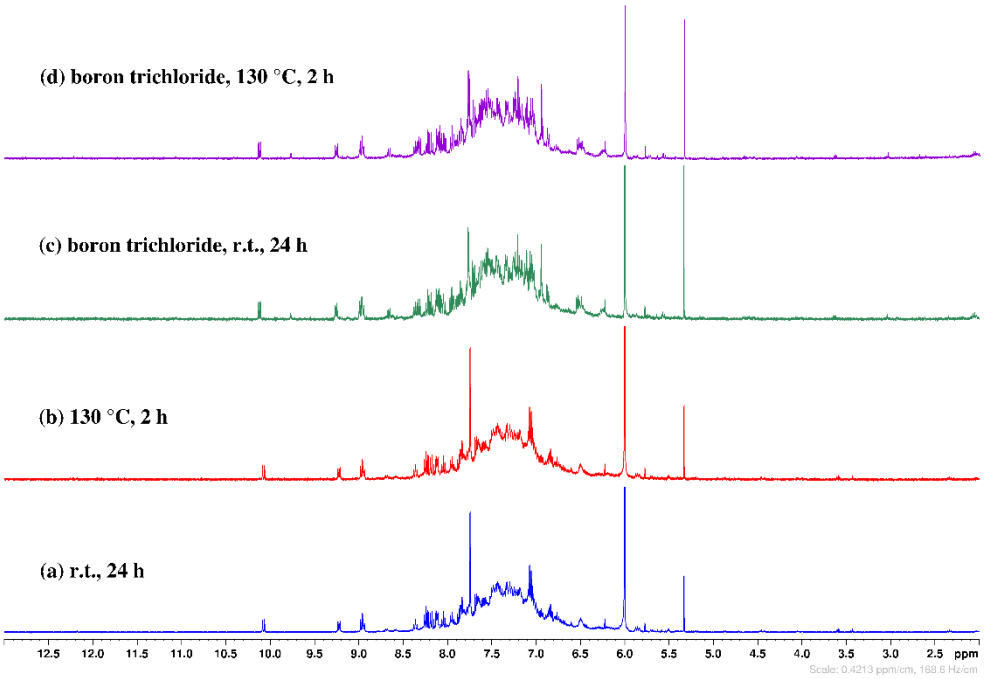


Figure S55: Reaction of compound **3** and 2-isocyanobiphenyl measured by ^{1}H NMR spectroscopy (400 MHz, TCE-d2, 298 K) after (a) 24 h at room temperature, (b) after a subsequent 2 h at 130 °C, (c) further reacted with boron trichloride at room temperature for 24 h and (d) after a subsequent 2 h at 130 °C.

6. EPR spectra

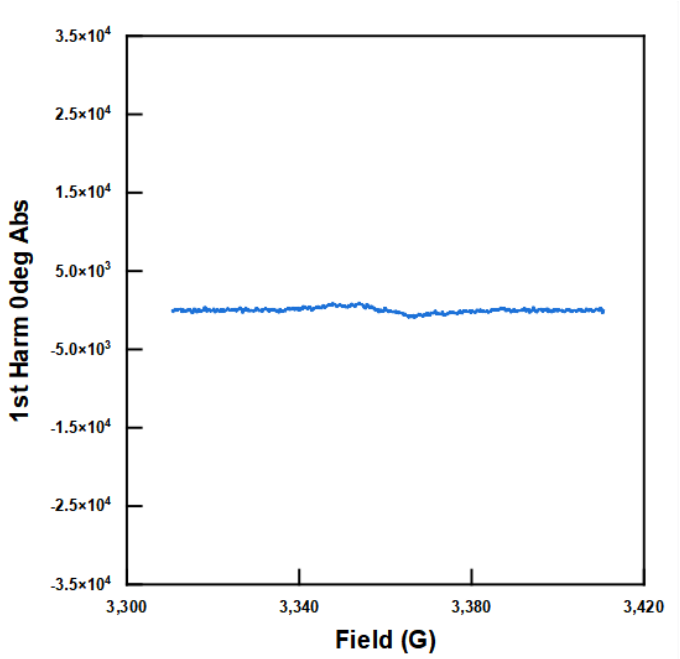


Figure S56: EPR spectrum ($C_2H_2Cl_4$, ν = 9423.24 MHz, 298 K) of compound **1** (0.015 M).

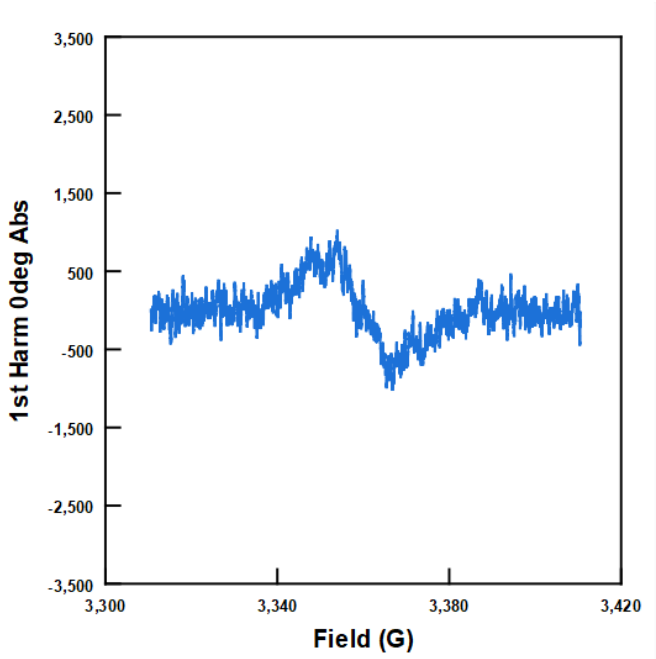


Figure S57: Magnified EPR spectrum ($C_2H_2Cl_4$, ν = 9423.24 MHz, 298 K) of compound **1** (0.015 M).

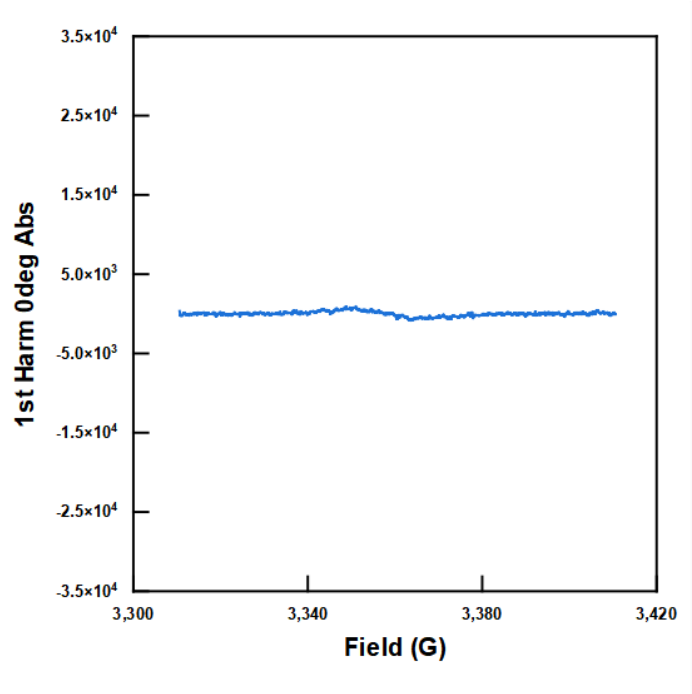


Figure S58: EPR spectrum ($C_2H_2Cl_4$, ν = 9418.99 MHz, 373 K) of compound **1** (0.015 M) at 373 K for 10 minutes.

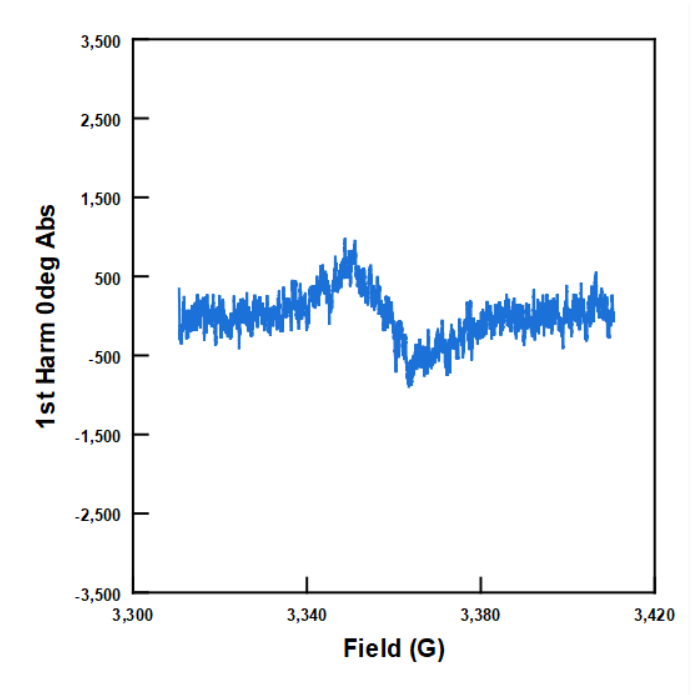


Figure S59: Magnified EPR spectrum ($C_2H_2Cl_4$, ν = 9418.99 MHz, 373 K) of compound **1** (0.015 M) at 373 K for 10 minutes.

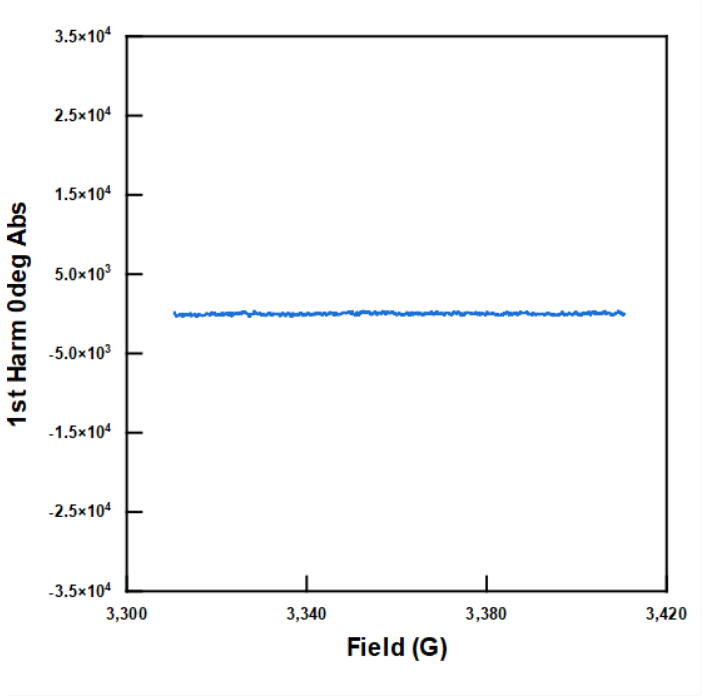


Figure S60: EPR spectrum ($C_2H_2Cl_4$, ν = 9422.97 MHz, 298 K) of compound **2** (0.013 M).

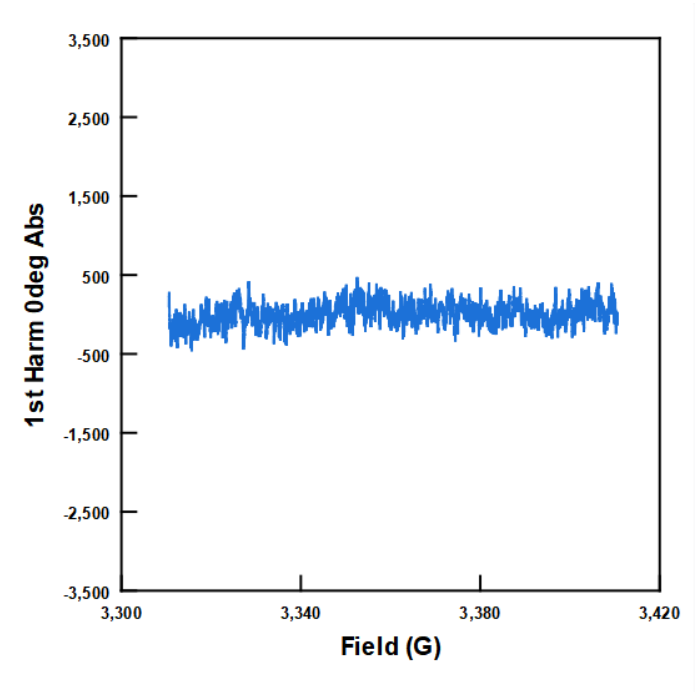


Figure S61: Magnified EPR spectrum ($C_2H_2Cl_4$, ν = 9422.97 MHz, 298 K) of compound **2** (0.013 M).

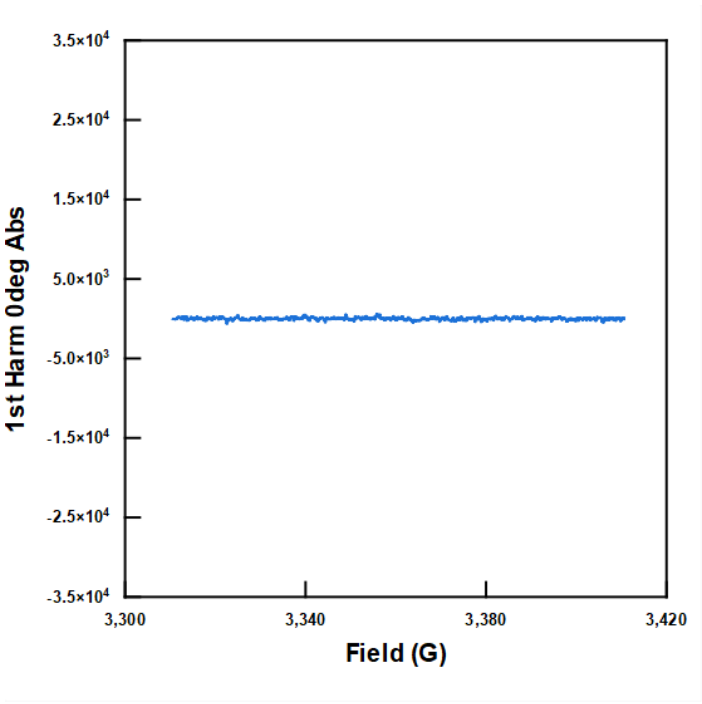


Figure S62: EPR spectrum ($C_2H_2Cl_4$, ν = 9419.38 MHz, 373 K) of compound **2** (0.013 M) at 373 K for 10 minutes.

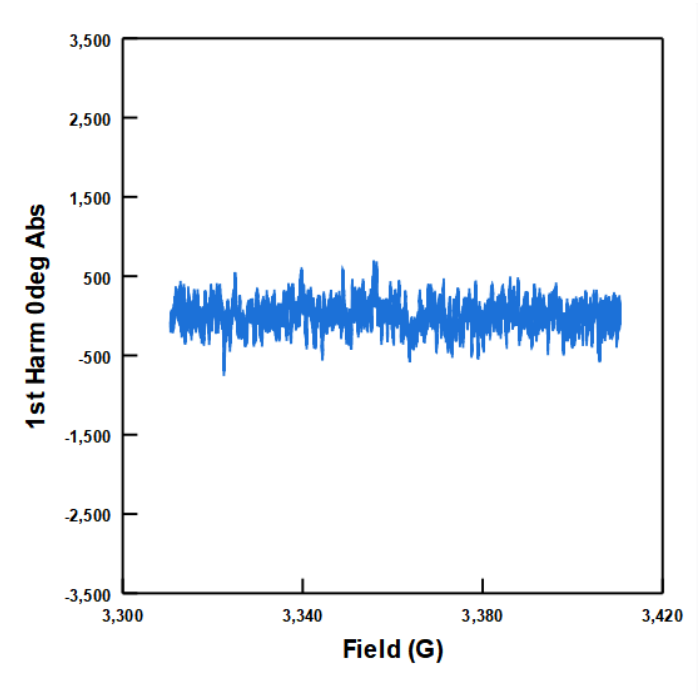


Figure S63: Magnified EPR spectrum ($C_2H_2Cl_4$, ν = 9419.38 MHz, 373 K) of compound **2** (0.013 M) at 373 K for 10 minutes.

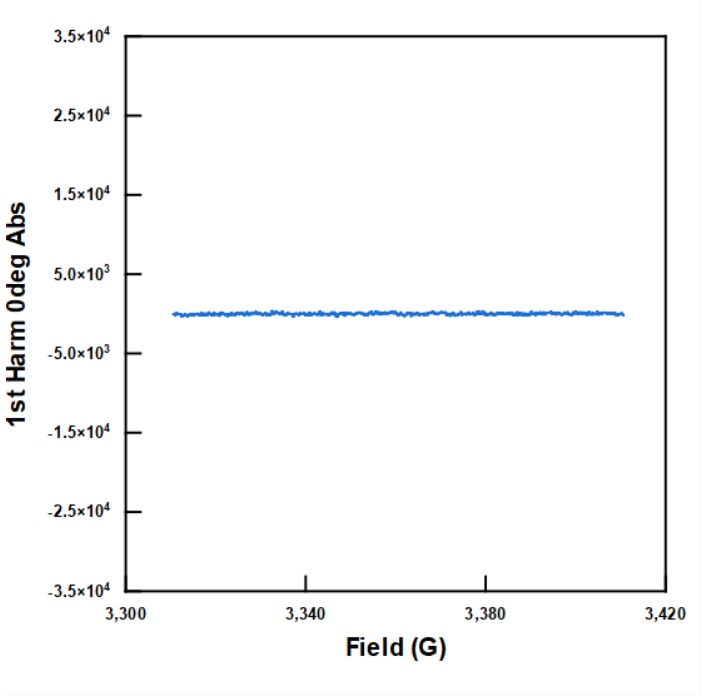


Figure S64: EPR spectrum ($C_2H_2Cl_4$, ν = 9423.05 MHz, 298 K) of compound **3** (0.016 M).

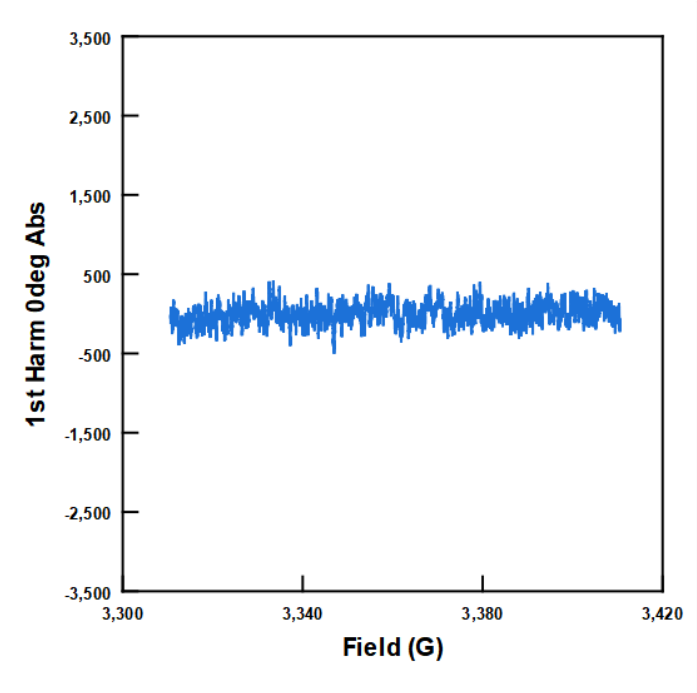


Figure S65: Magnified EPR spectrum ($C_2H_2Cl_4$, ν = 9423.05 MHz, 298 K) of compound **3** (0.016 M).

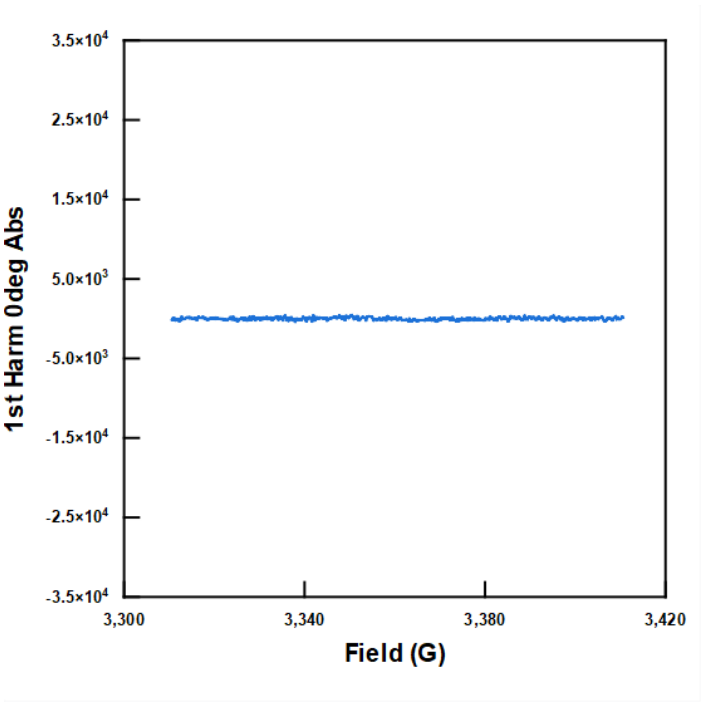


Figure S66: EPR spectrum ($C_2H_2Cl_4$, ν = 9418.02 MHz, 373 K) of compound **3** (0.016 M) at 373 K for 10 minutes.

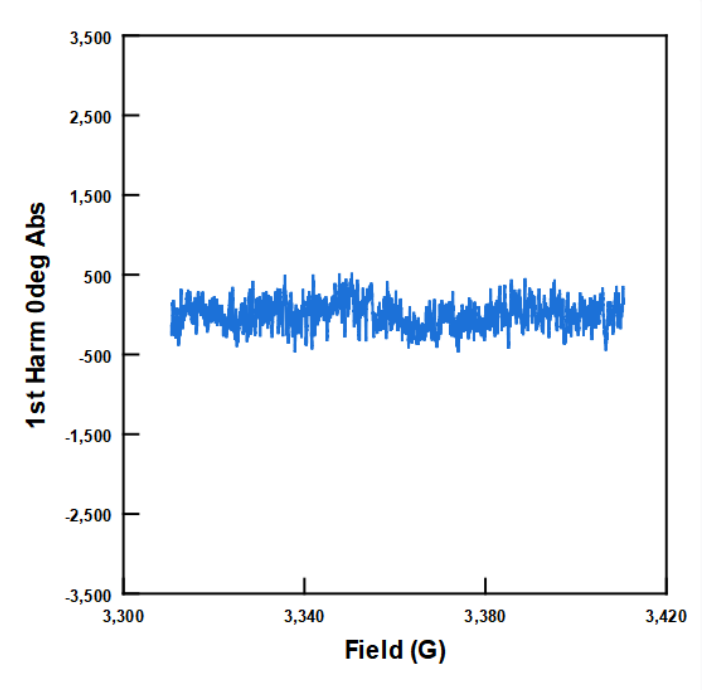


Figure S67: Magnified EPR spectrum ($C_2H_2Cl_4$, ν = 9418.02 MHz, 373 K) of compound **3** (0.016 M) at 373 K for 10 minutes.

7. X-ray crystallography

Crystal Data for **1** ($C_{13}H_9BI_3N$)：Mr = 570.72, 0.150 x 0.080 x 0.050 mm^3 , Monoclinic space group $P2_1/n$, a = 8.5624(3) Å, α = 90°, b = 10.9109(4) Å, β = 93.5760(15)°, c = 16.6083(6) Å, γ = 90°, V = 1548.58(10) $Å^3$, Z = 4, ρ(calcd) = 2.448 Mg/m^3 , μ = 6.037 mm^{-1} , F(000) = 1032, GooF(F^2) = 0.687, R_1 = 0.0200, wR^2 = 0.0756 for I>2σ(I), R_1 = 0.0219, wR^2 = 0.0805 for all data, 4748 unique reflections[θ ≤ 25.242°] with a completeness of 99.9% and 163 parameters, 0 restraints.

Crystal Data for **2** ($C_{13}H_9BBr_3N$): Mr = 429.75, 0.150 x 0.100 x 0.050 mm^3 , Monoclinic space group $P2_1/n$, a = 9.0581(4) Å, α = 90°, b = 10.2611(5) Å, β = 96.2352(13)°, c = 15.6575(7) Å, γ = 90°, V = 1446.69(12) $Å^3$, Z = 4, ρ(calcd) = 1.973 Mg/m^3 , μ = 10.172 mm^{-1} , F(000) = 816, GooF(F^2) = 1.066, R_1 = 0.0227, wR^2 = 0.0587 for I>2σ(I), R_1 = 0.0244, wR^2 = 0.0591 for all data, 2730 unique reflections[θ ≤ 67.679°] with a completeness of 99.6% and 163 parameters, 0 restraints.

Crystal Data for **3** ($C_{13}H_9BCl_3N$): Mr = 296.37, 0.200 x 0.100 x 0.020 mm^3 , Monoclinic space group $P2_1/n$, a = 9.3124(6) Å, α = 90°, b = 9.8992(6) Å, β = 98.038(2)°, c = 14.9871(8) Å, γ = 90°, V = 1368.02(14) $Å^3$, Z = 4, ρ(calcd) = 1.439 Mg/m^3 , μ = 0.648 mm^{-1} , F(000) = 600, GooF(F^2) = 1.031, R_1 = 0.0317, wR^2 = 0.0863 for I>2σ(I), R_1 = 0.0371, wR^2 = 0.0917 for all data, 3550 unique reflections[θ ≤ 25.242°] with a completeness of 100.0% and 163 parameters, 0 restraints.

Crystal Data for **4a** ($C_{13}H_9BI_3N$): Mr = 570.72, 0.150 x 0.100 x 0.080 mm^3 , Monoclinic

space group $P2_1/c$, a = 9.7914(6) Å, α = 90°, b = 10.8546(6) Å, β = 103.1323(19)°, c = 14.0091(8) Å, γ = 90°, V = 1449.97(15) $Å^3$, Z = 4, ρ(calcd) = 2.614 Mg/m^3 , μ = 6.447 mm^{-1} , F(000) = 1032, GooF(F^2) = 0.858, R_1 = 0.0241, wR^2 = 0.0958 for I>2σ(I), R_1 = 0.0249, wR^2 = 0.0978 for all data, 4361 unique reflections[θ ≤ 25.242°] with a completeness of 98.1% and 166 parameters, 0 restraints.

Crystal Data for **5a** ($C_{13}H_9BBr_3N$): Mr = 429.75, 0.150 x 0.025 x 0.010 mm^3 , Triclinic space group P-1, a = 7.1182(3) Å, α = 89.6056(14)°, b = 10.1195(5) Å, β = 88.8595(13)°, c = 18.3253(9) Å, γ = 89.3333(14)°, V = 1319.64(11) $Å^3$, Z = 4, ρ(calcd) = 2.163 Mg/m^3 , μ = 11.151 mm^{-1} , F(000) = 816, GooF(F^2) = 1.071, R_1 = 0.0261, wR^2 = 0.0692 for I>2σ(I), R_1 = 0.0265, wR^2 = 0.0696 for all data, 5088 unique reflections[θ ≤ 67.679°] with a completeness of 98.5% and 333 parameters, 0 restraints.

Crystal Data for **6a** ($C_{13}H_9BCl_3N$): Mr = 296.37, 0.100 x 0.100 x 0.050 mm^3 , Orthorhombic space group $Pna2_1$, a = 17.5560(6) Å, α = 90°, b = 13.5459(5) Å, β = 90°, c = 10.4412(3) Å, γ = 90°, V = 2483.04(14) $Å^3$, Z = 8, ρ(calcd) = 1.586 Mg/m^3 , μ = 6.479 mm^{-1} , F(000) = 1200, GooF(F^2) = 1.378, R_1 = 0.0847, wR^2 = 0.2433 for I>2σ(I), R_1 = 0.0850, wR^2 = 0.2434 for all data, 4650 unique reflections[θ ≤ 67.679°] with a completeness of 99.9% and 326 parameters, 376 restraints.

Crystal Data for **6b** ($C_{26}H_{16}B_2Cl_6N_2$): Mr = 590.73, 0.200 x 0.120 x 0.080 mm^3 , Monoclinic space group $P2_1/c$, a = 16.4478(6) Å, α = 90°, b = 10.7938(4) Å, β = 90.3459(13)°, c = 13.9976(5) Å, γ = 90°, V = 2485.01(16) $Å^3$, Z = 4, ρ(calcd) = 1.579

Mg/m^3 , $\mu = 0.713\ mm^{-1}$, F(000) = 1192, $GooF(F^2) = 1.051$, $R_1 = 0.0313$, $wR^2 = 0.0832$ for $I>2\sigma(I)$, $R_1 = 0.0349$, $wR^2 = 0.0863$ for all data, 7581 unique reflections[$\theta \leq 25.242°$] with a completeness of 99.9% and 325 parameters, 0 restraints.

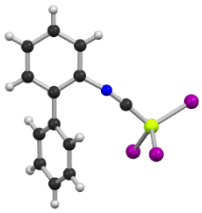


Figure S68: Solid-state structure of **1**. C: black, N: blue, B: yellow-green, I: purple, H: grey.

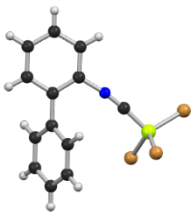


Figure S69: Solid-state structure of **2**. C: black, N: blue, B: yellow-green, Br: brown, H: grey.

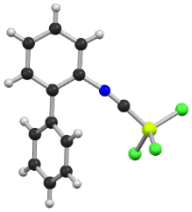


Figure S70: Solid-state structure of **3**. C: black, N: blue, B: yellow-green, Cl: green, H: grey.

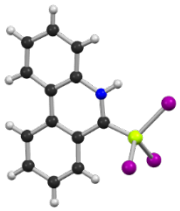


Figure S71: Solid-state structure of **4a**. C: black, N: blue, B: yellow-green, I: purple, H: grey.

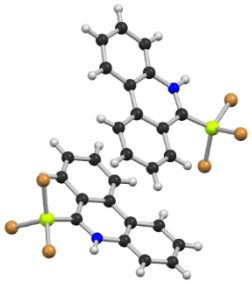


Figure S72: Solid-state structure of **5a**. C: black, N: blue, B: yellow-green, Br: brown, H: grey.

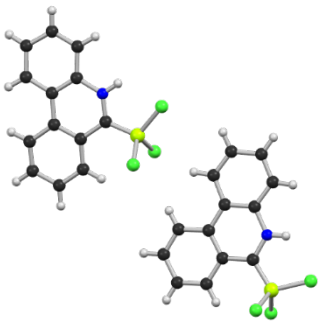


Figure S73: Solid-state structure of **6a**. C: black, N: blue, B: yellow-green, Cl: green, H: grey.

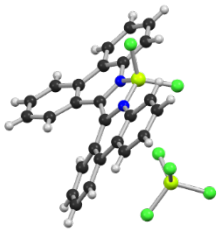


Figure S74: Solid-state structure of **6b**. C: black, N: blue, B: yellow-green, Cl: green, H: grey.

8. Computational details

Density Functional Theory (DFT) calculations were performed using Gaussian 16.[3] The B3LYP[4] functional with D3 dispersion corrections and Becke-Johnson damping[5] (B3LYP-D3BJ) was applied. Geometry optimizations and vibrational frequency analyses were conducted with the def2-SVP[6] basis set, a double-ζ quality basis. To confirm the nature of the stationary points, local minima were verified by the absence of imaginary frequencies, while transition states were characterized by a single imaginary frequency. Solvation free energy in tetrachloroethane was estimated within the conductor-like polarizable continuum model (CPCM).[7] For improved accuracy in electronic energy evaluations, the triple-ζ quality def2-TZVP[6] basis set was employed.

The Gibbs free energies were determining through the equation:

$$G = E_{elec} + G_{solv} + ZPE + H_{vib} + 4RT - TS$$

where E_{elec} denotes the electronic energy, G_{solv} represents the solvation free energy, ZPE corresponds to the zero-point vibrational energy, and H_{vib} includes the vibrational contribution to enthalpy. The term 4RT accounts for both translational and rotational thermal corrections, as well as the additional PV term.

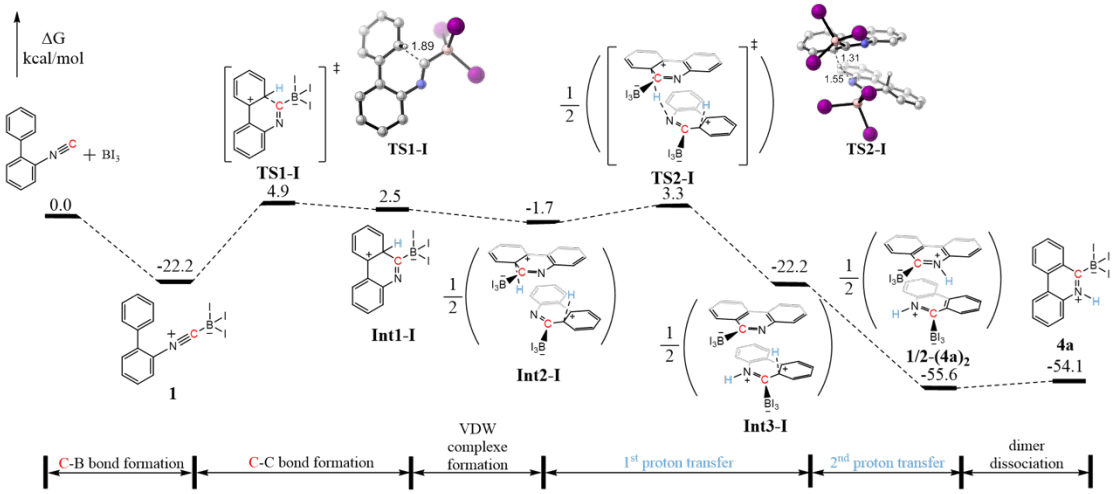


Figure S75. DFT-calculated Gibbs free energy profile of the formation of **4a**. The structures were optimized in CPCM solvation model in $C_2H_2Cl_4$.

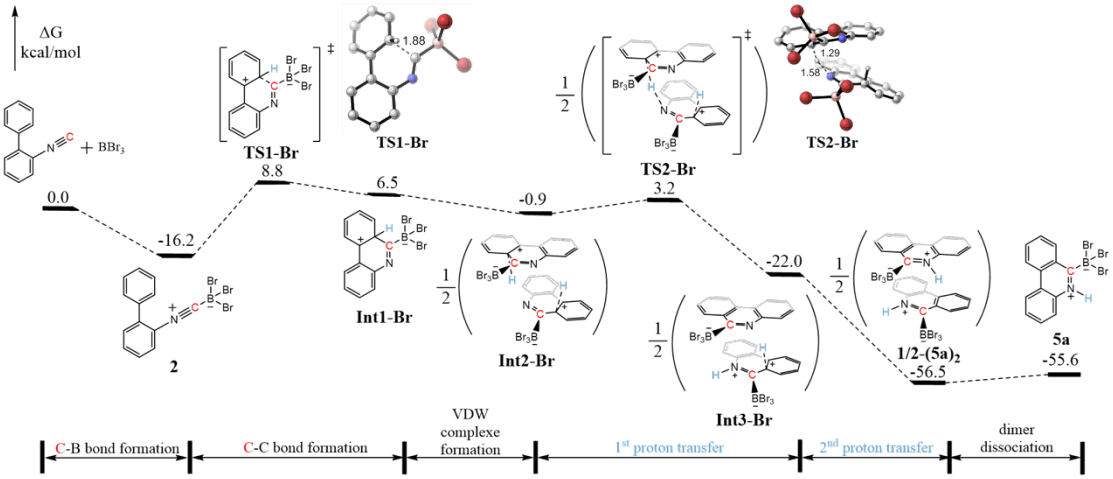


Figure S76. DFT-calculated Gibbs free energy profile of the formation of **5a**. The structures were optimized in CPCM solvation model in $C_2H_2Cl_4$.

Computed Gibbs free energy for each species:

Species	E_{elec}	$ZPE+H_{vib}+4RT-TS+G_{solv}$	G_{total}
2-isocyanobiphenyl	-555.7725	0.1429	-555.6296
BCl_3	-1405.6759	-0.0200	-1405.6959
3	-1961.4854	0.1428	-1961.3426
TS1-Cl	-1961.4504	0.1463	-1961.3041
Int1-Cl	-1961.4538	0.1465	-1961.3073
Int2-Cl	-3922.9302	0.3143	-3922.6159
TS2-Cl	-3922.9203	0.3157	-3922.6046
Int3-Cl	-3923.0067	0.3233	-3922.6834
1/2-$(6a)_2$	-3923.1242	0.3289	-3922.7953
6a	-1961.5488	0.1519	-1961.3969
BBr_3	-7747.5235	-0.0257	-7747.5492
2	-8303.3431	0.1384	-8303.2047
TS1-Br	-8303.3064	0.1416	-8303.1648
Int1-Br	-8303.3106	0.1421	-8303.1685
Int2-Br	-16606.6450	0.3051	-16606.3399
TS2-Br	-16606.6331	0.3064	-16606.3267
Int3-Br	-16606.7201	0.3132	-16606.4069

1/2-$(5a)_2$	-16606.8355	0.3186	-16606.5169
5a	-8303.4038	0.1469	-8303.2569
BI_3	-918.3579	-0.0286	-918.3865
1	-1474.1869	0.1355	-1474.0514
TS1-I	-1474.1465	0.1382	-1474.0083
Int1-I	-1474.1510	0.1389	-1474.0121
Int2-I	-2948.3287	0.2991	-2948.0296
TS2-I	-2948.3138	0.3000	-2948.0138
Int3-I	-2948.4009	0.3058	-2948.0951
1/2-$(4a)_2$	-2948.5126	0.3114	-2948.2012
4a	-1474.2418	0.1436	-1474.0982
TS3-Cl	-1961.4268	0.1439	-1961.2830
Int4-Cl	-1961.5196	0.1454	-1961.3742

Coordinates of optimized structures

2-isocyanobiphenyl

C	-0.84784900	-0.29517700	0.05703300
C	-1.53652800	0.65548900	0.83079900
C	-2.93185700	0.69933600	0.82594500
C	-3.66275300	-0.20280300	0.04632500
C	-2.98868300	-1.15441800	-0.72486300
C	-1.59304500	-1.20217400	-0.71720800
C	0.63456100	-0.38021700	0.07321800

C	1.46732500	0.74781200	-0.11569800
C	2.86641200	0.63578800	-0.09293200
C	3.46116300	-0.60642800	0.11300600
C	2.65800400	-1.73737800	0.28974000
C	1.26799800	-1.61898800	0.26782800
H	-0.97728700	1.35474600	1.45414800
H	-3.45092200	1.44002600	1.43870100
H	-4.75454100	-0.16479400	0.04097200
H	-3.55122800	-1.86122300	-1.33930200
H	-1.07118100	-1.93986000	-1.33071100
H	3.46931800	1.53140200	-0.24835800
H	4.54944400	-0.69033900	0.13218900
H	3.11555100	-2.71548600	0.45212700
H	0.64647500	-2.50266500	0.42387700
C	0.47253000	3.05768000	-0.59488200
N	0.91724300	1.99386500	-0.36764300

BCl_3

B	0.00000000	0.00000000	0.00000000
Cl	0.00000000	1.74982000	0.00000000

Cl	-1.51538900	-0.87491000	0.00000000
Cl	1.51538900	-0.87491000	0.00000000

3

C	-1.89422000	1.01550800	0.09071100
C	-0.88134900	1.46474100	0.95684600
C	-0.47382900	2.79931900	0.94101600
C	-1.07934100	3.70931500	0.06963700
C	-2.09835900	3.27720800	-0.78520900
C	-2.50322300	1.94138000	-0.77564100
C	-2.33128000	-0.40203400	0.07521400
C	-1.41547600	-1.48059500	0.00991300
C	-1.82737600	-2.82132400	-0.01902700
C	-3.18719400	-3.11347000	0.01358700
C	-4.11772800	-2.06963600	0.06714400
C	-3.69325300	-0.74031900	0.09552400
H	-0.41040200	0.77640100	1.65956300
H	0.32451900	3.12292600	1.61184900
H	-0.75740400	4.75302400	0.05576200

H	-2.57445900	3.98152300	-1.47109500
H	-3.28278900	1.60475000	-1.46224300
H	-1.07655400	-3.61018300	-0.07493100
H	-3.51949800	-4.15265900	-0.00553800
H	-5.18606700	-2.29342400	0.09340000
H	-4.42935300	0.06311600	0.15413000
C	1.05075100	-0.89723200	-0.10932900
N	-0.06228700	-1.20963100	-0.06287000
B	2.56544700	-0.37671800	-0.09019200
Cl	2.78246400	0.66899400	-1.60054600
Cl	2.70014800	0.61684400	1.47783500
Cl	3.64868400	-1.87358100	-0.08035700

TS1-Cl

C	0.55409100	3.31199300	-0.01783200
C	0.86366000	2.13769200	0.64257600
C	-0.08192300	1.06042100	0.70888500
C	-1.39760900	1.26659100	0.14554000
C	-1.68766900	2.46576500	-0.50221200

C	-0.72133900	3.47482500	-0.58264500
C	0.48461300	-0.53541000	-0.02956200
C	-2.33169100	0.14327200	0.14896200
C	-1.80729000	-1.15650400	-0.09113100
C	-2.66052800	-2.25572200	-0.22011100
H	-2.22569800	-3.23349500	-0.43081000
C	-4.03847600	-2.08651900	-0.07479900
C	-4.56644100	-0.81511200	0.17479700
C	-3.72074400	0.29163600	0.27220800
H	1.28716600	4.11763500	-0.08046700
H	1.81869900	2.01754100	1.15142000
H	-2.66236600	2.60718200	-0.97129100
H	-0.96680400	4.40591900	-1.09862600
H	-4.70235600	-2.94882300	-0.16122800
H	-5.64380000	-0.68336900	0.29204800
H	-4.13626900	1.28001600	0.47697700
N	-0.43443300	-1.32140900	-0.25714600
B	2.10672200	-0.70534500	-0.05020300
Cl	2.82664300	0.58508600	-1.18527900

Cl	2.69574200	-0.47706500	1.71519700
H	-0.03883100	0.50610000	1.66201900
Cl	2.50383700	-2.40859100	-0.66151000

Int1-Cl

C	0.34427800	3.41082100	-0.09972300
C	0.84332300	2.18620000	0.25022500
C	-0.03712200	1.01590500	0.40157300
C	-1.47284700	1.22209700	0.11114200
C	-1.93400500	2.50304900	-0.21067200
C	-1.04500700	3.56641600	-0.32329500
C	0.50260400	-0.40729500	0.00566500
C	-2.32416100	0.06151900	0.12397500
C	-1.70244100	-1.20888700	-0.07003600
C	-2.50307400	-2.35671800	-0.19240300
H	-2.00392100	-3.31160400	-0.36184600
C	-3.88616300	-2.26519300	-0.08709700
C	-4.50318100	-1.01882400	0.12645700
C	-3.73294800	0.13088300	0.21741800

H	1.00772400	4.27214700	-0.18863000
H	1.89265300	2.06306100	0.50671500
H	-2.99028200	2.66538000	-0.42289800
H	-1.43209700	4.55151900	-0.59448400
H	-4.49751500	-3.16629000	-0.16991500
H	-5.58865500	-0.95581900	0.22181600
H	-4.21692400	1.09135400	0.39905900
N	-0.32939800	-1.35480800	-0.19331800
B	2.10690700	-0.65844200	-0.01487100
Cl	2.81297300	0.40532400	-1.40587900
Cl	2.79148500	-0.10397200	1.65906300
H	0.02773200	0.81135300	1.50461200
Cl	2.52948400	-2.43576800	-0.31119600

Int2-Cl

C	4.52041100	-2.54223100	0.49391200
C	3.24038200	-2.21702200	0.14400900
C	2.84830100	-0.81632200	-0.09977800
C	3.93342700	0.19204400	-0.07292600

C	5.21693900	-0.19339500	0.33167900
C	5.50194600	-1.52569600	0.60290000
C	1.67881000	-0.50818300	-1.06974500
C	3.60702100	1.52836600	-0.48624700
C	2.43514300	1.70062600	-1.28319500
C	2.14238900	2.96807800	-1.81547300
H	1.25598500	3.06441100	-2.44271200
C	2.95123100	4.05848100	-1.52045000
C	4.08585700	3.90277200	-0.70085000
C	4.41903100	2.65182100	-0.20538400
H	4.78859400	-3.57894100	0.70168600
H	2.45885500	-2.97292700	0.12085400
H	6.01714000	0.54367600	0.38596700
H	6.51783400	-1.79878300	0.89798700
H	2.70339200	5.04319000	-1.92206100
H	4.70599200	4.76721200	-0.45775600
H	5.29411300	2.54324600	0.43598400
N	1.56462000	0.66513100	-1.57363600
B	0.57873800	-1.65443500	-1.38920300

Cl	1.43064100	-2.93799500	-2.45709700
Cl	-0.04402500	-2.41529300	0.21092800
H	2.26835700	-0.59155100	0.84279800
Cl	-0.88349900	-0.93474600	-2.31611000
C	-2.92821100	2.88589700	-1.41012200
C	-3.12349500	1.65182200	-0.84859100
C	-2.13648000	1.06769600	0.06655900
C	-0.99389700	1.92015500	0.44656700
C	-0.83430600	3.16764800	-0.16751600
C	-1.78017400	3.63786400	-1.07078800
C	-2.57809500	0.03639400	1.12084600
C	-0.08491500	1.40425400	1.43655500
C	-0.52257900	0.29200500	2.21314700
C	0.33421900	-0.24284300	3.19430900
H	-0.02503000	-1.09642800	3.76991100
C	1.59549700	0.29861600	3.40125000
C	2.02100100	1.41614600	2.65490400
C	1.18593600	1.96899100	1.69680400
H	-3.65115800	3.28847900	-2.12091500

H	-3.96389400	1.02948000	-1.14659700
H	0.01697600	3.79728400	0.08474300
H	-1.63168800	4.61890200	-1.52820200
H	2.25870100	-0.13587900	4.15205700
H	3.01083800	1.84315300	2.82441900
H	1.52971700	2.82707800	1.12150300
N	-1.78004900	-0.26771100	2.08197400
B	-4.02894400	-0.68232800	1.00218000
Cl	-5.31689500	0.69490000	1.20810700
Cl	-4.19736200	-1.47751600	-0.69912400
H	-1.66214400	0.31492200	-0.67263900
Cl	-4.28369100	-1.96918300	2.31351200

TS2-Cl

C	4.42154400	-2.42862500	0.73725400
C	3.11267700	-2.33013900	0.35714900
C	2.51342100	-1.01851700	0.03460300
C	3.44287200	0.13388700	-0.07333200
C	4.76134900	-0.02457600	0.36989200

C	5.23538700	-1.27061700	0.76103100
C	1.22435800	-0.94971700	-0.76384700
C	2.93980200	1.35650200	-0.63495200
C	1.64334600	1.33651700	-1.22160500
C	1.16674000	2.47403500	-1.88870600
H	0.19137300	2.42921800	-2.37182300
C	1.93110800	3.63273800	-1.93491300
C	3.19443200	3.67703900	-1.31926300
C	3.69698400	2.55003300	-0.68975400
H	4.83932100	-3.39354600	1.02670300
H	2.44887000	-3.19001700	0.40314800
H	5.44694200	0.82075500	0.36655600
H	6.27525400	-1.35941200	1.08392600
H	1.54506100	4.51372800	-2.45110900
H	3.78498700	4.59410100	-1.34712800
H	4.68240800	2.59288100	-0.22788400
N	0.83123500	0.20303900	-1.21530700
B	0.38169400	-2.29629700	-1.10664600
Cl	1.58685300	-3.23764300	-2.23368700

Cl	-0.00386300	-3.30933100	0.42077400
H	2.05332900	-0.82766600	1.06469800
Cl	-1.16250700	-1.90325000	-2.02797800
C	-2.32287900	3.25658600	-1.37925900
C	-2.36638800	1.89465800	-1.18750600
C	-1.55961000	1.25151600	-0.17120300
C	-0.72533800	2.11544400	0.66485400
C	-0.72185200	3.49819600	0.45089500
C	-1.52124200	4.05819100	-0.53949000
C	-2.09402600	0.01649100	0.55119400
C	0.11283400	1.44539600	1.63453300
C	-0.22957300	0.09987700	1.95962900
C	0.60675200	-0.62881800	2.83300400
H	0.33022900	-1.65808600	3.06126900
C	1.74767500	-0.04031600	3.37111500
C	2.07289800	1.29543900	3.06753100
C	1.25821700	2.02963600	2.21653600
H	-2.92807600	3.72130300	-2.15908000
H	-2.99775000	1.26117400	-1.80841500

H	-0.09770400	4.14484600	1.06723700
H	-1.51514000	5.14155900	-0.67874400
H	2.39403700	-0.62002400	4.03334500
H	2.97172400	1.74878600	3.48850900
H	1.53863500	3.05017100	1.95307100
N	-1.40181400	-0.48480600	1.52072300
B	-3.64687000	-0.46482300	0.36518200
Cl	-4.58618800	1.04968500	1.05267300
Cl	-4.24053800	-0.77958400	-1.38813900
H	-0.65296600	0.67574500	-0.86588800
Cl	-4.01961300	-1.96415200	1.39392700

Int3-Cl

C	4.69862600	1.36555000	0.56467400
C	3.86740800	0.29462500	0.39157000
C	2.50515800	0.48497900	-0.12520300
C	2.15130000	1.82281700	-0.65100800
C	3.03906400	2.88088600	-0.41802800
C	4.27716900	2.65769400	0.16928900

C	1.76820900	-0.68920200	-0.67151800
C	0.89616100	1.97807500	-1.33916700
C	0.14961200	0.81602000	-1.66164800
C	-1.06082000	0.89354700	-2.35828000
H	-1.62185800	-0.01767700	-2.56329700
C	-1.53989700	2.13818900	-2.74331600
C	-0.82334200	3.30620500	-2.42836400
C	0.37615500	3.22899100	-1.74085900
H	5.68748700	1.22574800	1.00257300
H	4.14892900	-0.69679900	0.73702100
H	2.77836400	3.89017400	-0.73063300
H	4.94795200	3.50582700	0.32209800
H	-2.48736200	2.20601900	-3.27870100
H	-1.21883100	4.28062900	-2.71802200
H	0.90927600	4.14511600	-1.49227600
N	0.66127700	-0.43946000	-1.31741300
B	2.28457300	-2.22855700	-0.53686900
Cl	3.89399500	-2.25502900	-1.50186800
Cl	2.55058300	-2.63262200	1.26376400

H	1.97569400	0.56467200	0.94244900
Cl	1.06016200	-3.38089000	-1.31200200
C	-4.35907300	1.97803600	-0.69081500
C	-3.79095300	0.77889100	-0.29819900
C	-2.59956200	0.74852100	0.46830100
C	-1.98145400	1.98967500	0.80947100
C	-2.58831700	3.20214700	0.40869000
C	-3.76035000	3.19900300	-0.32634300
C	-1.97385700	-0.50835100	0.88648200
C	-0.72562900	1.95259800	1.53279600
C	-0.21512600	0.67216100	1.87703000
C	1.03122800	0.57703700	2.56117700
H	1.37813300	-0.42162800	2.83231800
C	1.74547200	1.72291900	2.90422700
C	1.24312600	2.98736300	2.54812100
C	0.02994100	3.09575800	1.88128300
H	-5.27600900	1.97661800	-1.28422600
H	-4.26241800	-0.15720000	-0.58340200
H	-2.12768900	4.15434600	0.67057000

H	-4.21359600	4.14453000	-0.63209800
H	2.69827400	1.63671500	3.42995800
H	1.80905500	3.88760000	2.79380700
H	-0.33214800	4.08787300	1.61083000
N	-0.84209200	-0.49977900	1.55267900
B	-2.57816300	-1.97365800	0.51840500
Cl	-4.38600800	-2.13211900	1.03293200
Cl	-2.44984600	-2.17707700	-1.39447900
H	0.11501900	-1.26814200	-1.60909800
Cl	-1.62983400	-3.36364300	1.30538500

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C	-4.53876400	1.66906500	-0.71255300
C	-3.86278800	0.52690100	-0.33093200
C	-2.65225300	0.61368200	0.40431600
C	-2.12339400	1.90264300	0.73015900
C	-2.84265400	3.05047700	0.33258800
C	-4.02941600	2.93654600	-0.37015300
C	-1.94882900	-0.57432700	0.81362500

C	-0.86150900	1.99181700	1.44063000
C	-0.20492200	0.79025700	1.79321000
C	1.02789800	0.78889100	2.47191300
H	1.51397500	-0.16011500	2.69877300
C	1.61564100	1.99564700	2.80408600
C	0.98370800	3.20710500	2.46044100
C	-0.22938700	3.20607300	1.79305400
H	-5.46780900	1.58858200	-1.27976600
H	-4.25657700	-0.45029200	-0.59618000
H	-2.46000200	4.04145400	0.57108400
H	-4.56716400	3.83828100	-0.67046700
H	2.57790100	2.00671600	3.31759000
H	1.45924600	4.15605800	2.71421100
H	-0.69364100	4.15548200	1.53076400
N	-0.80221500	-0.41340900	1.45485400
B	-2.43381100	-2.10926100	0.53767300
Cl	-4.15380300	-2.36790900	1.20864500
Cl	-2.37952800	-2.38803200	-1.32565600
H	-1.51393000	-0.16037700	-2.69878000

Cl	-1.26587100	-3.30811200	1.37944000
C	4.53856400	1.66943400	0.71262500
C	3.86270300	0.52719600	0.33102300
C	2.65220800	0.61384500	-0.40430900
C	2.12325200	1.90275000	-0.73022700
C	2.84240200	3.05066000	-0.33267600
C	4.02913700	2.93685800	0.37013000
C	1.94892400	-0.57423800	-0.81364600
C	0.86137400	1.99179600	-1.44072700
C	0.20489100	0.79017300	-1.79328400
C	-1.02793700	0.78868700	-2.47198000
H	0.31823500	-1.28149200	-1.72307400
C	-1.61580300	1.99538500	-2.80414300
C	-0.98397000	3.20690300	-2.46052500
C	0.22913700	3.20598900	-1.79316200
H	5.46758200	1.58905400	1.27989700
H	4.25655400	-0.44995300	0.59634000
H	2.45968100	4.04159600	-0.57123900
H	4.56679900	3.83865000	0.67042700

H	-2.57808200	2.00636100	-3.31761500
H	-1.45960500	4.15581100	-2.71428400
H	0.69330600	4.15544300	-1.53088100
N	0.80231600	-0.41343600	-1.45490900
B	2.43399400	-2.10913100	-0.53764000
Cl	4.15411800	-2.36768100	-1.20830300
Cl	2.37940900	-2.38789000	1.32568300
H	-0.31803800	-1.28143300	1.72295300
Cl	1.26630200	-3.30809500	-1.37959900

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C	0.20954200	3.51376100	-0.00003200
C	0.77207800	2.25218800	-0.00003400
C	-0.04869200	1.09452200	-0.00010100
C	-1.47251700	1.24375500	-0.00005700
C	-2.01608700	2.54710700	-0.00002500
C	-1.19167000	3.65973700	-0.00003700
C	0.53356700	-0.22305900	-0.00011600
C	-2.31164900	0.05746600	-0.00003400

C	-1.67897300	-1.20678800	-0.00007300
C	-2.41369100	-2.40659900	-0.00006800
H	-1.88522200	-3.36195000	-0.00011600
C	-3.79698000	-2.35150800	-0.00001800
C	-4.45228800	-1.10385500	0.00005000
C	-3.72546800	0.07606000	0.00004800
H	0.85061800	4.39718000	0.00002400
H	1.85301300	2.13867500	0.00000000
H	-3.09623300	2.68680500	0.00000900
H	-1.63392900	4.65831600	0.00001100
H	-4.37855400	-3.27517400	-0.00001500
H	-5.54325700	-1.06555800	0.00012000
H	-4.25649500	1.02717900	0.00007300
N	-0.29564600	-1.25220700	-0.00011400
B	2.13179600	-0.56222600	-0.00000800
Cl	2.89875400	0.14942100	-1.54578300
Cl	2.89827600	0.14913300	1.54616700
Cl	2.37356600	-2.43802600	-0.00016100
H	0.15743100	-2.17458900	-0.00006900

BBr_3

B	0.00000000	0.00000000	0.00000000
Br	0.00000000	1.91072600	0.00000000
Br	-1.65473800	-0.95536300	0.00000000
Br	1.65473800	-0.95536300	0.00000000

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C	2.71583000	0.88252400	-0.09654000
C	1.77734300	1.37157000	-1.02266200
C	1.40349800	2.71570900	-1.01081800
C	1.96789700	3.59397700	-0.08107700
C	2.91409300	3.12162600	0.83372200
C	3.28705500	1.77619600	0.82632900
C	3.10790500	-0.54826800	-0.07631900
C	2.15071900	-1.59209700	-0.04245800
C	2.51092800	-2.94737300	-0.01363800
C	3.85993900	-3.28854400	-0.01225800
C	4.82969500	-2.27972100	-0.03088700

C	4.45609600	-0.93471000	-0.06041100
H	1.33988200	0.70401800	-1.76678300
H	0.66430400	3.07338600	-1.73046000
H	1.67069400	4.64499600	-0.06917600
H	3.35810700	3.80182500	1.56402500
H	4.01003600	1.40685700	1.55673800
H	1.73056300	-3.70839600	0.01709500
H	4.15350900	-4.33932600	0.00744500
H	5.88924700	-2.54329800	-0.02847300
H	5.22193200	-0.15781100	-0.09041300
C	-0.27500900	-0.86174300	0.04657800
N	0.81098300	-1.26176100	0.00561900
B	-1.72091400	-0.23109500	0.05222400
Br	-1.98831800	0.51338500	-1.81580400
Br	-1.66441600	1.22841300	1.45142500
Br	-3.01430900	-1.71177900	0.49815600

TS1-Br

C	-0.65629300	3.49588900	0.00562100

C	-0.20010600	2.37461500	0.67567300
C	-0.99097400	1.18063600	0.73318900
C	-2.31084500	1.20275500	0.14362200
C	-2.74946400	2.34849200	-0.51651600
C	-1.92993700	3.48163700	-0.58305300
C	-0.19898900	-0.35007800	-0.00564900
C	-3.08953100	-0.03398600	0.14344300
C	-2.39846000	-1.25594300	-0.08101300
C	-3.09808300	-2.45885200	-0.21099800
H	-2.53626000	-3.37229900	-0.40956300
C	-4.48773600	-2.47038900	-0.08135100
C	-5.17960500	-1.27710000	0.15265500
C	-4.48716700	-0.06837800	0.25084400
H	-0.03810400	4.39324200	-0.04755000
H	0.75211700	2.39176000	1.20391300
H	-3.72547900	2.35394800	-1.00376900
H	-2.29127600	4.36958500	-1.10683100
H	-5.03236600	-3.41252900	-0.16773600
H	-6.26625100	-1.28628400	0.25721900

H	-5.03093800	0.85816600	0.44358200
N	-1.01585700	-1.23992500	-0.23145400
B	1.42020600	-0.31929600	-0.02693000
H	-0.88648700	0.63103500	1.68367200
Br	2.04501400	-0.01590200	1.89392800
Br	2.03756800	1.16369900	-1.27054300
Br	2.08107900	-2.10969600	-0.70501100

Int1-Br

C	-0.82123900	3.54060800	-0.05403900
C	-0.18727800	2.38305000	0.30913700
C	-0.92408400	1.11372500	0.44465000
C	-2.37033400	1.15023800	0.12058100
C	-2.97183400	2.36695100	-0.21175600
C	-2.21238500	3.52941700	-0.30821700
C	-0.21662700	-0.23137100	0.05292900
C	-3.08038600	-0.10189400	0.12853000
C	-2.30988800	-1.29201900	-0.03313400
C	-2.96555600	-2.52934100	-0.14272400

H	-2.35365500	-3.42054300	-0.28752700
C	-4.35155200	-2.60103300	-0.05858700
C	-5.11546200	-1.43301000	0.11890500
C	-4.48865100	-0.19813600	0.19819000
H	-0.26283000	4.47468600	-0.12829300
H	0.85964500	2.39319100	0.60216500
H	-4.03571400	2.40484600	-0.44370100
H	-2.70871200	4.46171100	-0.58807200
H	-4.85017100	-3.56988000	-0.13129800
H	-6.20227600	-1.49754800	0.19609700
H	-5.08621600	0.70096300	0.35355500
N	-0.92834200	-1.27457000	-0.14425600
B	1.39848400	-0.30336300	-0.00163000
H	-0.87481600	0.93248400	1.55256700
Br	2.13826000	0.33723100	1.81117500
Br	1.98539500	0.95444700	-1.52952900
Br	2.07955600	-2.16665500	-0.38148500

Int2-Br

C	4.94102100	-1.49020700	2.10647500
C	3.73357700	-1.36084400	1.47939700
C	3.39763100	-0.15025600	0.70519600
C	4.48169300	0.84918600	0.53764800
C	5.68073800	0.68391400	1.23955600
C	5.90541000	-0.45854000	1.99818900
C	2.40327200	-0.25143600	-0.48113600
C	4.24546000	1.94217400	-0.36387000
C	3.21696800	1.77545800	-1.33918100
C	3.03263400	2.76039600	-2.32499900
H	2.25933400	2.59204700	-3.07469800
C	3.80191400	3.91727100	-2.31432600
C	4.78956700	4.10683600	-1.32831400
C	5.02061000	3.12491700	-0.37746800
H	5.16055000	-2.37820800	2.70056900
H	2.95624100	-2.10907400	1.61484200
H	6.47174300	1.42769400	1.15186600
H	6.86033400	-0.56776300	2.51757900
H	3.63711800	4.68647100	-3.07158600

H	5.37708000	5.02634100	-1.31467500
H	5.78219100	3.28447400	0.38624000
N	2.38907300	0.66885800	-1.37458400
B	1.35805700	-1.48076000	-0.57136700
H	2.68748600	0.36709000	1.41459400
C	-2.09921800	2.69092600	-2.71727400
C	-2.43523800	1.76469900	-1.76541300
C	-1.61239800	1.57207900	-0.56415700
C	-0.49264500	2.51734800	-0.36749100
C	-0.18533600	3.43402700	-1.37828600
C	-0.97064400	3.51847000	-2.52255100
C	-2.24471200	1.02055500	0.72390800
C	0.24715900	2.42059800	0.86344400
C	-0.33728600	1.66665800	1.92211600
C	0.35396900	1.53756100	3.14187900
H	-0.11698800	0.95196700	3.93191600
C	1.59588600	2.13277000	3.31462100
C	2.16416600	2.90452300	2.28095600
C	1.49203000	3.05776000	1.07849700

H	-2.69563300	2.78812900	-3.62537500
H	-3.25313700	1.06859600	-1.93484000
H	0.65474300	4.11590900	-1.26174800
H	-0.70742800	4.24947400	-3.29064200
H	2.13145200	2.01261400	4.25856600
H	3.13664600	3.37862500	2.42345500
H	1.94597700	3.65191400	0.28720700
N	-1.59120200	1.09227600	1.83045500
B	-3.71553900	0.34654200	0.70891800
H	-1.06034100	0.61333500	-0.90787700
Br	-5.01867700	1.85806000	0.14519100
Br	-3.77487400	-1.19909300	-0.64249300
Br	-4.27037000	-0.35024900	2.52660100
Br	-0.02155000	-1.16901200	-2.04127200
Br	0.35489600	-1.72674200	1.19254900
Br	2.47760400	-3.13634300	-1.03304300

TS2-Br

C	4.33892000	-1.82179200	2.23591500

C	3.13944700	-1.73493500	1.58204900
C	2.78859200	-0.53348500	0.80078000
C	3.85661800	0.48395300	0.60700100
C	5.04963000	0.34663400	1.32021300
C	5.28334400	-0.77790500	2.10709300
C	1.74912900	-0.63570100	-0.30195100
C	3.57524200	1.57842700	-0.28095800
C	2.40222200	1.50204400	-1.08442200
C	2.15337500	2.49362300	-2.04591900
H	1.29482700	2.37892400	-2.70543000
C	3.00460300	3.58445000	-2.16342500
C	4.13873000	3.69537000	-1.33787700
C	4.43022800	2.69573000	-0.42513000
H	4.56685100	-2.68890400	2.85663200
H	2.36359500	-2.48398000	1.72870200
H	5.82581500	1.10633700	1.24480900
H	6.23295900	-0.85418400	2.64188900
H	2.79538700	4.35474200	-2.90810300
H	4.79748400	4.56046800	-1.42742300

H	5.31898000	2.78461800	0.19837200
N	1.53251000	0.41488300	-1.03808900
B	0.99851200	-2.02868100	-0.64833800
H	2.16022600	0.01210500	1.58060800
C	-1.82163400	2.54878400	-2.82305200
C	-1.77712000	1.46129600	-1.97973900
C	-1.04428200	1.51070200	-0.73264300
C	-0.43136700	2.78899200	-0.35768600
C	-0.53923900	3.88248800	-1.22259000
C	-1.22681700	3.76391500	-2.42707600
C	-1.49674000	0.68067900	0.45893700
C	0.36488100	2.78379400	0.85010600
C	0.21535400	1.65838800	1.71460800
C	1.06920800	1.52553800	2.82947200
H	0.91401700	0.67379000	3.49444600
C	2.04549900	2.48457900	3.08529100
C	2.16443200	3.61488600	2.25796600
C	1.32447000	3.76844300	1.16256000
H	-2.34872500	2.48486400	-3.77596000

H	-2.25849300	0.52227100	-2.24884500
H	-0.07738900	4.83442000	-0.96216900
H	-1.29754200	4.63337500	-3.08457600
H	2.71008200	2.36630100	3.94354100
H	2.92696800	4.36693900	2.46679300
H	1.45452000	4.62960500	0.50680300
N	-0.81326400	0.75187600	1.55626200
B	-2.97918300	0.00485400	0.51935700
H	0.02508600	0.89203700	-1.09274100
Br	-4.19174800	1.69875200	0.26917500
Br	-3.46816300	-1.35558600	-0.91092500
Br	-3.37015600	-0.80903800	2.33665100
Br	-0.09197300	-1.87009900	-2.33860600
Br	-0.10291000	-2.75090100	0.88634500
Br	2.62276700	-3.27642200	-1.05454700

Int3-Br

C	4.70814400	2.08250500	1.05143300
C	3.90042400	1.00786500	0.80349000

C	2.59480600	1.18663900	0.14960200
C	2.29446800	2.52488600	-0.41811100
C	3.15194700	3.58520600	-0.10390400
C	4.32683800	3.36947800	0.60521100
C	1.93717800	0.00727800	-0.49213300
C	1.11292100	2.67801700	-1.22611500
C	0.40647000	1.51368300	-1.61998300
C	-0.73014900	1.58402800	-2.43124300
H	-1.26296400	0.66948600	-2.69288100
C	-1.17473600	2.82617000	-2.86346300
C	-0.49692300	3.99705700	-2.48103700
C	0.62976200	3.92607700	-1.67840700
H	5.64704200	1.94799600	1.58943000
H	4.14723500	0.02361600	1.19317900
H	2.92098400	4.59194600	-0.44653800
H	4.97704200	4.22072100	0.81798000
H	-2.06484700	2.88960400	-3.48998100
H	-0.86600700	4.96947200	-2.80939400
H	1.13134700	4.84504900	-1.37971900

N	0.89501600	0.26055600	-1.23979400
B	2.45929300	-1.52301200	-0.35243100
H	1.95529300	1.26458200	1.14348900
C	-4.19951500	2.78423300	-1.10941000
C	-3.70878000	1.57511500	-0.64858500
C	-2.59632100	1.51884900	0.22681300
C	-1.97557100	2.74679400	0.60989100
C	-2.50493600	3.97054100	0.13911300
C	-3.60118600	3.99212100	-0.70420300
C	-2.05239400	0.25159400	0.72590500
C	-0.79926300	2.68789100	1.45510100
C	-0.35749800	1.39965800	1.85929000
C	0.80413600	1.28192700	2.67445600
H	1.09606500	0.27851100	2.98922500
C	1.50644800	2.41313500	3.08112900
C	1.07606700	3.68601200	2.66355300
C	-0.05701200	3.81691400	1.87221800
H	-5.05585600	2.79977500	-1.78705800
H	-4.18158100	0.65160100	-0.96991300

H	-2.04169700	4.91207000	0.43232100
H	-3.99377400	4.94604400	-1.06301300
H	2.39490200	2.31004600	3.70698100
H	1.63482200	4.57492300	2.96145300
H	-0.36535800	4.81488300	1.56012700
N	-0.98384400	0.24092200	1.48863400
B	-2.69752500	-1.19888100	0.38323400
H	0.40611300	-0.56841000	-1.61856600
Br	-4.68939500	-1.25756300	0.91868900
Br	-2.51658800	-1.53869600	-1.67234300
Br	-1.76731800	-2.73372200	1.33494300
Br	1.26227700	-2.79029800	-1.37597700
Br	2.54711800	-2.05159100	1.60400400
Br	4.31140000	-1.47169600	-1.23436400

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C	4.49274800	2.46522700	1.17005700
C	3.88981000	1.30992000	0.71305700
C	2.75171000	1.36890700	-0.13242300

C	2.22081900	2.64858600	-0.49433000
C	2.86701200	3.81086900	-0.02002200
C	3.98333400	3.72247500	0.79252200
C	2.12472200	0.16679100	-0.62577100
C	1.03176000	2.71817200	-1.32221500
C	0.44125300	1.50554800	-1.74405600
C	-0.72057400	1.47935100	-2.53787700
H	-1.15773800	0.52030200	-2.81832300
C	-1.30231400	2.67419200	-2.91942100
C	-0.73401700	3.89719300	-2.51084800
C	0.40856800	3.91995400	-1.72889700
H	5.36541700	2.40192000	1.82249200
H	4.28766200	0.34311600	1.00810200
H	2.48027500	4.79330000	-0.28531200
H	4.46396100	4.63500100	1.15125400
H	-2.21072800	2.66691200	-3.52311800
H	-1.20446400	4.83672500	-2.80548900
H	0.82269200	4.87824000	-1.41960700
N	1.03590400	0.31401000	-1.36566900

B	2.64412900	-1.35622400	-0.36586500
H	1.15777100	0.52038200	2.81827200
C	-4.49285500	2.46512900	-1.17000600
C	-3.88986900	1.30984100	-0.71302000
C	-2.75174700	1.36886400	0.13242700
C	-2.22088500	2.64856000	0.49431900
C	-2.86712700	3.81082200	0.02002600
C	-3.98346700	3.72239200	-0.79248800
C	-2.12471100	0.16676800	0.62576100
C	-1.03181100	2.71818200	1.32217900
C	-0.44126200	1.50557600	1.74401400
C	0.72057700	1.47941600	2.53782000
H	-0.60399500	-0.55915000	1.70002700
C	1.30229000	2.67427600	2.91934700
C	0.73395400	3.89725900	2.51077600
C	-0.40864500	3.91998400	1.72884400
H	-5.36554000	2.40179400	-1.82241600
H	-4.28770000	0.34302400	-1.00805000
H	-2.48041200	4.79326500	0.28530400

H	-4.46413200	4.63490400	-1.15120800
H	2.21071300	2.66702500	3.52303200
H	1.20437800	4.83680500	2.80540500
H	-0.82280200	4.87825600	1.41955800
N	-1.03588500	0.31401900	1.36564100
B	-2.64409100	-1.35626000	0.36587200
H	0.60404300	-0.55917300	-1.70005900
Br	4.55658200	-1.54072300	-1.04507300
Br	1.47440800	-2.70087300	-1.37698200
Br	2.51056100	-1.75994200	1.63733500
Br	-2.51049000	-1.76001800	-1.63731800
Br	-4.55655400	-1.54076400	1.04505100
Br	-1.47437500	-2.70087900	1.37703400

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C	-0.96073300	3.63585900	-0.00013500
C	-0.25917100	2.44626800	-0.00016300
C	-0.93947600	1.20055200	-0.00008100
C	-2.37205800	1.18965500	0.00000400

C	-3.06007600	2.42313300	0.00004400
C	-2.36922200	3.62265500	-0.00000900
C	-0.21363800	-0.04703300	-0.00005300
C	-3.07658900	-0.08049000	0.00002200
C	-2.30854900	-1.26670400	-0.00000200
C	-2.90564800	-2.54100300	-0.00005500
H	-2.27586900	-3.43298000	-0.00006300
C	-4.28637900	-2.63873300	-0.00010000
C	-5.07557600	-1.47089300	-0.00006900
C	-4.48381700	-0.21791300	0.00000800
H	-0.42257200	4.58543500	-0.00019100
H	0.82724400	2.46266500	-0.00026000
H	-4.14903800	2.43825000	0.00011600
H	-2.92237600	4.56430000	0.00001400
H	-4.76236400	-3.62095900	-0.00020200
H	-6.16407800	-1.55336900	-0.00009900
H	-5.11667600	0.66854400	0.00005100
N	-0.92936900	-1.15990200	0.00000800
B	1.40808400	-0.20979200	-0.00003000

H	-0.38480100	-2.03238900	0.00003600
Br	2.16026400	0.64030400	-1.69168900
Br	1.92832700	-2.20773900	0.00010800
Br	2.16001700	0.64048300	1.69170200

BI_3

B	0.00000000	0.00000000	0.00000000
I	0.00000000	2.13529900	0.00000000
I	1.84922400	-1.06765000	0.00000000
I	-1.84922400	-1.06765000	0.00000000

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C	3.25979100	0.63872400	-0.10319700
C	2.39555800	1.20736500	-1.05563600
C	2.12510200	2.57587500	-1.03971800
C	2.71824700	3.39814500	-0.07723700
C	3.58867000	2.84481300	0.86682900
C	3.86009200	1.47518400	0.85370700
C	3.54363800	-0.81744900	-0.09479400

C	2.50754900	-1.78379700	-0.09653300
C	2.76297600	-3.16340200	-0.08780400
C	4.08173200	-3.60695600	-0.06819900
C	5.12644500	-2.67585400	-0.04838600
C	4.85765000	-1.30558100	-0.05973000
H	1.93705600	0.58116900	-1.82307100
H	1.44383200	2.99725800	-1.78170300
H	2.50115100	4.46852500	-0.06178100
H	4.05313400	3.48090700	1.62369500
H	4.52516200	1.04336300	1.60462000
H	1.92584900	-3.86230900	-0.08507200
H	4.29388400	-4.67735300	-0.06339800
H	6.16232300	-3.02050500	-0.03035400
H	5.68076500	-0.58893400	-0.06032900
C	0.14577500	-0.86698400	-0.00874800
N	1.19889900	-1.35202500	-0.05840100
B	-1.23268300	-0.15627400	0.03260000
I	-1.53891400	0.69243000	-2.03769100
I	-1.00837100	1.45338200	1.59505800

I	-2.74689100	-1.72500200	0.57546000

TS1-I

C	-1.38444300	3.52871000	0.04133400
C	-0.85053000	2.43556000	0.70214100
C	-1.55388300	1.18748700	0.74912900
C	-2.86862200	1.12057600	0.14905000
C	-3.38363400	2.23709800	-0.50511000
C	-2.64943200	3.42858200	-0.55521000
C	-0.65028700	-0.30102400	0.01432400
C	-3.56466600	-0.16404000	0.14291800
C	-2.79450300	-1.33940300	-0.07160700
C	-3.41401400	-2.58567500	-0.20593300
H	-2.79240000	-3.46114300	-0.39717700
C	-4.80092500	-2.68641400	-0.08937900
C	-5.57035300	-1.53946600	0.13549100
C	-4.95824300	-0.28855900	0.23749500
H	-0.83165500	4.46834300	0.00078400
H	0.09192700	2.52284700	1.24154900

H	-4.35464900	2.17656900	-0.99847900
H	-3.07233800	4.29334100	-1.07148600
H	-5.28304500	-3.66176100	-0.17846600
H	-6.65508100	-1.61843400	0.23008700
H	-5.56256700	0.60098800	0.42398700
N	-1.41694100	-1.23562400	-0.21146100
B	0.95168100	-0.18551800	-0.01156400
H	-1.42329000	0.64635000	1.70142600
I	1.78804300	-2.14375500	-0.78493400
I	1.66145500	0.15771600	2.11973700
I	1.56379400	1.48432800	-1.40804800

Int1-I

C	-1.48192200	3.54127700	0.03239600
C	-0.79203800	2.41411700	0.39758900
C	-1.46316900	1.10541500	0.52083100
C	-2.90574800	1.07033300	0.16461200
C	-3.56158400	2.25436800	-0.17295800
C	-2.86290300	3.45855900	-0.24692200

C	-0.68519800	-0.19587700	0.12251600
C	-3.55266800	-0.21626200	0.16963700
C	-2.72025400	-1.36764800	0.04297800
C	-3.30867000	-2.64016100	-0.04425000
H	-2.64978100	-3.50136500	-0.16190800
C	-4.69030700	-2.78189700	0.02368600
C	-5.51584800	-1.65106300	0.16000300
C	-4.95474400	-0.38348000	0.21932300
H	-0.97098800	4.50324300	-0.02489600
H	0.24102100	2.48685500	0.72891100
H	-4.62209800	2.23914200	-0.42231400
H	-3.40394900	4.36542300	-0.52724800
H	-5.13724900	-3.77672700	-0.03173400
H	-6.59906300	-1.76976100	0.22197400
H	-5.60061800	0.48640900	0.34444200
N	-1.34164100	-1.27892200	-0.06569500
B	0.92218100	-0.19073800	0.01881500
H	-1.43867800	0.93334000	1.63072000
I	1.77289700	-2.21460100	-0.49518200

I	1.81766700	0.50300600	2.00759800
I	1.42702700	1.26430300	-1.69597800

Int2-I

C	5.05168700	-0.02605400	2.47070900
C	3.94297800	-0.08249700	1.66808900
C	3.57950000	1.03610400	0.77797600
C	4.53404400	2.17420200	0.72934000
C	5.63164700	2.19019700	1.59085100
C	5.88793800	1.11160600	2.43464700
C	2.86021300	0.74285800	-0.57136900
C	4.25898600	3.22110600	-0.21844500
C	3.40917900	2.90118900	-1.31850400
C	3.17924500	3.86203800	-2.31788500
H	2.55162900	3.58078100	-3.16417500
C	3.73213900	5.13324000	-2.21031900
C	4.54899300	5.46334500	-1.11307200
C	4.82267200	4.51440000	-0.13876500
H	5.28272400	-0.85068400	3.14605200

H	3.24328900	-0.90884300	1.76184400
H	6.32265800	3.03233700	1.57961400
H	6.76345600	1.14854500	3.08699000
H	3.53228600	5.87940600	-2.98200100
H	4.96903600	6.46694500	-1.02776600
H	5.44557700	4.78387900	0.71475500
N	2.82188800	1.65728100	-1.47097700
B	2.14763500	-0.67492600	-0.84839500
H	2.69395200	1.48074900	1.31656300
C	-1.93647800	1.85683300	-2.97449500
C	-2.27327400	1.12178400	-1.86503900
C	-1.63736400	1.36652300	-0.56508400
C	-0.68441300	2.49944600	-0.49587500
C	-0.36585700	3.20056000	-1.65753200
C	-0.98567200	2.89078700	-2.86729700
C	-2.41431600	1.10361600	0.74414600
C	-0.08436200	2.75915300	0.78807400
C	-0.68728700	2.15663100	1.92979900
C	-0.10140900	2.33448500	3.19660300

H	-0.58534700	1.86335900	4.05294100
C	1.05483100	3.09092600	3.33797400
C	1.63029200	3.72459500	2.21937700
C	1.05737200	3.57360700	0.96449400
H	-2.39230700	1.63272900	-3.93954400
H	-2.93314500	0.26217900	-1.95597100
H	0.35898900	4.01229700	-1.62659300
H	-0.71624400	3.46202900	-3.75860400
H	1.51019900	3.21105200	4.32305400
H	2.52803500	4.33409600	2.33621300
H	1.51173500	4.06750200	0.10758500
N	-1.88616900	1.46569400	1.86045900
B	-3.83544000	0.34685200	0.73995100
H	-0.93578400	0.46241900	-0.46978400
I	-5.23475600	1.63240600	-0.56740500
I	-4.74107200	0.19301000	2.80383600
I	-3.60490400	-1.76068900	-0.11918200
I	1.04296700	-0.72079000	-2.81119000
I	0.62417100	-1.16076300	0.79781400

I	3.84569200	-2.21272200	-0.87562800

TS2-I

C	4.62835400	-0.39549700	2.77819100
C	3.50680900	-0.61108600	2.01745600
C	3.00111600	0.43048300	1.09975100
C	3.88169600	1.61310300	0.87768500
C	5.00185600	1.77552800	1.69165000
C	5.36332300	0.79664300	2.61737800
C	2.12379200	0.02604200	-0.07532900
C	3.48731000	2.55098100	-0.13873500
C	2.41705200	2.18799300	-1.00402900
C	2.07611200	3.02546800	-2.07766300
H	1.31321300	2.69304900	-2.77919800
C	2.72588100	4.23992300	-2.25250100
C	3.74970100	4.63228100	-1.37089400
C	4.13838100	3.78945200	-0.34279400
H	4.95281800	-1.14396200	3.50187700
H	2.87165400	-1.47700100	2.19665200

H	5.62500400	2.66311100	1.59706100
H	6.25001800	0.96098600	3.23401000
H	2.44586500	4.88660400	-3.08618300
H	4.25017400	5.59222000	-1.50697900
H	4.94451100	4.09678600	0.32222800
N	1.76279400	0.96158700	-0.91070500
B	1.72942000	-1.50589300	-0.37918600
H	2.21457200	0.90644700	1.77046600
C	-1.68956500	2.31223000	-3.14811300
C	-1.55383700	1.31648700	-2.20592600
C	-0.97845800	1.58629600	-0.90685300
C	-0.63484600	2.97817800	-0.59740700
C	-0.83758300	3.96771600	-1.56495700
C	-1.36004700	3.64038500	-2.81257200
C	-1.40799900	0.78828700	0.31312600
C	0.02527400	3.20703900	0.66930800
C	-0.00977000	2.13888400	1.61488500
C	0.73923000	2.24345800	2.80603400
H	0.67038400	1.42821200	3.52868700

C	1.50388000	3.37919400	3.05596400
C	1.50688600	4.44881800	2.14317100
C	0.76515600	4.36855400	0.97171600
H	-2.09237100	2.08212100	-4.13536000
H	-1.84225800	0.29181000	-2.43554200
H	-0.57551700	5.00326800	-1.34987900
H	-1.50858100	4.43218500	-3.55017300
H	2.09056600	3.44627200	3.97439300
H	2.10386400	5.33904000	2.34764700
H	0.80857700	5.18888300	0.25502500
N	-0.84791600	1.05734800	1.45107400
B	-2.76491100	-0.10501900	0.34113700
H	0.23528800	1.14613000	-1.11932400
I	-4.35584200	1.53983600	-0.17677600
I	-3.23409000	-0.88182100	2.42102200
I	-3.02686800	-1.82200900	-1.10849300
I	0.81195800	-1.74368900	-2.42381900
I	0.48812200	-2.48327400	1.20926700
I	3.86383800	-2.46253700	-0.51193800

Int3-I

C	4.66980400	2.64600400	1.37757500
C	3.91395000	1.54225900	1.09063300
C	2.64581000	1.66637200	0.35023900
C	2.34537300	2.99462400	-0.25361000
C	3.14713900	4.08271200	0.10128900
C	4.28036500	3.91314400	0.88932600
C	2.10351000	0.46036200	-0.36220500
C	1.21308400	3.10692000	-1.13529000
C	0.57784300	1.91712200	-1.56969600
C	-0.51130400	1.94236600	-2.44529700
H	-0.99060100	1.00772500	-2.74047600
C	-0.97841500	3.16606100	-2.90607000
C	-0.36811300	4.36171600	-2.48904200
C	0.71184000	4.33470300	-1.62097600
H	5.57342100	2.54688100	1.97975300
H	4.15969200	0.57769100	1.52750900
H	2.90745100	5.07804900	-0.26788000

H	4.88794500	4.78742600	1.13249900
H	-1.83289900	3.19458600	-3.58277600
H	-0.75381900	5.31907600	-2.84129500
H	1.15846700	5.27268100	-1.29527000
N	1.09905700	0.68438000	-1.17271800
B	2.69356000	-1.03431800	-0.22930500
H	1.93211500	1.71087500	1.27658300
C	-4.11892200	3.28371800	-1.35148200
C	-3.68695200	2.05978500	-0.87064900
C	-2.62786200	1.96682900	0.06468700
C	-1.99836000	3.17597000	0.49131100
C	-2.46903000	4.41602400	0.00065700
C	-3.51406000	4.47271700	-0.90373100
C	-2.15386900	0.68344000	0.59729100
C	-0.88164700	3.08525600	1.41116500
C	-0.49810600	1.78469100	1.83513100
C	0.59177700	1.63576300	2.73712600
H	0.84235300	0.62426500	3.06031300
C	1.28598100	2.74691100	3.20393500

C	0.91804600	4.03293900	2.76423100
C	-0.14788500	4.19520800	1.89044500
H	-4.93557500	3.32439500	-2.07538300
H	-4.16865800	1.15348500	-1.22586400
H	-2.00020000	5.34300500	0.32905000
H	-3.86106800	5.43901000	-1.27603900
H	2.12098600	2.61958200	3.89559000
H	1.47245000	4.90669000	3.11121800
H	-0.40990900	5.20179200	1.56431300
N	-1.13047900	0.64456400	1.41864300
B	-2.85070900	-0.74297600	0.27107700
H	0.69044700	-0.15477600	-1.61759700
I	-5.06909400	-0.68882800	0.90272300
I	-1.89566300	-2.47735500	1.38679200
I	-2.69320400	-1.24359600	-1.98685300
I	1.56387300	-2.50432300	-1.51832200
I	2.67092900	-1.73541300	1.91283100
I	4.81019900	-0.79218800	-1.07955900

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C	4.48516900	2.99561600	1.42758000
C	3.93853000	1.82507500	0.93952800
C	2.84234600	1.84887700	0.03927600
C	2.29511400	3.11521100	-0.34673700
C	2.88637900	4.29482100	0.15626300
C	3.96217600	4.23880500	1.02390600
C	2.27691700	0.62779900	-0.49131900
C	1.14483000	3.15859600	-1.22850400
C	0.60302100	1.93200000	-1.67216700
C	-0.52088300	1.87601100	-2.51747900
H	-0.91996200	0.90648600	-2.81911700
C	-1.11288100	3.05538600	-2.92974200
C	-0.59154300	4.29251300	-2.50148900
C	0.51359300	4.34432800	-1.66837600
H	5.32529300	2.95387400	2.12299000
H	4.35229600	0.87258400	1.25732800
H	2.48612100	5.26560400	-0.13052800
H	4.39921000	5.16424900	1.40451800

H	-1.99262100	3.02455800	-3.57387100
H	-1.06906700	5.21990200	-2.82168700
H	0.89080200	5.31314800	-1.34515100
N	1.21171900	0.75599800	-1.27168100
B	2.84875700	-0.87367700	-0.25075100
H	0.92018800	0.90648100	2.81877200
C	-4.48524300	2.99584800	-1.42736200
C	-3.93858300	1.82527000	-0.93941500
C	-2.84238200	1.84899800	-0.03917500
C	-2.29514900	3.11531600	0.34689500
C	-2.88643200	4.29496300	-0.15598900
C	-3.96225400	4.23900900	-1.02360300
C	-2.27694300	0.62788200	0.49136200
C	-1.14480400	3.15866800	1.22856500
C	-0.60293200	1.93205900	1.67209200
C	0.52107900	1.87603500	2.51726400
H	-0.81580600	-0.12082700	1.63949200
C	1.11311100	3.05539300	2.92952300
C	0.59169700	4.29253600	2.50140700

C	-0.51353700	4.34438500	1.66842600
H	-5.32538000	2.95415500	-2.12276000
H	-4.35235100	0.87280900	-1.25729100
H	-2.48615700	5.26572300	0.13086300
H	-4.39930600	5.16448000	-1.40412600
H	1.99293400	3.02454700	3.57353900
H	1.06924300	5.21991500	2.82160300
H	-0.89079700	5.31321600	1.34528700
N	-1.21167300	0.75607000	1.27163200
B	-2.84879600	-0.87361700	0.25074100
H	0.81586800	-0.12089200	-1.63957400
I	4.99973800	-0.96808900	-0.99271400
I	1.65804100	-2.42795800	-1.43789000
I	2.67876900	-1.41824900	1.95401900
I	-2.67862500	-1.41813600	-1.95401700
I	-1.65817600	-2.42800800	1.43792700
I	-4.99980400	-0.96817200	0.99259400

4a

C	-1.61673300	3.65316700	0.00006300
C	-0.86432000	2.49528100	0.00004900
C	-1.48484900	1.21896800	0.00011100
C	-2.91625900	1.14691800	0.00016200
C	-3.65825500	2.34909400	0.00016900
C	-3.02302200	3.57850800	0.00011300
C	-0.70344400	0.00113300	0.00009100
C	-3.56893800	-0.15010800	0.00017000
C	-2.75189600	-1.30231400	0.00004000
C	-3.29348600	-2.60157600	-0.00002800
H	-2.62551300	-3.46551800	-0.00016900
C	-4.66862600	-2.75756000	0.00006800
C	-5.50665100	-1.62399500	0.00023900
C	-4.96903600	-0.34684100	0.00028000
H	-1.11924500	4.62461300	0.00002000
H	0.21948200	2.56618800	0.00000600
H	-4.74672600	2.31464400	0.00016800
H	-3.61771200	4.49440900	0.00010000
H	-5.10285900	-3.75890000	-0.00000700

H	-6.59061700	-1.75277200	0.00032500
H	-5.63909800	0.51174900	0.00041900
N	-1.37922400	-1.13877000	0.00000600
B	0.91763800	-0.09447300	0.00010500
H	-0.80971000	-1.99541000	-0.00000200
I	1.72408400	0.86906000	-1.89331500
I	1.63148500	-2.28668600	0.00014700
I	1.72464700	0.86933800	1.89296800

TS3-Cl

C	-0.20826300	3.47287600	0.03085200
C	-0.77187200	2.22479400	-0.06694600
C	0.06483700	1.06322100	-0.06698900
C	1.50097000	1.21928300	-0.03153000
C	2.03237800	2.53066800	0.05056200
C	1.20028500	3.62874700	0.08583800
C	-0.51334000	-0.33101400	-0.05804900
C	2.31881300	0.04450200	-0.04398300
C	1.65796200	-1.23681700	0.00577300

C	2.43904100	-2.43299400	0.05635600
H	1.89925800	-3.37952600	0.10151700
C	3.81022500	-2.36790900	0.03412300
C	4.45856400	-1.10576000	-0.03350600
C	3.73563000	0.06953900	-0.06944600
H	-0.85122900	4.35411700	0.06584400
H	-1.84932800	2.10350900	-0.12858600
H	3.11079300	2.67407200	0.09115100
H	1.62917600	4.63050000	0.15067200
H	4.40824700	-3.28050800	0.06563500
H	5.54952100	-1.06525900	-0.05543400
H	4.26632500	1.01926300	-0.12131400
N	0.32579800	-1.37448000	0.02796400
B	-2.13005900	-0.61314200	0.01921000
Cl	-2.80849100	0.17678400	1.58002900
Cl	-2.92683200	0.17603500	-1.51658100
H	-0.34457200	0.25292700	-1.14574500
Cl	-2.48819800	-2.42910300	0.01456100

Int4-Cl

C	-3.97107800	-0.30097700	0.30874200
C	-3.38005800	0.43749900	-0.70128400
C	-2.05735700	0.91336000	-0.55560200
C	-1.32293900	0.63863900	0.63056000
C	-1.95066200	-0.11453100	1.64923000
C	-3.24775700	-0.57538400	1.48871400
C	-1.41549400	1.66816800	-1.59888300
C	0.03683300	1.13984600	0.70751200
C	0.54525400	1.87339600	-0.40722300
C	1.86730500	2.37523100	-0.36672500
H	2.22356900	2.92822500	-1.23767000
C	2.67188100	2.16274400	0.73807500
C	2.17432000	1.43703400	1.83992300
C	0.88359600	0.93615100	1.82300500
H	-4.99203900	-0.67207400	0.19677100
H	-3.92427400	0.65868000	-1.62288900
H	-1.41391600	-0.34473000	2.56930100
H	-3.71487200	-1.15900100	2.28528400

H	3.69275900	2.55063600	0.75699100
H	2.81152800	1.26351100	2.70977300
H	0.52080200	0.37201100	2.68233600
N	-0.19997200	2.12289300	-1.54196200
B	1.12654700	-1.73326100	-0.50131100
Cl	0.57165100	-2.54115000	0.95159600
Cl	0.03937900	-1.54552900	-1.86104400
H	-1.99136500	1.87291700	-2.51170700
Cl	2.77437100	-1.16103700	-0.61197400

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