Electronic Supplementary Information

Pd-Catalyzed Selective Tetrafunctionalization of Diiodo-*o*-Carboranes

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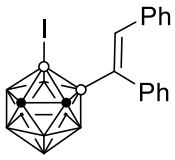
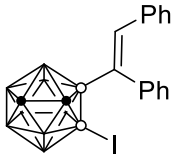
General Procedures.

All reactions were carried out in oven-dried glassware under an atmosphere of dry N_2 with the rigid exclusion of air and moisture using standard Schlenk techniques or in a glovebox. 4-I-*o*-carborane,[1] 9-I-*o*-carborane,[2] 4,5-I_2-*o*-carborane,[3] 4,7-I_2-*o*-carborane[1] and 3,6-I_2-*o*-carborane[4] were prepared according to literature procedures. Toluene was freshly distilled from sodium benzophenone ketyl immediately prior to use. All other chemicals were purchased from either Aldrich or J&K Chemical Co. and used as received unless otherwise specified. ^{1}H, ^{13}C{^{1}H}, ^{11}B and ^{19}F NMR spectra were recorded on a Bruker 400 spectrometer at 400, 101, 128 and 376 MHz, respectively. All chemical shifts were reported in ppm unit with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external $BF_3{\cdot}OEt_2$ (0.00) for boron chemical shifts and to external $CFCl_3$ (0.00) for fluorine chemical shifts. Mass spectra were obtained on a Thermo Fisher Scientific LTQ FTICR-MS spectrometer. Elemental analyses were performed with an elementary VARIO EL III elemental analyzer, Shanghai Institute of Organic Chemistry, CAS.

Synthesis of 2 and 3. An oven-dried Schlenk flask equipped with a stir bar was charged with 4-I-*o*-carborane (**1**; 27 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol), diphenylacetylene (89 mg, 0.5 mmol) and dry toluene (1 mL) under an atmosphere of dry nitrogen. The flask was closed, and then stirred at 80 ^{o}C for 72 h. After quenching with water (1 mL) and extraction with ethyl acetate (5 mL × 3), the organic portions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (300-400 mesh) using *n*-hexane as eluent to give the product **2** (22 mg, 49%) and **3** (23 mg, 50%).



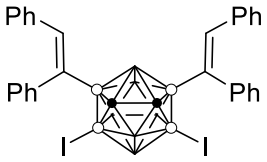
2: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33 (m, 2H), 7.28 (m, 1H), 7.23 (m, 2H), 7.09 (m, 3H), 6.94 (m, 3H) (aromatic and olefinic *H*), 3.87 (s, 1H), 3.57 (s, 1H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.0, 139.7, 137.4, 129.6, 128.9, 128.8, 128.0, 127.3, 126.7 (aromatic and olefinic *C*), 59.5, 57.8 (cage *C*), the B_{cage}-*C* was not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -0.4 (d, J_{BH} = 145 Hz, 1B) (*B*H), -2.7 (unresolved, 2B) (*B*H & *B*C), -8.0 (d, J_{BH} = 140 Hz, 1B), -11.0 (d, J_{BH} = 160 Hz, 2B), -12.7 (d, J_{BH} = 174 Hz, 1B), -14.2 (d, J_{BH} = 198 Hz, 1B), -15.7 (d, J_{BH} = 174 Hz, 1B) (*B*H), -27.0 (s, 1B) (*B*I). HRMS (DART-positive mode) calcd for $C_{16}H_{22}B_{10}I^{+}$ [M+H^{+}]: 449.1764. Found 449.1760.



3: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36 (m, 2H), 7.28 (m, 3H), 7.10 (m, 3H), 6.95 (m, 2H) (aromatic C*H*), 6.89 (s, 1H) (olefinic C*H*), 3.57 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 141.9, 140.1, 137.4, 129.6, 129.0, 128.7, 128.0, 127.4, 126.8 (aromatic and olefinic *C*), 55.2 (cage *C*), the B_{cage}-*C* was not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ -1.3 (d, J_{BH} = 145 Hz, 1B) (*B*H), -2.5 (unresolved, 2B) (*B*H & *B*C), -6.8 (d, J_{BH} = 155 Hz, 2B), -13.0 (d, J_{BH} = 164 Hz, 1B), -14.2 (d, J_{BH} = 119 Hz, 1B), -15.2 (d, J_{BH} = 153 Hz, 2B) (*B*H), -24.1 (s, 1B) (*B*I). HRMS (DART-positive mode) calcd for $C_{16}H_{22}B_{10}I^{+}$ [M+H^{+}]: 449.1764. Found 449.1761.

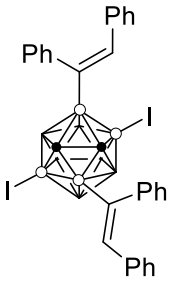
Synthesis of 5b. An oven-dried Schlenk flask equipped with a stir bar was charged with 4,7-I_2-*o*-carborane (**4b**; 40 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol), diphenylacetylene (143 mg, 0.8 mmol) and dry toluene (1 mL) under an atmosphere of dry nitrogen. The flask was closed, and then stirred at 80 ^{o}C for 120 h. After quenching with water (1 mL) and extraction with ethyl acetate (5 mL × 3), the organic portions were combined and concentrated to dryness in vacuo. The residue was

subjected to flash column chromatography on silica gel (300-400 mesh) using *n*-hexane as eluent to give the product **5b** (60 mg, 80%).



5b: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33 (m, 4H), 7.27 (m, 2H), 7.21 (m, 4H), 7.09 (m, 6H), 6.90 (m, 4H) (aromatic C*H*), 6.83 (s, 2H) (olefinic C*H*), 3.65 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 141.5, 140.2, 137.2, 129.6, 129.1, 128.6, 128.1, 127.5, 126.9 (aromatic and olefinic *C*), 56.5 (cage *C*), the B_{cage}-*C* was not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ -1.1 (d, J_{BH} = 116 Hz, 2B), -4.3 (unresolved, 4B) (*B*H), -12.3 (s, 2B) (*B*C), -24.7 (s, 2B) (*B*I). HRMS (DART-positive mode) calcd for $C_{30}H_{31}B_{10}I_2^+$ [M+H$^+$]: 753.1513. Found 753.1502.

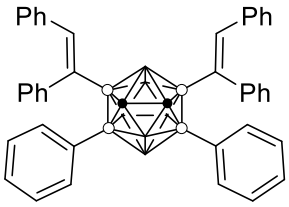
Synthesis of 5c. An oven-dried Schlenk flask equipped with a stir bar was charged with 3,6-I_2-*o*-carborane (**4c**; 40 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol), diphenylacetylene (143 mg, 0.8 mmol) and dry toluene (1 mL) under an atmosphere of dry nitrogen. The flask was closed, and then stirred at 100 ^{o}C for 96 h. After quenching with water (1 mL) and extraction with ethyl acetate (5 mL × 3), the organic portions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (300-400 mesh) using *n*-hexane as eluent to give the product **5c** (65 mg, 86%).



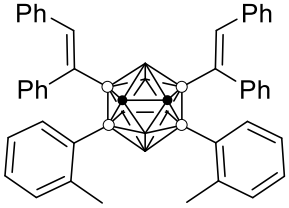
5c: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.23 (m, 6H), 7.17 (s, 2H), 7.10 (m, 6H), 6.89 (m, 8H) (aromatic and olefinic *H*), 3.34 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 144.2, 139.9, 136.5, 129.9, 129.7, 128.2, 128.2, 127.6, 127.2 (aromatic and olefinic *C*), 57.7 (cage *C*), the B_{cage}-*C* was not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ 0.1 (d, J_{BH} = 140 Hz, 2B) (*B*H), -3.8 (s, 2B) (*B*C), -8.4 (d, J_{BH} = 218 Hz, 2B), -

10.4 (d, J_{BH} = 143 Hz, 2B) (*B*H), -24.1 (s, 2B) (*B*I). Anal. Calcd for $C_{30}H_{30}B_{10}I_2$: C, 47.89; H, 4.02. Found C, 47.95; H, 4.26.

General procedure for syntheses of 7. An oven-dried Schlenk flask equipped with a stir bar was charged with 4,7-I_2-*o*-carborane (**4b**; 40 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol), diphenylacetylene (143 mg, 0.8 mmol) and dry toluene (1 mL) under an atmosphere of dry nitrogen. The flask was closed, and then stirred at 80 °C for 120 h. Then, the resulting solution was cooled to 0 °C, to which was slowly added RMgBr (0.5 mmol, 1.0 M in THF, 0.5 mL). After warming to room temperature, the reaction mixture was stirred at 80 °C for 24 h. After quenching with water (1 mL) and extraction with ethyl acetate (5 mL × 3), the organic portions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (300-400 mesh) using *n*-hexane as eluent to give the product **7**.

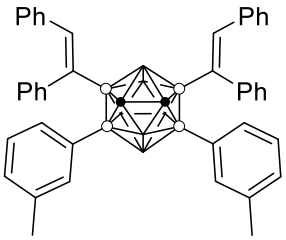


7a: Yield 86%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 (m, 4H), 7.28 (m, 6H), 7.11 (m, 6H), 7.03 (m, 6H), 6.89 (s, 2H), 6.79 (m, 4H), 6.44 (brs, 4H) (aromatic and olefinic *H*), 3.49 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.0, 139.2, 137.6, 133.2, 129.3, 128.7, 128.5, 128.0, 128.0, 127.9, 126.9, 126.2 (aromatic and olefinic *C*), 51.5 (cage *C*), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ -5.5 (unresolved, 8B) (*B*H *&* *B*C), -14.5 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{42}H_{44}B_{10}N^+$ [M+NH_4^+]: 670.4471. Found 670.4470.

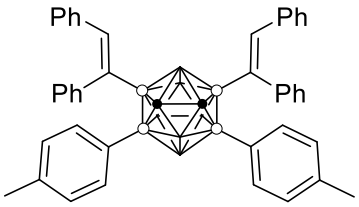


7b: Yield 82%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.28 (m, 2H), 7.16 (m, 8H), 7.04 (m, 10H), 6.85 (s, 2H), 6.76 (m, 4H), 6.55 (brs, 4H) (aromatic and olefinic *H*), 3.86 (s, 2H) (cage C*H*), 2.34 (s, 6H) (CH_3). ^{13}C{^{1}H}

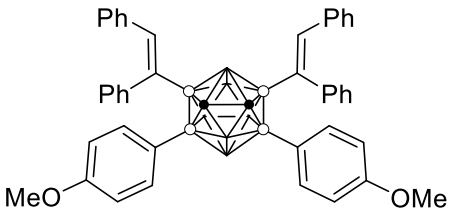
NMR ($CDCl_3$, 101 MHz): δ 142.8, 142.0, 138.8, 137.6, 134.8, 130.9, 129.3, 128.6, 128.3, 128.1, 127.9, 126.9, 126.3, 125.2 (aromatic and olefinic *C*), 51.6 (cage *C*), 23.4 (*C*H_3), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -4.5 (unresolved, 4B), -6.6 (unresolved, 4B) (*B*H *&* *B*C), -13.8 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}^+$ [M+H$^+$]: 681.4519. Found 681.4505.



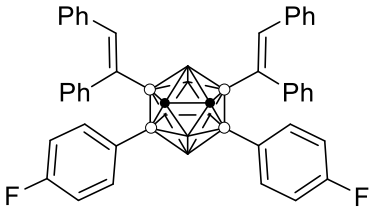
7c: Yield 88%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.20 (m, 4H), 7.10 (m, 8H), 7.02 (m, 8H), 6.88 (s, 2H), 6.78 (m, 4H), 6.44 (brs, 4H) (aromatic and olefinic *H*), 3.48 (s, 2H) (cage C*H*), 2.26 (s, 6H) (CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.0, 139.1, 137.7, 137.1, 134.1, 130.3, 129.3, 129.2, 128.6, 128.1, 127.9, 126.9, 126.2 (aromatic and olefinic *C*), 51.4 (cage *C*), 21.6 (*C*H_3), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -5.8 (unresolved, 8B) (*B*H *&* *B*C), -14.6 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}^+$ [M+H$^+$]: 681.4519. Found 681.4513.



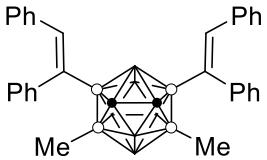
7d: Yield 87%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34 (d, J = 7.7 Hz, 4H), 7.11 (m, 10H), 7.06 (m, 6H), 6.90 (s, 2H), 6.82 (m, 4H), 6.50 (brs, 4H) (aromatic and olefinic *H*), 3.45 (s, 2H) (cage C*H*), 2.35 (s, 6H) (CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.1, 139.0, 138.2, 137.7, 133.2, 129.3, 128.8, 128.6, 128.0, 127.9, 126.9, 126.2 (aromatic and olefinic *C*), 51.5 (cage *C*), 21.5 (*C*H_3), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -5.8 (unresolved, 8B) (*B*H *&* *B*C), -14.3 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}^+$ [M+H$^+$]: 681.4519. Found 681.4514.



7e: Yield 93%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36 (d, J = 8.2 Hz, 4H), 7.12 (m, 6H), 7.04 (m, 6H), 6.90 (s, 2H), 6.82 (m, 8H), 6.48 (brs, 4H) (aromatic and olefinic *H*), 3.79 (s, 6H) (OC*H*$_3$), 3.41 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 160.2, 142.1, 138.9, 137.7, 134.5, 129.3, 128.7, 128.0, 127.9, 126.9, 126.2, 113.7 (aromatic and olefinic *C*), 55.2 (O*C*H$_3$), 51.5 (cage *C*), the four B$_{cage}$-*C* were not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ -5.9 (unresolved, 8B) (*B*H *&* *B*C), -15.1 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}O_2^+$ [M+H$^+$]: 713.4417. Found 713.4392.

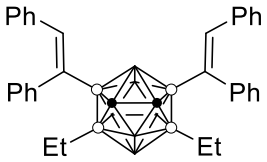


7f: Yield 81%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.38 (m, 4H), 7.14 (m, 6H), 7.05 (m, 6H), 6.98 (m, 4H), 6.91 (s, 2H), 6.80 (m, 4H), 6.47 (brs, 4H) (aromatic and olefinic *H*), 3.48 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 163.6 (d, $^{1}J_{CF}$ = 247.6 Hz), 141.8, 139.4, 137.5, 134.9 (d, $^{3}J_{CF}$ = 7.7 Hz), 129.3, 128.8, 128.0, 127.9, 127.1, 126.4, 115.1 (d, $^{2}J_{CF}$ = 20.2 Hz) (aromatic and olefinic *C*), 51.6 (cage *C*), the four B$_{cage}$-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -5.7 (unresolved, 8B) (*B*H *&* *B*C), -14.2 (unresolved, 2B) (*B*H). ^{19}F NMR (376 MHz, $CDCl_3$): -114.6 (m, 1F). HRMS (DART-positive mode) calcd for $C_{42}H_{39}B_{10}F_2^+$ [M+H$^+$]: 689.4018. Found 689.3992.

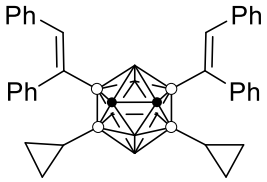


7g: Yield 85%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32 (m, 4H), 7.23 (m, 2H), 7.08 (m, 10H), 6.89 (m, 4H), 6.83 (s, 2H) (aromatic and olefinic *H*), 3.15 (s, 2H) (cage C*H*), 0.45 (s, 6H) (C*H*$_3$). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.7, 138.4, 137.6, 129.5, 129.0, 128.3, 128.0, 127.0, 126.4 (aromatic and olefinic *C*), 54.5 (cage *C*), the four B$_{cage}$-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -4.1 (d, J_{BH} = 146 Hz, 2B) (*B*H), -6.9 (unresolved, 6B) (*B*H *&* *B*C), -14.7 (unresolved, 2B) (*B*H). HRMS (DART-positive mode)

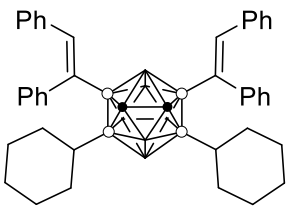
calcd for $C_{32}H_{37}B_{10}^+$ [M+H$^+$]: 529.3893. Found 529.3890.



7h: Yield 54% (70% using THF as the solvent). Light yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36 (m, 4H), 7.28 (m, 2H), 7.12 (m, 10H), 6.93 (m, 4H), 6.88 (s, 2H) (aromatic and olefinic *H*), 3.19 (s, 2H) (cage C*H*), 1.03 (m, 6H) (C*H*$_3$), 0.88 (m, 4H) (C*H*$_2$). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.6, 138.3, 137.6, 129.5, 129.0, 128.3, 128.0, 127.0, 126.4 (aromatic and olefinic *C*), 53.3 (cage *C*), 12.7 (*C*H$_2$), the four B$_{cage}$-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -4.7 (unresolved, 4B), -6.8 (unresolved, 3B) (*B*H *&* *B*C), -8.5 (d, J_{BH} = 121 Hz, 1B), -15.3 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{34}H_{41}B_{10}^+$ [M+H$^+$]: 557.4206. Found 557.4209.

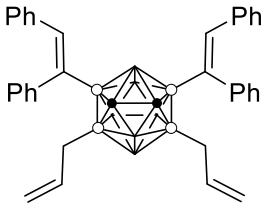


7i: Yield 81%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31 (m, 4H), 7.23 (m, 2H), 7.14 (d, J = 7.2 Hz, 4H), 7.06 (m, 6H), 6.88 (m, 6H) (aromatic and olefinic *H*), 3.18 (s, 2H), 0.67 (m, 2H), 0.55 (m, 2H), 0.44 (m, 2H), 0.23 (m, 2H), -0.05 (m, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.8, 138.4, 137.7, 129.5, 129.0, 128.3, 128.0, 126.9, 126.4 (aromatic and olefinic *C*), 53.4 (cage *C*), 6.8, 6.4 (*C*H$_2$), the four B$_{cage}$-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -5.2 (unresolved, 3B), -7.1 (unresolved, 3B) (*B*H *&* *B*C), -9.3 (d, J_{BH} = 135 Hz, 2B), -15.2 (unresolved, 1B), -16.5 (unresolved, 1B) (*B*H). HRMS (DART-positive mode) calcd for $C_{36}H_{41}B_{10}^+$ [M+H$^+$]: 581.4206. Found 581.4207.



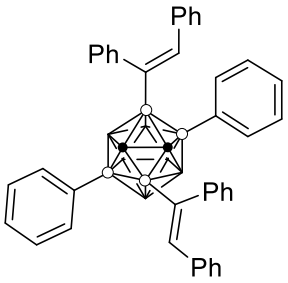
7j: Yield 48%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32 (m, 4H), 7.24 (m, 2H), 7.10 (m, 10H), 6.92 (m, 4H), 6.86 (s, 2H) (aromatic and olefinic *H*), 3.20 (s, 2H) (cage C*H*), 1.84 (m, 2H), 1.73 (m, 2H), 1.64 (m, 4H), 1.16 (m, 12H), 0.93 (m, 2H) (C*H*$_2$). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.5, 138.6, 137.7, 129.5, 128.9, 128.4, 128.0, 126.9, 126.5 (aromatic and olefinic *C*), 51.8 (cage *C*), 33.3, 32.6, 28.3, 28.0, 26.6 (*C*H$_2$),

the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ -4.9 (unresolved, 5B), -6.8 (unresolved, 2B) (*B*H *&* *B*C), -9.4 (unresolved, 1B), -16.1 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{42}H_{53}B_{10}^+$ [M+H$^+$]: 665.5145. Found 665.5142.

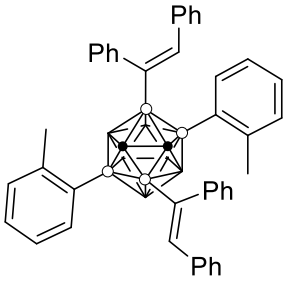


7k: Yield 79%. Light yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32 (m, 4H), 7.25 (m, 2H), 7.09 (m, 10H), 6.90 (m, 4H), 6.83 (s, 2H) (aromatic and olefinic *H*), 5.83 (m, 2H), 4.85 (m, 4H) (olefinic *H*), 3.26 (s, 2H) (cage C*H*), 1.91 (m, 2H), 1.79 (m, 2H) (CH_2). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.5, 138.6, 138.1, 137.5, 129.5, 129.0, 128.3, 128.0, 127.1, 126.5, 114.1 (aromatic and olefinic *C*), 53.2 (cage *C*), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -4.3 (unresolved, 2B), -6.6 (unresolved, 5B) (*B*H *&* *B*C), -8.1 (unresolved, 1B), -14.8 (unresolved, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{36}H_{41}B_{10}^+$ [M+H$^+$]: 581.4206. Found 581.4208.

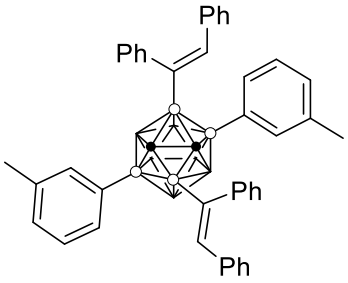
General procedure for syntheses of 8. An oven-dried Schlenk flask equipped with a stir bar was charged with 3,6-I_2-*o*-carborane (**4c**; 40 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol), diphenylacetylene (143 mg, 0.8 mmol) and dry toluene (1 mL) under an atmosphere of dry nitrogen. The flask was closed, and then stirred at 100 ^{o}C for 96 h. Then, the resulting solution was cooled to 0 ^{o}C, to which was slowly added RMgBr (0.5 mmol, 1.0 M in THF, 0.5 mL). After warming to room temperature, the reaction mixture was stirred at 80 ^{o}C for 24 h. After quenching with water (1 mL) and extraction with ethyl acetate (5 mL × 3), the organic portions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (300-400 mesh) using *n*-hexane as eluent to give the product **8**.



8a: Yield 95%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47 (m, 4H), 7.31 (m, 6H), 7.17 (m, 2H), 7.09 (m, 4H), 7.01 (m, 6H), 6.96 (s, 2H), 6.69 (m, 4H), 6.34 (brs, 4H) (aromatic and olefinic *H*), 3.38 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.7, 140.8, 136.9, 133.4, 129.5, 129.5, 128.5, 128.0, 128.0, 127.6, 127.1, 126.9 (aromatic and olefinic *C*), 56.5 (cage *C*), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -2.9 (d, J_{BH} = 140 Hz, 2B) (*B*H), -5.2 (s, 4B) (*B*C), -11.4 (d, J_{BH} = 228 Hz, 2B), -12.7 (d, J_{BH} = 148 Hz, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{42}H_{44}B_{10}N^+$ [M+NH_4^+]: 670.4471. Found 670.4469.

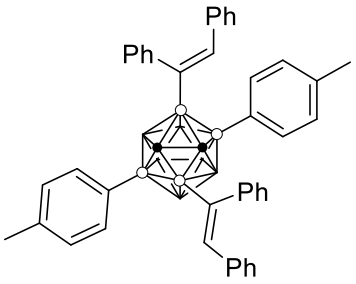


8b: Yield 91%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.38 (d, J = 6.9 Hz, 2H), 7.20 (m, 12H), 7.09 (d, J = 7.4 Hz, 2H), 6.99 (m, 6H), 6.67 (s, 2H), 6.56 (m, 6H) (aromatic and olefinic *H*), 3.58 (s, 2H) (cage C*H*), 2.33 (s, 6H) (CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.2, 141.7, 141.2, 136.8, 135.3, 130.8, 129.6, 129.4, 128.3, 128.0, 127.5, 127.2, 126.9, 125.5 (aromatic and olefinic *C*), 55.5 (cage *C*), 23.3 (*C*H_3), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 128 MHz): δ -2.8 (d, J_{BH} = 113 Hz, 2B) (*B*H), -4.8 (s, 4B) (*B*C), -11.7 (unresolved, 4B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}^+$ [M+H^+]: 681.4519. Found 681.4512.

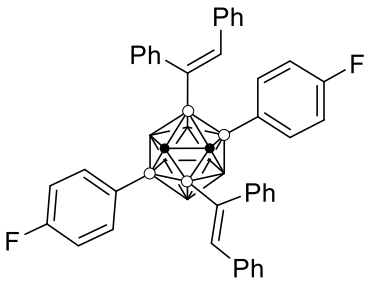


8c: Yield 86%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.24 (s, 2H), 7.12 (m, 12H), 6.99 (m, 8H), 6.70 (m, 4H), 6.32 (m, 4H) (aromatic and olefinic *H*), 3.36 (s, 2H) (cage C*H*), 2.29 (s, 6H) (CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.6, 140.8, 137.1, 136.9, 134.3, 130.4, 129.4, 129.4, 129.2, 128.0, 127.8, 127.5, 127.2, 126.8 (aromatic and olefinic *C*), 56.6 (cage *C*), 21.6 (*C*H_3), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -2.6 (d, J_{BH} = 152 Hz, 2B) (*B*H),

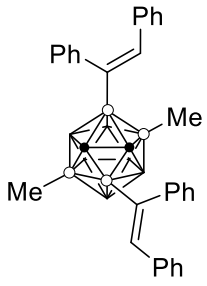
-4.5 (s, 4B) (*B*C), -11.9 (unresolved, 4B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}^+$ [M+H$^+$]: 681.4519. Found 681.4514.



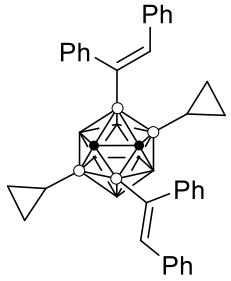
8d: Yield 93%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.37 (d, J = 7.6 Hz, 2H), 7.17 (m, 2H), 7.10 (m, 8H), 7.04 (m, 6H), 6.98 (s, 2H), 6.71 (m, 4H), 6.35 (brs, 4H) (aromatic and olefinic *H*), 3.35 (s, 2H) (cage C*H*), 2.34 (s, 6H) (CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.5, 140.9, 138.2, 137.0, 133.4, 129.5, 128.7, 128.0, 127.5, 127.1, 126.8 (aromatic and olefinic *C*), 56.5 (cage *C*), 21.5 (*C*H$_3$), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -2.9 (d, J_{BH} = 102 Hz, 2B) (*B*H), -5.1 (s, 4B) (*B*C), -11.3 (d, J_{BH} = 235 Hz, 2B), -12.8 (d, J_{BH} = 111 Hz, 2B) (*B*H). HRMS (DART-positive mode) calcd for $C_{44}H_{45}B_{10}^+$ [M+H$^+$]: 681.4519. Found 681.4518.



8e: Yield 92%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.45 (m, 4H), 7.18 (m, 2H), 7.11 (m, 4H), 7.01 (m, 12H), 6.72 (d, J = 7.0 Hz, 4H), 6.32 (brs, 4H) (aromatic and olefinic *H*), 3.37 (s, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 163.6 (d, $^1J_{CF}$ = 247.5 Hz), 143.0, 140.7, 136.7, 135.2 (d, $^3J_{CF}$ = 7.7 Hz), 129.6, 129.5, 128.1, 127.8, 127.0, 115.0 (d, $^2J_{CF}$ = 20.2 Hz) (aromatic and olefinic *C*), 56.8 (cage *C*), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -2.8 (d, J_{BH} = 108 Hz, 2B) (*B*H), -5.4 (s, 4B) (*B*C), -11.4 (d, J_{BH} = 166 Hz, 2B), -12.7 (d, J_{BH} = 153 Hz, 2B) (*B*H). ^{19}F NMR (376 MHz, $CDCl_3$): -113.5 (m, 1F). HRMS (DART-positive mode) calcd for $C_{42}H_{39}B_{10}F_2^+$ [M+H$^+$]: 689.4018. Found 689.4018.



8f: Yield 90%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.22 (m, 6H), 7.08 (m, 8H), 6.86 (m, 4H), 6.75 (m, 4H) (aromatic and olefinic *H*), 2.92 (s, 2H) (cage C*H*), 0.50 (s, 6H) (CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 141.7, 141.2, 136.9, 129.7, 129.6, 128.1, 127.6, 127.2, 127.0 (aromatic and olefinic *C*), 57.6 (cage *C*), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -2.9 (d, J_{BH} = 147 Hz, 2B) (*B*H), -6.1 (s, 4B) (*B*C), -11.2 (d, J_{BH} = 219 Hz, 2B), -12.5 (d, J_{BH} = 152 Hz, 2B) (*B*H). Anal. Calcd for $C_{32}H_{36}B_{10}$: C, 72.69; H, 6.86. Found C, 72.75; H, 7.07.



8g: Yield 66%. White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.23 (m, 6H), 7.16 (s, 2H), 7.09 (m, 6H), 6.88 (m, 4H), 6.80 (m, 4H) (aromatic and olefinic *H*), 3.00 (s, 2H), 0.69 (m, 2H), 0.56 (m, 2H), 0.45 (m, 2H), 0.24 (m, 2H), 0.08 (m, 2H) (cage C*H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 141.7, 141.2, 137.0, 129.7, 129.6, 128.1, 127.6, 127.2, 127.0 (aromatic and olefinic *C*), 57.1 (cage *C*), 6.5, 6.3 (*C*H_2), the four B_{cage}-*C* were not observed. ^{11}B NMR ($CDCl_3$, 193 MHz): δ -4.6 (d, J_{BH} = 119 Hz, 2B) (*B*H), -6.1 (s, 4B) (*B*C), -12.8 (d, J_{BH} = 153 Hz, 2B), -13.6 (d, J_{BH} = 117 Hz, 2B) (*B*H). Anal. Calcd for $C_{36}H_{40}B_{10}$: C, 74.45; H, 6.94. Found C, 73.97; H, 6.84.

X-ray Structure Determination. The data of **2**, **3**, **5c**, **7j**, **8a** and **8g** were collected at 170 K on a Bruker APEX DUO diffractometer. An empirical absorption correction was applied using the SADABS program.[5] All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least-squares on F^2 using the SHELXTL program package.[6] All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and structure refinements were given in Table S1.

CCDC 2091154-2091159 (**2**, **3**, **5c**, **7j**, **8a** and **8g**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal Data and Summary of Data Collection and Refinement for **2**, **3**, **5c**, **7j**, **8a** and **8g**.

Compound No.	**2**	**3**	**5c**	**7j**	**8a**	**8g**
formula	$C_{16}H_{21}B_{10}I$	$C_{16}H_{21}B_{10}I$	$C_{30}H_{30}B_{10}I_2$	$C_{42}H_{52}B_{10}$	$C_{42}H_{40}B_{10}$	$C_{36}H_{40}B_{10}$
crystal size(mm^3)	0.1 x 0.08 x 0.06	0.15 x 0.1 x 0.08	0.15 x 0.08 x 0.06	0.1 x 0.08 x 0.06	0.1 x 0.03 x 0.001	0.15 x 0.08 x 0.08
fw	448.33	448.33	752.44	664.93	652.84	580.78
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1$	$P2_1/n$	$C2/c$	$P2_1/c$	$C2/c$	$P2_1/c$
a, Å	8.418(1)	11.446(1)	24.055(1)	12.154(1)	17.353(2)	19.531(1)
b, Å	12.482(1)	12.797(1)	10.937(1)	18.859(1)	10.570(1)	21.599(1)
c, Å	10.406(1)	14.484(1)	17.081(1)	17.606(1)	19.807(1)	17.610(1)
β, deg	113.774(1)	99.139(1)	133.676(1)	99.467(1)	97.064(9)	116.151(1)
V, $Å^3$	1000.6(1)	2094.6(1)	3250.2(1)	3980.5(1)	3605.4(7)	6668.5(2)
Z	2	4	4	4	4	8
D_{calcd}, Mg/m^3	1.488	1.422	1.538	1.110	1.203	1.157
radiation(λ), Å	1.34139	1.34139	1.34139	1.34139	1.34139	1.34139
2θ range, deg	8.1 to 109.8	8.0 to 109.8	8.3 to 110.0	7.6 to 109.9	7.8 to 110.8	5.6 to 109.9
μ, mm^{-1}	8.382	8.008	10.273	0.274	0.302	0.285
F(000)	440	880	1464	1416	1368	2448
no. of obsd reflns	3331	3963	3099	7535	3340	12640
no. of params refnd	244	244	190	514	235	829
goodness of fit	1.092	1.065	1.074	1.282	1.055	1.026
R1	0.0229	0.0320	0.0412	0.0538	0.1009	0.0595
wR2	0.0544	0.0777	0.1046	0.1641	0.2362	0.1372

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1 (a) M. R. Bhaskar, B. K. Carolyn and M. F. Hawthorne, *Inorg. Chem.*, 2006, **45**, 336; (b) P. O. Frederic and M. F. Hawthorne, *Inorg. Chem.*, 1965, **4**, 1839.

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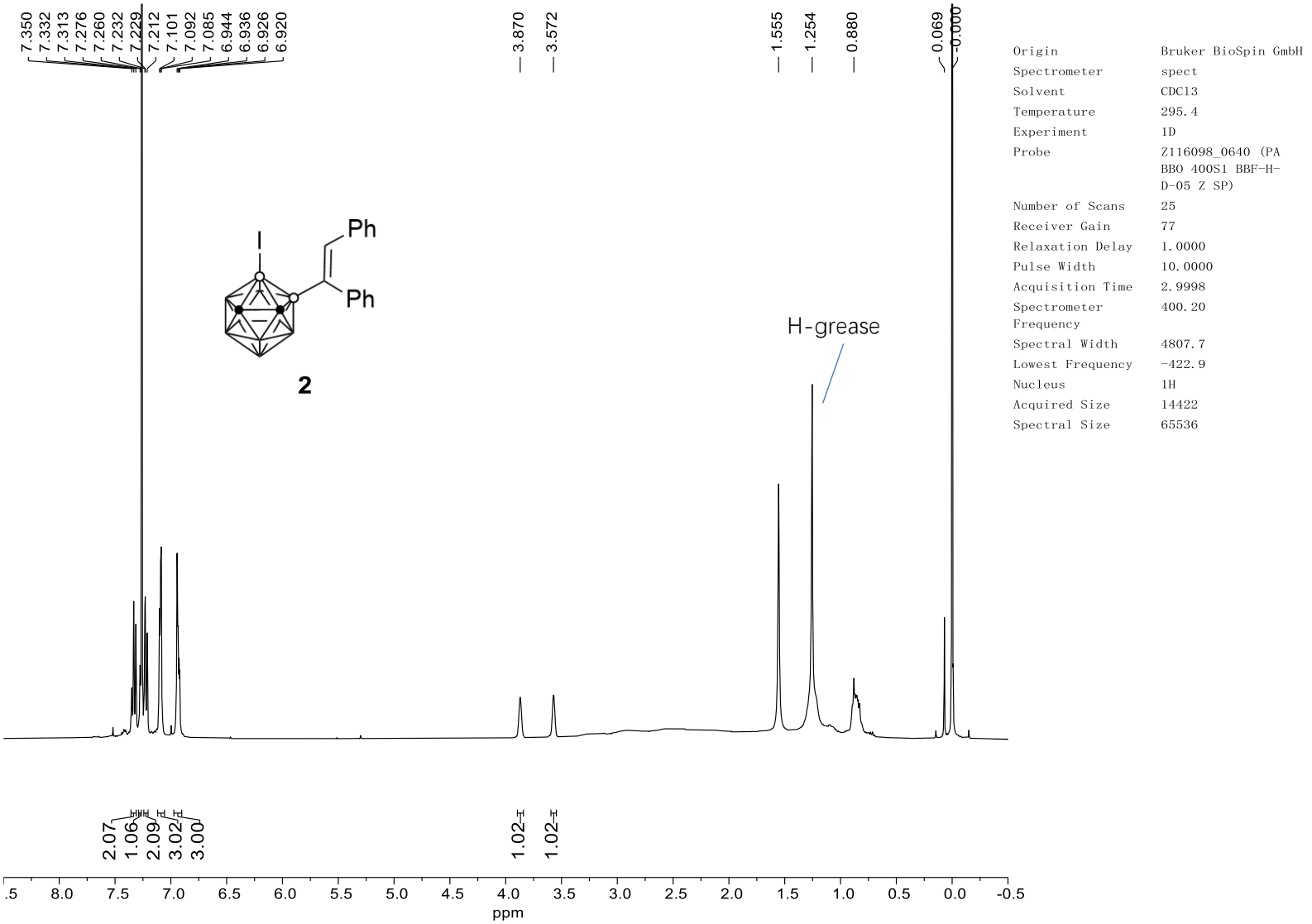

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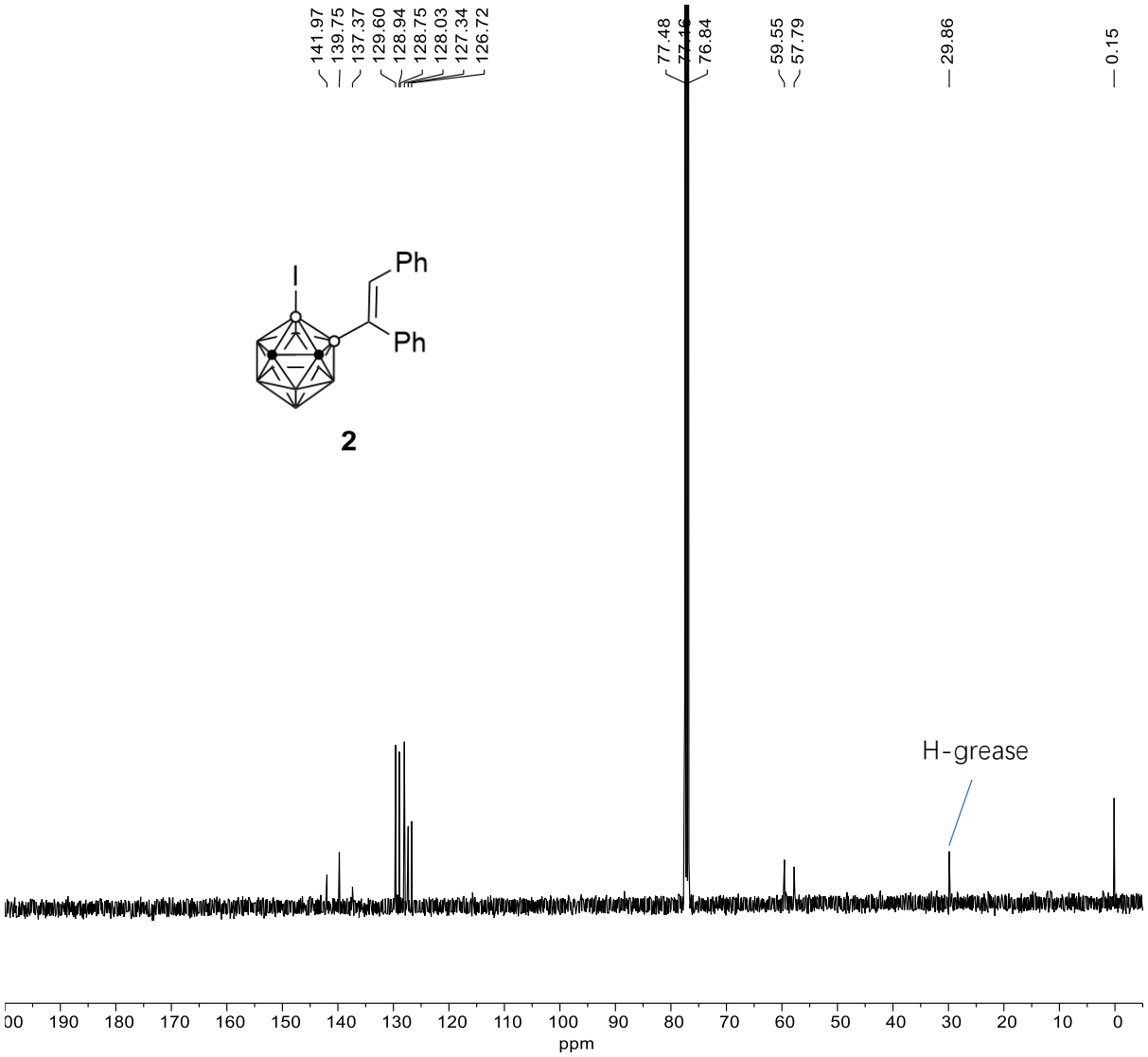

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Spectrometer	spect
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Experiment	1D
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Number of Scans	2000
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Pulse Width	10.0000
Acquisition Time	0.6999
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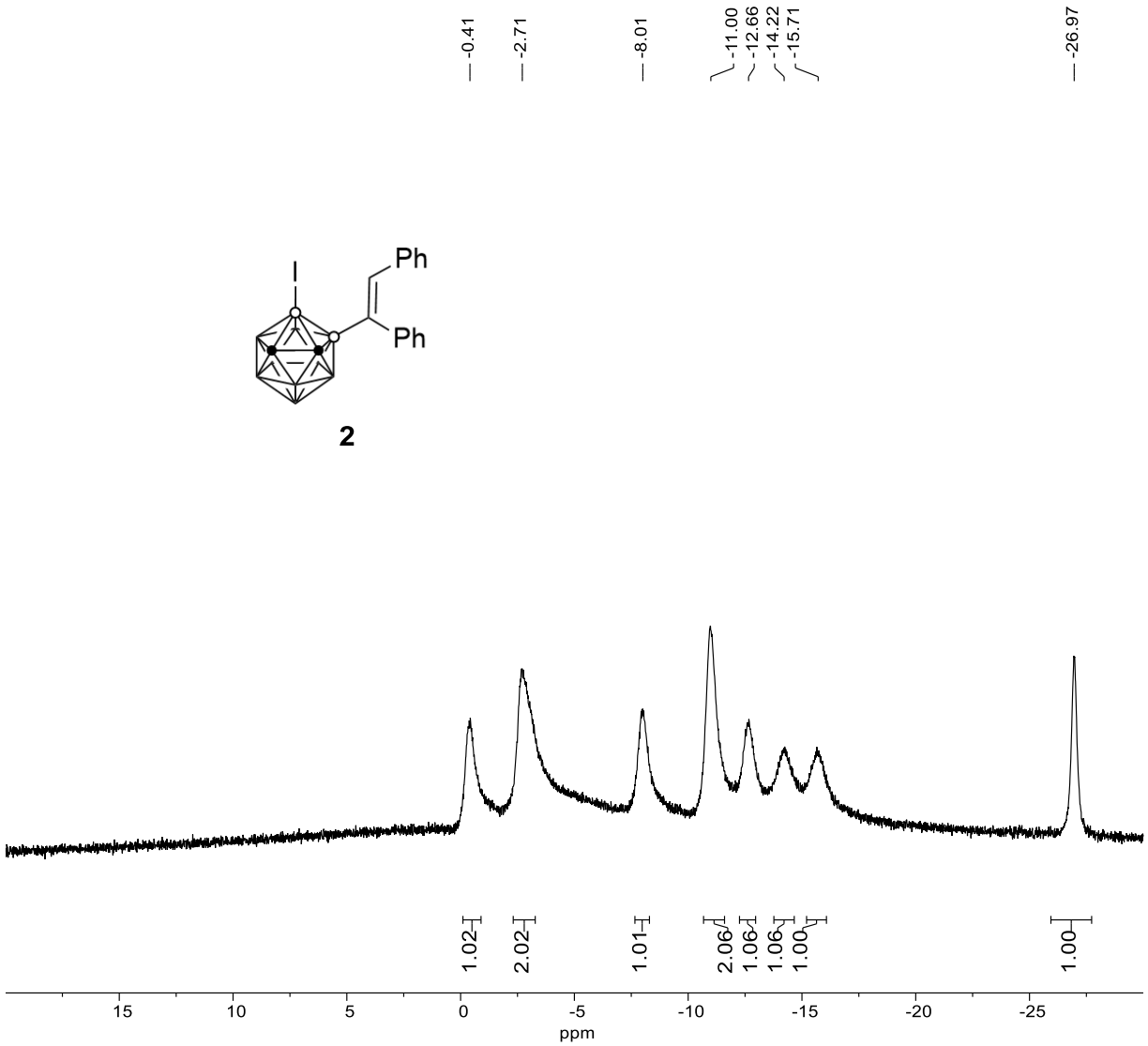
Nucleus	13C
Acquired Size	17675
Spectral Size	65536



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Solvent	CDCl3
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Experiment	1D
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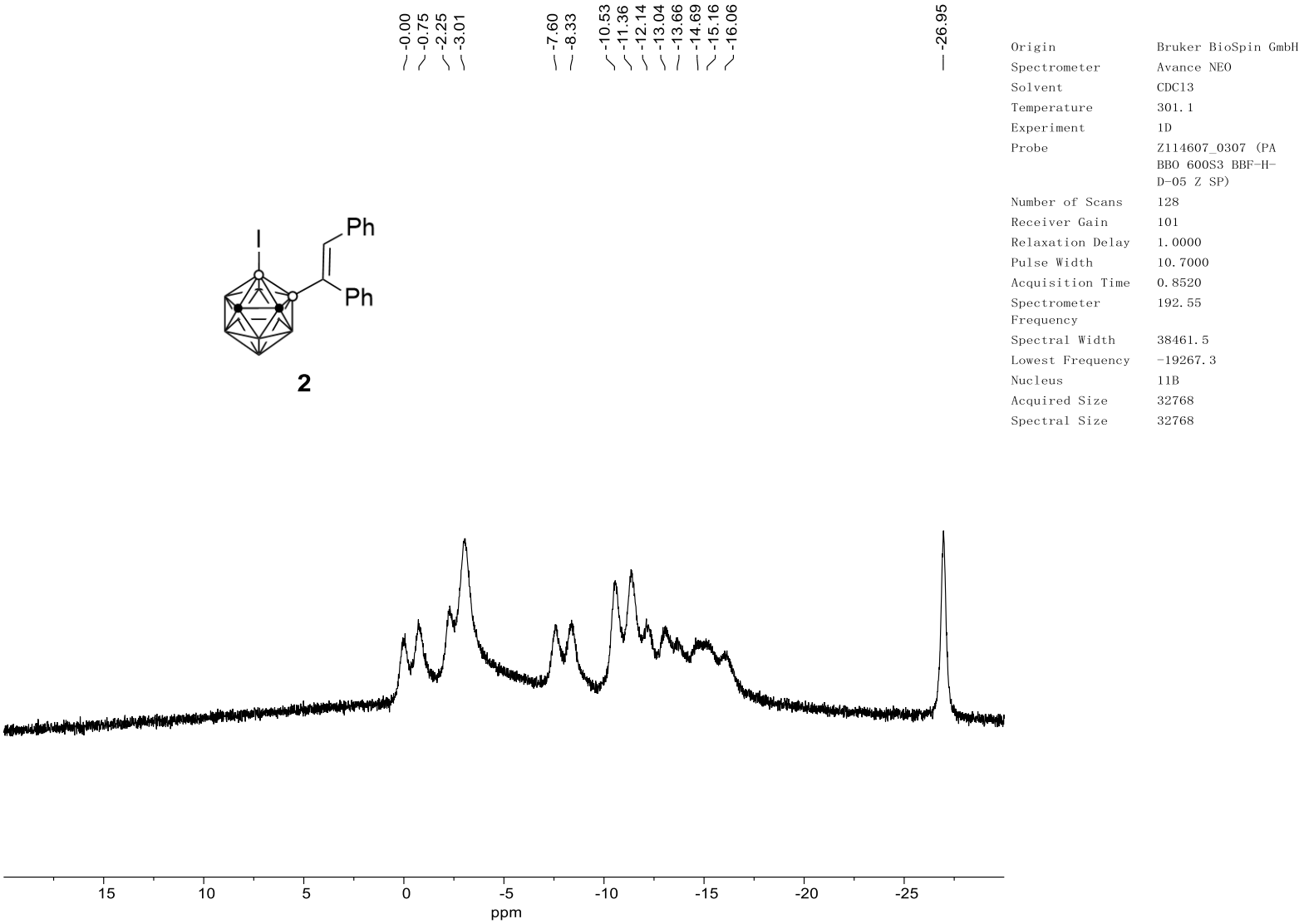

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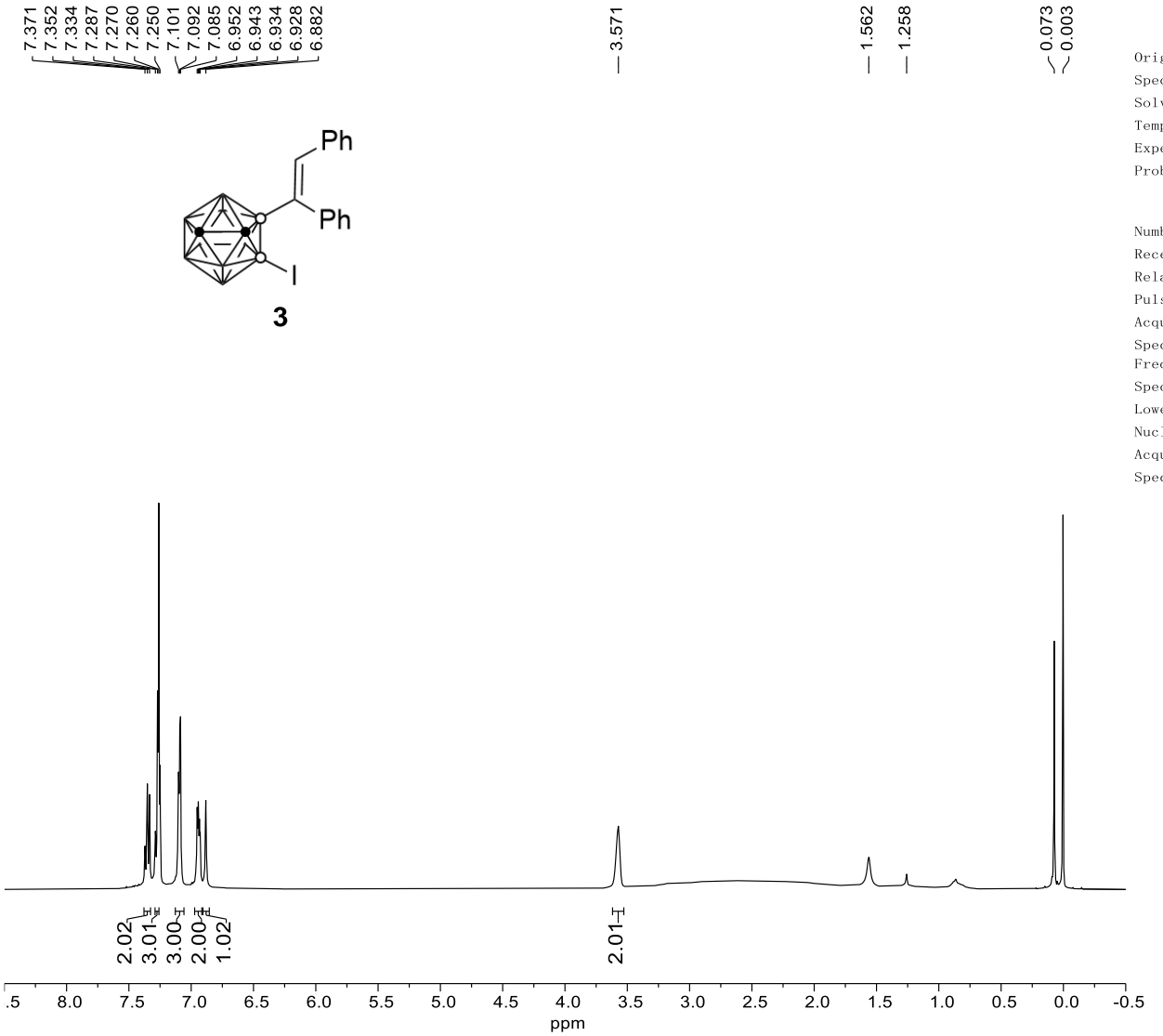
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Ph
Ph
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3
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 295.4
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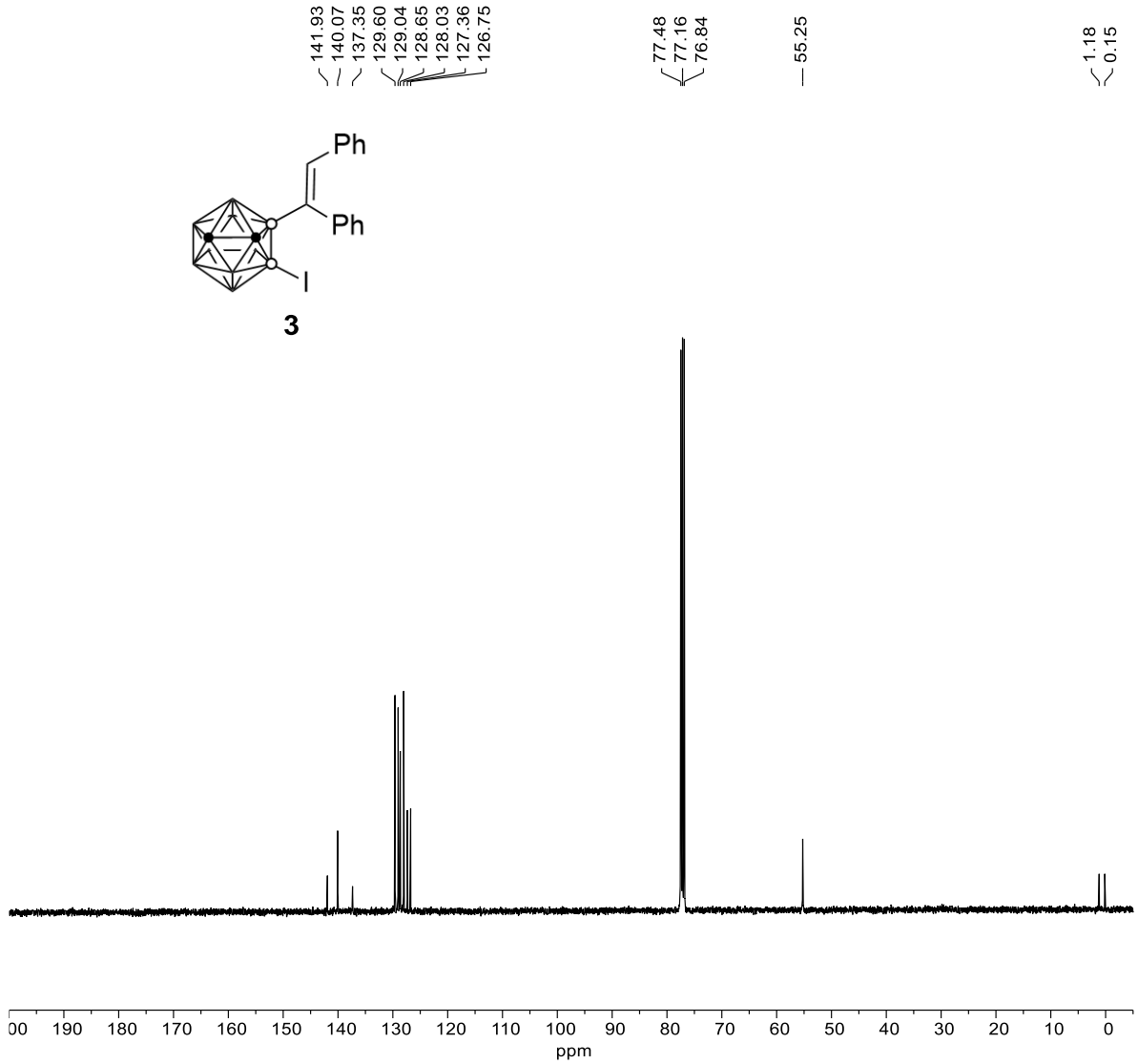

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Spectrometer	spect
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Experiment	1D
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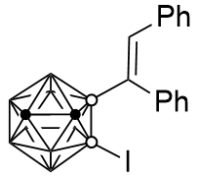
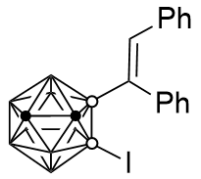
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	0.6999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1546.1
Nucleus	13C
Acquired Size	17675
Spectral Size	65536



3

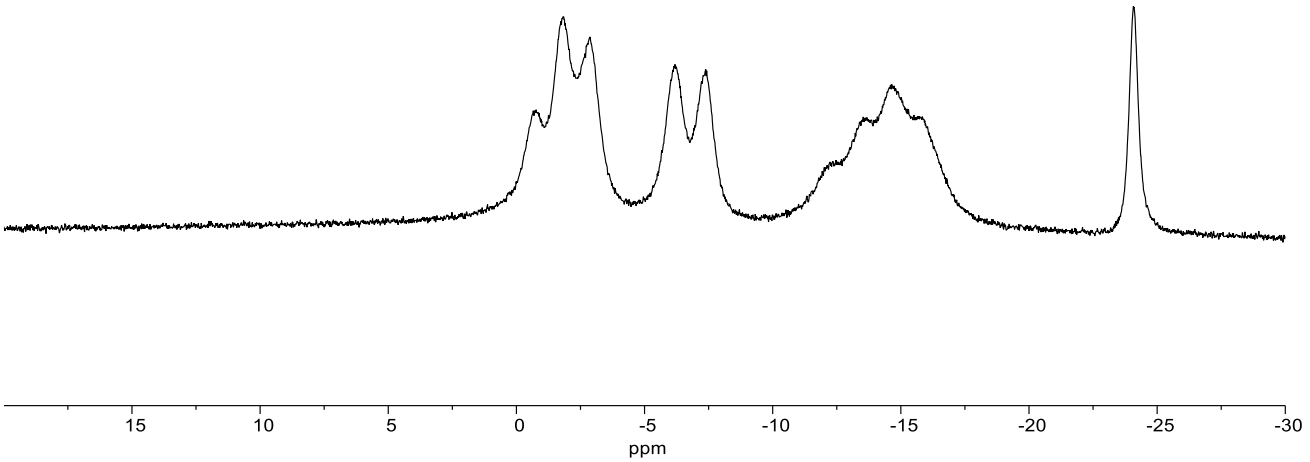
Solvent	CDCl3
Number of Scans	128
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19578.2
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

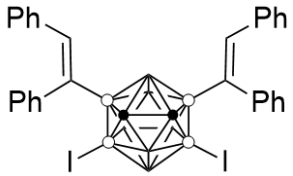


3

-0.67
-1.80
-2.85
-6.17
-7.38
-12.35
-13.63
-14.56
-15.75
-24.09

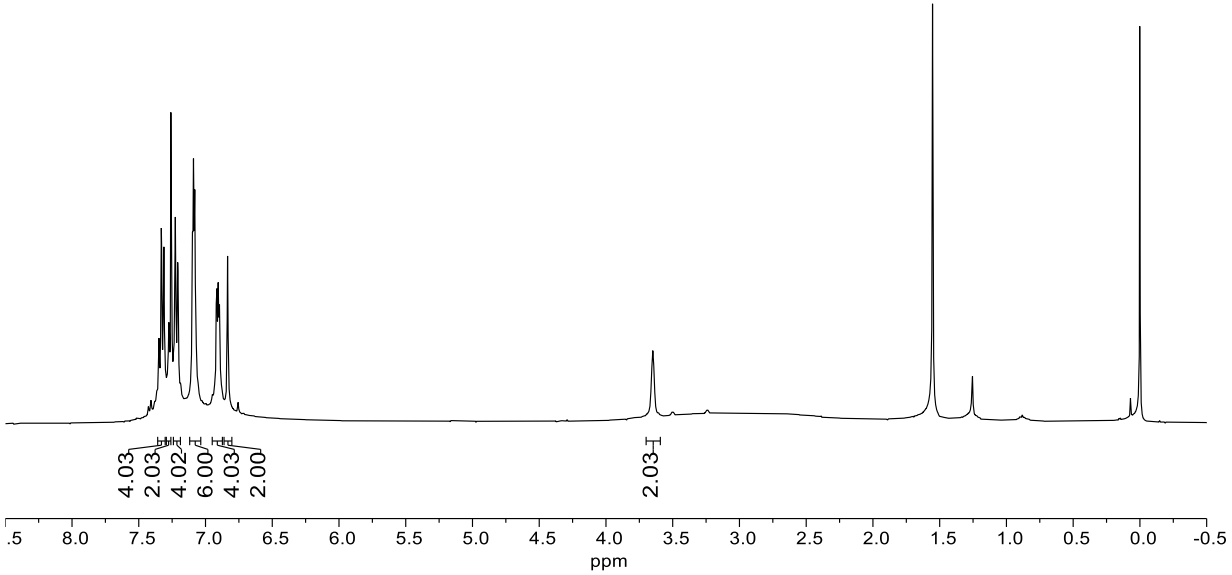
Solvent	CDCl3
Number of Scans	128
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19578.2
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

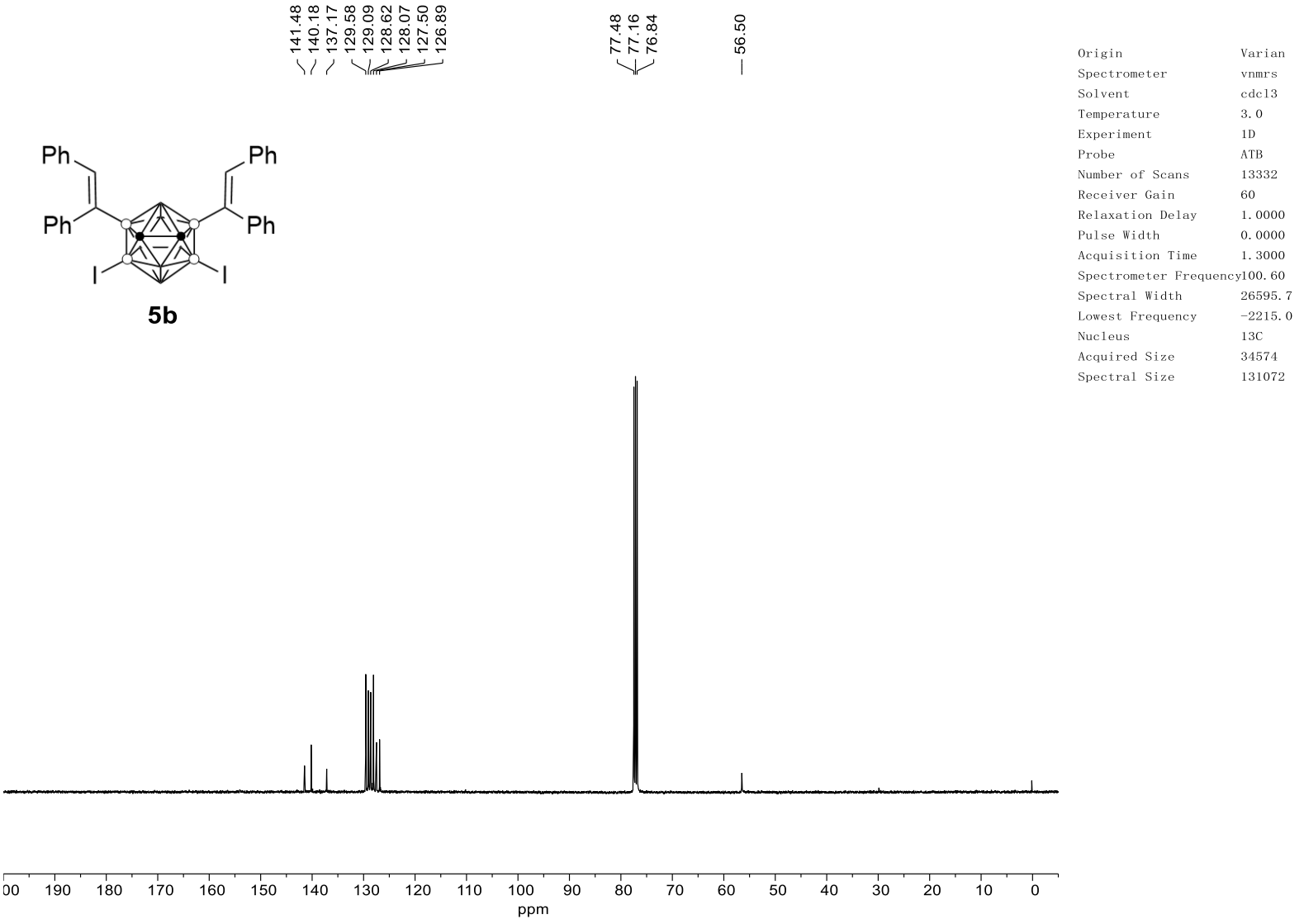


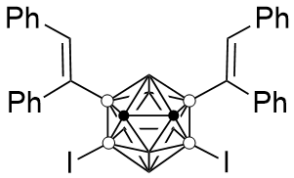


5b

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	295.6
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	11
Receiver Gain	126
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-413.3
Nucleus	1H
Acquired Size	14422
Spectral Size	65536

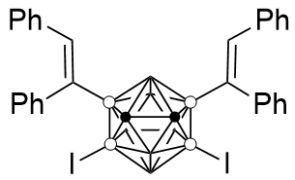



141.48
140.18
137.17
129.58
129.09
128.62
128.07
127.50
126.89
77.48
77.16
76.84
56.50
Ph
Ph
Ph
Ph
I
I
5b
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 3.0
Experiment 1D
Probe ATB
Number of Scans 13332
Receiver Gain 60
Relaxation Delay 1.0000
Pulse Width 0.0000
Acquisition Time 1.3000
Spectrometer Frequency 100.60
Spectral Width 26595.7
Lowest Frequency -2215.0
Nucleus 13C
Acquired Size 34574
Spectral Size 131072
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


Ph
Ph
Ph
Ph
I
I

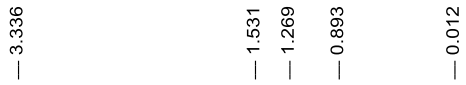
5b

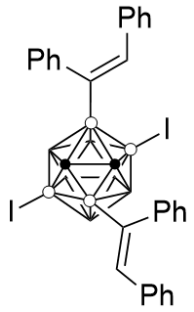
-1.08
-4.26
-12.26
-24.71
Solvent CDCl3
Number of Scans 128
Receiver Gain 362
Relaxation Delay 0.0000
Pulse Width 5.0000
Spectrometer Frequency 128.38
Spectral Width 38461.5
Lowest Frequency -19532.4
Nucleus 11B
Acquired Size 16384
Spectral Size 32768
2.05
4.09
2.35
2.00
15
10
5
0
-5
-10
-15
-20
-25
ppm



5b

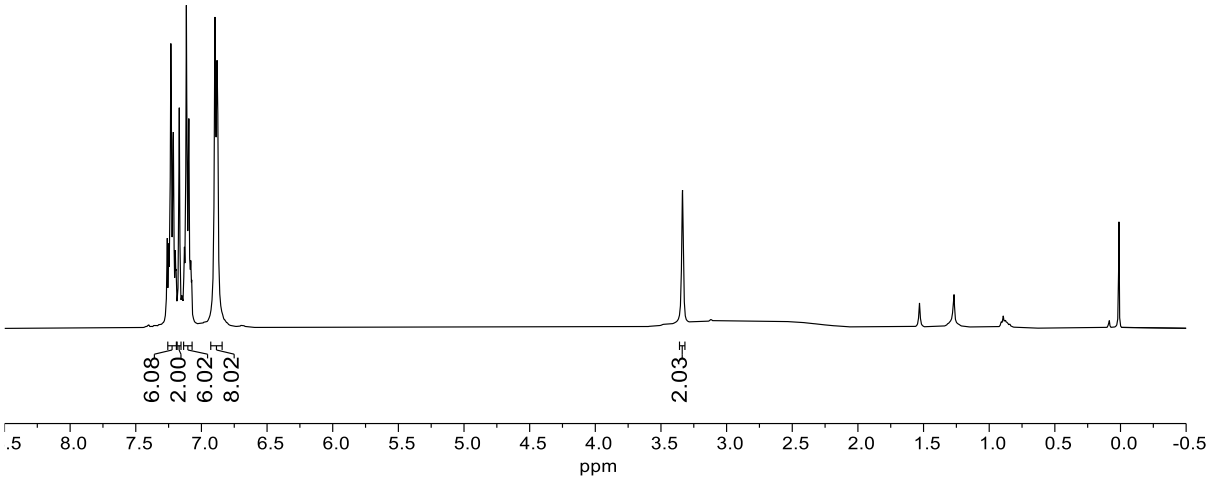
Solvent	CDCl3
Number of Scans	128
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19532.4
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

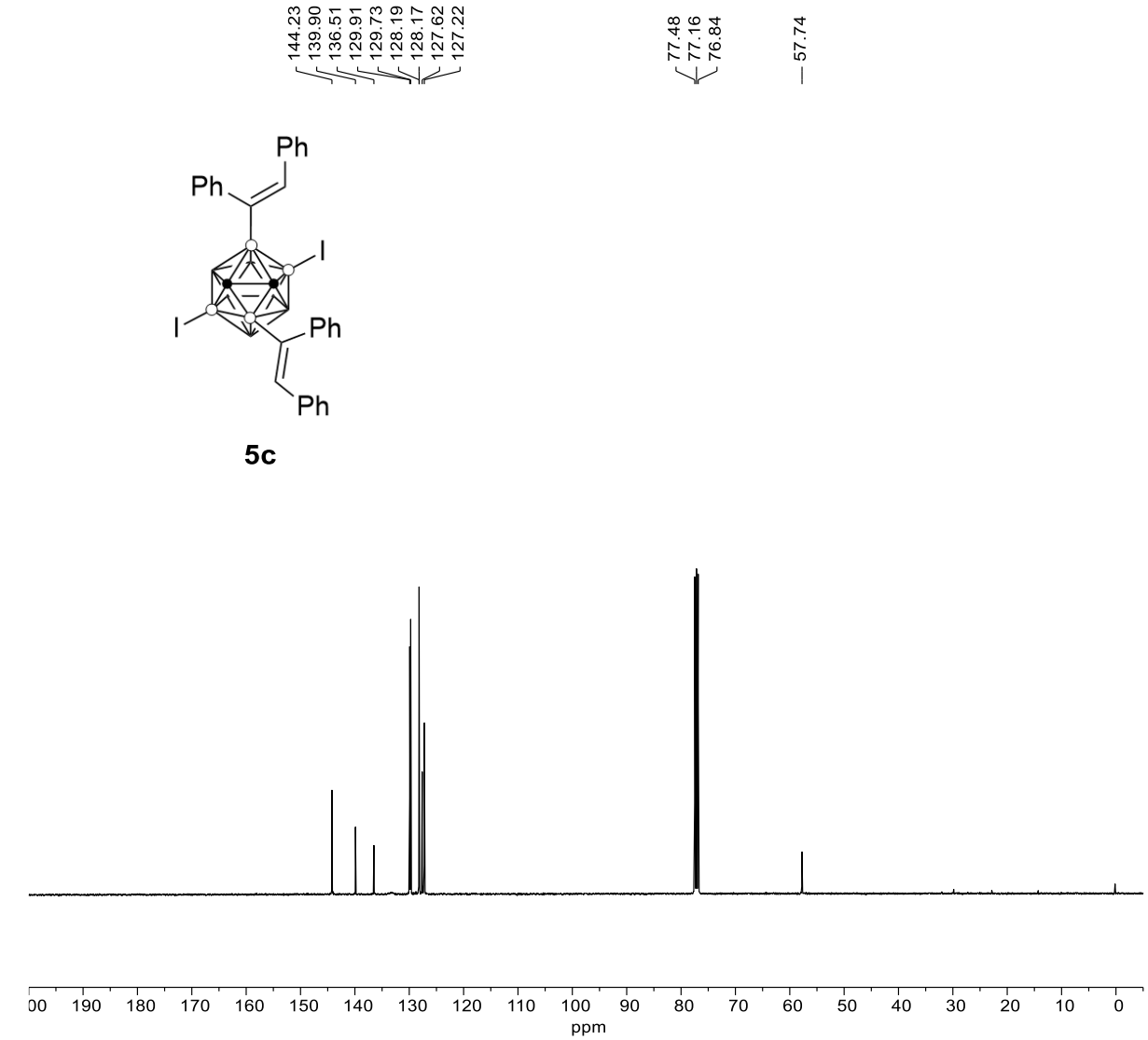


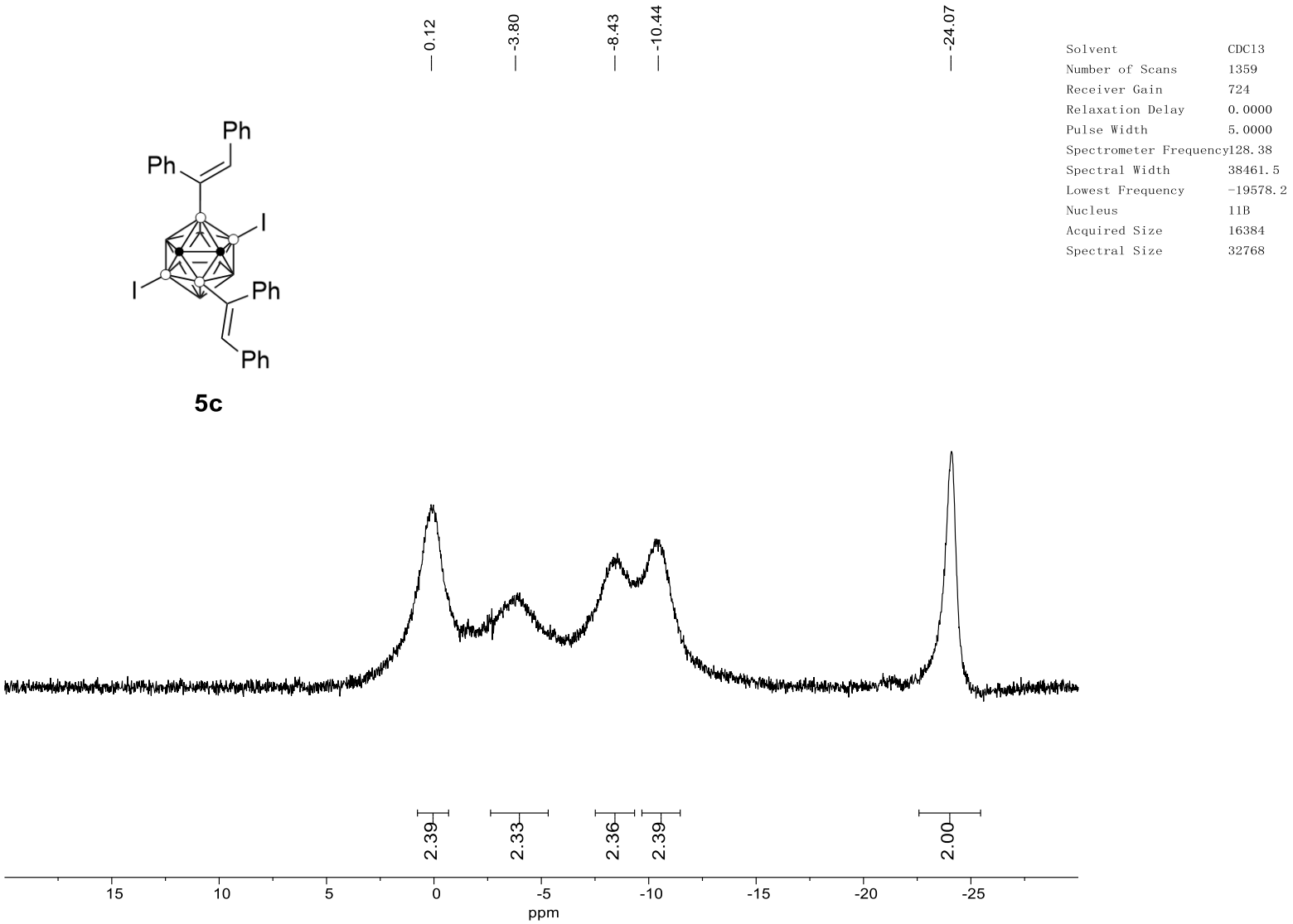


5c

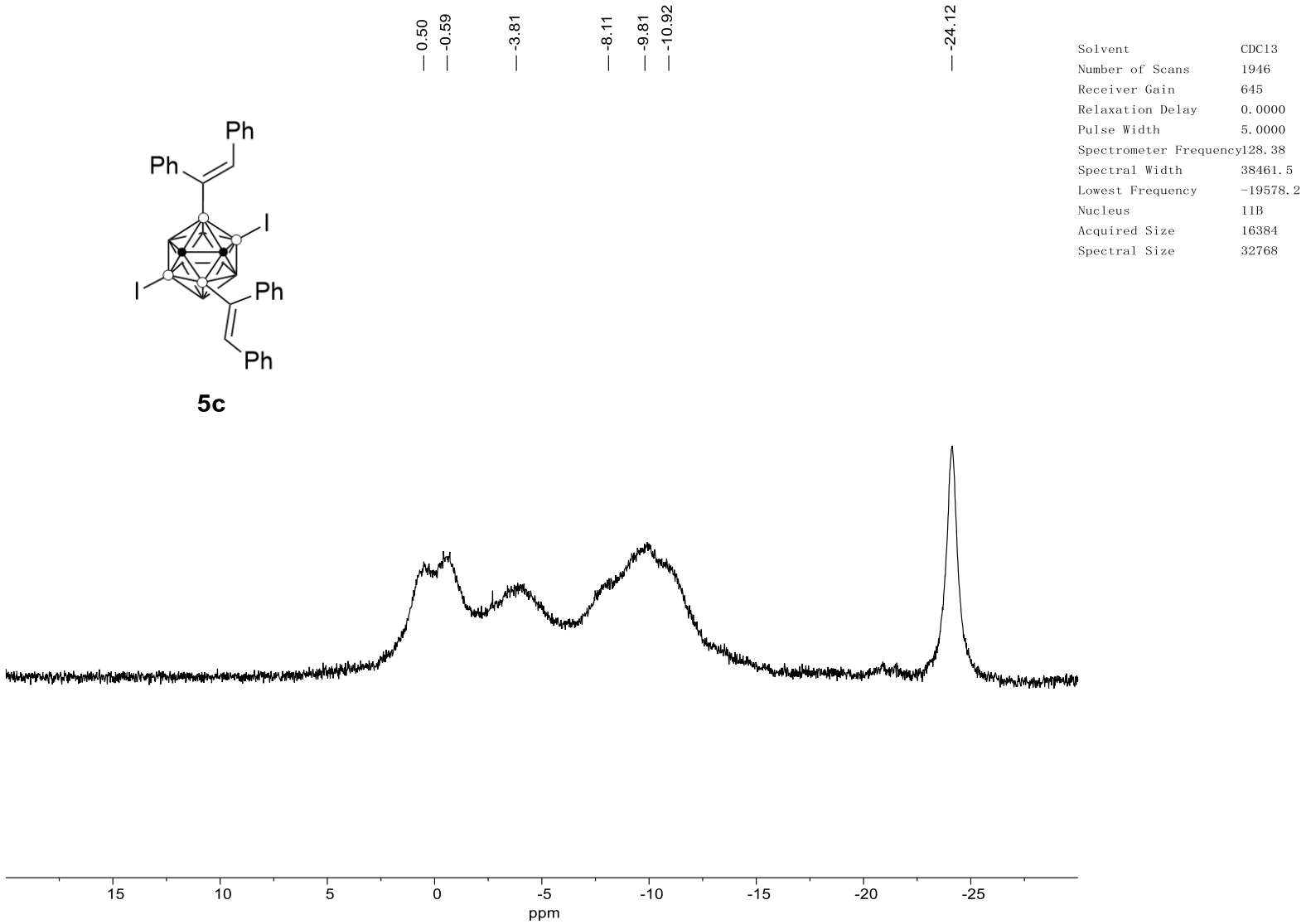
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	77
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-407.0
Nucleus	1H
Acquired Size	14385
Spectral Size	65536



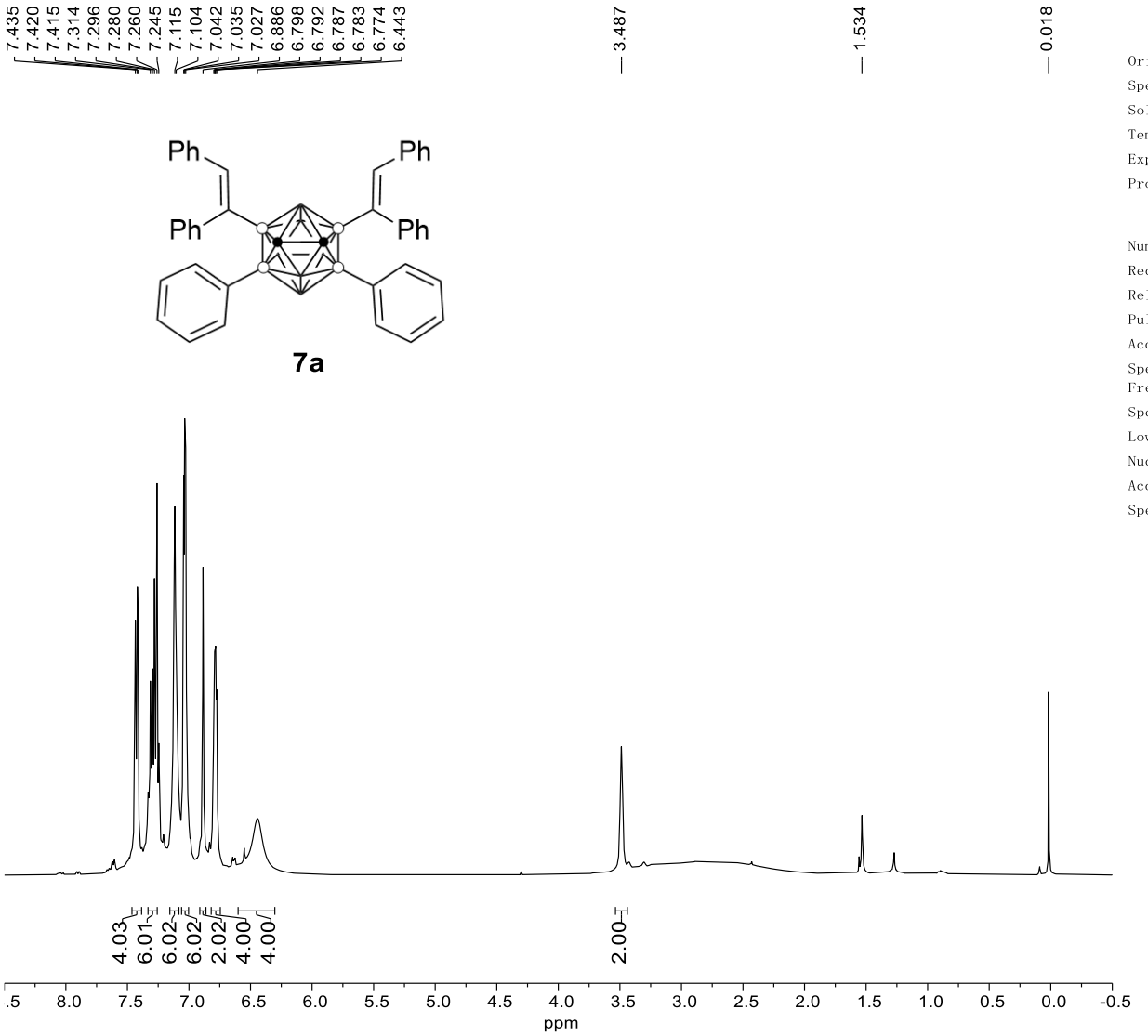

144.23
139.90
136.51
129.91
129.73
128.19
128.17
127.62
127.22
77.48
77.16
76.84
57.74
Ph
Ph
I
I
Ph
Ph
5c
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 298.1
Experiment 1D
Probe Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 4300
Receiver Gain 197
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.2999
Spectrometer Frequency 100.62
Spectral Width 25252.5
Lowest Frequency -1547.0
Nucleus 13C
Acquired Size 32827
Spectral Size 131072
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


0.12
-3.80
-8.43
-10.44
-24.07
Solvent CDCl3
Number of Scans 1359
Receiver Gain 724
Relaxation Delay 0.0000
Pulse Width 5.0000
Spectrometer Frequency 128.38
Spectral Width 38461.5
Lowest Frequency -19578.2
Nucleus 11B
Acquired Size 16384
Spectral Size 32768
Ph
Ph
I
I
Ph
Ph
2.39
2.33
2.36
2.39
2.00
15
10
5
0
-5
-10
-15
-20
-25
ppm

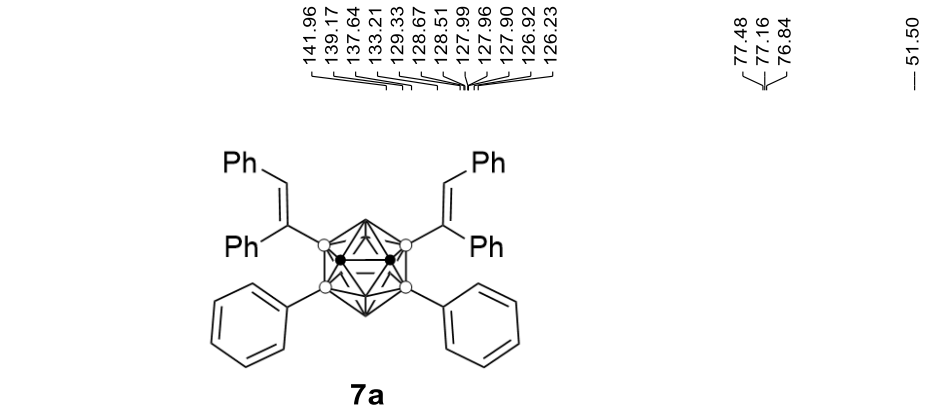
5c


0.50
-0.59
-3.81
-8.11
-9.81
-10.92
-24.12
Solvent CDCl3
Number of Scans 1946
Receiver Gain 645
Relaxation Delay 0.0000
Pulse Width 5.0000
Spectrometer Frequency 128.38
Spectral Width 38461.5
Lowest Frequency -19578.2
Nucleus 11B
Acquired Size 16384
Spectral Size 32768
Ph
Ph
I
I
Ph
Ph
15
10
5
0
-5
-10
-15
-20
-25
ppm

5c

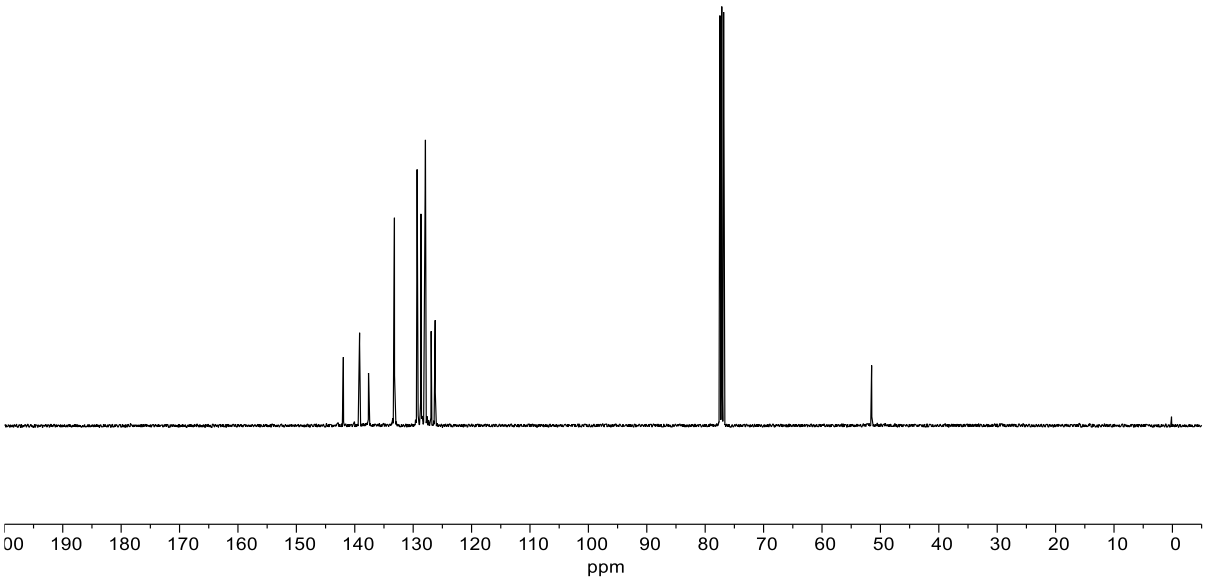


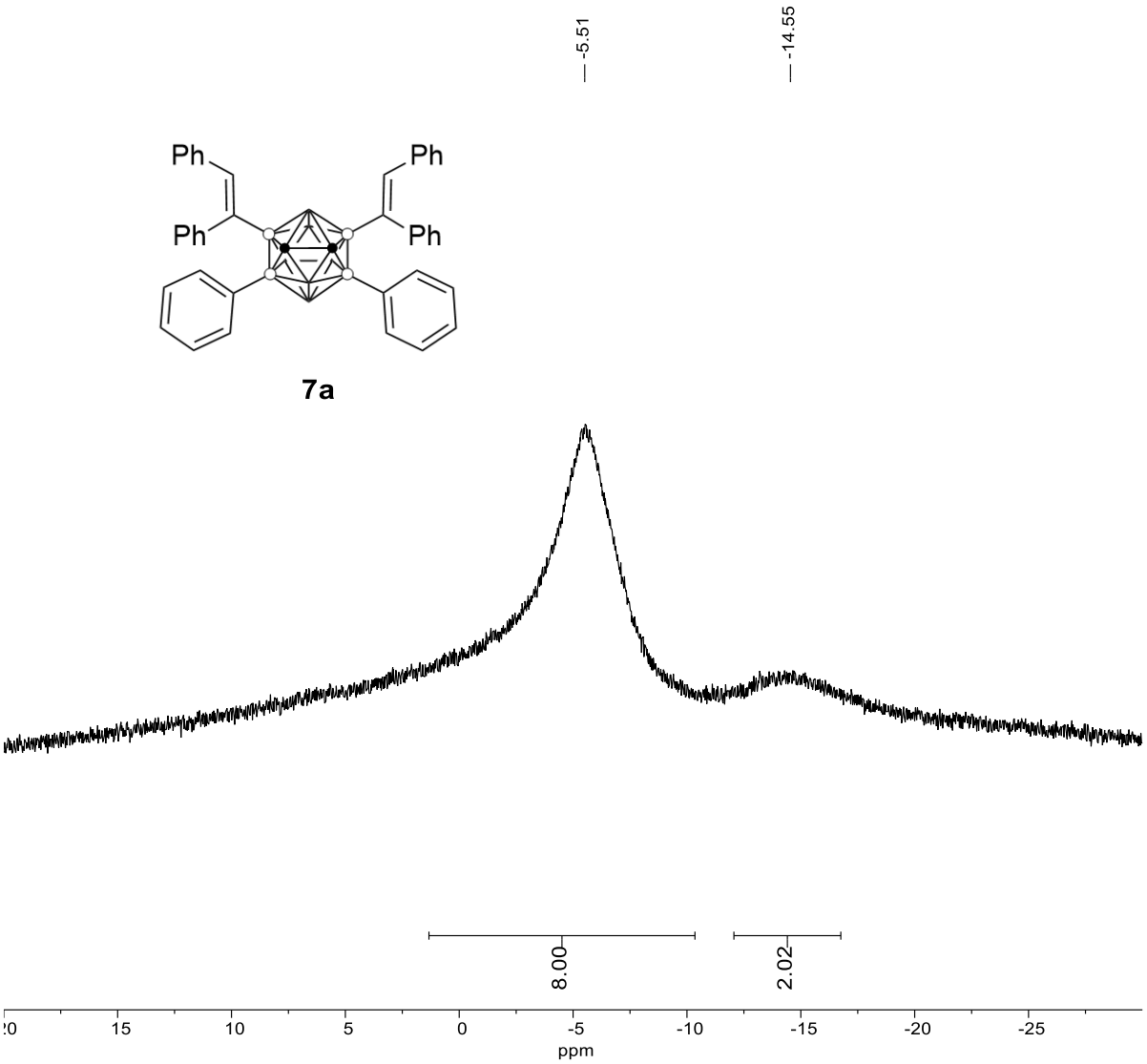
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.1
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	10
Receiver Gain	77
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-412.9
Nucleus	1H
Acquired Size	14422
Spectral Size	65536



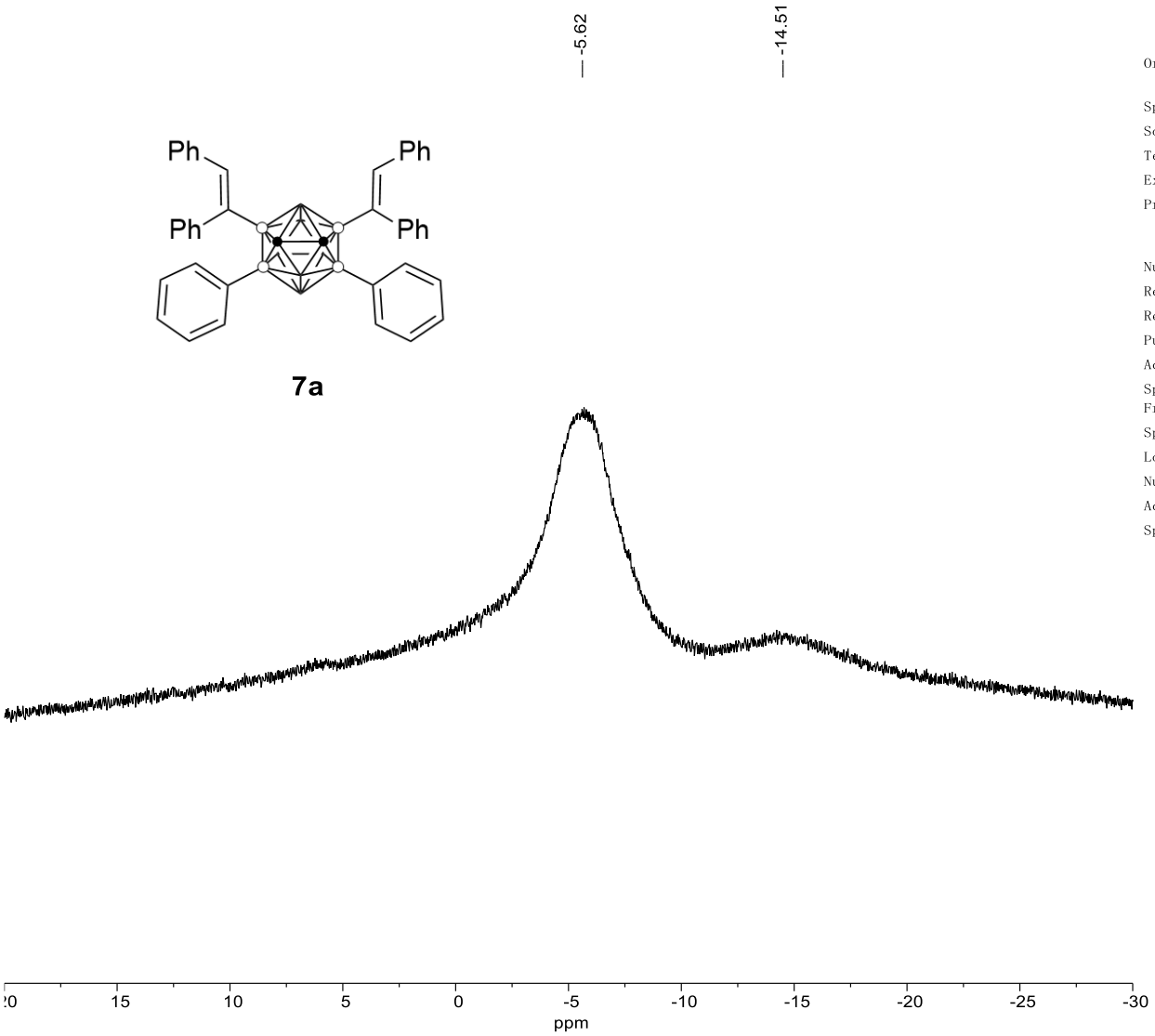
7a

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	2900
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1547.7
Nucleus	13C
Acquired Size	32827
Spectral Size	131072

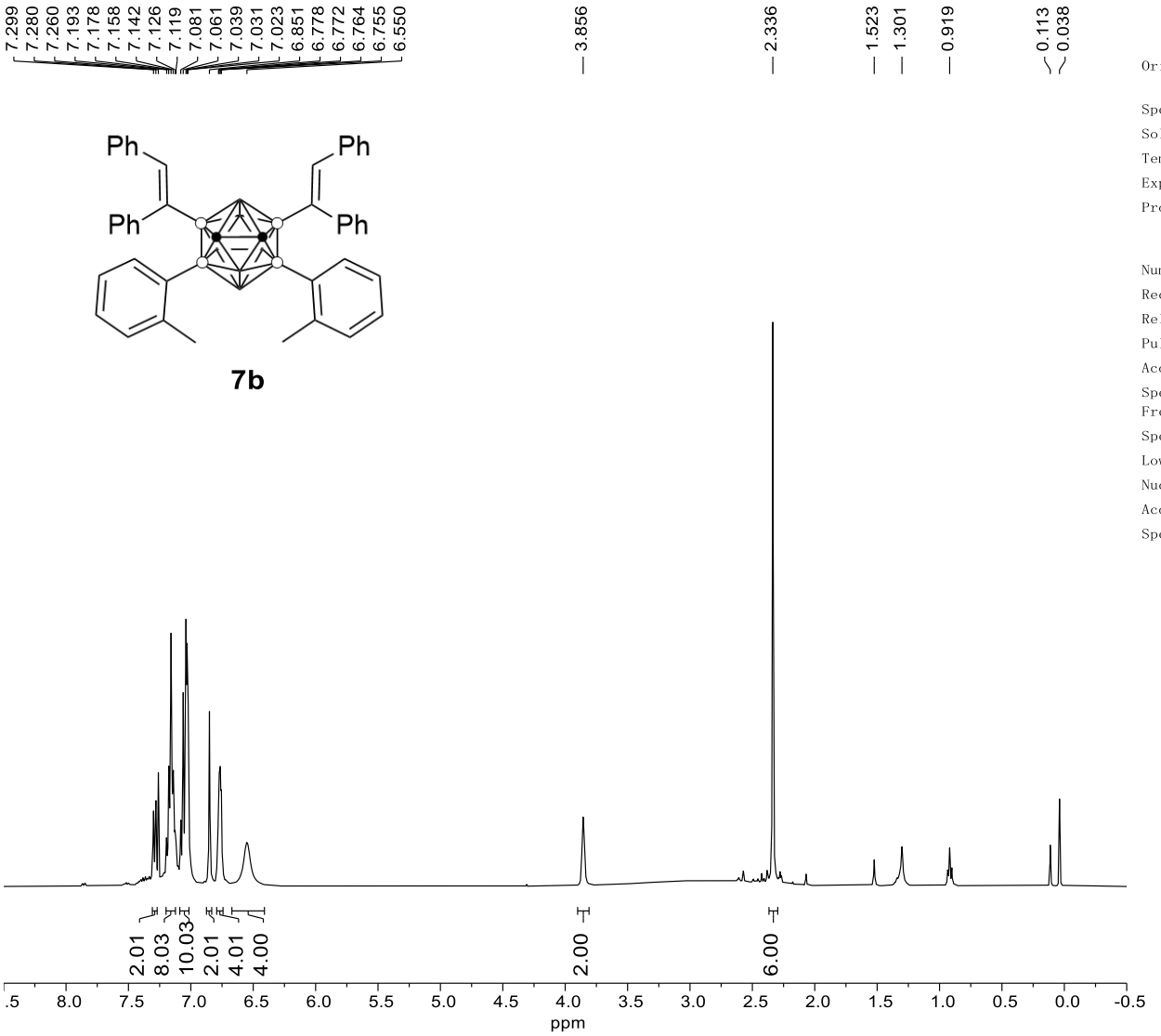




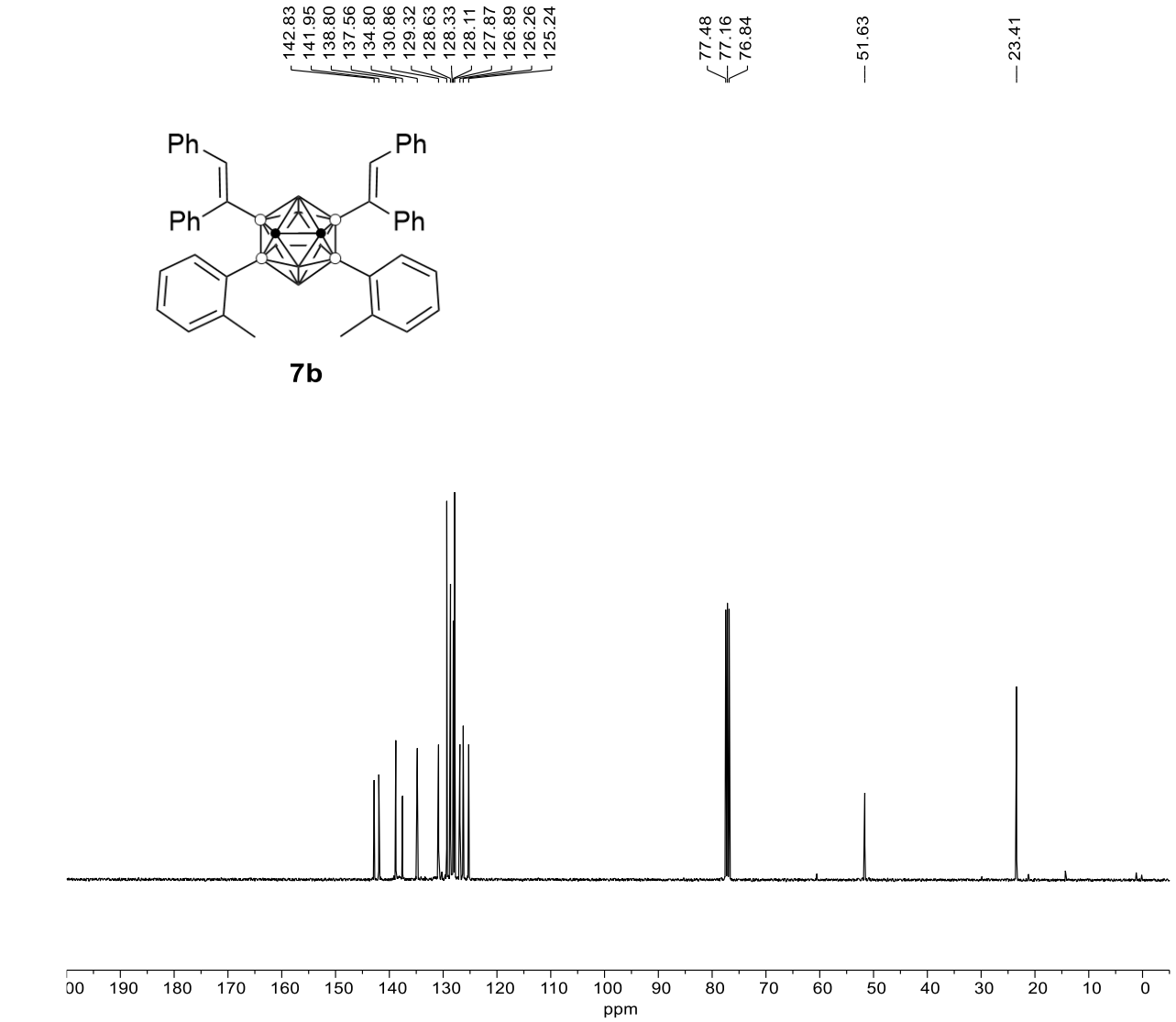
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	10
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2845
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12772.6
Nucleus	11B
Acquired Size	32768
Spectral Size	65536



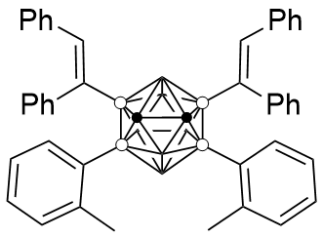
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	18
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	0.9999
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12772.6
Nucleus	11B
Acquired Size	25508
Spectral Size	65536



Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-406.8
Nucleus	1H
Acquired Size	14385
Spectral Size	65536

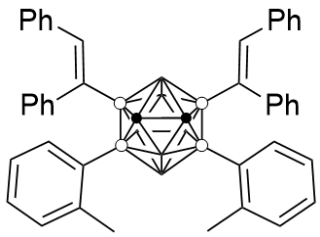


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1800
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1559.7
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



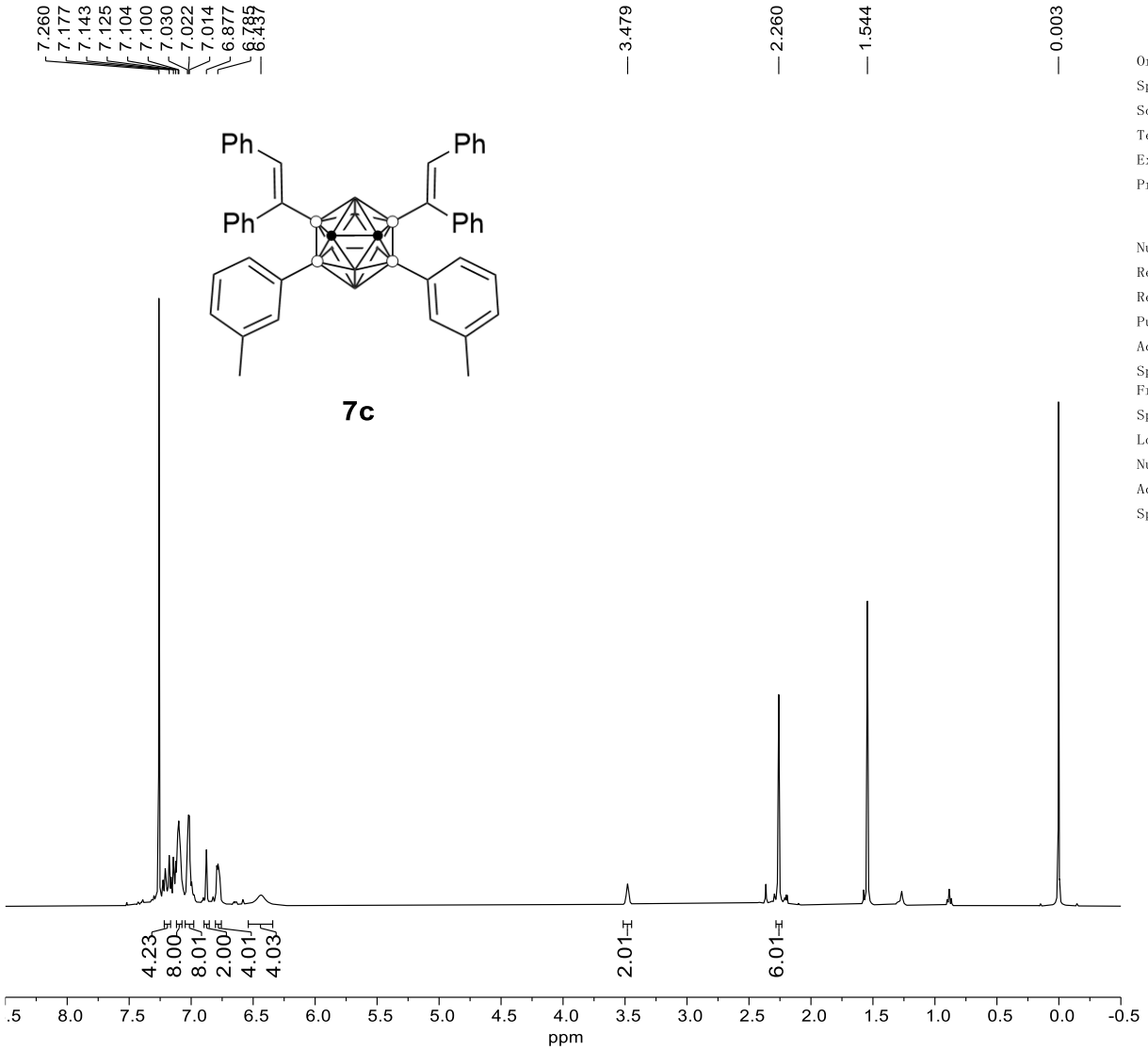
7b

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z114607_0307 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19230.8
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

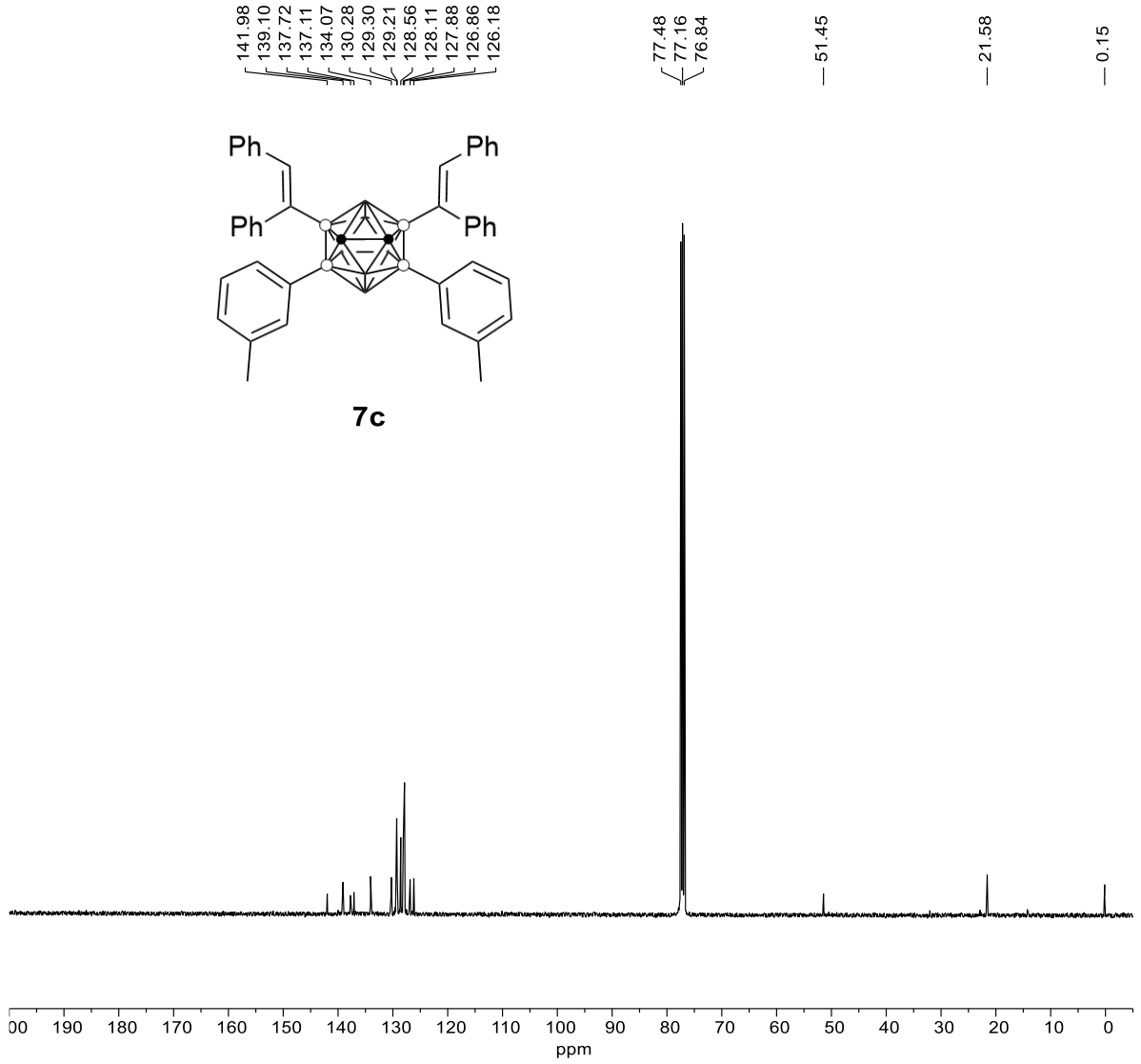


6b

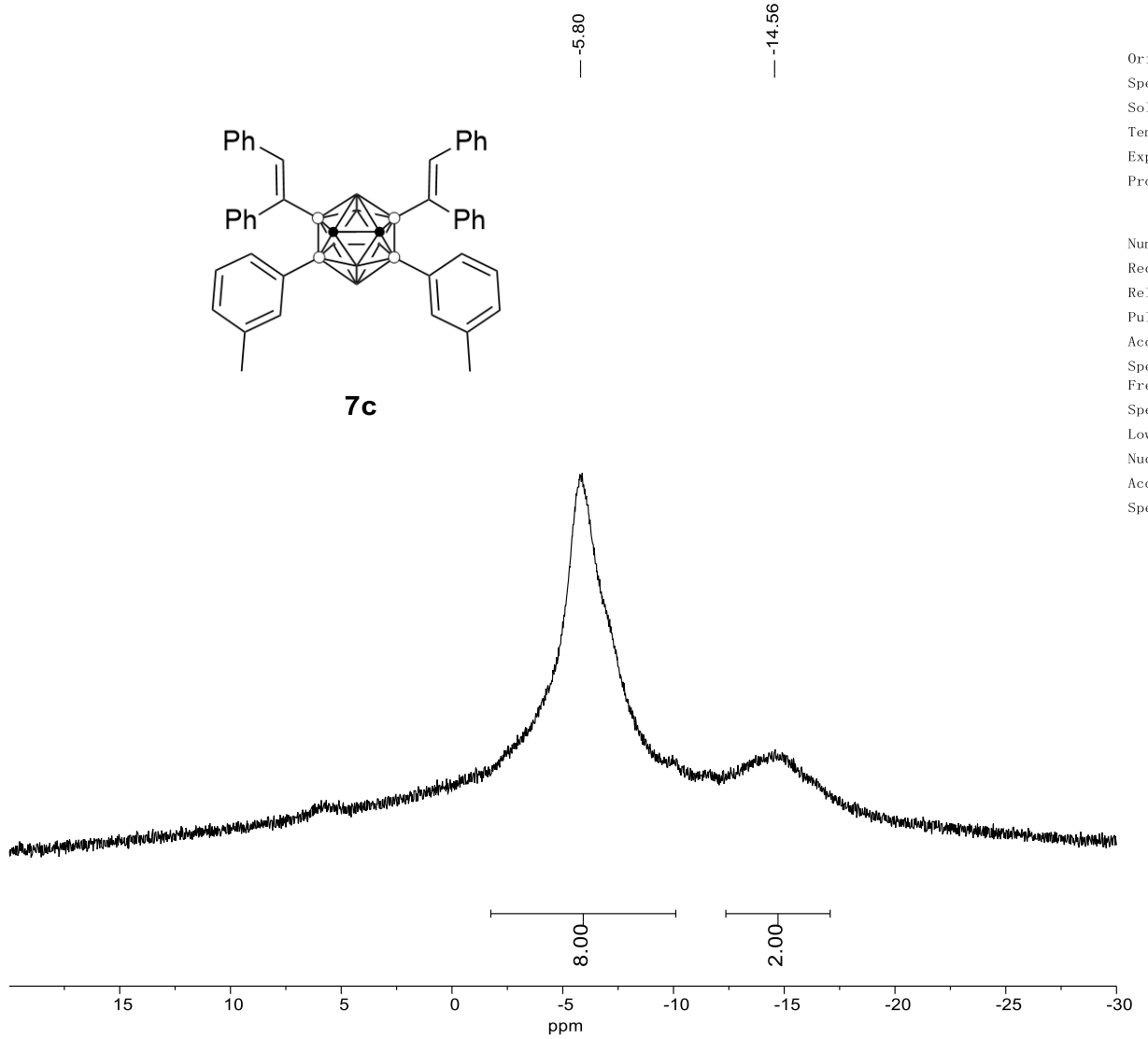
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.4
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-20959.5
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



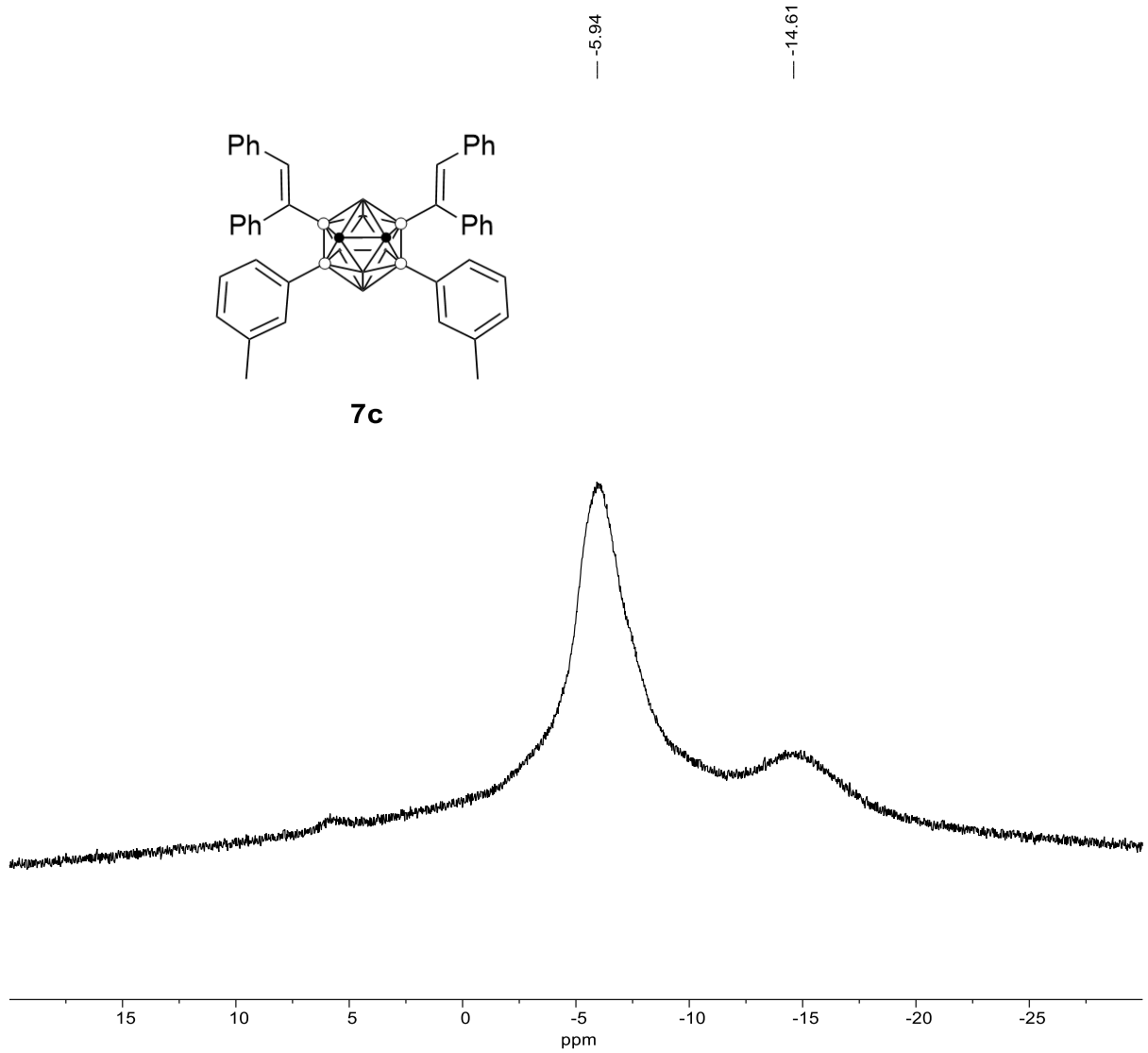
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	146
Receiver Gain	127
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-407.2
Nucleus	1H
Acquired Size	14385
Spectral Size	65536



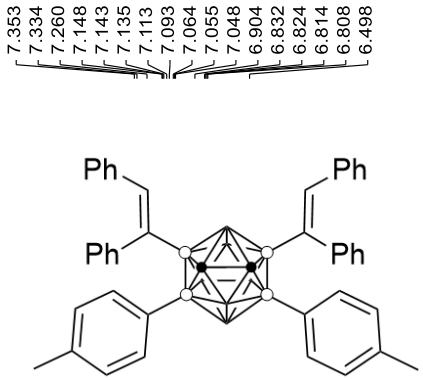
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	11600
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	0.6999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.4
Nucleus	13C
Acquired Size	17675
Spectral Size	65536



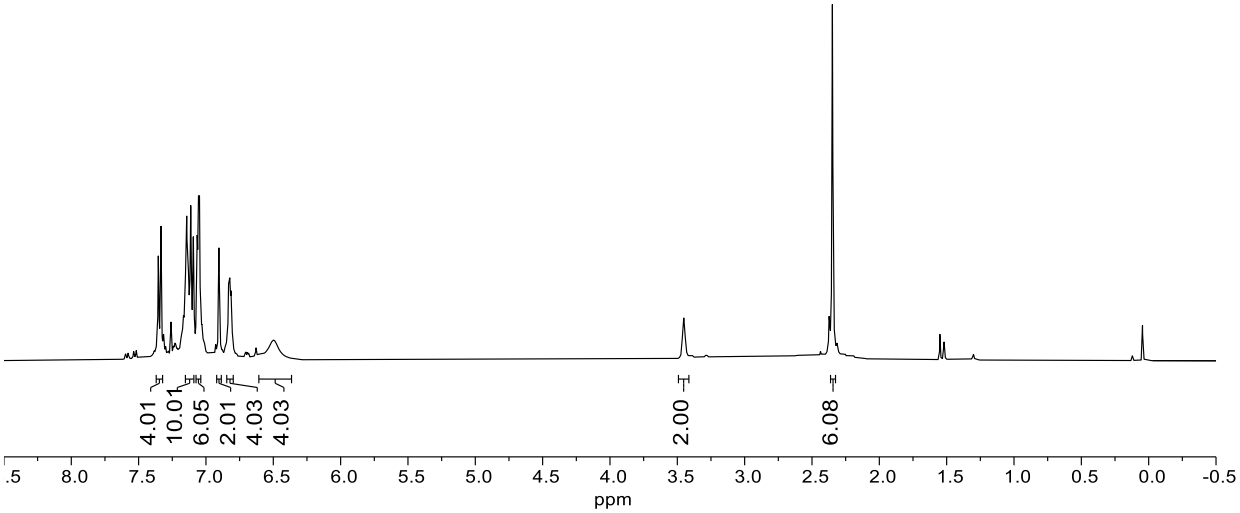
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.4
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-20994.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



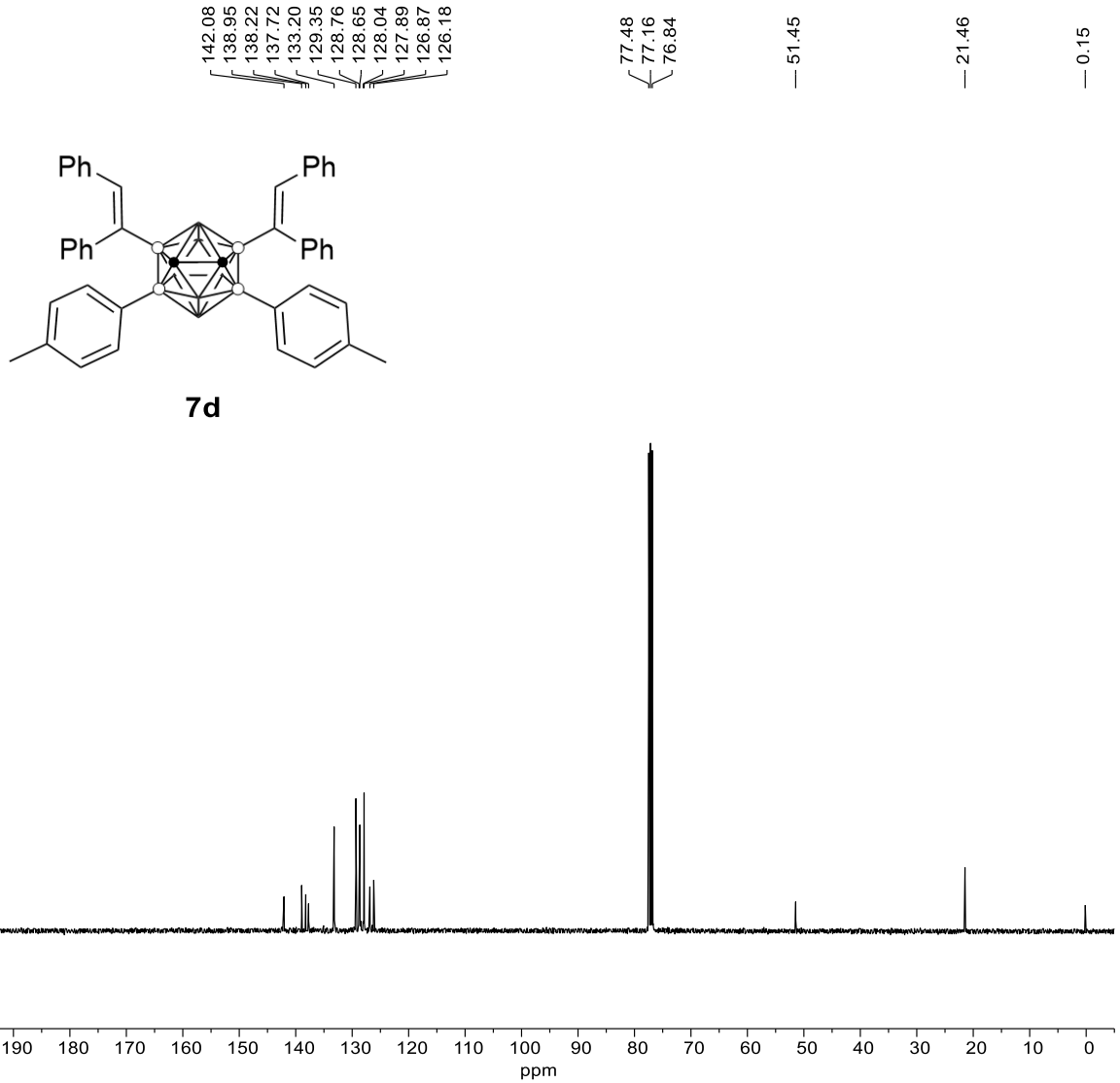
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19265.4
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

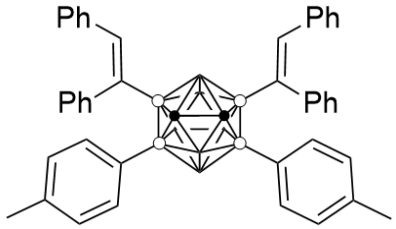


7d



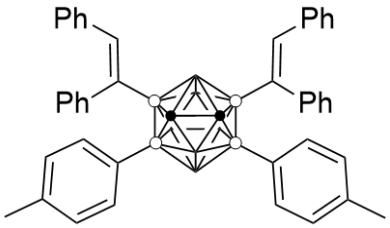
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.5
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	7
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-412.9
Nucleus	1H
Acquired Size	14422
Spectral Size	65536


142.08
138.95
138.22
137.72
133.20
129.35
128.76
128.65
128.04
127.89
126.87
126.18
77.48
77.16
76.84
51.45
21.46
0.15
Ph
Ph
Ph
Ph
7d
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 298.1
Experiment 1D
Probe Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 1600
Receiver Gain 197
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.2999
Spectrometer Frequency 100.62
Spectral Width 25252.5
Lowest Frequency -1546.0
Nucleus 13C
Acquired Size 32827
Spectral Size 131072
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm



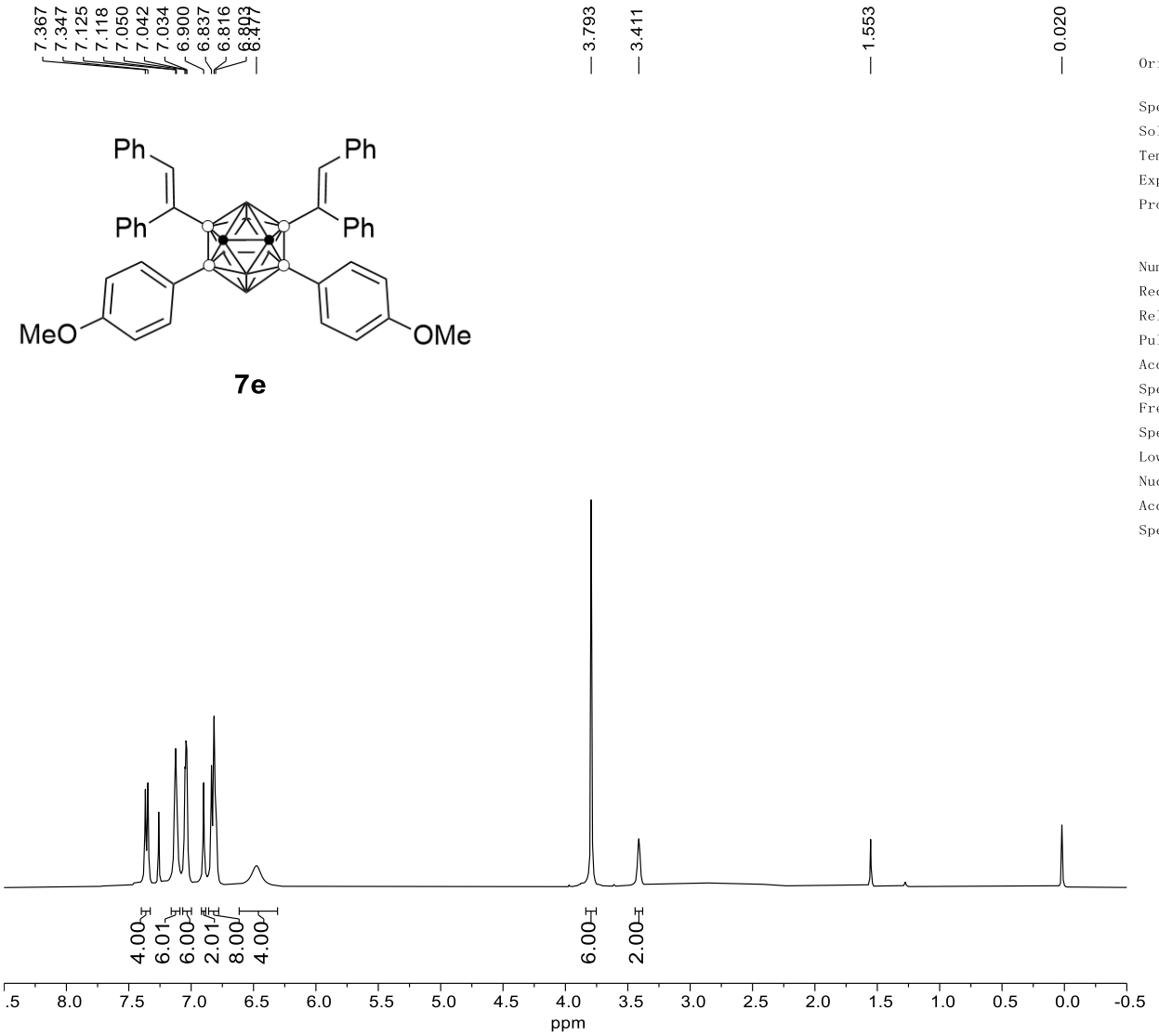
7d

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.3
Experiment	1D
Probe	Z114607_0307 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21000.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

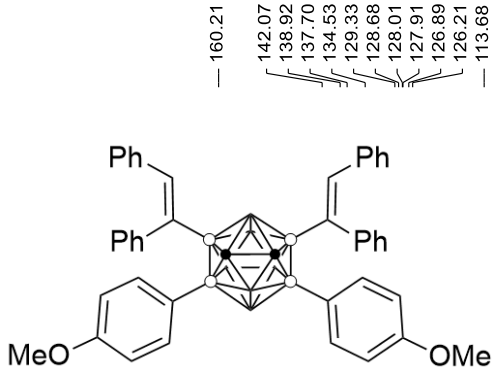


7d

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19271.4
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



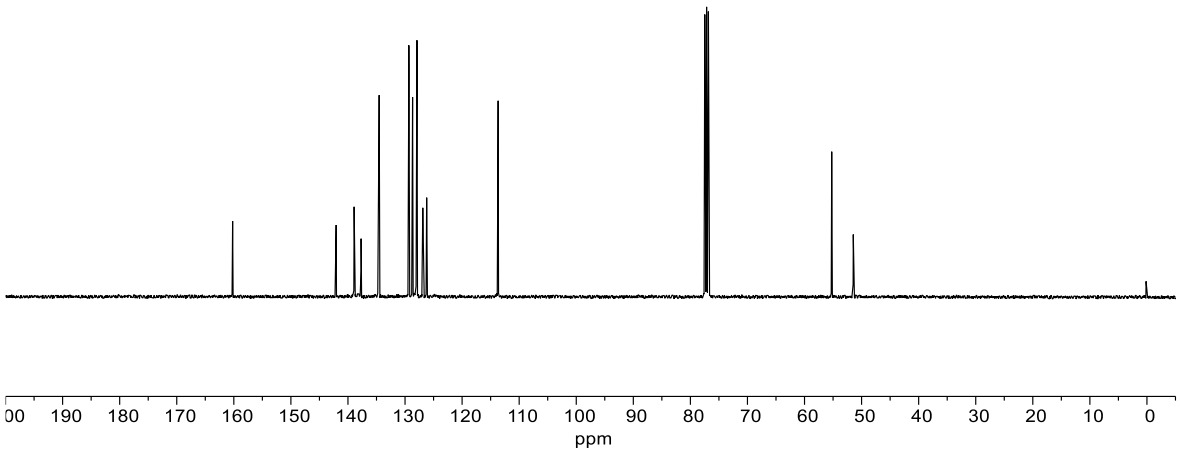
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.5
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	7
Receiver Gain	77
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-412.9
Nucleus	1H
Acquired Size	14422
Spectral Size	65536

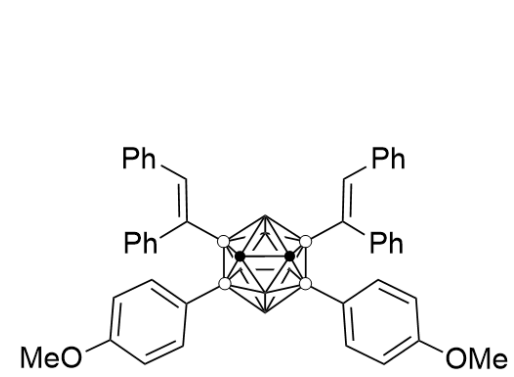


7e

160.21
142.07
138.92
137.70
134.53
129.33
128.68
128.01
127.91
126.89
126.21
113.68
77.48
77.16
76.84
55.24
51.46
0.15

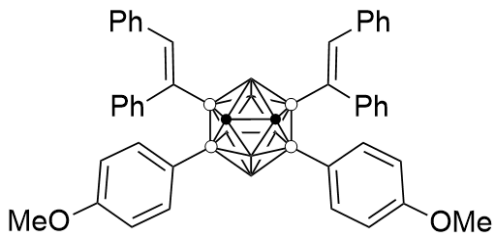
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1600
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1548.3
Nucleus	13C
Acquired Size	32827
Spectral Size	131072





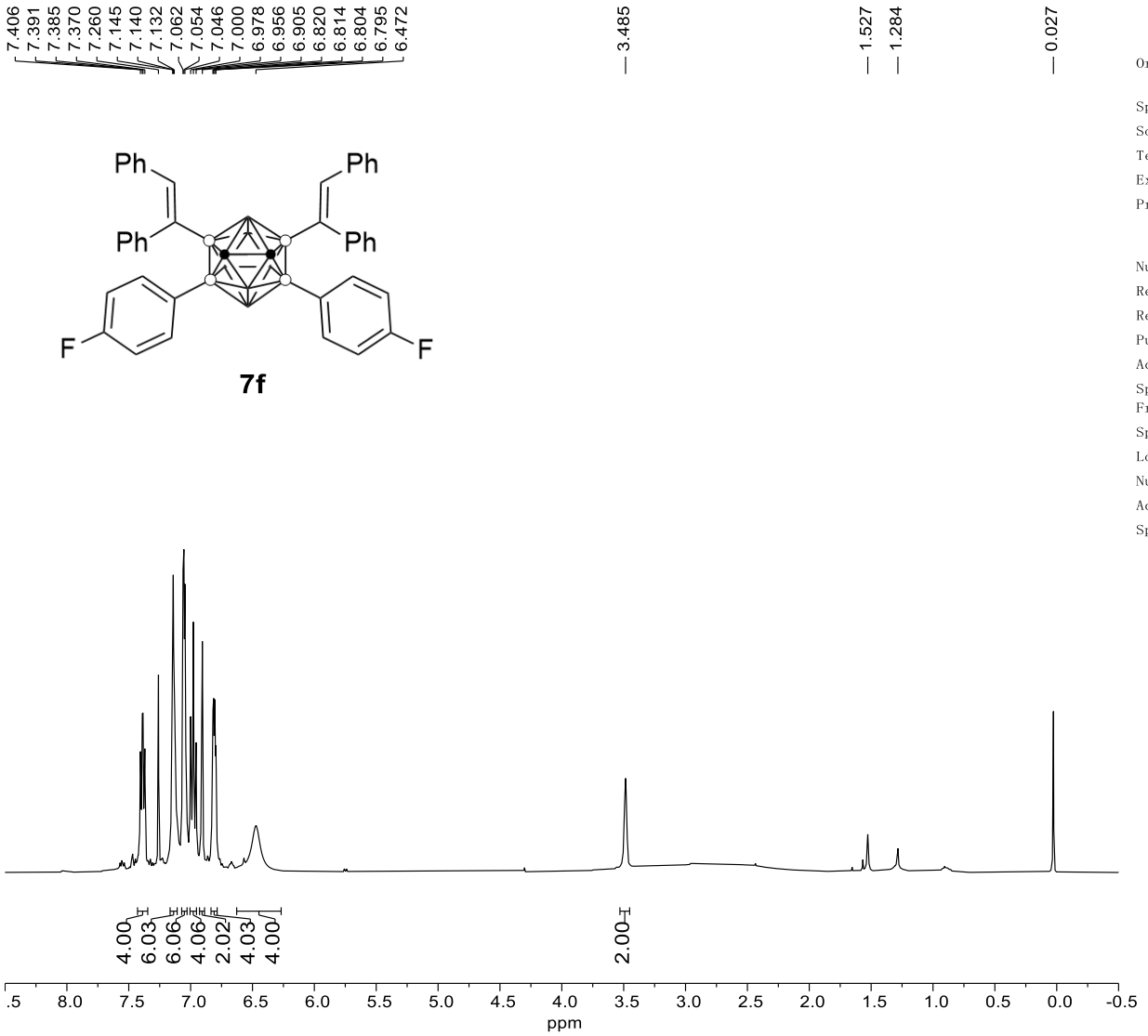
7e

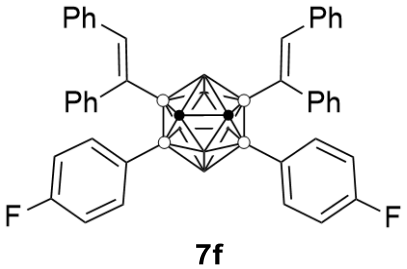
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	21
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2845
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12790.2
Nucleus	11B
Acquired Size	32768
Spectral Size	65536



7e

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.5
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	14
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	0.9999
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12790.2
Nucleus	11B
Acquired Size	25508
Spectral Size	65536


7.406
7.391
7.385
7.370
7.260
7.145
7.140
7.132
7.062
7.054
7.046
7.000
6.978
6.956
6.905
6.820
6.814
6.804
6.795
6.472
3.485
1.527
1.284
0.027
Ph
Ph
Ph
Ph
F
F
7f
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 298.1
Experiment 1D
Probe Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 16
Receiver Gain 50
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 2.9998
Spectrometer Frequency 400.10
Spectral Width 4795.4
Lowest Frequency -406.8
Nucleus 1H
Acquired Size 14385
Spectral Size 65536
4.00
6.03
6.06
4.06
2.02
4.03
4.00
2.00
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm



7f

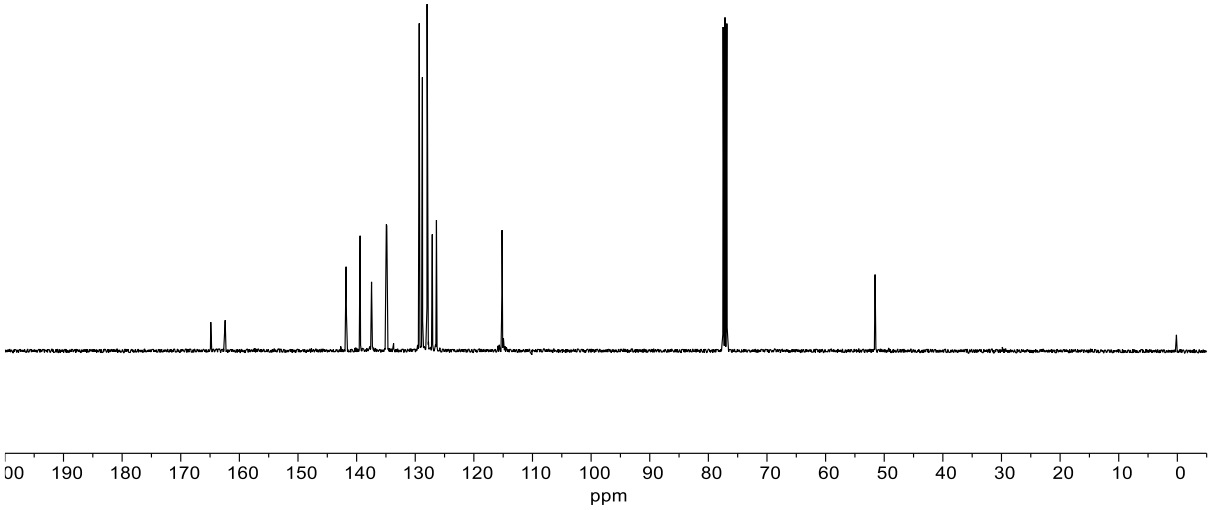
164.88
162.42
141.80
139.41
137.46
134.93
134.86
129.32
128.78
127.98
127.91
127.09
126.38
115.19
114.99

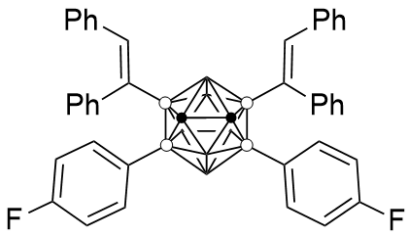
77.48
77.16
76.84

51.56

0.16

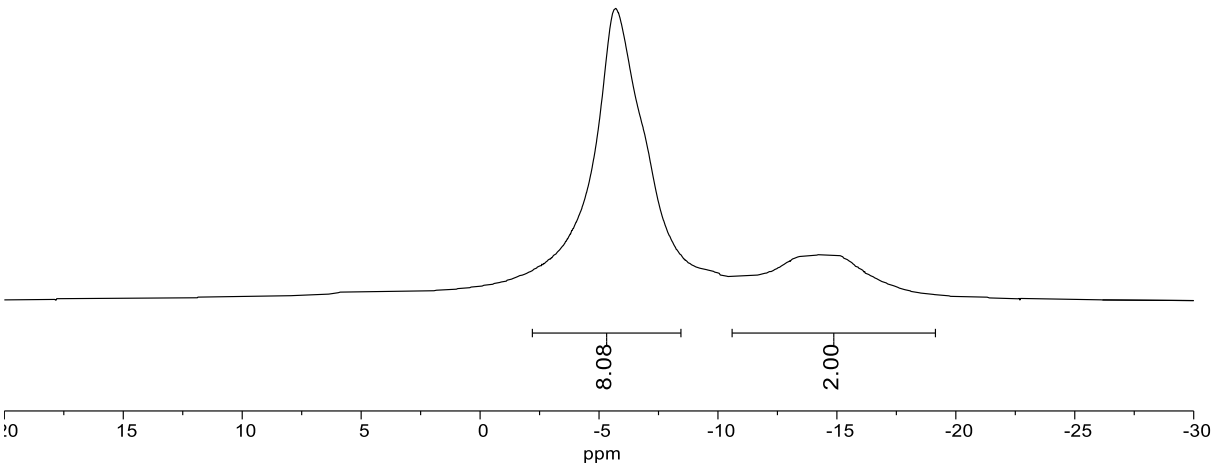
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1600
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1548.5
Nucleus	13C
Acquired Size	32827
Spectral Size	131072

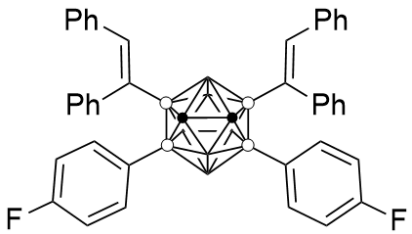




7f

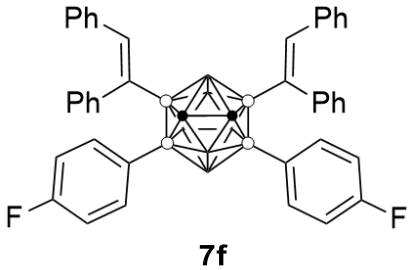
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	300.4
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21005.8
Nucleus	11B
Acquired Size	32768
Spectral Size	32768





7f

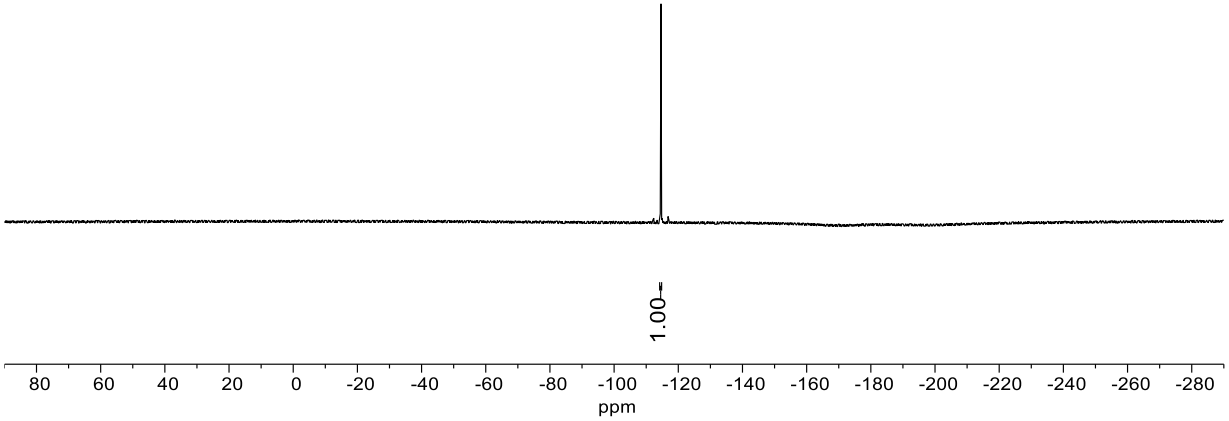
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	301.2
Experiment	1D
Probe	Z114607_0307 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19277.2
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

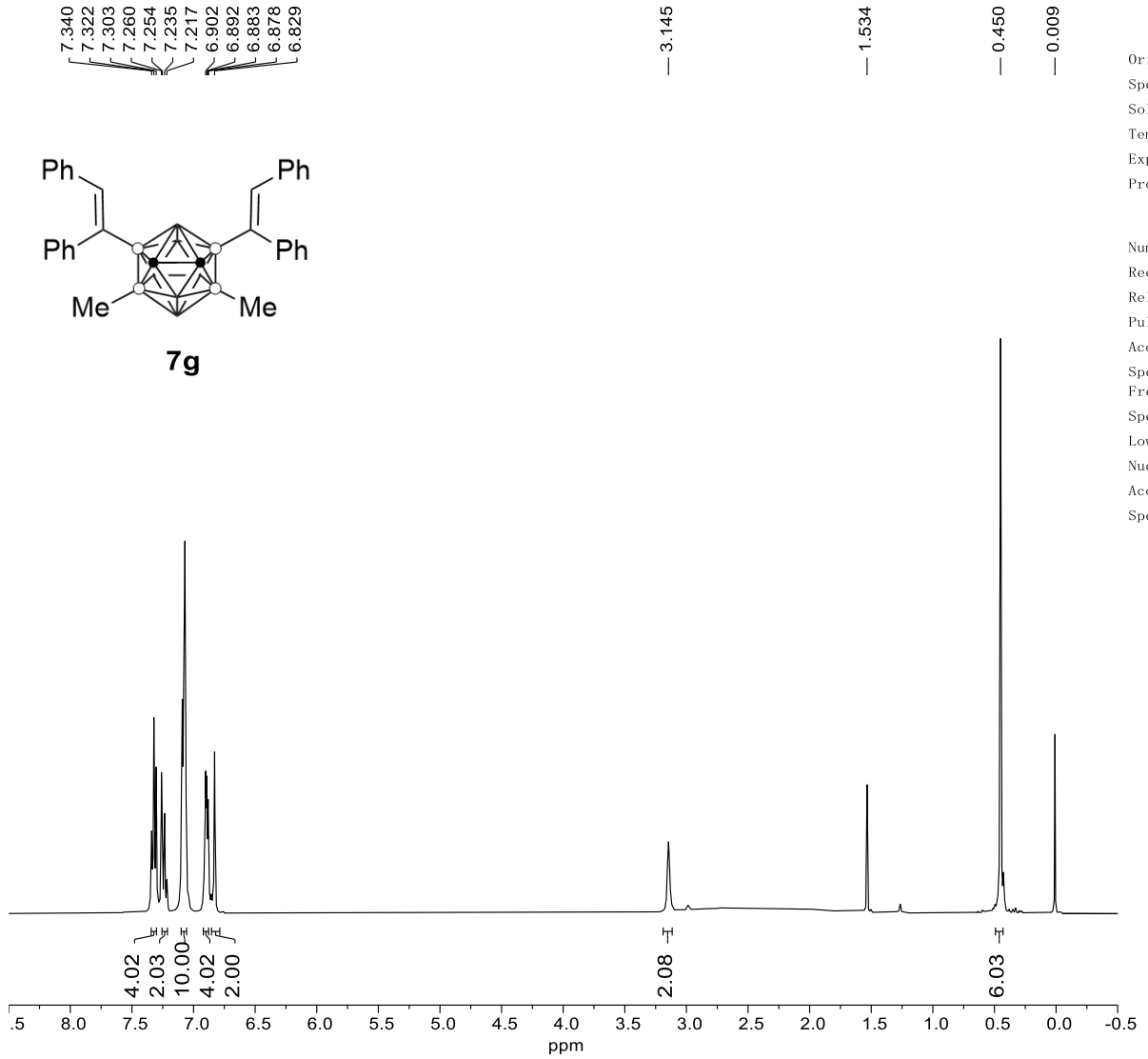


7f

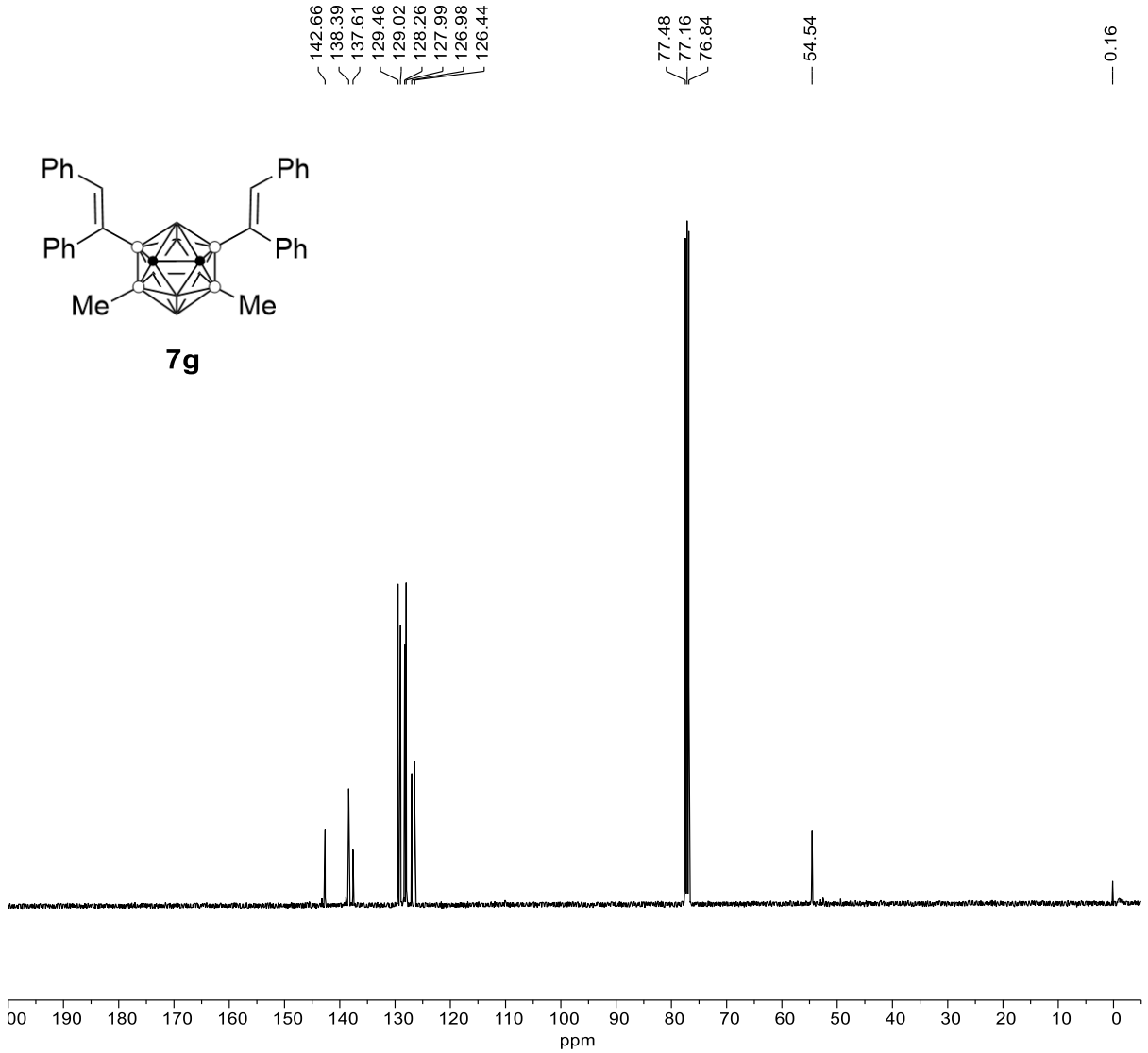
-114.56
-114.58
-114.61

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Temperature	293.8
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	10
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	18.0000
Acquisition Time	0.9999
Spectrometer Frequency	376.53
Spectral Width	150000.0
Lowest Frequency	-112656.4
Nucleus	19F
Acquired Size	149992
Spectral Size	524288

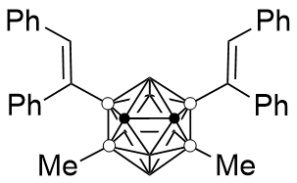




Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	98
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-407.0
Nucleus	1H
Acquired Size	14385
Spectral Size	65536

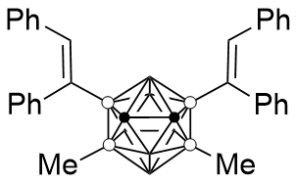


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	3000
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1546.0
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



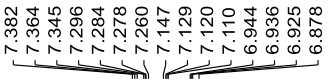
7g

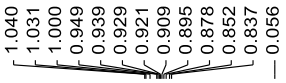
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	297.7
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	0.5000
Pulse Width	9.3500
Acquisition Time	0.9175
Spectrometer Frequency	192.55
Spectral Width	35714.3
Lowest Frequency	-19615.9
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

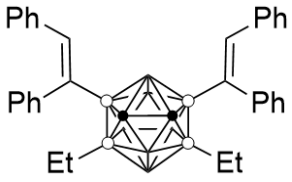


7g

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	297.5
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19260.9
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

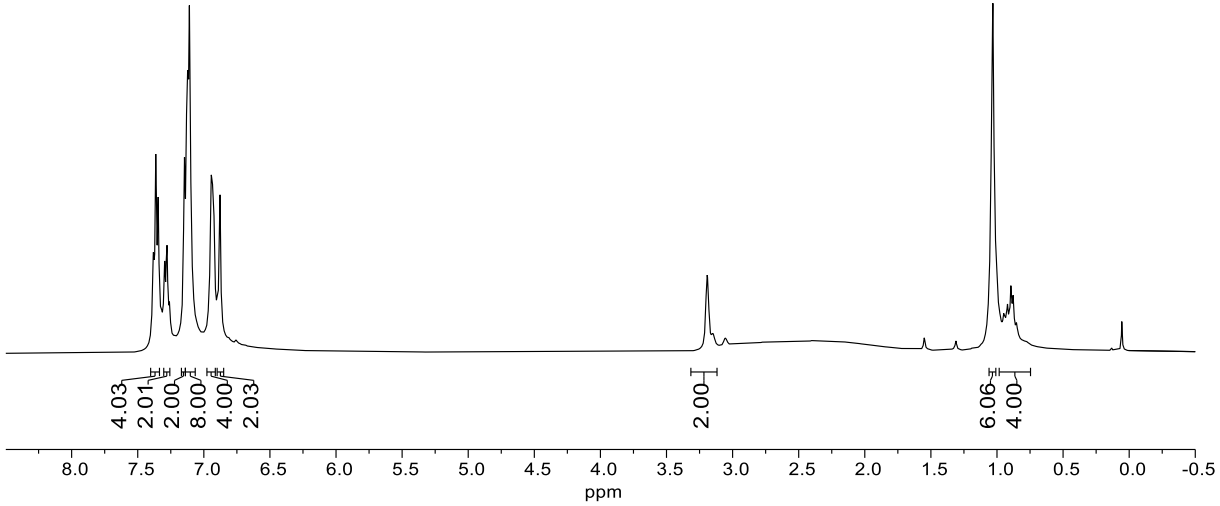


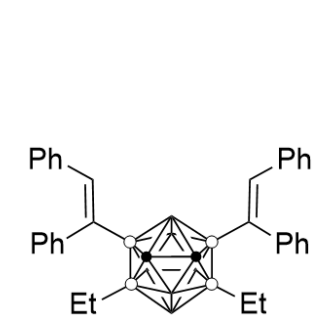




7h

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.1
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	12
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-402.8
Nucleus	1H
Acquired Size	14422
Spectral Size	65536

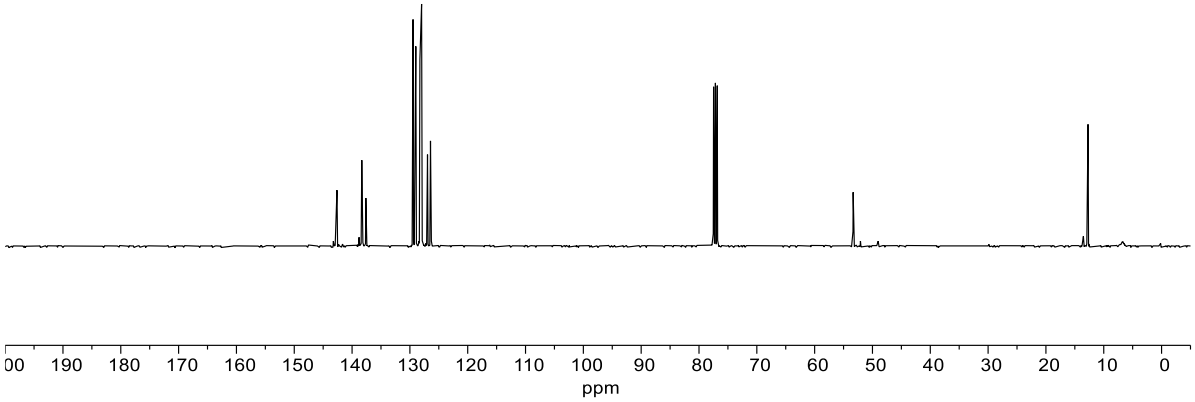


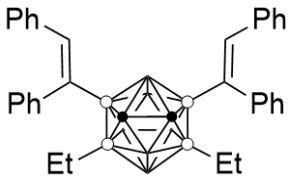


7h

142.61
138.32
137.62
129.46
128.98
128.27
127.98
126.95
126.44
77.48
77.16
76.84
53.34
12.72

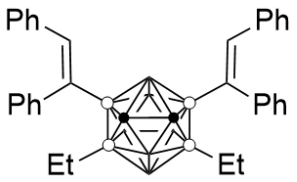
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	2000
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1549.7
Nucleus	13C
Acquired Size	32827
Spectral Size	131072





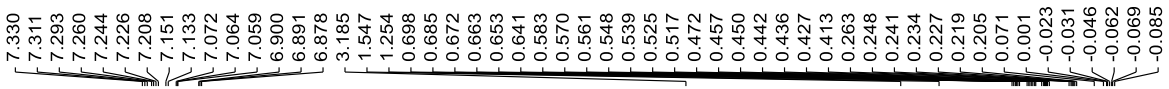
7h

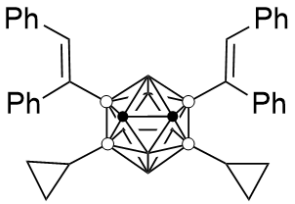
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	301.2
Experiment	1D
Probe	Z114607_0307 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-20987.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



7h

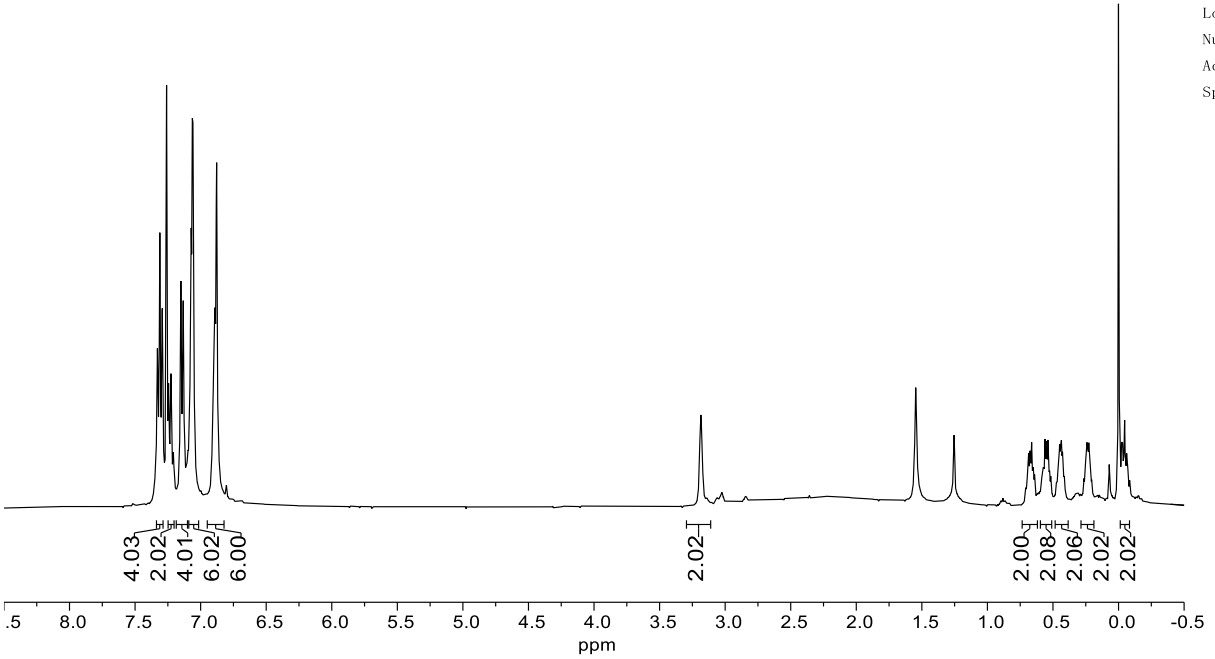
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	301.0
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19258.4
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

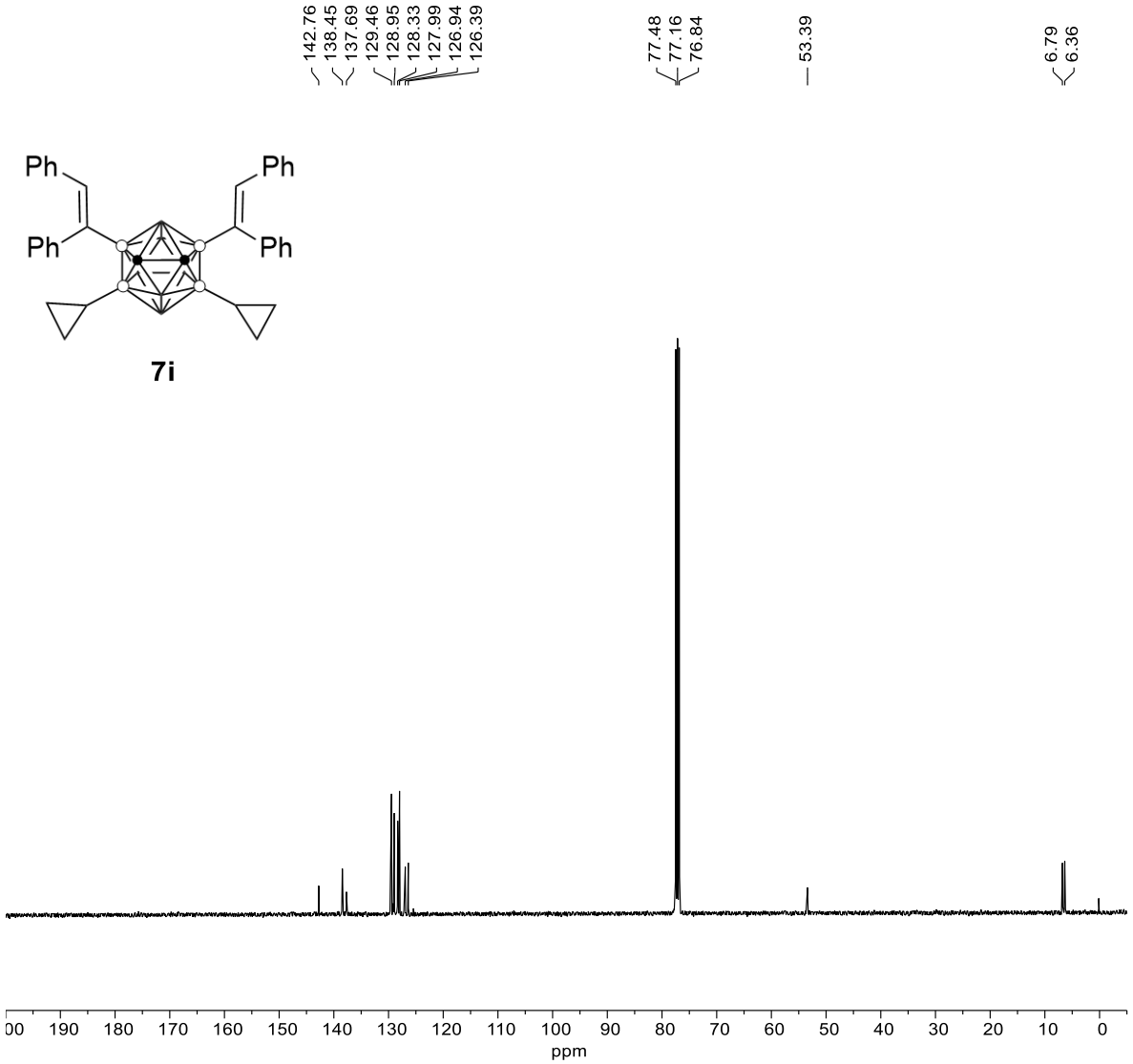




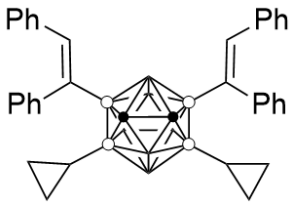
7i

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.1
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	10
Receiver Gain	77
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-412.9
Nucleus	1H
Acquired Size	14422
Spectral Size	65536



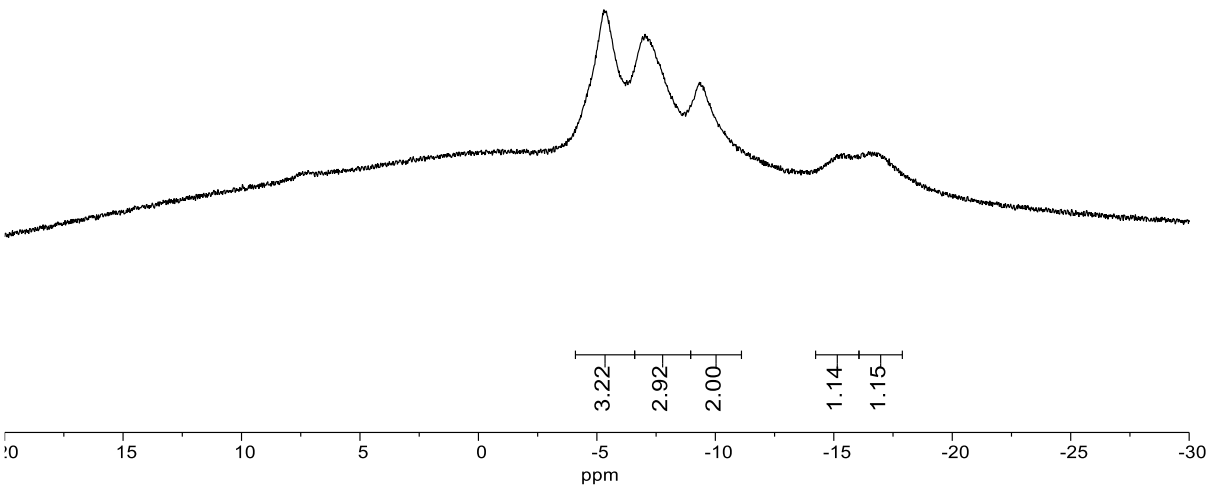


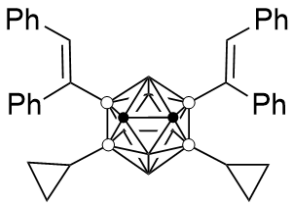
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	3600
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.5
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



7i

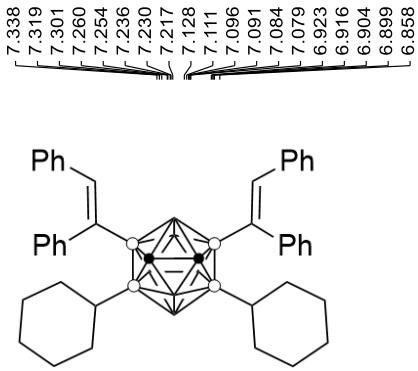
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.6
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	32
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21198.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768





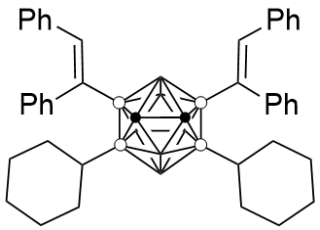
7i

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	96
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21198.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



7j

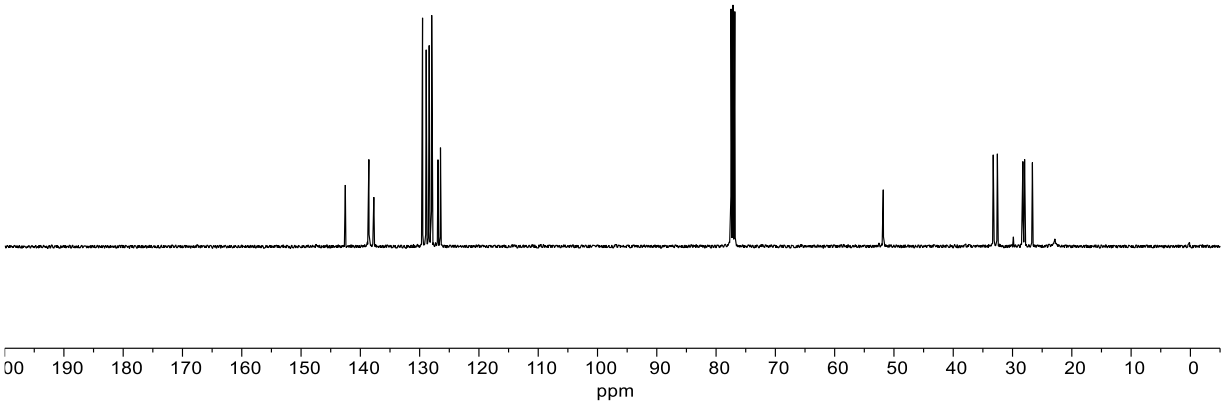
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	8
Receiver Gain	71
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-413.3
Nucleus	1H
Acquired Size	14422
Spectral Size	65536

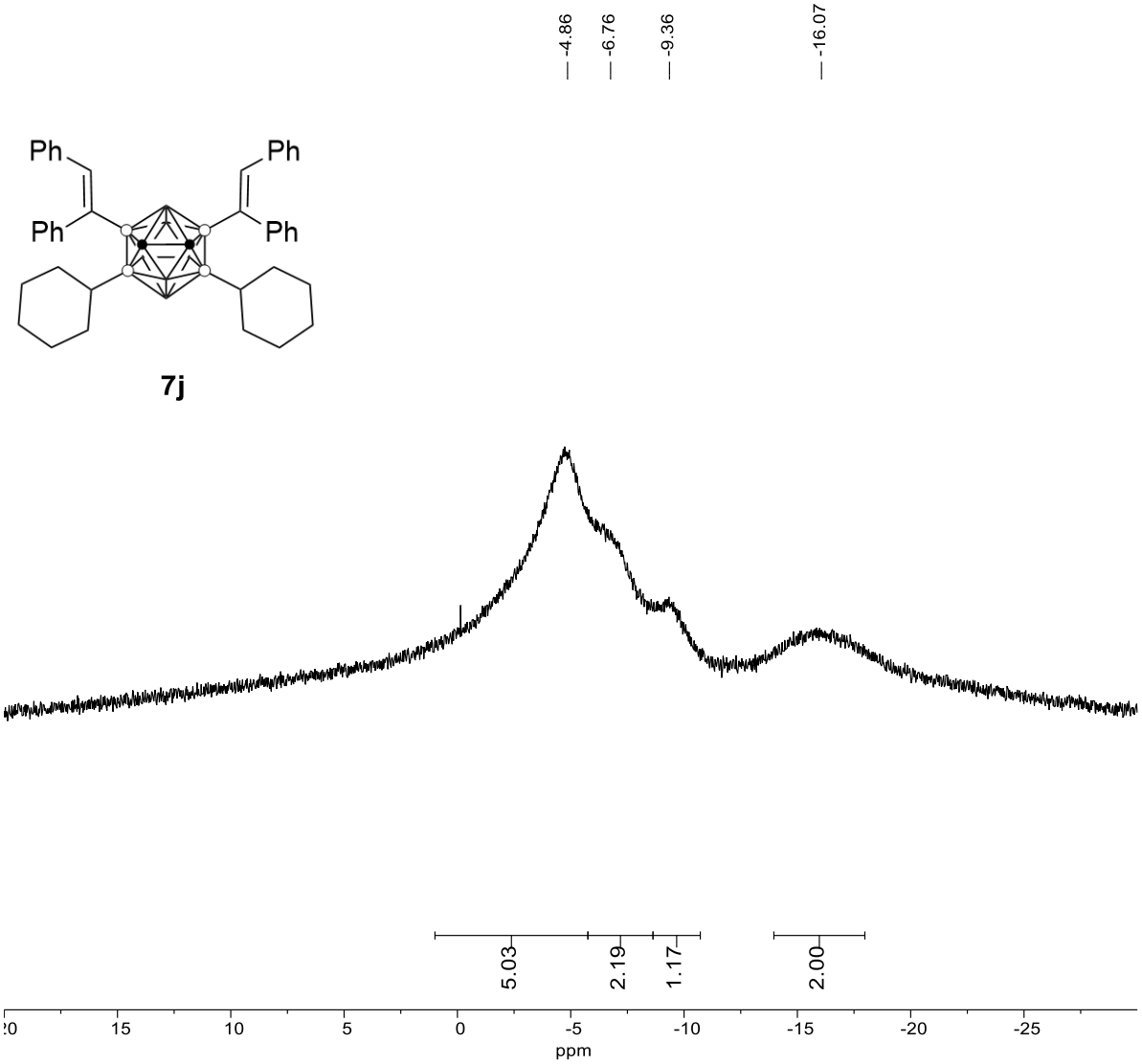


7j

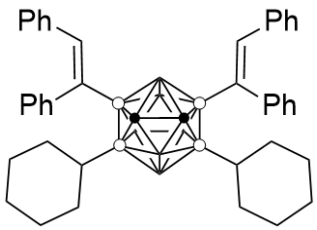
142.54
138.56
137.73
129.51
128.89
128.39
127.97
126.91
126.48
77.48
77.16
76.84
51.80
33.26
32.56
28.25
27.96
26.65

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	2000
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1547.8
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



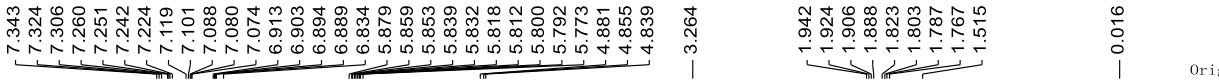


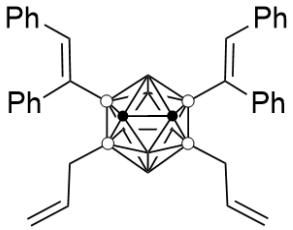
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.7
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	13
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2845
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12772.6
Nucleus	11B
Acquired Size	32768
Spectral Size	65536



7j

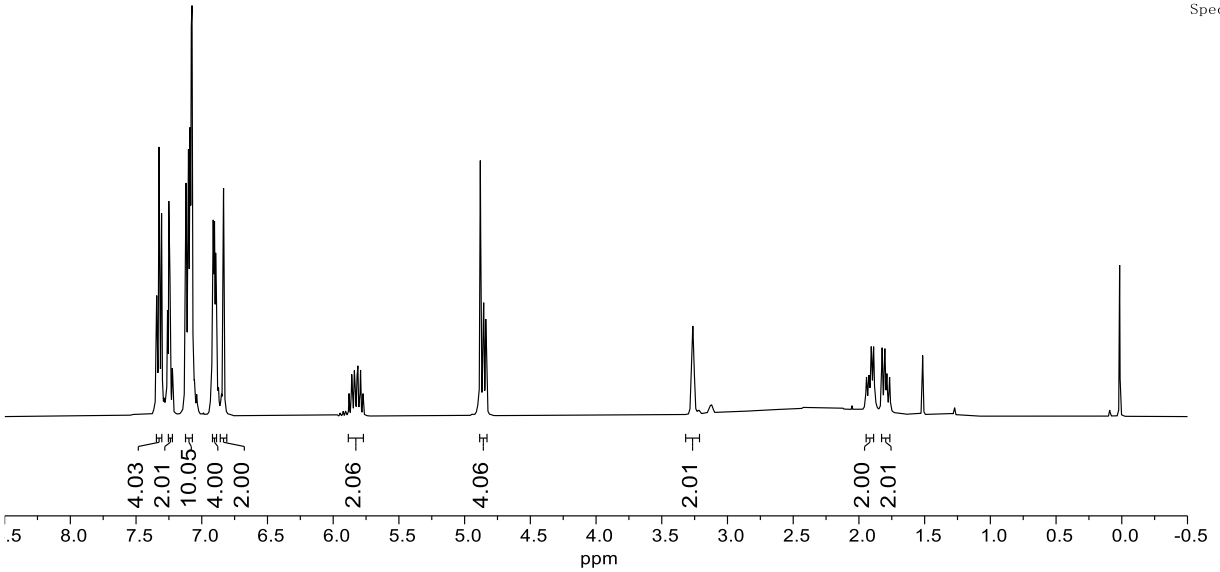
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	20
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	0.9999
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12772.6
Nucleus	11B
Acquired Size	25508
Spectral Size	65536

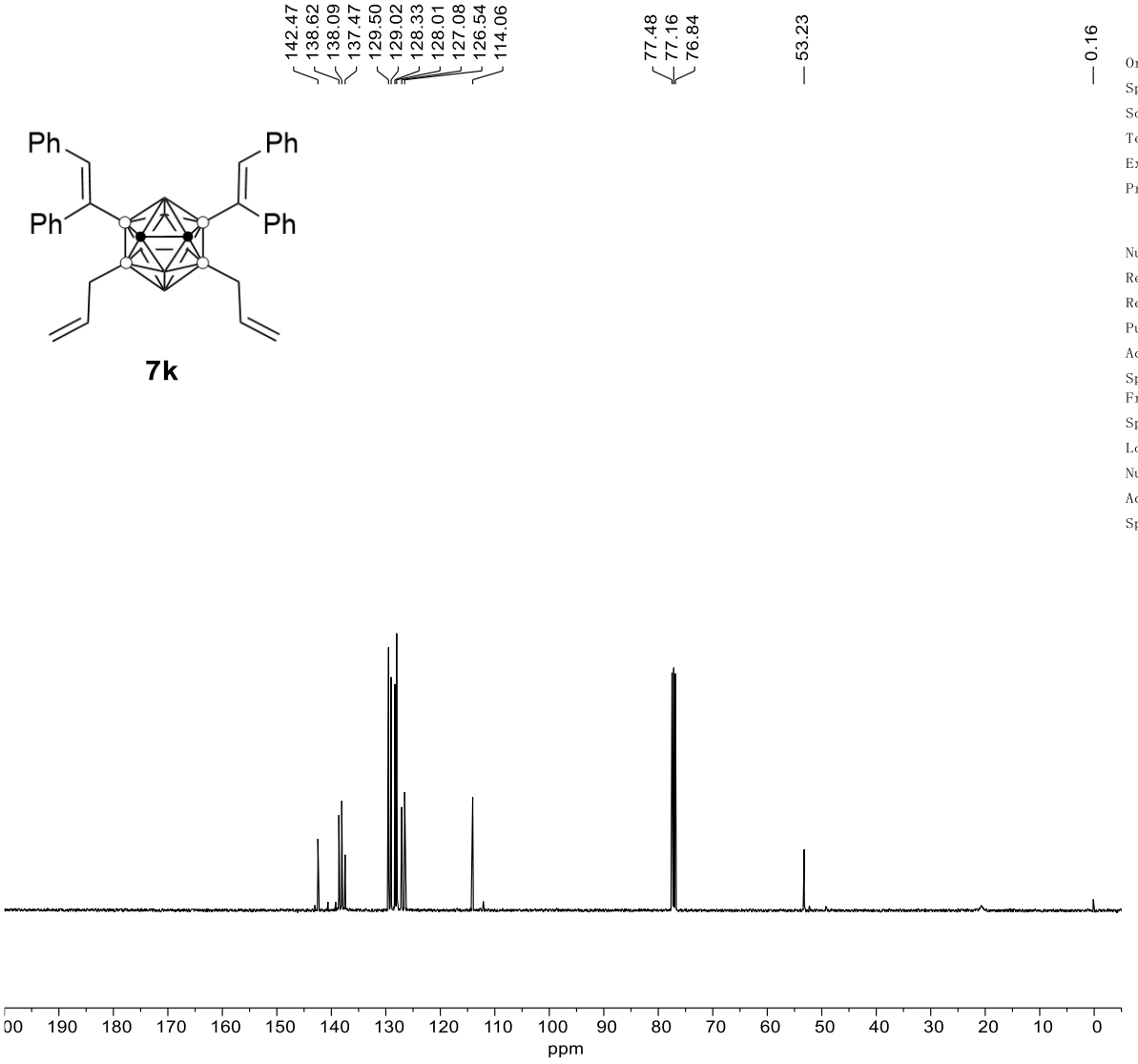


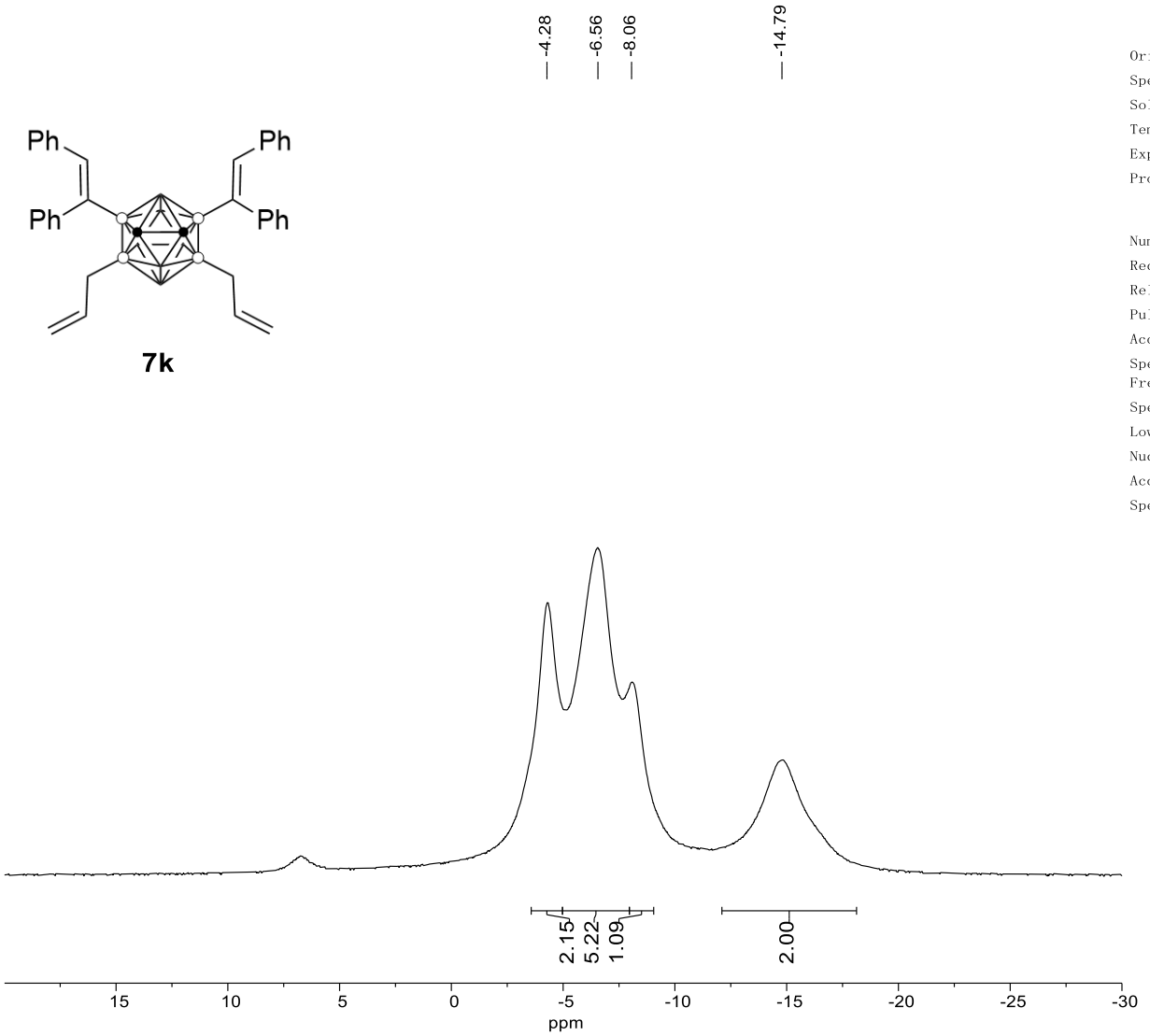


7k

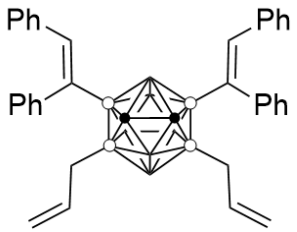
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-410.7
Nucleus	1H
Acquired Size	14385
Spectral Size	65536



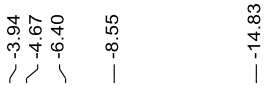

142.47
138.62
138.09
137.47
129.50
129.02
128.33
128.01
127.08
126.54
114.06
77.48
77.16
76.84
53.23
0.16
Ph
Ph
Ph
Ph
7k
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 298.1
Experiment 1D
Probe Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 1024
Receiver Gain 197
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.2999
Spectrometer Frequency 100.62
Spectral Width 25252.5
Lowest Frequency -1548.8
Nucleus 13C
Acquired Size 32827
Spectral Size 131072
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm



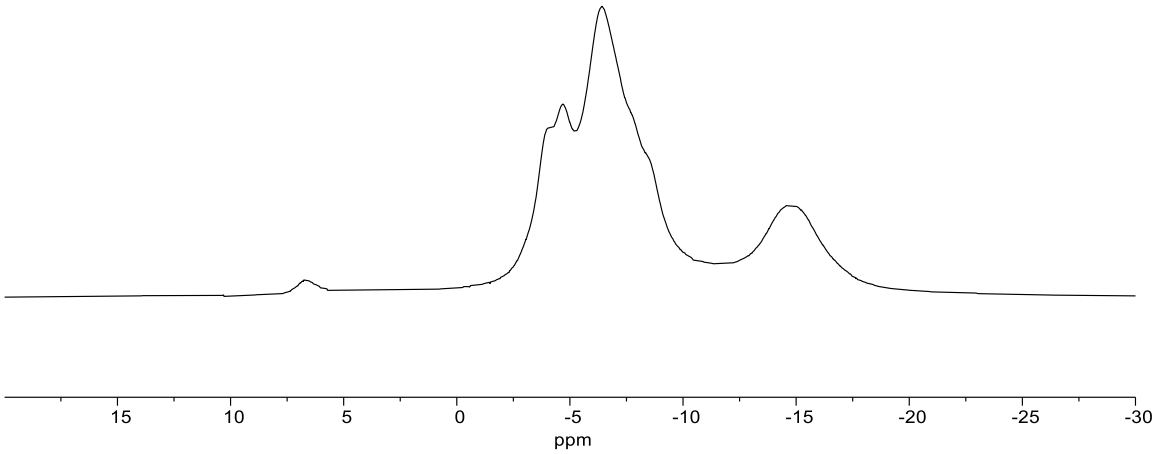
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	301.5
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	34
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-20987.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

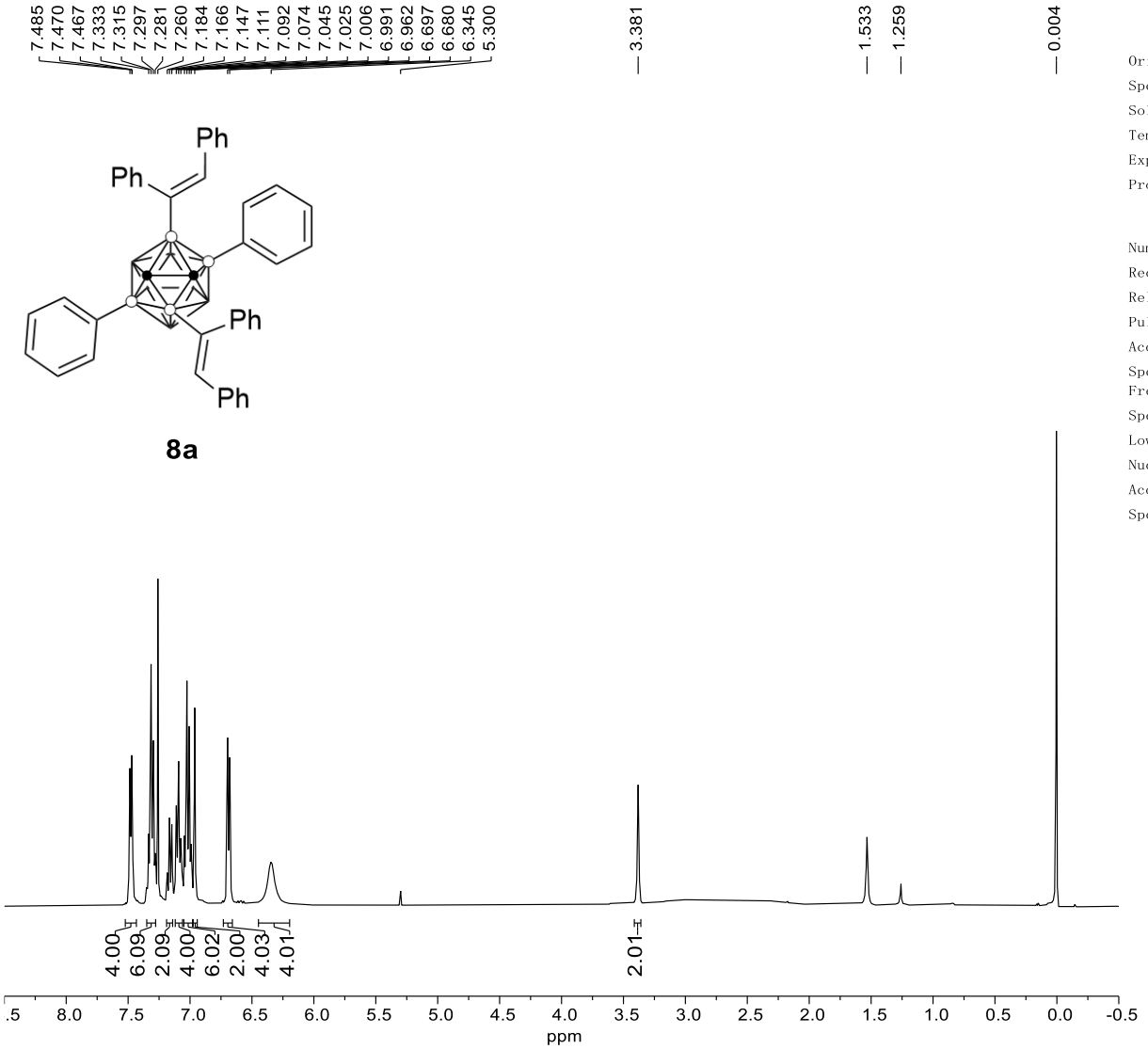


7k

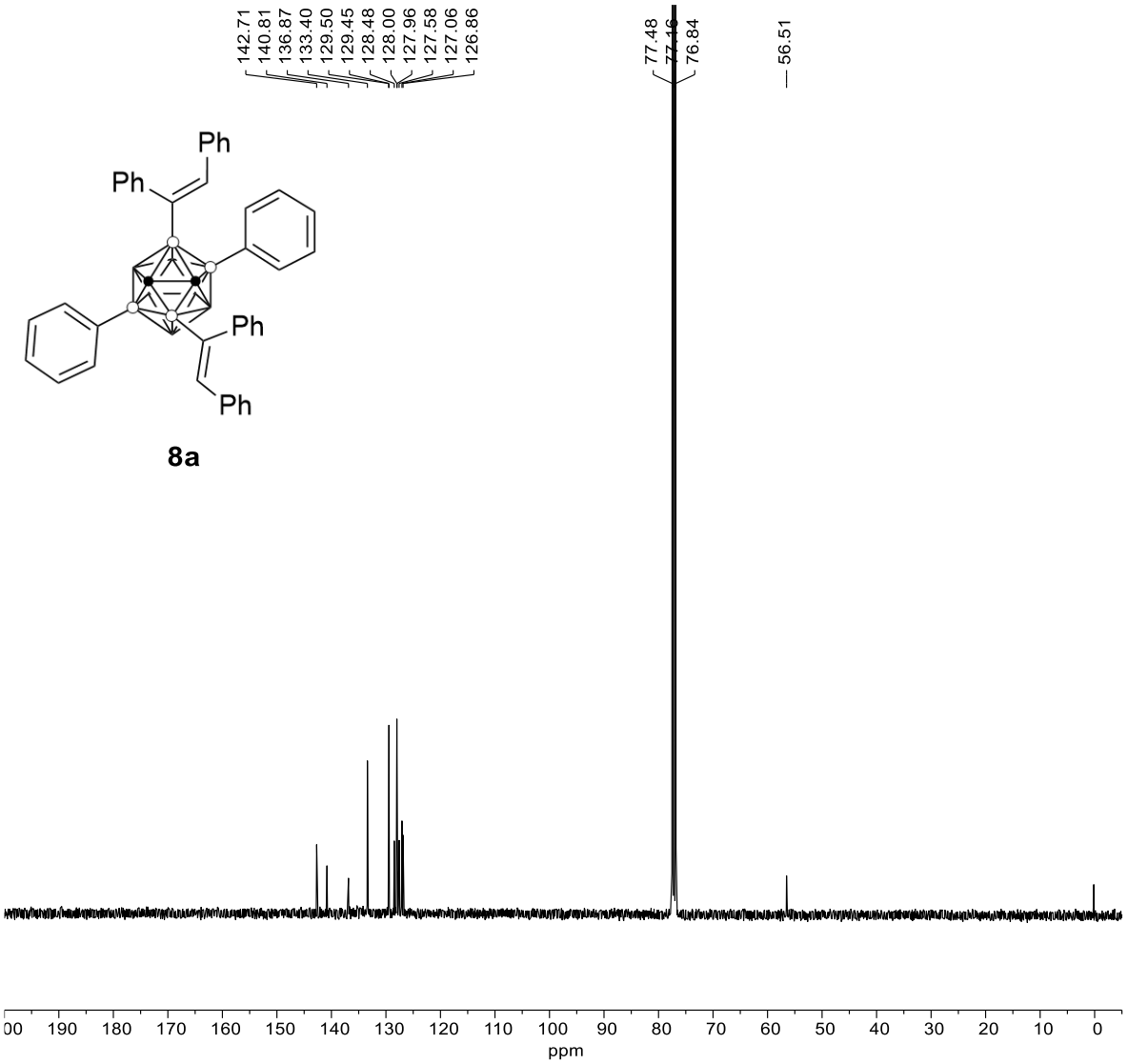


Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	301.1
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	54
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19258.4
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

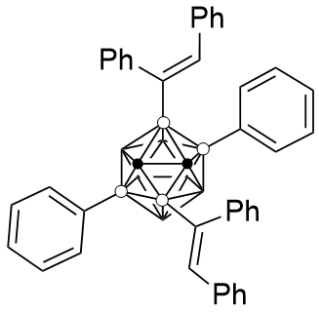




Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	127
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-406.9
Nucleus	1H
Acquired Size	14385
Spectral Size	65536

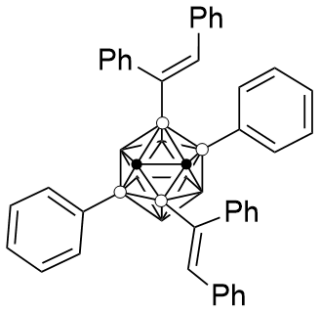


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	2000
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.4
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



8a

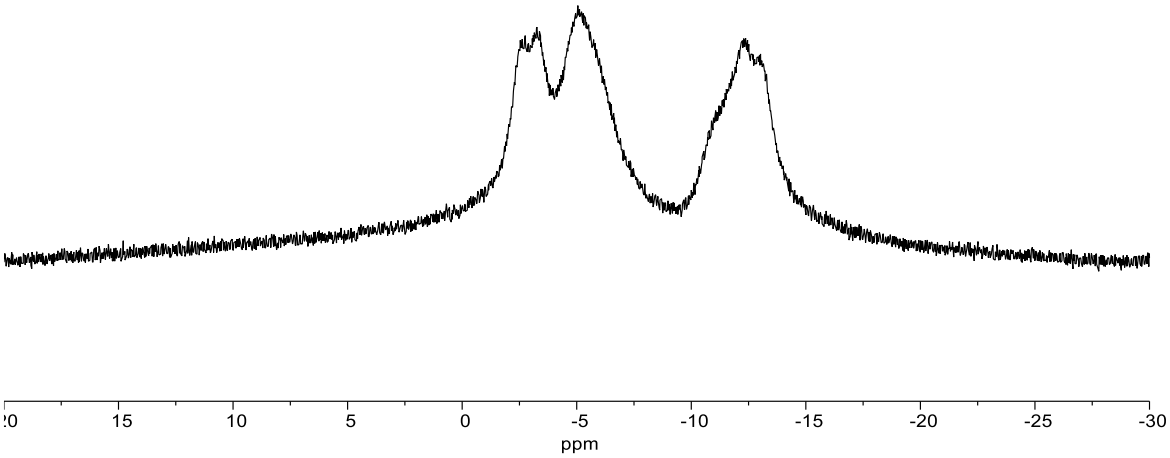
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	299.0
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-20997.2
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

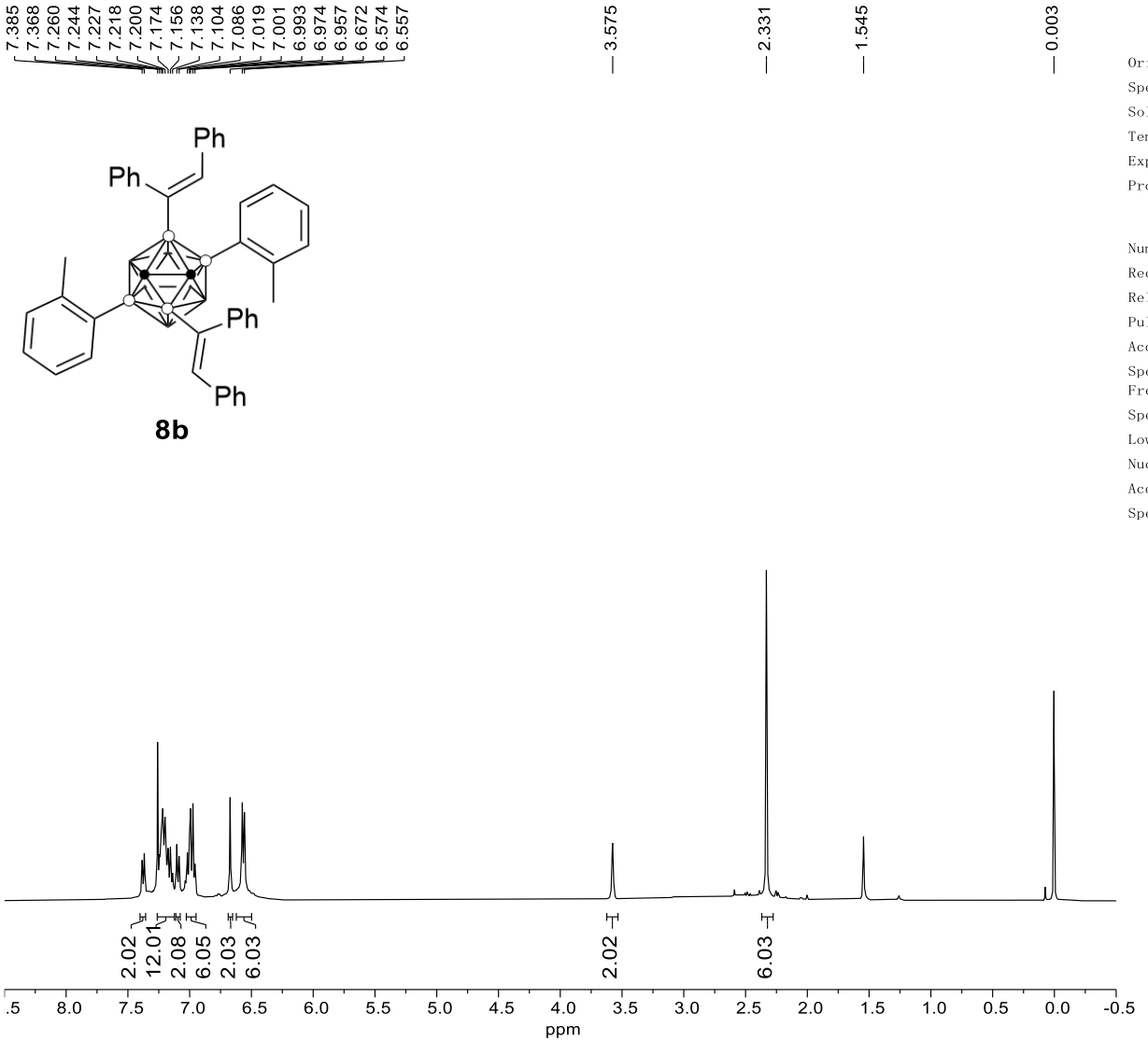


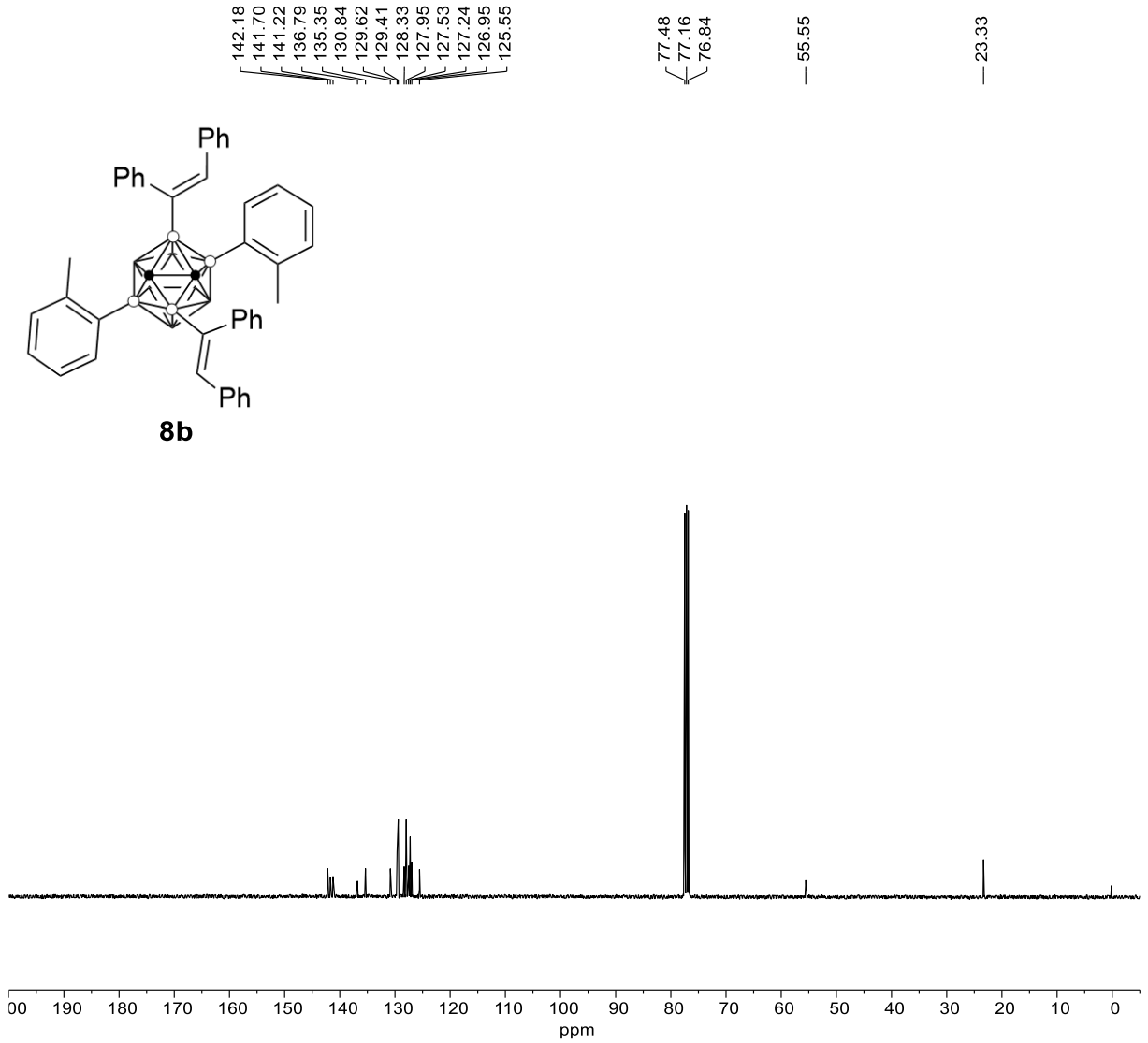
8a

-2.54
-3.26
-5.09
-11.11
-12.29
-13.06

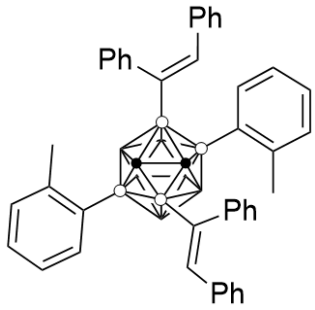
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.8
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19268.6
Nucleus	11B
Acquired Size	32768
Spectral Size	32768




7.385
7.368
7.260
7.244
7.227
7.218
7.200
7.174
7.156
7.138
7.104
7.086
7.019
7.001
6.993
6.974
6.957
6.672
6.574
6.557
3.575
2.331
1.545
0.003
Ph
Ph
Ph
Ph
8b
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 294.5
Experiment 1D
Probe Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 8
Receiver Gain 77
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 2.9998
Spectrometer Frequency 400.20
Spectral Width 4807.7
Lowest Frequency -412.9
Nucleus 1H
Acquired Size 14422
Spectral Size 65536
2.02
12.01
2.08
6.05
2.03
6.03
2.02
6.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

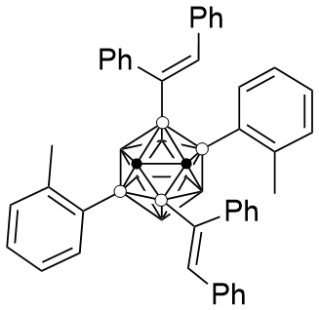


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1500
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.7
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



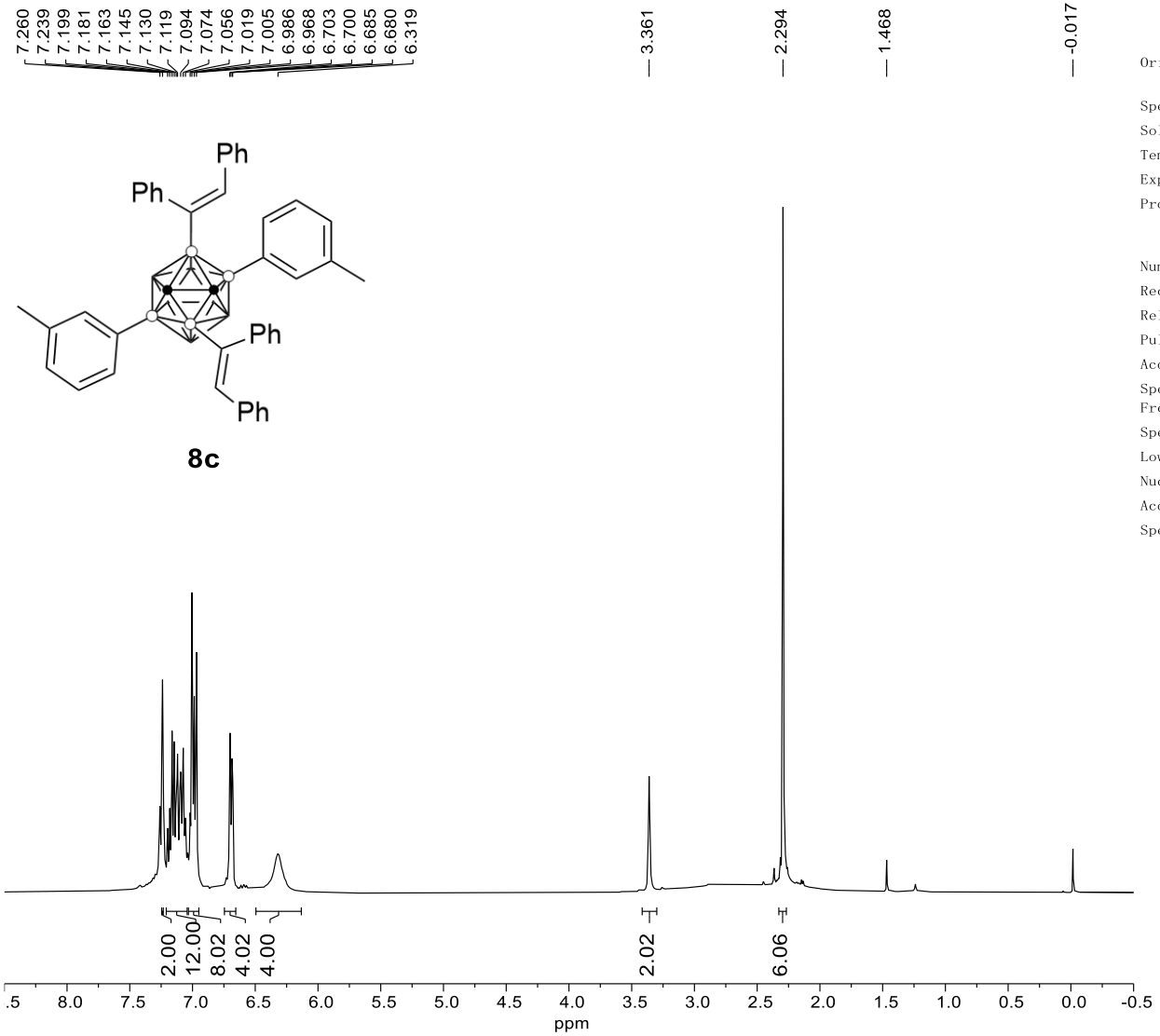
8b

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-20991.2
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

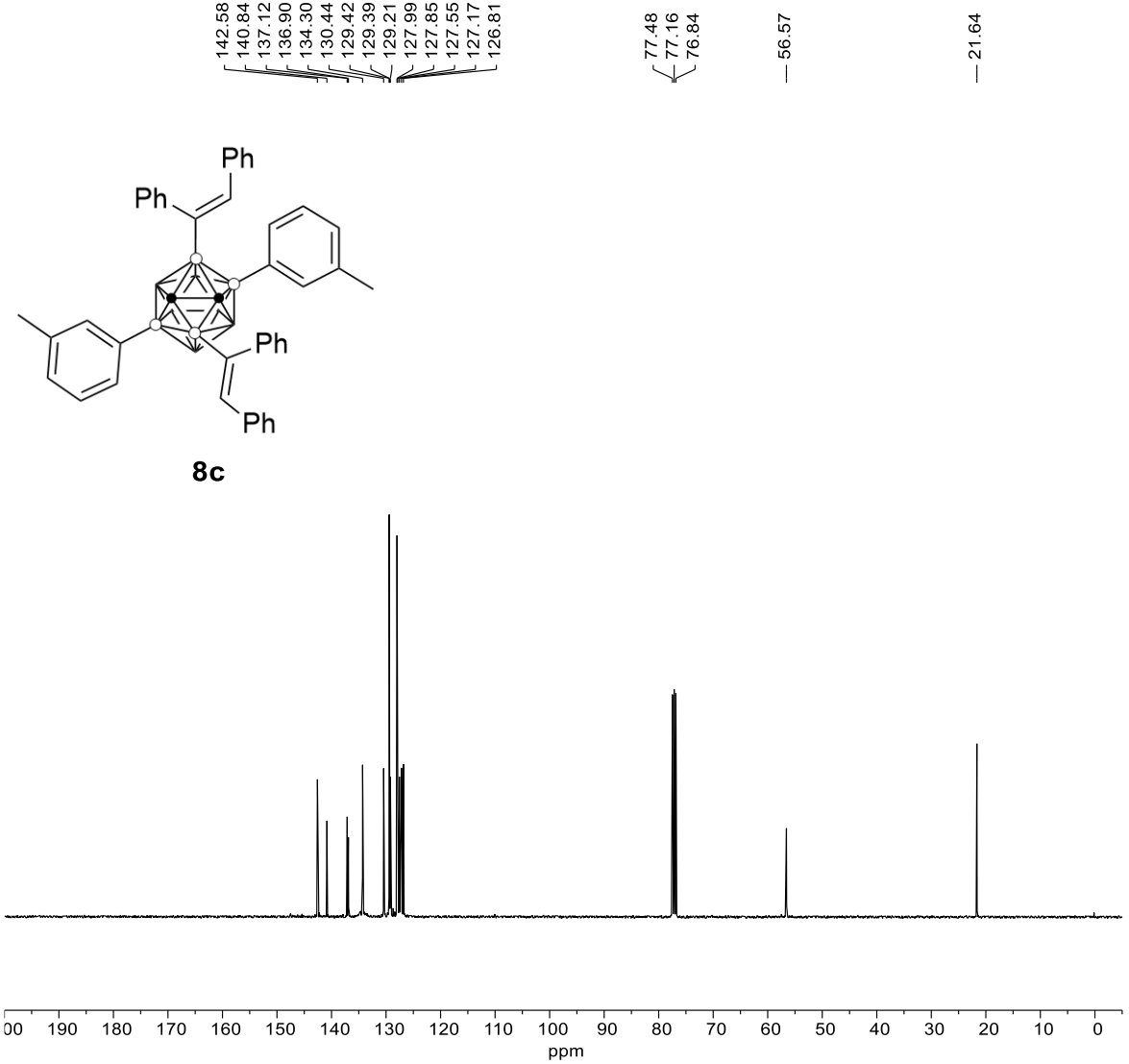


8b

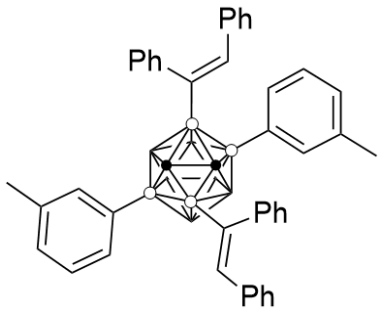
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z114607_0308 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19262.6
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.5
Experiment	1D
Probe	Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	8
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.20
Spectral Width	4807.7
Lowest Frequency	-437.3
Nucleus	1H
Acquired Size	14422
Spectral Size	65536

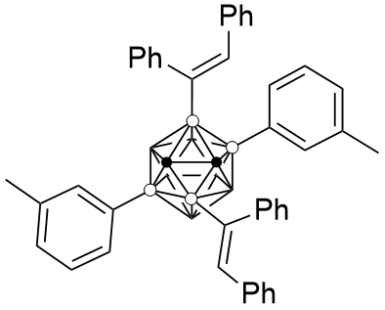


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1500
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1551.3
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



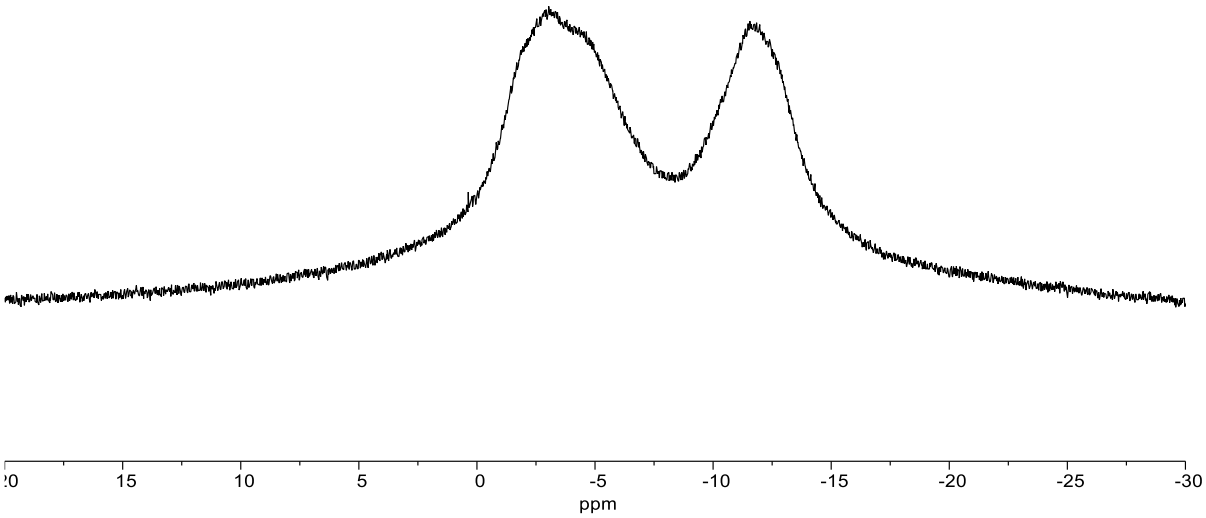
8c

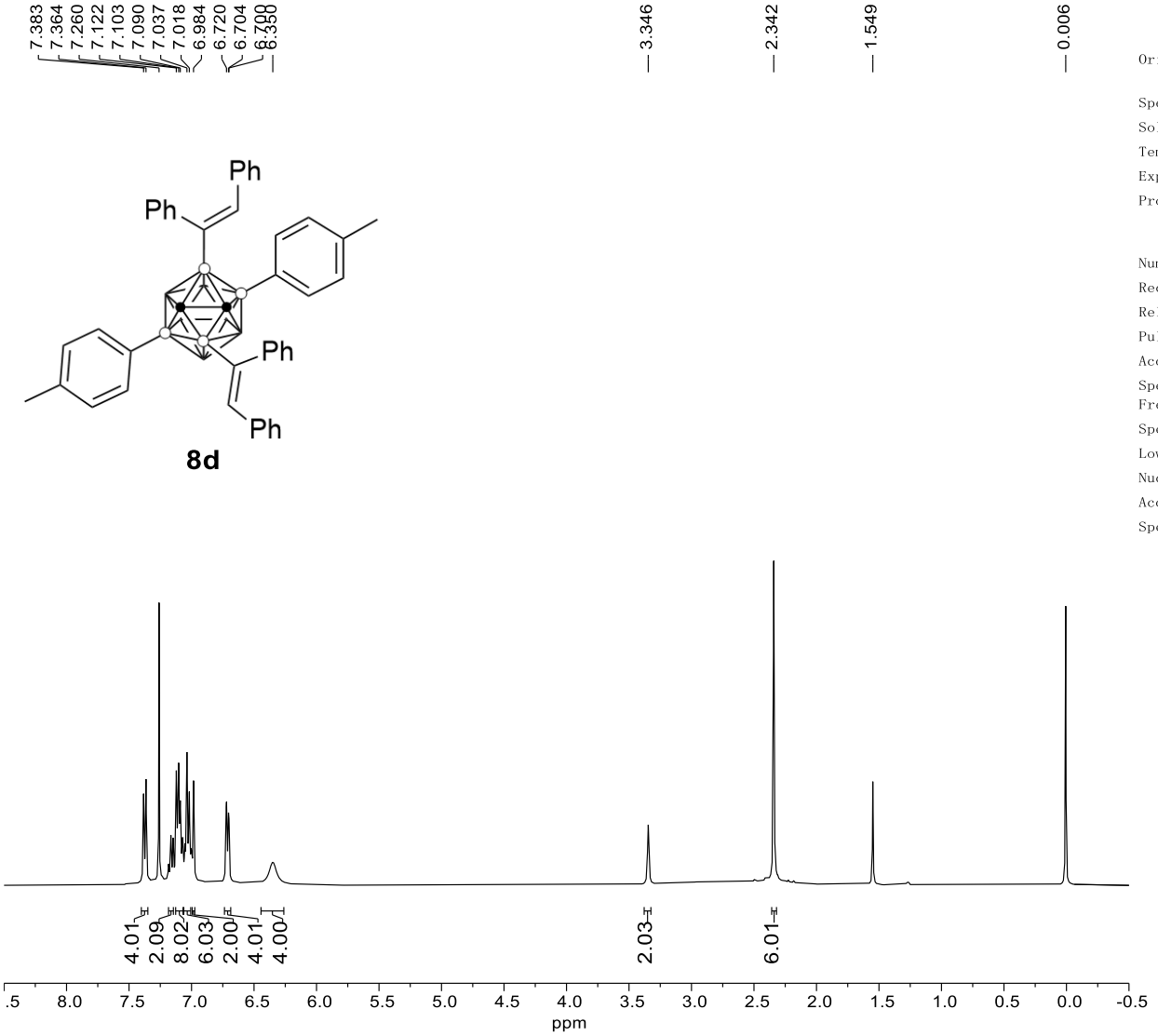
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.5
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	13
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2845
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12707.7
Nucleus	11B
Acquired Size	32768
Spectral Size	65536

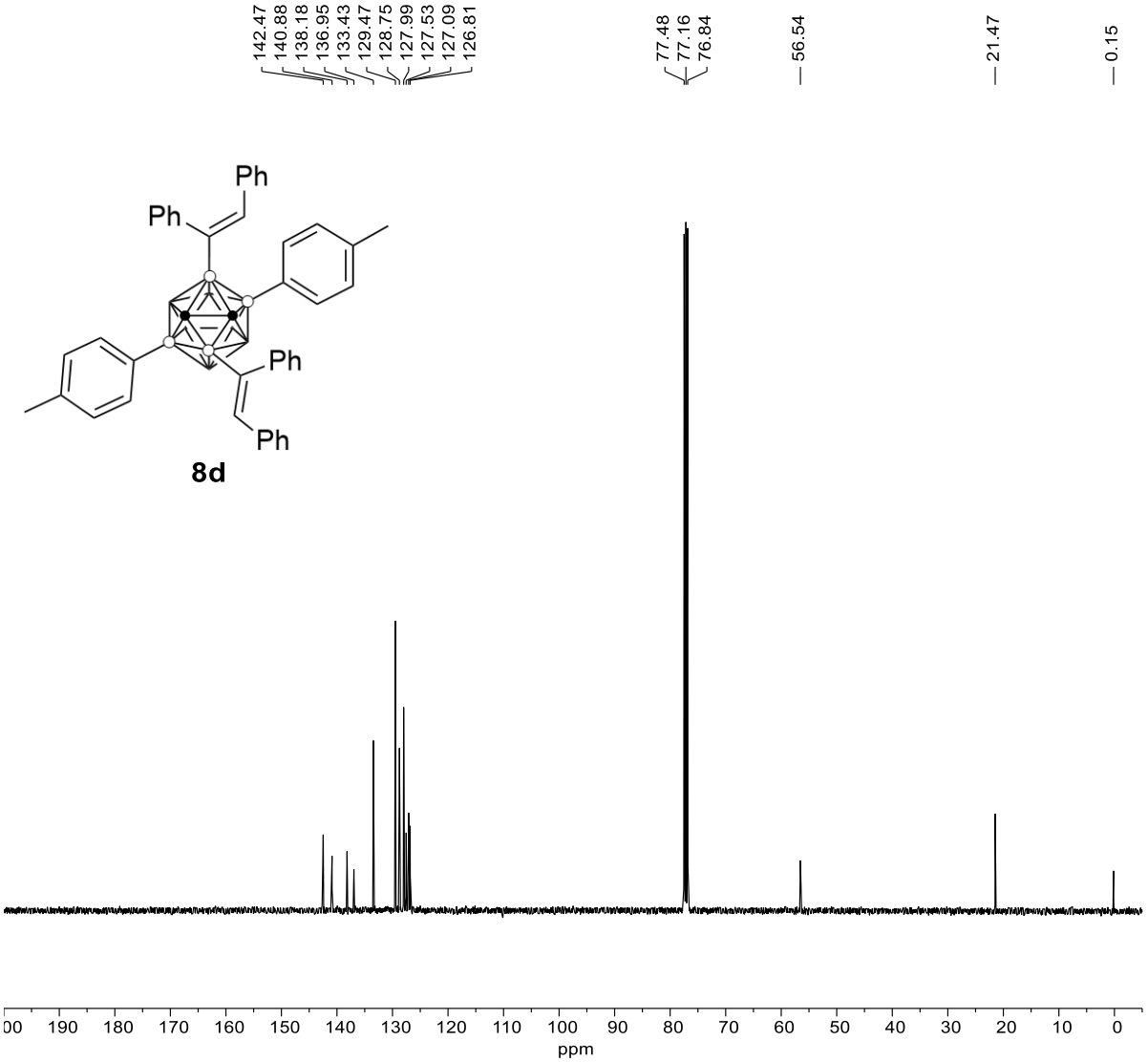


8c

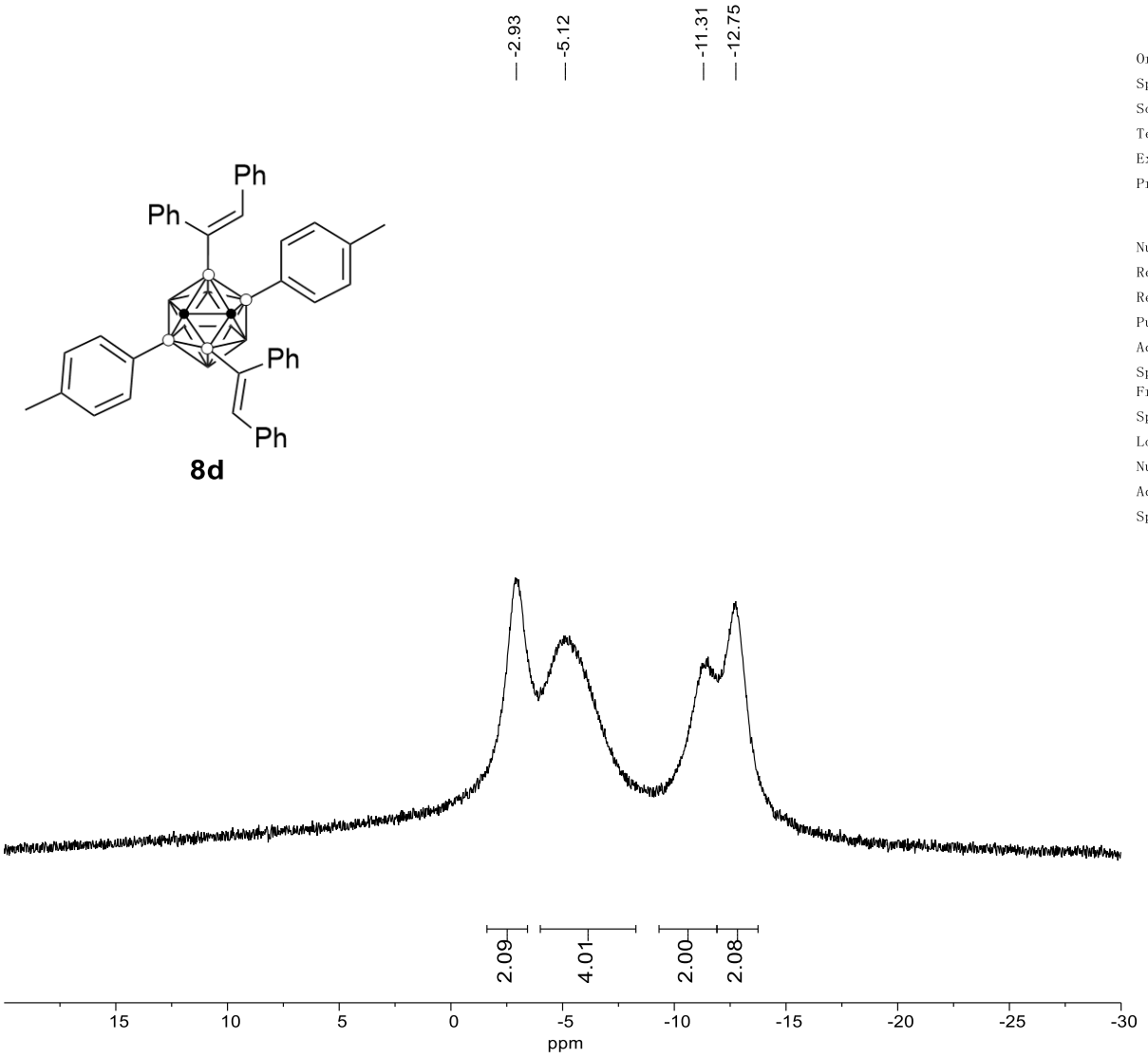
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.5
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	14
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	0.9999
Spectrometer Frequency	128.40
Spectral Width	25510.2
Lowest Frequency	-12707.7
Nucleus	11B
Acquired Size	25508
Spectral Size	65536



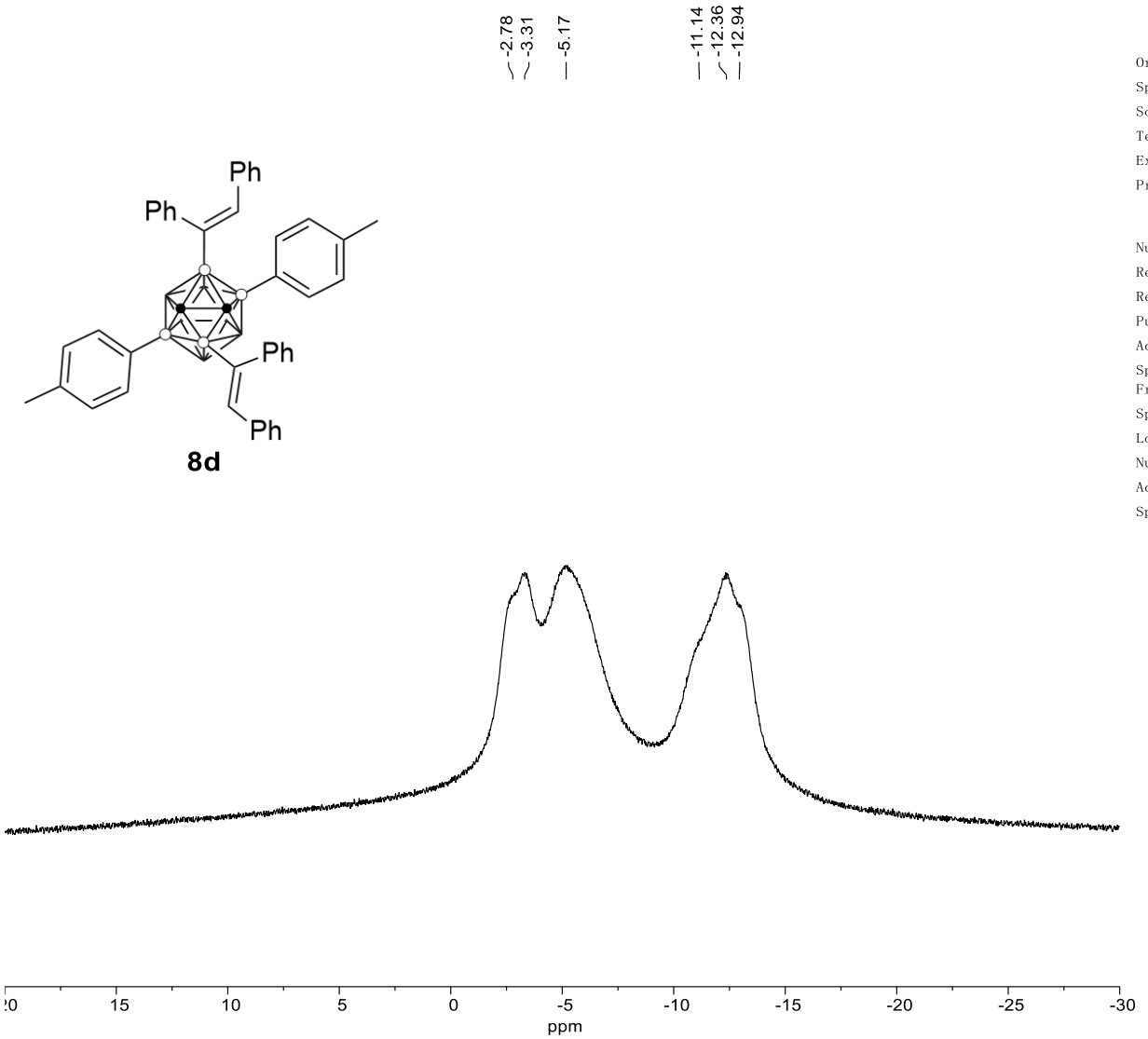

7.383
7.364
7.260
7.122
7.103
7.090
7.037
7.018
6.984
6.720
6.704
6.700
6.350
3.346
2.342
1.549
0.006
Ph
Ph
Ph
Ph
8d
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 294.4
Experiment 1D
Probe Z116098_0640 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 9
Receiver Gain 77
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 2.9998
Spectrometer Frequency 400.20
Spectral Width 4807.7
Lowest Frequency -412.9
Nucleus 1H
Acquired Size 14422
Spectral Size 65536
4.01
2.09
8.02
6.03
2.00
4.01
4.00
2.03
6.01
ppm

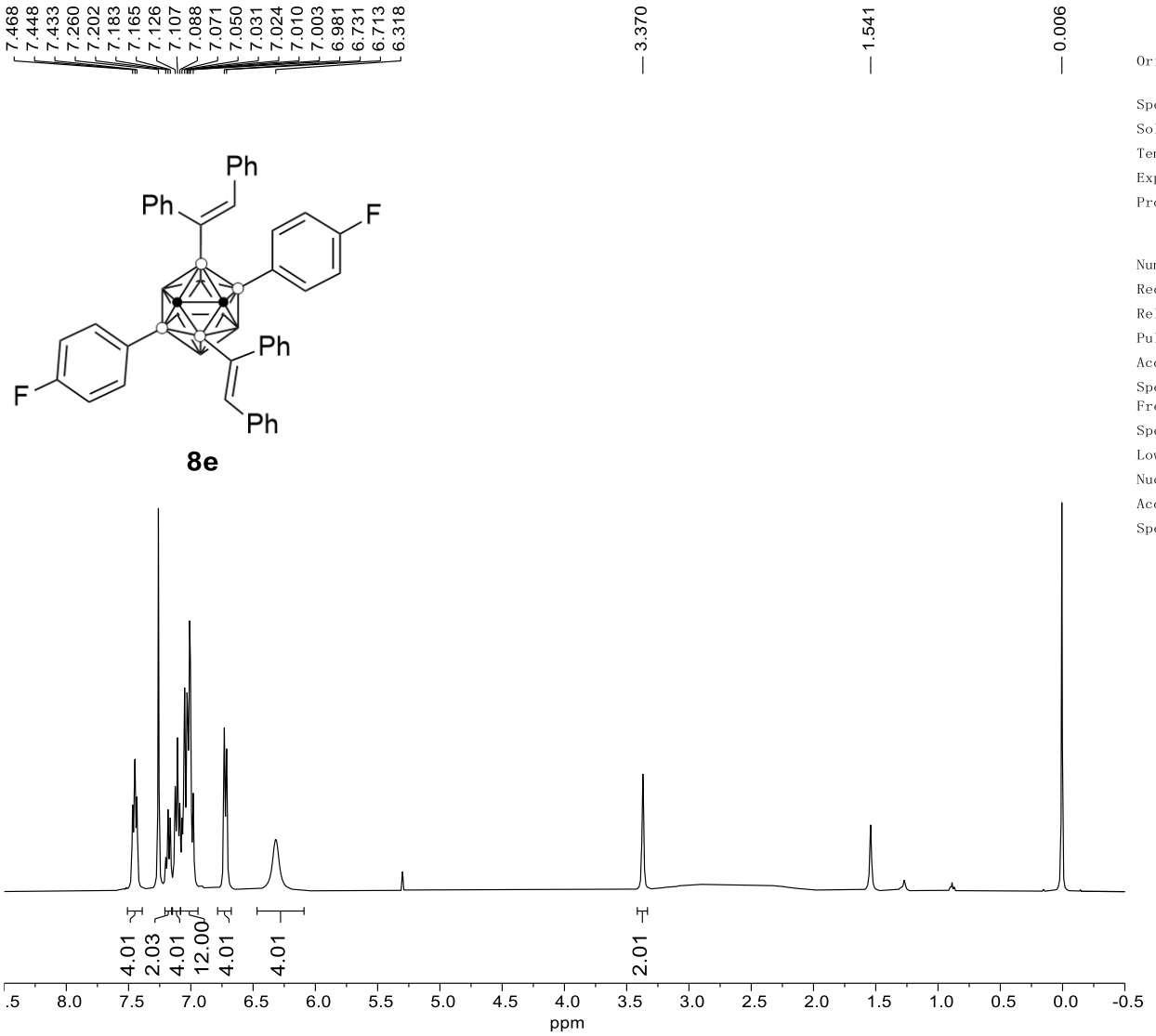


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1600
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.8
Nucleus	13C
Acquired Size	32827
Spectral Size	131072

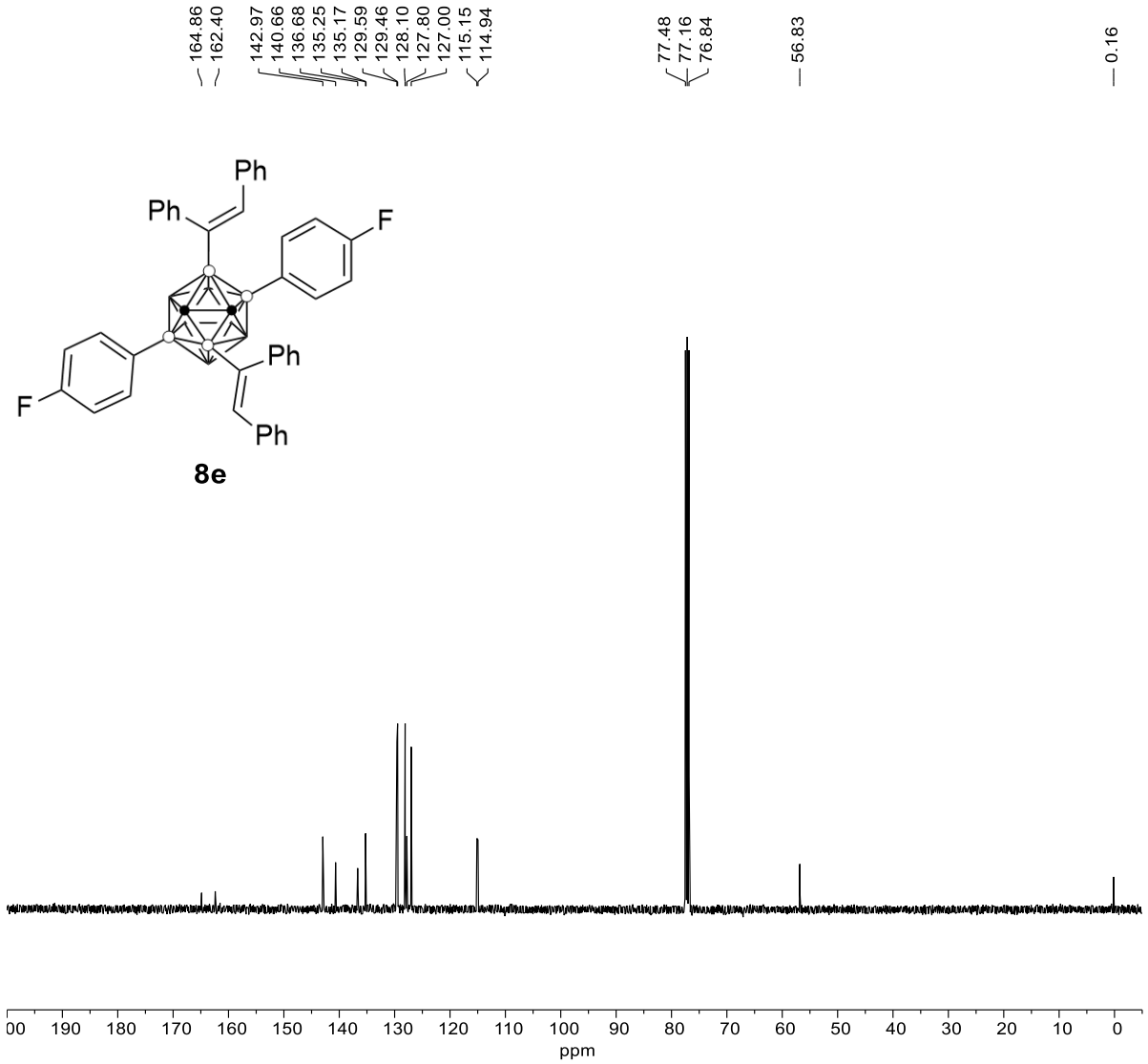


Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.3
Experiment	1D
Probe	Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21000.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

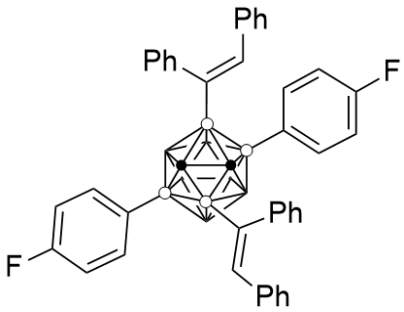

-2.78
-3.31
-5.17
-11.14
-12.36
-12.94
Ph
Ph
Ph
Ph
8d
Origin Bruker BioSpin GmbH
Spectrometer Avance NEO
Solvent CDCl3
Temperature 298.2
Experiment 1D
Probe Z114607_0307 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans 128
Receiver Gain 101
Relaxation Delay 1.0000
Pulse Width 10.7000
Acquisition Time 0.8520
Spectrometer Frequency 192.55
Spectral Width 38461.5
Lowest Frequency -19271.4
Nucleus 11B
Acquired Size 32768
Spectral Size 32768
20
15
10
5
0
-5
-10
-15
-20
-25
-30
ppm



Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	111
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-406.8
Nucleus	1H
Acquired Size	14385
Spectral Size	65536

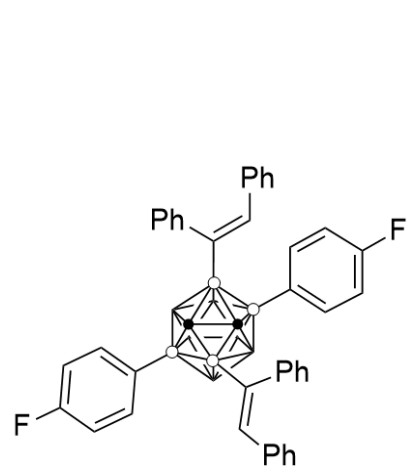


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	1024
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.3
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



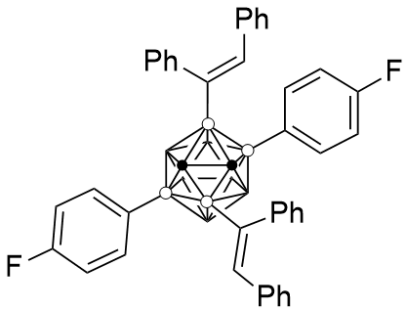
8e

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.3
Experiment	1D
Probe	Z114607_0307 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	64
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21000.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

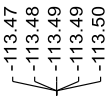


8e

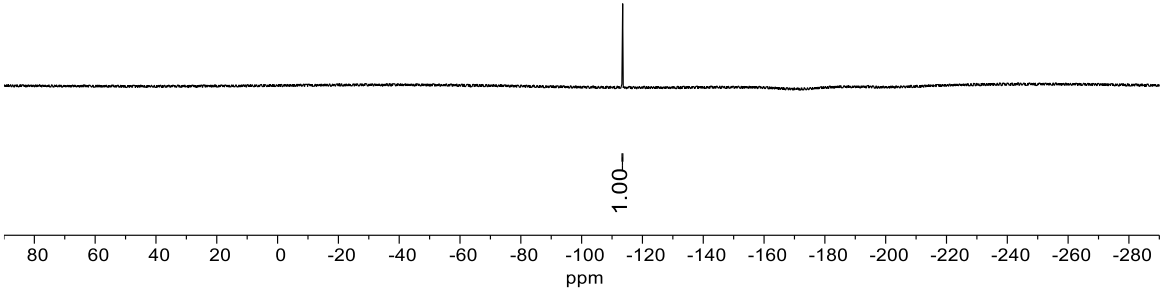
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z114607_0307 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	128
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.7000
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-19271.4
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

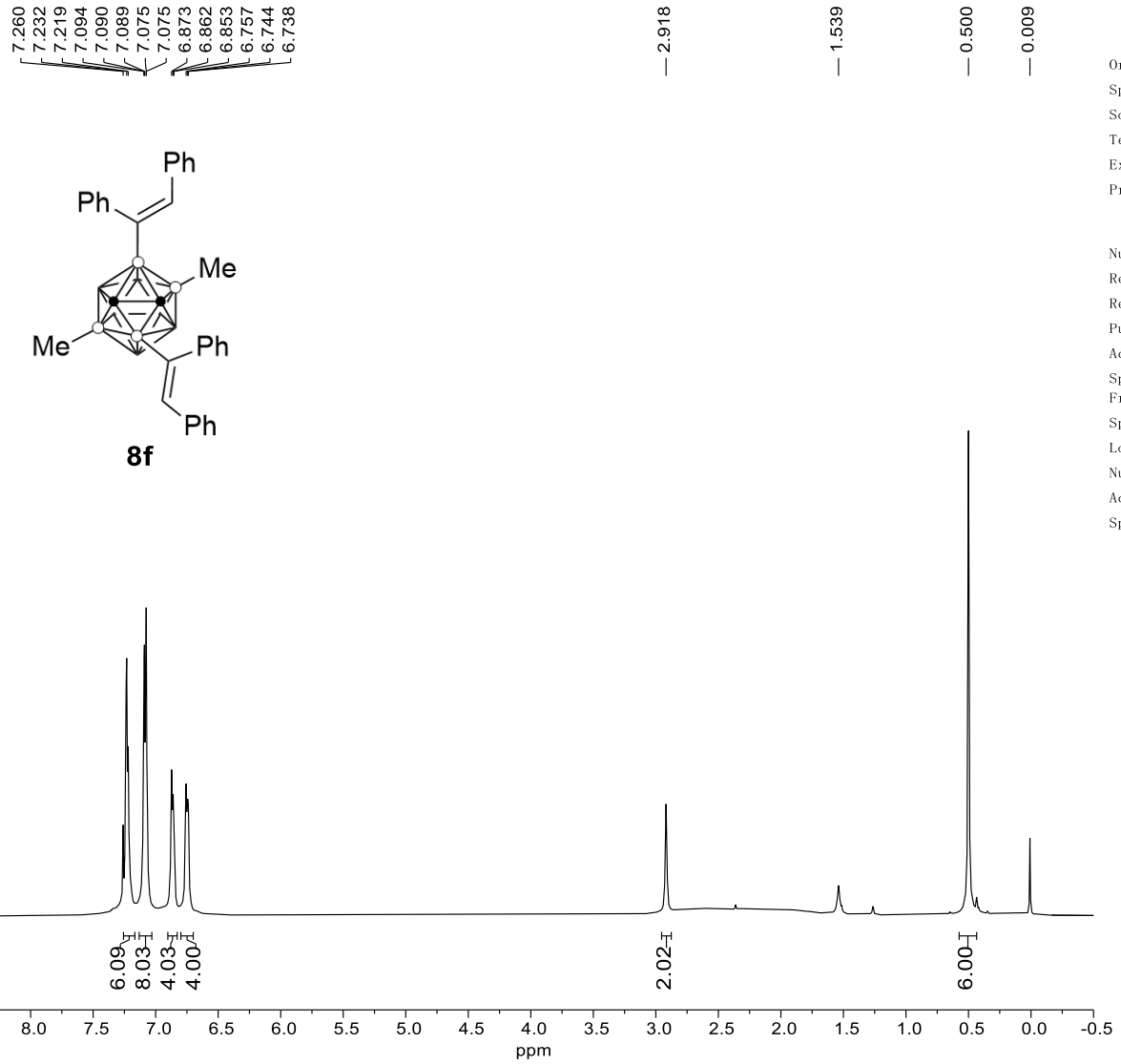


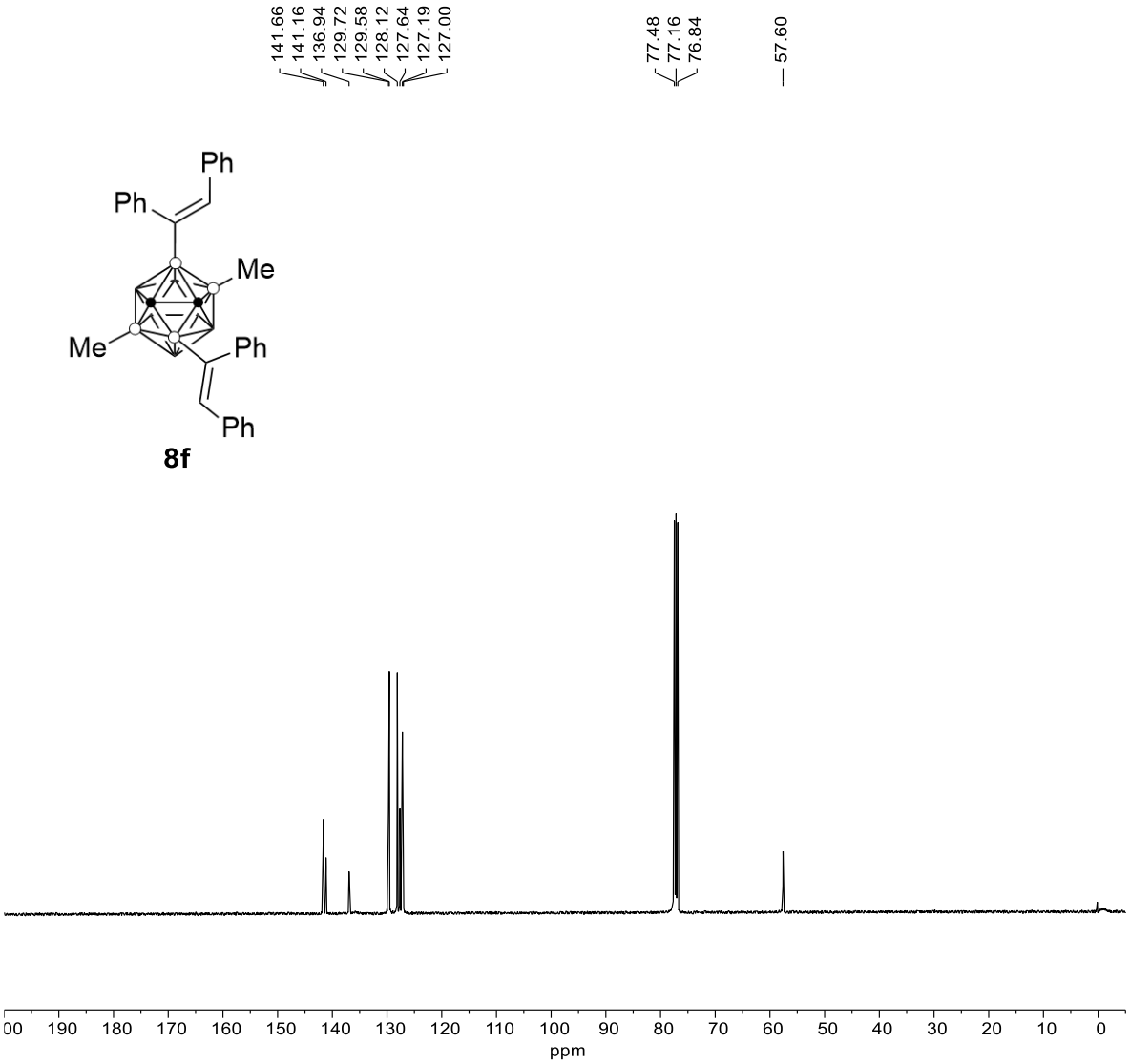
8e



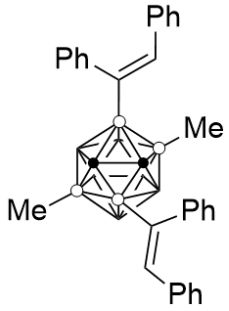
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	294.4
Experiment	1D
Probe	Z116098_0640 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	27
Receiver Gain	196
Relaxation Delay	1.0000
Pulse Width	18.0000
Acquisition Time	0.9999
Spectrometer Frequency	376.53
Spectral Width	150000.0
Lowest Frequency	-112656.4
Nucleus	19F
Acquired Size	149992
Spectral Size	524288




7.260
7.232
7.219
7.094
7.090
7.089
7.075
7.075
6.873
6.862
6.853
6.757
6.744
6.738
2.918
1.539
0.500
0.009
Ph
Ph
Me
Me
Ph
Ph
8f
Origin Bruker BioSpin GmbH
Spectrometer spect
Solvent CDCl3
Temperature 298.1
Experiment 1D
Probe Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans 16
Receiver Gain 87
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 2.9998
Spectrometer Frequency 400.10
Spectral Width 4795.4
Lowest Frequency -407.2
Nucleus 1H
Acquired Size 14385
Spectral Size 65536
6.09
8.03
4.03
4.00
2.02
6.00
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

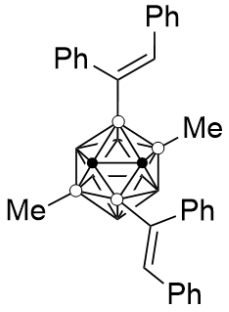


Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	6000
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1546.3
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



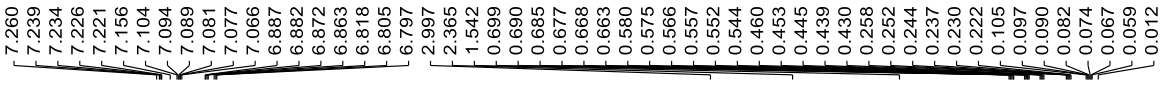
8f

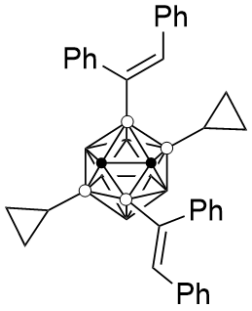
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.5
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	32
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21198.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



8f

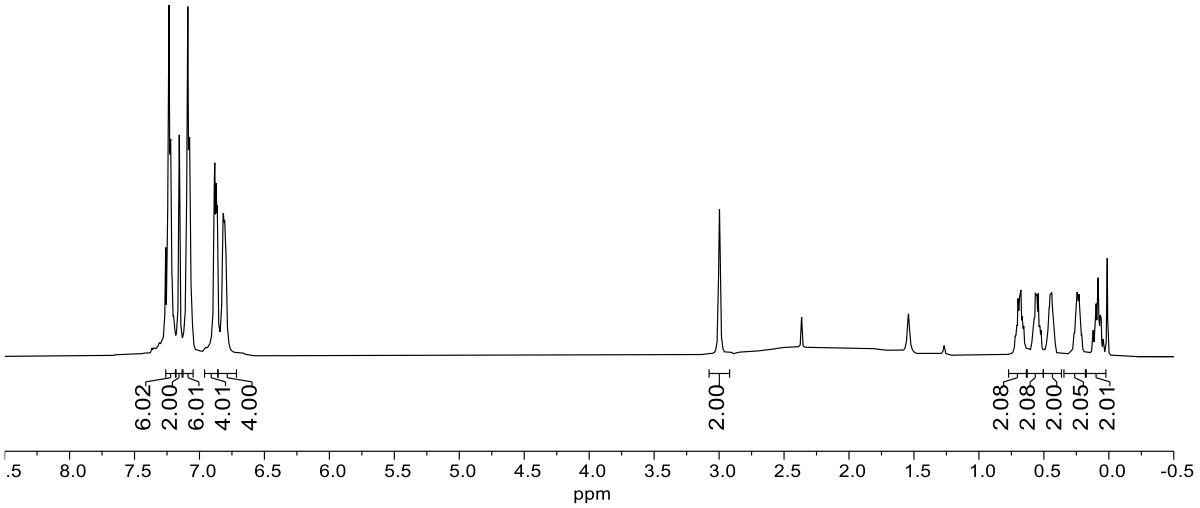
Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.0
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	32
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21198.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768

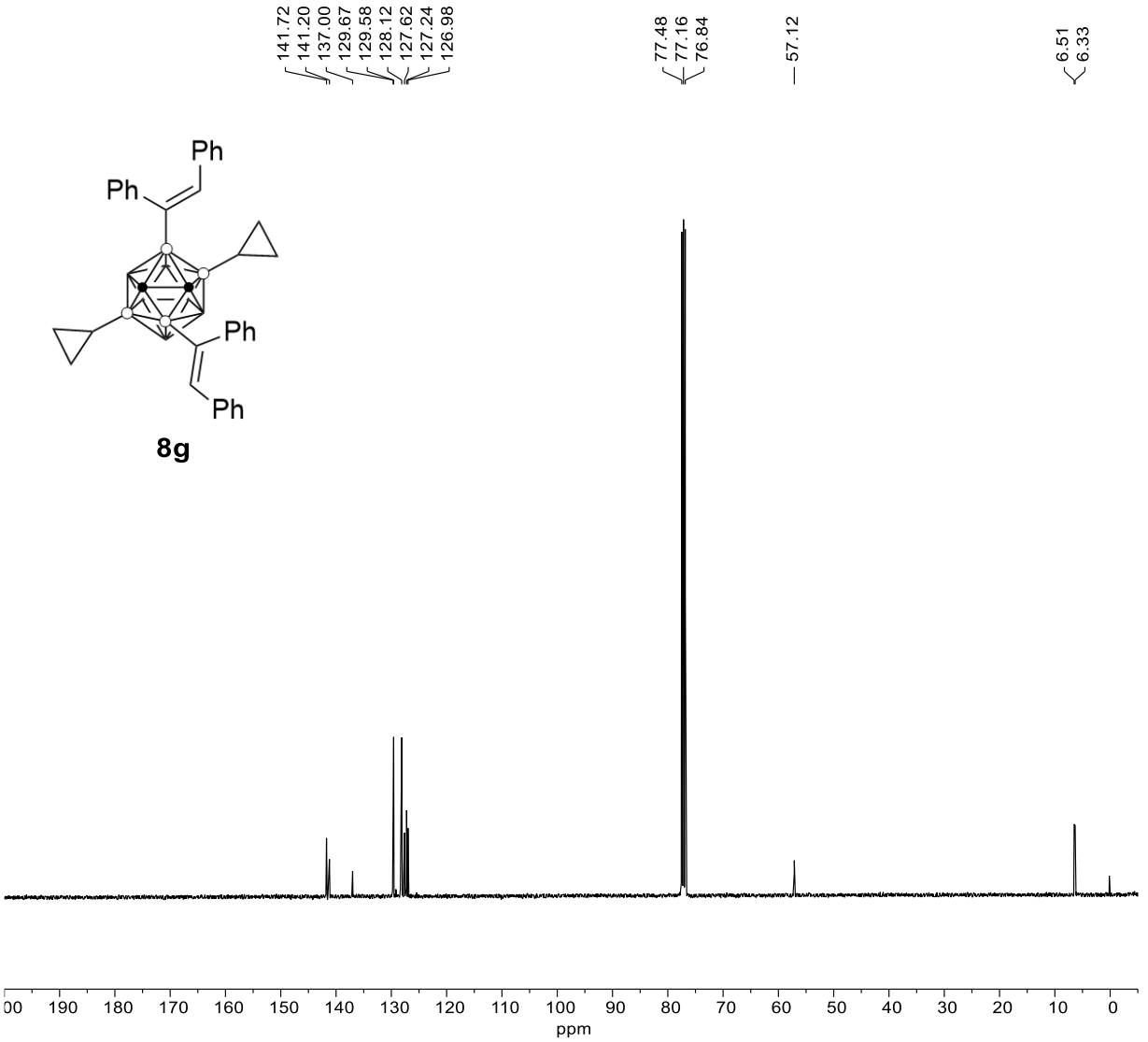




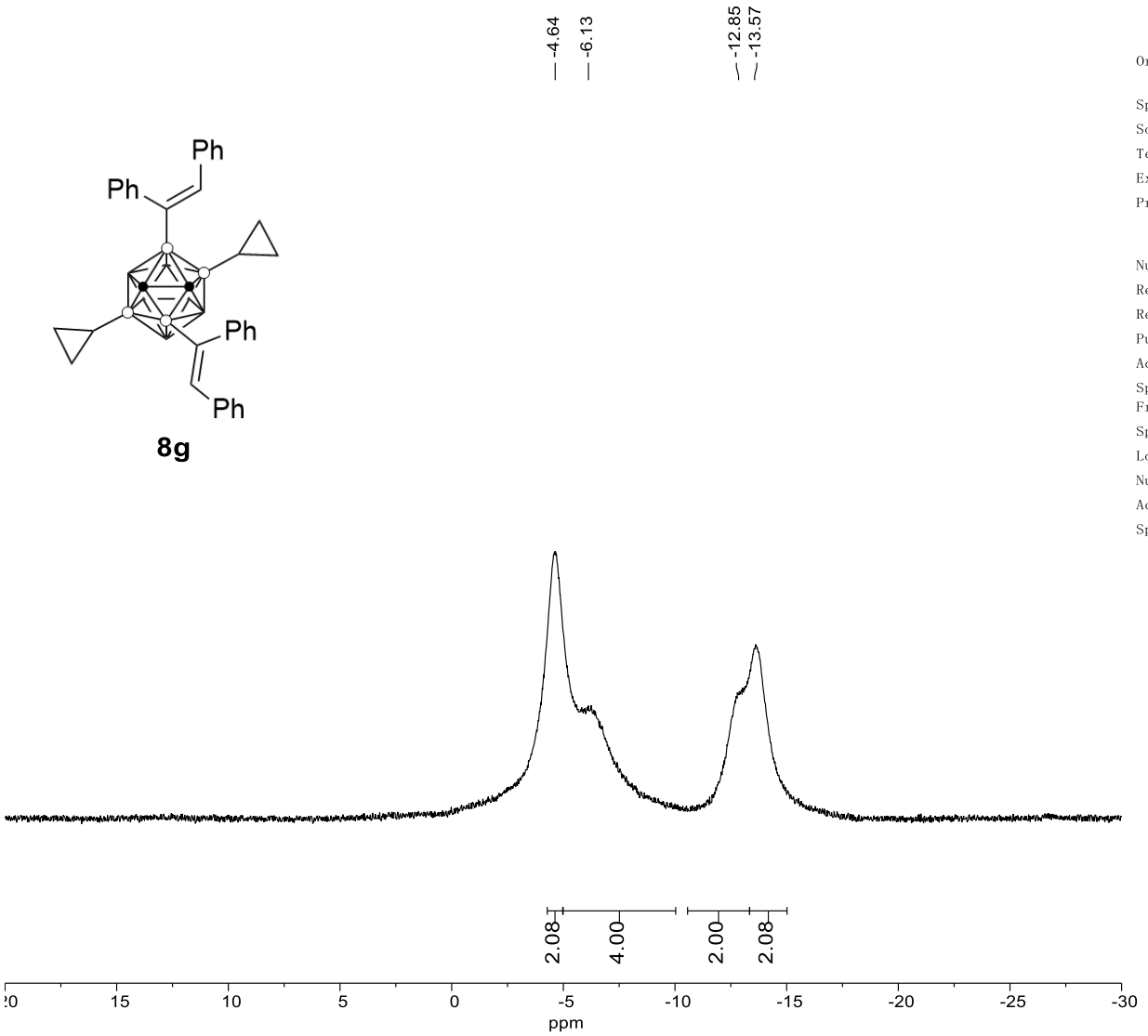
8g

Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.1
Experiment	1D
Probe	Z116098_0643 (PA BBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	16
Receiver Gain	70
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	2.9998
Spectrometer Frequency	400.10
Spectral Width	4795.4
Lowest Frequency	-406.8
Nucleus	1H
Acquired Size	14385
Spectral Size	65536

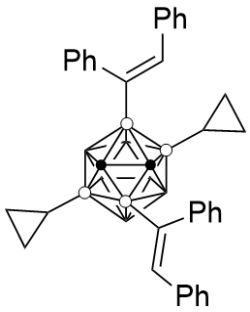




Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z116098_0643 (PABBO 400S1 BBF-H-D-05 Z SP)
Number of Scans	4000
Receiver Gain	197
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.2999
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-1545.4
Nucleus	13C
Acquired Size	32827
Spectral Size	131072



Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.6
Experiment	1D
Probe	Z114607_0308 (PABBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	32
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21198.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



8g

Origin	Bruker BioSpin GmbH
Spectrometer	Avance NEO
Solvent	CDCl3
Temperature	298.2
Experiment	1D
Probe	Z114607_0308 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	32
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	9.3500
Acquisition Time	0.8520
Spectrometer Frequency	192.55
Spectral Width	38461.5
Lowest Frequency	-21198.0
Nucleus	11B
Acquired Size	32768
Spectral Size	32768