Supplementary Information for

Carbene-stabilized 6,12-diboraanthanthrenes: unveiling the multistage redox properties of polycyclic aromatic hydrocarbons featuring electron-rich boron centers

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Contents

1. Synthesis of 1–11 and their spectral data

General considerations: All air and moisture experiments and manipulations were carried out under dry nitrogen using standard Schlenk techniques or in a Vigor inert atmosphere dry-box containing an atmosphere of purified nitrogen and equipped with a -25 ℃ freezer. Solvents including tetrahydrofuran (THF), toluene, hexane and pentane were dried by distilled over Na, K and benzophenone prior to use. *o*-Difluorobenzene (*o*-DFB), dichloromethane (DCM) and acetonitrile were dried by distilled over CaH_2. Deuterated solvents including DMF-d_7, CD_2Cl_2, CD_3CN were distilled over CaH_2 then soaked in 3 Å molecular sieves. The solution NMR spectra were recorded with Bruker AVANCE NEO 400MHz, Bruker AVANCE III HD 600 MHz, and JEOL-JNM-ECZ400S/L1 400 MHz spectrometers. Solid-state NMR spectra were obtained with a JEOL-JNM-ECZ400R/S1 400 MHz spectrometer. Proton and carbon signals chemical shifts are reported in ppm, referenced to residual solvent signals as internal standards (^1H and $^{13}C\{^1H\}$), and boron chemical shifts are collected in quartz NMR tube with an external reference ($BF_3{\cdot}OEt_2$ for ^{11}B). Abbreviations: s = singlet; d = doublet; t = triplet; m = multiplet; br = broad. The UV-Vis absorption spectra of the compounds were recorded on Perkin-Elmer Lambda-950 Spectrophotometer. The photoluminescence (PL) spectra, related emission lifetimes, and the absolute fluorescence quantum yields of the compounds were recorded on Edinburgh Instruments Ltd (FLSP980) steady state transient fluorescence spectrometer. Elemental analyses (C, H, N) were performed with a EuroVector EA3000 Elemental Analyzer. Melting points were measured on an SGW X-4B apparatus. EPR spectra were recorded on Bruker X-band spectrometer A300-9.5/12. Single crystal X-ray diffraction data were collected on Bruker D8-VENTURE diffractometer. The starting materials dinaphthosilole (DNSi),[1] 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (NHC)[2] and 2,6-(diisopropylphenyl)-2,2,4,4-tetramethyl-pyrrolidin-5-ylidene (CAAC)[3] were prepared according to literature procedures.

Synthesis of Compound 1 The synthesis of **1** was performed following the procedure reported in the literature with some modifications.[1] In a nitrogen atmosphere, BBr_3 (3 mL) was added to a mixture of DNSi (600 mg, 1.93 mmol) and $AlCl_3$ (12.9 mg, 0.097 mmol) to give a dark brown suspension, which was stirred at 50 ℃ in oil bath for 24 h. After the removal of the excess amount of BBr_3 under reduced pressure, an aqueous solution of potassium carbonate was added to give an orange-yellow suspension. The mixture was stirred for 2 hours, then the filtrate was decanted. The solid was dried and washed three times with dichloromethane to afford the orange product **1** (236.2 mg, 40%). M.p.: >300 ℃. ^{1}H NMR (400 MHz, DMSO-*d*$_6$, 25 ℃) δ (ppm) = 10.18 (s, 2H, B-O*H*), 8.62 (d, *J* = 6.8 Hz, 2H), 8.40 (d, *J* = 8.1 Hz, 2H), 8.22 (d, *J* = 8.0 Hz, 2H), 8.06 (d, *J* = 8.2 Hz, 2H), 7.77 (t, *J* = 7.8 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, DMSO-*d*$_6$, 25 ℃) δ (ppm) = 139.37, 134.60, 134.56, 134.31, 134.18, 133.68, 131.03, 128.80, 128.58, 126.72. ^{11}B{^{1}H} NMR (128 MHz, DMSO-*d*$_6$, 25 ℃) δ (ppm) = 40.11.

Synthesis of Compound 2 A solution of **1** (1.56 g, 5.10 mmol) in DCM was cooled to 0 ℃ before BBr_3 (1M in DCM, 11.5 mL, 11.5 mmol) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for 3 hours. Excess BBr_3 was removed under reduced pressure to obtain a crude solid. Dry toluene (50 mL) was added and the resulting suspension was stirred for 30 minutes. The solvent was then removed under vacuum to eliminate residual BBr_3. The solid was subsequently washed with toluene to yield the final product as a deep red powder (1.76 g, 80%). M.p.: >300 ℃. Note: Due to the extremely poor solubility of **2**, its NMR spectra were unable to be collected. Elemental analysis (%) calcd for $C_{20}H_{10}B_2Br_2$: C 55.64, H 2.33; found: C 55.31, H 2.22.

Synthesis of Compound 3 THF (20 mL) was added to a mixture of **2** (118 mg, 0.27 mmol), 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (NHC) (213.7 mg, 0.55 mmol) and potassium graphite (KC_8) (74.4 mg, 0.55 mmol) at −78 ℃. The reaction mixture was slowly allowed to reach room temperature and stirred for another 6 hours. All volatiles were then removed under vacuum, and the residue was washed with toluene (3×10 mL) before being extracted with a large volume of THF (300 mL). The extract was subsequently dried under vacuum, yielding **3** as a dark blue solid (226.6

mg, 80%). Alternative methods for the synthesis of compound **3** involve treating **6** with 1.0 equivalent of KC_8 or **8** with 2.0 equivalents of KC_8 in THF at −78 °C, affording yields of 76% and 72%, respectively. Single crystals suitable for X-ray diffraction were obtained by evaporation of a saturated THF solution of **3** at room temperature. M.p.: >300 °C (dec.). ^{1}H NMR (400 MHz, DMF-d_7, 25 °C) δ (ppm) = 8.33 (s, 4H), 7.74 (d, J = 7.3 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 6.8 Hz, 2H), 7.19 (t, J = 7.3 Hz, 2H), 7.05 (t, J = 7.6 Hz, 4H), 7.03 - 6.94 (m, 10H,), 3.46 - 3.38 (m, 8H, CH(CH$_3$)$_2$), 1.19 (dd, J = 12.6, 6.8 Hz, 24H, CH(CH_3)$_2$), 0.95 (d, J = 6.6 Hz, 12H, CH(CH_3)$_2$), 0.75 (d, J = 6.6 Hz, 12H, CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, DMF-d_7) δ (ppm) = 146.15, 136.25, 135.19, 135.05, 132.85, 130.29, 126.75, 126.52, 124.69, 124.61, 119.92, 119.26, 117.62, 29.59 (d, J = 13.6 Hz, CH(CH$_3$)$_2$), 26.40 (d, J = 4.7 Hz, CH(CH$_3$)$_2$), 22.42 (d, J = 13.9 Hz, CH(CH$_3$)$_2$). Note that carbon atoms directly bonded to boron are not always observed in the ^{13}C{^{1}H} NMR spectra due to quadrupolar relaxation leading to signal broadening. ^{11}B NMR (128 MHz, DMF-d_7, 25 °C) δ (ppm) = 22.88. Solid-state ^{1}H NMR (MAS, 12 kHz) δ (ppm) = 74.54, 41.63, 2.98, -30.16, -63.82. Solid-state ^{13}C NMR (CP/MAS, 12 kHz) δ (ppm) = 175.55, 150.80, 150.20, 147.40, 145.00, 142.98, 138.97, 138.36, 135.91, 135.27, 134.73, 133.81, 131.61, 129.00, 126.67, 124.45, 122.86, 121.69, 120.71, 32.88, 32.18, 31.13, 29.68, 28.21, 22.65, 20.98. Solid-state ^{11}B NMR (MAS, 12 kHz) δ (ppm) = 18.97. Elemental analysis (%) calcd for $C_{74}H_{82}B_2N_4$: C 84.72, H 7.88, N 5.34; found: C 84.53, H 7.96, N 5.45.

Synthesis of Compound 4 THF (20 mL) was added to a mixture of **2** (118 mg, 0.27 mmol), 2,6-(diisopropylphenyl)-2,2,4,4-tetramethyl-pyrrolidin-5-ylidene (CAAC) (157 mg, 0.55 mmol) and potassium graphite (KC_8) (74.4 mg, 0.55 mmol) at −78 °C. The reaction mixture was slowly allowed to reach room temperature and stirred for another 6 hours. The resulting dark purple reaction mixture was filtrated, and the residue was washed with THF (2×10 mL) before being extracted with trifluorotoluene (100 mL). The extract was subsequently dried under vacuum, yielding **4** as a dark purple solid (193.4 mg, 85%). Alternative methods for the synthesis of compound **4** involve treating **7** with 1.0 equivalent of KC_8 or **9** with 2.0 equivalents of KC_8 in THF at −78 °C, affording yields of 79% and 76%, respectively. Single crystals suitable for X-ray

diffraction were obtained by evaporation of a saturated *o*-DFB solution of **4** at room temperature. M.p.: 206 ℃ (dec.). Solid-state ^{1}H NMR (MAS, 12 kHz) δ (ppm) = 67.19, 36.11, 6.04, 4.22, 2.44, -27.67, -58.46. Solid-state ^{13}C NMR (CP/MAS, 12 kHz) δ (ppm) = 150.25, 149.01, 148.43, 141.83, 140.05, 139.71, 138.63, 138.07, 135.49, 132.94, 132.41, 130.82, 129.80, 128.75, 127.99, 121.28, 119.70, 118.95, 84.14, 83.40, 70.00, 59.99, 53.21, 52.43, 37.11, 36.11, 34.89, 33.03, 32.26, 30.75, 27.21, 26.17. Solid-state ^{11}B NMR (MAS, 12 kHz) δ (ppm) = 19.54. Elemental analysis (%) calcd for $C_{60}H_{72}B_2N_2$: C 85.50, H, 8.61, N 3.32; found: C 85.26, H 8.43, N 3.43.

Synthesis of Compound 5 THF (10mL) was added to the mixture of **3** (86 mg, 0.082mmol) and TEMPO (28.19 mg, 0.18 mmol) at room temperature. The reaction mixture was stirred for 6 hours, resulting in a pale yellow solid suspension. All volatiles were removed in vacuo and the residue was washed with Et_2O (3×10 mL) and dried, yielding **5** as a yellow green soild (35.94 mg, 75%). An alternative method for the synthesis of **5** from **4** using 2.0 equivalent of TEMPO following the procedure described above gave 80% yield. Single crystals suitable for X-ray diffraction were obtained by evaporation of a saturated toluene solution of **5** at room temperature. M.p.: >300 ℃. *Note: The NMR spectra showed the formation of an 83:17 mixture of anti-**5** and syn-**5**. The NMR resonances of the two atropisomers were assigned on the basis of COSY, HSQC and HMBC spectra.* ^{1}H NMR (400 MHz, $CDCl_3$, 25 ℃) for *anti*-**5**: δ 10.04 (dd, *J* = 15.8, 7.1 Hz, 1H), 8.50 (d, *J* = 8.1 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 1.84 (d, *J* = 7.9 Hz, 4H), 1.76 - 1.69 (m, 2H), 1.42 (s, 6H), 1.17 (s, 6H); for *syn*-**5**: δ 9.90 (dd, *J* = 13.9, 8.5 Hz, 1H), 8.62 (d, *J* = 6.8 Hz, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.68 (t, *J* = 3.3 Hz, 1H), 1.56 (m, 6H), 1.41 (s, 6H), 1.19 (s, 6H). ^{13}C {^{1}H} NMR (151 MHz, $CDCl_3$, 25 ℃) for *anti*-**5**: δ 140.11, 139.77, 135.19, 134.87, 134.55, 129.11, 128.52, 125.95, 60.59 (N*C*$(CH_3)_2$), 39.86 (CH_2), 32.55 (CH_3), 20.50 (CH_3), 17.53 (CH_2); for *syn*-**5**: δ 141.88, 140.18, 135.33, 134.91, 134.75, 134.72, 134.08, 133.64, 133.42, 133.40, 130.06, 130.03, 128.81, 128.64, 128.13, 126.59, 126.18, 60.49 (N*C*$(CH_3)_2$), 39.83 (CH_2), 32.09 (CH_3), 20.38 (CH_3), 17.53 (CH_2). Note that carbon atoms directly bonded to boron are not always observed in the ^{13}C{^{1}H} NMR spectra due to quadrupolar relaxation leading

to signal broadening. ^{11}B NMR (128 MHz, $CDCl_3$, 25 ℃) δ 39.21. Elemental analysis (%) calcd for for *anti*-$C_{38}H_{46}B_2N_2O_2$: C 78.10, H 7.93, N 4.79; found: C 78.04, H 7.85, N 4.75.

Synthesis of Compound 6 *o*-DFB (15 mL) was added to a mixture of **3** (116 mg, 0.11 mmol) and $AgSbF_6$ (37.8 mg, 0.11 mmol) at −78 ℃. The reaction mixture was slowly allowed to reach room temperature and stirred for another 6 hours. All volatiles were then removed under vacuum, and the residue was washed with THF (3×10 mL) before being extracted with *o*-DFB (3×20 mL). The combined extracts were subsequently dried under vacuum, yielding **6** as an NMR-silent dark brown solid (110 mg, 78%). An alternative method for the synthesis of **6** from **8** using 1.0 equivalent of KC_8 in THF at -78 ℃ gave 70% yield. Single crystals suitable for X-ray diffraction were obtained by the evaporation of a saturated *o*-DFB solution of **6** at room temperature. M.p.: 248 ℃ (dec.). Elemental analysis (%) calcd for $C_{74}H_{82}B_2N_4SbF_6$: C 69.18, H 6.43, N 4.36; found: C 69.41, H 6.29, N 4.52.

Synthesis of Compound 7 *o*-DFB (15 mL) was added to a mixture of **4** (116 mg, 0.13 mmol) and $AgSbF_6$ (44.7 mg, 0.13 mmol) at −78 ℃. The reaction mixture was slowly allowed to reach room temperature and stirred for another 6 hours. All volatiles were then removed under vacuum, and the residue was washed with THF (3×10 mL) before being extracted with *o*-DFB (3×20 mL). The combined extracts were subsequently dried under vacuum, yielding compound **7** as an NMR-silent dark brown solid (115 mg, 82%). An alternative method for the synthesis of **7** from **9** using 1.0 equivalent of KC_8 in THF at -78 ℃ gave 73% yield. Single crystals suitable for X-ray diffraction were obtained by gas-phase diffusion of pentane into a saturated *o*-DFB solution of **7** at room temperature. M.p.: 251 ℃ (dec.). Elemental analysis (%) calcd for $C_{60}H_{72}B_2N_2SbF_6$: C 66.81, H 6.73, N 2.60; found C 66.52, H 6.62, N 2.73.

Synthesis of Compound 8 *o*-DFB (15 mL) was added to a mixture of **3** (116 mg, 0.11 mmol) and $AgSbF_6$ (75.6 mg, 0.22 mmol) at −78 ℃. The reaction mixture was slowly allowed to reach room temperature, then the reaction mixture was stirred for 30 minutes. The mixture was filtered, and the residue was extracted with *o*-DFB (3 × 20 mL). The combined *o*-DFB extracts were concentrated to 30 mL, followed by the addition of

toluene (100 mL). The resulting solution was stirred for 3 hours, leading to the formation of compound **8** as a bright red solid (103.7 mg, 62%). An alternative method for the synthesis of **8** from **6** using 1.0 equivalent of $AgSbF_6$ following the procedure described above gave 70% yield. Single crystals suitable for X-ray diffraction were obtained by diffusion of hexane into a saturated DCM solution of **8** at room temperature. M.p.: 273 °C (dec.). ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C) δ (ppm) = 8.20 (d, *J* = 7.9 Hz, 2H), 8.01 (s, 4H), 7.92 (d, *J* = 7.4 Hz, 4H), 7.66 (d, *J* = 8.5 Hz, 4H), 7.32 (t, *J* = 7.7 Hz, 4H), 7.12 (d, *J* = 7.7 Hz, 8H), 2.94-2.79 (m, 8H, NHC C*H*$(CH_3)_2$), 1.23 (d, *J* = 6.3 Hz, 24H, NHC CH(C*H*$_3)_2$), 0.87 (d, *J* = 6.3 Hz, 24H, NHC CH(C*H*$_3)_2$). ^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2, 25 °C) δ (ppm) = 146.96, 145.22, 142.79, 139.73, 136.07, 134.33, 132.72, 132.14, 131.67, 131.35, 130.06, 128.56, 125.85, 29.93 (NHC *C*H$(CH_3)_2$), 27.04 (NHC CH(*C*H$_3)_2$), 22.14 (NHC CH(*C*H$_3)_2$). Note that carbon atoms directly bonded to boron are not always observed in the ^{13}C{^{1}H} NMR spectra due to quadrupolar relaxation leading to signal broadening. ^{11}B NMR (128 MHz, CD_2Cl_2, 25 °C) δ (ppm) = 51.92. Elemental analysis (%) calcd for $C_{74}H_{82}B_2N_4Sb_2F_{12}$: C 58.45, H 5.44, N 3.68; found: C 58.78, H 5.61, N 3.42.

Synthesis of Compound 9 *o*-DFB (15 mL) was added to a mixture of **4** (116 mg, 0.13 mmol) and $AgSbF_6$ (89.3 mg, 0.26 mmol) at −78 °C. The reaction mixture was slowly allowed to reach room temperature, then the reaction mixture was stirred for 30 minutes. The mixture was filtered, and the residue was extracted with *o*-DFB (3 × 20 mL). The combined *o*-DFB extracts were concentrated to 30 mL, followed by the addition of toluene (100 mL). The resulting solution was stirred for 3 hours, leading to the formation of compound **9** as a bright red solid (126 mg, 58%). An alternative method for the synthesis of **9** from **7** using 1.0 equivalent of $AgSbF_6$ following the procedure described above gave 69% yield. Single crystals suitable for X-ray diffraction were obtained by diffusion of hexane into a saturated *o*-DFB solution of **9** at −20 °C. M.p.: 226 °C (dec.). ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C) δ (ppm) = 8.49 (d, *J* = 6.9 Hz, 2H), 8.40 (d, *J* = 7.2 Hz, 2H), 8.22 (d, *J* = 2.2 Hz, 4H), 7.95 (t, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.8 Hz, 2H), 7.09 (dd, *J* = 13.4, 7.8 Hz, 4H), 2.96-2.86 (m, 4H, C*H*$(CH_3)_2$), 2.83 (s, 4H, $(CH_3)_2$CC*H*$_2$), 1.95 (d, *J* = 5.9 Hz, 12H, CH_2C(C*H*$_3)_2$), 1.69 (s, 12H, CH_2C(C*H*$_3)_2$), 1.35

(t, J = 6.4 Hz, 12H, CH(CH_3)$_2$), 0.22 (dd, J = 47.1, 6.4 Hz, 12H, CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2) δ (ppm) = 149.34, 145.80, 145.36, 142.90, 139.52, 136.76, 136.52, 132.21, 132.00, 131.32, 130.33, 130.32, 126.98, 126.94, 87.55 ((CH$_3$)$_2$*C*), 55.48 ((CH$_3$)$_2$*C*), 50.35 (C*C*H$_2$C), 31.54 (d, J = 30.0 Hz, C(*C*H$_3$)$_2$), 30.00 (d, J = 1.4 Hz), 29.95, 28.24 (d, J = 17.3 Hz, CH(*C*H$_3$)$_2$), 24.86 (d, J = 7.3 Hz, CH(*C*H$_3$)$_2$). Note that carbon atoms directly bonded to boron are not always observed in the ^{13}C{^{1}H} NMR spectra due to quadrupolar relaxation leading to signal broadening. ^{11}B NMR (128 MHz, CD_2Cl_2, 25 °C) δ (ppm) = 55.99. Elemental analysis (%) calcd for $C_{60}H_{72}B_2N_2Sb_2F_{12}$: C 54.83, H, 5.52, N, 2.13; found: C 54.48, H 5.76, N 2.38.

Synthesis of Compound 10 THF (10 mL) was added to a mixture of **3** (118 mg, 0.11 mmol) and potassium graphite (KC_8) (30.4 mg, 0.22 mmol) at −78 °C. The reaction mixture was slowly allowed to reach room temperature and stirred for another 6 hours. The resulting dark blue reaction mixture was filtered, and the residue was extracted with THF (2×10 mL). Then, [2.2.2]-cryptand (82.8 mg, 0.22 mmol) was added to the combined THF solution. The mixture was stirred for 30 minutes before concentrated to 10 mL, and then placed in the glovebox fridge at -20 °C to afford dark blue crystals of **10** after three days (113 mg, 66%). Single crystals suitable for X-ray diffraction were obtained by evaporation of a saturated THF solution of **10** at −20 °C. M.p.: >300 °C (dec.). ^{1}H NMR (600 MHz, CD_3CN, 25 °C) δ (ppm) = 7.78 (d, J = 7.1 Hz, 2H), 7.69 (d, J = 8.3 Hz, 2H), 7.38 (s, 2H), 7.21 (s, 2H), 7.04 - 6.99 (m, 4H), 6.95 (t, J = 7.6 Hz, 2H), 6.88 (br, 4H), 6.73 (d, J = 8.3 Hz, 2H), 3.54 (s, 24H, crypt OC*H*$_2$C*H*$_2$O), 3.50 (t, J = 4.6 Hz, 24H, crypt NCH$_2$C*H*$_2$O), 3.24 - 3.15 (m, 4H, C*H*(CH$_3$)$_2$), 2.51 (t, J = 4.7 Hz, 24H, crypt NC*H*$_2$CH$_2$O), 1.13 - 1.04 (br, 24H). ^{13}C{^{1}H} NMR (151 MHz, CD_3CN, 25 °C) δ (ppm) = 147.40, 138.44, 138.26, 137.75, 134.17, 130.79, 130.76, 128.62, 128.37, 127.84, 125.11, 124.68, 123.88, 122.43, 118.81, 115.95, 115.39, 71.18 (crypt O*C*H$_2$CH$_2$O), 68.39 (crypt NCH$_2$*C*H$_2$O), 54.65 (crypt N*C*H$_2$CH$_2$O), 29.00 (d, J = 4.5 Hz, *C*H(CH$_3$)$_2$), 26.94 (*C*H$_3$), 24.41 (*C*H$_3$), 24.32 (*C*H$_3$).^{11}B NMR (128 MHz, CD_3CN, 25 °C) δ (ppm) = 28.06. Elemental analysis (%) calcd for $C_{86}H_{120}B_2N_8O_{12}K_2$: C 66.31, H 7.76, N 7.19; found: C 66.57, H 7.62 N 7.49.

Synthesis of Compound 11 THF (15 mL) was added to a mixture of **4** (118 mg, 0.14 mmol) and potassium graphite (KC_8) (37.9 mg, 0.28 mmol) at -78 ℃. The reaction mixture was slowly allowed to reach room temperature and stirred for another 6 hours. The resulting dark red reaction mixture was filtered, and the residue was extracted with THF (10 mL). [2.2.2]-cryptand (105.4 mg, 0.28 mmol) was added to the combined THF solution. The mixture was stirred for 30 minutes before concentrated to 5 mL, and then hexane (10 mL) was added before placed in the glovebox fridge at -20 ℃ to afford pale yellow crystals of **11** after one day (84.3 mg, 36%). Single crystals suitable for X-ray diffraction were obtained by diffusion of hexane into a saturated THF solution of **11** at -20 ℃. M.p.: 265 ℃ (dec.). ^{1}H NMR (400 MHz, CD_3CN, 25 ℃) δ (ppm) = 7.54 (d, *J* = 7.7 Hz, 1H), 7.33 (d, *J* = 6.6 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 6.8 Hz, 1H), 6.92 (t, *J* = 7.2 Hz, 1H), 6.67 (dd, *J* = 14.7, 7.4 Hz, 2H), 6.46 (t, *J* = 7.5 Hz, 1H), 3.75 - 3.67 (m, 2H, C*H*$(CH_3)_2$), 3.56 (s, 12H, crypt OC*H*$_2$C*H*$_2$O), 3.52 (t, *J* = 4.6 Hz, 12H, crypt NCH$_2$C*H*$_2$O), 2.53 (t, *J* = 4.7 Hz, 12H, crypt NC*H*$_2$CH$_2$O), 1.55 (q, *J* = 12.5 Hz, 2H), 1.30 (d, *J* = 3.8 Hz, 6H, C(C*H*$_3$)$_2$), 1.09 (d, *J* = 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), 1.02 (d, *J* = 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), 0.84 (d, *J* = 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), 0.62 (d, *J* = 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), -0.02 (d, *J* = 36.5 Hz, 6H, C(C*H*$_3$)$_2$).^{13}C{^{1}H} NMR (151 MHz, CD_3CN, 25 ℃) δ (ppm) = 151.91, 138.54, 136.67, 136.03, 135.75, 135.15, 132.21, 130.55, 122.79, 122.26, 121.93, 121.79, 119.87, 71.19 (crypt OC*H*$_2$C*H*$_2$O), 68.40 (crypt NCH$_2$C*H*$_2$O), 58.34 (C*C*H$_2$C), 54.65 (crypt NC*H*$_2$CH$_2$O), 49.30 (*C*$(CH_3)_2$), 33.87 (C(*C*H$_3$)$_2$), 32.80 (C(*C*H$_3$)$_2$), 30.42 (C(*C*H$_3$)$_2$), 30.05 (C(*C*H$_3$)$_2$), 28.53 (*C*H$(CH_3)_2$), 28.23 (*C*H$(CH_3)_2$), 23.11 (CH(*C*H$_3$)$_2$), 22.91 (CH(*C*H$_3$)$_2$). ^{11}B NMR (128 MHz, CD_3CN, 25 ℃) δ (ppm) = -8.03. Elemental analysis (%) calcd for $C_{96}H_{144}B_2N_6O_{12}K_2$: C 68.88, H 8.67, N 5.02; found: C 68.51, H 8.46, N 5.18.

NMR Spectra:

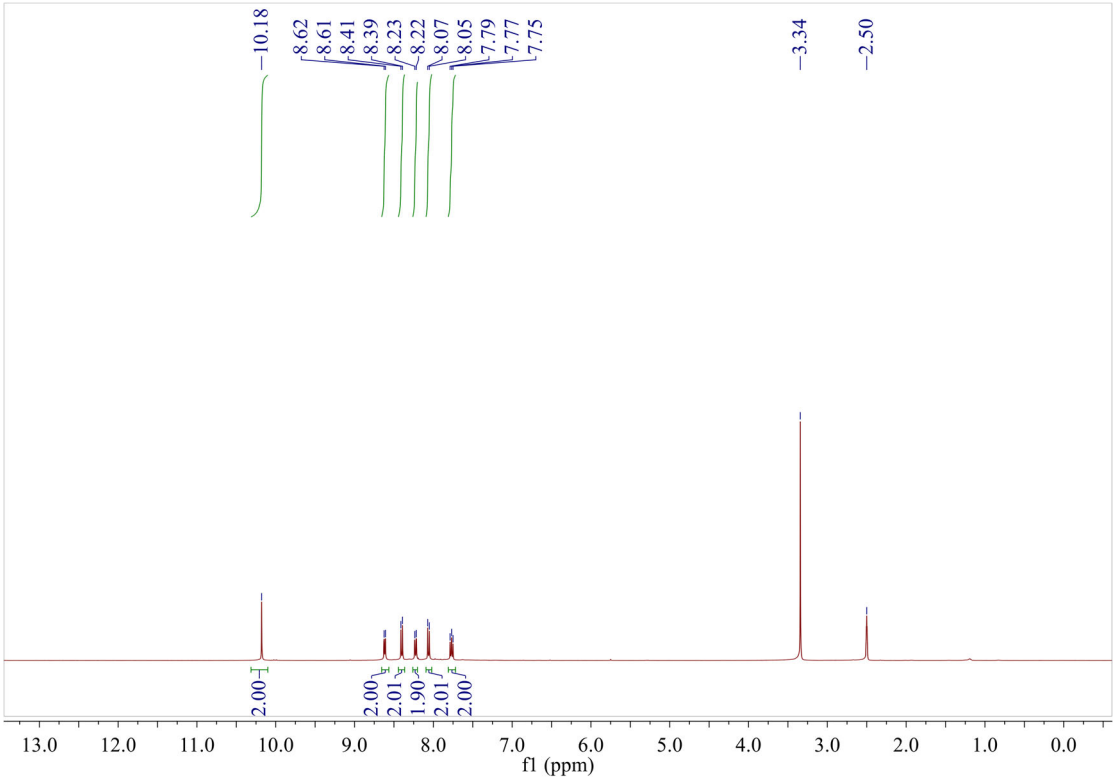


Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6, 25 ℃) spectrum of **1**.

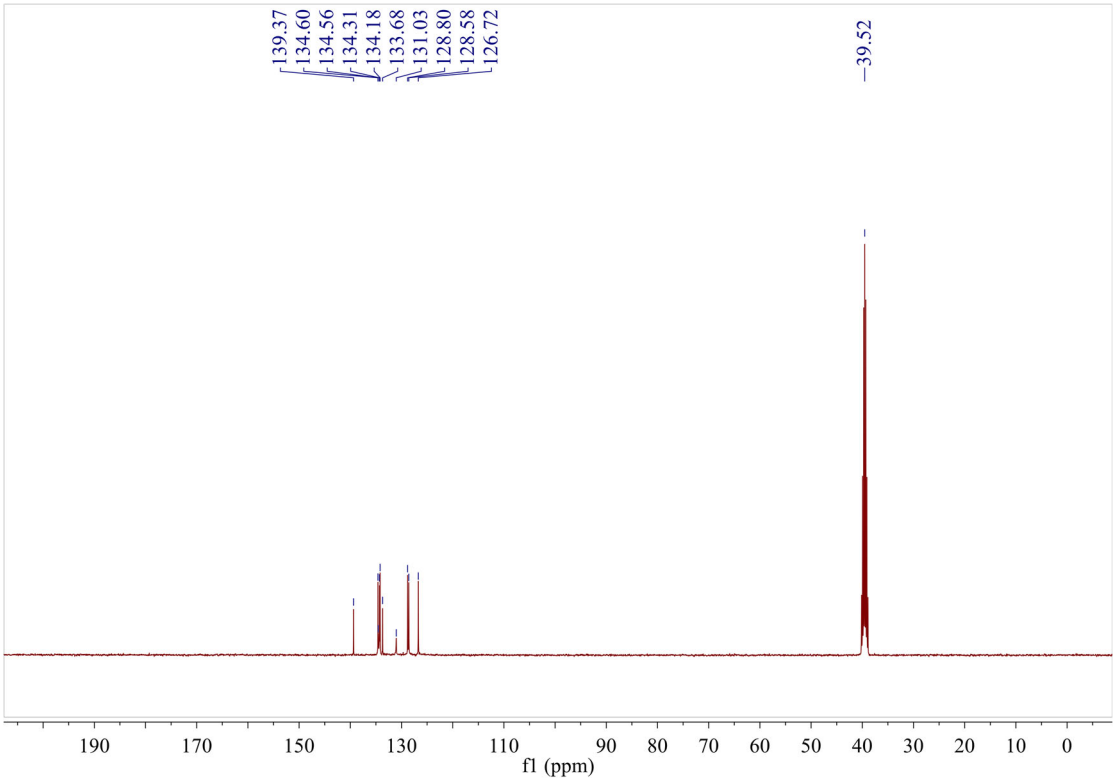


Figure S2. ^{13}C NMR (101 MHz, DMSO-d_6, 25 ℃) spectrum of **1**.

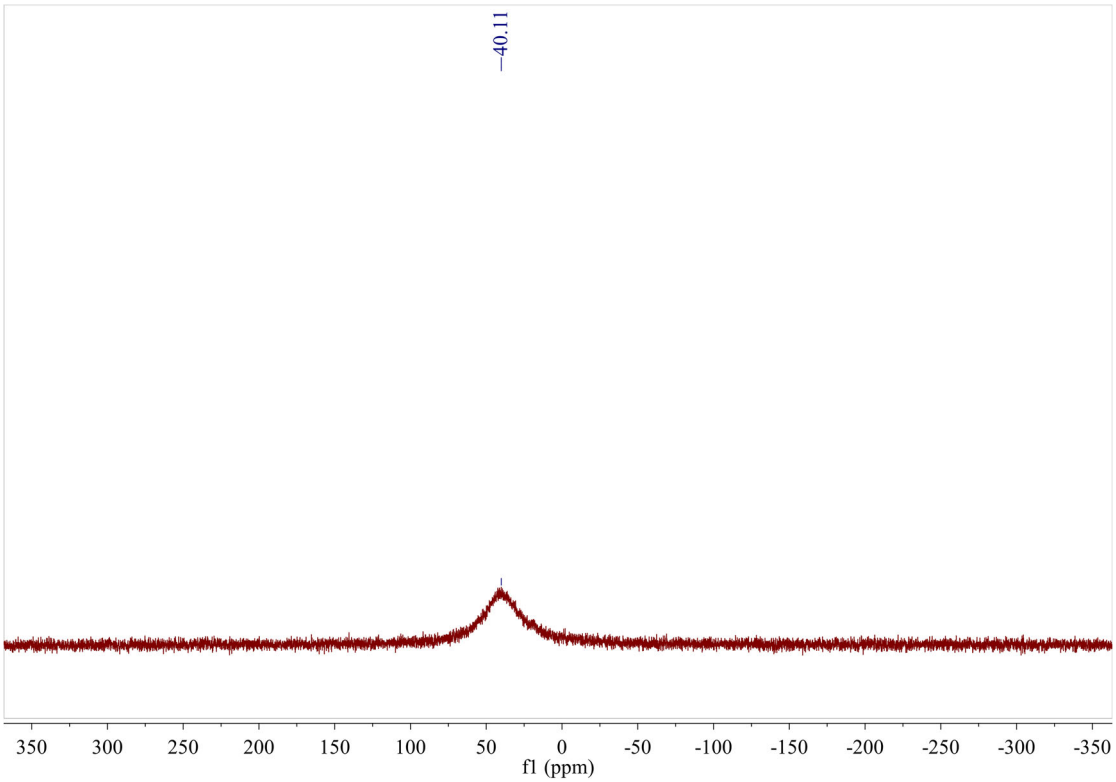


Figure S3. ^{11}B NMR (128 MHz, DMSO-d_6, 25 ℃) spectrum of **1**.

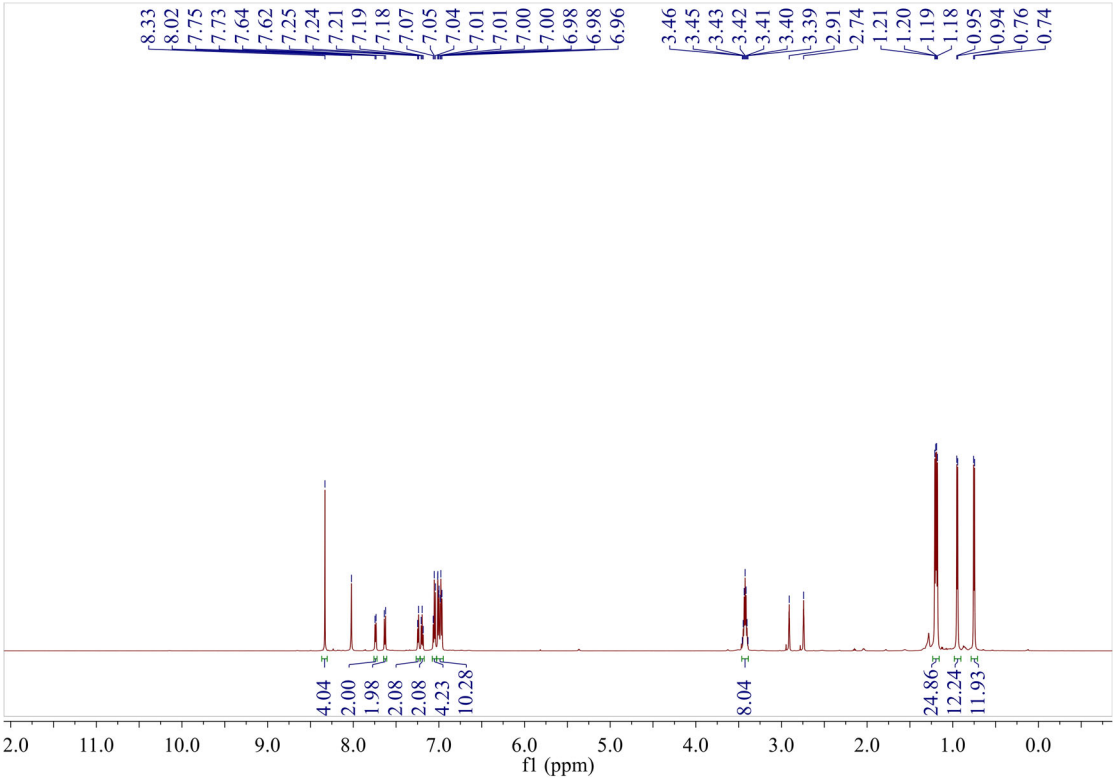


Figure S4. ^{1}H NMR (600 MHz, DMF-d_7, 25 ℃) spectrum of **3**.

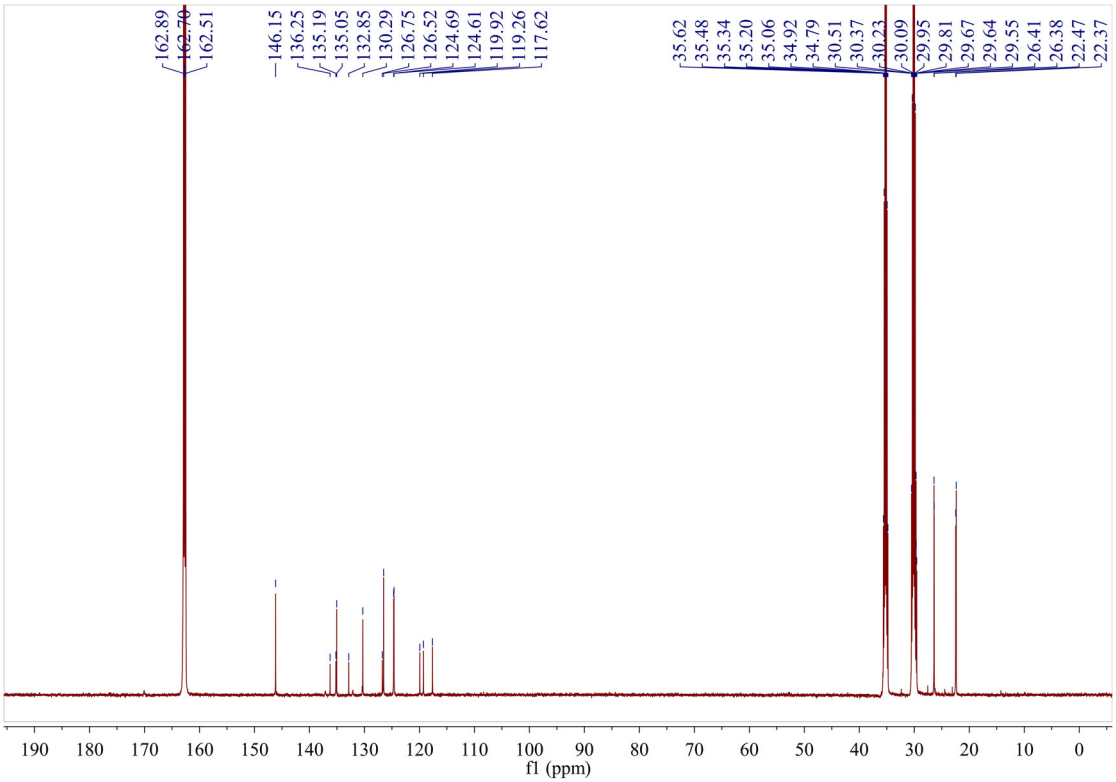


Figure S5. ^{13}C NMR (151 MHz, DMF-d_7, 25 °C) spectrum of **3**.

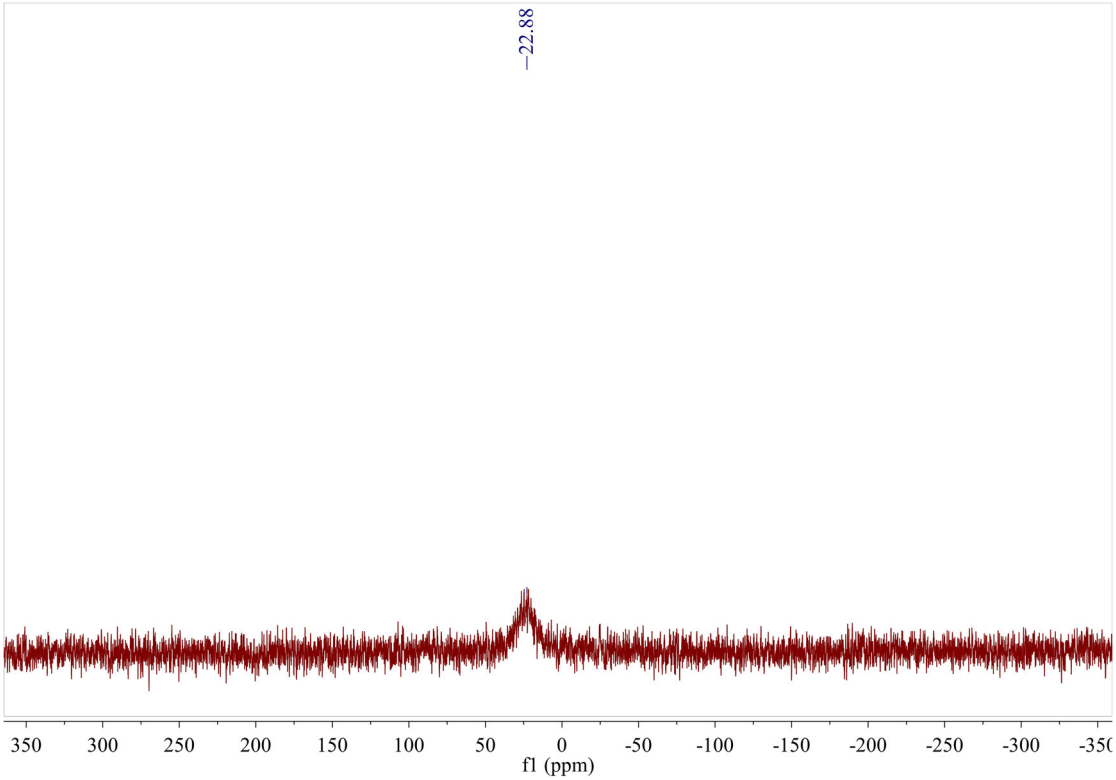


Figure S6. ^{11}B NMR (128 MHz, DMF-d_7, 25 °C) spectrum of **3**.

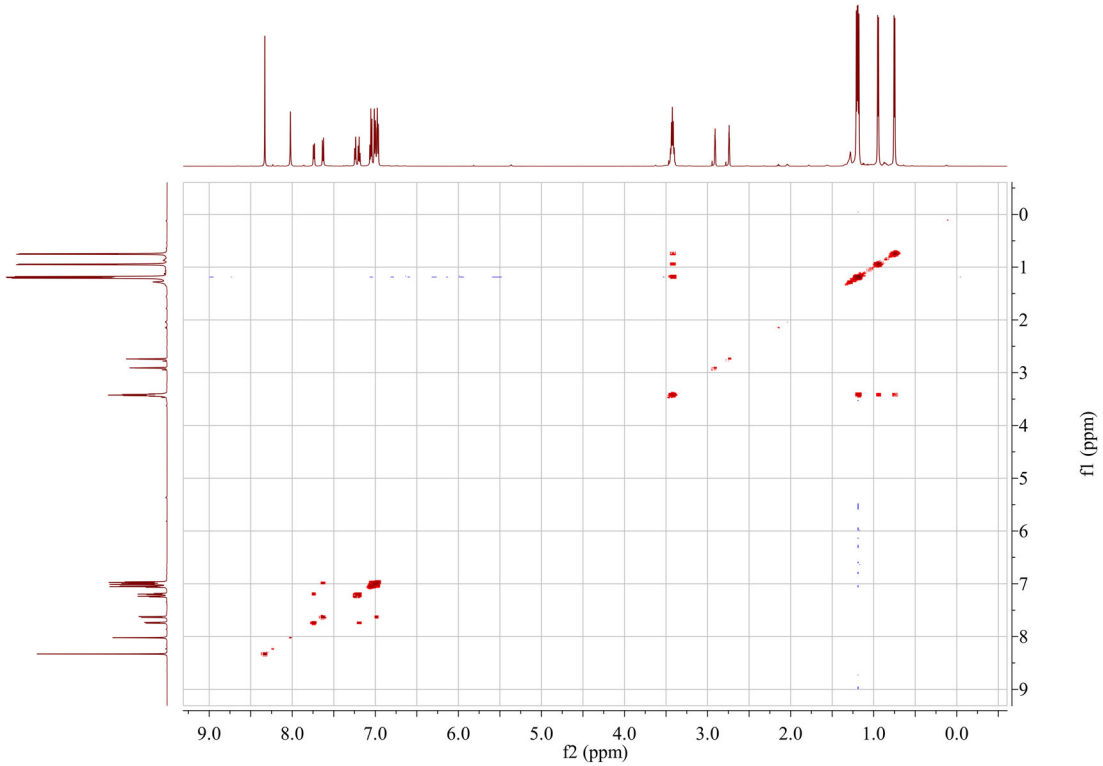


Figure S7. ^{1}H-^{1}H Correlated Spectroscopy [COSY] (DMF-d_7, 25 °C) spectrum of **3**.

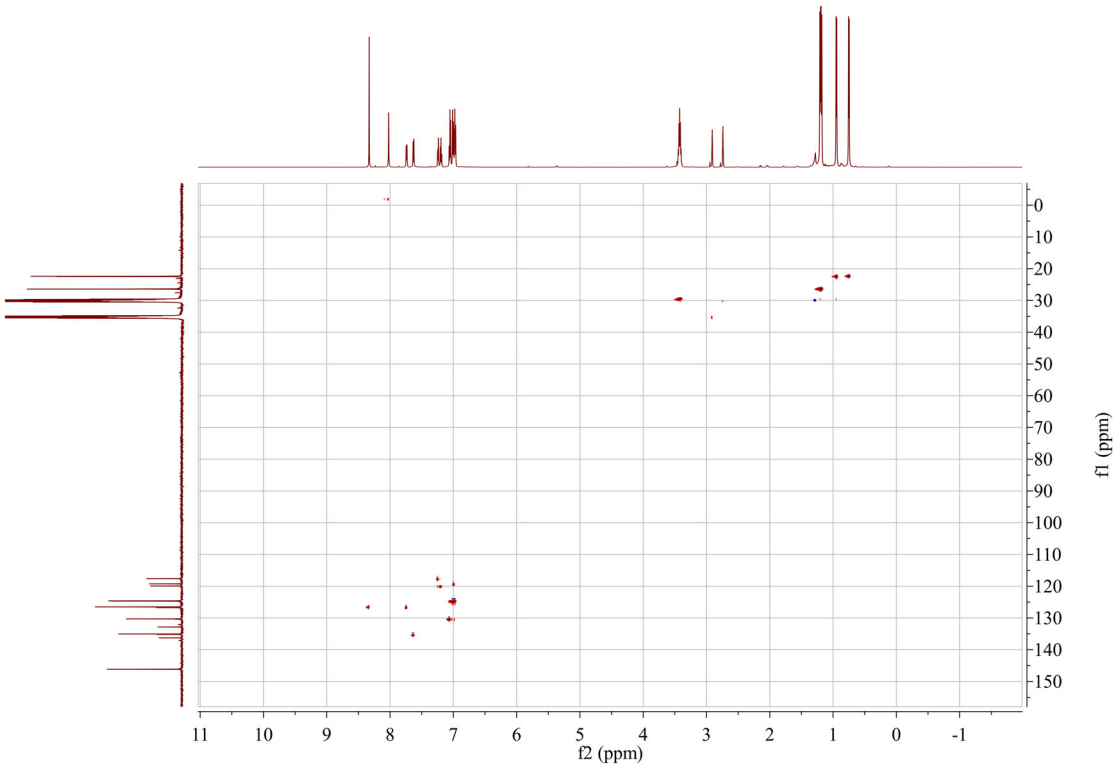


Figure S8. Heteronuclear Single Quantum Coherence Spectroscopy [HSQC] (DMF-d_7, 25 °C) spectrum of **3**.

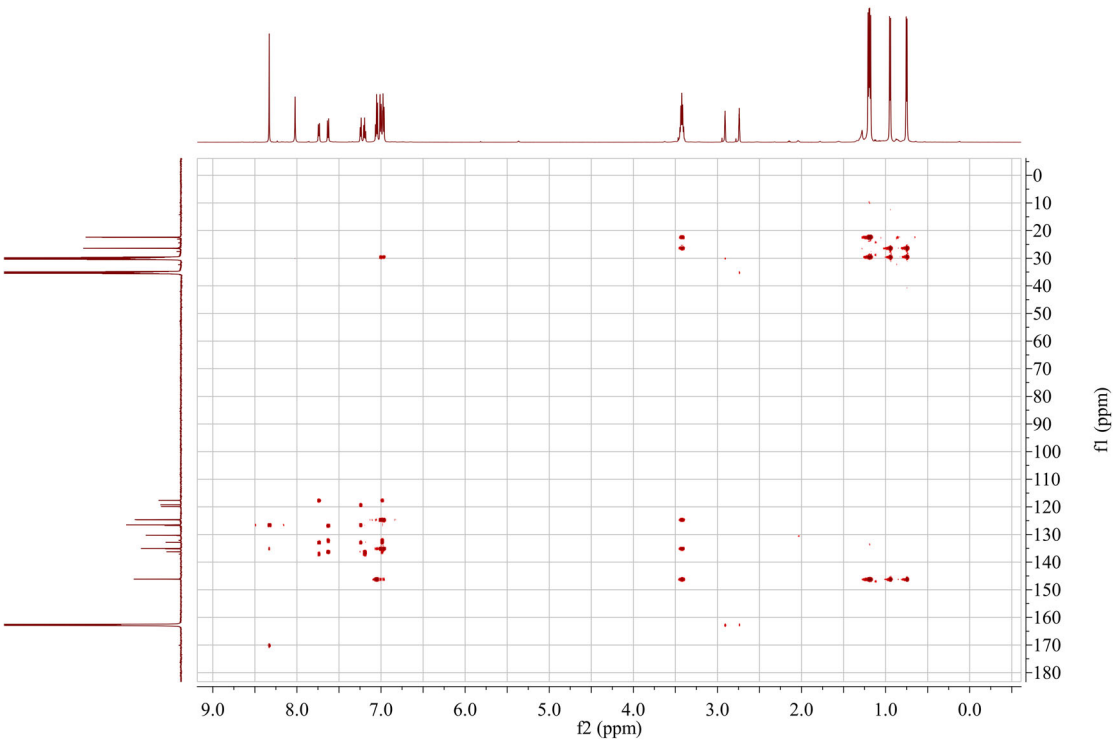


Figure S9. Heteronuclear Multiple Bond Correlation Spectroscopy [HMBC] (DMF-d_7, 25 °C) spectrum of **3**.

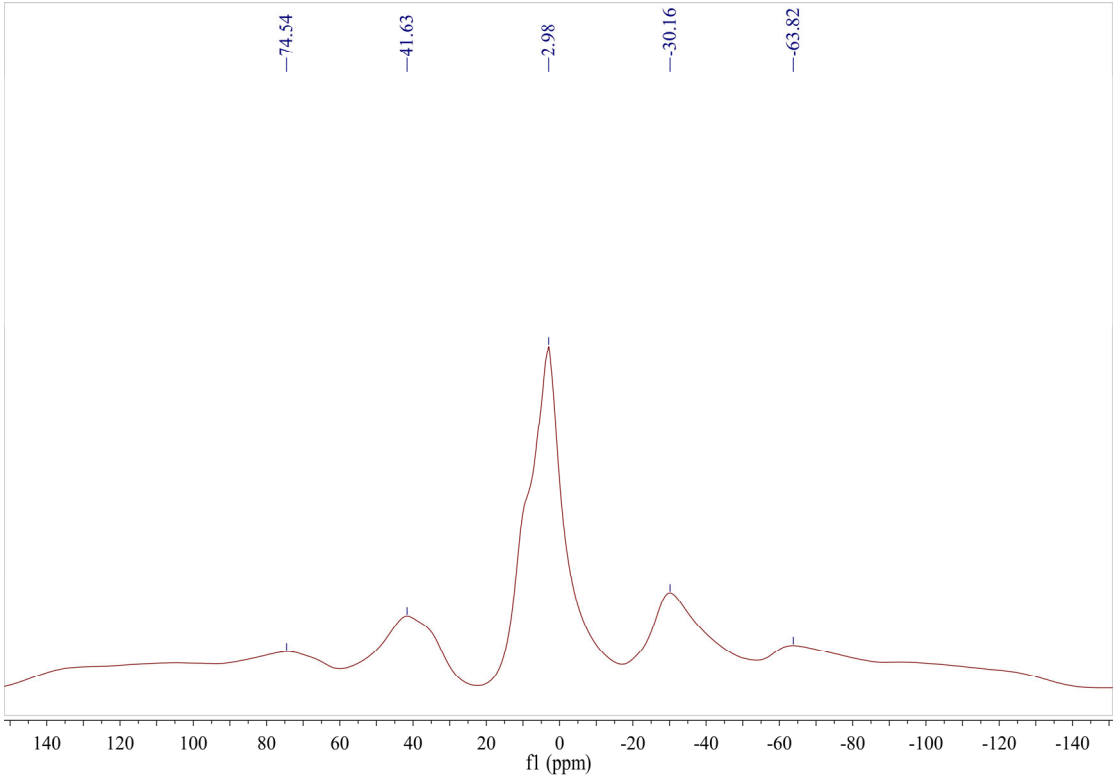


Figure S10. Solid-state ^{1}H NMR (MAS, 12 kHz) spectrum of **3**.

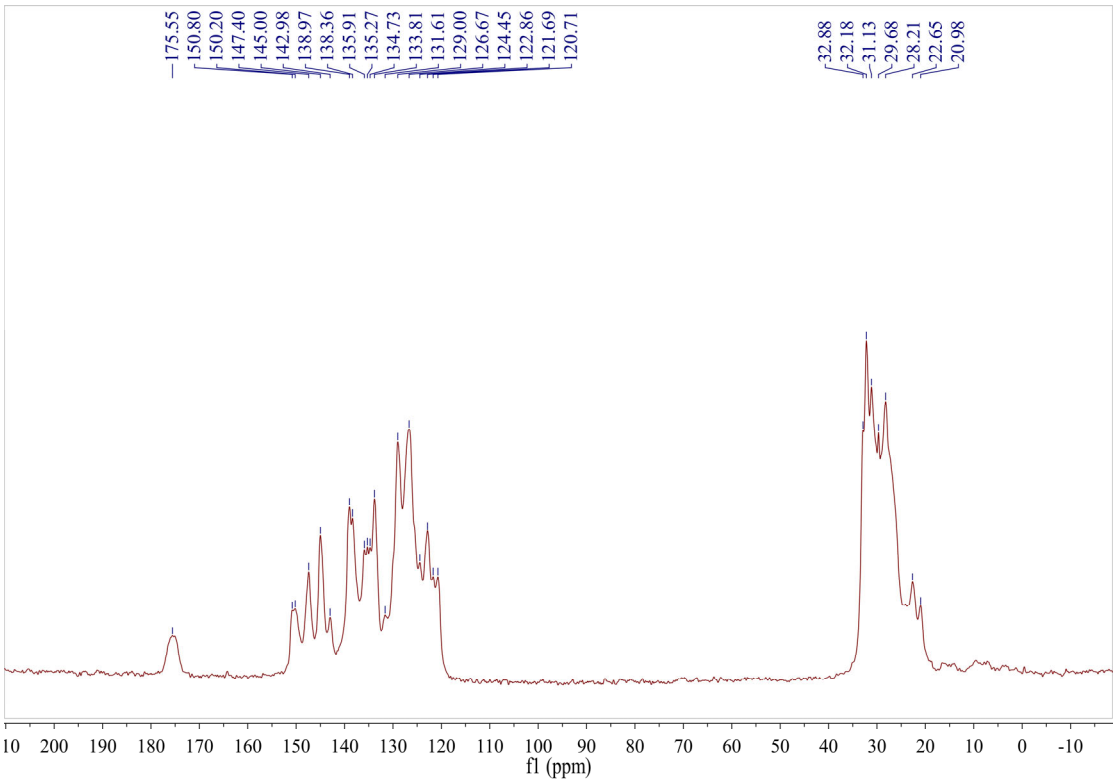


Figure S11. Solid-state ^{13}C NMR (CP/MAS, 12 kHz) spectrum of **3**.

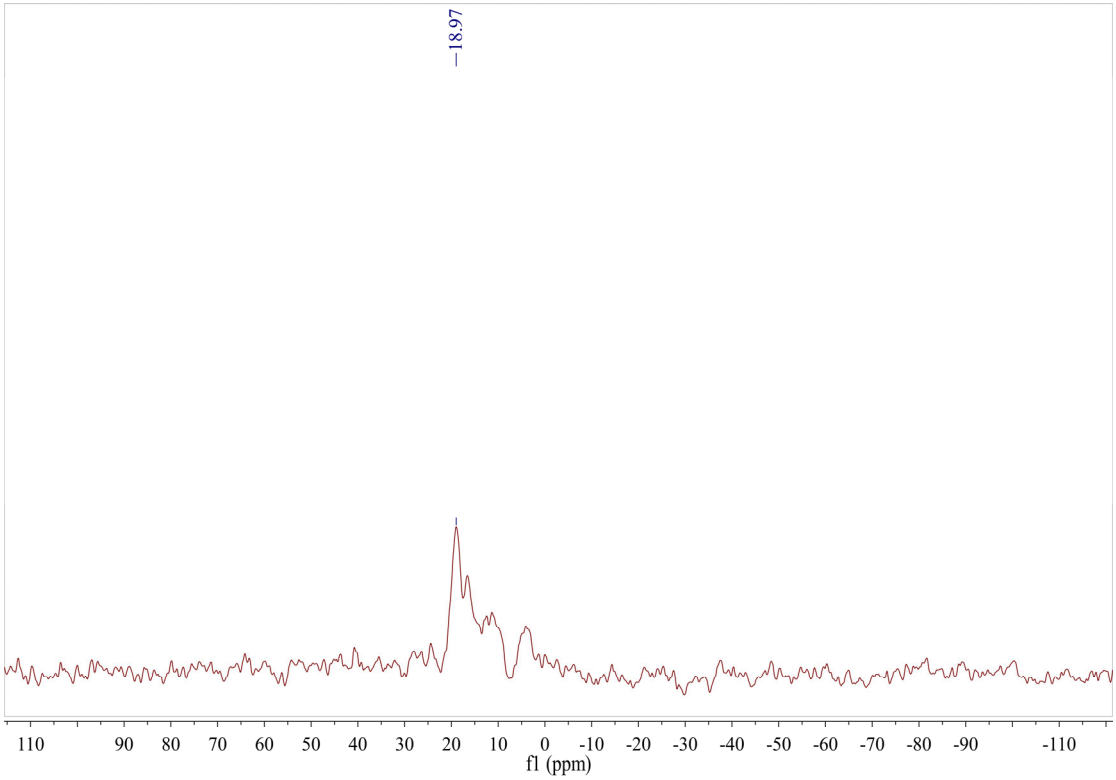


Figure S12. Solid-state ^{11}B NMR (MAS, 12 kHz) spectrum of **3**.

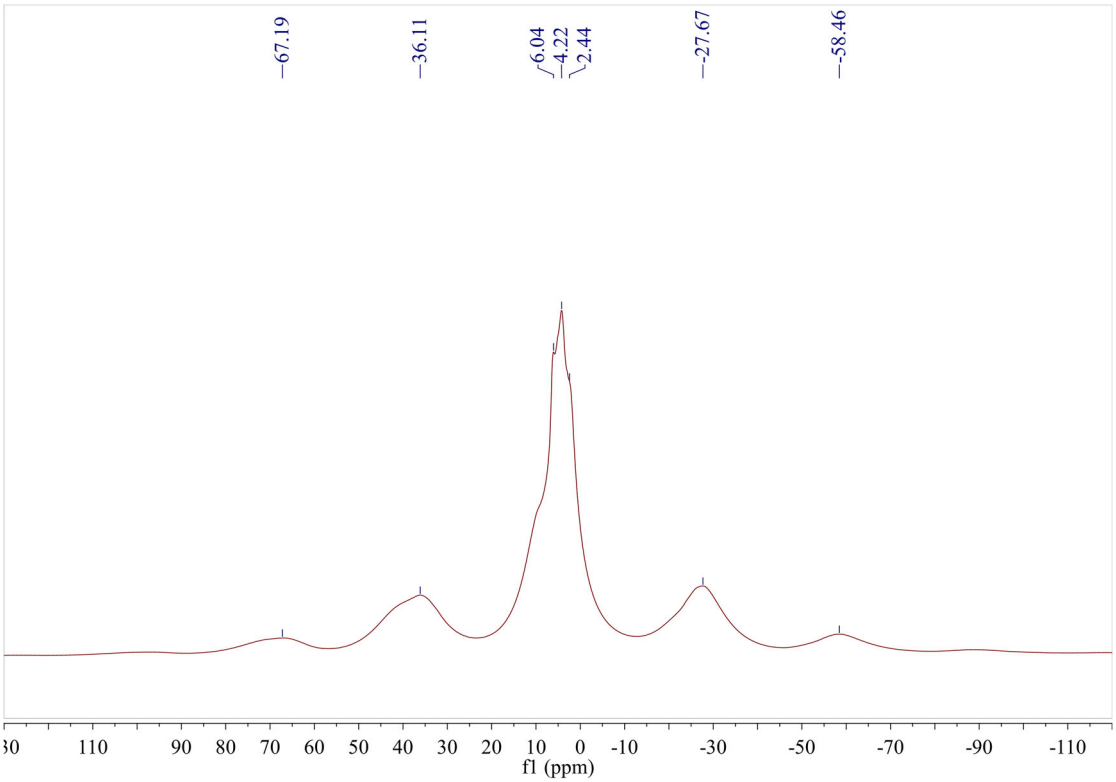


Figure S13. Solid-state ^{1}H NMR (MAS, 12 kHz) spectrum of **4**.

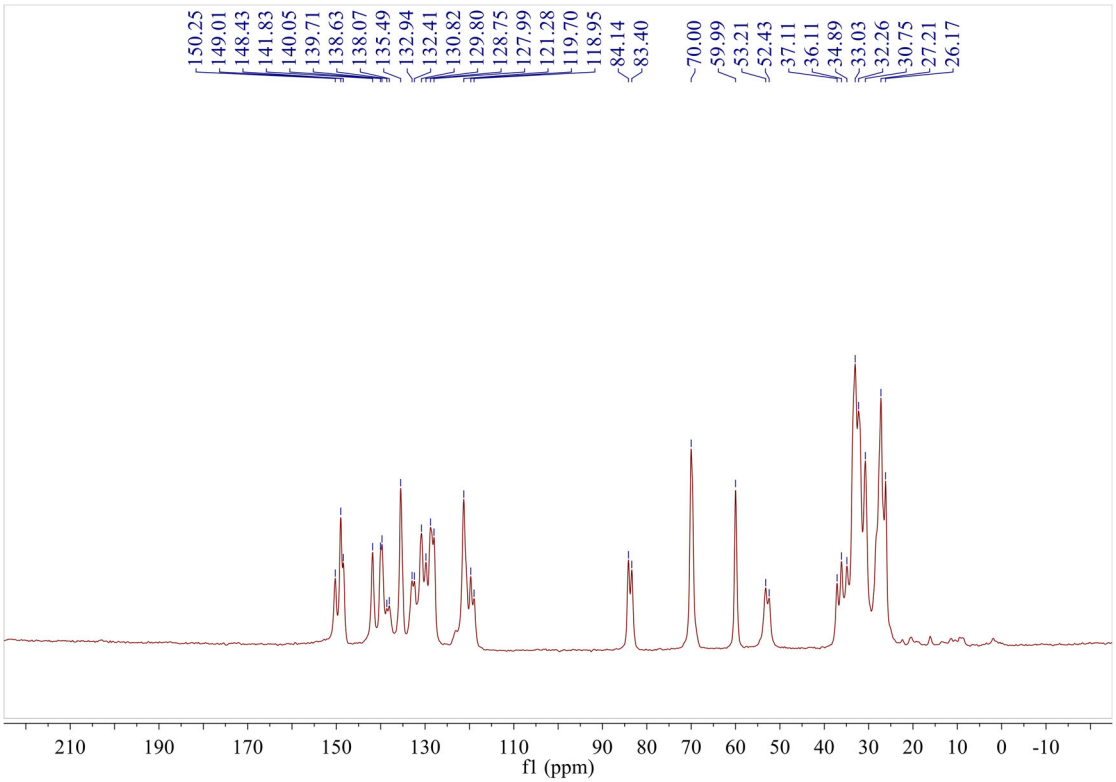


Figure S14. Solid-state ^{13}C NMR (CP/MAS, 12 kHz) spectrum of **4**.

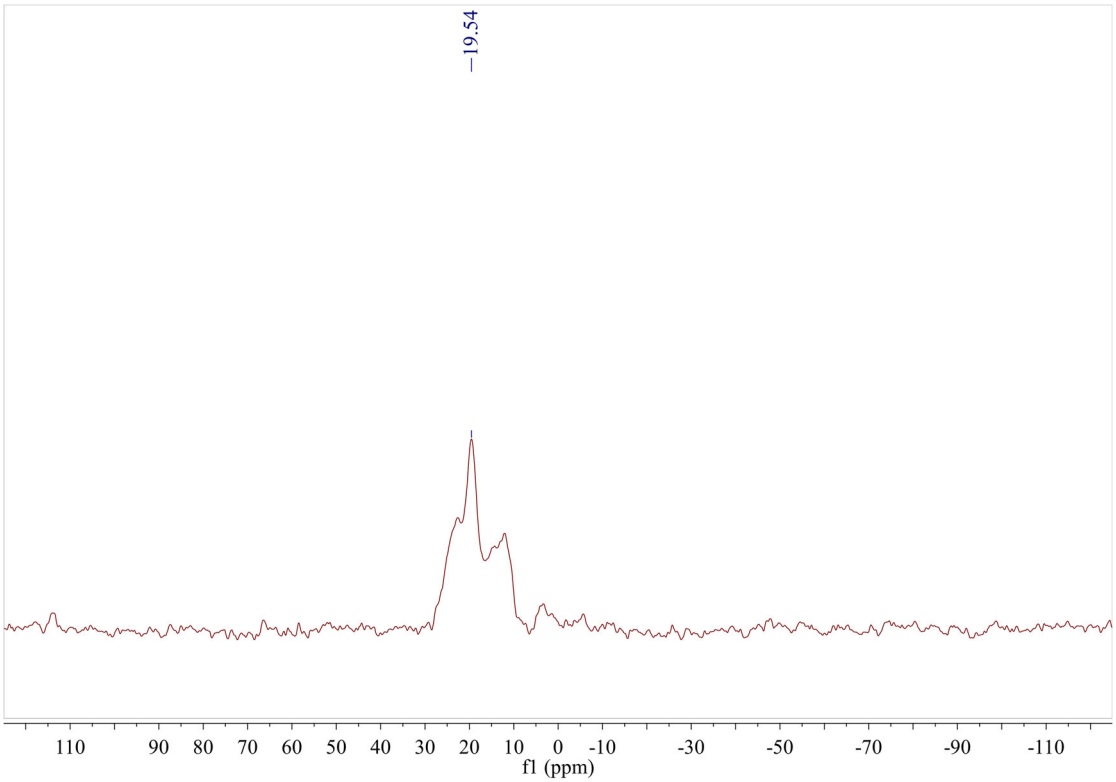


Figure S15. Solid-state ^{11}B NMR (MAS, 12 kHz) spectrum of **4**.

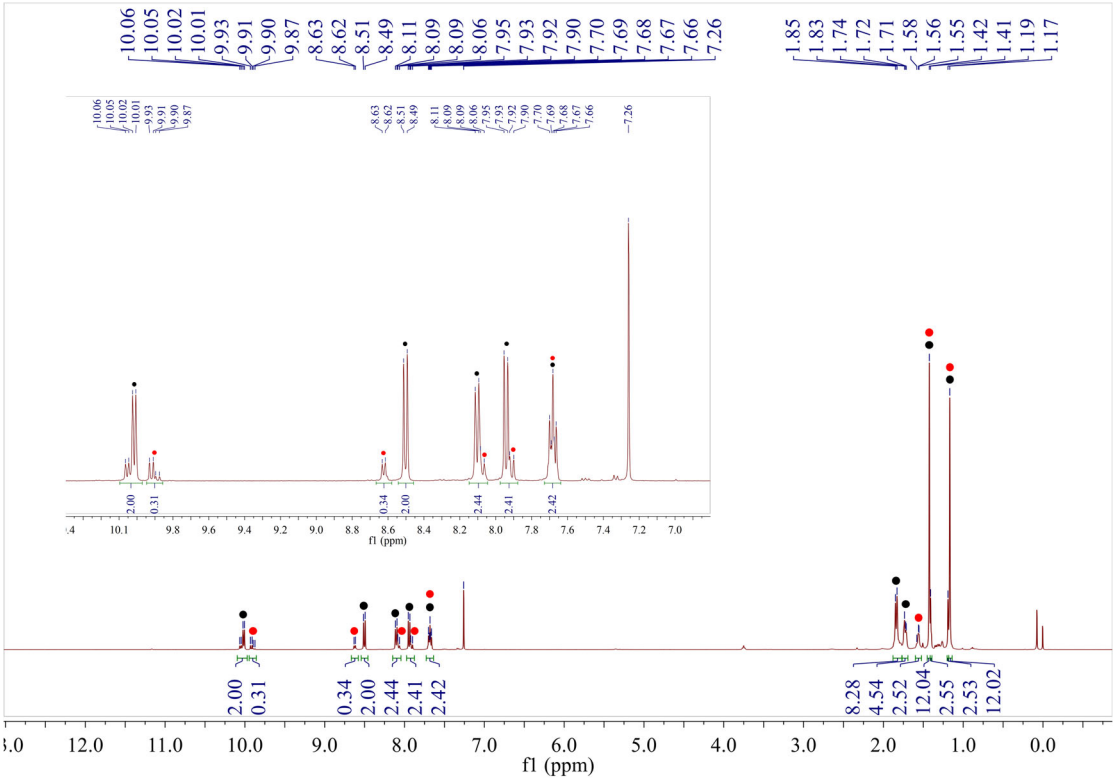


Figure S16. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectrum of **5** (●*anti*-**5**, ●*syn*-**5**).

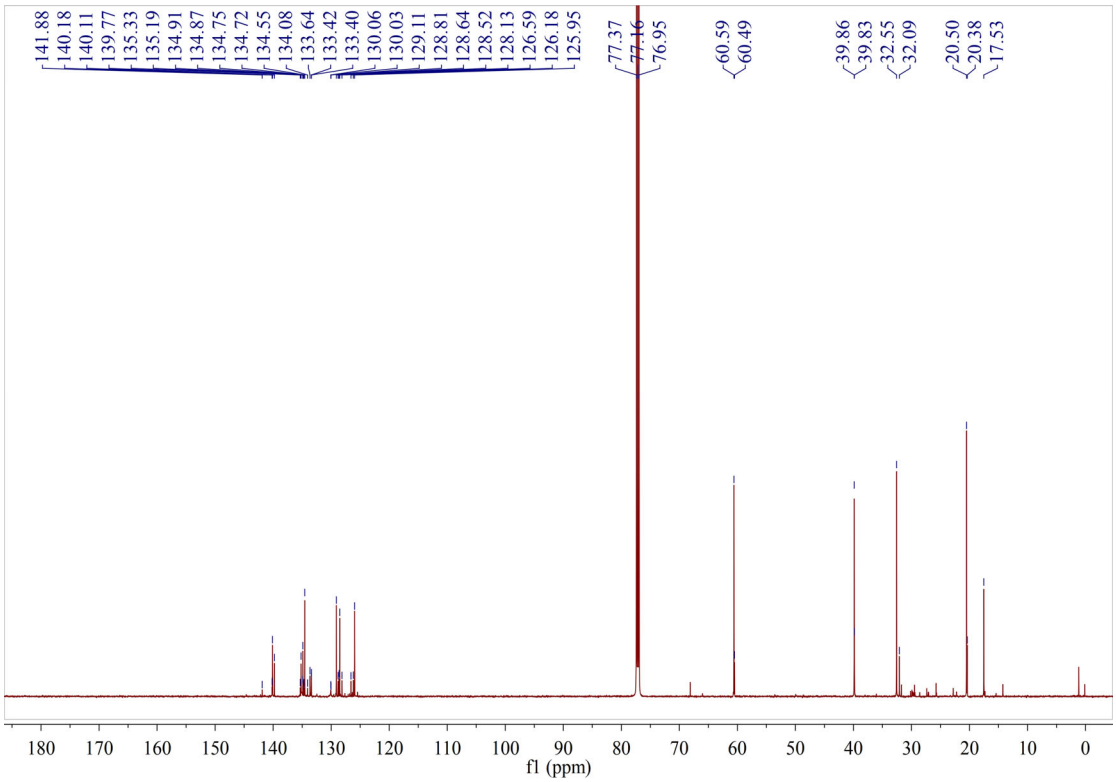


Figure S17. ^{13}C NMR (151 MHz, $CDCl_3$, 25 °C) spectrum of **5**.

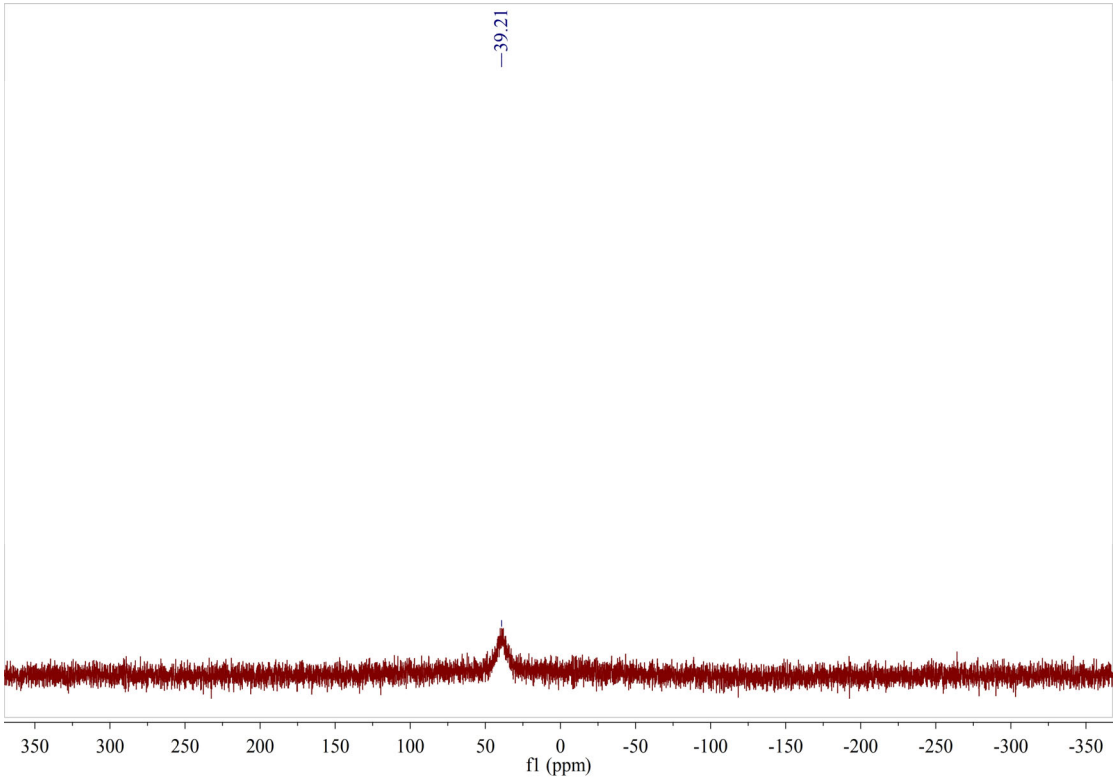


Figure S18. ^{11}B NMR (128 MHz, $CDCl_3$, 25 °C) spectrum of **5**.

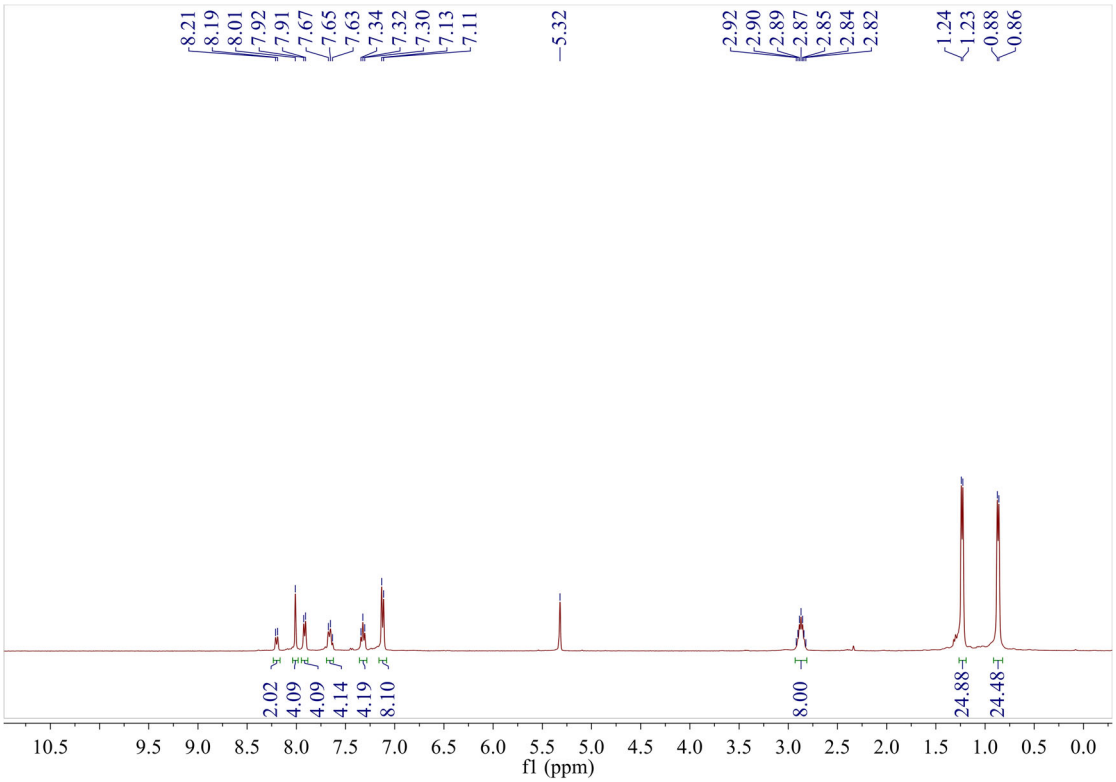


Figure S19. ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C) spectrum of **8**.

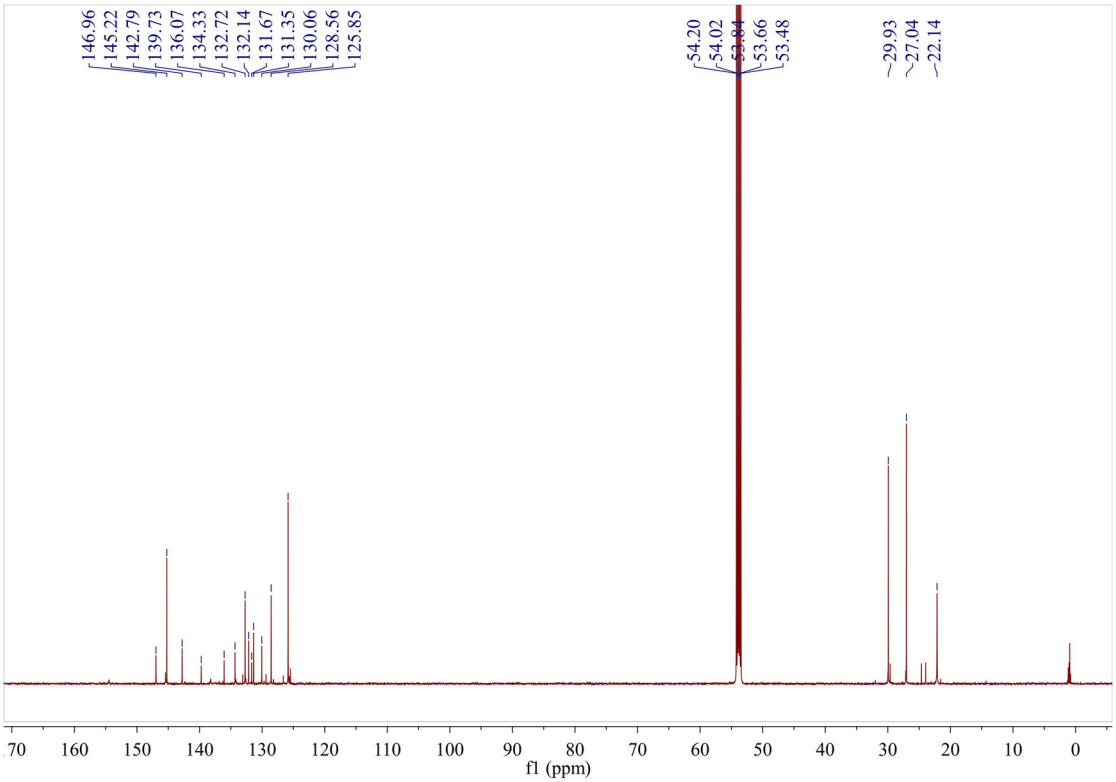


Figure S20. ^{13}C NMR (151 MHz, CD_2Cl_2, 25 °C) spectrum of **8**.

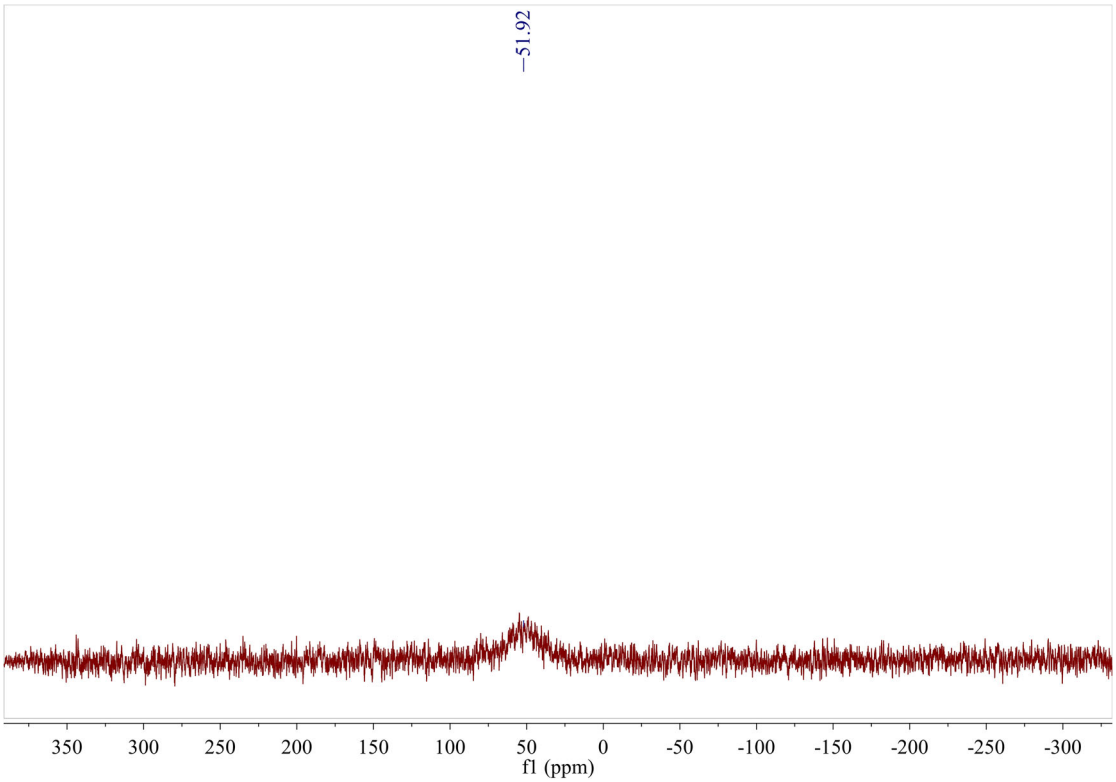


Figure S21. ^{11}B NMR (128 MHz, CD_2Cl_2, 25 °C) spectrum of **8**.

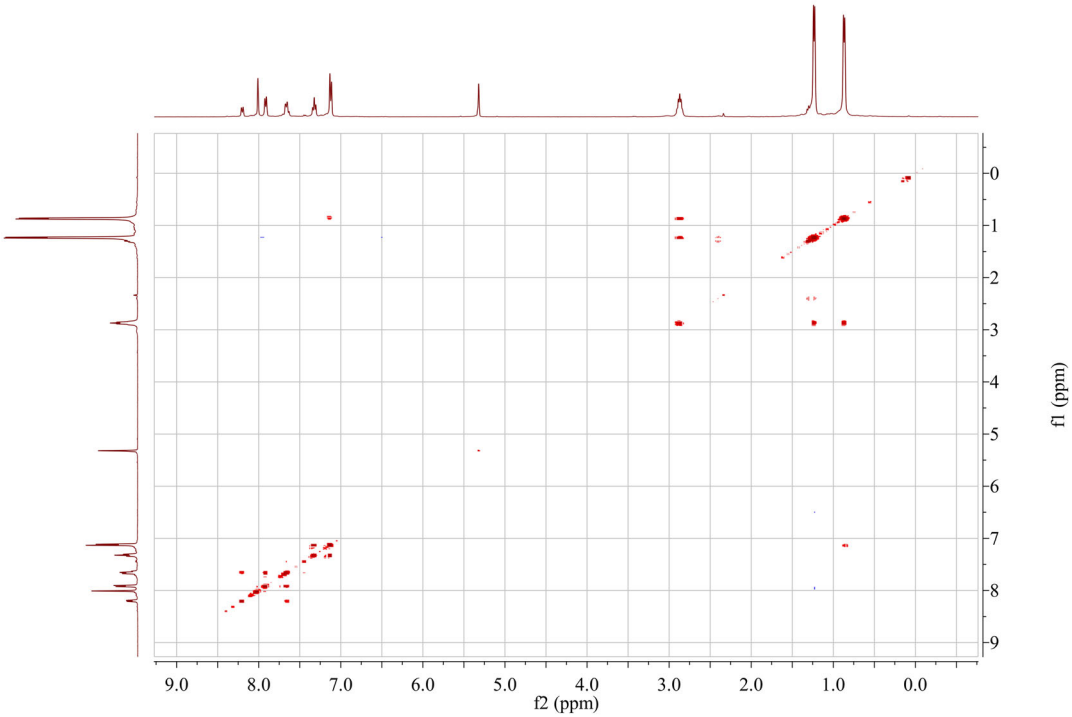


Figure S22. ^{1}H-^{1}H Correlated Spectroscopy [COSY] (CD_2Cl_2, 25 °C) spectrum of **8**.

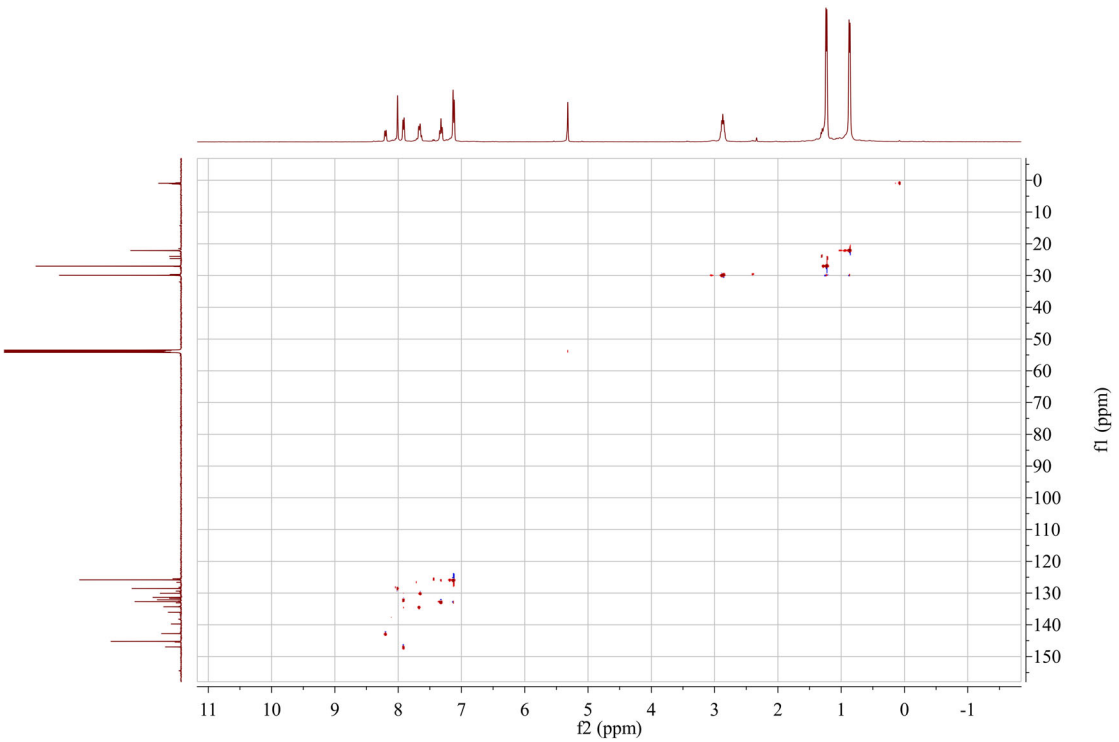


Figure S23. Heteronuclear Single Quantum Coherence Spectroscopy [HSQC] (CD_2Cl_2, 25 °C) spectrum of **8**.

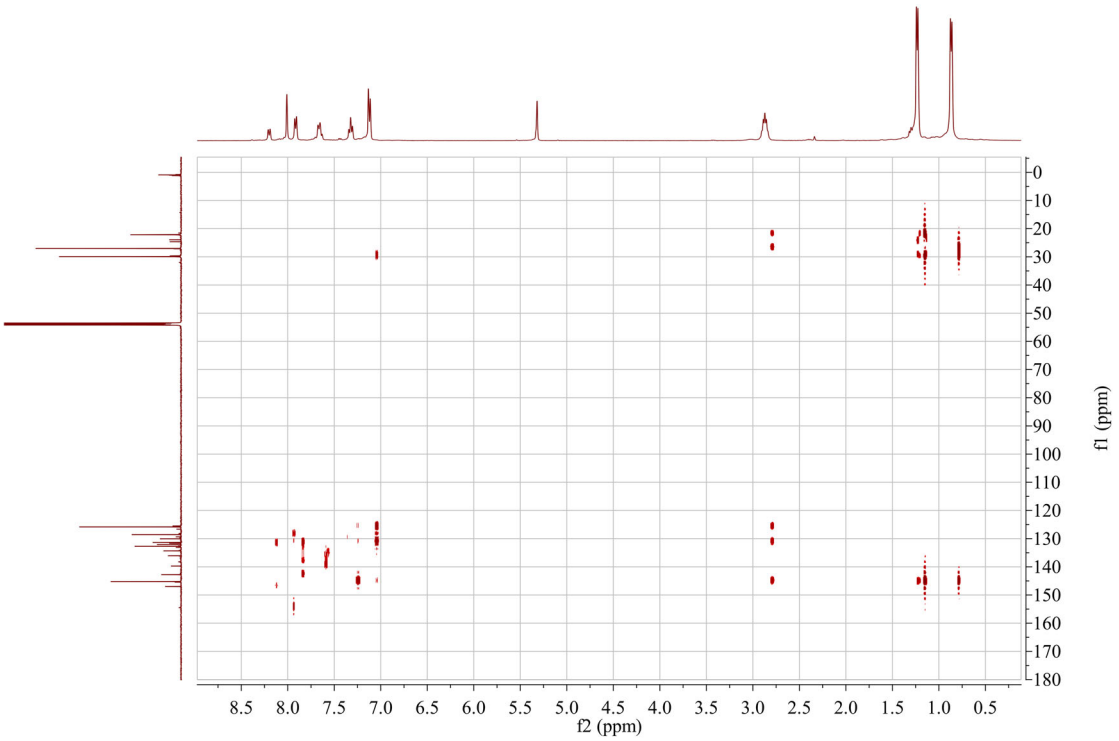


Figure S24. Heteronuclear Multiple Bond Correlation Spectroscopy [HMBC] (CD_2Cl_2, 25 °C) spectrum of **8**.

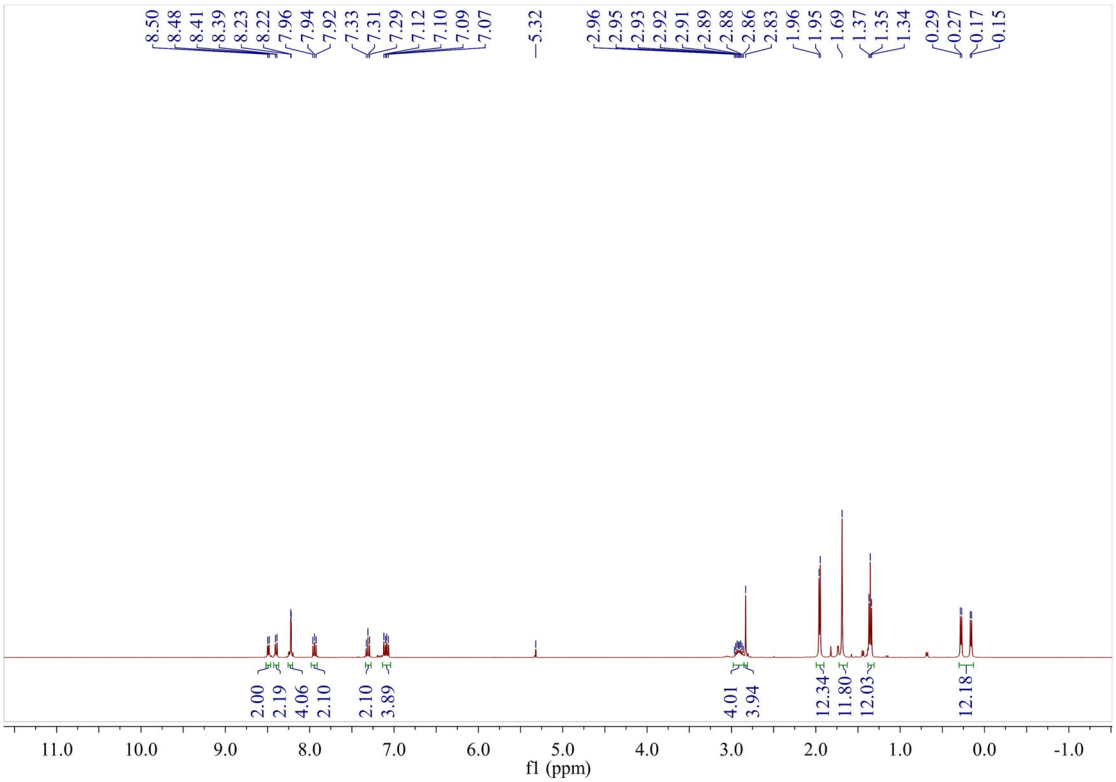


Figure S25. ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C) spectrum of **9**.

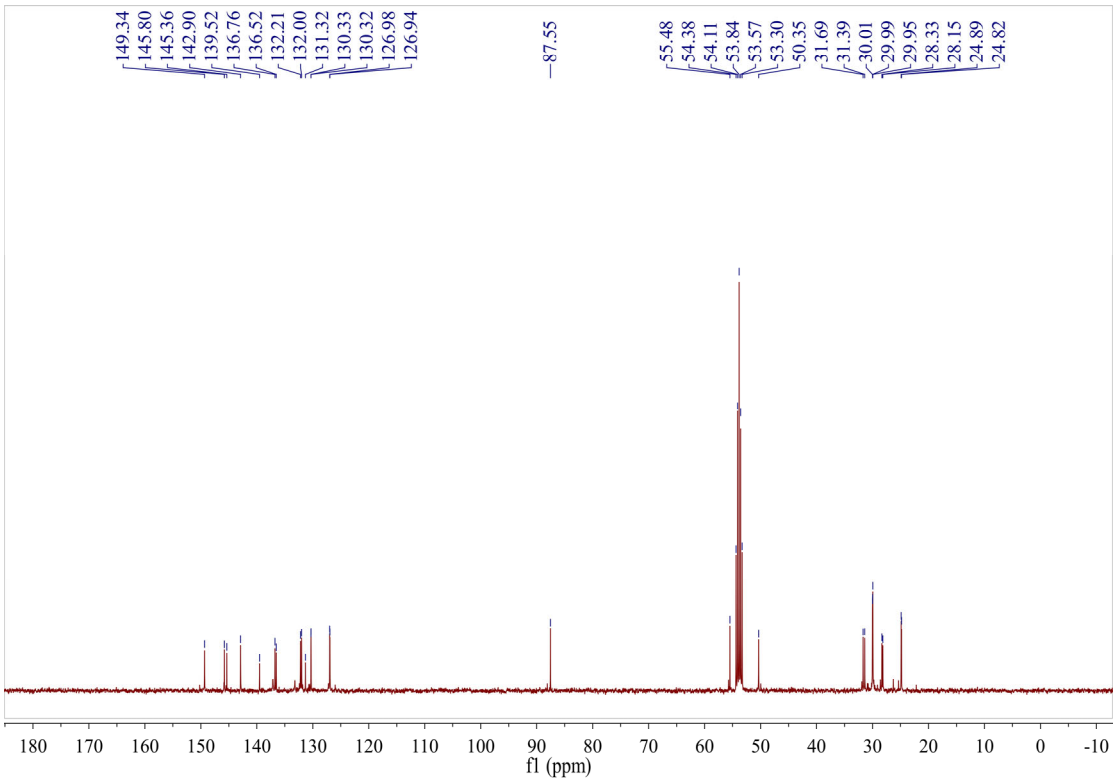


Figure S26. ^{13}C NMR (151 MHz, CD_2Cl_2, 25 °C) spectrum of **9**.

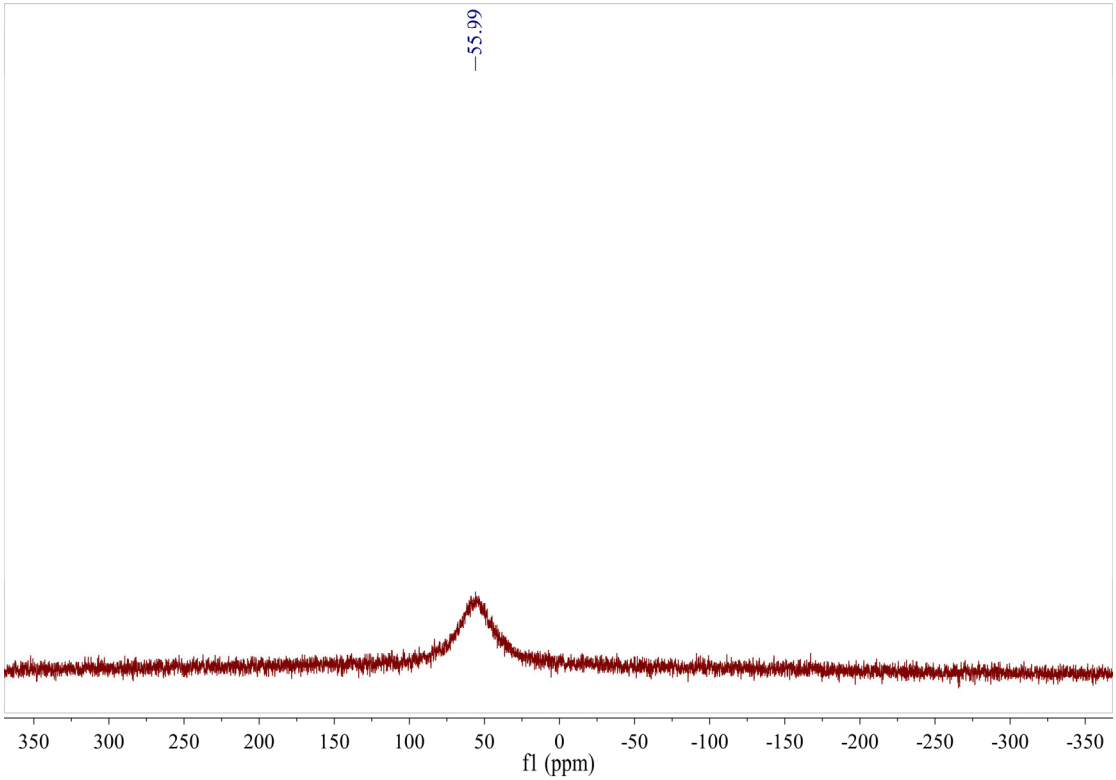


Figure S27. ^{11}B NMR (128 MHz, CD_2Cl_2, 25 °C) spectrum of **9**.

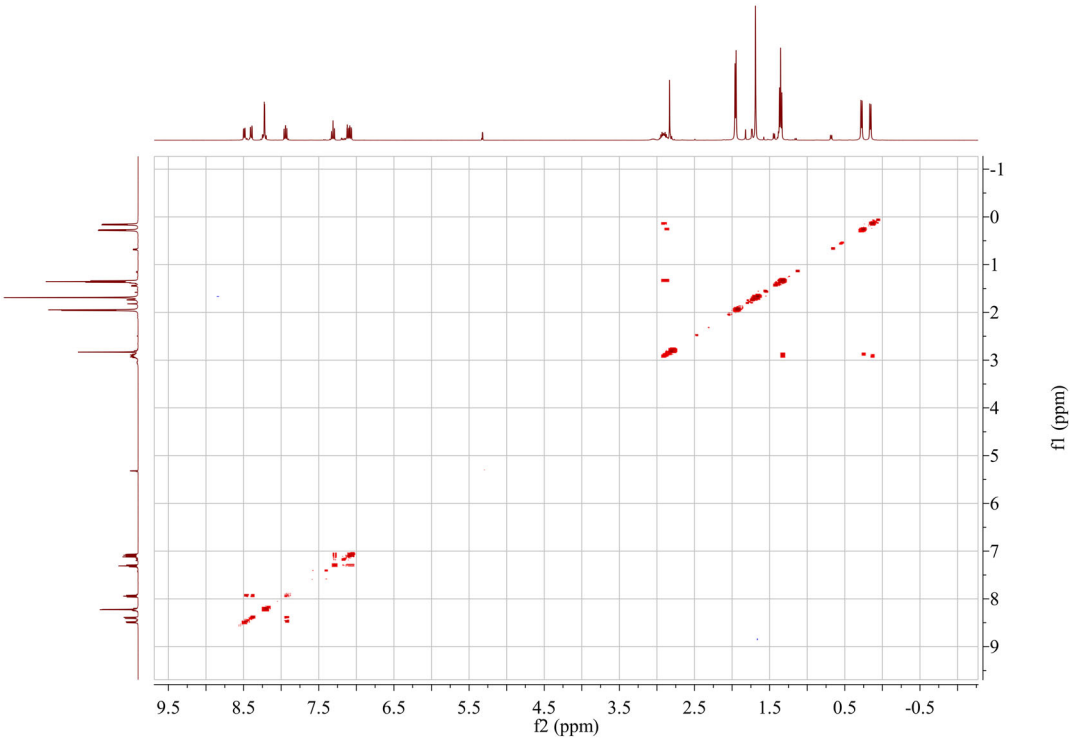


Figure S28. ^{1}H-^{1}H Correlated Spectroscopy [COSY] (CD_2Cl_2, 25 °C) spectrum of **9**.

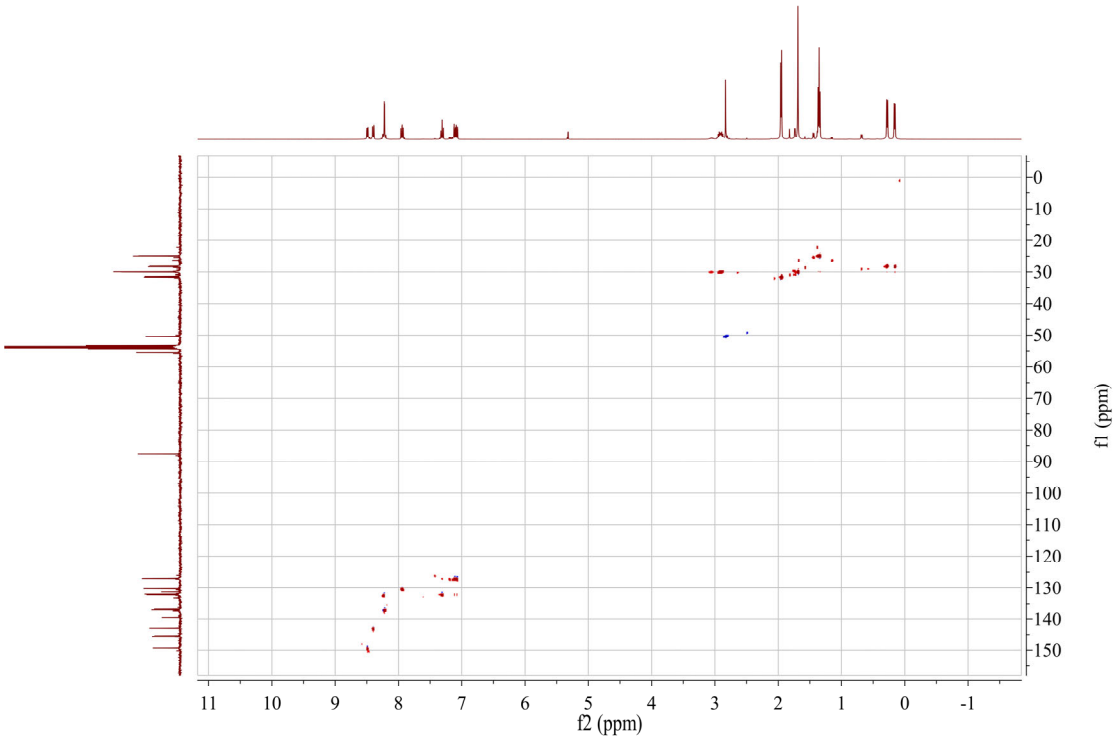


Figure S29. Heteronuclear Single Quantum Coherence Spectroscopy [HSQC] (CD_2Cl_2, 25 °C) spectrum of **9**.

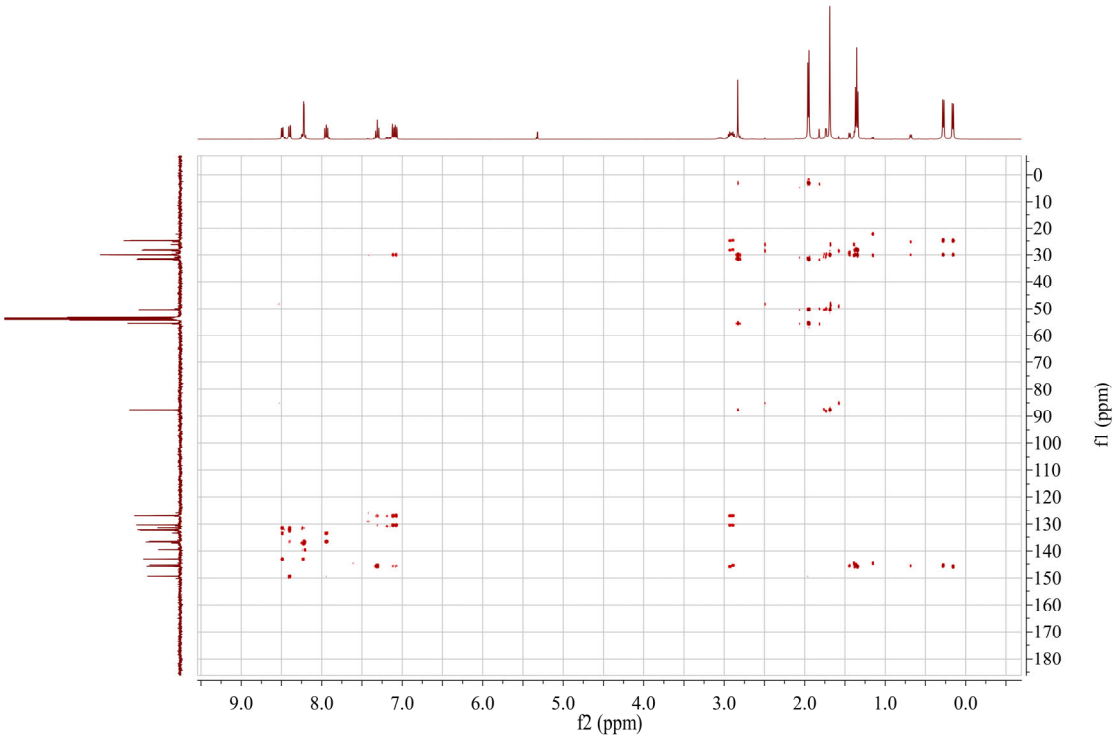


Figure S30. Heteronuclear Multiple Bond Correlation Spectroscopy [HMBC] (CD_2Cl_2, 25 °C) spectrum of **9**.

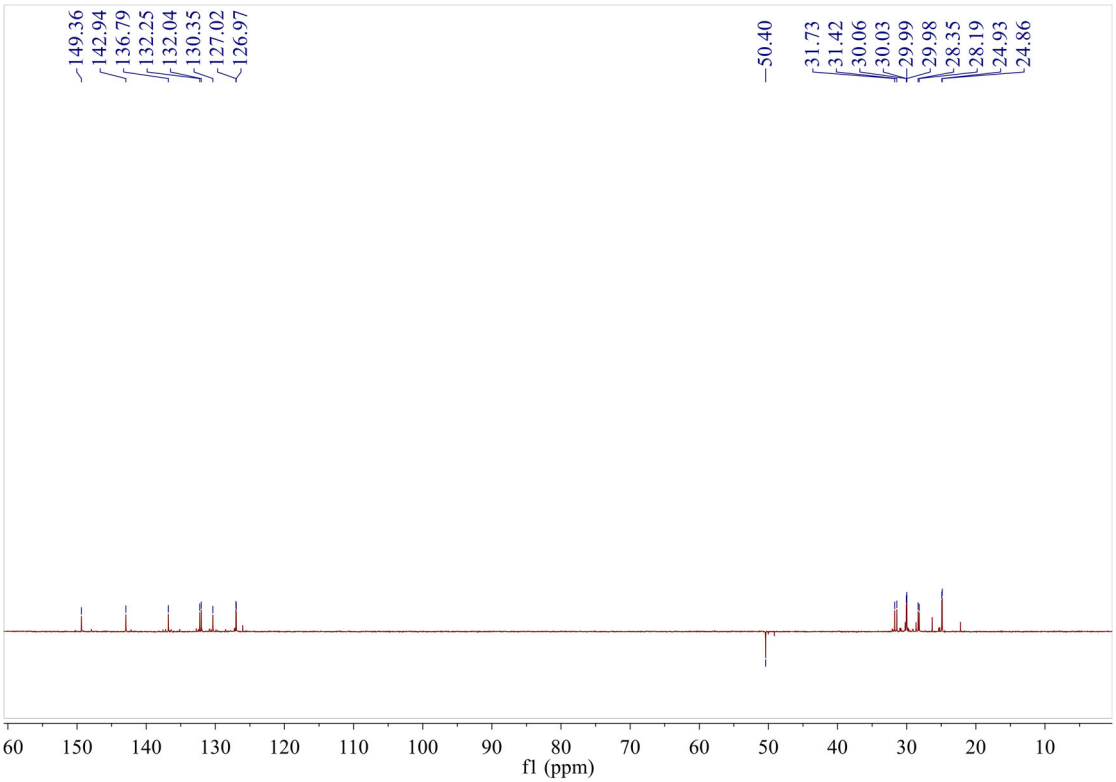


Figure S31. Distortionless Enhancement by Polarization Transfer [DEPT] 135º (101 MHz, CD_2Cl_2, 25 °C) spectrum of **9**.

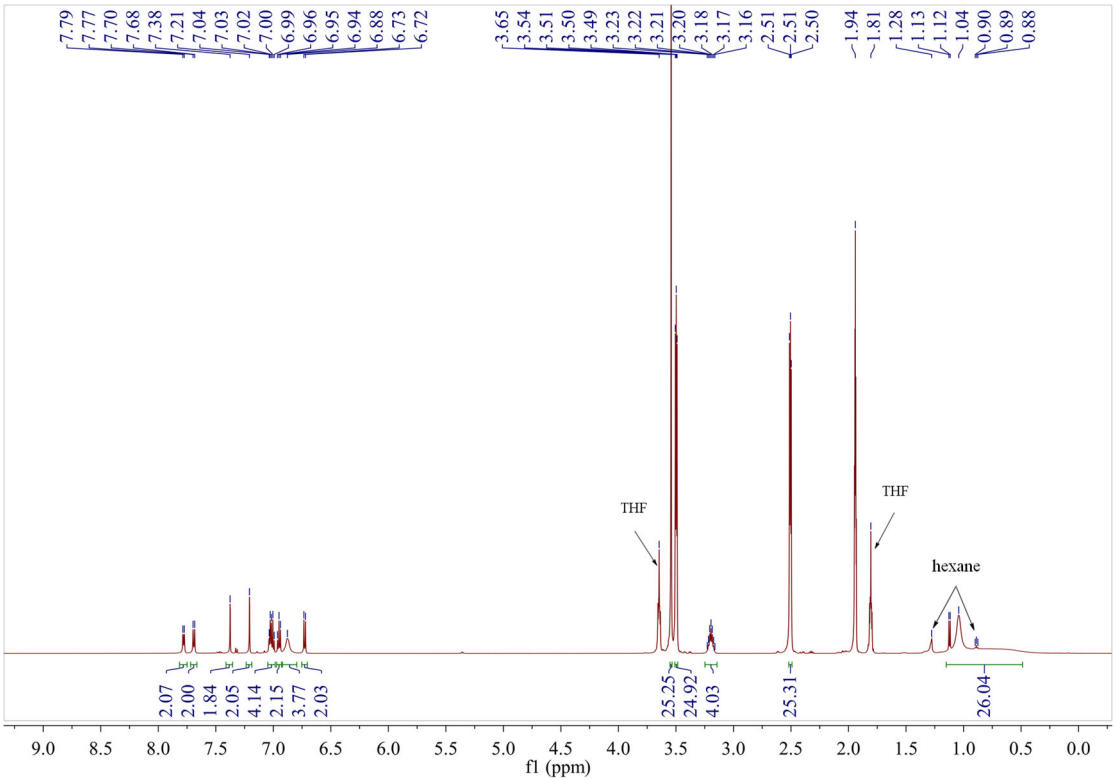


Figure S32. ^1H NMR (600 MHz, CD_3CN, 25 °C) spectrum of **10**.

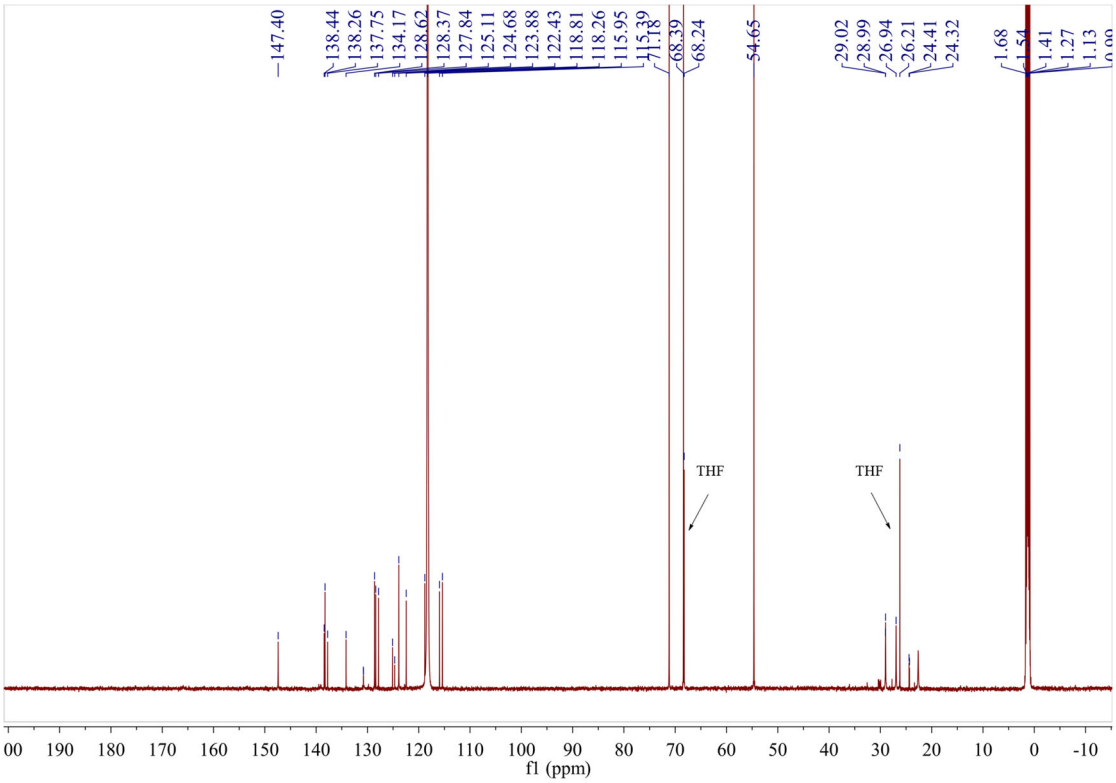


Figure S33. ^{13}C NMR (151 MHz, CD_3CN, 25 °C) spectrum of **10**.

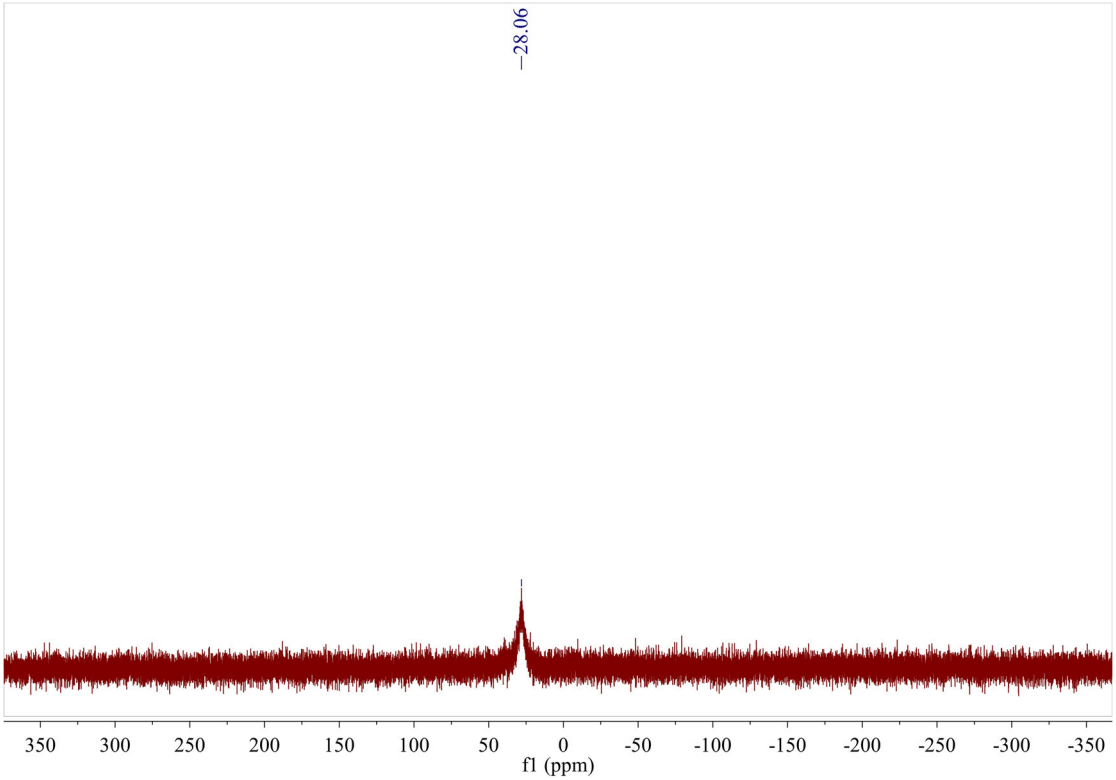


Figure S34. ^{11}B NMR (128 MHz, CD_3CN, 25 °C) spectrum of **10**.

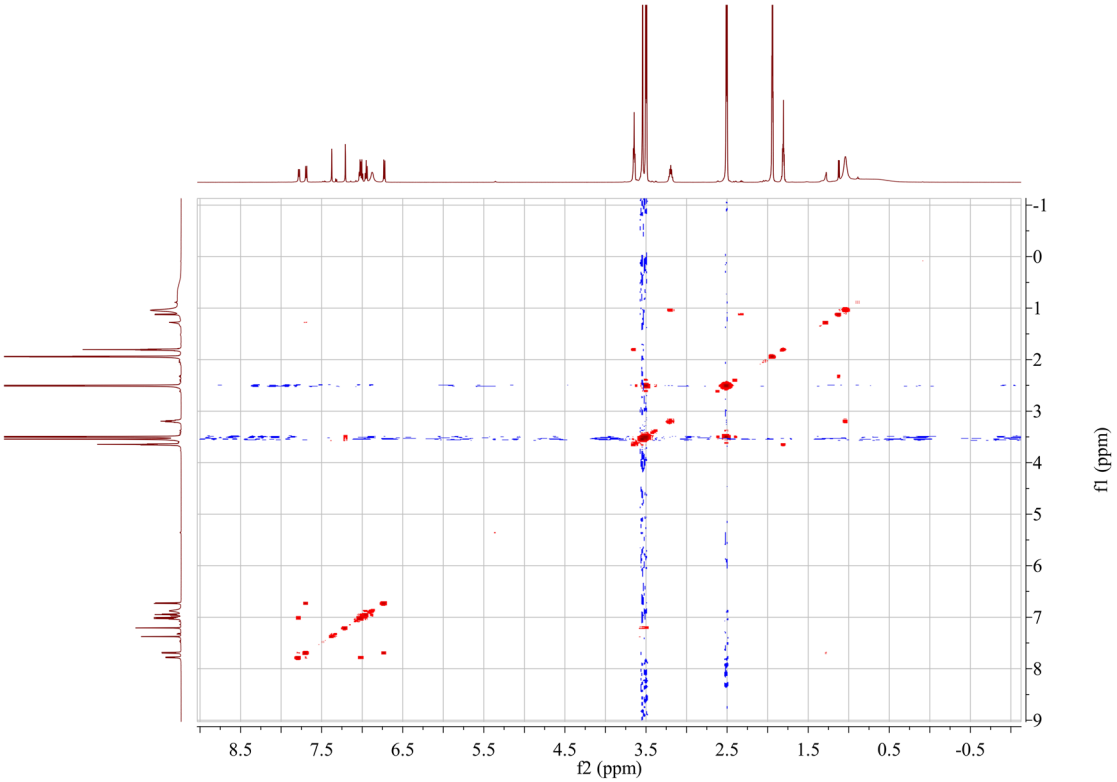


Figure S35. ^{1}H-^{1}H Correlated Spectroscopy [COSY] (CD_3CN, 25 °C) spectrum of **10**.

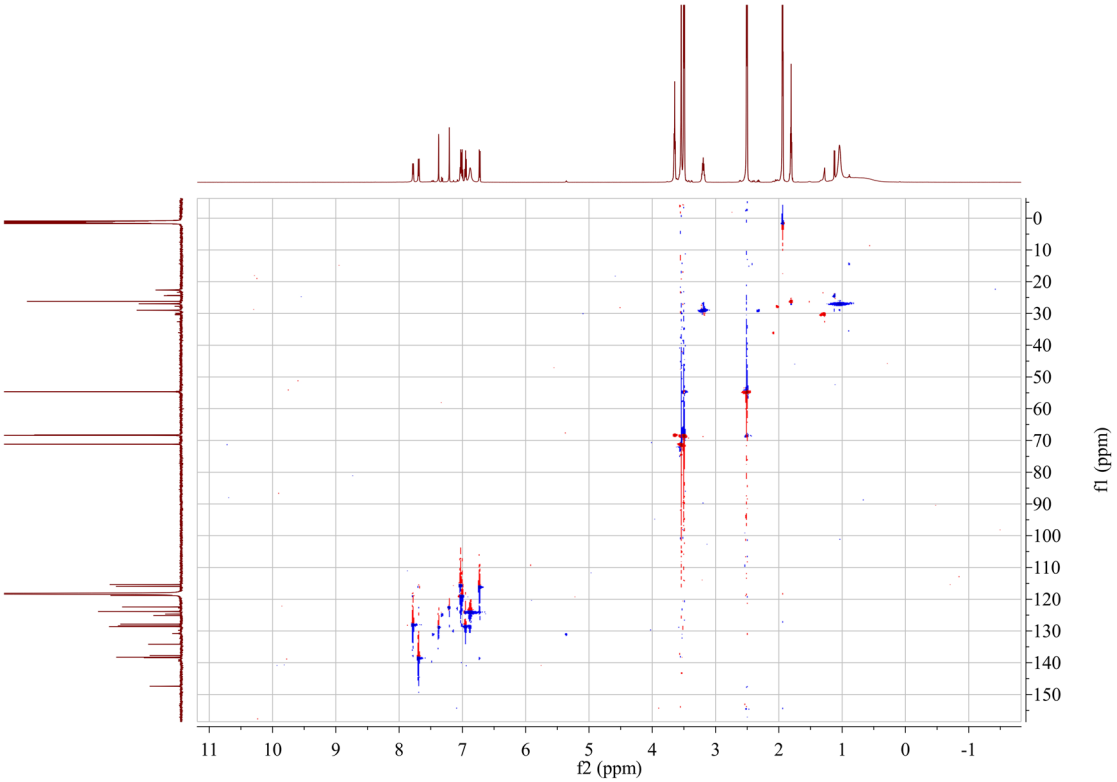


Figure S36. Heteronuclear Single Quantum Coherence Spectroscopy [HSQC] (CD_3CN, 25 °C) spectrum of **10**.

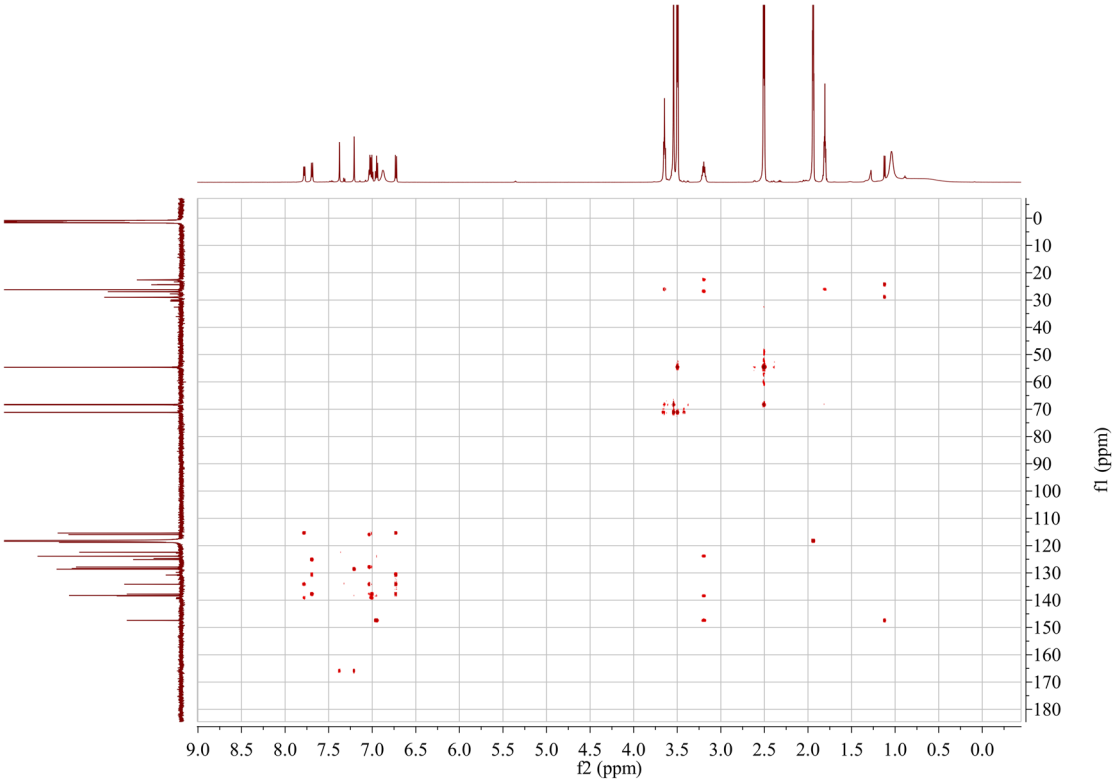


Figure S37. Heteronuclear Multiple Bond Correlation Spectroscopy [HMBC] (CD_3CN, 25 °C) spectrum of **10**.

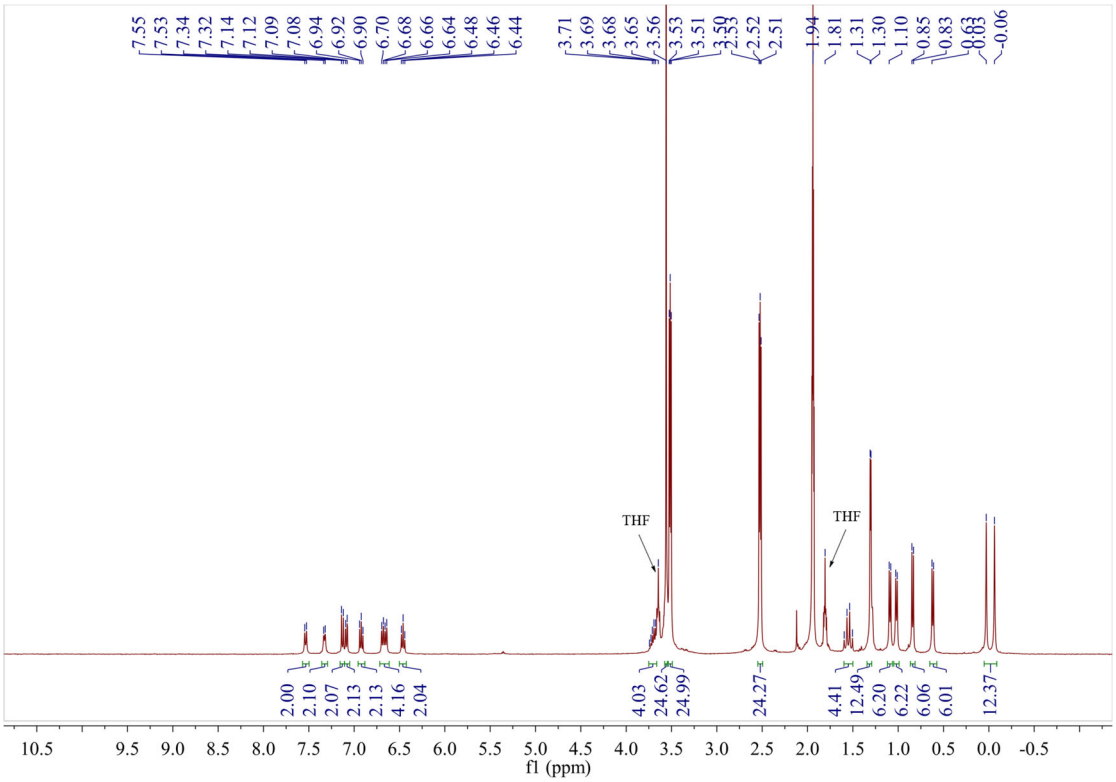


Figure S38. ^1H NMR (400 MHz, CD_3CN, 25 °C) spectrum of **11**.

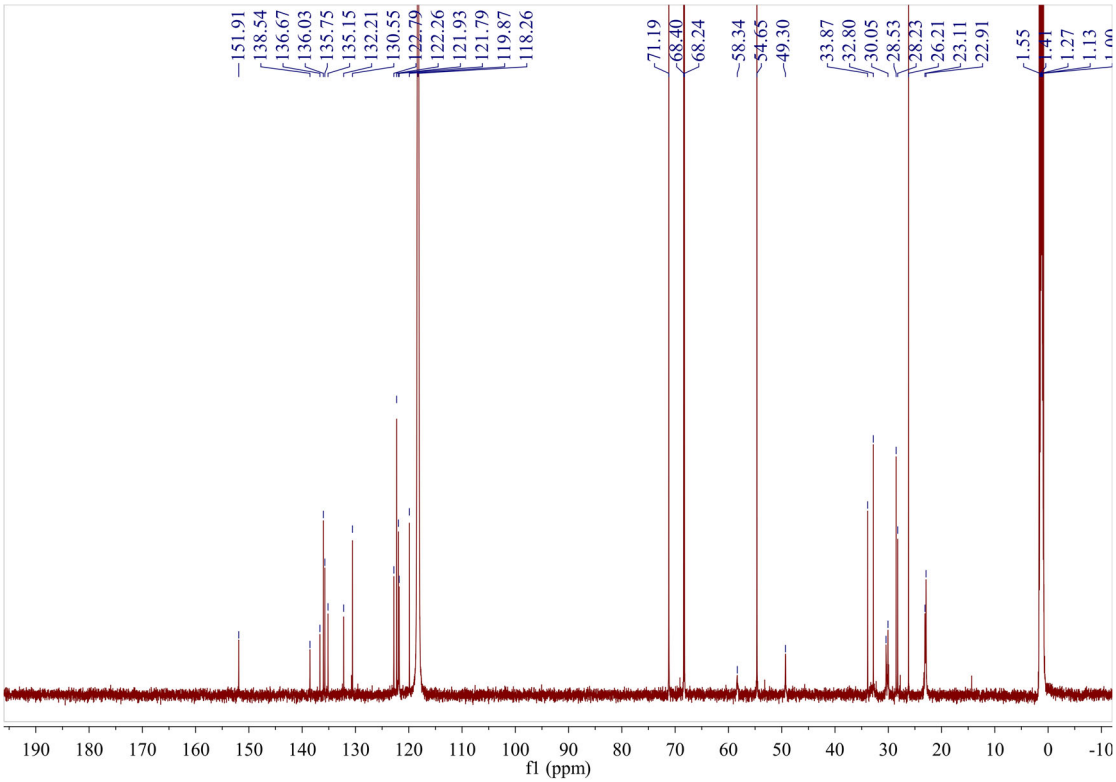


Figure S39. ^{13}C NMR (151 MHz, CD_3CN, 25 °C) spectrum of **11**.

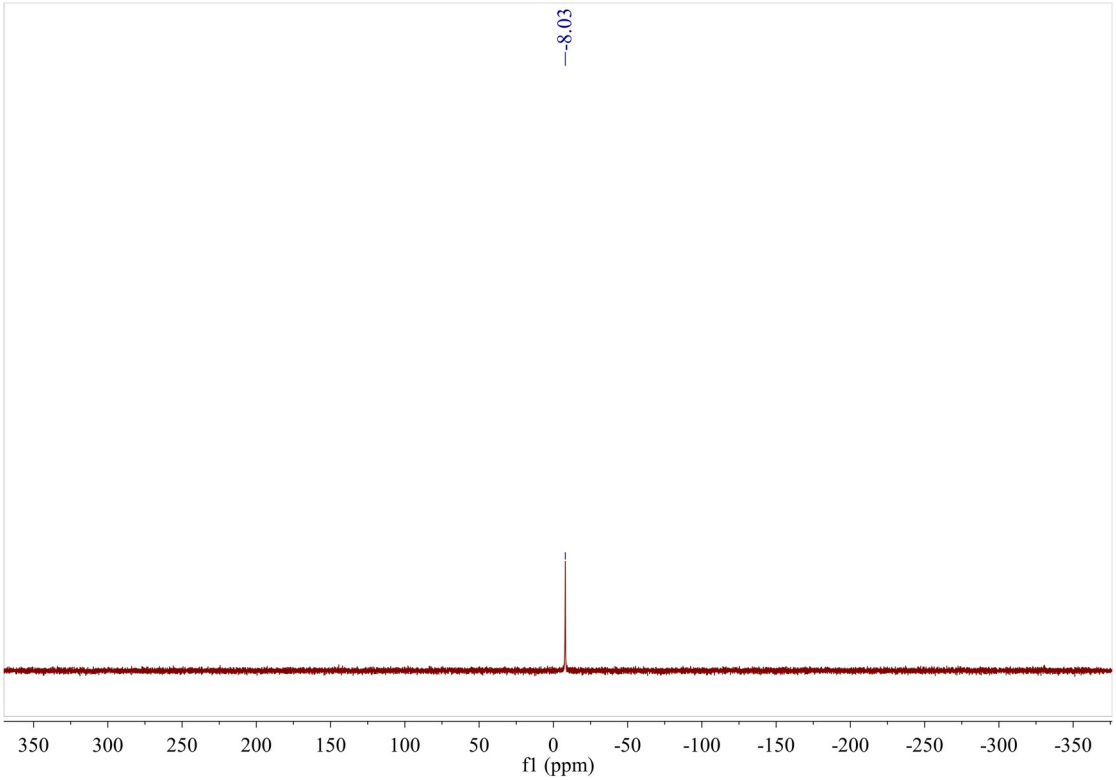


Figure S40. ^{11}B NMR (128 MHz, CD_3CN, 25 °C) spectrum of **11**.

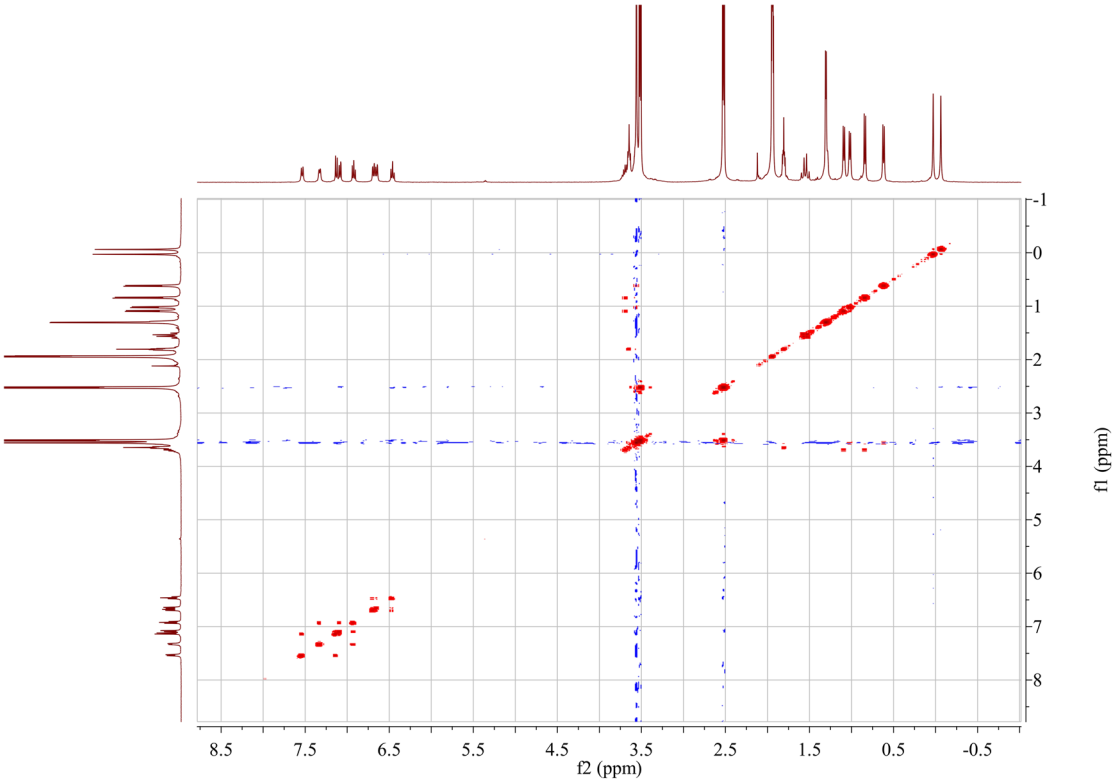


Figure S41. ^{1}H-^{1}H Correlated Spectroscopy [COSY] (CD_3CN, 25 °C) spectrum of **11**.

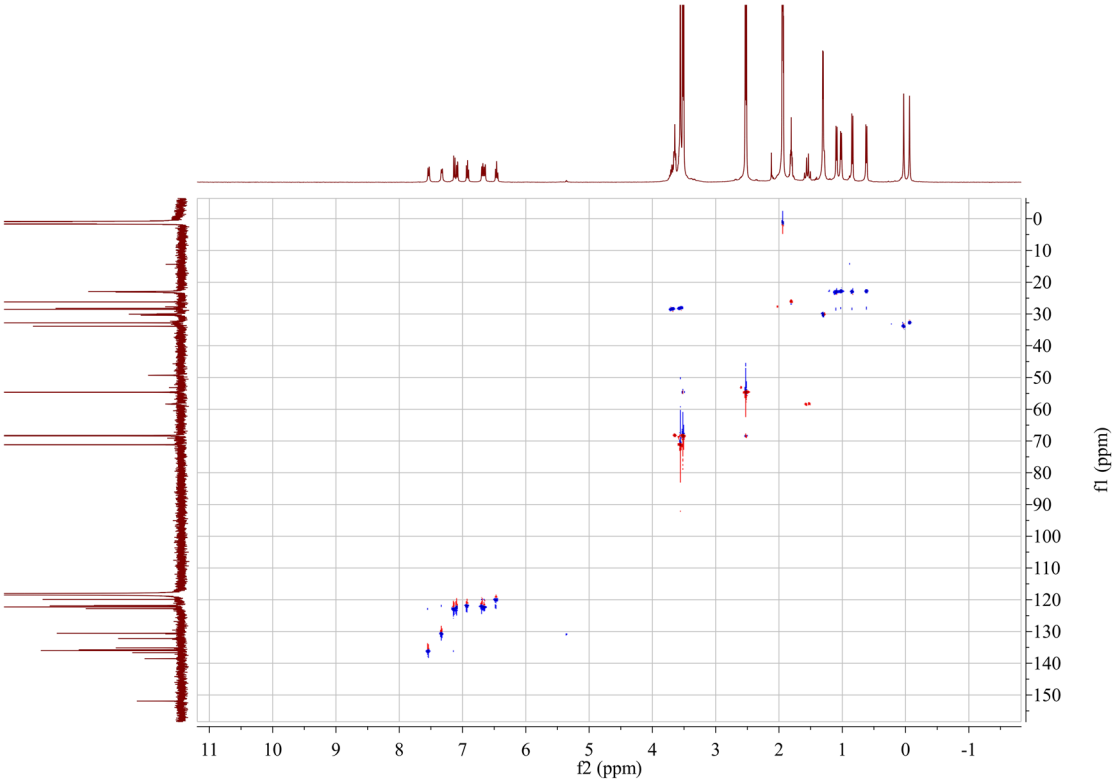


Figure S42. Heteronuclear Single Quantum Coherence Spectroscopy [HSQC] (CD_3CN, 25 °C) spectrum of **11**.

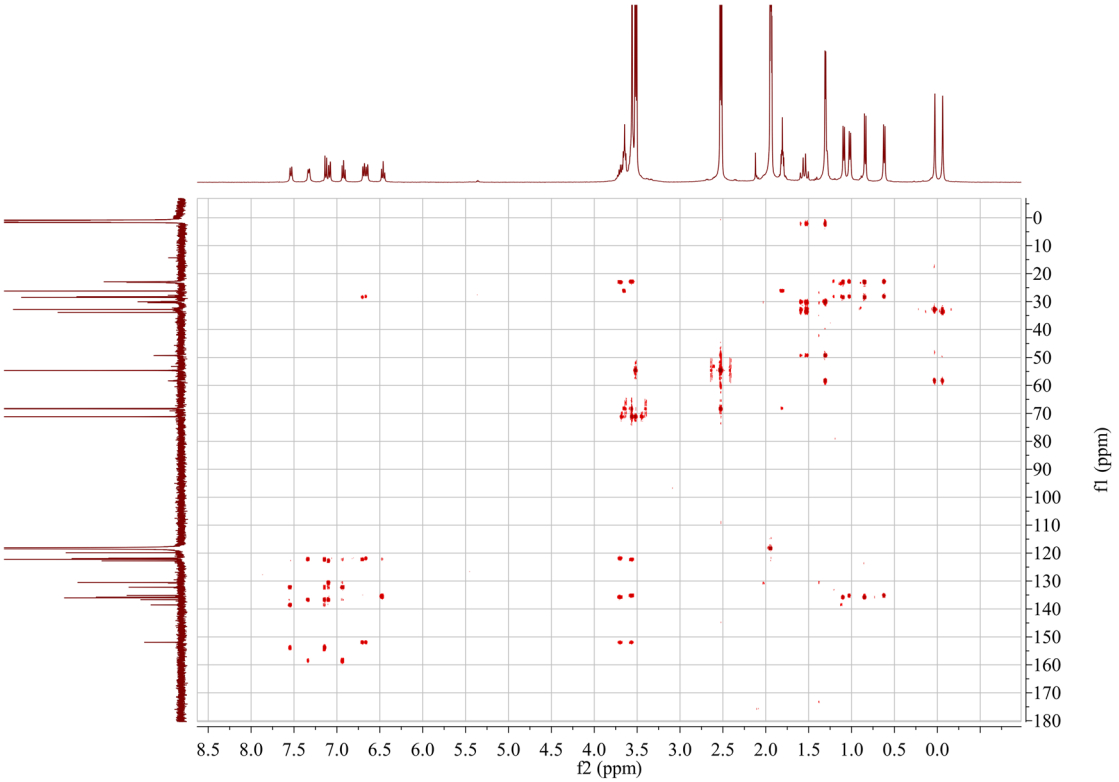


Figure S43. Heteronuclear Multiple Bond Correlation Spectroscopy [HMBC] (CD_3CN, 25 °C) spectrum of **11**.

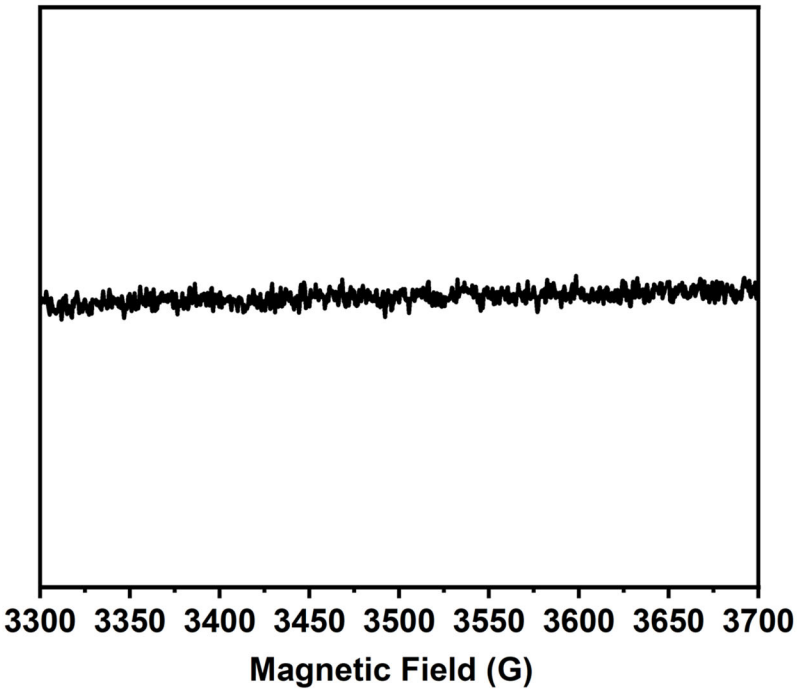


Figure S44. The powder EPR spectra of **4** at room temperature.

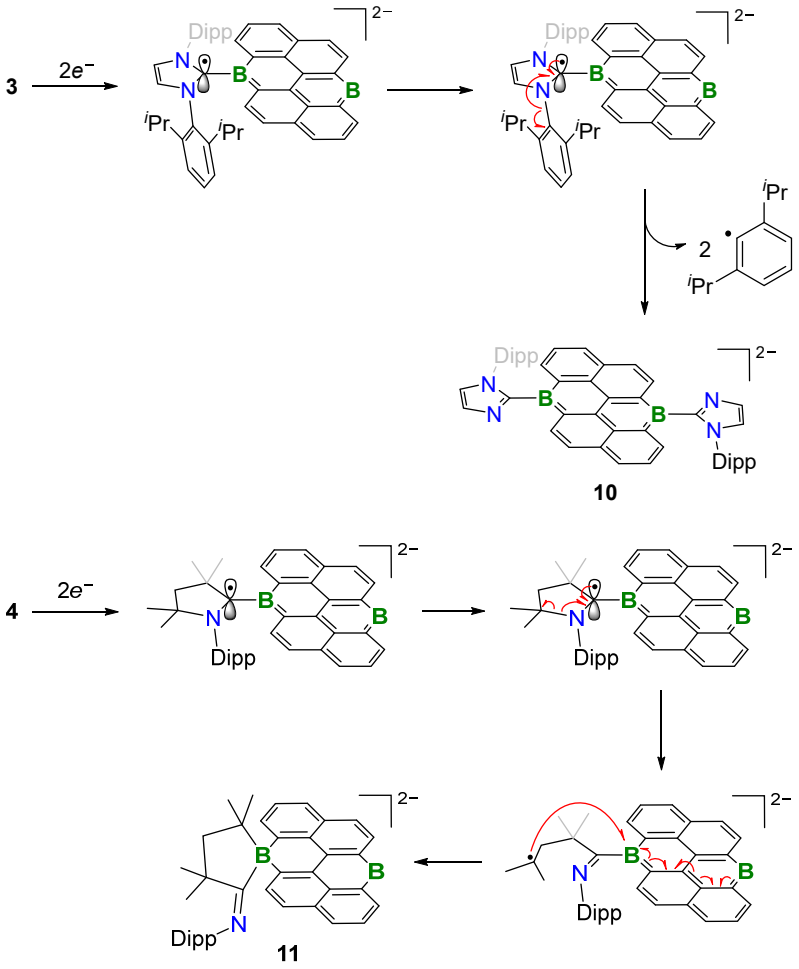
Table S1. Experimental EPR spectra parameter list for **4** in the solid state at room temperature.

Parameter	**4** (solid)
Center Field(G)	3517.134
Sweep Width(G)	400
Microwave Frequency(GHz)	9.85
Power(mW)	1
Receiver Gain	2×10^4
Modulation Frequency(kHz)	100
Modulation Amplitude(G)	10
Modulation Phase	0
Harmonic	1
Sweep time(s)	80
Number of X-Scans	3
Resolution in X	1024

Table S2. Experimental EPR spectra parameter list for **6** and **7** in *o*-DFB at room temperature.

Parameter	**6**	**7**
Center Field(G)	3515.163	3515.594
Sweep Width(G)	50	50
Microwave Frequency(GHz)	9.85	9.85
Power(mW)	1	1
Receiver Gain	10^4	10^4
Modulation Frequency(kHz)	100	100
Modulation Amplitude(G)	1	1
Modulation Phase	0	0
Harmonic	1	1
Sweep time(s)	320	320
Number of X-Scans	1	1
Resolution in X	1024	1024

Scheme S1. Proposed mechanisms for the generation of the dianionic species **10** and **11** (For clarity, only the substitution on one boron center is depicted).



2. Crystal structural parameters for 3-11

Single-Crystal X-ray Structure Determinations: Crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of all compounds were collected on a Bruker D8-VENTURE diffractometer. The structures were solved by direct methods and refined on F^2 with the SHELX-97[4]and X-Seed software packages.[5] The positions of the H atoms were calculated and considered isotropically according to a riding model. CCDC: 2413196-2413204 contain the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif

Table S3. Crystallographic data for **3** and **4**.

Compounds	**3•(THF)$_4$**	**4**
Empirical formula	$C_{90}H_{114}B_2N_4O_4$	$C_{60}H_{72}B_2N_2$
Formula weight	1335.45	842.81
Temperature	150(2) K	150(2) K
Wavelength	0.71073 Å	1.54178 Å
Crystal system	Triclinic	Orthorhombic
Space group	P-1	Pbca
Unit cell dimensions	a = 11.1662(5) Å	a = 10.5812(5) Å
	b = 11.7494(6) Å	b = 19.2594(11) Å
	c = 15.5317(8) Å	c = 29.9453(16) Å
	α = 71.647(2)°	α = 90°
	β = 84.332(2)°	β = 90°
	γ = 88.761(2)°	γ = 90°
Volume	1924.50(17) Å^3	6102.5(6) Å^3
Z	1	4
Density (calculated)	1.154 Mg/m^3	0.917 Mg/m^3
Absorption coefficient	0.069 mm^{-1}	0.385 mm^{-1}
F(000)	724	1824
Crystal size	0.120 x 0.090 x 0.040 mm^3	0.130 x 0.100 x 0.090 mm^3
Theta range for data collection	2.404 to 27.536°.	2.951 to 67.499°.
Index ranges	-12<=h<=14, -15<=k<=15,	-12<=h<=12, -23<=k<=23,
	-20<=l<=20	-35<=l<=35
Reflections collected	44655	64031
Independent reflections	8812 [R_{int} = 0.0813]	5479 [R_{int} = 0.1098]
Completeness to theta	25.242° 99.5 %	67.499° 99.6 %
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	8812 / 12 / 479	5479 / 6 / 307
Goodness-of-fit on F^2	1.055	1.060
Final R indices [I>2sigma(I)]	R_1 = 0.0847, wR_2 = 0.2291	R_1 = 0.0642, wR_2 = 0.1653
R indices (all data)	R_1 = 0.1228, wR_2 = 0.2634	R_1 = 0.0864, wR_2 = 0.1852
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	0.583 and -0.633 e.Å^{-3}	0.288 and -0.235 e.Å^{-3}

Table S4. Crystallographic data for **5**.

Compound	**5**
Empirical formula	$C_{38}H_{46}B_2N_2O_2$
Formula weight	584.39
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 14.2417(12) Å
	b = 14.4218(12) Å
	c = 16.5090(15) Å
	α = 90°
	β = 103.326(4)°
	γ = 90°
Volume	3299.5(5) $Å^3$
Z	4
Density (calculated)	1.176 Mg/m^3
Absorption coefficient	0.071 mm^{-1}
F(000)	1256
Crystal size	0.140 x 0.120 x 0.090 mm^3
Theta range for data collection	2.038 to 27.506°.
Index ranges	-18<=h<=18, -18<=k<=18,
	-21<=l<=21
Reflections collected	25849
Independent reflections	3779 [$R_{(int)}$ = 0.0727]
Completeness to theta = 25.242°	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3779 / 1 / 203
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R_1 = 0.0527, wR_2 = 0.1312
R indices (all data)	R_1 = 0.0766, wR_2 = 0.1478
Extinction coefficient	n/a
Largest diff. peak and hole	0.296 and -0.249 e.$Å^{-3}$

Table S5. Crystallographic data for **6** and **7**.

Compounds	**[6• (*o*-DFB)]$_2$**	**7**
Empirical formula	$C_{160}H_{172}B_4F_{16}N_8Sb_2$	$C_{60}H_{72}B_2F_6N_2Sb$
Formula weight	2797.79	1078.56
Temperature	150(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic
Space group	P-1	P2/n
Unit cell dimensions	a = 12.3898(6) Å	a = 16.4468(10) Å
	b = 17.0733(8) Å	b = 9.5691(6) Å
	c = 19.6357(9) Å	c = 19.4316(12) Å
	α = 109.541(2)°	α = 90°
	β = 106.403(2)°	β = 109.712(2)°
	γ = 93.078(2)°	γ = 90°
Volume	3704.3(3) Å^3	2879.0(3) Å^3
Z	1	2
Density (calculated)	1.254 Mg/m^3	1.244 Mg/m^3
Absorption coefficient	0.437 mm^{-1}	0.536 mm^{-1}
F(000)	1454	1122
Crystal size	0.090 x 0.080 x 0.060 mm^3	0.070 x 0.060 x 0.060 mm^3
Theta range for data collection	2.021 to 27.539°.	2.502 to 27.551°.
Index ranges	-15<=h<=16, -22<=k<=21,	-21<=h<=21, -10<=k<=12,
	-25<=l<=24	-25<=l<=25
Reflections collected	77669	40651
Independent reflections	16955 [R_{int} = 0.0616]	6517 [R_{int} = 0.0540]
Completeness to theta	25.242° 99.8 %	25.242° 98.0 %
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	16955 / 0 / 875	6517 / 7 / 329
Goodness-of-fit on F^2	1.034	1.073
Final R indices [I>2sigma(I)]	R_1 = 0.0542, wR_2 = 0.1376	R_1 = 0.0799, wR_2 = 0.2112
R indices (all data)	R_1 = 0.0833, wR_2 = 0.1574	R_1 = 0.1028, wR_2 = 0.2291
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	0.988 and -0.534 e.Å^{-3}	2.1o6 and -1.350 e.Å^{-3}

Table S6. Crystallographic data for **8** and **9**.

Compounds	**8•(DCM)$_2$**	**9•(o-DFB)$_2$**
Empirical formula	$C_{76}H_{86}B_2Cl_4F_{12}N_4Sb_2$	$C_{72}H_{80}B_2F_{16}N_2Sb_2$
Formula weight	1690.40	1542.50
Temperature	150(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$
Unit cell dimensions	a = 12.4457(7) Å	a = 11.1837(11) Å
	b = 27.8277(17) Å	b = 32.500(3) Å
	c = 13.0240(8) Å	c = 21.1355(19) Å
	α = 90°.	α= 90°
	β = 95.719(2)°	β= 92.894(3)°
	γ = 90°	γ = 90°
Volume	4488.2(5) Å^3	7672.4(12) Å^3
Z	2	4
Density (calculated)	1.251 Mg/m^3	1.335 Mg/m^3
Absorption coefficient	0.784 mm^{-1}	0.782 mm^{-1}
F(000)	1716	3128
Crystal size	0.800 x 0.100 x 0.090 mm^3	0.120 x 0.110 x 0.090 mm^3
Theta range for data collection	2.148 to 26.999°.	1.928 to 27.572°.
Index ranges	-14<=h<=15, -35<=k<=35,	-13<=h<=14, -42<=k<=38,
	-16<=l<=16	-27<=l<=22
Reflections collected	54885	60352
Independent reflections	9776 [R_{int} = 0.0798]	17553 [R_{int} = 0.0612]
Completeness to theta = 25.242°	99.7 %	99.6 %
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	9776 / 0 / 459	17553 / 0 / 863
Goodness-of-fit on F^2	1.119	1.032
Final R indices [I>2sigma(I)]	R_1 = 0.0817, wR_2 = 0.1734	R_1 = 0.0640, wR_2 = 0.1579
R indices (all data)	R_1 = 0.0982, wR_2 = 0.1819	R_1 = 0.0824, wR_2 = 0.1694
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	2.521 and -1.874 e.Å^{-3}	1.838 and -1.352 e.Å^{-3}

Table S7. Crystallographic data for **10** and **11**.

Compounds	**10•(THF)$_2$**	**11•(THF)$_2$**
Empirical formula	$C_{94}H_{136}B_2K_2N_8O_{14}$	$C_{104}H_{160}B_2K_2N_6O_{14}$
Formula weight	1701.92	1818.19
Temperature	150(2) K	150(2) K
Wavelength	1.54178 Å	1.54178 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/c$
Unit cell dimensions	a = 13.2016(3) Å	a = 14.9184(6) Å
	b = 13.5917(3) Å	b = 17.1615(7) Å
	c = 27.9529(8) Å	c = 20.7225(9) Å
	$\alpha = 90°$	$\alpha = 90°$
	$\beta = 91.891(2)°$	$\beta = 106.128(2)°$
	$\gamma = 90°$	$\gamma = 90°$
Volume	5012.9(2) Å^3	5096.6(4) Å^3
Z	2	2
Density (calculated)	1.128 Mg/m^3	1.185 Mg/m^3
Absorption coefficient	1.319 mm^{-1}	1.320 mm^{-1}
F(000)	1832	1972
Crystal size	0.120 x 0.100 x 0.090 mm^3	0.140 x 0.120 x 0.090 mm^3
Theta range for data collection	3.164 to 68.521°.	3.400 to 66.687°.
	-15<=h<=15, -16<=k<=16,	-17<=h<=17, -20<=k<=20,
	-33<=l<=33	-24<=l<=24
Reflections collected	51540	48818
Independent reflections	9192 [R_{int} = 0.1375]	8985 [R_{int} = 0.0451]
Completeness to theta	67.679° 99.8 %	66.687° 99.6 %
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	9192 / 0 / 547	8985 / 0 / 585
Goodness-of-fit on F^2	1.086	1.035
Final R indices [I>2sigma(I)]	R_1 = 0.0679, wR_2 = 0.1767	R_1 = 0.0455, wR_2 = 0.1276
R indices (all data)	R_1 = 0.0937, wR_2 = 0.1962	R_1 = 0.0509, wR_2 = 0.1328
Extinction coefficient	0.0024(3)	n/a
Largest diff. peak and hole	0.467 and -0.557 e.Å^{-3}	0.693 and -0.345 e.Å^{-3}

3. Photophysical properties of compounds 6-9

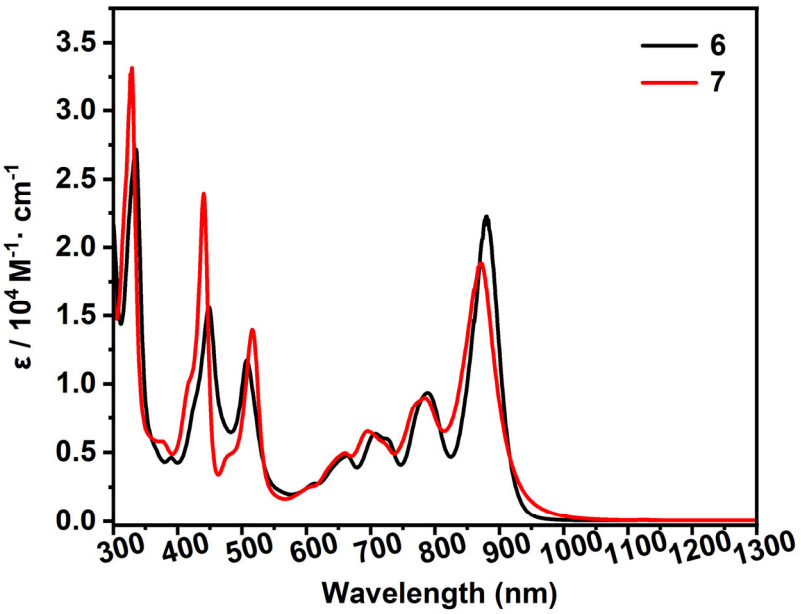


Figure S45. UV-Vis absorption spectra of **6** and **7** in *o*-difluorobenzene.

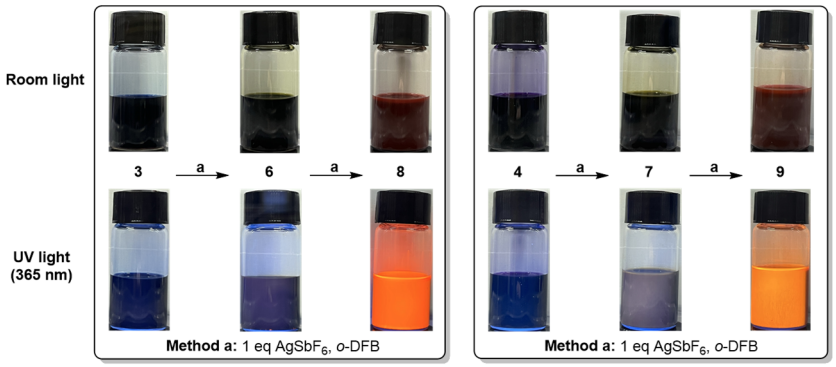


Figure S46. Images illustrating the stepwise oxidation process of compounds **3** and **4** in *o*-difluorobenzene under room light and UV light.

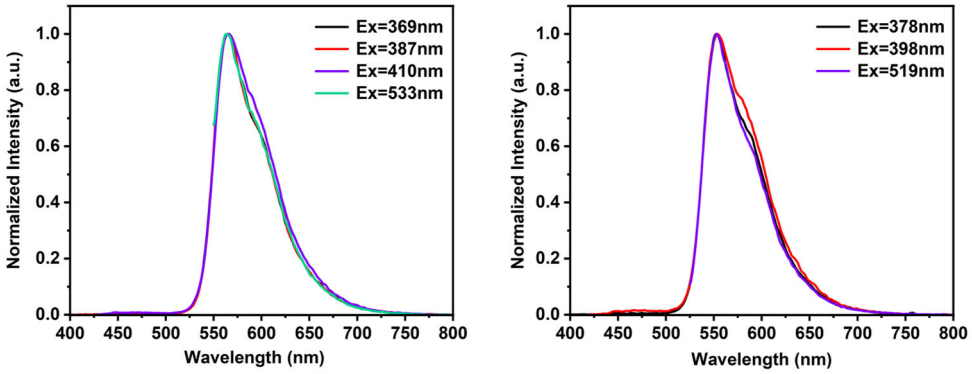


Figure S47. Fluorescence spectra of **8** (left) and **9** (right) at various excitation wavelengths.

4. Computational Details

All quantum chemical calculations were carried out using Gaussian 09.[6] The geometries of all compounds including the triplet states of **3** and **4** were optimized by using the hybrid functional (U)B3LYP with the 6-311G(d,p) basis set, according to the best agreement with the metric data from X-ray structure analyses. For **3** and **4**, the open-shell singlet (OS) state was considered using the UB3LYP and UBH&HLYP functionals with the 6-311G(d,p) basis set, as well as the UB3LYP, UBH&HLYP, and UM06-2X functionals with the def2-TZVP basis-sets. All attempts to optimize **3** and **4** as singlet broken symmetry state showed no spin contamination and collapsed into the closed-shell singlet electronic structure. Time-dependent DFT (TD-DFT) was utilized at the (U)CAM-B3LYP/6-311G(d,p) level to calculate the excitation energies. In addition, frequency calculations are carried out at the same level of theory to confirm the stationary points are minima with no imaginary frequencies. The NBO analysis,[7] the anisotropy of the induced current density (ACID)[8], and nucleus-independent chemical shifts (NICS)[9] using the gauge invariant atomic orbital (GIAO) approach, and were calculated at the same level of theory.

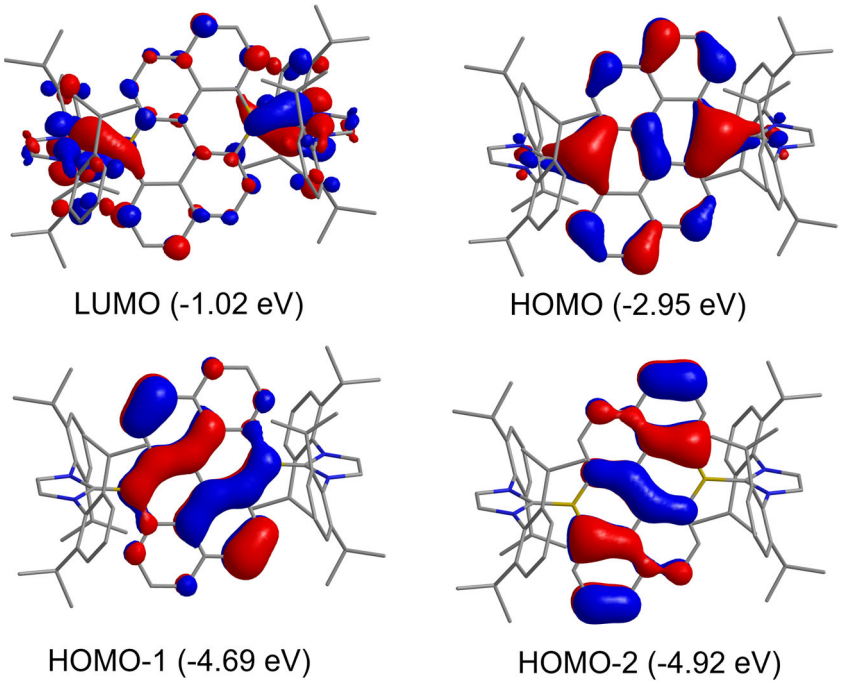


Figure S48. Plots of MOs of **3-closed-shell singlet** (isovalue = 0.03, hydrogen atoms are omitted for clarity).

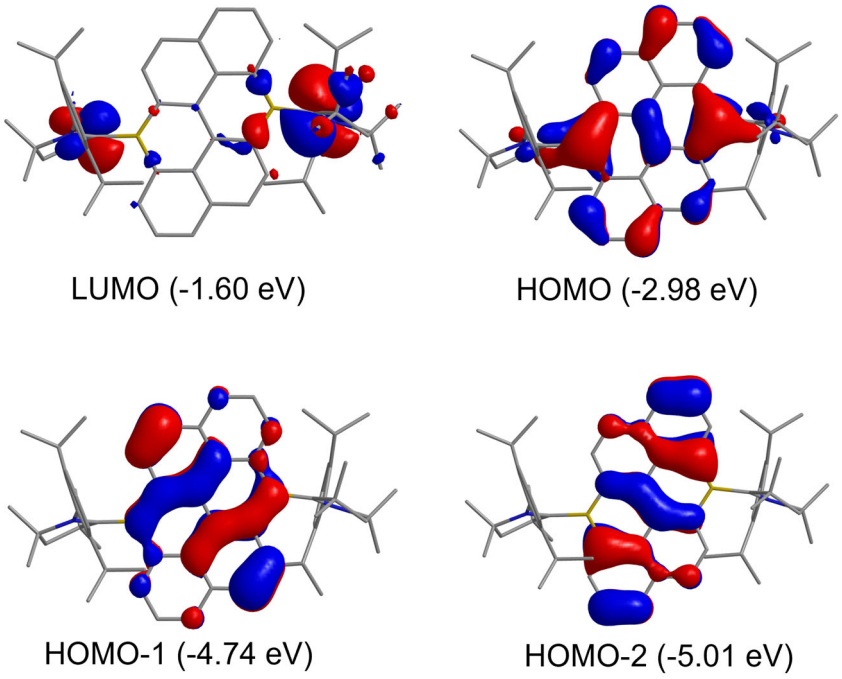


Figure S49. Plots of MOs of **4-closed-shell singlet** (isovalue = 0.03, hydrogen atoms are omitted for clarity).

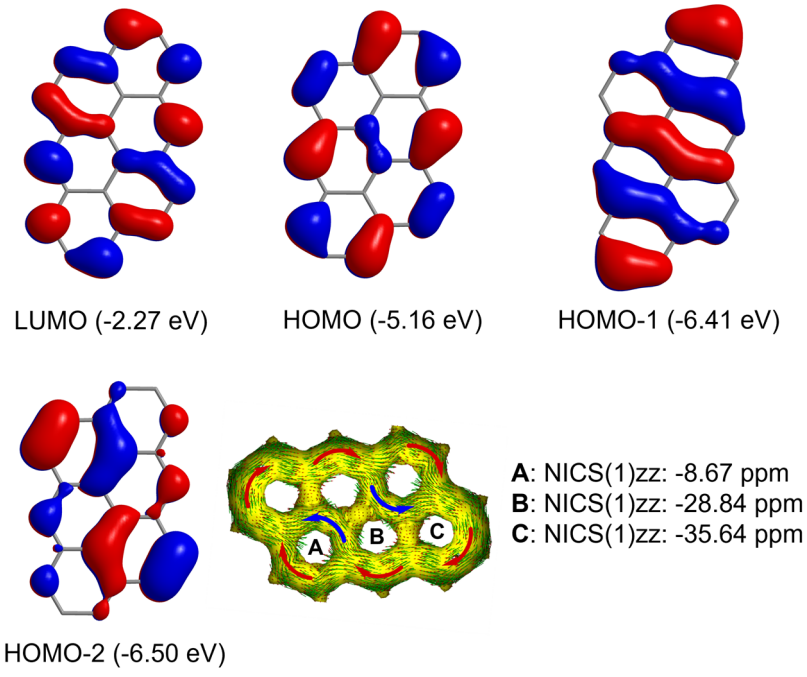
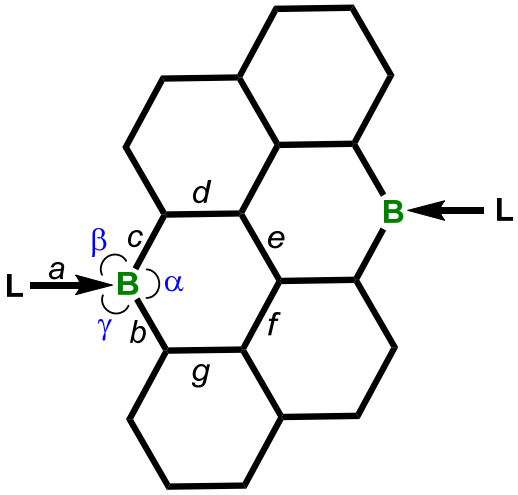


Figure S50. Plots of the MOs of **all-carbon anthanthrene VI** (isovalue = 0.03, hydrogen atoms are omitted for clarity), and the ACID, and NICS(1)$_{zz}$ values (the external magnetic field is applied orthogonal to the plane, and the red and blue arrows indicate the clockwise (diamagnetic) and counter-clockwise (paramagnetic) current flow, respectively).

Table S8. Experimental and calculated bond lengths (Å) and angles (°) of **3** and **4** at the (U)B3LYP/6-311G(d, p) level.



	3_{exp}	$3_{calcd\text{-}singlet}$	$3_{calcd\text{-}triplet}$	4_{exp}	$4_{calcd\text{-}singlet}$	$4_{calcd\text{-}triplet}$
a	1.590(3)	1.59813	1.57835	1.610(3)	1.59153	1.56142
b	1.516(4)	1.52088	1.52693	1.517(4)	1.53118	1.55934
c	1.485(4)	1.49543	1.54018	1.491(4)	1.49304	1.56554
d	1.456(3)	1.45149	1.42791	1.459(3))	1.44965	1.42162
e	1.431(4)	1.44150	1.46738	1.436(5))	1.43810	1.47061
f	1.443(3)	1.44432	1.44876	1.443(3)	1.44512	1.44044
g	1.444(3)	1.44163	1.44304	1.440(3)	1.44172	1.42919
α	119.4(2)	118.15	117.32	117.9(2)	117.67	111.77
β	120.6(2)	121.32	121.79	122.7(2)	125.36	130.59
γ	120.0(2)	120.53	120.89	118.4(2)	116.60	117.25

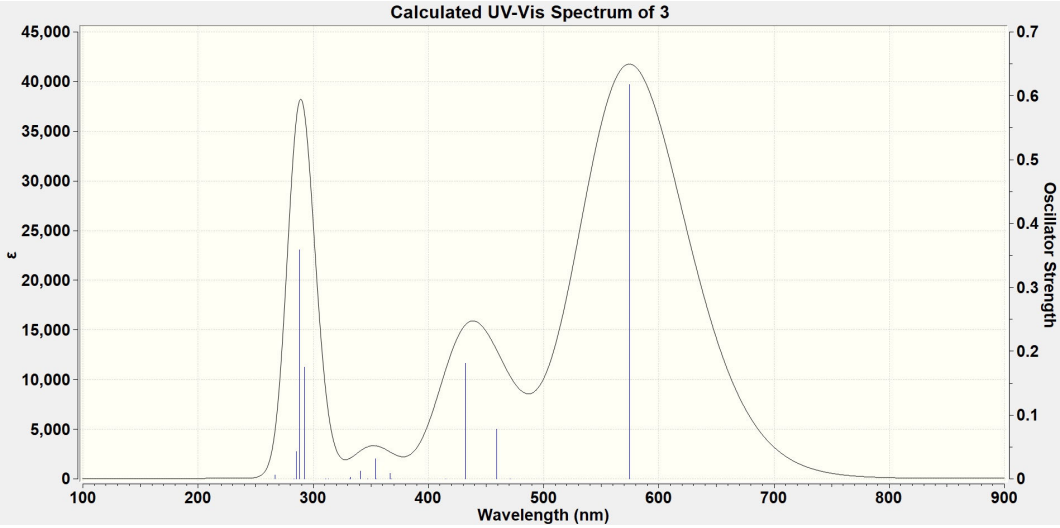


Figure S51. Calculated UV-Vis spectrum of **3** at CAM-B3LYP/6-311 G(d, p) (PCM, *o*-difluorobenzene) level of theory.

Table S9. TD-DFT description of first 5 electronically excited states in **3**. The highest occupied molecular orbital of **3** is MO 282.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.1570 eV 574.81 nm f=0.6181 <S**2>=0.000

282 → 283 0.69289

Excited State 2: Singlet-A 2.6337 eV 470.76 nm f=0.0000 <S**2>=0.000

282 → 284 0.63675

282 → 293 -0.25542

Excited State 3: Singlet-A 2.7008 eV 459.07 nm f=0.0779 <S**2>=0.000

282 → 285 0.65979

282 → 294 -0.20151

Excited State 4: Singlet-A 2.8686 eV 432.21 nm f=0.1811 <S**2>=0.000

280 → 283 0.15840

282 → 286 0.42350

282 → 291 -0.41261

282 → 292 0.28348

282 → 294 0.15465

Excited State 5: Singlet-A 2.9873 eV 415.03 nm f=0.0000 <S**2>=0.000

282 → 284 0.19450

282 → 287 -0.25156

282 → 288 -0.25665

282 → 290 -0.20973

282 → 293 0.28142

282 → 295 0.43885

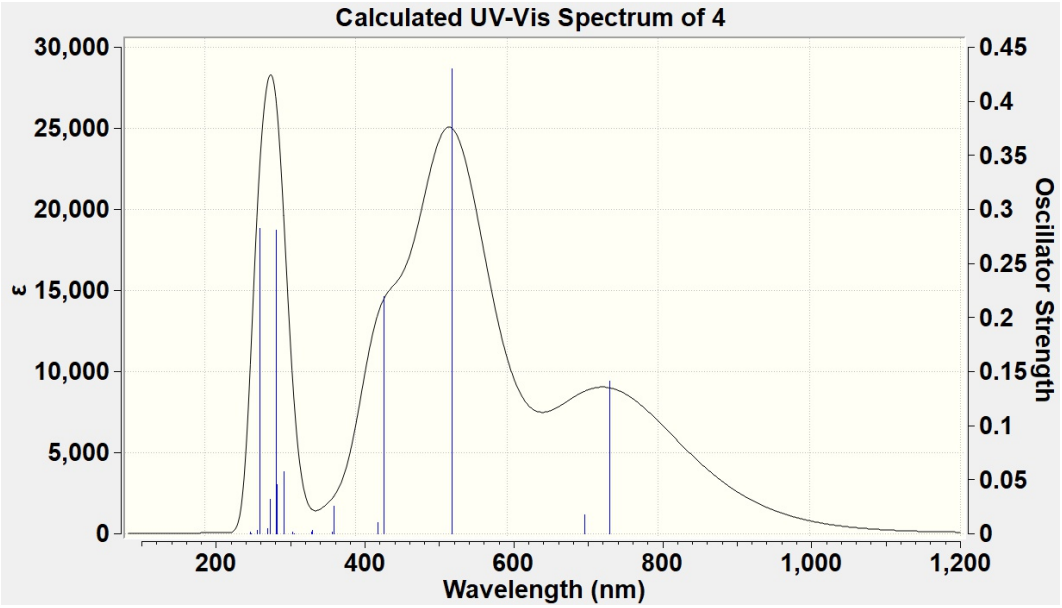


Figure S52. Calculated UV-Vis spectrum of **4** at CAM-B3LYP/6-311 G(d, p) (PCM, *o*-difluorobenzene) level of theory.

Table S10. TD-DFT description of first 5 electronically excited states in **4**. The highest occupied molecular orbital of **4** is MO 228.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.6856 eV 735.55 nm f=0.1412 <S**2>=0.000

227 → 230 -0.10034

228 → 229 0.65044

228 → 230 0.15089

228 → 231 -0.16860

Excited State 2: Singlet-A 1.7627 eV 703.38 nm f=0.0173 <S**2>=0.000

228 → 229 -0.13689

228 → 230 0.66918

Excited State 3: Singlet-A 2.3496 eV 527.68 nm f=0.4304 <S**2>=0.000

228 → 229 0.18846

228 → 231 0.66011

Excited State 4: Singlet-A 2.8365 eV 437.11 nm f=0.2194 <S**2>=0.000

226 → 229 0.10159

226 → 231 0.11168

228 → 231 0.10639

228 → 232 0.12042

228 → 234 0.55139

228 → 236 -0.33764

228 → 237 0.10009

Excited State 5: Singlet-A 2.8889 eV 429.17 nm f=0.0106 <S**2>=0.000

228 → 235 -0.18151

228 → 237 0.65935

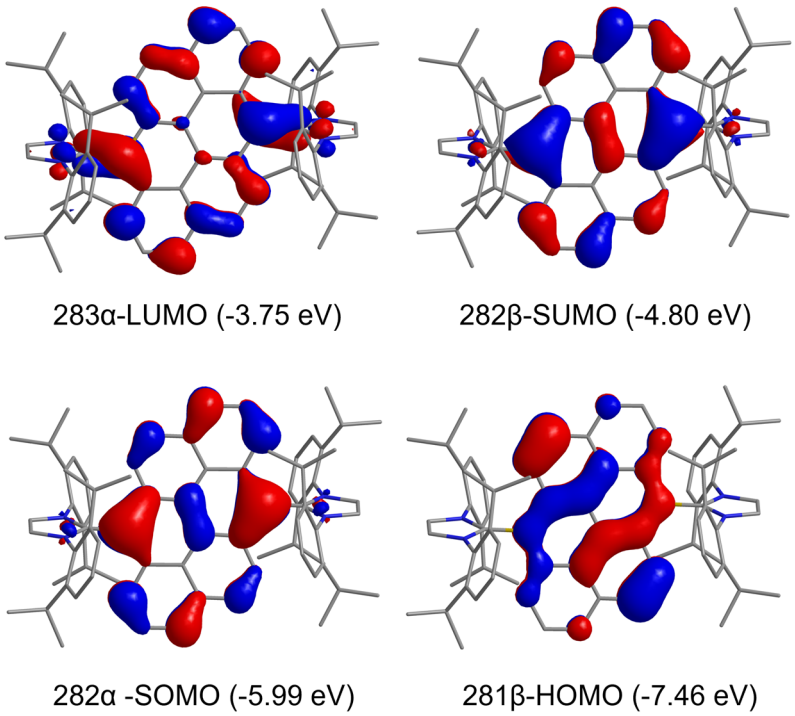


Figure S53. Plots of MOs of **6** (isovalue = 0.03, hydrogen atoms are omitted for clarity).

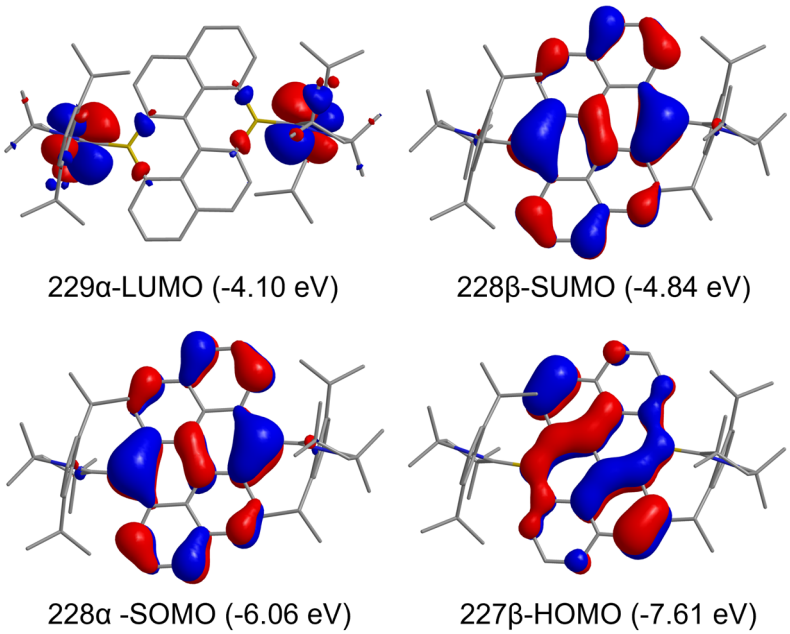
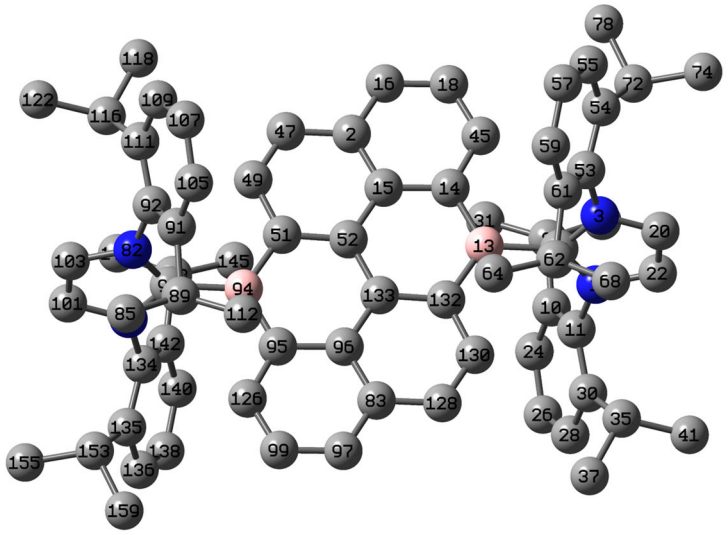


Figure S54. Plots of MOs of **7** (isovalue = 0.03, hydrogen atoms are omitted for clarity).

Table S11. Mulliken spin populations and SOMO atomic contributions of **6**.



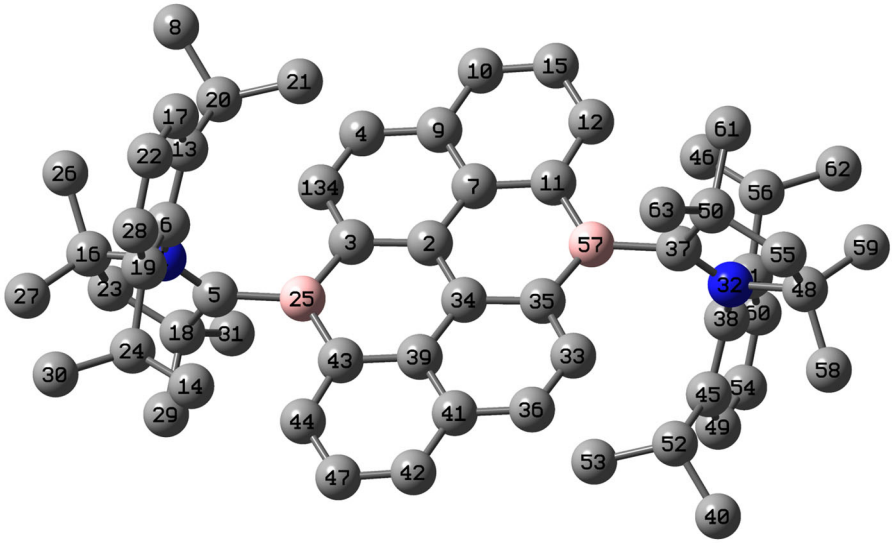
Mulliken spin population:

1	N	0.00569
2	C	-0.02121
3	N	0.00595
4	C	0.00013
8	C	-0.00067
10	C	-0.00036
11	C	0.00002
12	C	-0.00067
13	B	0.22573
14	C	-0.04528
15	C	-0.00051
16	C	0.11076
18	C	-0.03507
20	C	0.00135
22	C	0.00218
24	C	0.00049
26	C	0.00056
28	C	0.00056
30	C	0.00098
31	C	0.00000
35	C	-0.00010
37	C	0.00058
41	C	0.00004
45	C	0.11808
47	C	0.06086
49	C	-0.02420
51	C	0.05069

52	C	0.04137
53	C	-0.00051
54	C	0.00015
55	C	0.00129
57	C	-0.00013
59	C	0.00122
61	C	-0.00082
62	C	-0.00030
64	C	-0.00023
68	C	0.00029
72	C	0.00011
74	C	0.00007
78	C	0.00090
82	N	0.00569
83	C	-0.02121
84	N	0.00595
85	C	0.00013
89	C	-0.00067
91	C	-0.00036
92	C	0.00002
93	C	-0.00067
94	B	0.22574
95	C	-0.04528
96	C	-0.00050
97	C	0.11076
99	C	-0.03507
101	C	0.00135

103	C	0.00218
105	C	0.00049
107	C	0.00056
109	C	0.00056
111	C	0.00098
112	C	0.00000
116	C	-0.00010
118	C	0.00058
122	C	0.00004
126	C	0.11809
128	C	0.06086
130	C	-0.02420
132	C	0.05070
133	C	0.04137
134	C	-0.00051
135	C	0.00015
136	C	0.00129
138	C	-0.00013
140	C	0.00122
142	C	-0.00082
143	C	-0.00030
145	C	-0.00023
149	C	0.00029
153	C	0.00011
155	C	0.00007
159	C	0.00090

Table S12. Mulliken spin populations and SOMO atomic contributions of **7**.



Mulliken spin population:

1	N	0.00199
2	C	0.04526
3	C	0.06568
4	C	0.06368
5	C	-0.00528
6	C	0.00003
7	C	-0.00248
8	C	0.00007
9	C	-0.02068
10	C	0.10953
11	C	-0.04082
12	C	0.11863
13	C	0.00007
14	C	0.00036
15	C	-0.03308
16	C	0.00012
17	C	-0.00014
18	C	0.00349
19	C	0.00065
20	C	-0.00043
21	C	-0.00012
22	C	0.00048

23	C	0.00146
24	C	-0.00001
25	B	0.21673
26	C	0.00006
27	C	0.00017
28	C	-0.00015
29	C	0.00012
30	C	0.00000
31	C	0.00160
32	N	0.00199
33	C	-0.02698
34	C	0.04526
35	C	0.06568
36	C	0.06368
37	C	-0.00528
38	C	0.00003
39	C	-0.00248
40	C	0.00007
41	C	-0.02068
42	C	0.10953
43	C	-0.04082
44	C	0.11863

45	C	0.00007
46	C	0.00036
47	C	-0.03308
48	C	0.00012
49	C	-0.00014
50	C	0.00349
51	C	0.00065
52	C	-0.00043
53	C	-0.00012
54	C	0.00048
55	C	0.00146
56	C	-0.00001
57	B	0.21673
58	C	0.00006
59	C	0.00017
60	C	-0.00015
61	C	0.00012
62	C	0.00000
63	C	0.00160
134	C	-0.02698

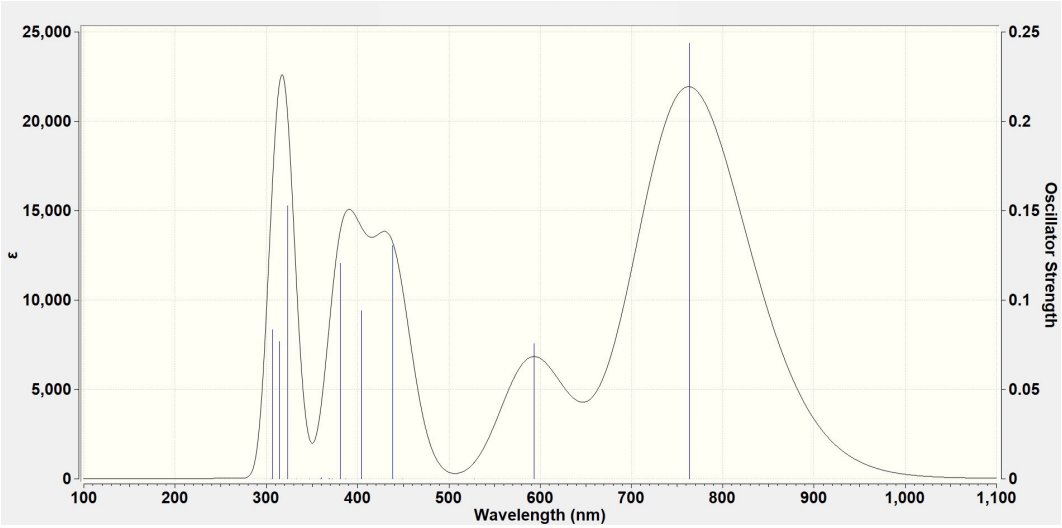


Figure S55. Calculated UV-Vis spectrum of **6** at UCAM-B3LYP/6-311 G(d, p) (PCM, *o*-difluorobenzene) level of theory.

Table S13. TD-DFT description of first 5 electronically excited states in **6**. The highest occupied molecular orbital of **6** is MO 282α.

Excited State 1: 2.136-A 1.6247 eV 763.10 nm f=0.2436 <S**2>=0.890

282α → 283α 0.95711

279β → 282β 0.11719

282α ← 283α 0.10339

Excited State 2: 2.154-A 2.0906 eV 593.06 nm f=0.0755 <S**2>=0.910

282α → 285α -0.12551

282α → 286α 0.11671

281β → 282β 0.93522

Excited State 3: 2.448-A 2.3490 eV 527.81 nm f=0.0000 <S**2>=1.249

281α → 283α 0.25917

282α → 284α -0.25788

282α → 287α -0.21115

282α → 288α -0.10321

282α → 292α 0.11703

269β → 283β 0.10968

280β → 282β 0.78501

281β → 283β -0.20698

Excited State 4: 2.195-A 2.7580 eV 449.54 nm f=0.0000 <S**2>=0.955

281α → 283α	-0.23796
282α → 284α	0.61354
282α → 287α	0.42246
282α → 288α	0.17353
282α → 292α	-0.23573
278β → 282β	-0.12812
280β → 282β	0.48076
281β → 283β	0.10649

Excited State 5: 2.084-A 2.8275 eV 438.49 nm f=0.1306 <S**2>=0.836

280α → 283α	0.17379
282α → 285α	0.68750
282α → 286α	-0.61540
282α → 289α	-0.18986
281β → 282β	0.13440

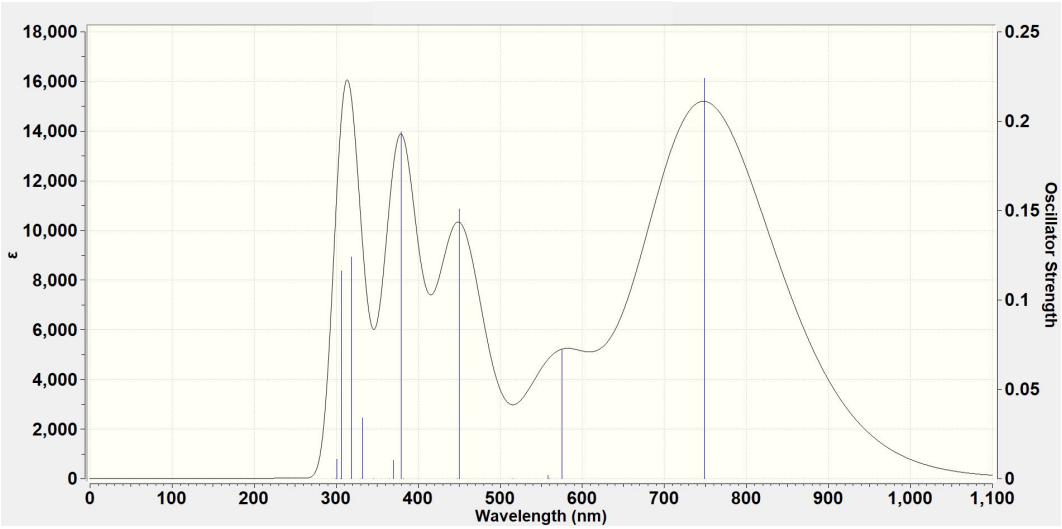


Figure S56. Calculated UV-Vis spectrum of **7** at UCAM-B3LYP/6-311 G(d, p) (PCM, *o*-difluorobenzene) level of theory.

Table S14. TD-DFT description of first 5 electronically excited states in **7**. The highest occupied molecular orbital of **7** is MO 228α.

Excited State 1: 2.142-A 1.6552 eV 749.06 nm f=0.2242 <S**2>=0.897

223α → 238α -0.10259

226α → 232α -0.12209

228α → 229α 0.95574

225β → 228β 0.12110

228α → 229α 0.10049

Excited State 2: 2.153-A 2.1558 eV 575.13 nm f=0.0720 <S**2>=0.909

228α → 232α 0.21207

224β → 231β 0.10695

227β → 228β 0.92268

Excited State 3: 2.082-A 2.2134 eV 560.14 nm f=0.0000 <S**2>=0.833

223α → 231α 0.12002

227α → 231α 0.13911

228α → 230α 0.97245

Excited State 4: 2.082-A 2.2226 eV 557.83 nm f=0.0020 <S**2>=0.834

223α → 230α 0.12071

227α → 230α 0.14066

228α → 231α 0.96476

Excited State 5: 2.474-A 2.4060 eV 515.32 nm f=0.0000 <S**2>=1.280

227α → 229α -0.27840

228α → 233α -0.41234

228α → 235α 0.18840

219β → 231β 0.12090

225β → 231β 0.10804

226β → 228β 0.73081

227β → 231β 0.22617

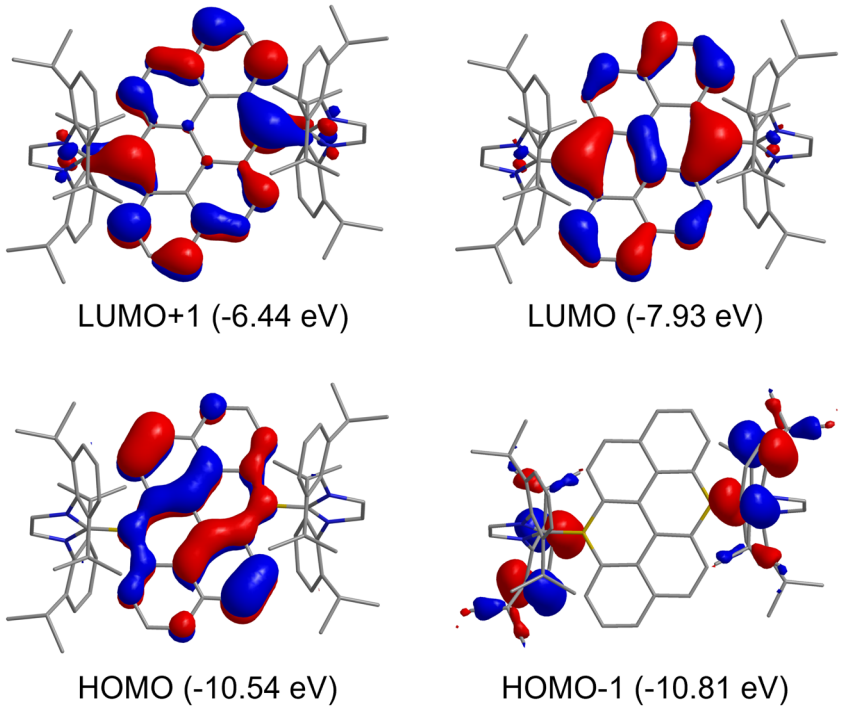


Figure S57. Plots of MOs of **8** (isovalue = 0.03, hydrogen atoms are omitted for clarity).

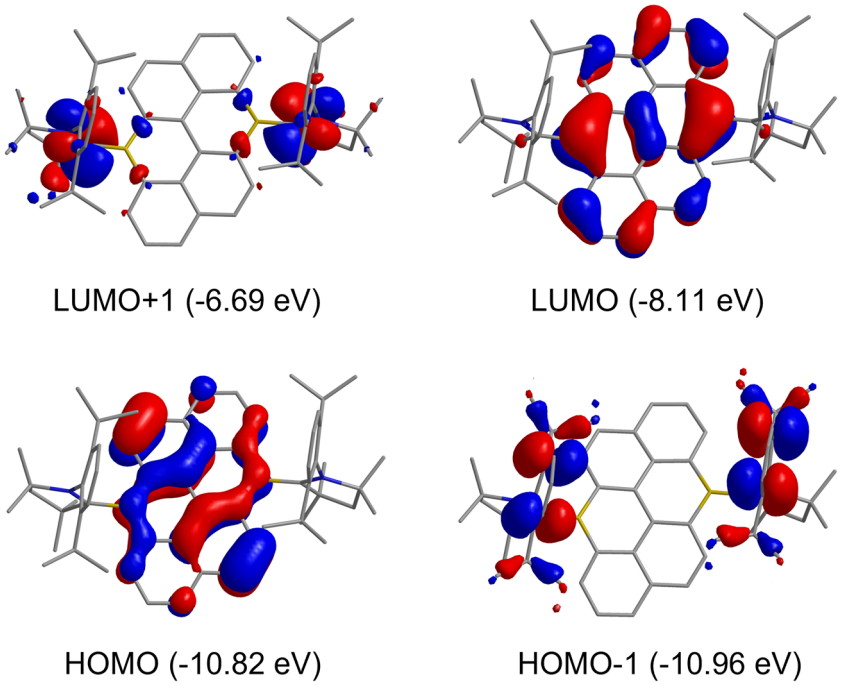


Figure S58. Plots of MOs of **9** (isovalue = 0.03, hydrogen atoms are omitted for clarity).

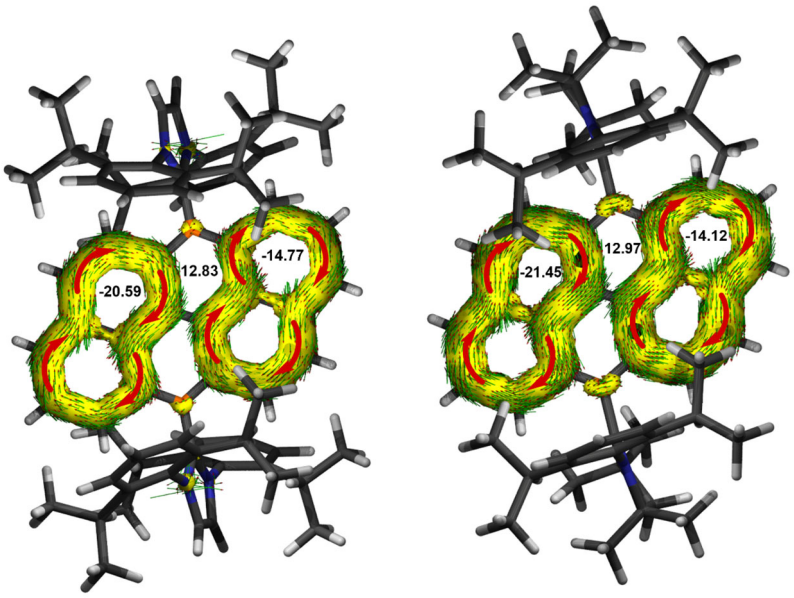


Figure S59. The ACID plots (π-electron only) of **8** (left) and **9** (right) (the external magnetic field is applied orthogonal to the plane, and the red and blue arrows indicate the clockwise (diamagnetic) and counter-clockwise (paramagnetic) current flow, respectively.), and calculated NICS(1)$_{zz}$ values.

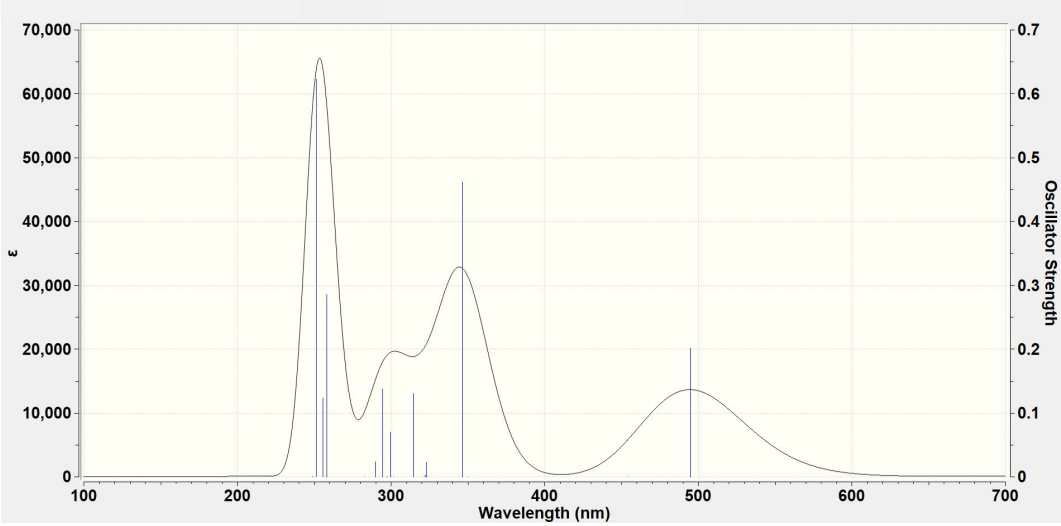


Figure S60. Calculated UV-Vis spectrum of **8** at CAM-B3LYP/6-311 G(d, p) (PCM, *o*-difluorobenzene) level of theory.

Table S15. TD-DFT description of first 5 electronically excited states in **8**. The highest occupied molecular orbital of **8** is MO 281.

Excited State 1:	Singlet-A	2.5060 eV	494.75 nm	f=0.2014	<S**2>=0.000
267 → 282	0.10108				
281 → 282	0.68876				

Excited State 2:	Singlet-A	2.7307 eV	454.04 nm	f=0.0000	<S**2>=0.000
274 → 282	-0.11473				
280 → 282	0.67802				
Excited State 3:	Singlet-A	3.5400 eV	350.23 nm	f=0.0000	<S**2>=0.000
270 → 282	0.38534				
274 → 282	0.50713				
278 → 282	0.18782				
280 → 282	0.14052				
Excited State 4:	Singlet-A	3.5791 eV	346.41 nm	f=0.4623	<S**2>=0.000
271 → 282	0.36114				
275 → 282	0.54111				
279 → 282	0.17322				
Excited State 5:	Singlet-A	3.8362 eV	323.20 nm	f=0.0000	<S**2>=0.000
277 → 282	0.64501				
278 → 282	-0.24284				
279 → 283	0.11695				

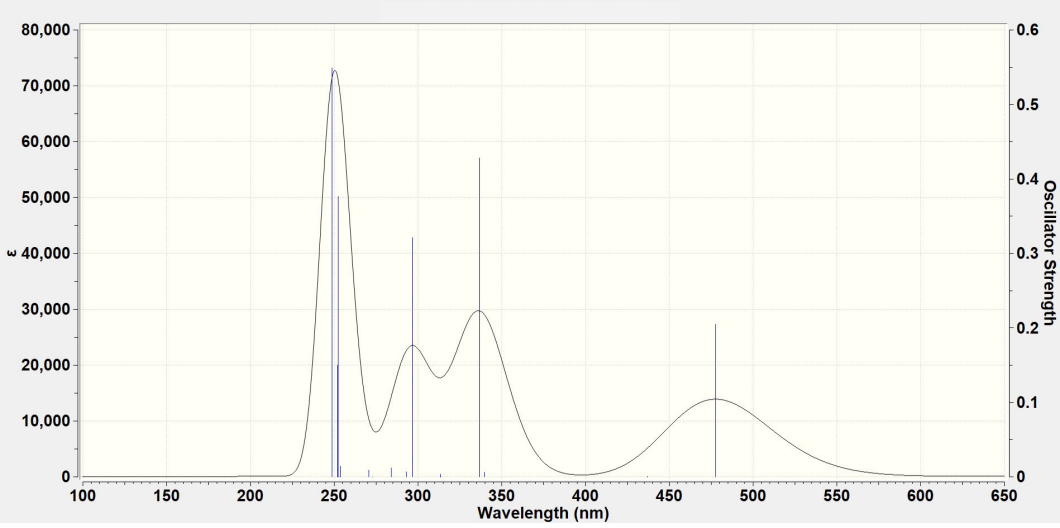


Figure S61. Calculated UV-Vis spectrum of **9** at CAM-B3LYP/6-311 G(d, p) (PCM, *o*-difluorobenzene) level of theory

Table S16. TD-DFT description of first 5 electronically excited states in **9**. The highest occupied molecular orbital of **9** is MO 227.

Excited State 1:	Singlet-A	2.5948 eV	477.82 nm	f=0.2047	<S**2>=0.000
219 → 228	0.10501				
227 → 228	0.68982				
Excited State 2:	Singlet-A	2.8375 eV	436.95 nm	f=0.0006	<S**2>=0.000
226 → 228	0.68064				
Excited State 3:	Singlet-A	3.6511 eV	339.58 nm	f=0.0061	<S**2>=0.000
220 → 228	0.54857				
222 → 228	0.37212				
226 → 228	0.12276				
227 → 233	-0.11014				
Excited State 4:	Singlet-A	3.6819 eV	336.74 nm	f=0.4279	<S**2>=0.000
221 → 228	0.18872				
223 → 228	0.64232				
227 → 232	-0.12653				
Excited State 5:	Singlet-A	3.9528 eV	313.66 nm	f=0.0002	<S**2>=0.000
224 → 228	0.69343				

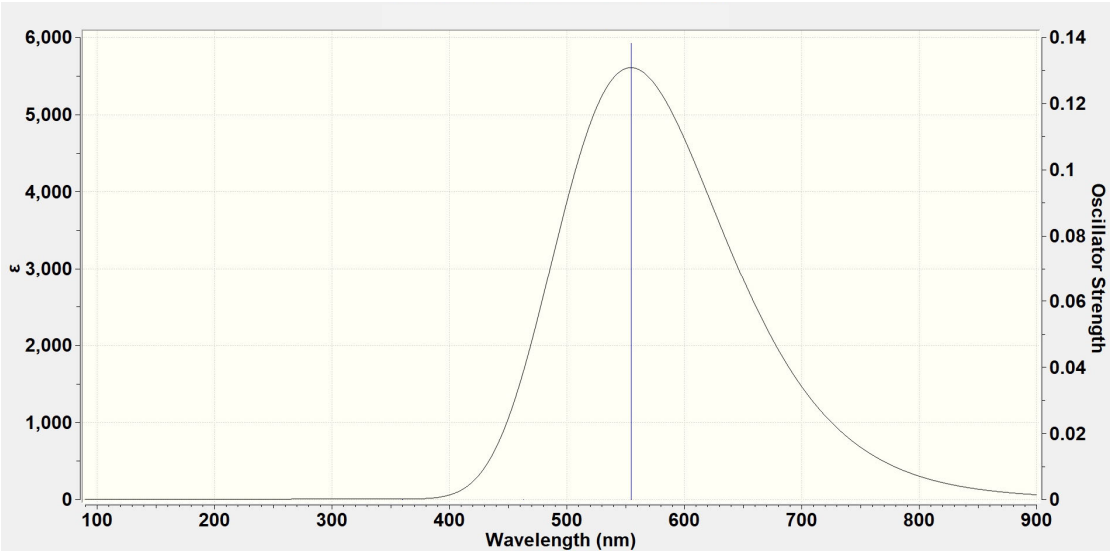


Figure S62. Calculated emission spectrum for **8** at CAM-B3LYP/6-311 G(d, p) level of theory.

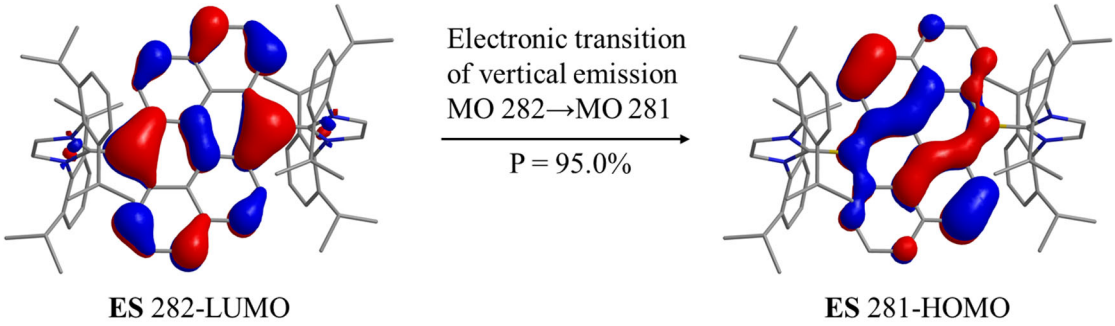


Figure S63. The calculated orbitals HOMO and LUMO of the excited state (ES) most likely involved in the vertical transition of emission for compound **8**.

Table S17. Output for TDDFT excitations for emission of **8**. The highest occupied molecular orbital of **8** is MO 282. Excitation energies and oscillator strengths:

Excited State 1:	**Singlet-A**	**2.2349 eV**	**554.76 nm**	**f=0.1383**	**<S**2>=0.000**
267 → 282	**0.10331**				
281 → 282	**0.68902**				
Excited State 2:	Singlet-A	2.6759 eV	463.33 nm	f=0.0000	<S**2>=0.000
274 → 282	0.14269				
276 → 282	0.60897				
280 → 282	0.27605				
Excited State 3:	Singlet-A	3.4424 eV	360.16 nm	f=0.0000	<S**2>=0.000
270 → 282	-0.40321				
274 → 282	0.41097				
276 → 282	-0.13886				
278 → 282	-0.33083				

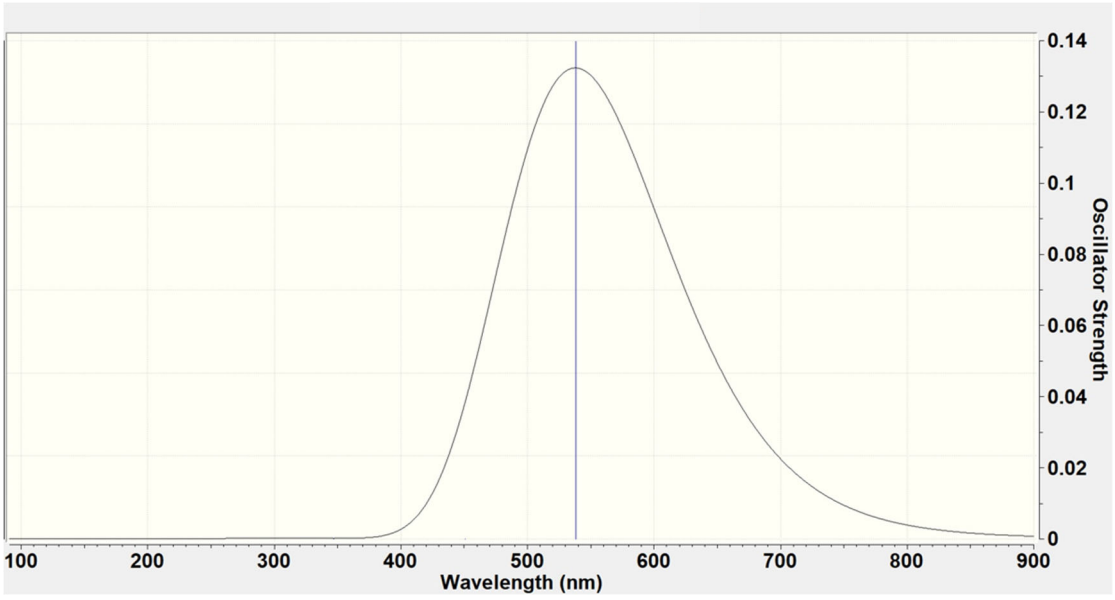


Figure S64. Calculated emission spectrum for **9** at CAM-B3LYP/6-311 G(d, p) level of theory.

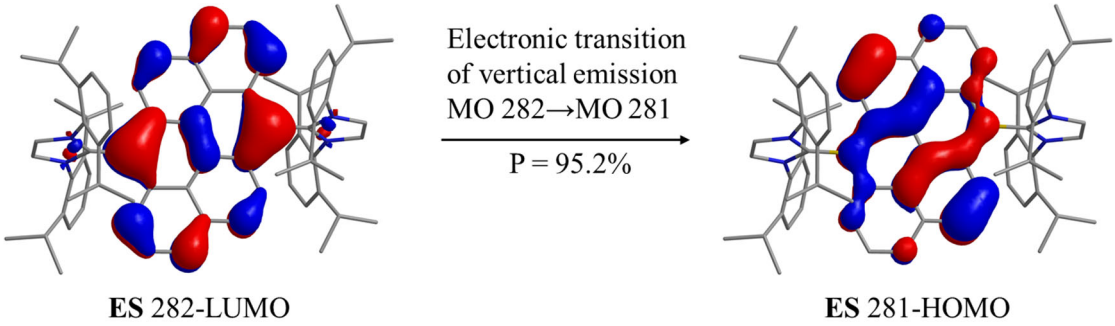


Figure S65. The calculated orbitals HOMO and LUMO of the excited state (ES) most likely involved in the vertical transition of emission for compound **9**.

Table S18. Output for TDDFT excitations for emission of **9**. The highest occupied molecular orbital of **9** is MO 227. Excitation energies and oscillator strengths:

Excited State 1:	**Singlet-A**	**2.3040 eV**	**538.12 nm**	**f=0.1399**	**<S**2>=0.000**
219 → 228	**0.11091**				
227 → 228	**0.68976**				
Excited State 2:	Singlet-A	2.7517 eV	450.57 nm	f=0.0007	<S**2>=0.000
220 → 228	-0.12658				
224 → 228	0.67863				
Excited State 3:	Singlet-A	3.5730 eV	347.01 nm	f=0.0223	<S**2>=0.000
221 → 228	0.16710				
225 → 228	-0.67623				

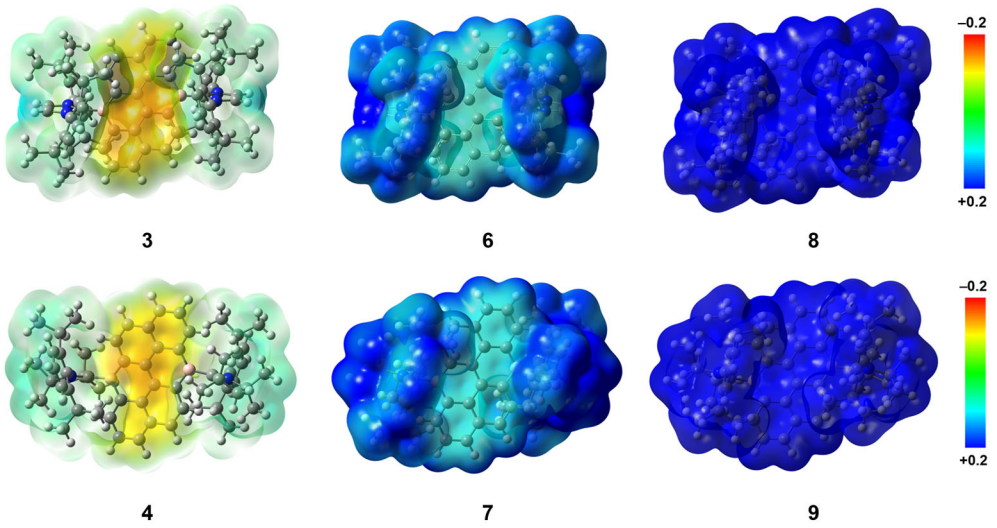
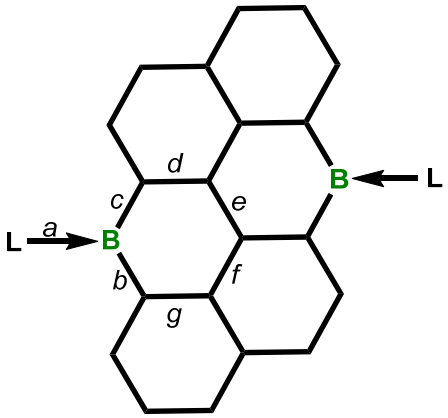


Figure S66. Electrostatic potential (ESP) surfaces (isosurface = 0.002 au) showing charge density distributions in the neutral species **3** and **4**, radicals **6** and **7**, and dications **8** and **9**, reveal that positive charge accumulates significantly over the hexacyclic frameworks upon sequential oxidation.

Table S19. Wiberg bond index values of 3-4 and 6-9



	3	4	6	7	8	9
a	0.891	0.892	0.861	0.849	0.856	0.848
b	1.054	1.038	1.022	1.025	0.981	0.979
c	1.174	1.169	1.063	1.053	0.966	0.954
d	1.200	1.199	1.268	1.267	1.339	1.346
e	1.250	1.252	1.186	1.186	1.127	1.122
f	1.247	1.242	1.235	1.235	1.231	1.229
g	1.233	1.236	1.229	1.227	1.219	1.219

Table S20. Cartesian Coordinates for 3-(closed-shell singlet)

N	5.13313	0.79966	-0.46476	H	-3.15447	-2.90593	-3.89235
N	4.97138	-1.28999	0.11407	C	4.88805	2.18510	-0.83781
C	2.06365	-1.52863	-1.77037	C	-1.10243	-2.57997	-3.33391
H	3.12544	-1.68555	-1.92379	H	-0.69758	-3.19240	-4.13384
C	-0.21732	-1.95038	-2.45377	C	1.19252	-2.12870	-2.61781
C	4.22397	-0.15047	-0.06498	H	1.53968	-2.75096	-3.43716
C	4.53536	-2.60356	0.56588	C	-2.97086	-1.64302	-2.16220
C	1.65474	-0.67286	-0.69854	H	-4.04455	-1.52427	-2.07167
C	6.40610	0.25173	-0.53657	C	4.65130	-3.69337	-0.32562
H	7.25388	0.82977	-0.85393	C	4.12281	-2.77433	1.90256
C	-0.70603	-1.11499	-1.38634	C	4.19806	2.46536	-2.03426
C	0.23277	-0.44529	-0.51674	C	5.44947	3.20725	-0.04059
C	6.30840	-1.03994	-0.16463	C	3.76359	-4.06233	2.30924
H	7.05911	-1.80131	-0.06332	H	3.43298	-4.21777	3.32857
C	-2.13314	-0.97236	-1.24041	C	4.29203	-4.29245	-2.78249
C	-2.47870	-2.42349	-3.19323	H	4.34007	-5.37967	-2.67741

H	4.62486	-4.04996	-3.79578
H	3.25081	-3.98983	-2.67785
C	5.19156	-3.58441	-1.75163
H	5.23057	-2.52876	-2.02750
C	6.30995	2.95572	1.19749
H	6.18865	1.91271	1.49661
C	4.13420	-1.65875	2.93987
H	4.22881	-0.70663	2.42370
C	4.01837	3.80860	-2.37719
H	3.48102	4.05125	-3.28532
C	4.28832	-4.95788	0.14667
H	4.35781	-5.80996	-0.51821
C	3.73051	1.39403	-3.01186
H	3.74849	0.43202	-2.50530
C	3.83565	-5.14352	1.44390
H	3.54949	-6.13272	1.78349
B	2.65285	0.04263	0.15479
C	5.24578	4.52932	-0.44580
H	5.65623	5.33421	0.15128
C	7.80515	3.18647	0.88995
H	8.16412	2.56917	0.06341
H	8.41434	2.95800	1.76940
H	7.98602	4.23025	0.61840
C	2.28506	1.61011	-3.48836
H	1.60281	1.69385	-2.64145
H	1.96318	0.75588	-4.08802
H	2.18885	2.50708	-4.10743
C	5.89603	3.82728	2.39821
H	6.15624	4.87745	2.24053
H	6.42233	3.49546	3.29784
H	4.82403	3.76917	2.58237
C	4.52551	4.83221	-1.59132
H	4.37083	5.86636	-1.87836
C	5.35789	-1.80544	3.86766
H	5.31416	-2.73867	4.43708
H	5.39110	-0.97722	4.58148
H	6.29462	-1.80414	3.30275
C	6.62499	-4.14882	-1.84865
H	7.31669	-3.65875	-1.15968
H	7.01546	-4.02338	-2.86278
H	6.63558	-5.21707	-1.61496
C	2.83018	-1.58658	3.75095
H	1.96400	-1.51053	3.09245
H	2.84033	-0.69843	4.38669
H	2.70288	-2.45954	4.39817
C	4.70166	1.30684	-4.20765
H	4.71579	2.24176	-4.77578
H	4.39324	0.50589	-4.88585
H	5.72530	1.10012	-3.88191
N	-5.13313	-0.79966	0.46476
N	-4.97138	1.28999	-0.11407
C	-2.06365	1.52863	1.77037
H	-3.12544	1.68555	1.92379
C	0.21732	1.95038	2.45377
C	-4.22397	0.15047	0.06498
C	-4.53536	2.60356	-0.56588
C	-1.65474	0.67286	0.69854
C	-6.40610	-0.25173	0.53657
H	-7.25388	-0.82977	0.85393
C	0.70603	1.11499	1.38634
C	-0.23277	0.44529	0.51674
C	-6.30840	1.03994	0.16463
H	-7.05911	1.80131	0.06332
C	2.13314	0.97236	1.24041
C	2.47870	2.42349	3.19323
H	3.15447	2.90593	3.89235
C	-4.88805	-2.18510	0.83781
C	1.10243	2.57997	3.33391
H	0.69758	3.19240	4.13384
C	-1.19252	2.12870	2.61781
H	-1.53968	2.75096	3.43716
C	2.97086	1.64302	2.16219
H	4.04455	1.52427	2.07167
C	-4.65130	3.69337	0.32562
C	-4.12281	2.77433	-1.90256
C	-4.19806	-2.46536	2.03426
C	-5.44947	-3.20725	0.04059
C	-3.76359	4.06233	-2.30924
H	-3.43298	4.21777	-3.32857
C	-4.29203	4.29245	2.78249
H	-4.34007	5.37967	2.67741
H	-4.62486	4.04996	3.79578
H	-3.25081	3.98983	2.67785
C	-5.19156	3.58441	1.75163
H	-5.23057	2.52876	2.02750
C	-6.30995	-2.95572	-1.19749
H	-6.18865	-1.91271	-1.49661
C	-4.13420	1.65875	-2.93986

H	-4.22881	0.70663	-2.42370
C	-4.01836	-3.80860	2.37719
H	-3.48102	-4.05125	3.28532
C	-4.28832	4.95788	-0.14667
H	-4.35781	5.80996	0.51821
C	-3.73051	-1.39403	3.01186
H	-3.74848	-0.43202	2.50530
C	-3.83565	5.14352	-1.44390
H	-3.54949	6.13272	-1.78349
B	-2.65285	-0.04263	-0.15479
C	-5.24577	-4.52932	0.44580
H	-5.65622	-5.33422	-0.15128
C	-7.80515	-3.18647	-0.88995
H	-8.16412	-2.56917	-0.06341
H	-8.41434	-2.95800	-1.76940
H	-7.98602	-4.23025	-0.61840
C	-2.28506	-1.61011	3.48836
H	-1.60281	-1.69385	2.64145
H	-1.96318	-0.75588	4.08802
H	-2.18885	-2.50708	4.10743
C	-5.89603	-3.82728	-2.39821
H	-6.15624	-4.87745	-2.24053
H	-6.42233	-3.49546	-3.29784
H	-4.82403	-3.76917	-2.58237
C	-4.52551	-4.83221	1.59132
H	-4.37083	-5.86637	1.87836
C	-5.35789	1.80544	-3.86766
H	-5.31416	2.73867	-4.43708
H	-5.39110	0.97722	-4.58148
H	-6.29462	1.80414	-3.30275
C	-6.62499	4.14882	1.84865
H	-7.31669	3.65875	1.15968
H	-7.01546	4.02338	2.86278
H	-6.63558	5.21707	1.61497
C	-2.83018	1.58659	-3.75095
H	-1.96400	1.51053	-3.09245
H	-2.84033	0.69843	-4.38669
H	-2.70289	2.45954	-4.39817
C	-4.70166	-1.30684	4.20765
H	-4.71578	-2.24176	4.77578
H	-4.39324	-0.50590	4.88585
H	-5.72530	-1.10012	3.88191

Table S21. Cartesian Coordinates for 3-(triplet)

N	5.18134	0.73808	-0.41349
N	4.93449	-1.37450	0.11159
C	2.02567	-1.66375	-1.66815
H	3.08485	-1.81977	-1.83056
C	-0.25290	-2.13984	-2.29386
C	4.21921	-0.19585	-0.05387
C	4.46206	-2.65329	0.60449
C	1.62147	-0.74926	-0.66215
C	6.43495	0.14066	-0.46609
H	7.31133	0.69063	-0.75409
C	-0.72966	-1.23316	-1.29134
C	0.22643	-0.50049	-0.48636
C	6.28459	-1.15494	-0.13364
H	7.01170	-1.93860	-0.03009
C	-2.15601	-1.07159	-1.14365
C	-2.51626	-2.64566	-3.00691
H	-3.20494	-3.15671	-3.67167
C	4.98439	2.10978	-0.83813
C	-1.16047	-2.83348	-3.13762
H	-0.75941	-3.50137	-3.89323
C	1.13626	-2.32731	-2.46597
H	1.47666	-2.99428	-3.25187
C	-2.99842	-1.78003	-2.01970
H	-4.06851	-1.63193	-1.94671
C	4.56921	-3.78391	-0.23764
C	4.01555	-2.76307	1.93832
C	4.29734	2.37224	-2.04237
C	5.58598	3.14534	-0.08651
C	3.61056	-4.02335	2.38629
H	3.25641	-4.13055	3.40411
C	4.26332	-4.47299	-2.67961
H	4.28691	-5.55607	-2.53199
H	4.62668	-4.27589	-3.69227
H	3.22531	-4.14950	-2.61498
C	5.14793	-3.74221	-1.65192
H	5.21538	-2.69839	-1.96533
C	6.44166	2.91070	1.15823
H	6.28694	1.88307	1.49345

C	4.04972	-1.61171	2.93703
H	4.19396	-0.68337	2.38913
C	4.16427	3.70583	-2.43769
H	3.63422	3.93192	-3.35460
C	4.16427	-5.01957	0.27556
H	4.23018	-5.90007	-0.35190
C	3.79103	1.28154	-2.97979
H	3.79062	0.33646	-2.44129
C	3.67397	-5.14099	1.56659
H	3.35433	-6.10804	1.93862
B	2.67114	0.04513	0.13740
C	5.43125	4.45744	-0.54458
H	5.87772	5.26936	0.01647
C	7.94320	3.08217	0.84259
H	8.27982	2.42854	0.03499
H	8.54701	2.86134	1.72777
H	8.15745	4.11055	0.53823
C	2.34732	1.52131	-3.45110
H	1.67436	1.65635	-2.60323
H	1.99495	0.65747	-4.01961
H	2.27048	2.39935	-4.09920
C	6.06096	3.83755	2.32823
H	6.35330	4.87269	2.13211
H	6.57876	3.52191	3.23857
H	4.98840	3.82308	2.51713
C	4.71485	4.74190	-1.69653
H	4.59828	5.76856	-2.02546
C	5.24790	-1.77393	3.89520
H	5.15551	-2.68372	4.49583
H	5.30128	-0.92273	4.58040
H	6.19397	-1.82984	3.34935
C	6.57142	-4.33829	-1.68999
H	7.25408	-3.83927	-0.99876
H	6.99248	-4.25616	-2.69637
H	6.55266	-5.39786	-1.41966
C	2.73446	-1.46082	3.71885
H	1.88355	-1.36986	3.04232
H	2.76917	-0.55627	4.33061
H	2.55773	-2.30827	4.38784
C	4.74681	1.12719	-4.18103
H	4.77964	2.04107	-4.78164
H	4.41132	0.31140	-4.82820
H	5.76732	0.90515	-3.85636
N	-5.18135	-0.73807	0.41348
N	-4.93449	1.37450	-0.11158
C	-2.02567	1.66375	1.66815
H	-3.08485	1.81977	1.83056
C	0.25290	2.13983	2.29387
C	-4.21921	0.19585	0.05387
C	-4.46205	2.65330	-0.60448
C	-1.62147	0.74926	0.66216
C	-6.43495	-0.14065	0.46608
H	-7.31133	-0.69062	0.75408
C	0.72967	1.23315	1.29134
C	-0.22643	0.50049	0.48636
C	-6.28458	1.15494	0.13365
H	-7.01169	1.93861	0.03010
C	2.15601	1.07159	1.14365
C	2.51626	2.64565	3.00691
H	3.20494	3.15670	3.67167
C	-4.98439	-2.10978	0.83812
C	1.16048	2.83348	3.13763
H	0.75941	3.50136	3.89324
C	-1.13626	2.32730	2.46598
H	-1.47665	2.99427	3.25188
C	2.99843	1.78002	2.01970
H	4.06852	1.63193	1.94671
C	-4.56920	3.78392	0.23766
C	-4.01554	2.76308	-1.93831
C	-4.29735	-2.37225	2.04235
C	-5.58600	-3.14533	0.08650
C	-3.61055	4.02335	-2.38628
H	-3.25640	4.13056	-3.40409
C	-4.26331	4.47298	2.67962
H	-4.28690	5.55607	2.53200
H	-4.62667	4.27589	3.69229
H	-3.22530	4.14949	2.61499
C	-5.14792	3.74221	1.65194
H	-5.21537	2.69839	1.96534
C	-6.44167	-2.91069	-1.15825
H	-6.28695	-1.88306	-1.49346
C	-4.04971	1.61172	-2.93702
H	-4.19396	0.68337	-2.38913
C	-4.16428	-3.70584	2.43767
H	-3.63424	-3.93194	3.35459
C	-4.16426	5.01957	-0.27554
H	-4.23017	5.90007	0.35191
C	-3.79104	-1.28156	2.97978

H	-3.79062	-0.33648	2.44129	C	-4.71487	-4.74191	1.69651
C	-3.67396	5.14100	-1.56658	H	-4.59831	-5.76857	2.02543
H	-3.35433	6.10805	-1.93860	C	-5.24789	1.77394	-3.89520
B	-2.67114	-0.04513	-0.13740	H	-5.15550	2.68374	-4.49582
C	-5.43127	-4.45744	0.54456	H	-5.30127	0.92275	-4.58040
H	-5.87775	-5.26935	-0.01649	H	-6.19396	1.82986	-3.34934
C	-7.94321	-3.08215	-0.84262	C	-6.57141	4.33830	1.69001
H	-8.27983	-2.42853	-0.03501	H	-7.25407	3.83927	0.99877
H	-8.54702	-2.86132	-1.72779	H	-6.99247	4.25617	2.69638
H	-8.15747	-4.11053	-0.53825	H	-6.55265	5.39787	1.41968
C	-2.34733	-1.52134	3.45109	C	-2.73445	1.46083	-3.71883
H	-1.67436	-1.65637	2.60321	H	-1.88354	1.36987	-3.04231
H	-1.99495	-0.65750	4.01960	H	-2.76916	0.55628	-4.33060
H	-2.27048	-2.39938	4.09918	H	-2.55771	2.30828	-4.38782
C	-6.06098	-3.83753	-2.32825	C	-4.74681	-1.12721	4.18102
H	-6.35331	-4.87267	-2.13214	H	-4.77965	-2.04109	4.78163
H	-6.57877	-3.52189	-3.23859	H	-4.41131	-0.31142	4.82820
H	-4.98842	-3.82307	-2.51715	H	-5.76732	-0.90516	3.85636

Table S22. Cartesian Coordinates for 4-(closed-shell singlet)

N	5.12015	-0.16137	0.59599	C	6.24703	0.79505	-2.85710
C	5.31995	-0.22715	-0.86733	C	5.80682	2.35195	-0.98029
C	4.08226	0.33086	1.25685	C	4.45754	0.52627	2.73915
C	6.31639	-0.53551	1.49510	H	-0.21962	-5.15305	1.03311
C	0.07180	-3.04962	0.73324	H	1.77961	-4.00200	1.67719
C	-0.48129	-1.80100	0.26928	H	-2.53086	-5.16041	0.10137
C	-0.67092	-4.23356	0.67314	C	3.33181	0.13323	3.71127
C	1.39980	-3.07167	1.26462	C	4.81439	2.00840	3.02546
C	5.19153	-1.45217	-1.57021	C	5.69097	-0.38818	2.89144
C	5.80565	0.92891	-1.53677	H	3.17288	-2.02015	1.63073
C	0.32459	-0.60217	0.31102	H	6.62427	1.67018	-3.37114
C	1.71801	-0.69990	0.70505	C	6.20047	-0.41425	-3.52781
C	-0.24275	0.67148	-0.04125	H	5.55353	-2.44445	-3.43180
C	-1.83731	-1.80466	-0.22038	H	6.55987	-0.49199	-4.54781
C	-2.52521	-3.04349	-0.26148	H	4.24260	-2.55521	-0.00433
B	-2.47637	-0.45935	-0.57570	C	3.13286	-2.85199	-1.80153
C	2.16817	-1.95626	1.22625	C	5.29632	-3.99367	-1.19299
B	2.59307	0.52445	0.72107	H	5.46825	2.32442	0.05486
H	-3.54743	-3.06811	-0.62528	C	4.80389	3.21316	-1.77764
C	-1.96493	-4.23569	0.15911	C	7.19078	3.03183	-1.01194
C	5.64996	-1.51161	-2.89075	C	7.50593	0.40475	1.27047
C	4.47542	-2.69677	-1.05601	C	6.78050	-1.97146	1.24621

H	5.13683	3.33072	-2.81263
H	4.72333	4.20933	-1.33601
H	3.80873	2.77082	-1.78323
C	1.92657	1.86980	0.46893
H	3.30132	-3.03521	-2.86698
H	2.51690	-1.95878	-1.69646
H	2.57006	-3.69356	-1.39270
H	5.44696	-4.26841	-2.24032
H	4.75577	-4.81853	-0.72035
H	6.27976	-3.92303	-0.72477
H	8.31202	0.11200	1.94774
H	7.25978	1.44540	1.47359
H	7.88277	0.32501	0.25032
H	7.20906	-2.09322	0.25103
H	5.96988	-2.68782	1.37550
H	7.55840	-2.20913	1.97724
H	7.95987	2.45483	-0.49800
H	7.12939	4.01437	-0.53505
H	7.52977	3.19370	-2.03836
H	3.68280	0.27066	4.73905
H	3.02617	-0.90558	3.58857
H	2.45099	0.75849	3.55945
H	3.92868	2.63925	2.96815
H	5.56582	2.40970	2.34382
H	5.21464	2.07454	4.04144
H	6.41114	0.00400	3.61214
H	5.36933	-1.36909	3.25090
N	-5.13178	-0.25605	-0.64849
C	-5.42593	0.38046	0.65019
C	-3.94431	-0.50761	-1.18872
C	-6.31315	-0.85114	-1.44868
C	-0.05224	3.14496	-0.27909
C	0.54656	1.87648	0.05025
C	0.66098	4.33759	-0.11713
C	-1.39315	3.18212	-0.77586
C	-5.88710	1.72611	0.68609
C	-5.36768	-0.38311	1.84397
C	-1.62602	0.76289	-0.46516
C	2.58623	3.11404	0.60894
C	-2.12291	2.04319	-0.86276
H	3.62385	3.12457	0.91449
C	1.97217	4.32586	0.34760
C	-6.36451	2.22805	1.90183
C	-5.81978	2.74278	-0.45903
C	-5.84746	0.19064	3.02600
C	-4.75030	-1.77042	1.97225
C	-4.15642	-0.95455	-2.64639
H	0.17173	5.27563	-0.36106
H	-1.80885	4.14133	-1.06908
H	2.51422	5.25691	0.48187
C	-4.05612	0.34894	-3.49089
C	-3.14511	-1.94314	-3.24185
C	-5.58822	-1.51285	-2.63743
H	-3.13331	2.09622	-1.24971
H	-5.80273	-0.38890	3.93959
C	-6.36761	1.47178	3.06045
H	-6.72294	3.24921	1.93880
H	-6.74657	1.88789	3.98720
H	-5.42275	2.24471	-1.34445
C	-4.85434	3.89237	-0.08821
C	-7.17964	3.37704	-0.82293
H	-4.47180	-2.12238	0.98344
C	-3.45309	-1.69531	2.80431
C	-5.70525	-2.81052	2.59025
C	-7.03642	-1.89742	-0.59305
C	-7.33583	0.19169	-1.89737
H	-3.67113	-1.43002	3.84341
H	-2.94803	-2.66378	2.79589
H	-2.76292	-0.95689	2.39679
H	-5.29989	4.53577	0.67524
H	-3.90417	3.52584	0.29269
H	-4.65641	4.51383	-0.96676
H	-7.56450	3.97451	0.00731
H	-7.05226	4.05353	-1.67322
H	-7.94539	2.64973	-1.08634
H	-7.81496	-2.36241	-1.20385
H	-6.35698	-2.68149	-0.25996
H	-7.51505	-1.44971	0.27914
H	-7.83365	0.64427	-1.04139
H	-6.89843	0.97540	-2.51407
H	-8.09967	-0.31468	-2.49309
H	-6.65615	-2.87582	2.05771
H	-5.23423	-3.79717	2.56622
H	-5.92722	-2.58338	3.63647
H	-4.76450	1.11483	-3.17208
H	-3.05179	0.77010	-3.43053
H	-4.26779	0.10452	-4.53562
H	-2.12719	-1.55916	-3.16391

H	-3.17147	-2.91511	-2.75355	H	-5.55266	-2.59561	-2.49318
H	-3.38059	-2.08418	-4.30132	H	-6.11145	-1.32634	-3.57762

Table S23. Cartesian Coordinates for 4-(triplet)

N	4.97900	-0.20867	0.08753	C	4.74410	-4.01318	-1.68835
C	4.62968	-0.25659	-1.32806	H	4.99812	2.27621	-0.48821
C	4.28462	0.50480	1.05219	C	3.62626	3.18442	-1.85086
C	6.40236	-0.53594	0.50572	C	6.12471	3.06378	-2.13761
C	0.36865	-3.01411	1.94301	C	7.44062	0.32158	-0.23876
C	-0.28536	-1.86559	1.40009	C	6.77007	-2.00548	0.27808
C	-0.39817	-4.14234	2.32136	H	3.49092	3.33719	-2.92540
C	1.77826	-2.99625	2.10299	H	3.71396	4.16902	-1.38296
C	4.31050	-1.48903	-1.96184	H	2.72838	2.70681	-1.45930
C	4.70962	0.92693	-2.11838	C	1.90717	1.90191	1.24586
C	0.47034	-0.66310	1.15964	H	2.20852	-3.27792	-2.46885
C	1.87842	-0.70145	1.24388	H	1.82639	-2.21728	-1.10523
C	-0.24955	0.60843	0.99336	H	2.13683	-3.93214	-0.82597
C	-1.68344	-1.93193	1.11101	H	4.51000	-4.28358	-2.72166
C	-2.39032	-3.05900	1.52640	H	4.48495	-4.87405	-1.06483
B	-2.36801	-0.71699	0.41330	H	5.82247	-3.86447	-1.62299
C	2.49344	-1.89771	1.72075	H	8.44335	0.04464	0.09750
B	2.72555	0.59378	1.11087	H	7.31001	1.38600	-0.05731
H	-3.46139	-3.09986	1.35852	H	7.38959	0.14618	-1.31506
C	-1.76325	-4.15241	2.14741	H	6.83458	-2.24107	-0.78419
C	4.20272	-1.52463	-3.35697	H	6.05721	-2.68166	0.75024
C	3.94069	-2.77936	-1.23230	H	7.75406	-2.19289	0.71829
C	4.57386	0.82450	-3.50570	H	7.04214	2.49007	-2.00036
C	4.88712	2.34108	-1.56878	H	6.25179	4.03203	-1.64364
C	5.23524	0.83563	2.22223	H	6.01495	3.25920	-3.20780
H	0.11056	-4.99436	2.76131	H	5.28557	0.80125	4.39758
H	2.27302	-3.86648	2.52372	H	4.13834	-0.35467	3.70123
H	-2.35041	-5.00759	2.46531	H	3.74743	1.36653	3.73324
C	4.55779	0.64744	3.59377	H	5.12522	3.00764	2.53245
C	5.85170	2.26136	2.21085	H	6.23527	2.56004	1.23550
C	6.34198	-0.22581	2.01009	H	6.68470	2.29731	2.92076
H	3.57007	-1.90666	1.83606	H	7.31197	0.10069	2.39197
H	4.64709	1.72359	-4.10584	H	6.06893	-1.13698	2.55023
C	4.35306	-0.38997	-4.13380	N	-4.75296	-0.45996	-0.82293
H	3.97152	-2.46702	-3.83876	C	-5.29892	0.67878	-0.11355
H	4.27124	-0.44532	-5.21373	C	-3.51092	-1.02774	-0.60416
H	4.11325	-2.63047	-0.16922	C	-5.67258	-1.32291	-1.68107
C	2.43512	-3.06467	-1.42001	C	-0.26795	3.07032	1.26118

C	0.46992	1.84657	1.17062
C	0.40519	4.29886	1.46218
C	-1.67689	3.04570	1.13701
C	-5.40060	1.92926	-0.78238
C	-5.73234	0.55343	1.23141
C	-1.65175	0.63115	0.76029
C	2.50779	3.15587	1.37927
C	-2.32684	1.87658	0.85725
H	3.58582	3.21909	1.35969
C	1.77838	4.34444	1.51615
C	-5.98008	3.00503	-0.10314
C	-4.85030	2.20481	-2.18375
C	-6.29586	1.67048	1.85766
C	-5.57775	-0.71091	2.07583
C	-3.29790	-2.02564	-1.77195
H	-0.18527	5.20550	1.54894
H	-2.23055	3.97418	1.23632
H	2.29509	5.28966	1.64471
C	-2.67812	-1.20935	-2.94211
C	-2.40307	-3.25773	-1.58279
C	-4.73468	-2.47032	-2.09979
H	-3.39773	1.89954	0.73985
H	-6.62753	1.58505	2.88566
C	-6.43335	2.88295	1.20149
H	-6.06096	3.96248	-0.60409
H	-6.87763	3.73235	1.70861
H	-4.54868	1.25353	-2.61285
C	-3.59084	3.09331	-2.15159
C	-5.89686	2.84472	-3.11807
H	-5.15698	-1.49064	1.44197
C	-4.59071	-0.48543	3.23954
C	-6.92340	-1.21847	2.63124
C	-6.85047	-1.85664	-0.85057
C	-6.26204	-0.60143	-2.90138
H	-4.97708	0.25607	3.94482
H	-4.43529	-1.41911	3.78709
H	-3.61892	-0.13956	2.88623
H	-3.80098	4.06488	-1.69457
H	-2.77950	2.62989	-1.59215
H	-3.24150	3.27490	-3.17273
H	-6.11530	3.87506	-2.82422
H	-5.51355	2.87649	-4.14208
H	-6.84153	2.29840	-3.12782
H	-7.45231	-2.52208	-1.47568
H	-6.50561	-2.42898	0.01018
H	-7.49759	-1.04897	-0.50249
H	-6.87484	0.24967	-2.60554
H	-5.50007	-0.26573	-3.60363
H	-6.91090	-1.30340	-3.43188
H	-7.66426	-1.37305	1.84523
H	-6.77772	-2.16921	3.15261
H	-7.34725	-0.51470	3.35273
H	-2.63181	-1.82760	-3.84487
H	-3.25110	-0.31121	-3.17289
H	-1.66203	-0.89772	-2.69041
H	-1.37754	-2.99045	-1.32742
H	-2.77582	-3.93060	-0.81234
H	-2.37938	-3.80878	-2.52916
H	-4.96777	-3.36788	-1.52042
H	-4.85700	-2.72464	-3.15561

Table 24. Cartesian Coordinates for 6

N	-4.97943	1.28240	-0.09306
C	-0.22554	-1.78860	-2.56860
N	-5.12958	-0.80502	0.49426
C	-5.60996	1.98536	-3.75466
H	-5.74303	1.19788	-4.50171
H	-5.57236	2.94350	-4.28002
H	-6.49363	1.99433	-3.11087
C	-4.31761	1.74381	-2.94640
H	-4.41499	0.77293	-2.46382
C	-4.17320	2.80874	-1.86572
C	-4.53138	2.60587	-0.51831
C	-4.23776	0.14783	0.08648
B	-2.65355	-0.03975	-0.14646
C	-2.13307	-0.88800	-1.29810
C	-0.71040	-1.02108	-1.45892
C	-1.12425	-2.37338	-3.48106
H	-0.72359	-2.93860	-4.31593
C	-2.49021	-2.23401	-3.32066
H	-3.17251	-2.68336	-4.03287
C	-6.40203	-0.26201	0.57440
H	-7.24487	-0.84378	0.89855
C	-6.31192	1.02918	0.19194
H	-7.06486	1.78879	0.09192
C	-3.76506	4.09345	-2.23619

H	-3.47538	4.27935	-3.26250
C	-3.74636	5.13779	-1.32441
H	-3.42584	6.12524	-1.63606
C	-4.16571	4.92433	-0.01949
H	-4.17837	5.75465	0.67504
C	-4.57722	3.66261	0.41811
C	-3.09656	1.66002	-3.87691
H	-2.17401	1.51860	-3.31134
H	-2.99085	2.55800	-4.49114
H	-3.20570	0.81157	-4.55620
C	-5.11341	3.52770	1.84328
H	-5.16437	2.46634	2.09791
C	-4.21371	4.20964	2.89131
H	-3.16988	3.91778	2.77913
H	-4.54496	3.93928	3.89747
H	-4.26685	5.29858	2.81814
C	-6.54275	4.10291	1.94789
H	-7.23741	3.63541	1.24689
H	-6.54197	5.17548	1.73712
H	-6.93671	3.95961	2.95767
C	-2.97520	-1.50791	-2.23656
H	-4.04735	-1.40908	-2.12277
C	1.17312	-1.96180	-2.75349
H	1.51728	-2.54195	-3.60277
C	2.05152	-1.40582	-1.87663
H	3.11147	-1.55766	-2.03514
C	1.63599	-0.61471	-0.76652
C	0.23227	-0.40874	-0.55459
C	-4.87666	-2.20435	0.82735
C	-5.40151	-3.20276	-0.02300
C	-5.16563	-4.53397	0.33066
H	-5.54521	-5.32467	-0.30391
C	-4.46037	-4.86497	1.47839
H	-4.28528	-5.90569	1.72570
C	-4.00430	-3.86403	2.32247
H	-3.49032	-4.13341	3.23623
C	-4.21423	-2.51277	2.03198
C	-3.82667	-1.46855	3.07246
H	-3.83213	-0.48883	2.59795
C	-2.41490	-1.68035	3.64308
H	-1.66919	-1.73881	2.84841
H	-2.35139	-2.59116	4.24414
H	-2.14832	-0.84243	4.29104
C	-4.87741	-1.43625	4.20244
H	-4.62908	-0.65773	4.92921
H	-4.91403	-2.39162	4.73294
H	-5.87995	-1.23214	3.81682
C	-6.26516	-2.92031	-1.25218
H	-6.15430	-1.86718	-1.52164
C	-7.75752	-3.16928	-0.94262
H	-8.11617	-2.58015	-0.09596
H	-7.92986	-4.22147	-0.70175
H	-8.37247	-2.91882	-1.81123
C	-5.85556	-3.75583	-2.47989
H	-4.78334	-3.70267	-2.66685
H	-6.38191	-3.39480	-3.36748
H	-6.12161	-4.80830	-2.35577
N	4.97943	-1.28240	0.09306
C	0.22554	1.78860	2.56860
N	5.12959	0.80502	-0.49426
C	5.60996	-1.98536	3.75466
H	5.74303	-1.19788	4.50171
H	5.57235	-2.94350	4.28002
H	6.49363	-1.99433	3.11087
C	4.31761	-1.74381	2.94640
H	4.41499	-0.77293	2.46382
C	4.17320	-2.80874	1.86572
C	4.53138	-2.60587	0.51831
C	4.23776	-0.14783	-0.08648
B	2.65355	0.03975	0.14646
C	2.13307	0.88800	1.29809
C	0.71040	1.02108	1.45892
C	1.12425	2.37338	3.48106
H	0.72359	2.93860	4.31593
C	2.49021	2.23401	3.32066
H	3.17251	2.68336	4.03287
C	6.40203	0.26201	-0.57440
H	7.24487	0.84378	-0.89855
C	6.31192	-1.02918	-0.19194
H	7.06486	-1.78879	-0.09192
C	3.76506	-4.09345	2.23619
H	3.47538	-4.27935	3.26250
C	3.74636	-5.13779	1.32441
H	3.42583	-6.12524	1.63606
C	4.16571	-4.92433	0.01949
H	4.17837	-5.75465	-0.67504
C	4.57722	-3.66261	-0.41811
C	3.09656	-1.66002	3.87691

H	2.17401	-1.51860	3.31134
H	2.99085	-2.55800	4.49114
H	3.20570	-0.81157	4.55620
C	5.11341	-3.52770	-1.84328
H	5.16437	-2.46634	-2.09791
C	4.21371	-4.20964	-2.89131
H	3.16988	-3.91778	-2.77913
H	4.54496	-3.93928	-3.89747
H	4.26685	-5.29858	-2.81814
C	6.54275	-4.10292	-1.94789
H	7.23741	-3.63541	-1.24689
H	6.54197	-5.17548	-1.73712
H	6.93671	-3.95961	-2.95767
C	2.97520	1.50791	2.23656
H	4.04735	1.40908	2.12277
C	-1.17312	1.96180	2.75348
H	-1.51728	2.54195	3.60277
C	-2.05152	1.40582	1.87663
H	-3.11147	1.55766	2.03514
C	-1.63599	0.61471	0.76652
C	-0.23227	0.40874	0.55459
C	4.87666	2.20435	-0.82735
C	5.40151	3.20276	0.02300
C	5.16563	4.53397	-0.33065
H	5.54521	5.32467	0.30391
C	4.46038	4.86498	-1.47839
H	4.28528	5.90569	-1.72570
C	4.00430	3.86403	-2.32247
H	3.49032	4.13341	-3.23622
C	4.21423	2.51277	-2.03198
C	3.82667	1.46855	-3.07245
H	3.83213	0.48883	-2.59795
C	2.41490	1.68035	-3.64308
H	1.66919	1.73881	-2.84841
H	2.35139	2.59117	-4.24414
H	2.14832	0.84243	-4.29104
C	4.87741	1.43625	-4.20244
H	4.62908	0.65773	-4.92921
H	4.91403	2.39163	-4.73294
H	5.87995	1.23214	-3.81682
C	6.26516	2.92031	1.25218
H	6.15430	1.86718	1.52164
C	7.75752	3.16928	0.94262
H	8.11617	2.58015	0.09596
H	7.92987	4.22146	0.70175
H	8.37247	2.91882	1.81123
C	5.85557	3.75583	2.47989
H	4.78335	3.70266	2.66685
H	6.38191	3.39480	3.36748
H	6.12161	4.80829	2.35577

Table S25. Cartesian Coordinates for 7

N	5.10172	0.30811	0.69244
C	0.22522	0.64696	0.24173
C	1.56147	0.81284	0.73661
C	1.11604	3.16890	1.23651
C	4.01301	-0.09313	1.30377
C	5.38240	0.35423	-0.76391
C	-0.65536	1.78979	0.20510
C	5.10391	4.08654	-1.14272
C	-0.18242	3.06227	0.66750
C	-0.98743	4.21206	0.55284
C	-2.00383	1.71282	-0.29201
C	-2.74899	2.90083	-0.39212
C	5.15619	1.54578	-1.49820
C	5.32426	-3.16099	-1.60573
C	-2.25253	4.13983	0.00181
C	6.23357	0.75245	1.66329
C	5.64102	1.61505	-2.80841
C	4.27106	-0.21870	2.81702
C	6.01940	-0.75997	-1.37504
C	4.34686	2.74875	-1.02275
C	3.02667	2.83229	-1.81797
C	6.32376	0.56535	-3.39529
C	5.51237	0.67044	3.01904
C	6.16745	-2.16281	-0.78138
B	2.54044	-0.35257	0.71092
C	6.67405	2.18330	1.35206
C	7.45511	-0.16323	1.57677
C	6.48636	-0.61057	-2.68503
C	4.57885	-1.71029	3.12574
C	7.62185	-2.67661	-0.73880
C	3.10607	0.19697	3.73050
N	-5.10176	-0.30813	-0.69245

C	-1.93713	-2.08624	-1.25932
C	-0.22525	-0.64697	-0.24171
C	-1.56150	-0.81285	-0.73659
C	-1.11607	-3.16890	-1.23652
C	-4.01304	0.09313	-1.30376
C	-5.38243	-0.35425	0.76390
C	0.65533	-1.78980	-0.20510
C	-5.10385	-4.08656	1.14277
C	0.18239	-3.06227	-0.66752
C	0.98742	-4.21206	-0.55288
C	2.00380	-1.71283	0.29201
C	2.74897	-2.90084	0.39209
C	-5.15619	-1.54580	1.49820
C	-5.32425	3.16097	1.60586
C	2.25251	-4.13984	-0.00186
C	-6.23359	-0.75245	-1.66331
C	-5.64099	-1.61506	2.80842
C	-4.27106	0.21869	-2.81701
C	-6.01939	0.75996	1.37505
C	-4.34684	-2.74875	1.02275
C	-3.02664	-2.83223	1.81795
C	-6.32372	-0.56535	3.39531
C	-5.51238	-0.67043	-3.01905
C	-6.16738	2.16282	0.78141
B	-2.54047	0.35256	-0.71090
C	-6.67409	-2.18330	-1.35212
C	-7.45514	0.16324	-1.57680
C	-6.48632	0.61057	2.68505
C	-4.57883	1.71030	-3.12573
C	-7.62177	2.67663	0.73872
C	-3.10607	-0.19698	-3.73048
H	1.43916	4.12663	1.63089
H	5.27432	4.35962	-2.18671
H	6.07392	4.06865	-0.64420
H	4.50844	4.88693	-0.69518
H	-0.59117	5.16081	0.89886
H	-3.75555	2.85675	-0.78424
H	5.75684	-3.29883	-2.59952
H	4.29621	-2.82469	-1.72981
H	5.30915	-4.13852	-1.11646
H	-2.85894	5.03237	-0.10088
H	5.47206	2.51981	-3.37800
H	4.08951	2.60487	0.02398
H	3.22418	3.02341	-2.87598
H	2.40843	3.64816	-1.43780
H	2.45101	1.90948	-1.74085
H	6.70510	0.65361	-4.40589
H	5.19517	1.66966	3.32752
H	6.17099	0.28377	3.79801
H	5.78042	-2.15661	0.23859
H	7.15216	2.25988	0.37528
H	7.40646	2.48111	2.10661
H	5.84250	2.88542	1.40047
H	7.91961	-0.10465	0.59338
H	7.22448	-1.20317	1.80099
H	8.18911	0.18083	2.30887
H	6.97990	-1.44850	-3.16027
H	3.69324	-2.33121	2.99151
H	4.88583	-1.78296	4.17189
H	5.38321	-2.11792	2.51237
H	8.02279	-2.80584	-1.74661
H	7.65129	-3.65626	-0.25394
H	8.29771	-2.01525	-0.19884
H	2.84225	1.24788	3.62293
H	3.40327	0.03005	4.76931
H	2.21225	-0.39799	3.53596
H	-1.43918	-4.12663	-1.63092
H	-5.27422	-4.35963	2.18677
H	-6.07388	-4.06870	0.64428
H	-4.50837	-4.88694	0.69522
H	0.59116	-5.16081	-0.89892
H	3.75553	-2.85676	0.78420
H	-5.75693	3.29878	2.59962
H	-4.29622	2.82465	1.73004
H	-5.30908	4.13851	1.11663
H	2.85893	-5.03237	0.10081
H	-5.47201	-2.51980	3.37801
H	-4.08952	-2.60488	-0.02399
H	-3.22413	-3.02333	2.87597
H	-2.40839	-3.64810	1.43780
H	-2.45099	-1.90941	1.74079
H	-6.70503	-0.65360	4.40592
H	-5.19519	-1.66964	-3.32754
H	-6.17099	-0.28374	-3.79802
H	-5.78026	2.15665	-0.23853
H	-7.15222	-2.25989	-0.37534
H	-7.40650	-2.48109	-2.10668
H	-5.84255	-2.88543	-1.40053

H	-7.91966	0.10463	-0.59341
H	-7.22450	1.20318	-1.80099
H	-8.18912	-0.18081	-2.30892
H	-6.97983	1.44851	3.16030
H	-3.69320	2.33119	-2.99150
H	-4.88579	1.78297	-4.17188
H	-5.38318	2.11794	-2.51237
H	-8.02279	2.80586	1.74650
H	-7.65116	3.65629	0.25387
H	-8.29760	2.01529	0.19870
H	-2.84226	-1.24790	-3.62289
H	-3.40326	-0.03007	-4.76929
H	-2.21224	0.39797	-3.53593
C	1.93709	2.08623	1.25932
H	2.92569	2.20671	1.68501
H	-2.92573	-2.20671	-1.68500

Table S26. Cartesian Coordinates for 8

N	-4.98335	-1.28035	0.05393
C	-0.23365	1.71122	2.61718
N	-5.12497	0.81557	-0.51717
C	-5.82482	-2.08008	3.63211
H	-6.04626	-1.31796	4.38396
H	-5.78945	-3.04861	4.13691
H	-6.65553	-2.10656	2.92245
C	-4.48322	-1.77138	2.93258
H	-4.58574	-0.79326	2.46191
C	-4.21927	-2.80677	1.84436
C	-4.52622	-2.60255	0.48363
C	-4.24685	-0.14418	-0.10807
B	-2.66173	0.03668	0.13985
C	-2.13299	0.85055	1.31819
C	-0.71365	0.97909	1.48926
C	-1.14751	2.27160	3.54775
H	-0.75151	2.81173	4.40081
C	-2.50211	2.13746	3.37732
H	-3.19262	2.56440	4.09362
C	-6.39382	0.27348	-0.61935
H	-7.23222	0.85841	-0.95060
C	-6.30970	-1.02267	-0.24393
H	-7.06547	-1.78163	-0.15691
C	-3.77532	-4.07971	2.21517
H	-3.52565	-4.27259	3.25045
C	-3.68384	-5.11021	1.29163
H	-3.34189	-6.08974	1.60467
C	-4.07066	-4.89963	-0.02447
H	-4.03939	-5.72589	-0.72287
C	-4.51472	-3.64988	-0.46464
C	-3.34584	-1.66722	3.96220
H	-2.38121	-1.48648	3.48323
H	-3.26095	-2.57402	4.56511
H	-3.54227	-0.84324	4.65226
C	-5.04031	-3.52253	-1.89435
H	-5.09954	-2.46161	-2.15353
C	-4.13506	-4.20519	-2.93719
H	-3.08881	-3.92225	-2.81823
H	-4.45842	-3.93282	-3.94493
H	-4.19368	-5.29357	-2.86802
C	-6.46619	-4.10785	-2.00150
H	-7.16667	-3.64472	-1.30378
H	-6.45811	-5.17945	-1.78809
H	-6.85769	-3.97005	-3.01247
C	-2.97897	1.43660	2.25897
H	-4.04945	1.34504	2.13284
C	1.15342	1.88394	2.81793
H	1.49531	2.44020	3.68284
C	2.04062	1.35168	1.92506
H	3.09875	1.50021	2.08785
C	1.61938	0.59770	0.80079
C	0.23221	0.39623	0.57357
C	-4.85546	2.22032	-0.82717
C	-5.35080	3.20784	0.05332
C	-5.08013	4.54017	-0.27021
H	-5.43585	5.32612	0.38341
C	-4.37833	4.87994	-1.41829
H	-4.18137	5.92157	-1.64321
C	-3.96392	3.89004	-2.29669
H	-3.46497	4.17182	-3.21486
C	-4.20774	2.53775	-2.03795
C	-3.89210	1.51014	-3.11967
H	-3.91263	0.51661	-2.67107
C	-2.50079	1.69734	-3.74714
H	-1.71491	1.71810	-2.98899
H	-2.43847	2.62129	-4.32645

H	-2.28902	0.87391	-4.43312
C	-4.98894	1.53994	-4.20590
H	-4.79548	0.77589	-4.96354
H	-5.01695	2.51037	-4.70763
H	-5.98082	1.35583	-3.78555
C	-6.22771	2.91475	1.27062
H	-6.12999	1.85575	1.52669
C	-7.71480	3.17835	0.94504
H	-8.06727	2.60402	0.08602
H	-7.87618	4.23459	0.71652
H	-8.34207	2.92107	1.80215
C	-5.83082	3.73218	2.51475
H	-4.75947	3.68536	2.71291
H	-6.36431	3.35756	3.39182
H	-6.09949	4.78503	2.40543
N	4.98336	1.28035	-0.05392
C	0.23366	-1.71123	-2.61717
N	5.12499	-0.81557	0.51717
C	5.82480	2.08010	-3.63209
H	6.04625	1.31798	-4.38395
H	5.78943	3.04863	-4.13690
H	6.65551	2.10659	-2.92243
C	4.48321	1.77139	-2.93257
H	4.58574	0.79326	-2.46190
C	4.21925	2.80677	-1.84435
C	4.52621	2.60255	-0.48362
C	4.24686	0.14418	0.10808
B	2.66173	-0.03668	-0.13984
C	2.13299	-0.85055	-1.31818
C	0.71365	-0.97910	-1.48925
C	1.14752	-2.27161	-3.54774
H	0.75152	-2.81173	-4.40080
C	2.50211	-2.13747	-3.37731
H	3.19262	-2.56440	-4.09361
C	6.39383	-0.27347	0.61935
H	7.23223	-0.85840	0.95059
C	6.30971	1.02268	0.24393
H	7.06547	1.78164	0.15692
C	3.77527	4.07970	-2.21515
H	3.52560	4.27258	-3.25043
C	3.68379	5.11020	-1.29161
H	3.34183	6.08973	-1.60465
C	4.07063	4.89963	0.02449
H	4.03935	5.72589	0.72289
C	4.51471	3.64988	0.46465
C	3.34584	1.66721	-3.96219
H	2.38120	1.48646	-3.48322
H	3.26094	2.57401	-4.56510
H	3.54227	0.84324	-4.65225
C	5.04031	3.52254	1.89436
H	5.09956	2.46161	2.15353
C	4.13507	4.20519	2.93721
H	3.08882	3.92224	2.81827
H	4.45845	3.93282	3.94494
H	4.19368	5.29357	2.86804
C	6.46619	4.10787	2.00149
H	7.16667	3.64476	1.30376
H	6.45810	5.17948	1.78808
H	6.85770	3.97008	3.01245
C	2.97898	-1.43661	-2.25896
H	4.04946	-1.34505	-2.13283
C	-1.15341	-1.88394	-2.81792
H	-1.49530	-2.44020	-3.68283
C	-2.04062	-1.35168	-1.92506
H	-3.09874	-1.50021	-2.08785
C	-1.61938	-0.59770	-0.80079
C	-0.23221	-0.39623	-0.57357
C	4.85547	-2.22032	0.82716
C	5.35081	-3.20784	-0.05333
C	5.08013	-4.54017	0.27018
H	5.43586	-5.32611	-0.38345
C	4.37833	-4.87995	1.41825
H	4.18136	-5.92157	1.64317
C	3.96392	-3.89005	2.29665
H	3.46496	-4.17184	3.21482
C	4.20774	-2.53776	2.03793
C	3.89210	-1.51016	3.11966
H	3.91264	-0.51662	2.67106
C	2.50079	-1.69736	3.74712
H	1.71491	-1.71810	2.98897
H	2.43846	-2.62131	4.32642
H	2.28902	-0.87392	4.43311
C	4.98894	-1.53997	4.20589
H	4.79548	-0.77593	4.96354
H	5.01695	-2.51040	4.70761
H	5.98082	-1.35586	3.78555
C	6.22773	-2.91473	-1.27063
H	6.13002	-1.85573	-1.52669

C	7.71482	-3.17834	-0.94504	C	5.83085	-3.73216	-2.51477
H	8.06728	-2.60401	-0.08600	H	4.75951	-3.68533	-2.71294
H	7.87620	-4.23458	-0.71652	H	6.36436	-3.35753	-3.39183
H	8.34210	-2.92105	-1.80213	H	6.09952	-4.78500	-2.40545

Table S27. Cartesian Coordinates for 8-S_1 (first excited state)

N	-4.95848	1.30340	-0.07871	H	-4.41071	3.98049	3.85710
C	-0.26037	-1.79963	-2.54399	H	-4.14767	5.32907	2.76735
N	-5.12779	-0.76942	0.51455	C	-6.41455	4.16991	1.91376
C	-5.63888	1.99402	-3.71350	H	-7.12159	3.70956	1.22281
H	-5.82554	1.20959	-4.44993	H	-6.38530	5.23658	1.68296
H	-5.56472	2.94335	-4.24792	H	-6.80990	4.05709	2.92506
H	-6.50686	2.05275	-3.05362	C	-2.98928	-1.53367	-2.20384
C	-4.34932	1.70179	-2.93279	H	-4.05987	-1.44125	-2.08236
H	-4.48405	0.74232	-2.43530	C	1.12153	-1.96710	-2.71867
C	-4.13686	2.77098	-1.87479	H	1.47199	-2.55152	-3.56115
C	-4.47995	2.60324	-0.52617	C	2.02342	-1.40661	-1.84086
C	-4.24235	0.16816	0.10147	H	3.07666	-1.57563	-2.01486
B	-2.66907	-0.03791	-0.14091	C	1.62992	-0.62052	-0.75486
C	-2.15011	-0.90055	-1.27803	C	0.22057	-0.40624	-0.53696
C	-0.74426	-1.02982	-1.43995	C	-4.86469	-2.16143	0.84884
C	-1.15389	-2.39580	-3.45290	C	-5.37184	-3.15891	-0.00102
H	-0.75184	-2.96187	-4.28440	C	-5.11085	-4.48046	0.34573
C	-2.51005	-2.26409	-3.28309	H	-5.47988	-5.27666	-0.28691
H	-3.19613	-2.72218	-3.98356	C	-4.40172	-4.79897	1.48928
C	-6.38788	-0.21581	0.60119	H	-4.21263	-5.83637	1.73614
H	-7.23455	-0.78756	0.93409	C	-3.96730	-3.79699	2.33576
C	-6.28623	1.06880	0.21255	H	-3.45765	-4.06138	3.25275
H	-7.03089	1.83703	0.11277	C	-4.20262	-2.45580	2.04873
C	-3.68865	4.02891	-2.26741	C	-3.85050	-1.40862	3.09174
H	-3.41423	4.19458	-3.30069	H	-3.90547	-0.42442	2.62803
C	-3.61990	5.07857	-1.37153	C	-2.43435	-1.57425	3.64836
H	-3.27519	6.05068	-1.70187	H	-1.68829	-1.59750	2.85224
C	-4.02591	4.89918	-0.06188	H	-2.33564	-2.49122	4.23153
H	-4.00541	5.74043	0.61818	H	-2.19570	-0.74388	4.31592
C	-4.47552	3.66447	0.39445	C	-4.88663	-1.43342	4.22469
C	-3.15996	1.55735	-3.88526	H	-4.66584	-0.65870	4.96212
H	-2.22743	1.39051	-3.34358	H	-4.87981	-2.39639	4.73924
H	-3.03554	2.44187	-4.51212	H	-5.89847	-1.26606	3.85027
H	-3.31924	0.71007	-4.55453	C	-6.25060	-2.88197	-1.21344
C	-5.00677	3.56139	1.81759	H	-6.14397	-1.83060	-1.49222
H	-5.08374	2.50560	2.08919	C	-7.72920	-3.12678	-0.87413
C	-4.09494	4.24208	2.84534	H	-8.07328	-2.53218	-0.02712
H	-3.05100	3.95591	2.71919	H	-7.89377	-4.17572	-0.62007

H	-8.36071	-2.88757	-1.73185
C	-5.86925	-3.72804	-2.43397
H	-4.79812	-3.70431	-2.63102
H	-6.39554	-3.36471	-3.31866
H	-6.15632	-4.77217	-2.30084
N	4.95851	-1.30338	0.07869
C	0.26035	1.79958	2.54402
N	5.12774	0.76947	-0.51451
C	5.63889	-1.99410	3.71349
H	5.82549	-1.20968	4.44995
H	5.56476	-2.94345	4.24788
H	6.50689	-2.05277	3.05363
C	4.34934	-1.70190	2.93275
H	4.48404	-0.74241	2.43529
C	4.13695	-2.77107	1.87471
C	4.48004	-2.60326	0.52610
C	4.24233	-0.16816	-0.10146
B	2.66905	0.03785	0.14094
C	2.15010	0.90050	1.27805
C	0.74424	1.02977	1.43998
C	1.15387	2.39576	3.45293
H	0.75182	2.96182	4.28442
C	2.51003	2.26404	3.28311
H	3.19611	2.72214	3.98358
C	6.38785	0.21591	-0.60114
H	7.23451	0.78772	-0.93401
C	6.28626	-1.06871	-0.21254
H	7.03095	-1.83690	-0.11277
C	3.68881	-4.02903	2.26728
H	3.41440	-4.19475	3.30056
C	3.62013	-5.07867	1.37137
H	3.27546	-6.05081	1.70167
C	4.02613	-4.89921	0.06173
H	4.00568	-5.74043	-0.61837
C	4.47568	-3.66446	-0.39456
C	3.15994	-1.55755	3.88519
H	2.22743	-1.39073	3.34348
H	3.03554	-2.44210	4.51201
H	3.31917	-0.71028	4.55450
C	5.00692	-3.56130	-1.81769
H	5.08385	-2.50550	-2.08926
C	4.09511	-4.24199	-2.84547
H	3.05117	-3.95587	-2.71930
H	4.41087	-3.98035	-3.85722
H	4.14789	-5.32898	-2.76752
C	6.41472	-4.16977	-1.91389
H	7.12175	-3.70943	-1.22292
H	6.38551	-5.23645	-1.68314
H	6.81007	-4.05690	-2.92519
C	2.98926	1.53362	2.20386
H	4.05985	1.44121	2.08237
C	-1.12155	1.96705	2.71869
H	-1.47201	2.55148	3.56116
C	-2.02344	1.40657	1.84088
H	-3.07668	1.57560	2.01487
C	-1.62994	0.62047	0.75488
C	-0.22058	0.40618	0.53699
C	4.86458	2.16147	-0.84876
C	5.37172	3.15895	0.00111
C	5.11071	4.48050	-0.34562
H	5.47974	5.27670	0.28703
C	4.40156	4.79901	-1.48915
H	4.21245	5.83642	-1.73599
C	3.96714	3.79704	-2.33564
H	3.45749	4.06144	-3.25262
C	4.20250	2.45586	-2.04864
C	3.85041	1.40869	-3.09168
H	3.90540	0.42448	-2.62799
C	2.43425	1.57430	-3.64830
H	1.68819	1.59752	-2.85219
H	2.33553	2.49127	-4.23146
H	2.19563	0.74393	-4.31588
C	4.88654	1.43354	-4.22462
H	4.66578	0.65883	-4.96207
H	4.87970	2.39652	-4.73915
H	5.89839	1.26619	-3.85020
C	6.25051	2.88200	1.21351
H	6.14384	1.83064	1.49232
C	7.72911	3.12674	0.87413
H	8.07313	2.53209	0.02714
H	7.89372	4.17565	0.62004
H	8.36064	2.88751	1.73185
C	5.86924	3.72812	2.43403
H	4.79812	3.70445	2.63111
H	6.39554	3.36480	3.31871
H	6.15635	4.77224	2.30086

Table S28. Cartesian Coordinates for 9

N	-4.94528	0.45214	-0.02905	H	0.69792	5.18364	-1.94625
N	4.94516	-0.45223	-0.02922	C	-1.18861	3.35984	-1.59609
C	-4.21856	0.20773	-1.08519	H	-1.54570	4.37406	-1.73477
C	4.21839	-0.20752	-1.08526	C	6.36414	-1.01305	-0.37271
C	-0.23961	0.69451	-1.30482	C	-5.35376	-2.32063	1.20904
C	4.09216	-1.25372	2.19606	H	-5.44306	-2.08278	0.14735
C	0.69559	1.78425	-1.40966	C	-3.57574	2.60127	1.69473
C	-0.69573	-1.78392	-1.40995	H	-3.77532	2.67677	0.62600
C	1.62736	-0.98097	-1.27178	C	-4.93239	-1.05850	1.96459
C	0.23948	-0.69421	-1.30494	C	3.97676	-1.02985	3.57153
C	2.11772	1.58955	-1.35059	H	3.59076	-1.82340	4.19809
C	-2.11787	-1.58923	-1.35084	C	-6.64650	2.30041	0.39833
C	2.06077	-2.32553	-1.40786	H	-5.90898	3.07446	0.19198
H	3.11886	-2.54423	-1.38116	H	-6.70318	2.12950	1.47330
C	-0.20214	-3.11103	-1.59510	H	-7.61940	2.67560	0.07180
C	0.20199	3.11139	-1.59459	C	-4.79669	-1.20052	3.34941
C	1.18847	-3.35948	-1.59669	H	-5.05228	-2.14912	3.80336
H	1.54555	-4.37368	-1.73556	C	-2.46068	-3.99072	-1.75411
C	-1.62749	0.98126	-1.27157	H	-3.14592	-4.81696	-1.89756
C	2.94955	2.69758	-1.51345	C	-3.97637	1.02931	3.57166
H	4.01975	2.56784	-1.45305	H	-3.59032	1.82279	4.19827
C	5.03664	-0.41108	-2.37863	C	-6.21034	1.27772	-1.87752
C	-4.60311	0.20068	1.39367	H	-5.97803	2.33290	-2.04148
C	2.46053	3.99110	-1.75347	H	-7.13327	1.06186	-2.41632
H	3.14578	4.81736	-1.89679	C	-1.10452	-4.19131	-1.78282
C	-5.03691	0.41153	-2.37846	H	-0.69806	-5.18323	-1.94710
C	4.93279	1.05810	1.96464	C	4.26961	3.40885	1.36909
C	4.60320	-0.20094	1.39357	H	3.27586	3.04348	1.10981
C	-2.06091	2.32585	-1.40740	H	4.50005	4.27056	0.73726
H	-3.11899	2.54455	-1.38059	H	4.23231	3.76538	2.40058
C	-6.36438	1.01284	-0.37232	C	4.79734	1.19991	3.34950
C	5.35430	2.32027	1.20923	H	5.05311	2.14841	3.80357
H	5.44353	2.08254	0.14750	C	-4.28161	1.08017	-3.54152
C	-4.09205	1.25341	2.19624	H	-3.96110	2.09477	-3.30963
C	-2.94969	-2.69724	-1.51389	H	-4.95259	1.13651	-4.40179
H	-4.01989	-2.56750	-1.45346	H	-3.40625	0.50260	-3.84705
C	5.52964	0.96895	-2.89593	C	4.34514	0.16960	4.15449
H	4.71216	1.55291	-3.31853	H	4.26604	0.30597	5.22644
H	6.24977	0.78665	-3.69643	C	2.04735	-2.68494	1.89867
H	6.02965	1.56458	-2.13177	H	1.80122	-2.68495	2.96294
C	3.57560	-2.60143	1.69437	H	1.65825	-3.61119	1.46945
H	3.77516	-2.67681	0.62564	H	1.52539	-1.84676	1.43521
C	1.10438	4.19169	-1.78214	C	7.45591	0.00452	-0.03730

H	8.41475	-0.41548	-0.34797
H	7.50878	0.17896	1.03628
H	7.33057	0.95760	-0.54764
C	6.20998	-1.27755	-1.87796
H	5.97751	-2.33265	-2.04216
H	7.13291	-1.06170	-2.41678
B	2.65671	0.17051	-1.16502
C	-5.52974	-0.96839	-2.89615
H	-4.71218	-1.55217	-3.31887
H	-6.24985	-0.78593	-3.69663
H	-6.02973	-1.56428	-2.13218
C	-2.04750	2.68504	1.89902
H	-1.80136	2.68502	2.96330
H	-1.65858	3.61141	1.46990
H	-1.52538	1.84701	1.43549
C	4.28125	-1.07927	-3.54188
H	3.96068	-2.09393	-3.31030
H	4.95219	-1.13537	-4.40218
H	3.40591	-0.50154	-3.84719
C	-7.45595	-0.00499	-0.03708
H	-7.50876	-0.17964	1.03646
H	-7.33045	-0.95796	-0.54760
H	-8.41488	0.41488	-0.34765
C	-4.26892	-3.40910	1.36874
H	-3.27524	-3.04362	1.10935
H	-4.49935	-4.27081	0.73692
H	-4.23147	-3.76563	2.40023
C	6.70395	2.90309	1.67845
H	6.64127	3.26246	2.70762
H	6.97316	3.75981	1.05527
H	7.52098	2.18491	1.63132
C	6.64608	-2.30084	0.39763
H	5.90845	-3.07474	0.19110
H	6.70276	-2.13019	1.47264
H	7.61893	-2.67609	0.07104
C	4.24160	-3.80935	2.38535
H	5.32962	-3.78032	2.33338
H	3.90553	-4.73688	1.91445
H	3.96456	-3.86724	3.44001
C	-6.70332	-2.90366	1.67826
H	-6.64042	-3.26354	2.70723
H	-6.97269	-3.76007	1.05472
H	-7.52036	-2.18545	1.63168
C	-4.24195	3.80898	2.38588
H	-5.32996	3.77979	2.33392
H	-3.90602	4.73664	1.91511
H	-3.96491	3.86676	3.44054
C	-4.34449	-0.17028	4.15449
H	-4.26517	-0.30682	5.22640
B	-2.65686	-0.17023	-1.16504

Table S29. Cartesian Coordinates for 9-S_1 (first excited state)

N	-4.93022	0.42461	-0.01807
N	4.93020	-0.42463	-0.01811
C	-4.22173	0.17718	-1.07712
C	4.22174	-0.17704	-1.07715
C	-0.23401	0.66727	-1.32994
C	4.05601	-1.29803	2.15317
C	0.71022	1.77750	-1.42826
C	-0.71022	-1.77732	-1.42841
C	1.64859	-0.94065	-1.29061
C	0.23402	-0.66710	-1.33001
C	2.12015	1.60441	-1.34498
C	-2.12014	-1.60424	-1.34508
C	2.06554	-2.26473	-1.45464
H	3.12082	-2.49514	-1.43750
C	-0.20023	-3.09761	-1.63745
C	0.20023	3.09782	-1.63717
C	1.18740	-3.30608	-1.65932
H	1.56250	-4.31061	-1.81889
C	-1.64858	0.94082	-1.29048
C	2.93299	2.73669	-1.49599
H	4.00317	2.62430	-1.41392
C	5.06443	-0.34900	-2.34850
C	-4.55167	0.21743	1.39358
C	2.43140	4.00667	-1.74789
H	3.10508	4.84404	-1.87718
C	-5.06440	0.34928	-2.34847
C	4.82541	1.02956	1.99669
C	4.55164	-0.21759	1.39356
C	-2.06554	2.26492	-1.45435
H	-3.12081	2.49533	-1.43714
C	-6.35719	0.92775	-0.33178
C	5.21627	2.31357	1.27516

H	5.33934	2.09795	0.21320
C	-4.05608	1.29781	2.15331
C	-2.93298	-2.73650	-1.49615
H	-4.00316	-2.62412	-1.41404
C	5.51437	1.04173	-2.84823
H	4.68176	1.60229	-3.27085
H	6.24672	0.89214	-3.64289
H	5.98763	1.64569	-2.07460
C	3.59655	-2.64049	1.60247
H	3.82574	-2.67802	0.53821
C	1.07249	4.18846	-1.81284
H	0.65161	5.17018	-1.99287
C	-1.18739	3.30629	-1.65896
H	-1.56250	4.31083	-1.81843
C	6.35717	-0.92776	-0.33185
C	-5.21612	-2.31377	1.27490
H	-5.33908	-2.09807	0.21294
C	-3.59666	2.64034	1.60273
H	-3.82584	2.67795	0.53847
C	-4.82537	-1.02981	1.99657
C	3.90092	-1.11480	3.52391
H	3.52572	-1.93457	4.12175
C	-6.66713	2.21005	0.42411
H	-5.96445	3.00650	0.18794
H	-6.68964	2.05301	1.50176
H	-7.65985	2.54452	0.11778
C	-4.65435	-1.13685	3.37427
H	-4.86924	-2.08168	3.85507
C	-2.43140	-4.00646	-1.74817
H	-3.10508	-4.84383	-1.87752
C	-3.90099	1.11444	3.52403
H	-3.52582	1.93416	4.12196
C	-6.25198	1.17579	-1.83769
H	-6.06348	2.23577	-2.02064
H	-7.17863	0.91856	-2.34968
C	-1.07250	-4.18825	-1.81318
H	-0.65161	-5.16995	-1.99331
C	4.09053	3.34870	1.42886
H	3.12023	2.94898	1.13731
H	4.29869	4.23145	0.82096
H	4.01552	3.67982	2.46581
C	4.65440	1.13646	3.37440
H	4.86936	2.08122	3.85531
C	-4.34683	1.03441	-3.51529
H	-4.06708	2.06305	-3.29383
H	-5.02369	1.05992	-4.37108
H	-3.45169	0.48952	-3.81950
C	4.21694	0.07737	4.14063
H	4.10776	0.18554	5.21248
C	2.07513	-2.77393	1.77012
H	1.81095	-2.82368	2.82776
H	1.71864	-3.69286	1.30012
H	1.53903	-1.93168	1.33306
C	7.39911	0.11853	0.04237
H	8.37883	-0.26039	-0.25129
H	7.41948	0.27645	1.11878
H	7.25022	1.07427	-0.45494
C	6.25199	-1.17559	-1.83780
H	6.06349	-2.23555	-2.02090
H	7.17865	-0.91830	-2.34974
B	2.66206	0.19437	-1.16006
C	-5.51432	-1.04140	-2.84837
H	-4.68170	-1.60188	-3.27108
H	-6.24670	-0.89173	-3.64299
H	-5.98754	-1.64548	-2.07481
C	-2.07525	2.77381	1.77041
H	-1.81108	2.82348	2.82805
H	-1.71878	3.69280	1.30050
H	-1.53912	1.93162	1.33328
C	4.34685	-1.03398	-3.51540
H	4.06709	-2.06265	-3.29407
H	5.02372	-1.05941	-4.37120
H	3.45172	-0.48905	-3.81956
C	-7.39912	-0.11863	0.04227
H	-7.41951	-0.27669	1.11866
H	-7.25018	-1.07429	-0.45516
H	-8.37884	0.26030	-0.25137
C	-4.09037	-3.34889	1.42863
H	-3.12005	-2.94912	1.13722
H	-4.29845	-4.23159	0.82063
H	-4.01547	-3.68010	2.46556
C	6.52295	2.93582	1.78722
H	6.42011	3.27013	2.82053
H	6.77199	3.81546	1.19015
H	7.36926	2.25363	1.74638
C	6.66704	-2.21018	0.42386
H	5.96435	-3.00657	0.18755
H	6.68951	-2.05329	1.50153

H	7.65976	-2.54464	0.11753	H	-7.36916	-2.25392	1.74588
C	4.27869	-3.83993	2.27518	C	-4.27886	3.83970	2.27553
H	5.36510	-3.77688	2.25375	H	-5.36526	3.77661	2.25407
H	3.98391	-4.76455	1.77436	H	-3.98409	4.76438	1.77480
H	3.97613	-3.93219	3.31921	H	-3.97633	3.93188	3.31958
C	-6.52284	-2.93608	1.78677	C	-4.21694	-0.07782	4.14061
H	-6.42011	-3.27047	2.82007	H	-4.10775	-0.18612	5.21245
H	-6.77180	-3.81569	1.18961	B	-2.66204	-0.19421	-1.16004

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