Supporting Information

Cation Radicals, Borenium Cations, and Dication from Oxidation of B-Tolyl B^{III} Subporphyrins

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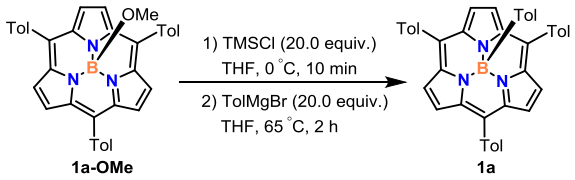
1. Instruments and Materials

^{1}H NMR (700 MHz) and ^{13}C NMR (176 MHz) were taken on a Bruker AVANCE NEO spectrometer, ^{13}C NMR (101 MHz) were taken on a Bruker AVANCE-400 spectrometer, ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectra were taken on a Bruker AVANCE-500 spectrometer or a Q.One Instruments Quantum-I spectrometer. Chemical shifts were reported as the delta scale in ppm relative to the internal standards for $CHCl_3$ (δ = 7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR) and CH_2Cl_2 (δ = 5.32 ppm for ^{1}H NMR and 53.84 ppm for ^{13}C NMR). UV-Vis-NIR absorption spectra were recorded on a Shimadzu UV-3600 spectrometer. MALDI-TOF mass spectra were obtained with a Bruker ultrafleXtreme MALDI-TOF/TOF spectrometer with DCTB as matrix. X-Ray data were taken on an Agilent Supernova X-Ray diffractometer equipped with a large area CCD detector. Redox potentials were measured by cyclic voltammetry and differential pulse voltammetry on a CHI900 scanning electrochemical microscope. Dichloromethane and dichlorobenzene were distilled in the presence of CaH_2, hexane, THF, and toluene were distilled in the presence of Na and stored over 3 Å molecular sieves overnight. HN^{n}Bu$_2$, $CHCl_3$ and CD_2Cl_2 were stored over 3 Å molecular sieves overnight. Unless otherwise noted, chemicals obtained from commercial suppliers were used without further purification.

2. Experimental Procedures

Synthesis of 1a



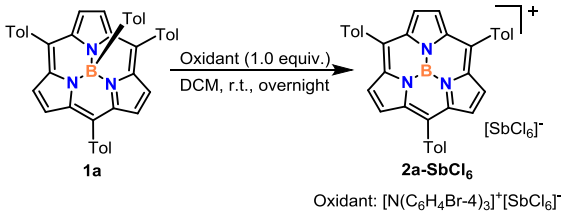
1a-OMe **1a**

Synthesis of *p*-$CH_3C_6H_4MgBr$: Under an argon atmosphere, *p*-$CH_3C_6H_4Br$ (2.5 mL, 20.317 mmol) was added to a solution of Mg (442.0 mg, 18.610 mmol) in dry tetrahydrofuran (15 mL) at 65 °C for 1 h. The majority of Mg dissolved and a gray suspension formed, which could be used as the THF solution of *p*-$CH_3C_6H_4MgBr$.

Under an argon atmosphere, trimethylchlorosilane (2.2 mL, 18 mmol) was added to a solution of **1a-OMe** (505.7 mg, 0.930 mmol) in dry tetrahydrofuran (15 mL) at 0 °C. After 10 min, *p*-$CH_3C_6H_4MgBr$ in THF was added to the solution, and the resulting mixture was heated at 65 °C for 2 h. After cooling to room temperature, the reaction mixture was washed with water (50 mL × 3) and the organic phase was dried over Na_2SO_4. After removal of the solvents in vacuo, the residue was purified through a silica gel column (CH_2Cl_2: *n*-hexane = 1:5 as eluent). Recrystallization from CH_2Cl_2/MeOH gave **1a** as orange solids (366 mg, 0.562 mmol, 66% yield). ^{1}H NMR (700 MHz, $CDCl_3$, 298 K) δ = 8.13 (s, 6H, *β*-H), 7.97 (d, *J* = 7.7 Hz, 6H, *meso*-C_6H_4Me), 7.51 (d, *J* = 7.7 Hz, 6H, *meso*-C_6H_4Me), 6.17 (d, *J* = 8.4 Hz, 2H, *axial*-C_6H_4Me), 4.60 (d, *J* = 8.4 Hz, 2H, *axial*-C_6H_4Me), 2.58 (s, 9H, *meso*-C_6H_4Me), and 1.80 (s, 3H, *axial*-C_6H_4Me) ppm. ^{13}C NMR (176 MHz, $CDCl_3$) δ

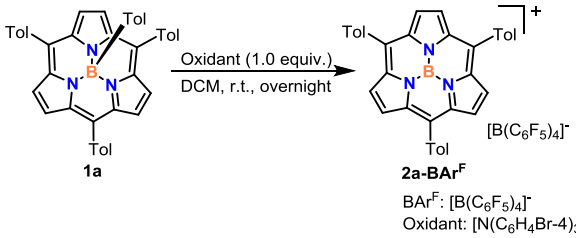
= 140.5, 137.6, 135.1, 134.8, 133.3, 129.5, 128.9, 127.1, 122.1, 120.4, 21.5, and 20.9 ppm. (The signal of the carbon connecting to B atom was not observed.) UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 386 (130000), and 511 (17000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 512.2301, calcd for $(C_{36}H_{27}BN_3)^+$ = 512.2299 ([*M*-Tol]$^+$).

Synthesis of 2a-$SbCl_6$



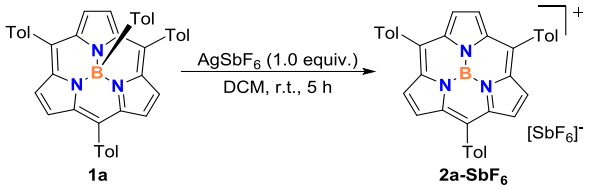
In a glovebox, to a CH_2Cl_2 (5 mL) solution of **1a** (16.3 mg, 0.033 mmol) was added $[N(C_6H_4Br\text{-}4)_3]^+[SbCl_6]^-$ (22.0 mg, 0.033 mmol) at room temperature. The resulting mixture was stirred overnight and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **2a-$SbCl_6$** as brown solids (20.0 mg, 0.0249 mmol, 89% yield). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 8.89 (s, 6H, *β*-H), 8.14 (d, *J* = 7.3 Hz, 6H, C_6H_4Me), 7.66 (d, *J* = 7.3 Hz, 6H, C_6H_4Me), and 2.64 (s, 9H, C_6H_4Me) ppm. ^{13}C NMR (101 MHz, CD_2Cl_2) δ = 141.1, 137.1, 133.5, 132.0, 131.1, 129.6, 126.9, 21.6 ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 374 (140000), 463 (11000), and 489 (14000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 512.2293, calcd for $(C_{36}H_{27}BN_3)^+$ = 512.2299 ([*M*-$SbCl_6$]$^+$).

Synthesis of 2a-BAr^F



In a glovebox, to a CH_2Cl_2 (5 mL) solution of **1a** (57.8 mg, 0.096 mmol) was added a solution of $[N(C_6H_4Br\text{-}4)_3]^+[B(C_6F_5)_4]^-$ (111.0 mg, 0.096 mmol) in CH_2Cl_2 (4 mL) at room temperature. The resulting mixture was stirred overnight and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **2a-BAr^F** as yellow solids (106 mg, 0.090 mmol, 88% yield). ^{1}H NMR (500 MHz, $CDCl_3$, 298 k) δ = 9.03 (s, 6H, *β*-H), 8.10 (d, *J* = 7.8 Hz, 6H, C_6H_4Me), 7.70 (d, *J* = 7.8 Hz, 6H, C_6H_4Me), 2.65 (s, 9H, C_6H_4Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 141.6, 136.6, 133.2, 131.4, 131.3, 130.4, 129.4, 128.5, 127.8, 125.6, and 21.8 ppm. (Some signals of $[B(C_6F_5)_4]^-$ are not observed due to complicated coupling of F atoms.) ^{19}F NMR (471 MHz, $CDCl_3$) δ = -132.70 – -132.75 (m), -163.42 (t, *J* = 20.7 Hz), -167.00 – -167.09 (m) ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 376 (130000), 461 (10000), and 488 (17000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 512.2293, calcd for $(C_{36}H_{27}BN_3)^+$ = 512.2299 ([*M*-$B(C_6F_5)_4$]$^+$).

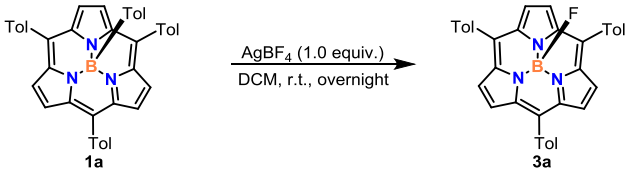
Synthesis of 2a-SbF_6



In a glovebox, to a CH_2Cl_2 (6 mL) solution of **1a** (100 mg, 0.166 mmol) was added a CH_2Cl_2 (2 mL) solution of $AgSbF_6$ (56.9 mg, 0.166 mmol) at room temperature. The resulting mixture was stirred for 5 h and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **2a-SbF$_6$** as brown solids (88 mg, 0.118 mmol, 71% yield).

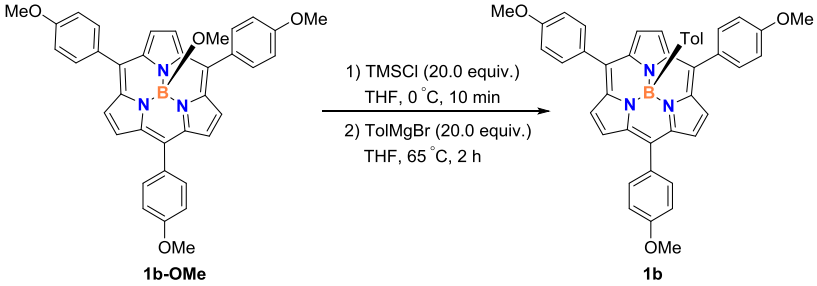
Gram scale synthesis: In a glovebox, to a CH_2Cl_2 (30 mL) solution of **1a** (1.0142 g, 1.680 mmol) was added a solution of $AgSbF_6$ (580 mg, 1.680 mmol) in CH_2Cl_2 (20 mL) at room temperature. The resulting mixture was stirred overnight and filtered. Similar to the procedure above, **2a-SbF$_6$** was afforded as brown solids (1.218 g, 1.628 mmol, 97% yield). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 8.99 (s, 6H, *β*-H), 8.15 (d, *J* = 8.0 Hz, 6H, C_6H_4Me), 7.67 (d, *J* = 8.0 Hz, 6H, C_6H_4Me), and 2.63 (s, 9H, C_6H_4*Me*) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 140.8, 136.7, 133.2, 131.6, 130.9, 129.9, 127.1, and 21.6 ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 373 (140000), 460 (12000), and 487 (15000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 512.2293, calcd for $(C_{36}H_{27}BN_3)^+$ = 512.2299 ([*M*-SbF_6]$^+$).

Synthesis of 3a



In a glovebox, to a solution of **1a** (25 mg, 0.041 mmol) in CH_2Cl_2 (5 mL) was added $AgBF_4$ (9.6 mg, 0.041 mmol) at room temperature. The resulting mixture was stirred overnight and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **3a** as yellow solids (17.7 mg, 0.033 mmol, 81% yield). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 8.21 (s, 6H, *β*-H), 7.98 (d, *J* = 7.8 Hz, 6H, C_6H_4Me), 7.54 (d, *J* = 7.8 Hz, 6H, C_6H_4Me), and 2.60 (s, 9H, C_6H_4*Me*) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 140.6, 138.2, 134.4, 133.4, 129.9, 123.0, 121.0, and 21.7 ppm. ^{19}F NMR (471 MHz, $CDCl_3$) δ = -156.73– -156.98 (m) ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 376 (110000), 461 (11000), and 488 (12000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 512.2293, calcd for $(C_{36}H_{27}BN_3)^+$ = 512.2299 ([*M*-F]$^+$).

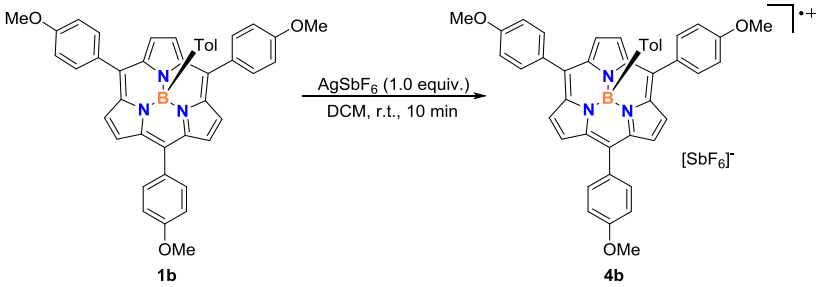
Synthesis of 1b



Under an argon atmosphere, trimethylchlorosilane (2.2 mL, 16.880 mmol) was added to a solution

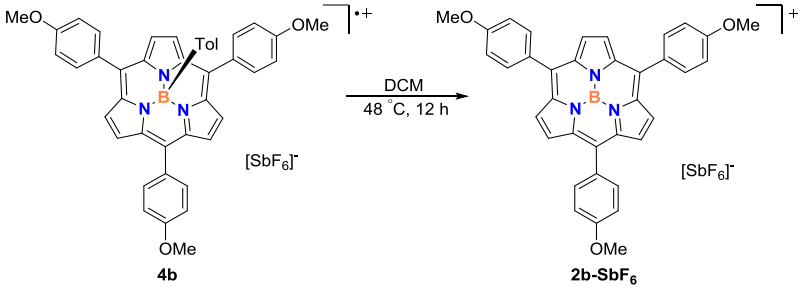
of **1b-OMe** (500 mg, 0.844 mmol) in dry tetrahydrofuran (15 mL) at 0 °C. After 10 min, *p*-$CH_3C_6H_4MgBr$ prepared from *p*-$CH_3C_6H_4Br$ (2.3 mL, 18.691 mmol) and Mg (412 mg, 16.948 mmol) in tetrahydrofuran (15 mL) was added to the solution, and the resulting mixture was heated at 65 °C for 2 h. After cooling to room temperature, the reaction mixture was washed with water (50 mL × 3) and the organic phase was dried over Na_2SO_4. After removal of the solvent in vacuo, the residue was purified through a silica gel column (CH_2Cl_2: *n*-hexane = 1:5 as eluent). Recrystallization from CH_2Cl_2/MeOH gave **1b** as orange solids (366 mg, 0.562 mmol, 66% yield). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 8.11 (s, 6H, *β*-H), 8.00 (d, *J* = 8.8 Hz, 6H, *meso*-C_6H_4OMe), 7.24 (d, *J* = 8.8 Hz, 6H, *meso*-C_6H_4OMe), 6.16 (d, *J* = 7.8 Hz, 2H, *axial*-C_6H_4Me), 4.59 (d, *J* = 7.8 Hz, 2H, *axial*-C_6H_4Me), 4.00 (s, 9H, C_6H_4OMe), and 1.79 (s, 3H, C_6H_4Me) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 159.6, 140.3, 135.1, 134.3, 130.1, 128.9, 127.1, 122.0, 120.0, 114.3, 55.7, and 20.9 ppm. (The signal of the carbon connecting to B atom was not observed.) UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 388 (130000), and 518 (22000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 560.2138, calcd for $(C_{36}H_{27}BN_3O_3)^+$ = 560.2146 ([*M*-Tol]$^+$).

Synthesis of 4b



In a glovebox, a solution of **1b** (50.5 mg, 0.078 mmol) in CH_2Cl_2 (2 mL) was added a solution of $AgSbF_6$ (26.6mg, 0.078 mmol) in CH_2Cl_2 (2 mL) at room temperature. The resulting mixture was stirred for 10 min and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **4b** as black solids (67.8 mg, 0.075 mmol, 96% yield). UV-Vis-NIR (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 389 (110000), 479 (25000), 510 (17000), 619 (39000), and 937 (24000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 560.2125, calcd for $(C_{36}H_{27}BN_3O_3)^+$ = 560.2146 ([*M*-Tol-SbF_6]$^+$).

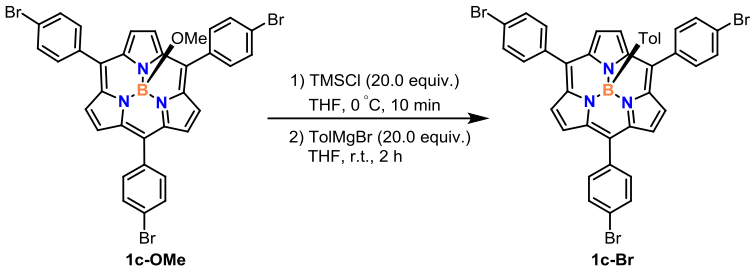
Synthesis of 2b-SbF_6



In a glovebox, a solution of **4b** (28.6 mg, 0.032 mmol) in CH_2Cl_2 (8 mL) was added to a Schlenk tube. The Schlenk tube was sealed and moved outside the glovebox. After heating for 12 h at reflux and cooling to room temperature, the Schlenk tube was moved inside the glovebox. The solution was concentrated to ca. 1 mL and hexane (5 mL) was added to the solution for recrystallization. **2b-SbF_6** was obtained as red solids (26.8 mg, 0.034 mmol, 85% yield). ^{1}H NMR (500 MHz, CD_2Cl_2,

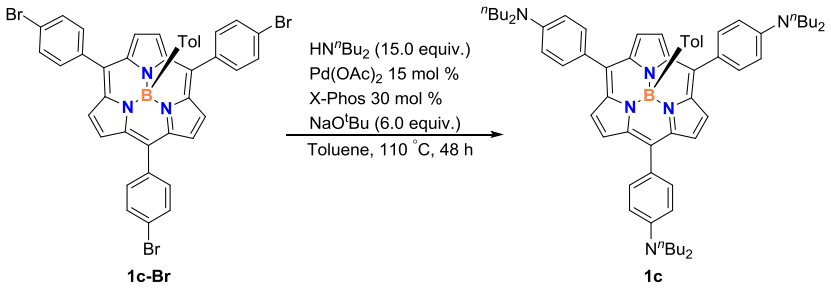
298 K) δ = 9.05 (s, 6H, *β*-H), 8.26 (d, *J* = 7.5 Hz, 6H, C_6H_4OMe), 7.45 (d, *J* = 7.5 Hz, 6H, C_6H_4OMe), and 4.06 (s, 9H, C_6H_4O*Me*) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 162.4, 136.6, 135.0, 130.4, 127.3, 127.1, 116.4, and 56.4 ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 380 (110000), and 503 (20000) nm, HR-MS (MALDI-TOF-MS): *m/z* = 560.2148, calcd for $(C_{36}H_{27}BN_3O_3)^+$ = 560.2146 ([*M*-SbF_6]$^+$).

Synthesis of 1c-Br



Under an argon atmosphere, trimethylchlorosilane (1.61 mL, 13.55 mmol) was added to a solution of **1c-OMe** (500 mg, 0.678 mmol) in dry THF (15 mL) at 0 °C. After 10 min, a THF (15 mL) solution of *p*-$CH_3C_6H_4MgBr$ prepared from *p*-$CH_3C_6H_4Br$ (1.65 mL, 13.55 mmol) and Mg (325.2 mg, 13.55 mmol) was added to the reaction and the resulting mixture was stirred at room temperature for 2 h. The reaction mixture was washed with water (50 mL × 3) and the organic phase was dried over Na_2SO_4. After removal of the solvent in vacuo, the residue was purified through a silica gel column (CH_2Cl_2: *n*-hexane = 1:5 as eluent). Recrystallization from CH_2Cl_2/MeOH gave **1c-Br** as orange solids (458.5 mg, 0.577 mmol, 85.1% yield). ^{1}H NMR (700 MHz, $CDCl_3$) δ = 8.12 (s, 6H, *β*-H), 7.92 (d, *J* = 8.4 Hz, 6H, C_6H_4Br), 7.84 (d, *J* = 8.4 Hz, 6H, C_6H_4Br), 6.17 (d, *J* = 7.7 Hz, 2H, C_6H_4Me), 4.55 (d, *J* = 7.7 Hz, 2H, C_6H_4Me), 1.80 (s, 3H, C_6H_4*Me*) ppm. ^{13}C NMR (176 MHz, $CDCl_3$) δ = 140.5, 136.3, 135.5, 134.6, 132.0, 128.7, 127.2, 122.8, 122.3, 119.5, 20.9 ppm. (The signal of the carbon connecting to B atom was not observed.) HR-MS (MALDI-TOF-MS): *m/z* = 705.9123, calcd for $(C_{33}H_{18}BBr_3N_3)^+$ = 705.9125 ([*M*-Tol]$^+$).

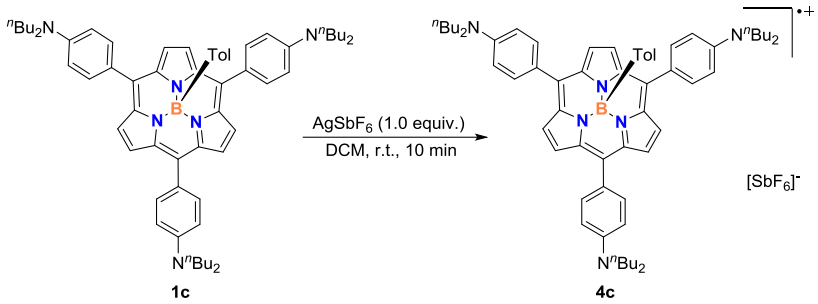
Synthesis of 1c



Dibutylamine (0.33 mL, 1.9 mmol) was added to a toluene (6 mL) solution of **1c-Br** (101.3 mg, 0.130 mmol), $Pd(OAc)_2$ (4.4 mg, 0.019 mmol), X-Phos (18.5 mg, 0.038 mmol), and NaO^{t}Bu (74.5 mg, 0.76 mmol) in a Schlenk tube. This mixture was deoxygenated via three freeze-pump-thaw cycles and heated at 110 °C for 48 h. After cooling to room temperature, the reaction mixture was washed by water (50 mL × 3) and the organic phase was dried over Na_2SO_4. After removal of the volatile in vacuo, the residue was purified by silica gel column (CH_2Cl_2: *n*-hexane = 1:4 as eluent). Further recrystallization from CH_2Cl_2/MeOH gave purple solids (52.7 mg, 0.056 mmol, 44% yield). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 8.13 (s, 6H, *β*-H), 7.95 (d, *J* = 8.8 Hz, 6H, $C_6H_4N^nBu_2$),

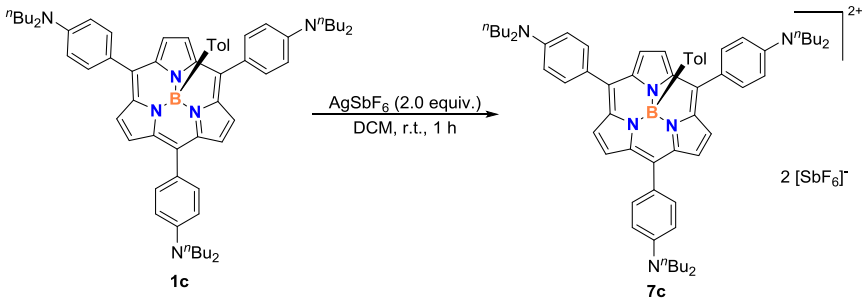
6.94 (d, J = 8.8 Hz, 6H, $C_6H_4N^nBu_2$), 6.11 (d, J = 7.8 Hz, 2H, C_6H_4Me), 4.59 (d, J = 7.8 Hz, 2H, C_6H_4Me), 3.42 (t, J = 7.8 Hz, 12H, $C_6H_4N(CH_2CH_2CH_2CH_3)_2$), 1.76 (s, 3H, C_6H_4Me), 1.74-1.68 (m, 12H, $C_6H_4N^nBu_2$), 1.48-1.41 (m, 12H, $C_6H_4N^nBu_2$), and 1.02 (t, J = 7.5 Hz, 18H, $C_6H_4N(CH_2CH_2CH_2CH_3)_2$) ppm. (Trace NH_2NH_2•H_2O was added in the sample to avoid oxidation by air.) ^{13}C NMR (176 MHz, $CDCl_3$) δ = 147.7, 139.5, 134.5, 134.2, 129.0, 126.8, 124.8, 121.7, 120.3, 111.9, 51.1, 29.8, 20.8, 20.5, and 14.2 ppm. (The signal of the carbon connecting to B atom was not observed. Trace NH_2NH_2•H_2O was added in the sample to avoid oxidation by air.) UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 416 (56000) and 563 (41000) nm. HR-MS (MALDI-TOF-MS): m/z = 851.5908, calcd for $(C_{57}H_{72}BN_6)^+$ = 851.5915 ([M-Tol]$^+$).

Synthesis of 4c



In a glovebox, to a CH_2Cl_2 (6 mL) solution of **1c** (47.1 mg, 0.050 mmol) was added a CH_2Cl_2 (2 mL) solution of $AgSbF_6$ (17.2 mg, 0.050 mmol) at room temperature. The resulting mixture was stirred for 10 min and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **4c** as black solids (39.3 mg, 0.033 mmol, 66% yield). UV-Vis-NIR (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 360 (26000), 412 (74000), 484 (60000), 758 (96000), and 1394 (71000) nm. HR-MS (MALDI-TOF-MS): m/z = 942.6443, calcd for $(C_{64}H_{79}BN_6)^+$ = 942.6464 ([M-SbF_6]$^+$).

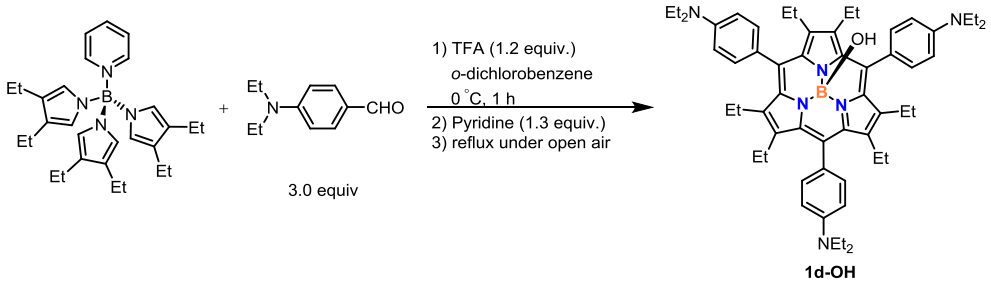
Synthesis of dication 7c



In a glovebox, a CH_2Cl_2 (2 mL) solution of $AgSbF_6$ (34.6 mg, 0.100 mmol) was added to a CH_2Cl_2 (6 mL) solution of **1c** (47.1 mg, 0.050 mmol) at room temperature. The resulting mixture was stirred for 1 h and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **7c** as black solids (67.6 mg, 0.046 mmol, 93% yield). ^1H NMR (500 MHz, CD_2Cl_2, 298 K) δ = 8.46 (d, J = 9.5 Hz, 6H, $C_6H_4^nNBu_2$), 7.44 (s, 6H, β-H), 7.15 (d, J = 9.5 Hz, 6H, $C_6H_4^nNBu_2$), 6.84 (d, J = 7.5 Hz, 2H, C_6H_4Me), 6.69 (d, J = 7.5 Hz, 2H, C_6H_4Me), 3.73 (t, J = 7.8 Hz, 12H, $C_6H_4N(CH_2CH_2CH_2CH_3)_2$), 2.12 (s, 3H, C_6H_4Me), 1.83-1.77 (m, 12H, $C_6H_4N^nBu_2$), 1.53-1.47 (m, 12H, $C_6H_4N^nBu_2$), and 1.04 (t, J = 7.3 Hz, 18H, $C_6H_4N(CH_2CH_2CH_2CH_3)_2$). ^{13}C NMR

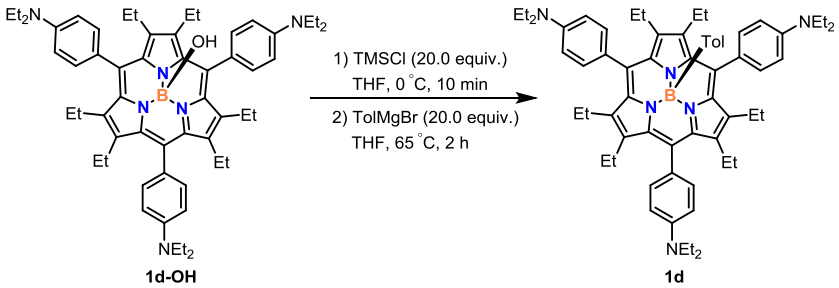
(101 MHz, CD_2Cl_2) δ = 156.9, 142.6, 138.7, 138.6, 138.1, 130.3, 130.0, 129.0, 128.1, 125.3, 117.2, 30.9, 21.2, 20.7, and 13.9 ppm. (The signal of $N(CH_2CH_2CH_2CH_3)_2$ overlaps with signals of CD_2Cl_2, which has been further confirmed by phase sensitive HSQC.) UV-Vis-NIR (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 416 (40000), 484 (30000), 562 (40000), and 972 (81000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 1177.5392, calcd for $(C_{64}H_{79}BF_6N_6Sb)^+$ = 1177.5407 ([*M*-SbF_6]$^+$).

Synthesis of 1d-OH



A mixture of borane pyridine complex (1.52 mL, 0.015 mmol) and 3,4-diethyl-1H-pyrrole (5.1 g, 0.042 mol) was heated at 100 °C for 3 h under an argon atmosphere. After the mixture cooling to room temperature volatile was removed the in vacuo to give the crude pyridine-tri-*N*-(3,4-diethylpyrrolyl)borane. This solid was dissolved in 1,2-dichlorobenzene (375 mL) and 4-Diethylaminobenzaldehyde (7.53 g, 0.042 mol) was then added. The solution was cooled to 0 °C and trifluoroacetic acid (1.25 mL, 0.017 mol) was added thereafter. The solution was stirred at 0 °C for 1 h then pyridine (1.48 mL, 0.018 mol) was added and the reaction mixture was refluxed under open air for 5 h. After removal of the volatile in vacuo, the residue was purified by Al_2O_3 column (CH_2Cl_2: *n*-hexane = 1:1 as eluent) and gel permeation chromatography ($CHCl_3$ as eluent). Further recrystallization from CH_2Cl_2/hexane gave **1d-OH** as green solids (556.6 mg, 0.640 mmol, 5% yield). ^{1}H NMR (700 MHz, $CDCl_3$, 298 k) δ = 8.02 (br, 3H, $C_6H_4NEt_2$), 7.22 (br, 3H, $C_6H_4NEt_2$), 6.96 (br, 3H, $C_6H_4NEt_2$), 6.78 (br, 3H, $C_6H_4NEt_2$), 3.52 (q, *J* = 7.0 Hz, 12H, $C_6H_4N(CH_2CH_3)_2$), 2.72 (q, *J* = 7.7 Hz, 12H, *β*-$N(CH_2CH_3)_2$), 1.29 (t, *J* = 7.0 Hz, 18H, $C_6H_4N(CH_2CH_3)_2$), 1.08 (t, *J* = 7.7 Hz, 18H, *β*-$N(CH_2CH_3)_2$), and -3.22 (br, 1H, *axial*-O*H*) ppm. ^{13}C NMR (176 MHz, $CDCl_3$) δ = 147.9, 137.9, 136.4, 133.5(br), 132.7(br), 125.0, 117.5, 111.5(br), 111.2(br), 44.8, 19.2, 17.2, and 12.6 ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 358 (89000), and 450 (18000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 851.5872, calcd for $(C_{57}H_{72}BN_6)^+$ = 851.5915 ([*M*-OH]$^+$).

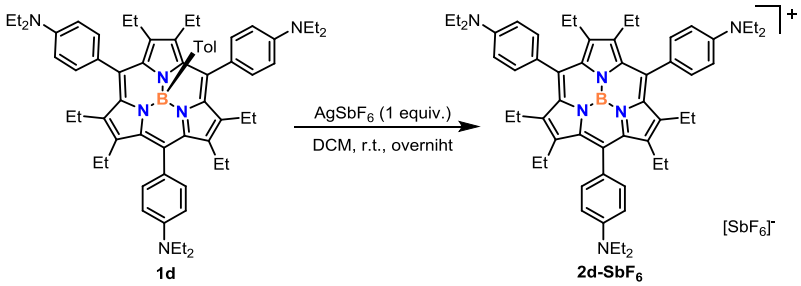
Synthesis of 1d



Under an argon atmosphere, trimethylchlorosilane (0.42 mL, 3.26 mmol) was added to a solution of **1d-OH** (141.7 mg, 0.163 mmol) in dry THF (5 mL) at 0 °C. After 10 min, a THF (4 mL) solution of *p*-$CH_3C_6H_4MgBr$ prepared from *p*-$CH_3C_6H_4Br$ (0.60 mL, 4.876 mmol) and Mg (84.7 mg, 3.484

mmol) was added to the reaction and the resulting mixture was heated at 65 °C for 2 h. After cooling to room temperature, the reaction mixture was washed with water (50 mL × 3) and the organic phase was dried over Na_2SO_4. After removal of the solvent in vacuo, the residue was purified through a silica gel column (CH_2Cl_2: *n*-hexane = 1:5 as eluent). Recrystallization from CH_2Cl_2/MeOH gave **1d** as yellow solids (38.2 mg, 0.041 mmol, 25% yield). ^{1}H NMR (700 MHz, $CDCl_3$, 298 K) δ = 7.88 (br, 3H, $C_6H_4NEt_2$), 7.36 (br, 3H, $C_6H_4NEt_2$), 6.86 (br, 6H, $C_6H_4NEt_2$), 6.13 (d, *J* = 8.1 Hz, 2H, C_6H_4Me), 4.36 (d, *J* = 8.1 Hz, 2H, C_6H_4Me), 3.51 (q, *J* = 7.0 Hz, 12H, $C_6H_4N(CH_2CH_3)_2$), 2.77-2.70 (m, 12H, *β*-$N(CH_2CH_3)_2$), 1.81 (s, 3H, C_6H_4Me), 1.28 (t, *J* = 7.0 Hz, 18H, $C_6H_4N(CH_2CH_3)_2$), and 1.04 (t, *J* = 7.4 Hz, 18H, *β*-$N(CH_2CH_3)_2$) ppm. ^{13}C NMR (176 MHz, $CDCl_3$) δ = 147.8, 137.7, 136.5, 133.7, 129.1, 126.6, 125.5, 117.5, 111.3, 44.9, 20.9, 19.3, 17.2, and 12.6 ppm. (The signals of the two carbons were observed as broad peaks, whose chemical shifts were difficult to note.) UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 314 (50000), 382 (102000) and 466 (16000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 851.5927, calcd for $(C_{57}H_{72}BN_6)^+$ = 851.5915 ([*M*-Tol]$^+$).

Synthesis of 2d-SbF_6



In a glovebox, a CH_2Cl_2 (2 mL) solution of $AgSbF_6$ (7.60 mg, 0.022 mmol) was added to a CH_2Cl_2 (2 mL) solution of **1d** (20.8 mg, 0.022 mmol) at room temperature. The resulting mixture was stirred overnight and filtered. The solvent was then removed under reduced pressure. Recrystallization from CH_2Cl_2/hexane gave **2d-SbF_6** as orange solids (16.4 mg, 0.015 mmol, 68% yield). ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K) δ = 7.66 (d, *J* = 8.3 Hz, 6H, $C_6H_4NEt_2$), 6.99 (d, *J* = 8.3 Hz, 6H, $C_6H_4NEt_2$), 3.58 (q, *J* = 6.5 Hz, 12H, $C_6H_4N(CH_2CH_3)_2$), 3.08 (q, *J* = 7.0 Hz, 12H, *β*-$N(CH_2CH_3)_2$), 1.32 (t, *J* = 6.5 Hz, 18H, $C_6H_4N(CH_2CH_3)_2$), and 1.17 (t, *J* = 7.0 Hz, 18H, *β*-$N(CH_2CH_3)_2$). ^{13}C NMR (101 MHz, CD_2Cl_2) δ = 149.4, 145.9, 134.3, 132.8, 125.1, 119.9, 111.4, 45.0, 20.0, 16.7, and 12.6 ppm. UV-Vis (CH_2Cl_2): λ_{max} (ε [M^{-1} cm^{-1}]) = 344 (126000), 420 (28000), and 512 (15000) nm. HR-MS (MALDI-TOF-MS): *m/z* = 851.5906, calcd for $(C_{57}H_{72}BN_6)^+$ = 851.5915 ([*M*-SbF_6]$^+$).

3. Copy of ^{1}H NMR and ^{13}C NMR spectra

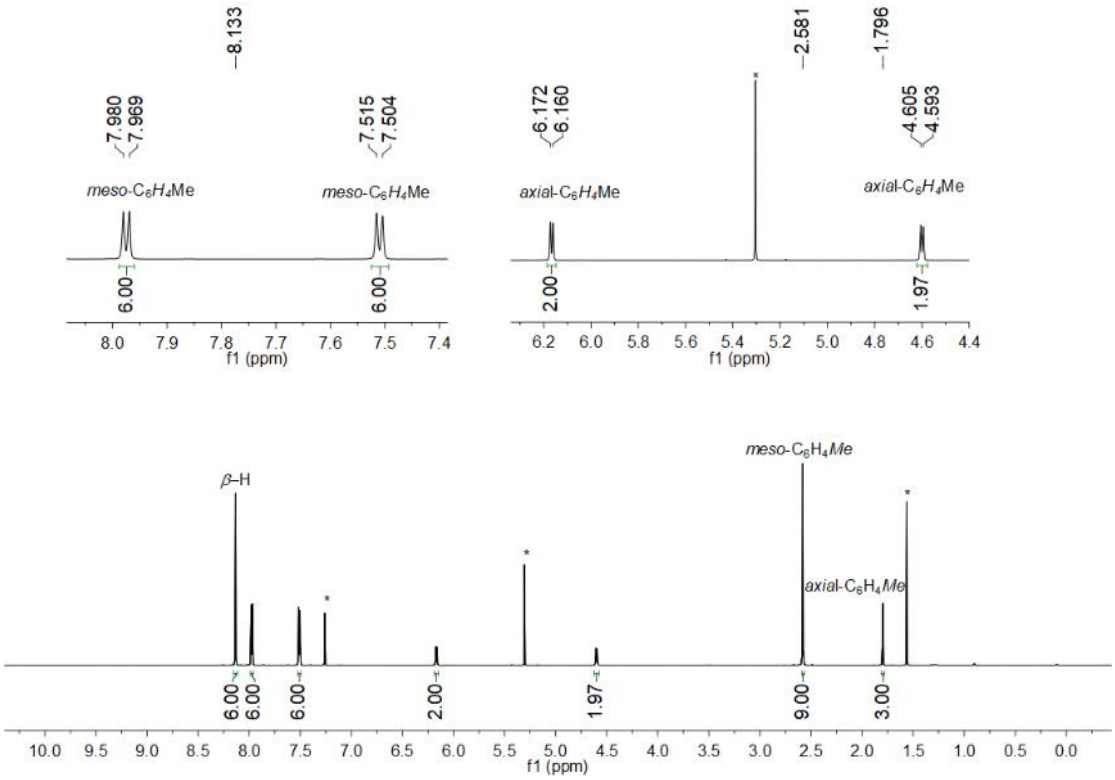


Fig. S1 ^{1}H NMR spectrum of **1a** in $CDCl_3$. *Solvents or impurities

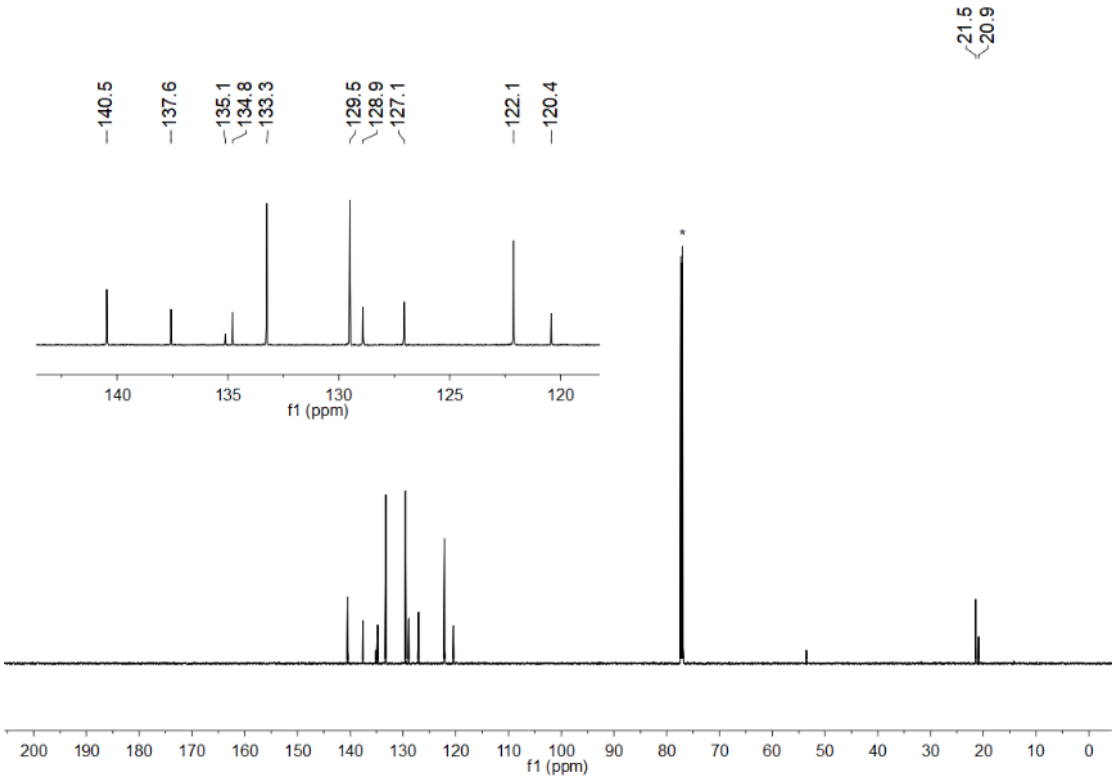


Fig. S2 ^{13}C NMR spectrum of **1a** in $CDCl_3$. *Solvents or impurities

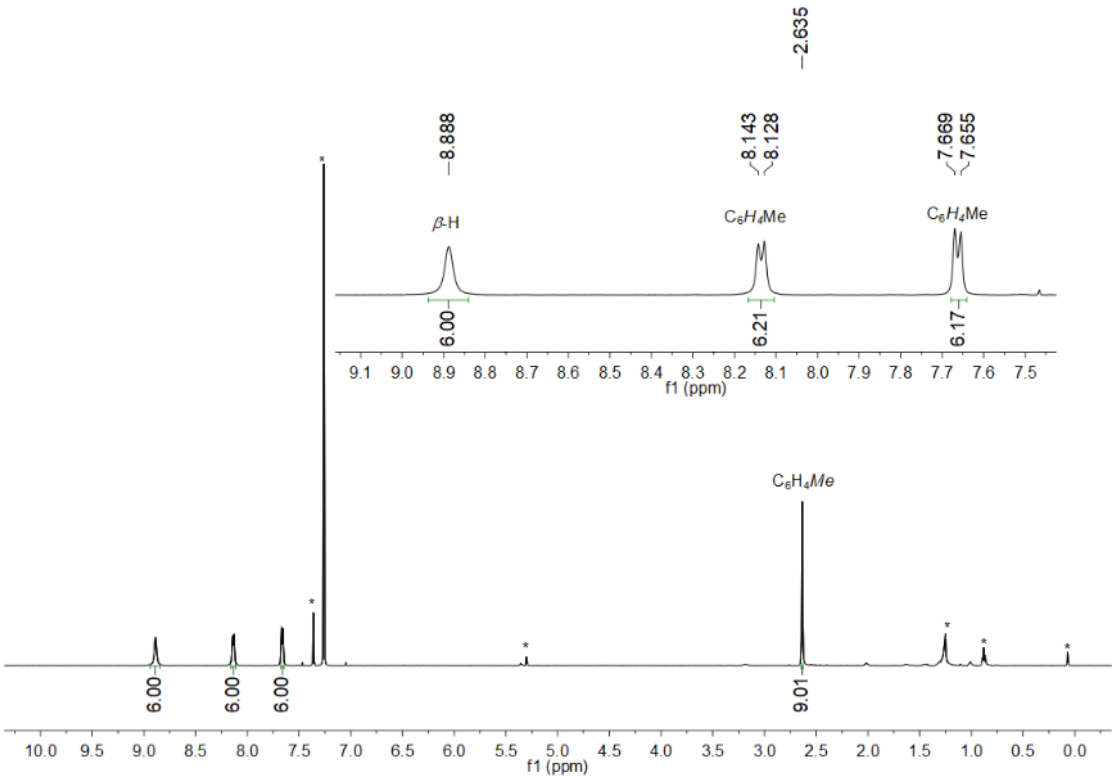


Fig. S3 ^{1}H NMR spectrum of **2a-SbCl$_6$** in $CDCl_3$. *Solvents or impurities

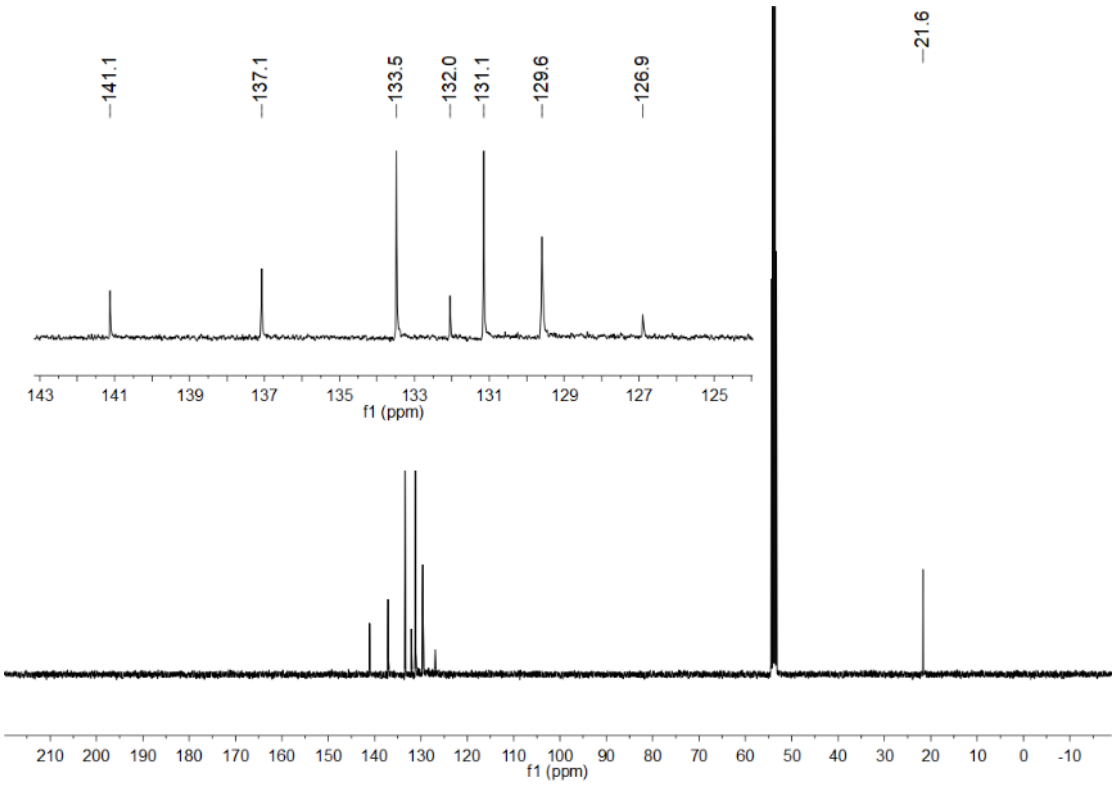


Fig. S4 ^{13}C NMR spectrum of **2a-SbCl$_6$** in CD_2Cl_2. *Solvents or impurities

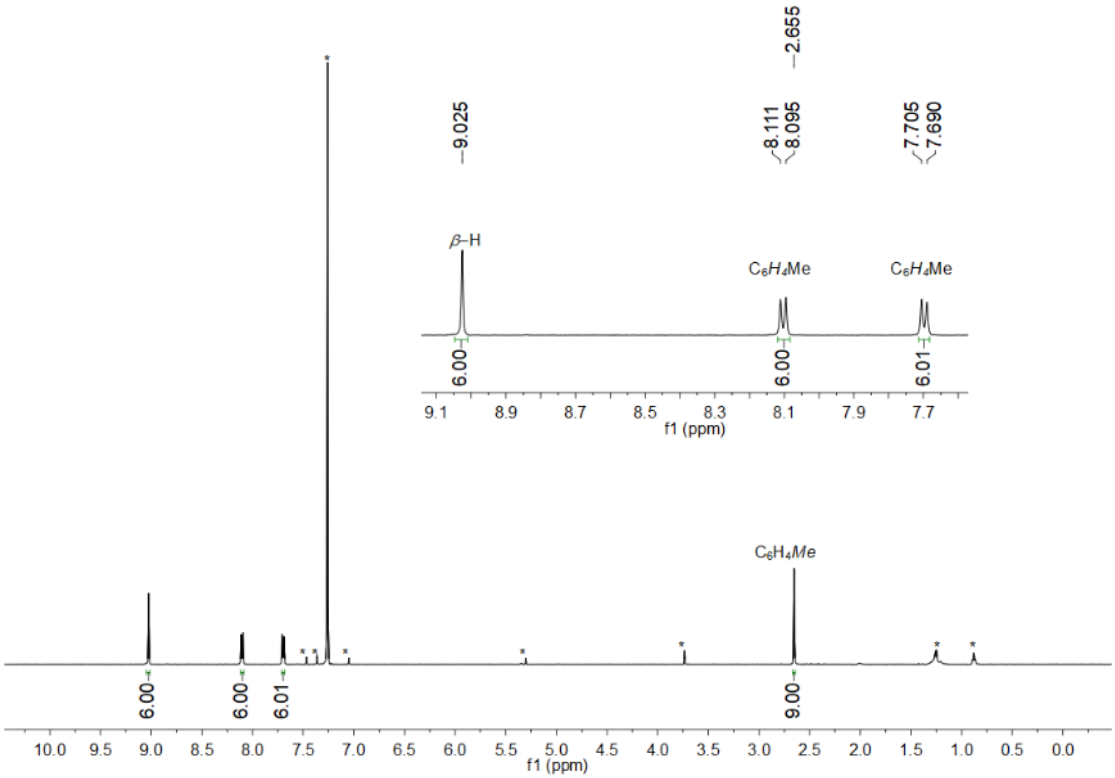


Fig. S5 ^{1}H NMR spectrum of **2a-BAr^{F}** in $CDCl_3$. *Solvents or impurities

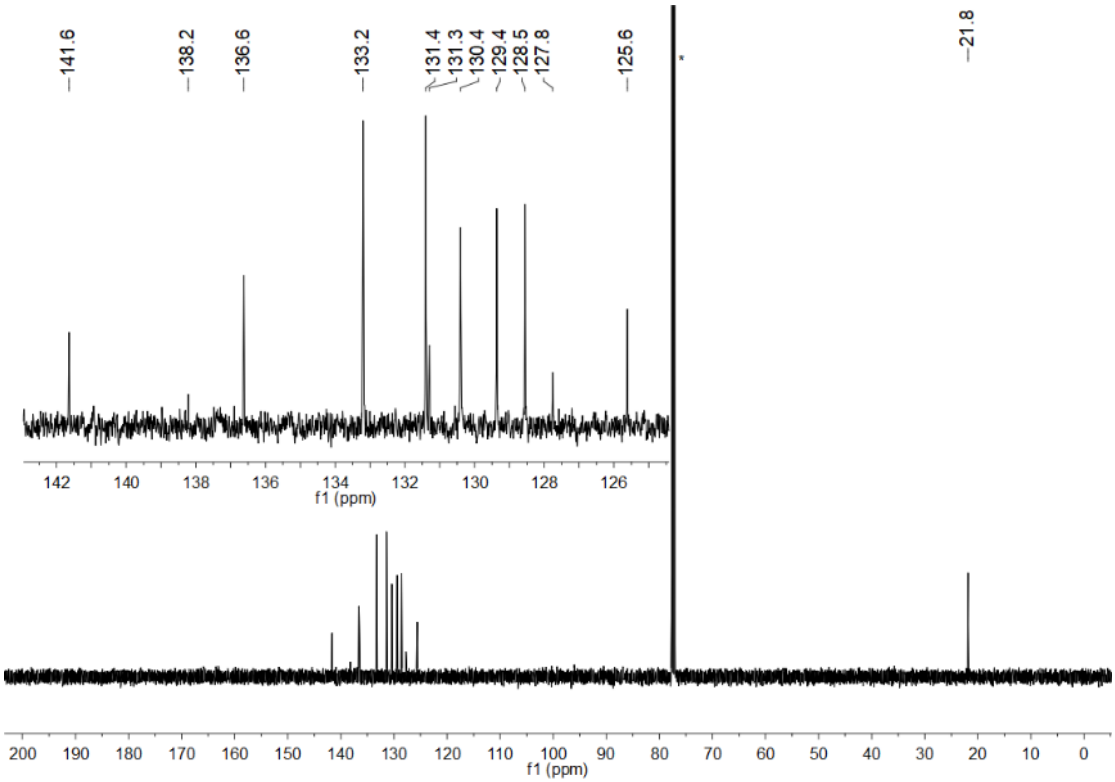


Fig. S6 ^{13}C NMR spectrum of **2a-BAr^{F}** in $CDCl_3$. *Solvents or impurities

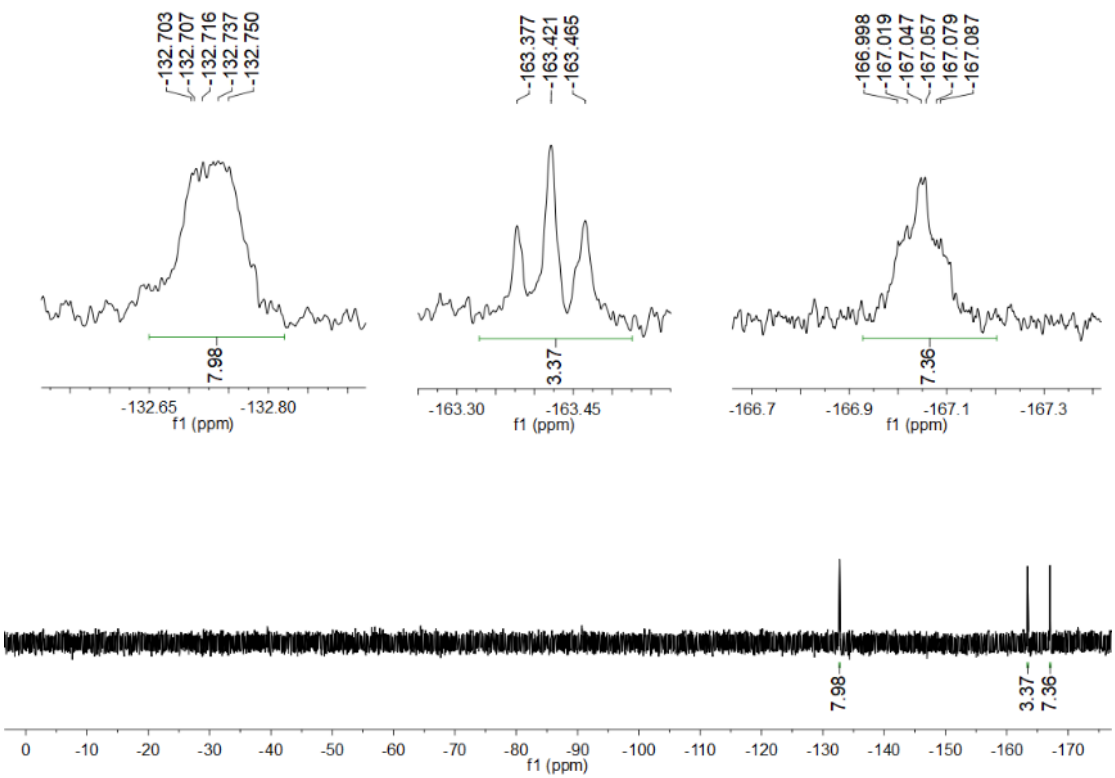


Fig. S7 ^{19}F NMR spectrum of **2a-BAr^{F}** in $CDCl_3$. *Solvents or impurities

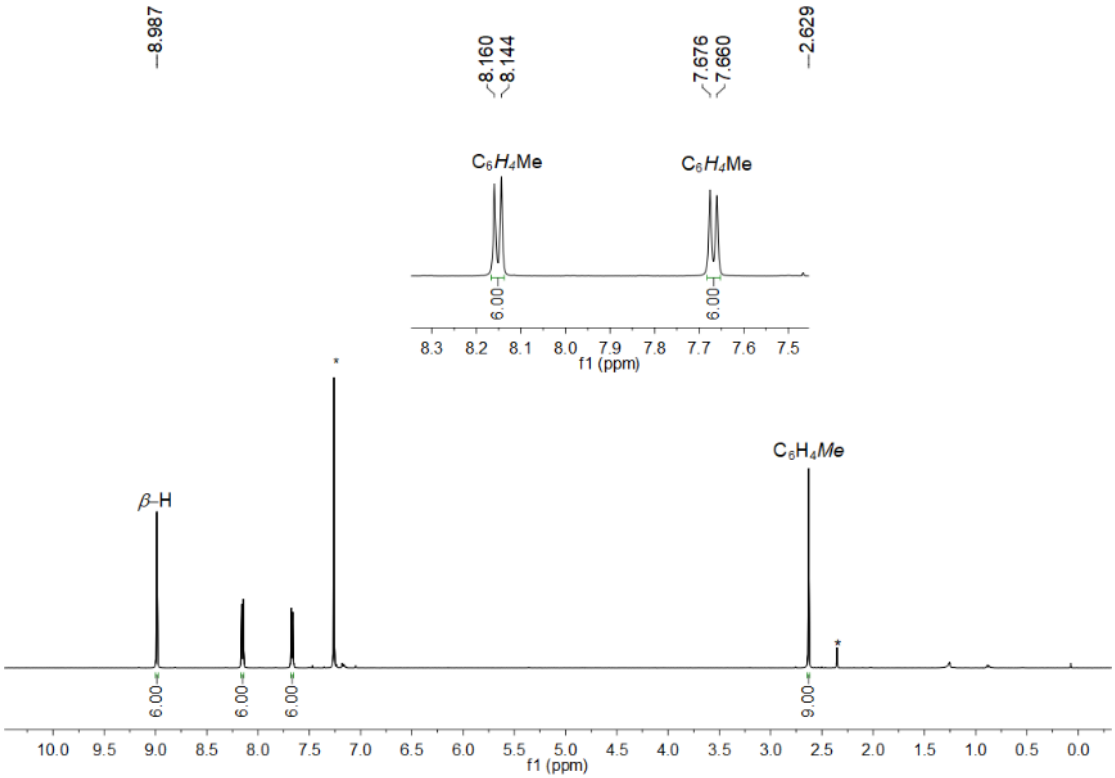


Fig. S8 ^{1}H NMR spectrum of **2a-SbF$_6$** in $CDCl_3$. *Solvents or impurities

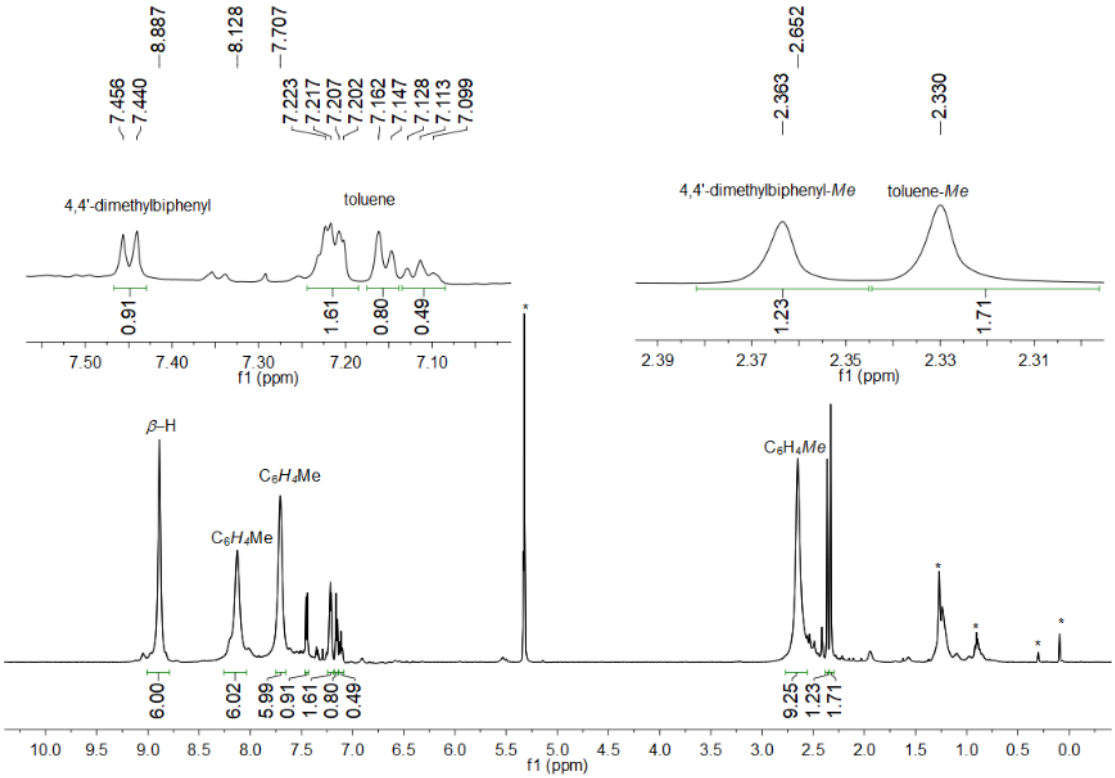


Fig. S9 *In situ* ^{1}H NMR spectrum of **1a** with $AgSbF_6$ (1 eq.) in CD_2Cl_2. *Solvents or impurities

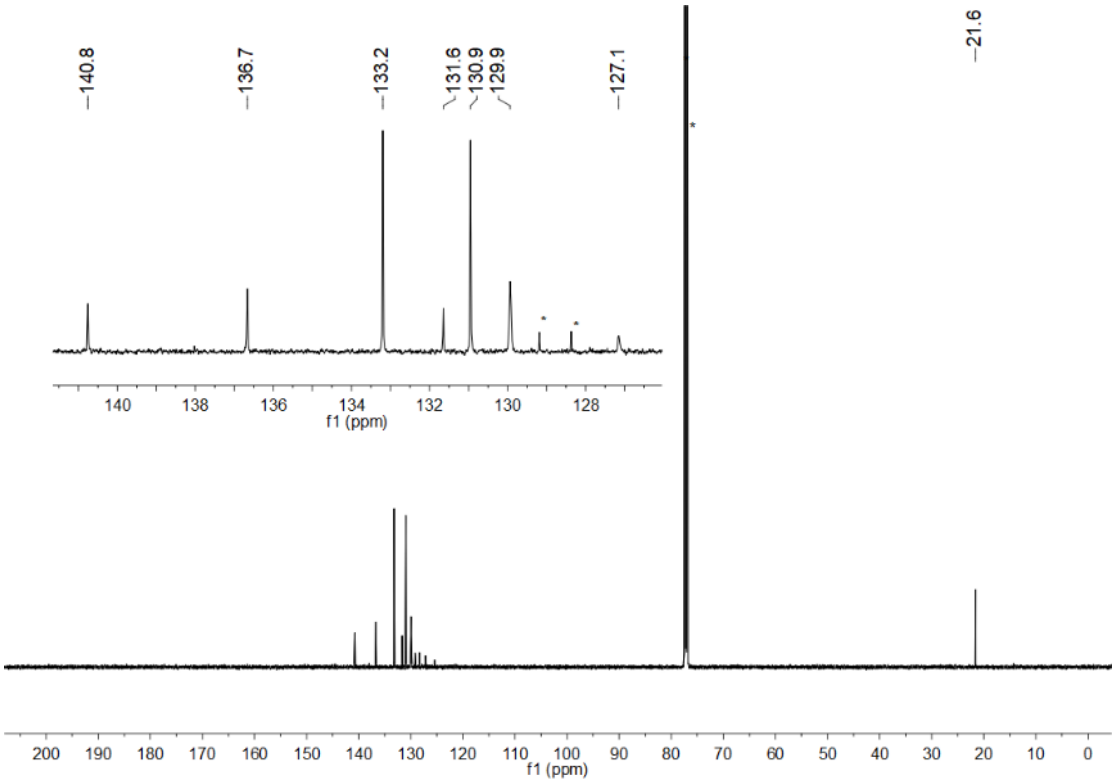


Fig. S10 ^{13}C NMR spectrum of **2a-SbF$_6$** in $CDCl_3$. *Solvents or impurities

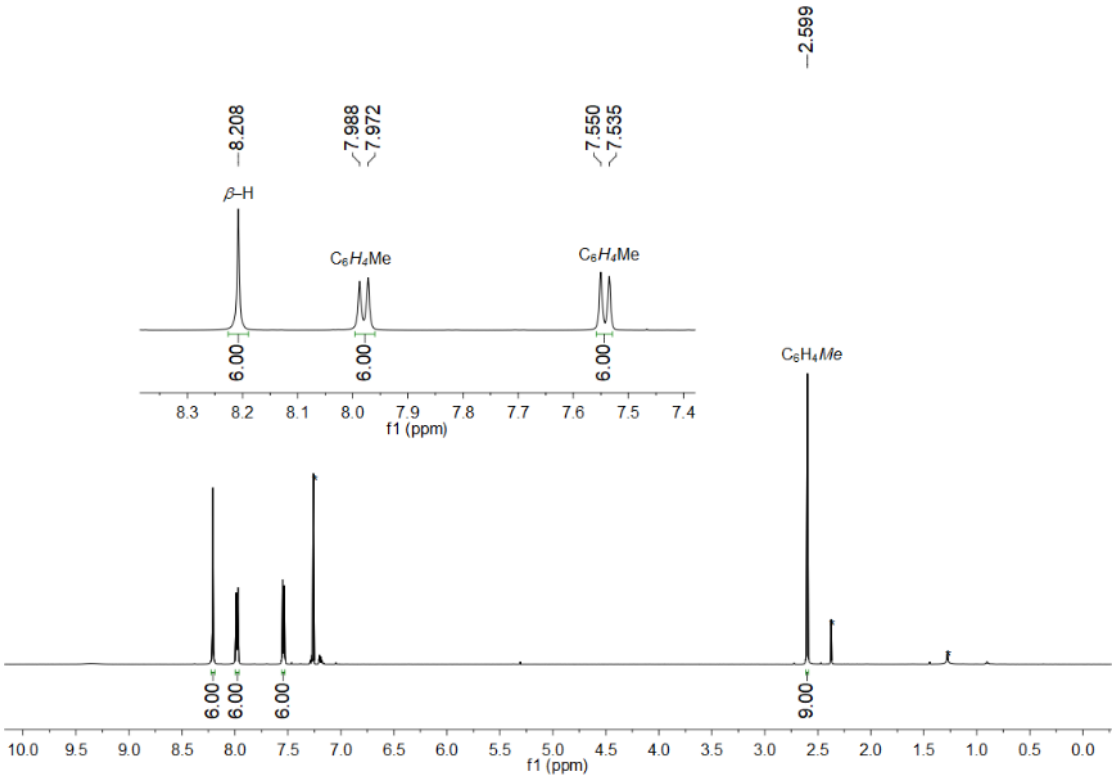


Fig. S11 ^{1}H NMR spectrum of **3a** in $CDCl_3$. *Solvents or impurities

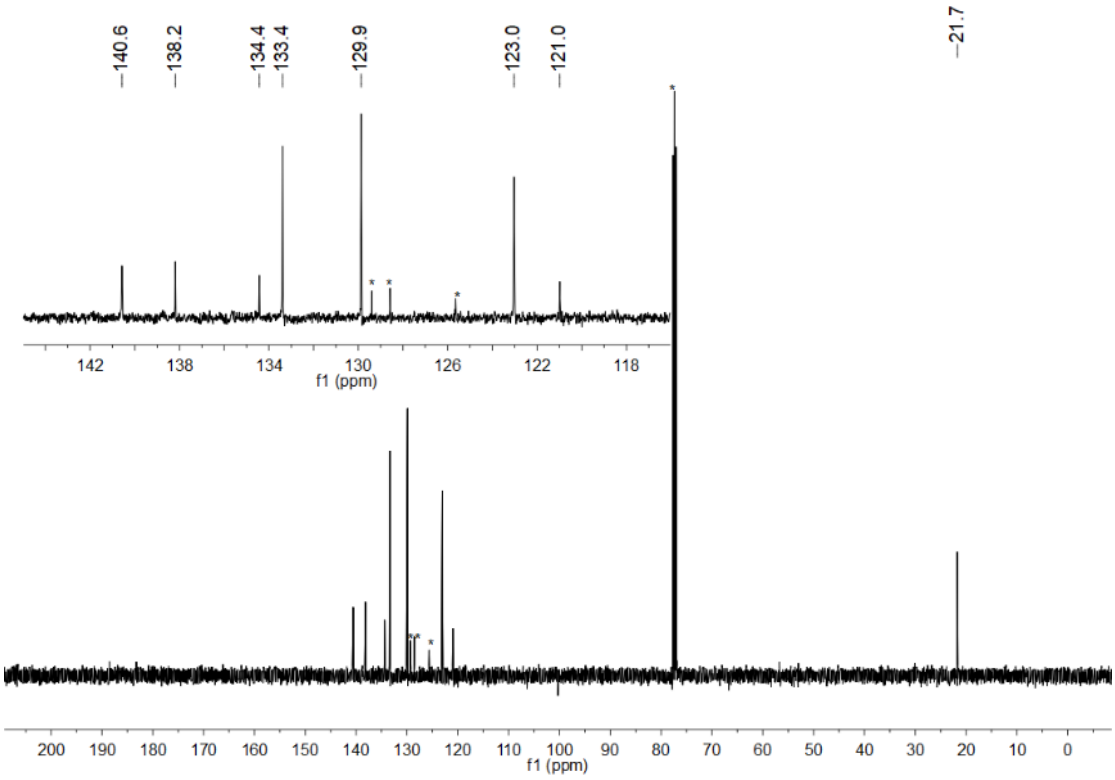


Fig. S12 ^{13}C NMR spectrum of **3a** in $CDCl_3$. *Solvents or impurities

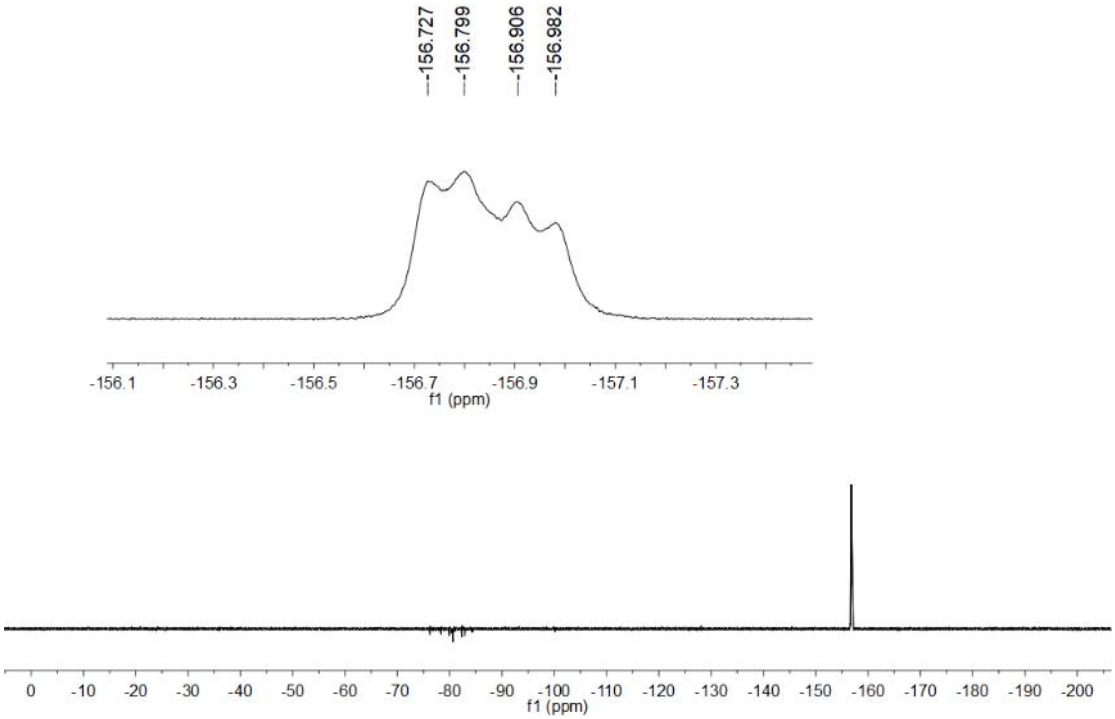


Fig. S13 ^{19}F NMR spectrum of **3a** in $CDCl_3$. *Solvents or impurities

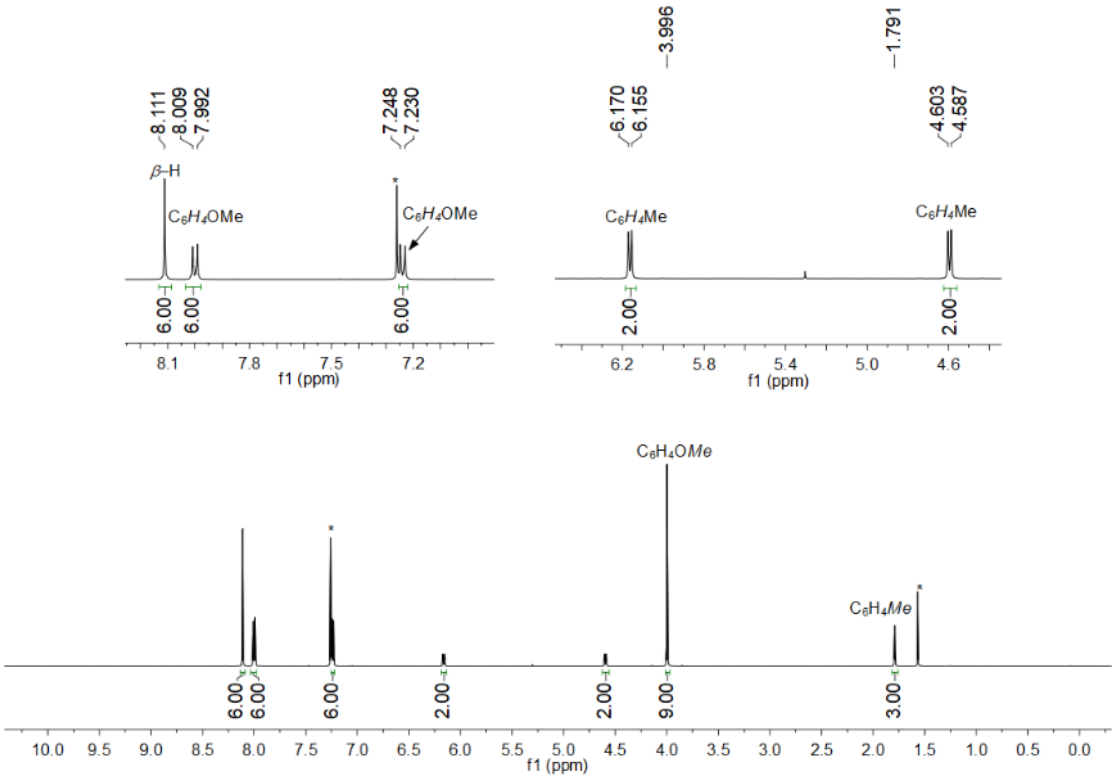


Fig. S14 ^{1}H NMR spectrum of **1b** in $CDCl_3$. *Solvents or impurities

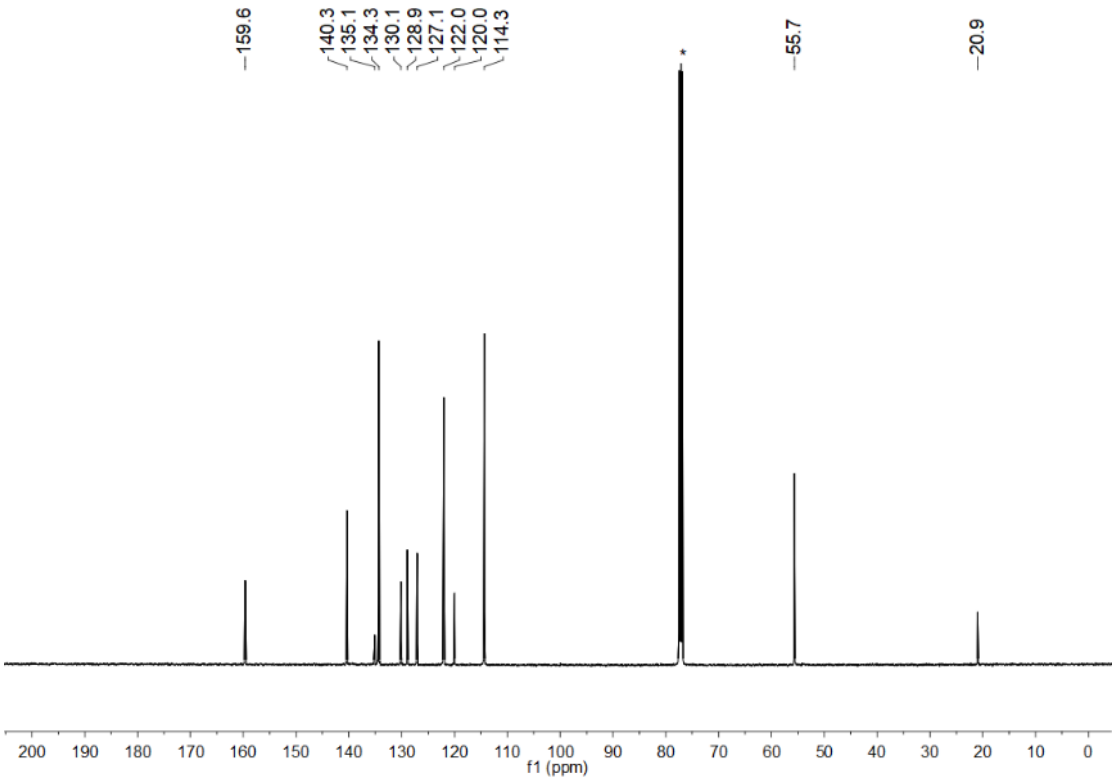


Fig. S15 ^{13}C NMR spectrum of **1b** in $CDCl_3$. *Solvents or impurities

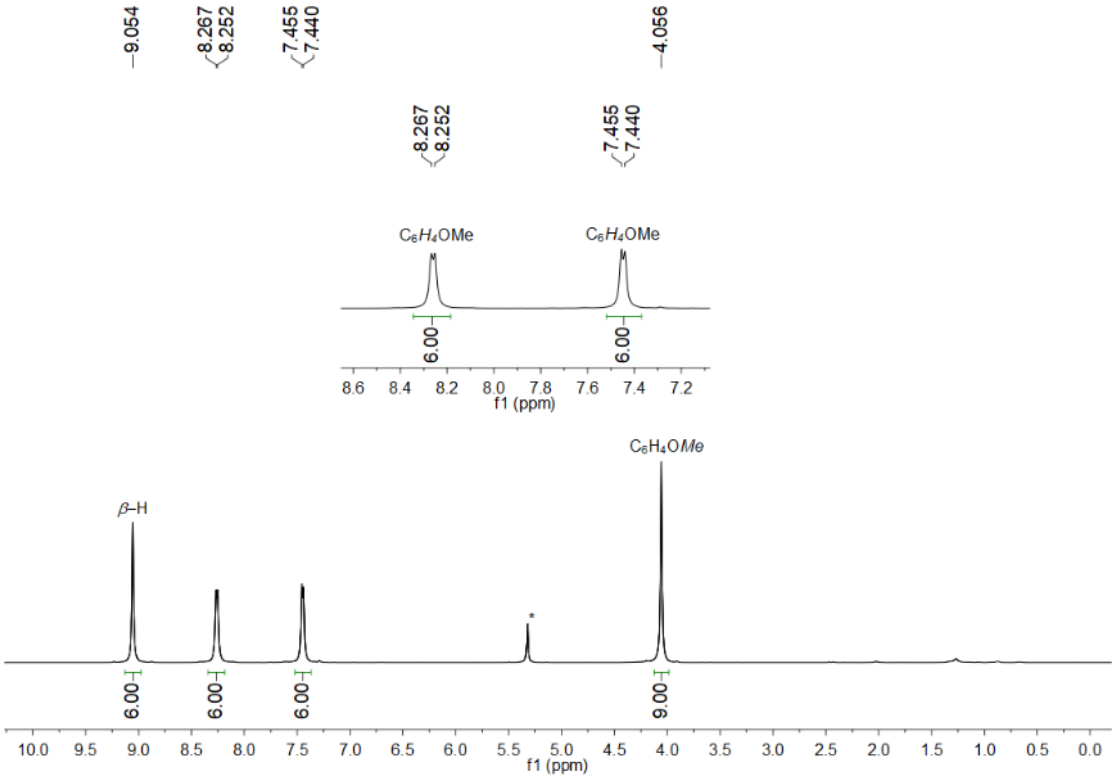


Fig. S16 ^{1}H NMR spectrum of **2b-SbF$_6$** in CD_2Cl_2. *Solvents or impurities

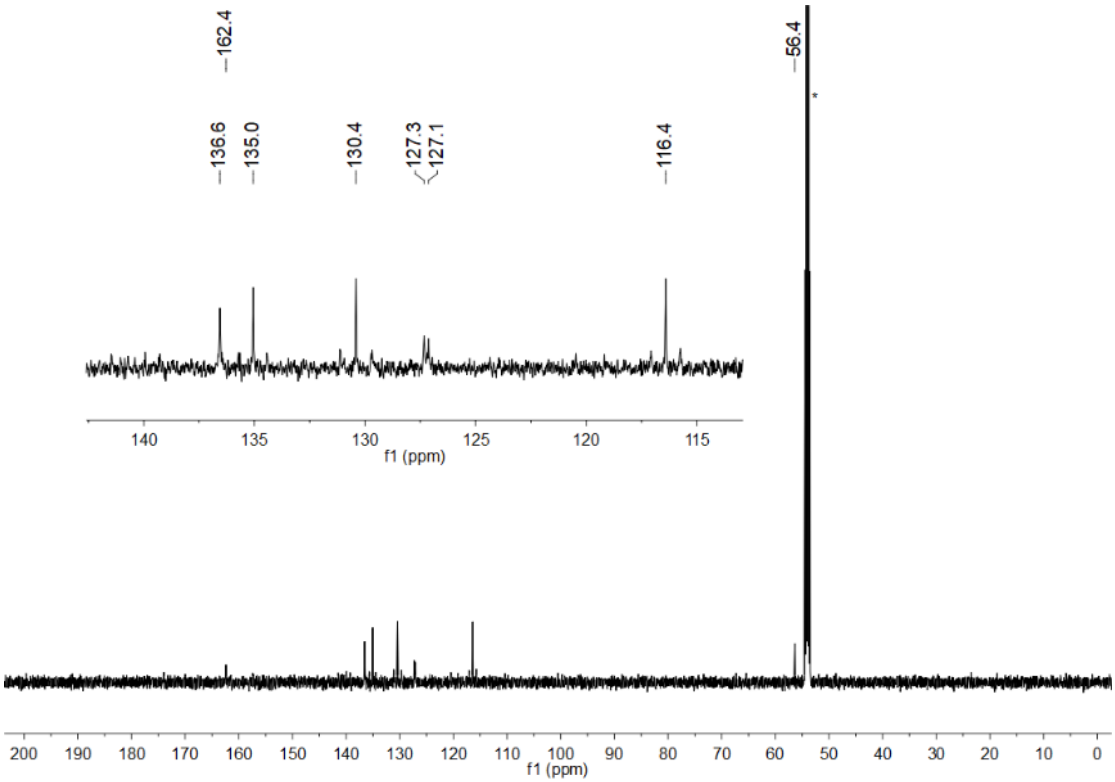


Fig. S17 ^{13}C NMR spectrum of **2b-SbF$_6$** in CD_2Cl_2. *Solvents or impurities

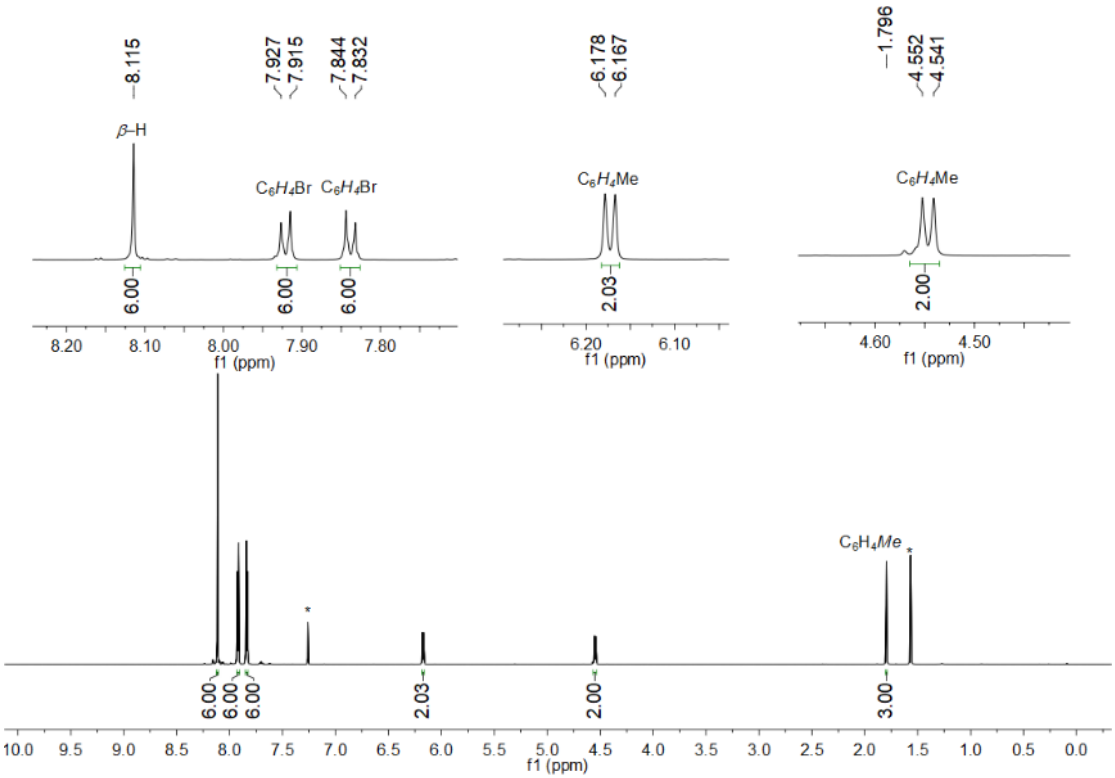


Fig. S18 ^{1}H NMR spectrum of **1c-Br** in $CDCl_3$. *Solvents or impurities

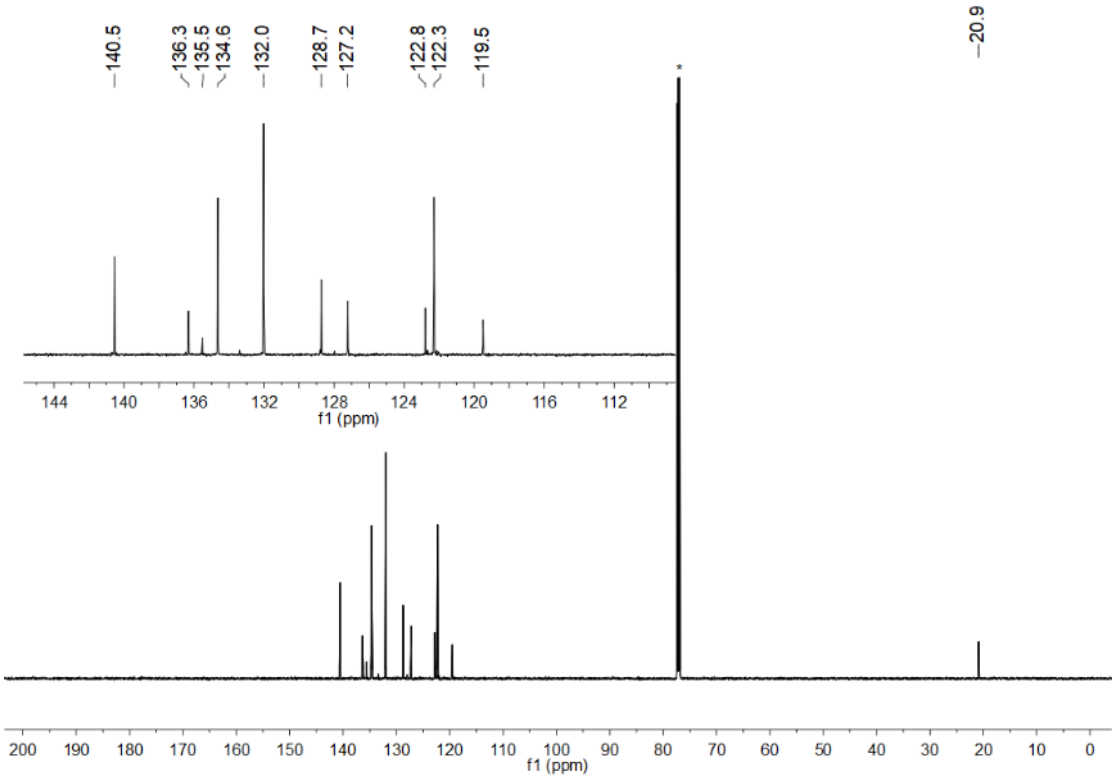


Fig. S19 ^{13}C NMR spectrum of **1c-Br** in $CDCl_3$. *Solvents or impurities

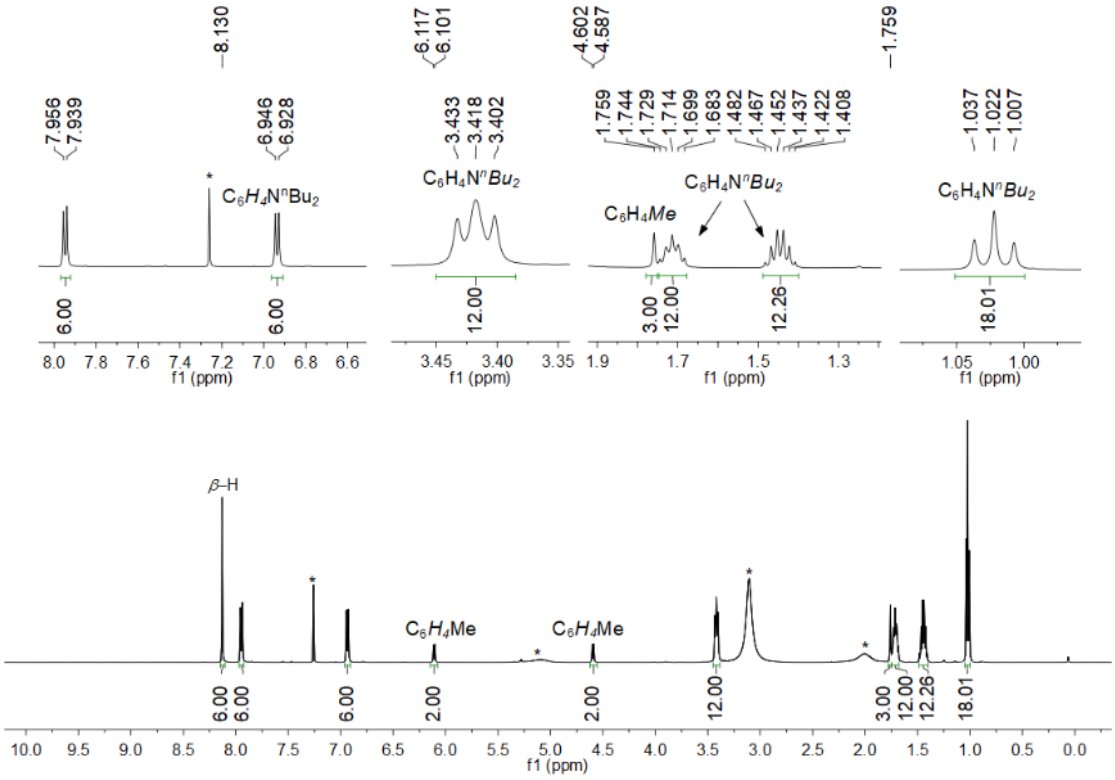


Fig. S20 ^{1}H NMR spectrum of **1c** in $CDCl_3$ ($NH_2NH_2{\cdot}H_2O$). *Solvents or impurities

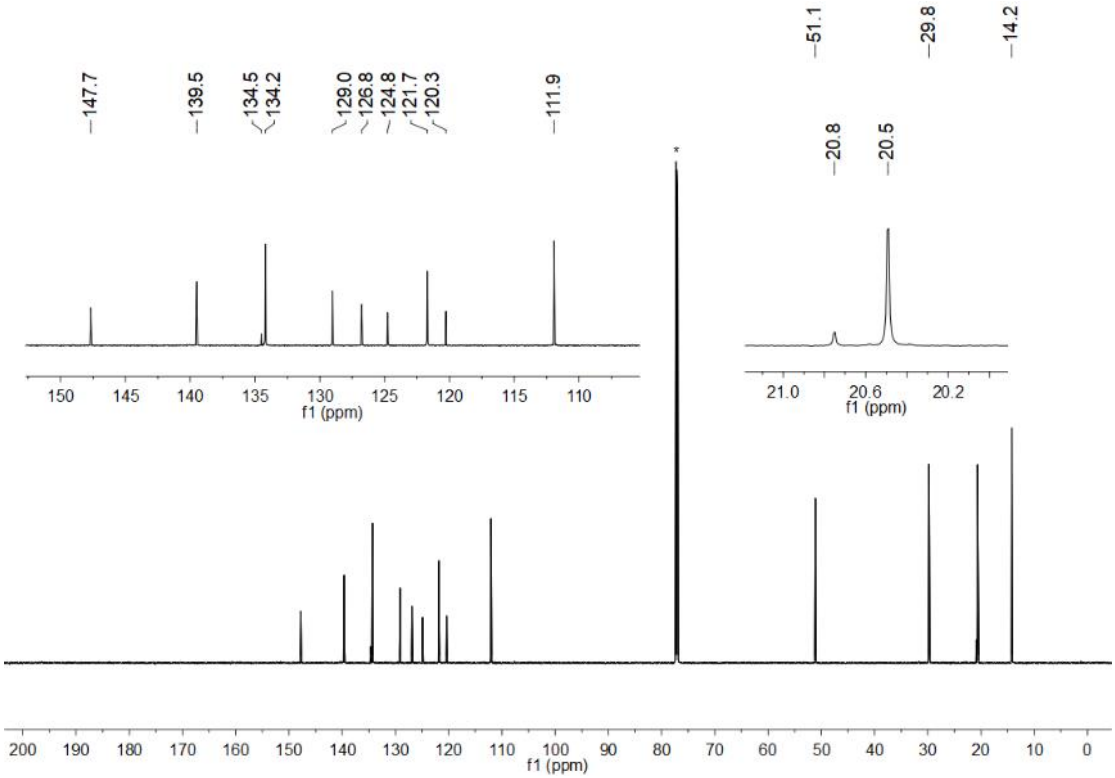


Fig. S21 ^{13}C NMR spectrum of **1c** in $CDCl_3$ ($NH_2NH_2{\cdot}H_2O$). *Solvents or impurities

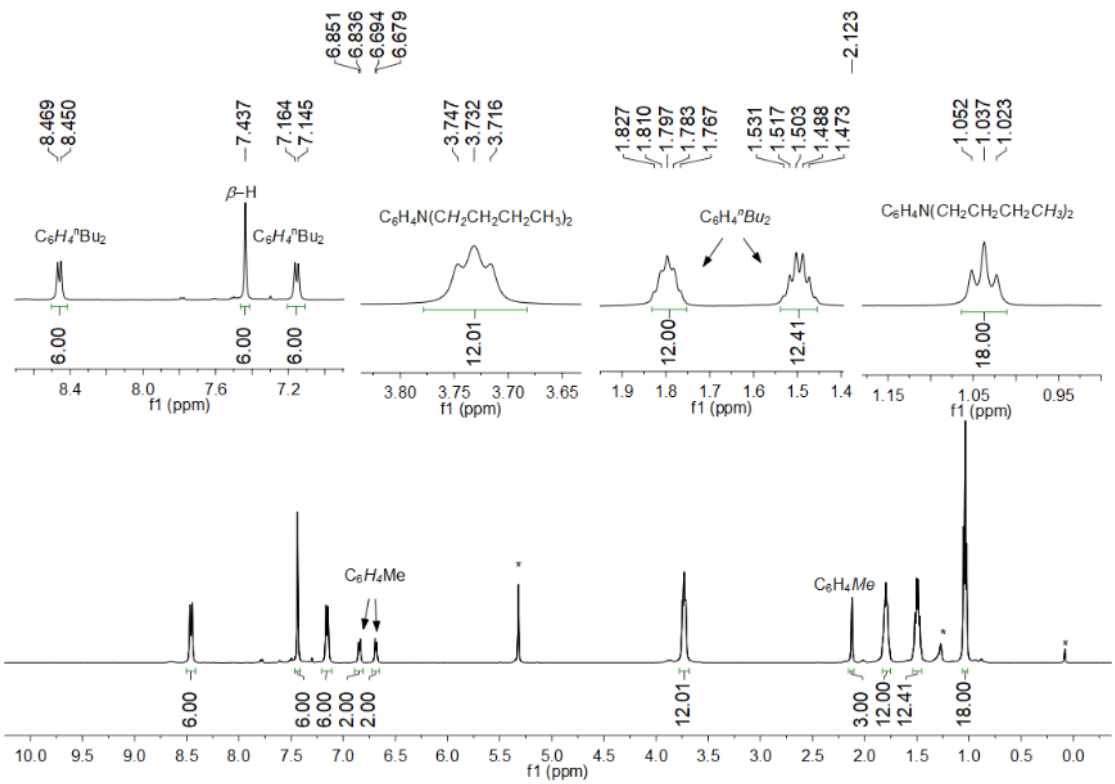


Fig. S22 ^{1}H NMR spectrum of **7c** in CD_2Cl_2. *Solvents or impurities

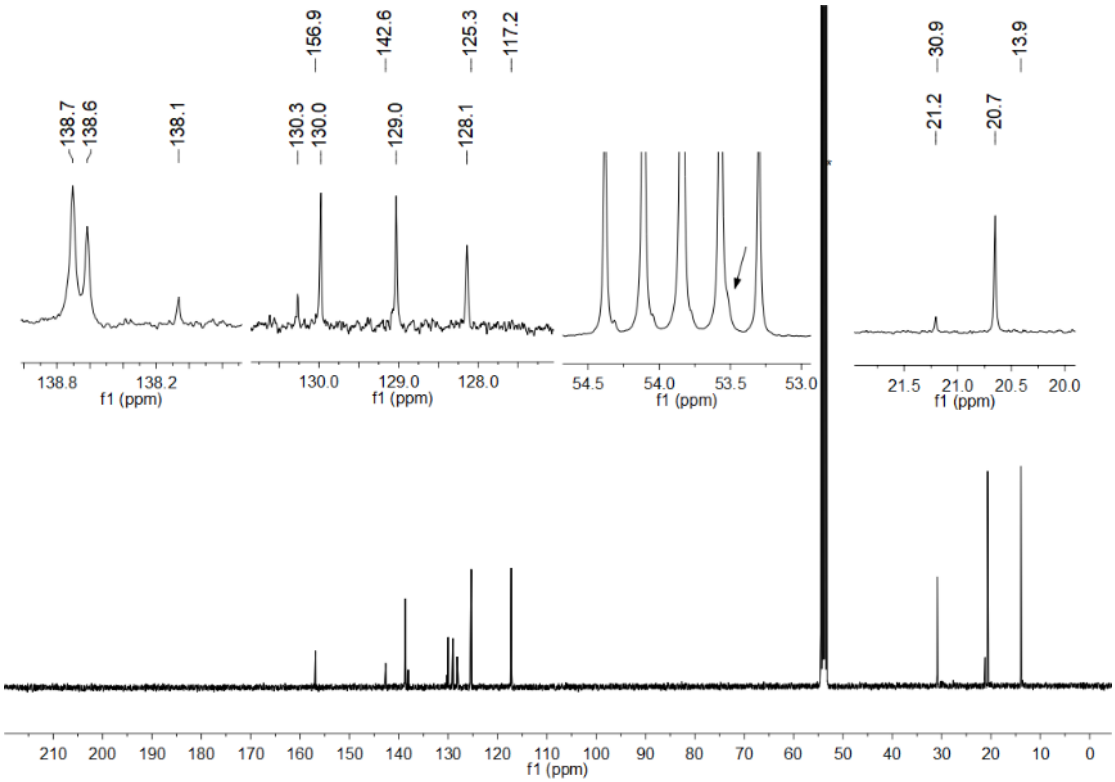
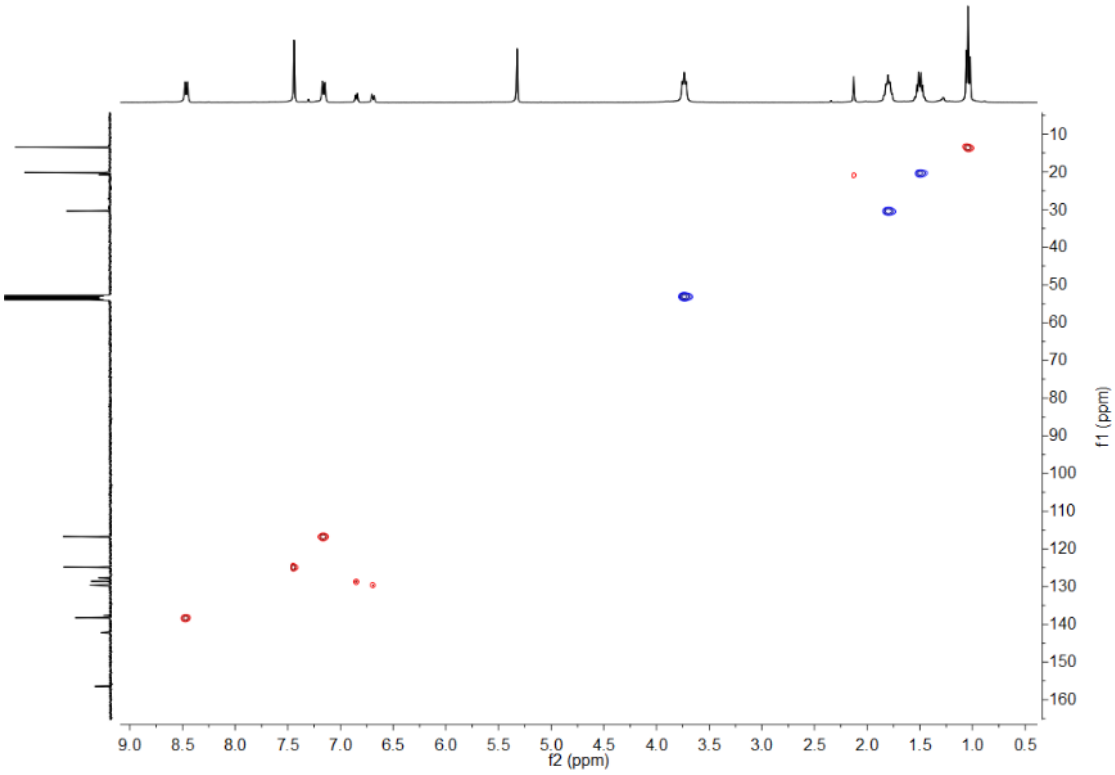


Fig. S23 ^{13}C NMR spectrum of **7c** in CD_2Cl_2. *Solvents or impurities



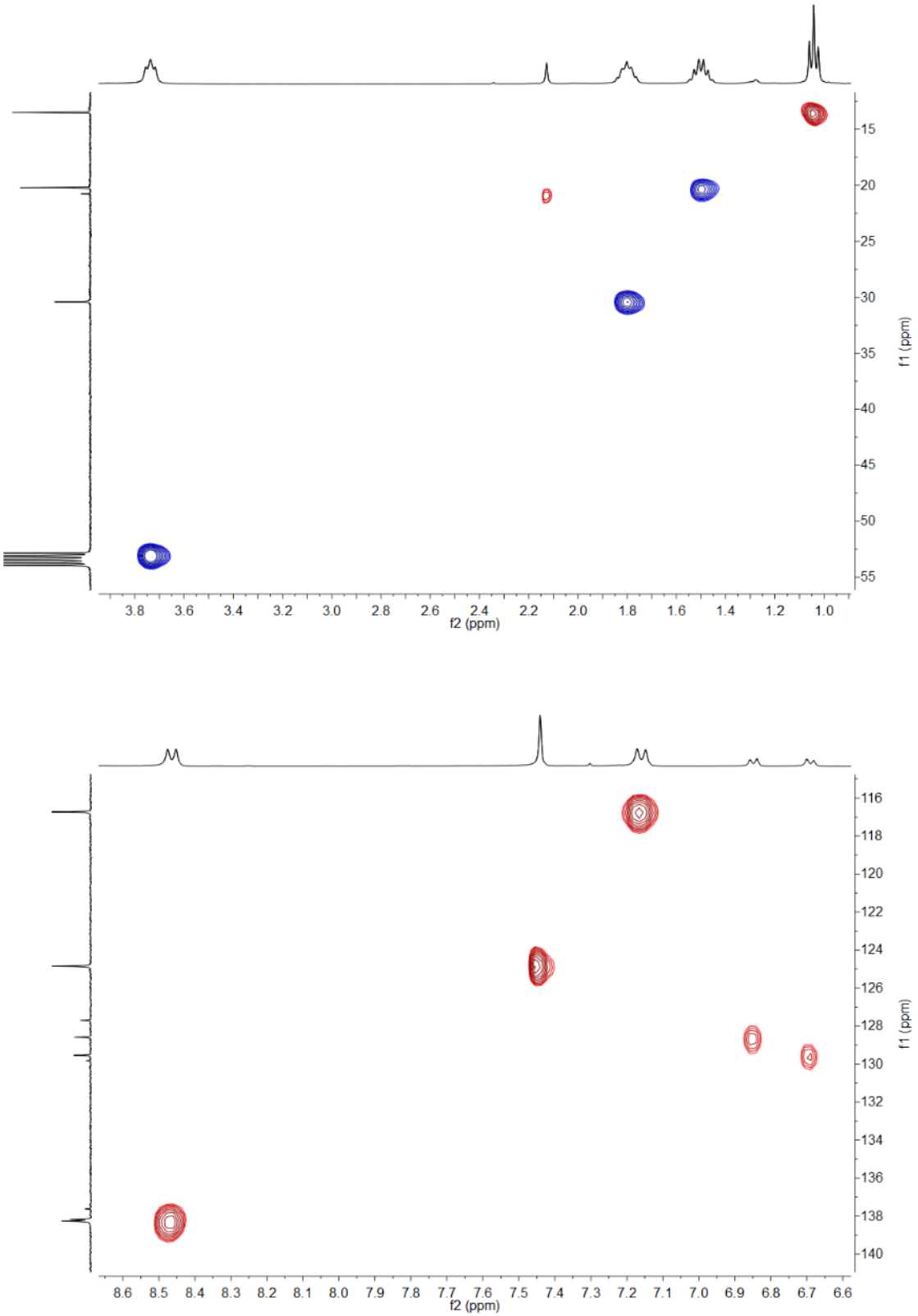


Fig. S24 Phase sensitive HSQC spectrum of **7c** in CD_2Cl_2. Red signals indicate the signals of CH and CH_3 while blue signals indicate signals of CH_2.

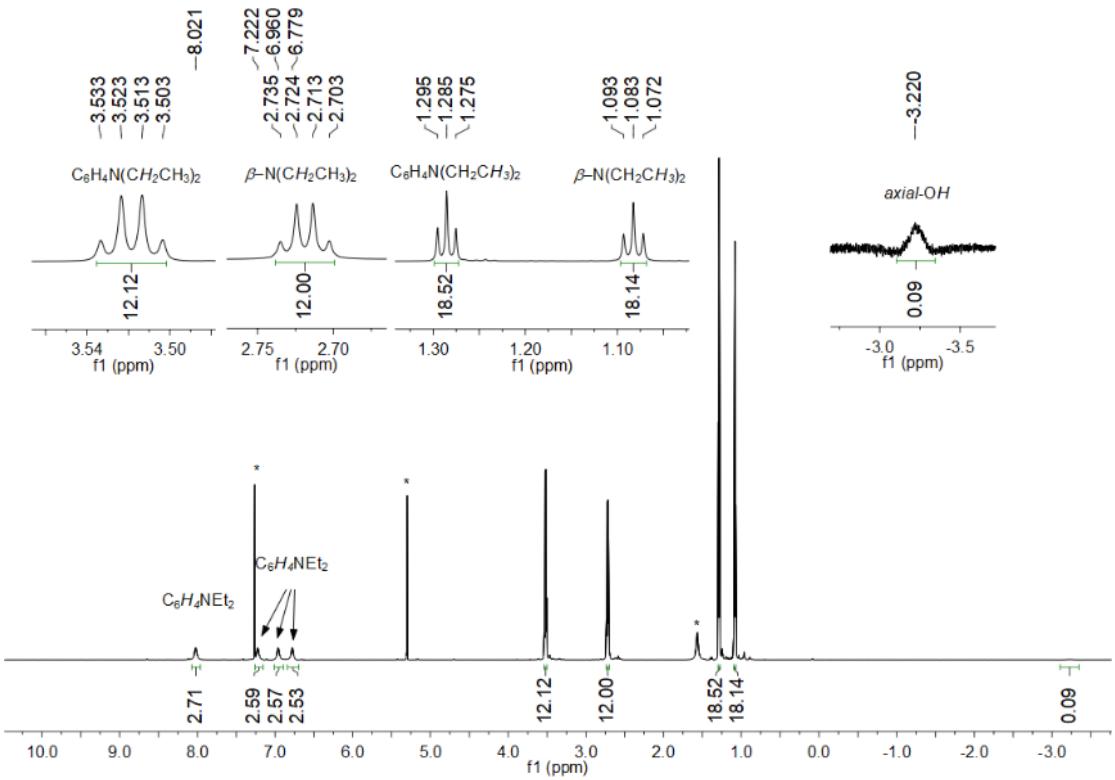


Fig. S25 ^{1}H NMR spectrum of **1d-OH** in $CDCl_3$. *Solvents or impurities

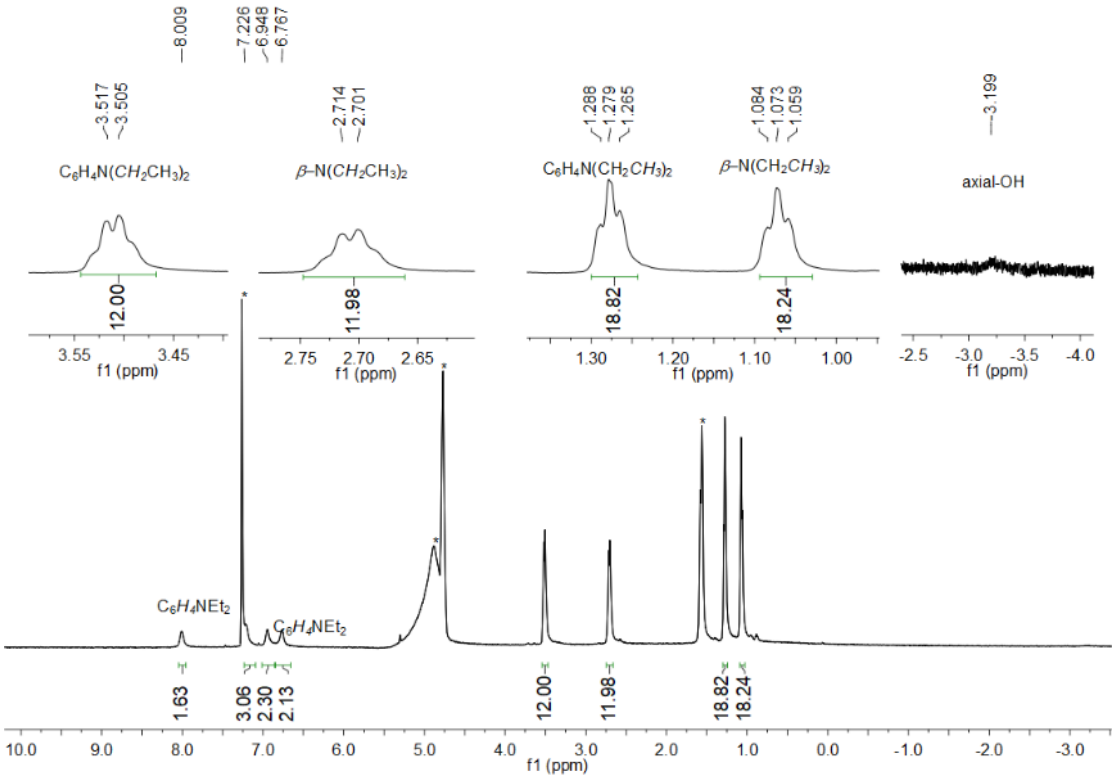


Fig. S26 ^{1}H NMR spectrum of **1d-OH** (D_2O exchange) in $CDCl_3$. *Solvents or impurities

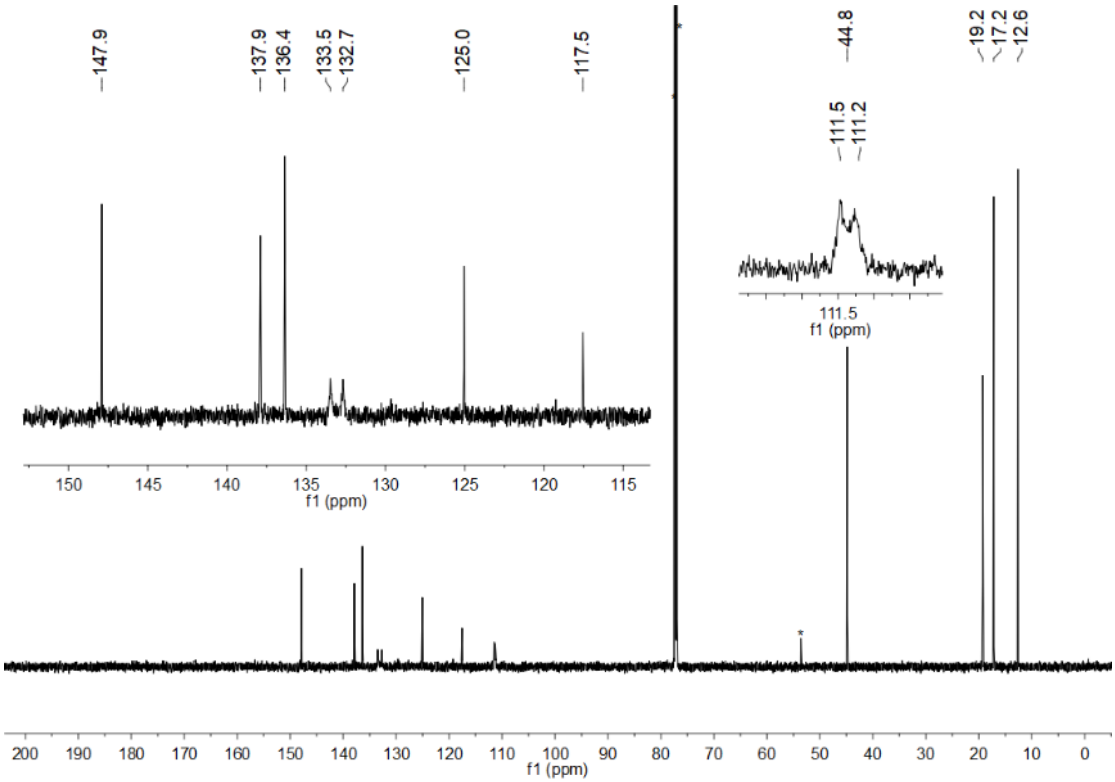


Fig. S27 ^{13}C NMR spectrum of **1d-OH** in $CDCl_3$. *Solvents or impurities

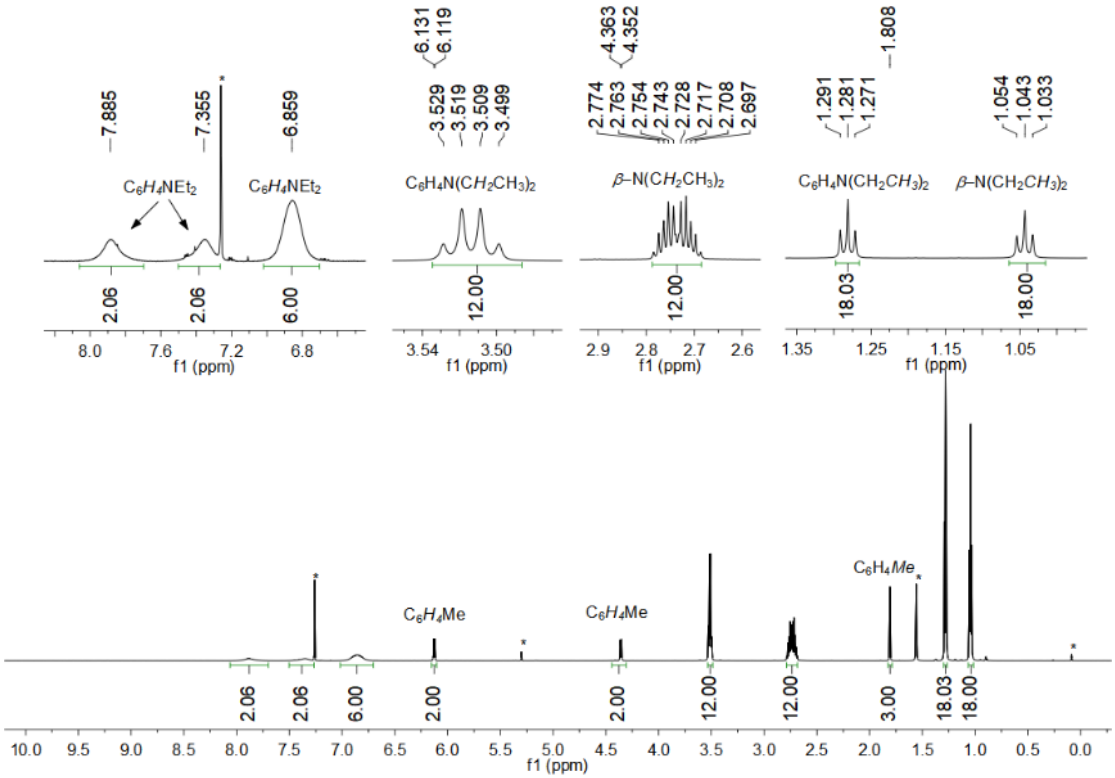


Fig. S28 ^{1}H NMR spectrum of **1d** in $CDCl_3$. *Solvents or impurities

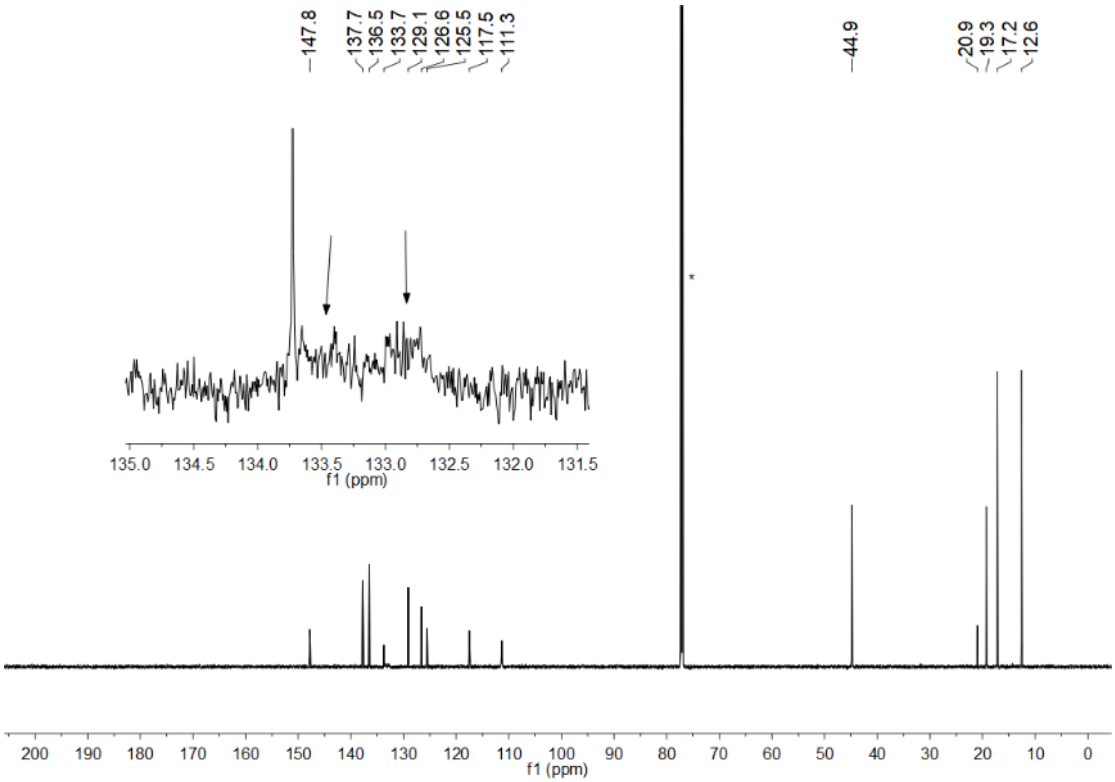


Fig. S29 ^{13}C NMR spectrum of **1d** in $CDCl_3$. *Solvents or impurities

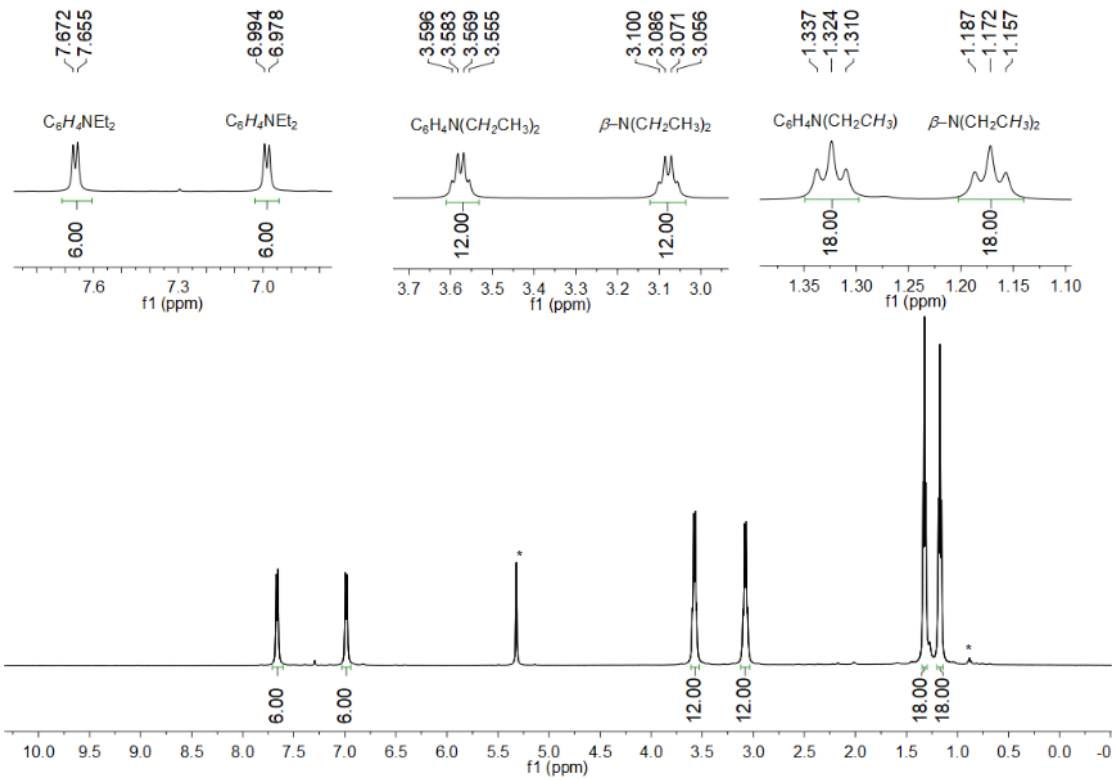


Fig. S30 ^{1}H NMR spectrum of **2d-SbF$_6$** in CD_2Cl_2. *Solvents or impurities

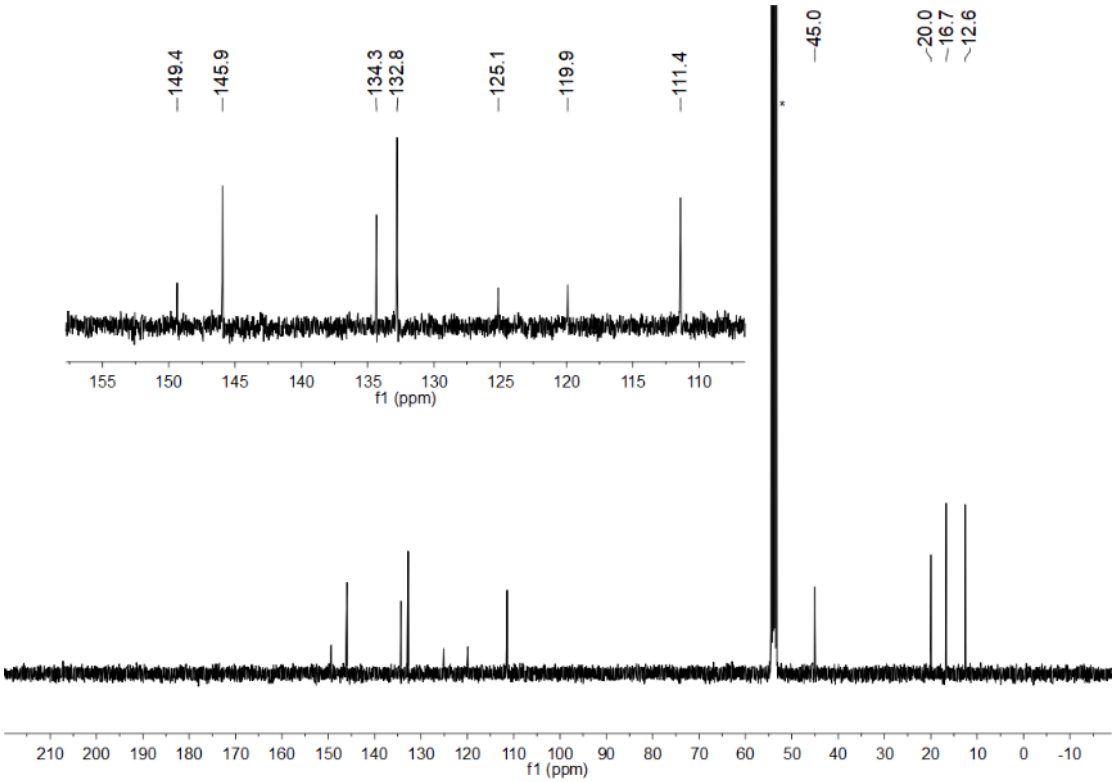


Fig. S31 ^{13}C NMR spectrum of **2d-SbF$_6$** in CD_2Cl_2. *Solvents or impurities

4. UV-Vis-NIR Absorption Spectra

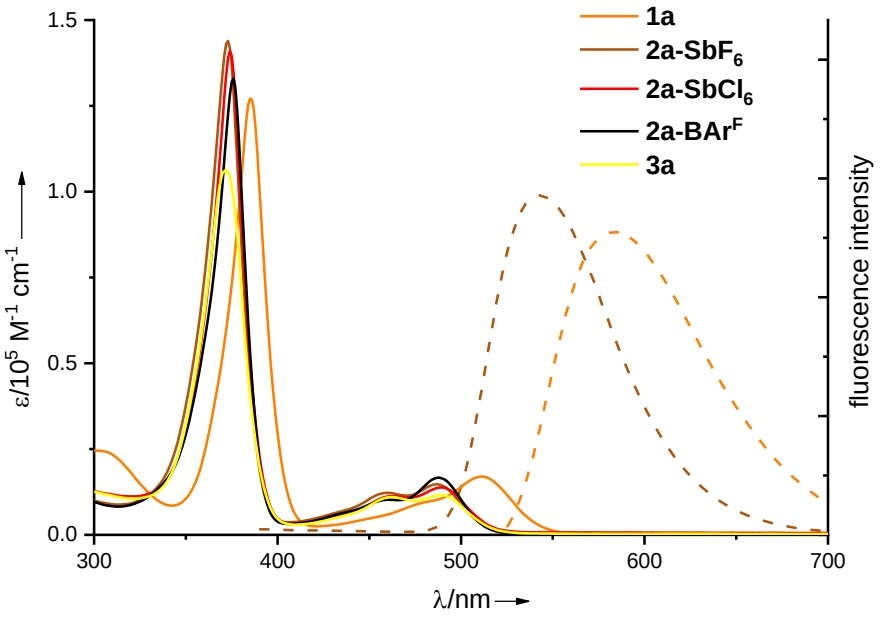


Fig. S32 UV-Vis absorption spectra of 1a, 2a-SbF$_6$, 2a-SbCl$_6$, 2a-BAr^F and **3a** and fluorescence emission spectra of **1a** and **2a-SbF$_6$**. Solid lines represent UV-Vis absorption spectra and dashed lines represent fluorescence emission spectra.

Table S1 UV-Vis absorption spectra data of **1a**, **2a-SbF$_6$**, **2a-SbCl$_6$**, **2a-BAr^F**, and **3a**.

Compound	λ/nm	$\varepsilon/10^5$ M^{-1} cm^{-1}
1a	386, 511	1.3, 0.17
2a-SbF$_6$	373, 460, 487	1.4, 0.12, 0.15
2a-BAr^F	376, 461, 488	1.3, 0.10, 0.17
3a	376, 461, 488	1.1, 0.11, 0.12
2a-SbCl$_6$	374, 463, 489	1.4, 0.11, 0.14

Table S2 Fluorescence emission spectra data of **1a** and **2a-SbF$_6$**.

Compound	λ/nm
1a	583
2a-SbF$_6$	541

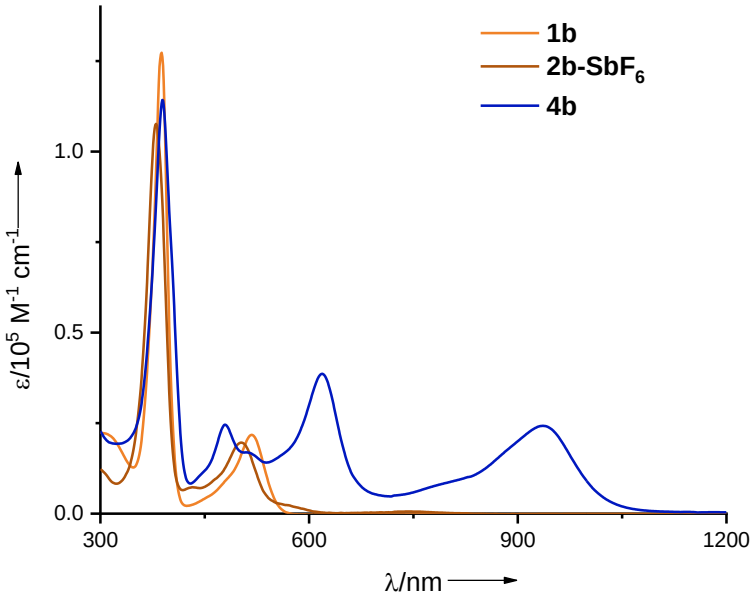


Fig. S33 UV-Vis absorption spectra of **1b**, **2b-SbF$_6$** and **4b**.

Table S3. UV-Vis absorption spectra data of **1b**, **2b-SbF$_6$** and **4b**.

Compound	λ/nm	ε / 10^5 M/cm^{-1}
1b	388, 518	1.3, 0.22
2b-SbF$_6$	380, 503	1.1, 0.20
4b	389, 479, 510, 619, 937	1.1, 0.25, 0.17, 0.39, 0.24

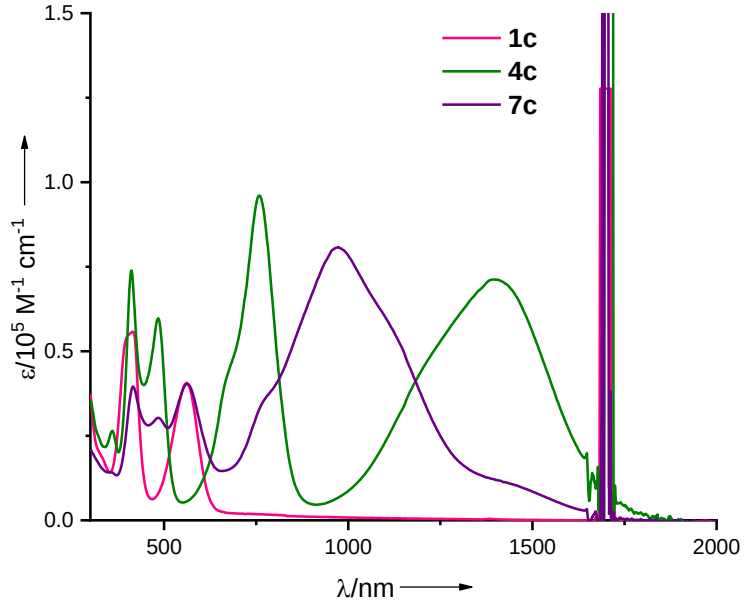


Fig. S34 UV-Vis absorption spectra of **1c**, **4c** and **7c**.

Table S4 UV-Vis absorption spectra data of **1c**, **4c** and **7c**.

Compound	λ/nm	ε / 10^5 M/cm^{-1}
1c	416, 563	0.56, 0.41
4c	360, 412, 484, 758, 1394	0.26, 0.74, 0.60, 0.96, 0.71
7c	416, 484, 562, 972	0.40, 0.30, 0.40, 0.81

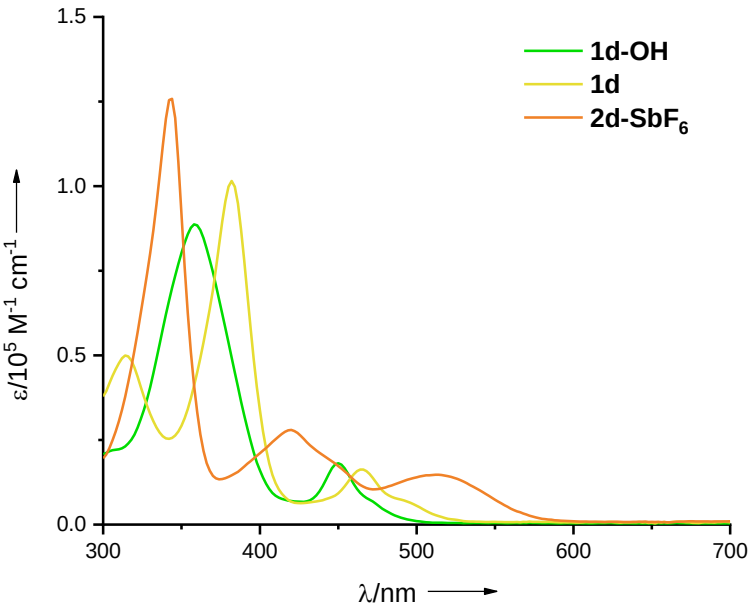


Fig. S35 UV-Vis absorption spectra of **1d-OH**, **1d** and **2d-SbF$_6$**.

Table S5 UV-Vis absorption spectra data of **1d-OH**, **1d** and **2d-SbF$_6$**.

Compound	λ/nm	ε / 10^5 M/cm^{-1}
1d-OH	358, 450	0.89, 0.18
1d	314, 382, 466	0.50, 1.02, 0.16
2d-SbF$_6$	344, 420, 512	1.26, 0.28, 0.15

5. X-ray Crystallographic Data

Using Olex2[1], structures of compound **2a-SbCl$_6$**, **2a-BAr^F**, **2a-SbF$_6$**, **3a**, **1b**, **2b-SbF$_6$**, **4b**, **1c**, **7c** and **2d-SbF$_6$** were solved with the ShelXT[2] structure solution program using intrinsic phasing and refined with the ShelXL[3] refinement package using least squares minimisation. Twin law of **2b-SbF$_6$** was found by using Platon. Disordered solvent molecules in **4b** and **7c** were treated by SQUEEZE[4] program of Platon.

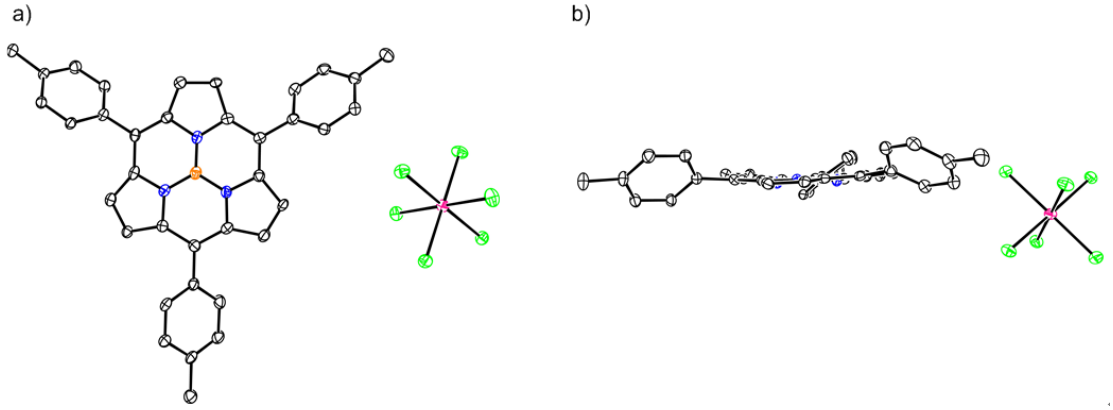


Fig. S36 X-ray crystal structure of **2a-SbCl$_6$**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

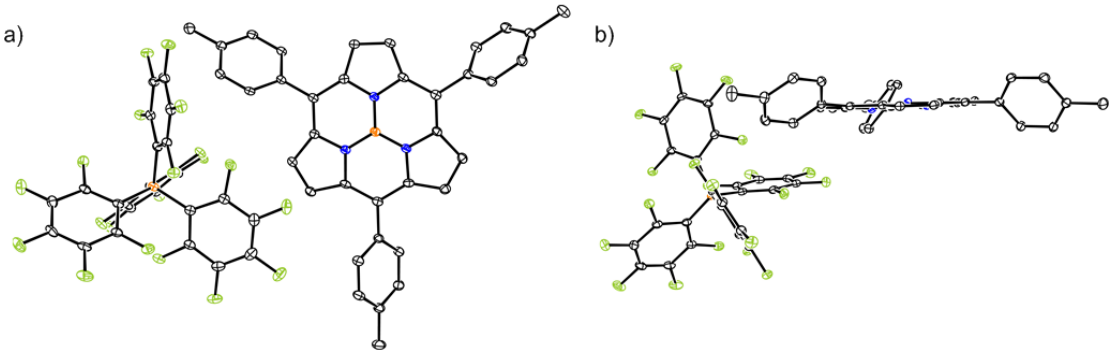


Fig. S37 X-ray crystal structure of **2a-BAr^F**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

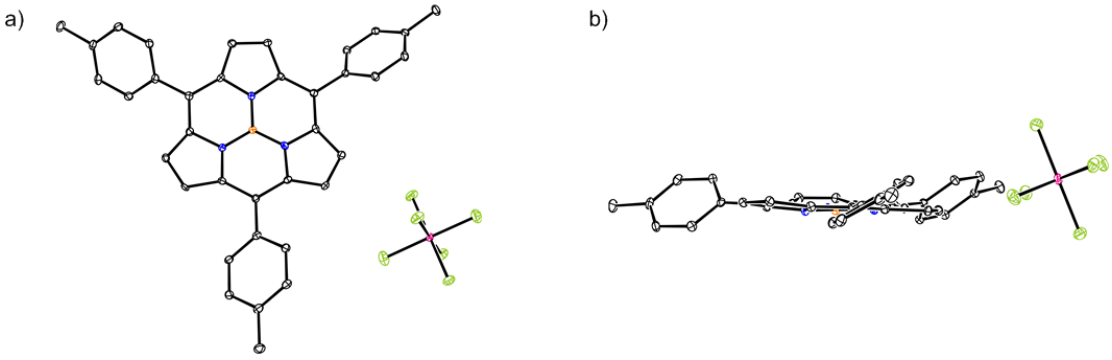


Fig. S38 X-ray crystal structure of **2a-SbF$_6$**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

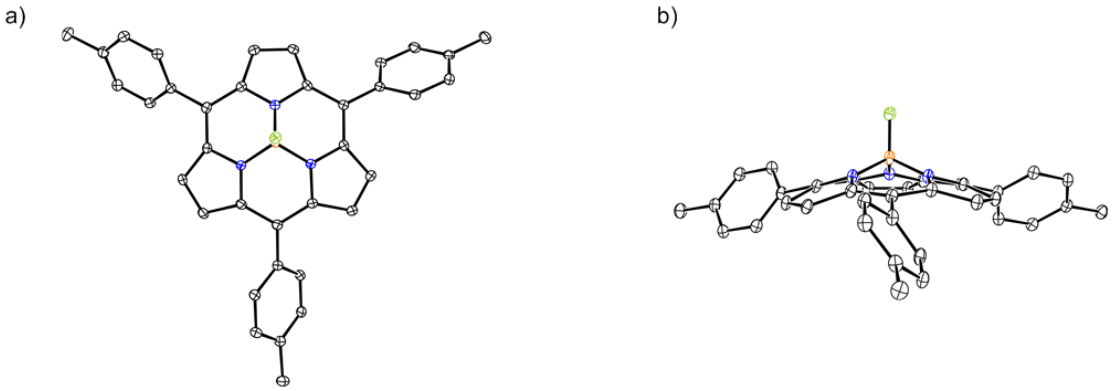


Fig. S39 X-ray crystal structure of **3a**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

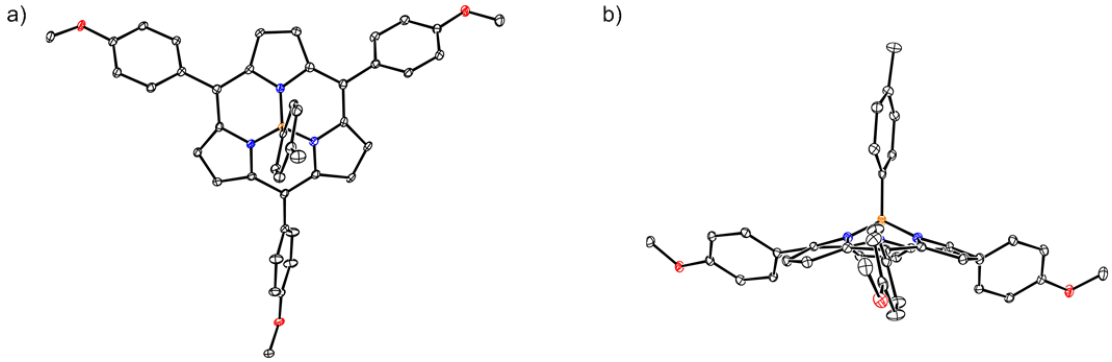


Fig. S40 X-ray crystal structure of **1b**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

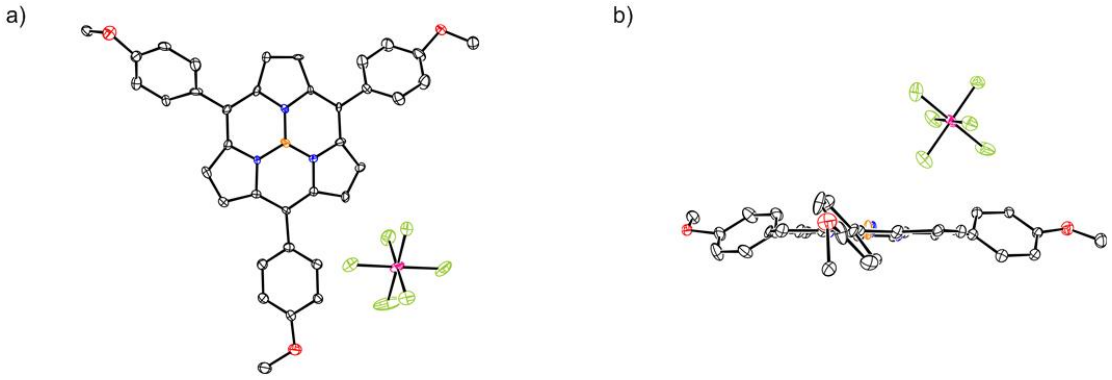


Fig. S41 X-ray crystal structure of **2b-SbF$_6$**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

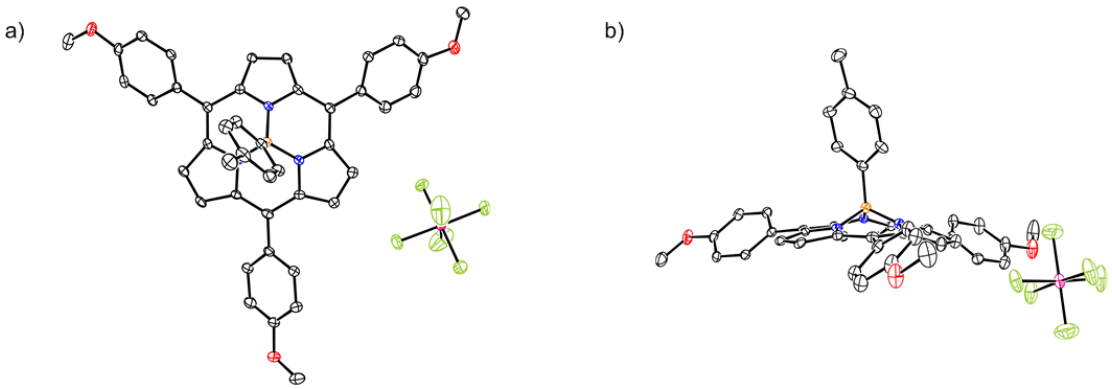


Fig. S42 X-ray crystal structure of **4b**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

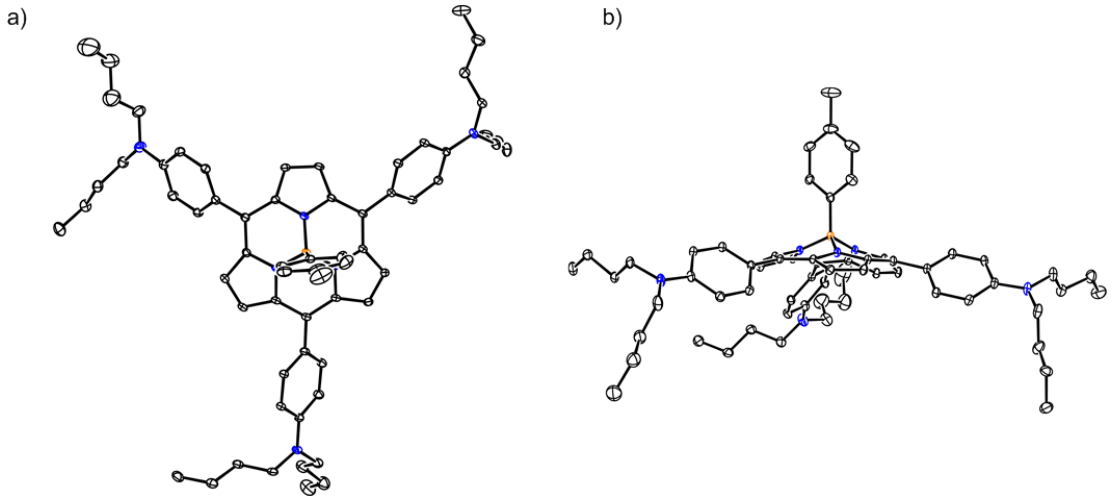


Fig. S43 X-ray crystal structure of **1c**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

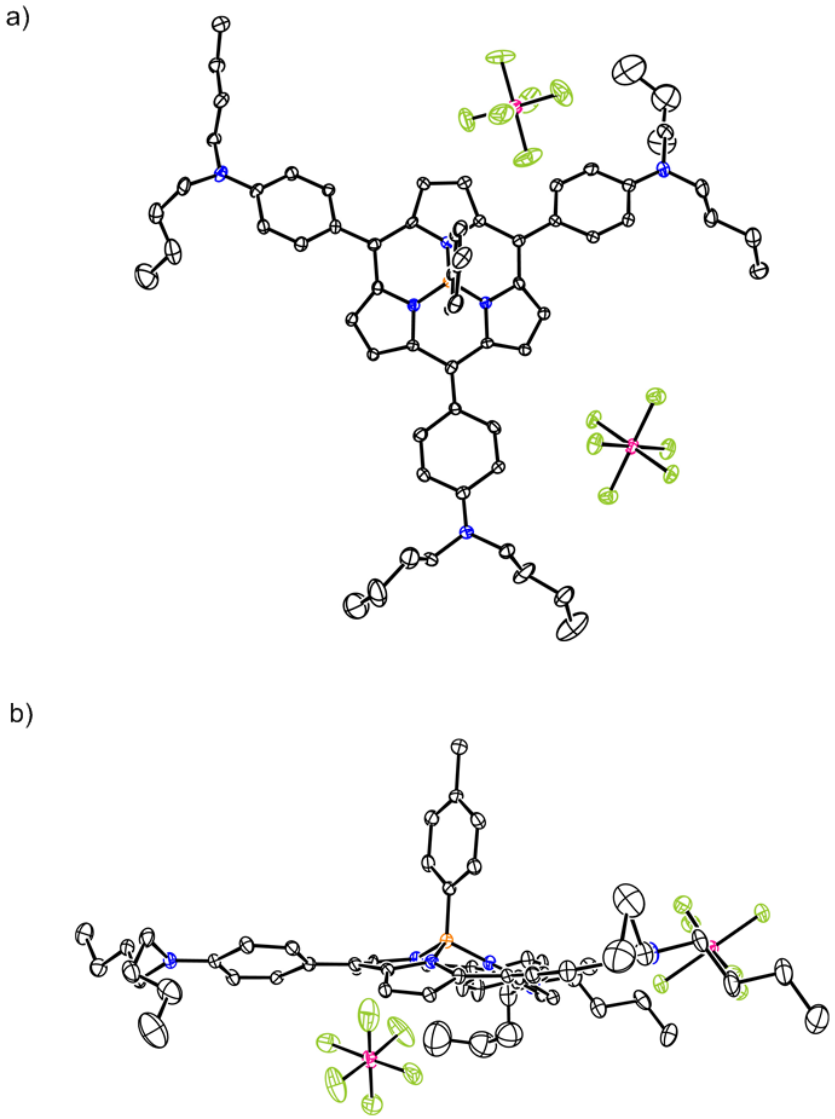


Fig. S44 X-ray crystal structure of **7c**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

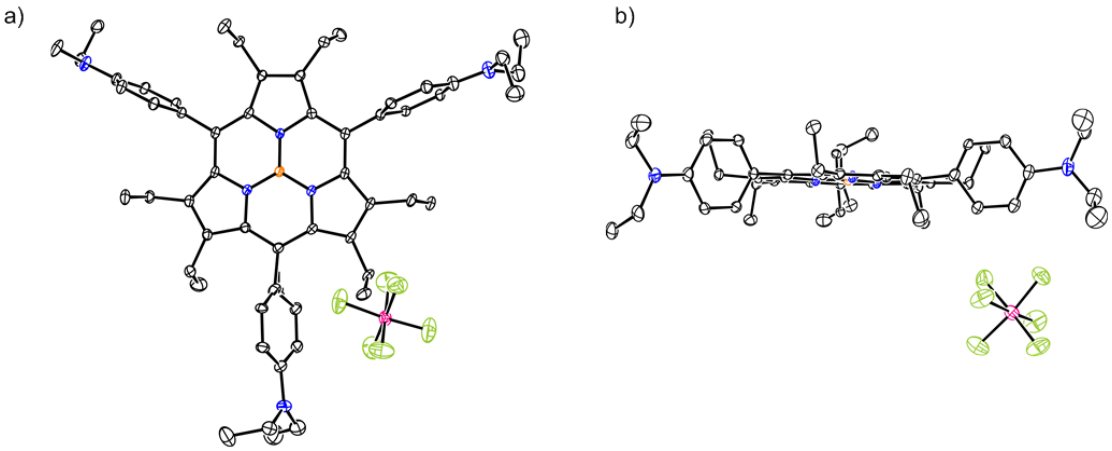


Fig. S45 X-ray crystal structure of **2d-SbF$_6$**. a) Top view and b) side view. Thermal ellipsoids are scaled to 30% probability. Hydrogen atoms are omitted for clarity.

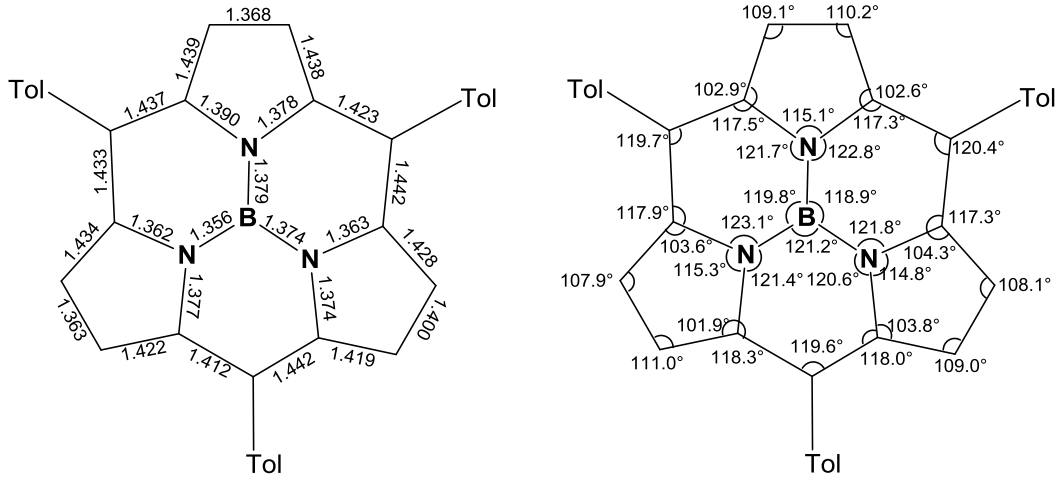


Fig. S46 Selected bond lengths and bond angles of **2a-SbCl$_6$**. Bond lengths and bond angles are measured based on single crystal data.

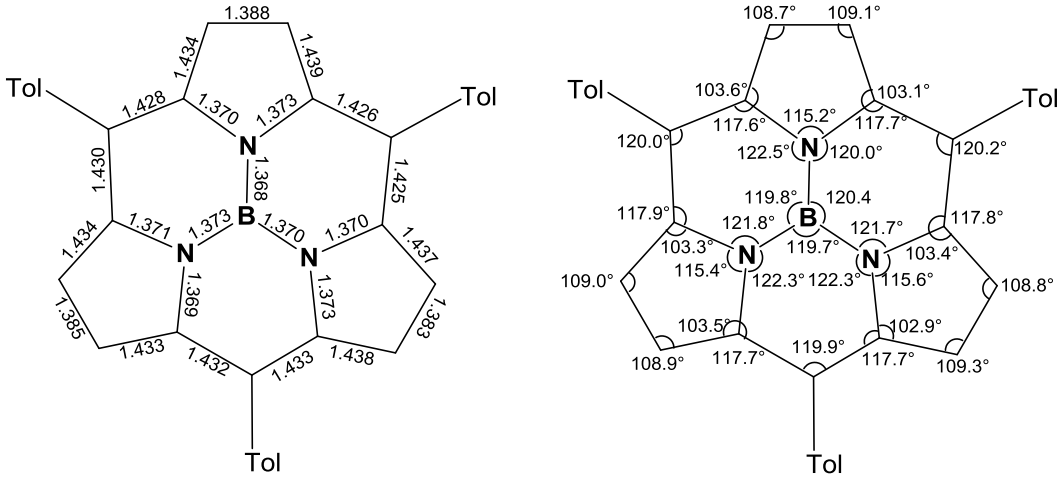


Fig. S47 Selected bond lengths and bond angles of **2a-BAr^F**. Bond lengths and bond angles are measured based on single crystal data.

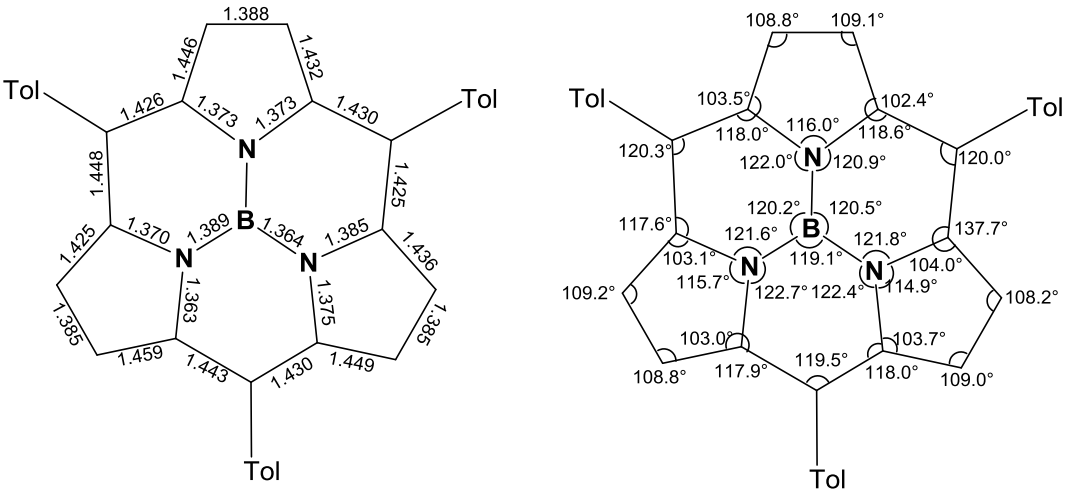


Fig. S48 Selected bond lengths and bond angles of **2a-SbF$_6$**. Bond lengths and bond angles are measured based on single crystal data.

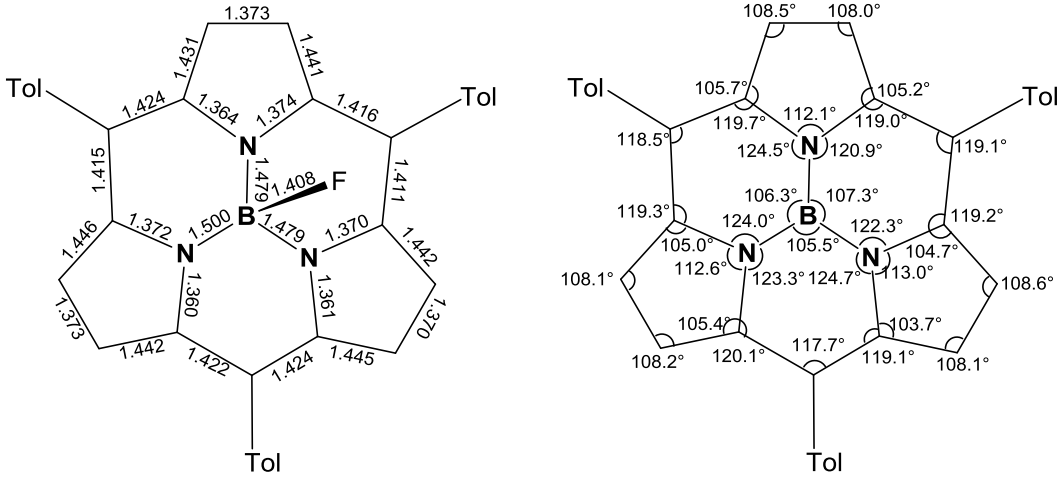


Fig. S49 Selected bond lengths and bond angles of **3a**. Bond lengths and bond angles are measured based on single crystal data.

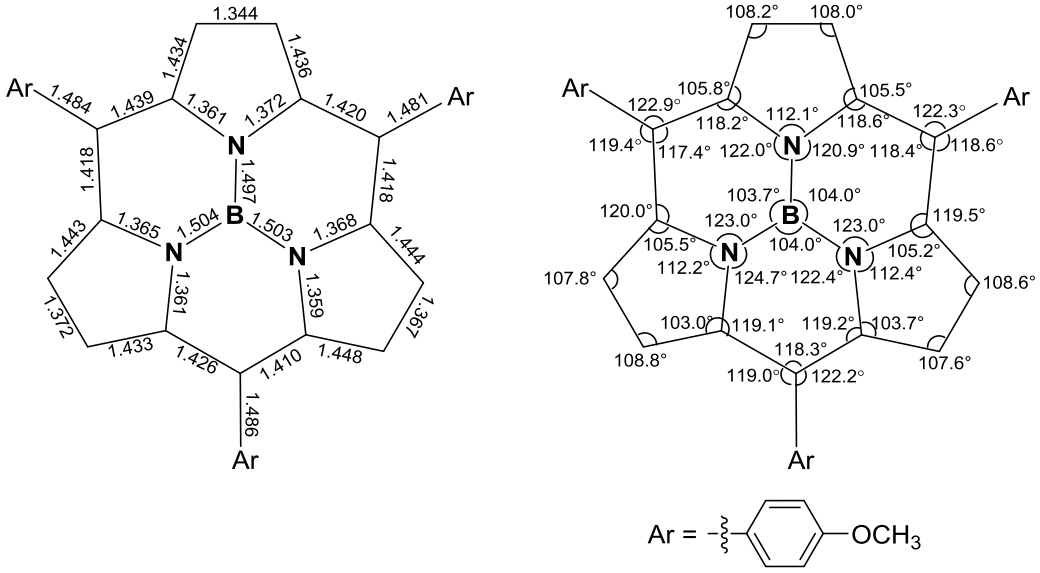


Fig. S50 Selected bond lengths and bond angles of **1b**. Bond lengths and bond angles are measured based on single crystal data.

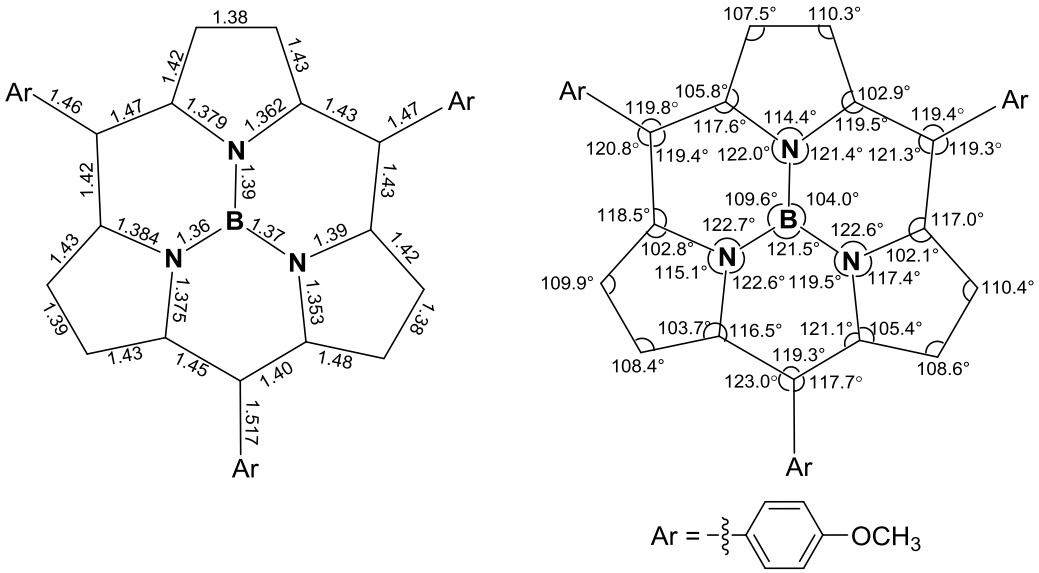


Fig. S51 Selected bond lengths and bond angles of **2b-SbF$_6$**. Bond lengths and bond angles are measured based on single crystal data.

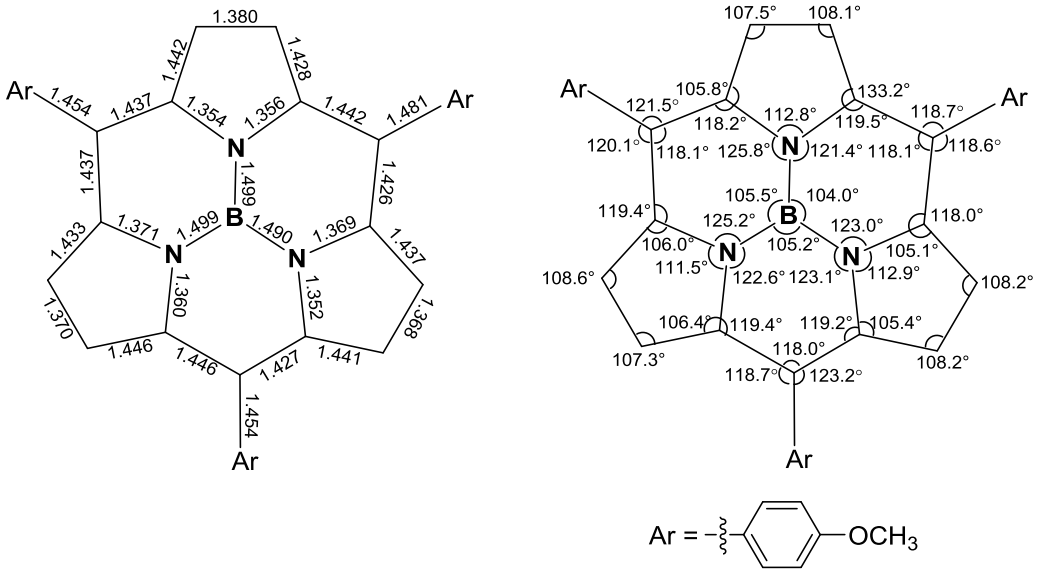


Fig. S52 Selected bond lengths and bond angles of **4b**. Bond lengths and bond angles are measured based on single crystal data.

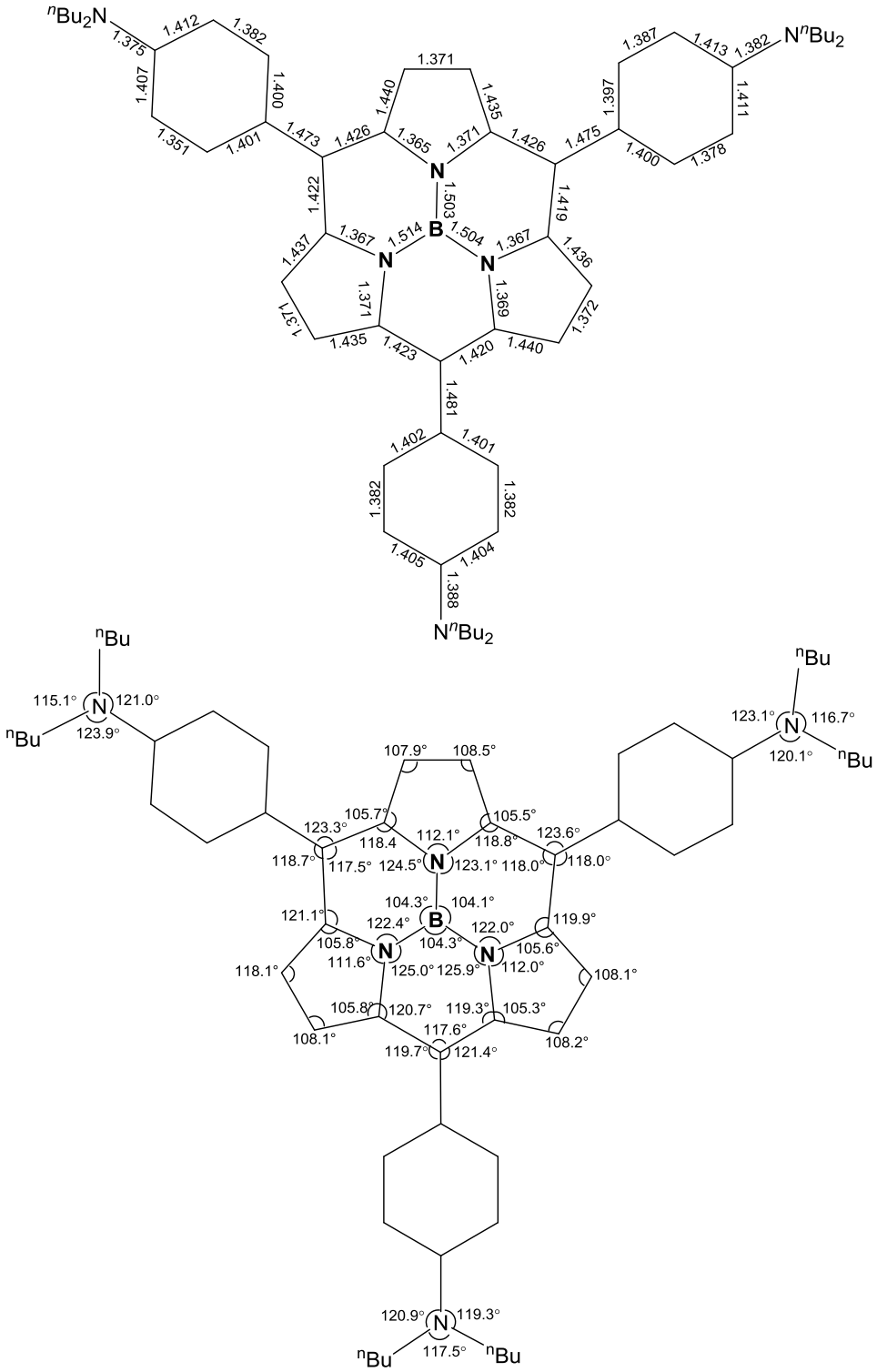


Fig. S53 Selected bond lengths and bond angles of **1c**. Bond lengths and bond angles are measured based on single crystal data.

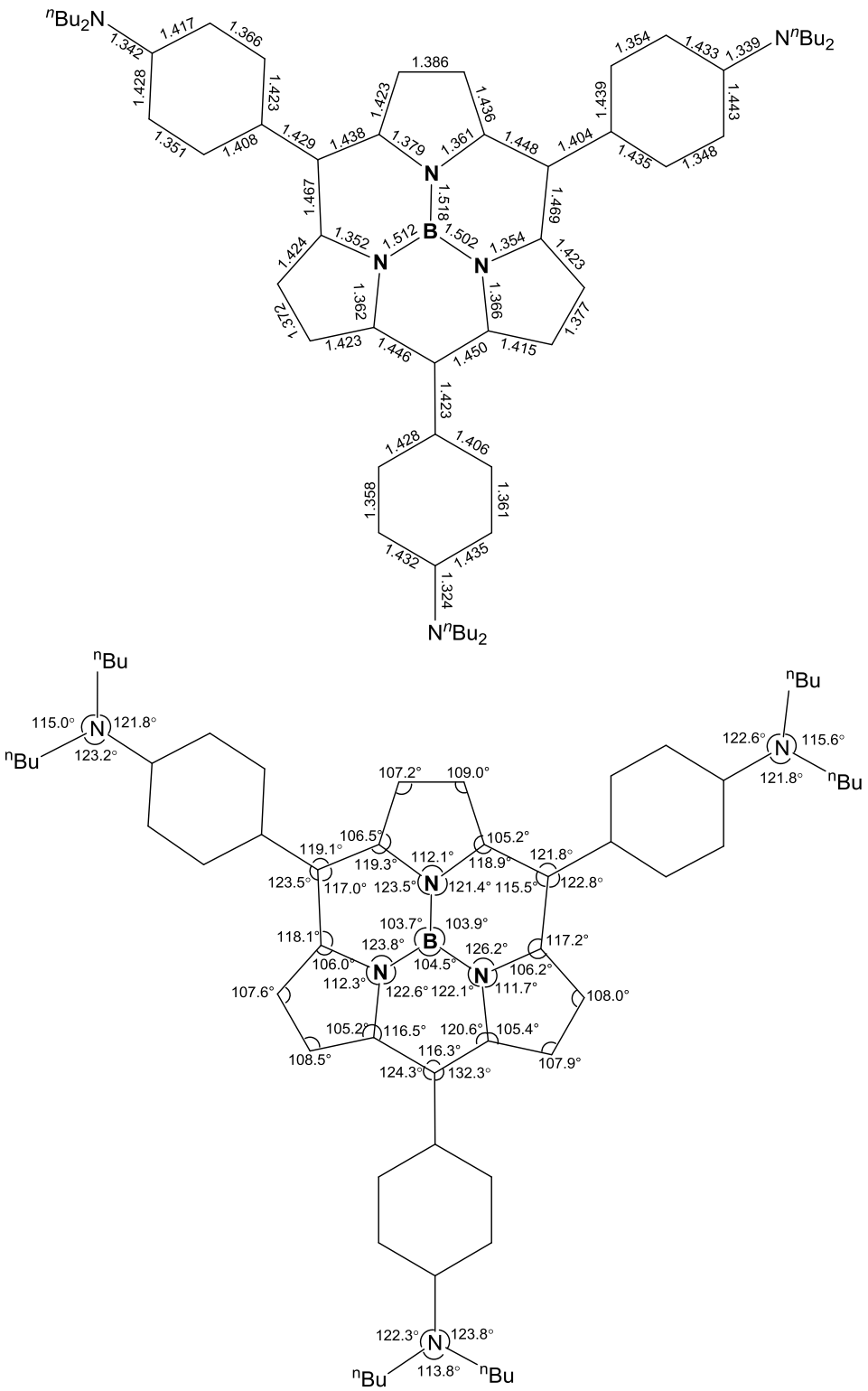


Fig. S54 Selected bond lengths and bond angles of **7c**. Bond lengths and bond angles are measured based on single crystal data.

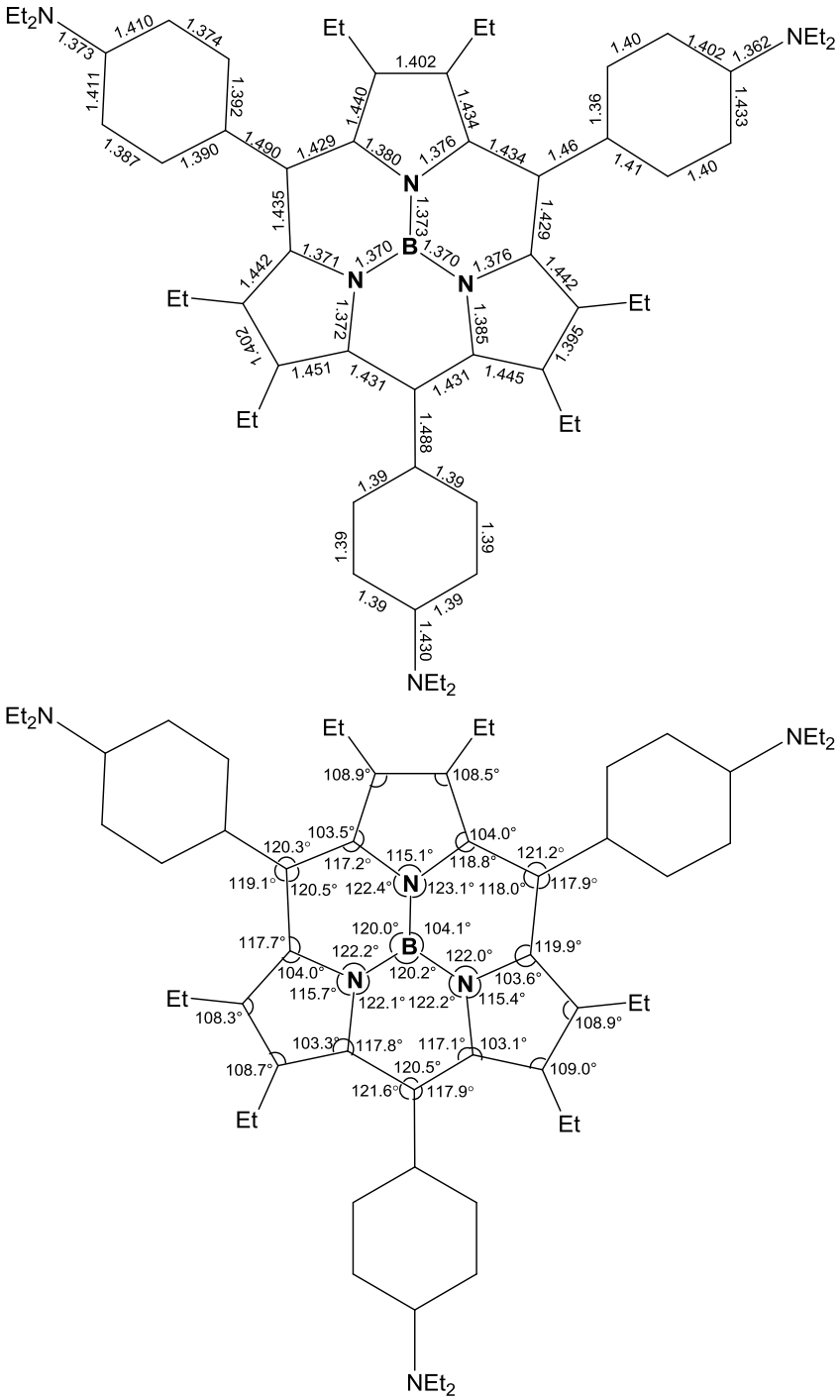


Fig. S55 Selected bond lengths and bond angles of **2d-SbF$_6$**. Bond lengths and bond angles are measured based on single crystal data.

Table S6 Crystal data and refinement results for compound **2a-$SbCl_6$**.

Identification code	**2a-$SbCl_6$**	
Empirical formula	C_{36} H_{27} B Cl_6 N_3 Sb	
Formula weight	846.86	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 12.2079(3) Å	α= 90 °.
	b = 33.4621(9) Å	β= 100.125(2) °.
	c = 17.1132(4) Å	γ = 90 °.
Volume	6881.9(3) $Å^3$	
Z	8	
Density (calculated)	1.635 Mg/m^3	
Absorption coefficient	10.899 mm^{-1}	
F(000)	3376	
Crystal size	0.25 x 0.1 x 0.02 mm^3	
Theta range for data collection	2.641 to 66.600 °.	
Index ranges	-14<=h<=13, -39<=k<=38, -13<=l<=20	
Reflections collected	25814	
Independent reflections	12121 [R(int) = 0.0626]	
Completeness to theta = 66.600 °	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.30136	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12121 / 0 / 856	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1421	
R indices (all data)	R1 = 0.0781, wR2 = 0.1675	
Largest diff. peak and hole	1.632 and -1.217 e.$Å^{-3}$	
CCDC number	2381939	

Table S7 Crystal data and refinement results for compound **2a-BAr^F**.

Identification code	**2a-BAr^F**	
Empirical formula	C_{74} H_{43} B_2 F_{20} N_3	
Formula weight	1375.73	
Temperature	101(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 15.2317(3) Å	α= 90 °.
	b = 12.8913(2) Å	β= 90.302(2) °.
	c = 31.0070(8) Å	γ = 90 °.
Volume	6088.3(2) Å^3	
Z	4	
Density (calculated)	1.501 Mg/m^3	
Absorption coefficient	1.133 mm^{-1}	
F(000)	2792	
Crystal size	0.3 x 0.15 x 0.02 mm^3	
Theta range for data collection	3.713 to 66.600 °.	
Index ranges	-9<=h<=18, -15<=k<=15, -36<=l<=36	
Reflections collected	23268	
Independent reflections	10735 [R(int) = 0.0384]	
Completeness to theta = 66.600 °	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.72332	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10735 / 0 / 897	
Goodness-of-fit on F^2	1.008	
Final R indices [I>2sigma(I)]	R1 = 0.0477, wR2 = 0.1094	
R indices (all data)	R1 = 0.0665, wR2 = 0.1202	
Largest diff. peak and hole	0.228 and -0.276 e.Å^{-3}	
CCDC number	2381940	

Table S8 Crystal data and refinement results for compound **2a-SbF$_6$**.

Identification code	**2a-SbF$_6$**	
Empirical formula	$C_{75}H_{60}B_2Cl_6F_{12}N_6Sb_2$	
Formula weight	1751.11	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 7.79716(14) Å	α= 90 °.
	b = 24.2551(4) Å	β= 94.9370(17) °.
	c = 36.7052(6) Å	γ = 90 °.
Volume	6916.0(2) Å^3	
Z	4	
Density (calculated)	1.682 Mg/m^3	
Absorption coefficient	9.041 mm^{-1}	
F(000)	3496	
Crystal size	0.3 x 0.12 x 0.03 mm^3	
Theta range for data collection	2.186 to 66.600 °.	
Index ranges	-8<=h<=9, -28<=k<=17, -43<=l<=38	
Reflections collected	29830	
Independent reflections	12218 [R(int) = 0.0546]	
Completeness to theta = 66.600 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.43791	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12218 / 0 / 954	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0484, wR2 = 0.1109	
R indices (all data)	R1 = 0.0578, wR2 = 0.1170	
Largest diff. peak and hole	0.980 and -0.928 e.Å^{-3}	
CCDC number	2381941	

Table S9 Crystal data and refinement results for compound **3a**.

Identification code	**3a**	
Empirical formula	C_{42} H_{33} B F N_3	
Formula weight	609.52	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 20.2522(6) Å	α= 90 °.
	b = 13.9389(4) Å	β= 104.932(4) °.
	c = 23.0024(9) Å	γ = 90 °.
Volume	6274.2(4) $Å^3$	
Z	8	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.619 mm^{-1}	
F(000)	2560	
Crystal size	0.2 x 0.14 x 0.1 mm^3	
Theta range for data collection	3.743 to 66.587 °.	
Index ranges	-24<=h<=24, -15<=k<=16, -27<=l<=27	
Reflections collected	40930	
Independent reflections	11069 [R(int) = 0.0615]	
Completeness to theta = 66.587 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.50278	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11069 / 0 / 853	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0652, wR2 = 0.1622	
R indices (all data)	R1 = 0.0866, wR2 = 0.1762	
Largest diff. peak and hole	0.273 and -0.268 $e.Å^{-3}$	
CCDC number	2381942	

Table S10 Crystal data and refinement results for compound **1b**.

Identification code	**1b**	
Empirical formula	$C_{43}H_{34}BN_3O_3$	
Formula weight	651.54	
Temperature	99.98(18) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.9203(3) Å	α= 77.130(4) °.
	b = 11.6190(6) Å	β= 87.008(3) °.
	c = 18.9943(8) Å	γ = 71.179(4) °.
Volume	1612.58(13) $Å^3$	
Z	2	
Density (calculated)	1.342 Mg/m^3	
Absorption coefficient	0.665 mm^{-1}	
F(000)	684	
Crystal size	0.2 x 0.04 x 0.02 mm^3	
Theta range for data collection	2.387 to 66.595 °.	
Index ranges	-9<=h<=7, -12<=k<=13, -20<=l<=22	
Reflections collected	9587	
Independent reflections	5668 [R(int) = 0.0947]	
Completeness to theta = 66.595 °	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.19508	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5668 / 0 / 455	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0696, wR2 = 0.1808	
R indices (all data)	R1 = 0.1037, wR2 = 0.2039	
Largest diff. peak and hole	0.331 and -0.391 e.$Å^{-3}$	
CCDC number	2381943	

Table S11 Crystal data and refinement results for compound **4b**.

Identification code	**4b**	
Empirical formula	$C_{87}H_{70}B_2Cl_2F_{12}N_6O_6Sb_2$	
Formula weight	1859.51	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 2/n 1	
Unit cell dimensions	a = 12.5687(2) Å	α= 90 °.
	b = 18.9045(4) Å	β= 98.6600(10) °.
	c = 18.1252(2) Å	γ = 90 °.
Volume	4257.54(12) $Å^3$	
Z	2	
Density (calculated)	1.451 Mg/m^3	
Absorption coefficient	6.307 mm^{-1}	
F(000)	1872	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	2.337 to 66.595 °.	
Index ranges	-9<=h<=14, -22<=k<=19, -21<=l<=18	
Reflections collected	15936	
Independent reflections	7520 [R(int) = 0.0409]	
Completeness to theta = 66.595 °	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.36202	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7520 / 0 / 534	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0630, wR2 = 0.1603	
R indices (all data)	R1 = 0.0745, wR2 = 0.1695	
Largest diff. peak and hole	3.914 and -1.365 e.$Å^{-3}$	
CCDC number	2381944	

Table S12 Crystal data and refinement results for compound **2b-SbF_6**.

Identification code	**2b-SbF_6**	
Empirical formula	$C_{36}H_{27}BF_6N_3O_3Sb$	
Formula weight	796.16	
Temperature	100.01(10) K	
Wavelength	0.710 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 17.917 Å	α= 90 °.
	b = 21.981 Å	β= 90 °.
	c = 8.366 Å	γ = 90 °.
Volume	3294.9 $Å^3$	
Z	4	
Density (calculated)	1.605 Mg/m^3	
Absorption coefficient	0.899 mm^{-1}	
F(000)	1592	
Crystal size	0.3 x 0.07 x 0.06 mm^3	
Theta range for data collection	1.465 to 25.000 °.	
Index ranges	-11<=h<=21, -26<=k<=26, -9<=l<=9	
Reflections collected	19951	
Independent reflections	5696 [R(int) = 0.0772]	
Completeness to theta = 25.000 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.40204	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5696 / 202 / 545	
Goodness-of-fit on F^2	1.170	
Final R indices [I>2sigma(I)]	R1 = 0.0835, wR2 = 0.1912	
R indices (all data)	R1 = 0.0850, wR2 = 0.1921	
Largest diff. peak and hole	1.532 and -1.916 e.$Å^{-3}$	
CCDC	2382017	

Table S13 Crystal data and refinement results for compound **1c**

Identification code	**1c**	
Empirical formula	C_{64} H_{79} B N_6	
Formula weight	943.14	
Temperature	99.97(18) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.4008(3) Å	α= 112.584(2) °.
	b = 15.0857(4) Å	β= 96.219(2) °.
	c = 16.5388(3) Å	γ = 110.308(2) °.
Volume	2780.22(12) $Å^3$	
Z	2	
Density (calculated)	1.127 Mg/m^3	
Absorption coefficient	0.495 mm^{-1}	
F(000)	1020	
Crystal size	0.3 x 0.3 x 0.1 mm^3	
Theta range for data collection	3.014 to 66.595 °.	
Index ranges	-15<=h<=15, -17<=k<=16, -15<=l<=19	
Reflections collected	18006	
Independent reflections	9802 [R(int) = 0.0281]	
Completeness to theta = 66.595 °	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.38896	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9802 / 141 / 725	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0724, wR2 = 0.1973	
R indices (all data)	R1 = 0.0784, wR2 = 0.2041	
Largest diff. peak and hole	0.981 and -0.525 e.$Å^{-3}$	
CCDC number	2381946	

Table S14 Crystal data and refinement results for compound **7c**.

Identification code	**7c**	
Empirical formula	$C_{64}H_{77}BF_{12}N_6Sb_2$	
Formula weight	1412.62	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.1950(12) Å	α= 70.971(9) °.
	b = 14.7581(16) Å	β= 78.991(8) °.
	c = 19.694(2) Å	γ = 79.512(8) °.
Volume	3796.4(7) $Å^3$	
Z	2	
Density (calculated)	1.236 Mg/m^3	
Absorption coefficient	6.209 mm^{-1}	
F(000)	1436	
Crystal size	0.15 x 0.03 x 0 mm^3	
Theta range for data collection	2.397 to 66.601 °.	
Index ranges	-16<=h<=16, -12<=k<=17, -20<=l<=23	
Reflections collected	26991	
Independent reflections	13402 [R(int) = 0.0861]	
Completeness to theta = 66.601 °	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.51554	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13402 / 206 / 883	
Goodness-of-fit on F^2	0.984	
Final R indices [I>2sigma(I)]	R1 = 0.0712, wR2 = 0.1731	
R indices (all data)	R1 = 0.1144, wR2 = 0.2056	
Largest diff. peak and hole	1.195 and -0.684 e.$Å^{-3}$	
CCDC number	2381948	

Table S15 Crystal data and refinement results for compound **2d-SbF_6**

Identification code	**2d-SbF_6**	
Empirical formula	C_{58} H_{74} B Cl_2 F_6 N_6 Sb	
Formula weight	1172.69	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 12.12180(10) Å	α= 90 °.
	b = 13.8905(2) Å	β= 97.8130(10) °.
	c = 32.6445(5) Å	γ = 90 °.
Volume	5445.59(12) $Å^3$	
Z	4	
Density (calculated)	1.430 Mg/m^3	
Absorption coefficient	5.458 mm^{-1}	
F(000)	2432	
Crystal size	0.3 x 0.25 x 0.08 mm^3	
Theta range for data collection	2.733 to 66.595 °.	
Index ranges	-9<=h<=14, -16<=k<=16, -38<=l<=38	
Reflections collected	32778	
Independent reflections	9614 [R(int) = 0.0394]	
Completeness to theta = 66.595 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.18654	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9614 / 465 / 896	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1563	
R indices (all data)	R1 = 0.0638, wR2 = 0.1597	
Largest diff. peak and hole	0.876 and -1.097 e.$Å^{-3}$	
CCDC number	2381949	

6. Copy of MALDI-TOF-MS

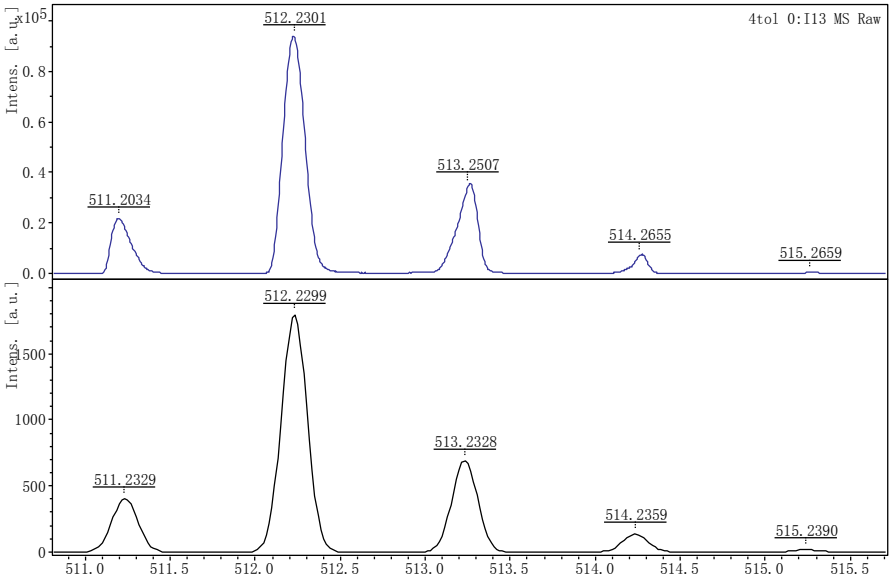


Fig. S56 MALDI-TOF-MS spectrum of **1a**

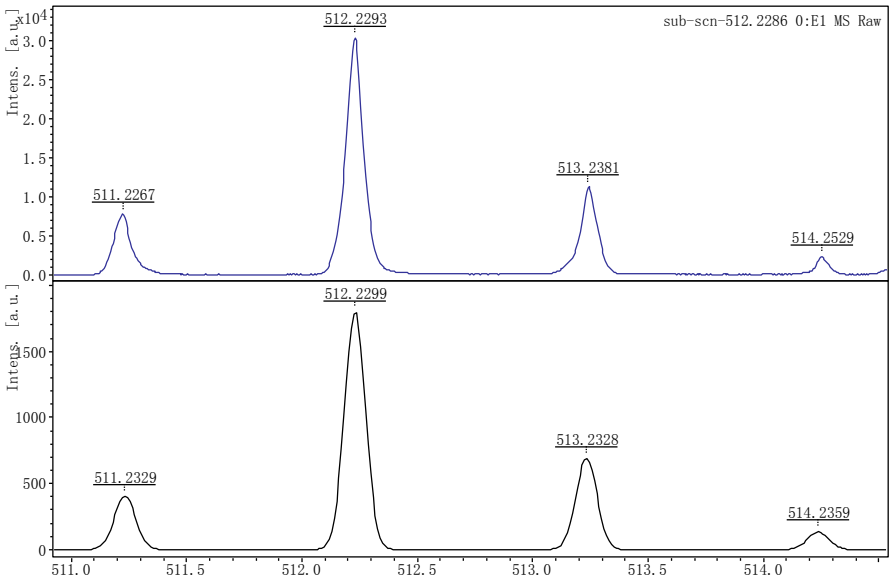


Fig. S57 MALDI-TOF-MS spectrum of **2a-SbCl$_6$**.

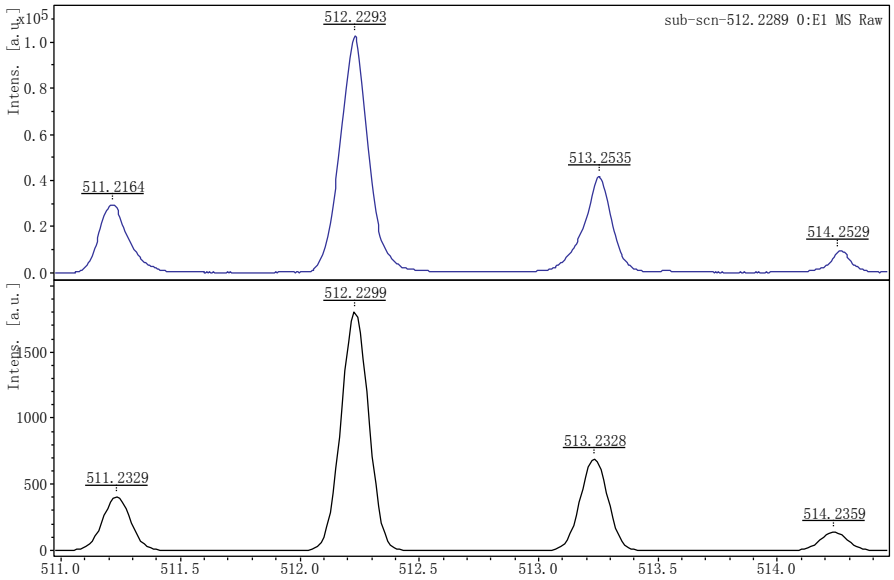


Fig. S58 MALDI-TOF-MS spectrum of **2a-BAr^{F}**.

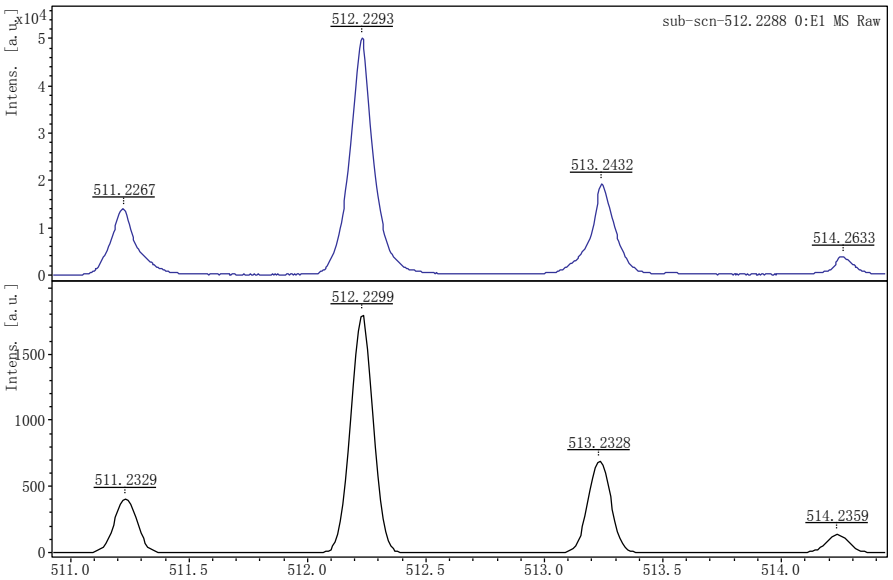


Fig. S59 MALDI-TOF-MS spectrum of **2a-SbF$_6$**.

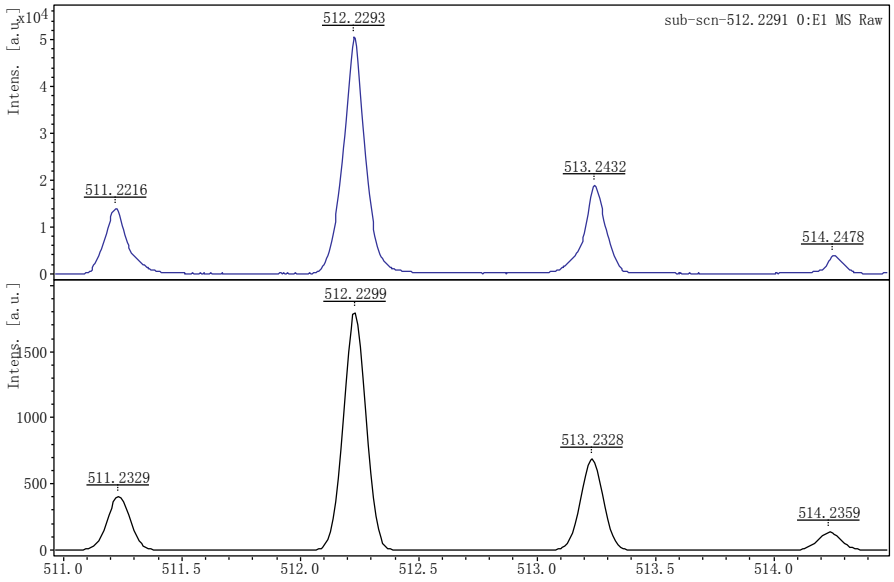


Fig. S60 MALDI-TOF-MS spectrum of **3a**.

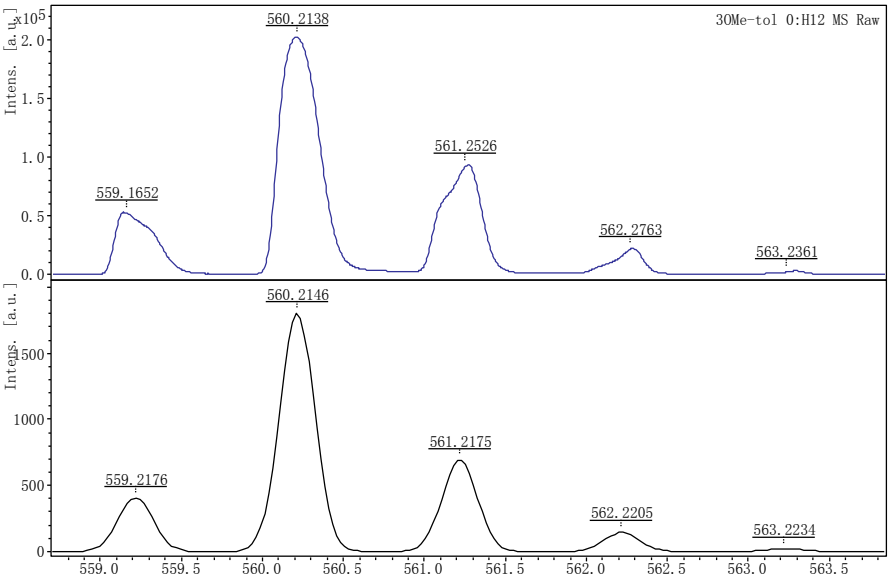


Fig. S61 MALDI-TOF-MS spectrum of **1b**.

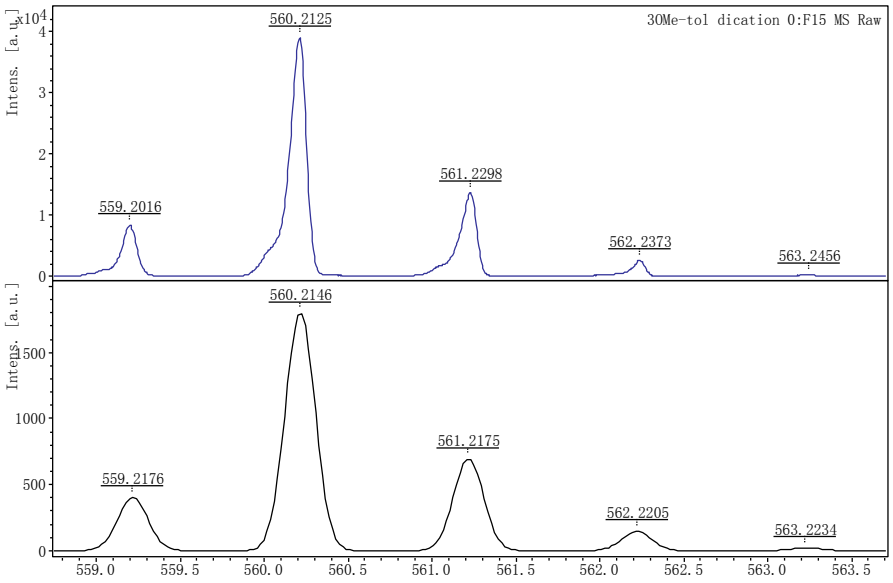


Fig. S62 MALDI-TOF-MS spectrum of **4b**.

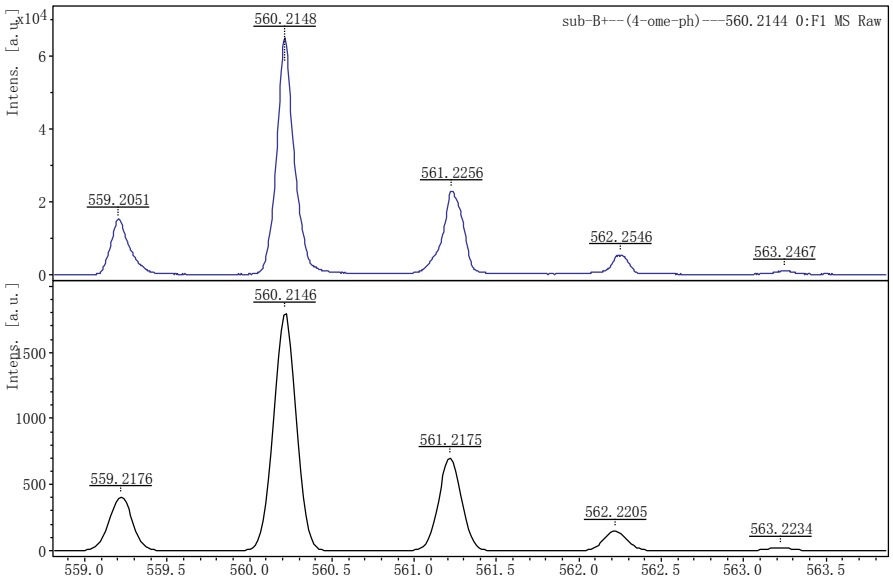


Fig. S63 MALDI-TOF-MS spectrum of **2b-SbF$_6$**.

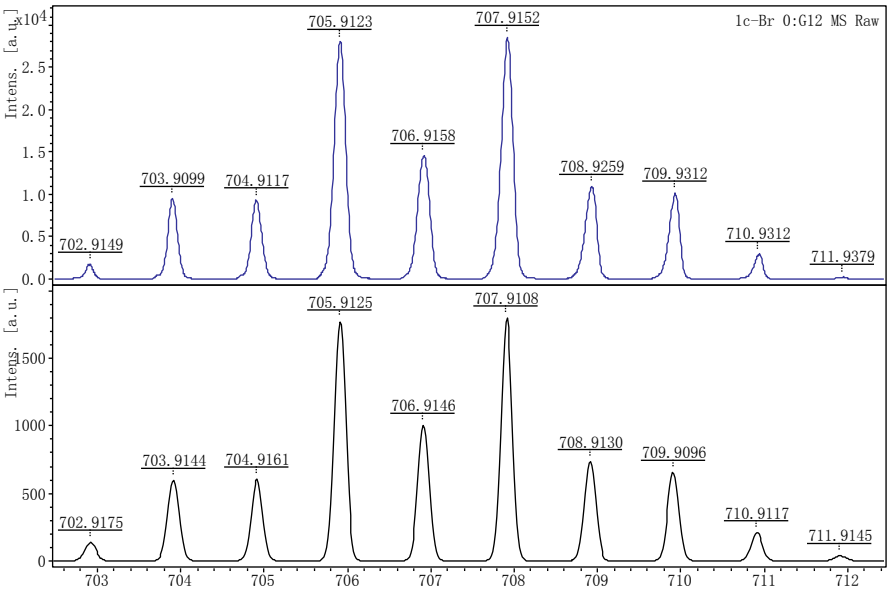


Fig. S64 MALDI-TOF-MS spectrum of **1c-Br**.

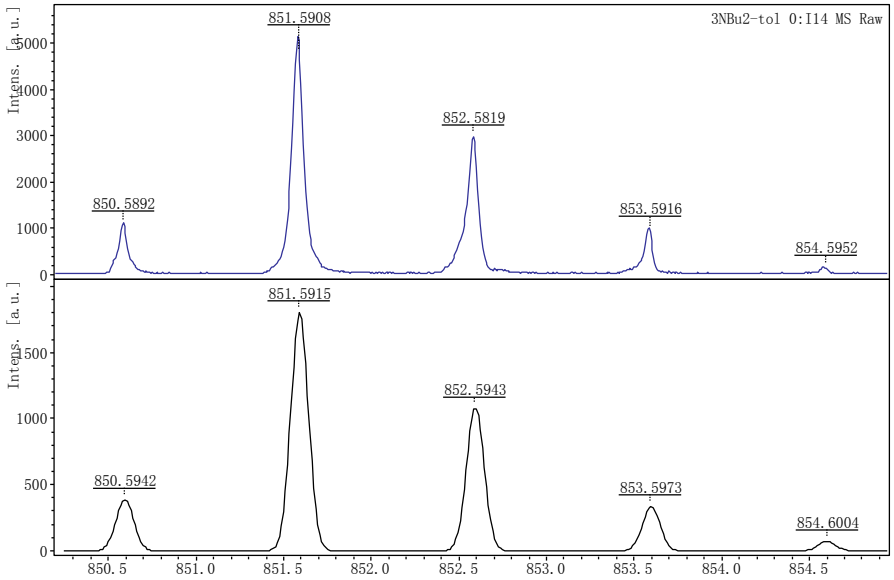


Fig. S65 MALDI-TOF-MS spectrum of **1c**.

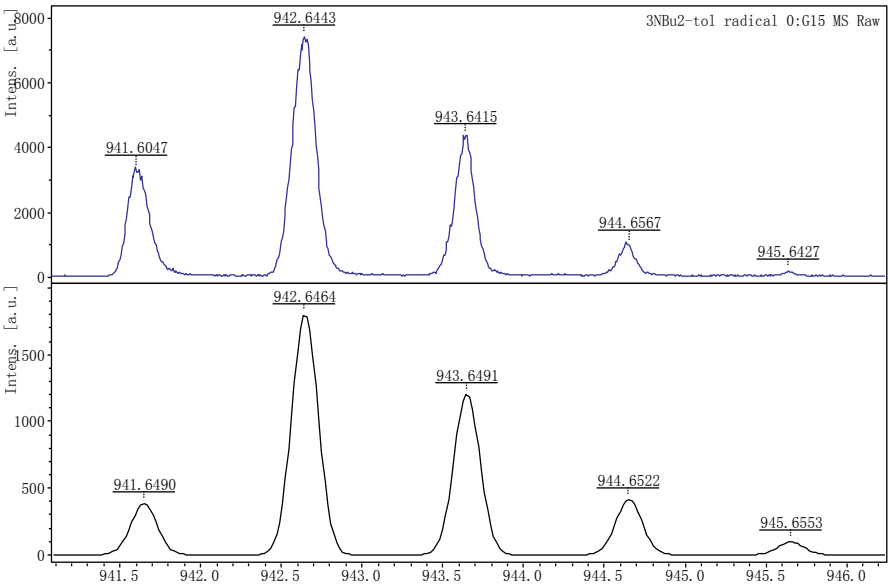


Fig. S66 MALDI-TOF-MS spectrum of **4c**.

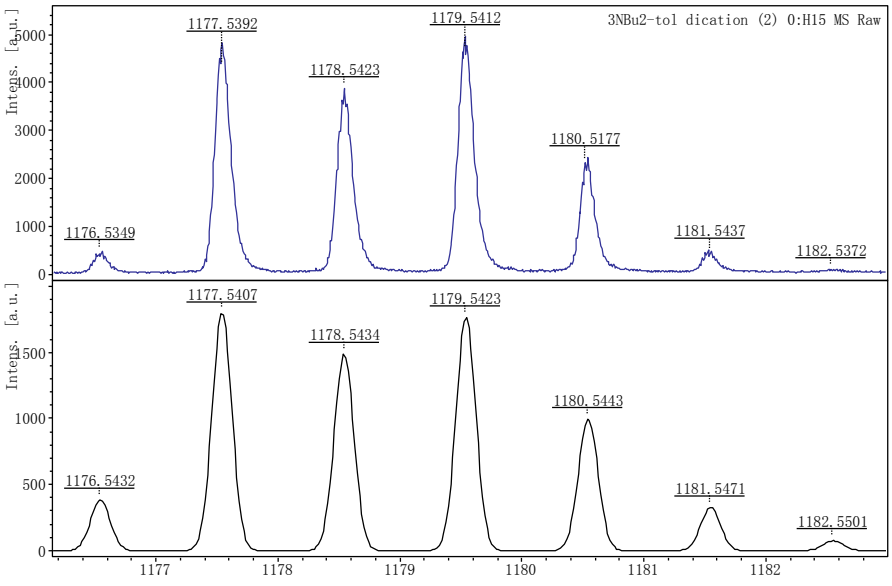


Fig. S67 MALDI-TOF-MS spectrum of **7c**.

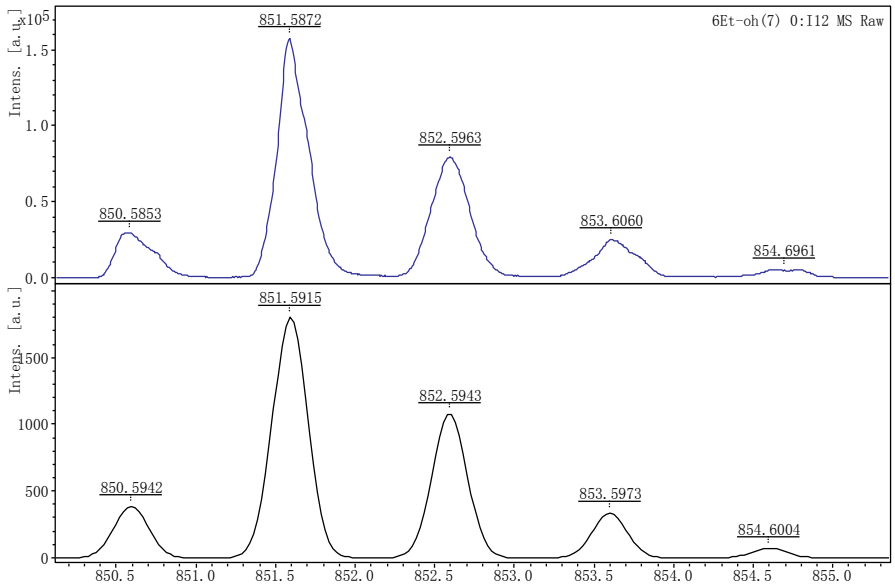


Fig. S68 MALDI-TOF-MS spectrum of **1d-OH**.

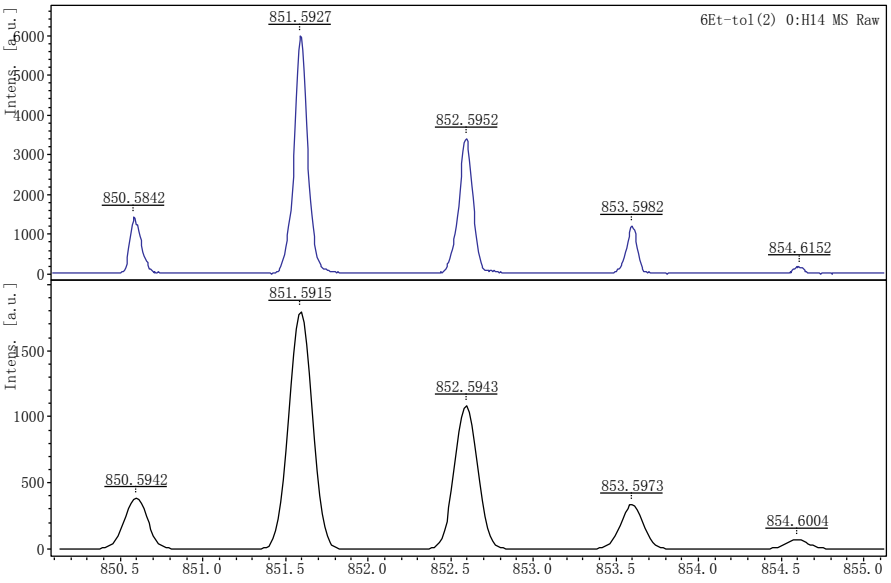


Fig. S69 MALDI-TOF-MS spectrum of **1d**.

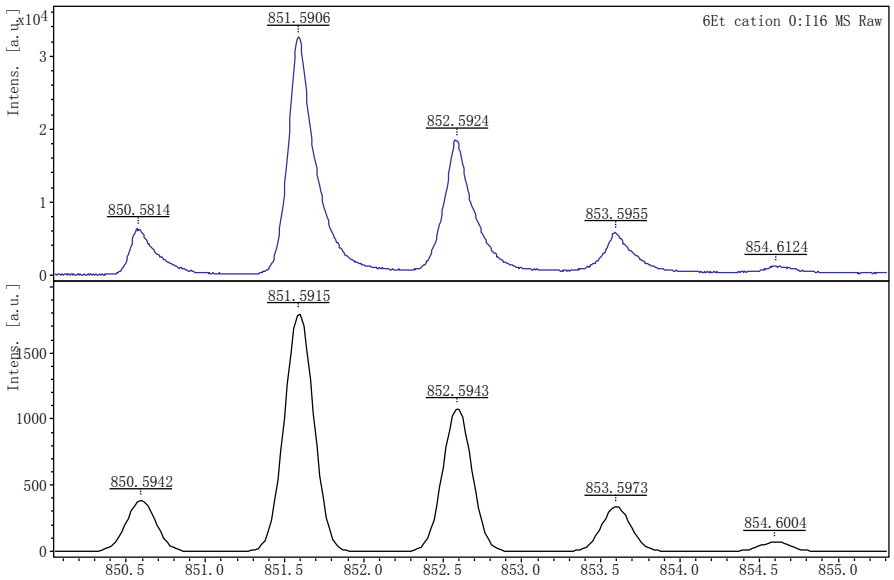


Fig. S70 MALDI-TOF-MS spectrum of **2d-SbF$_6$**.

7. Cyclic Voltammetry and Differential Pulse Voltammogram

Conditions: 0.1M $^{n}Bu_4NPF_6$ as electrolyte. Working electrode: Glassy carbon, counter electrode: Pt wire. Reference electrode: $Ag/AgNO_3$. Scan rate: 0.05 V/s. Potentials (V) vs. ferrocene/ferrocenium ion couple.

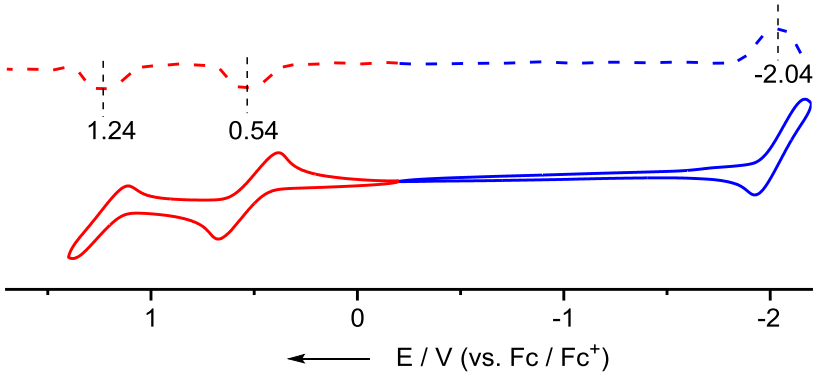


Fig. S71 Cyclic voltammogram and differential-pulse voltammogram of **1a**.

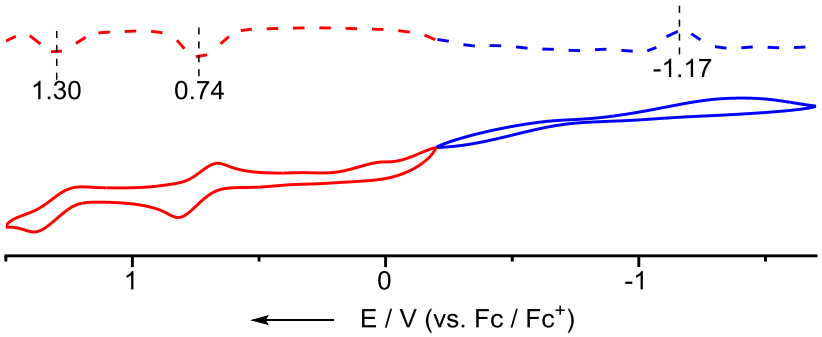


Fig. S72 Cyclic voltammogram and differential-pulse voltammogram of **2a-SbCl$_6$**.

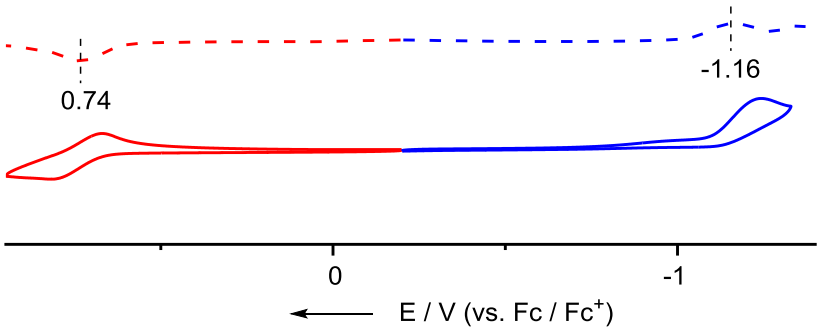


Fig. S73 Cyclic voltammogram and differential-pulse voltammogram of **2a-BAr^F**.

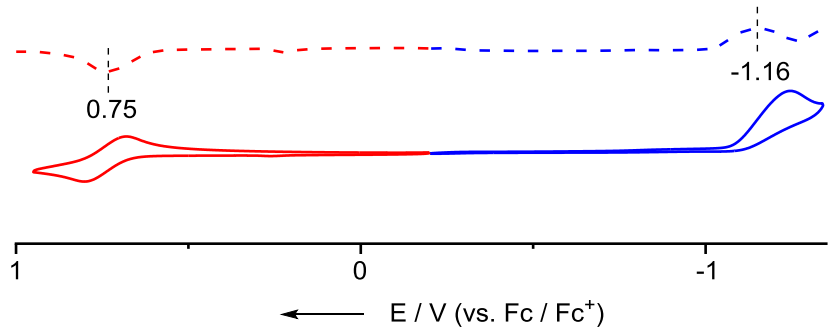


Fig. S74 Cyclic voltammogram and differential-pulse voltammogram of **2a-SbF$_6$**.

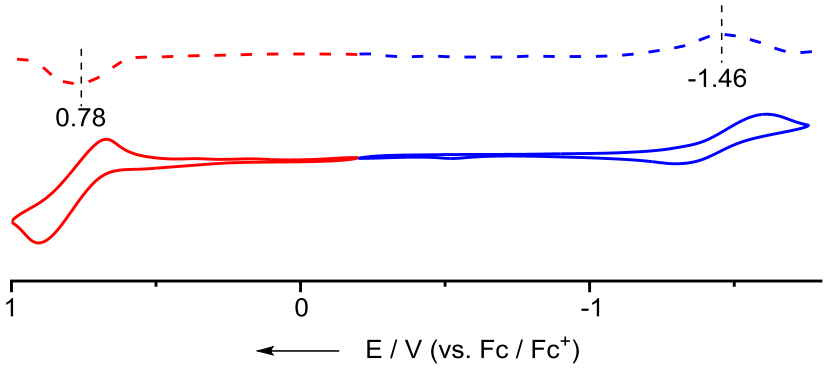


Fig. S75 Cyclic voltammogram and differential-pulse voltammogram of **3a**.

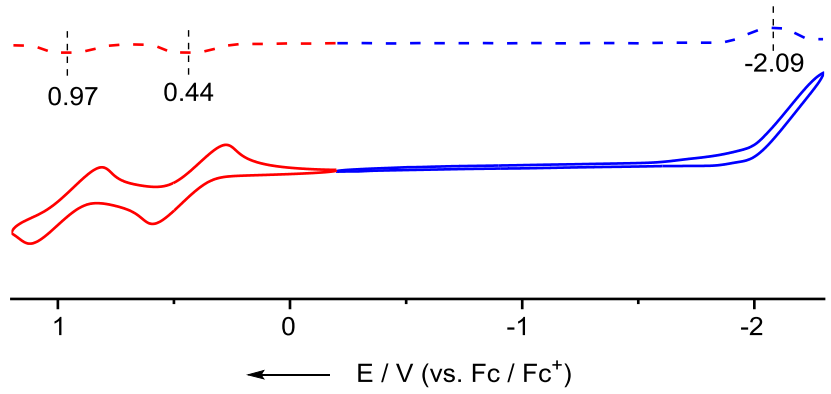


Fig. S76 Cyclic voltammogram and differential-pulse voltammogram of **1b**.

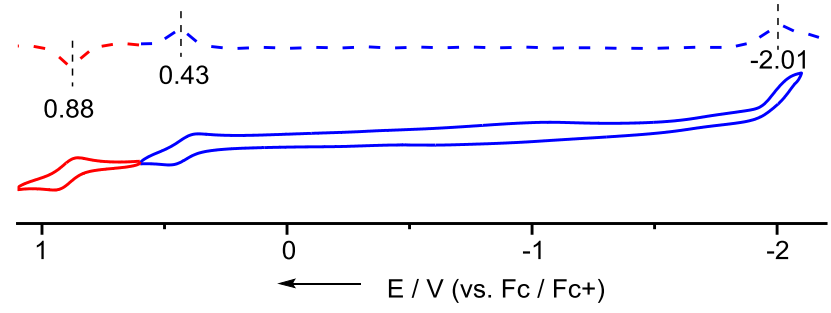


Fig. S77 Cyclic voltammogram and differential-pulse voltammogram of **4b**.

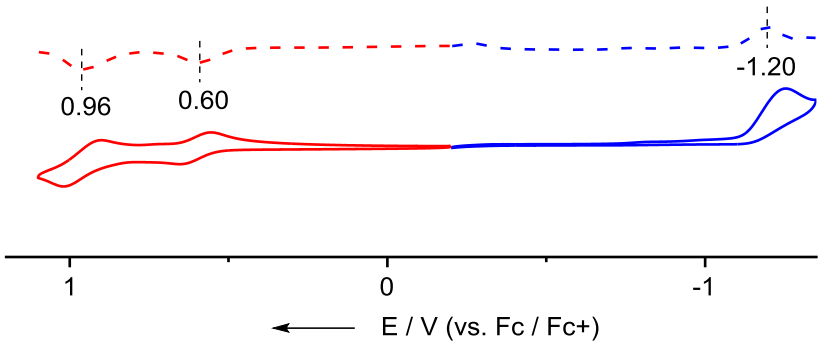


Fig. S78 Cyclic voltammogram and differential-pulse voltammogram of **2b-SbF$_6$**.

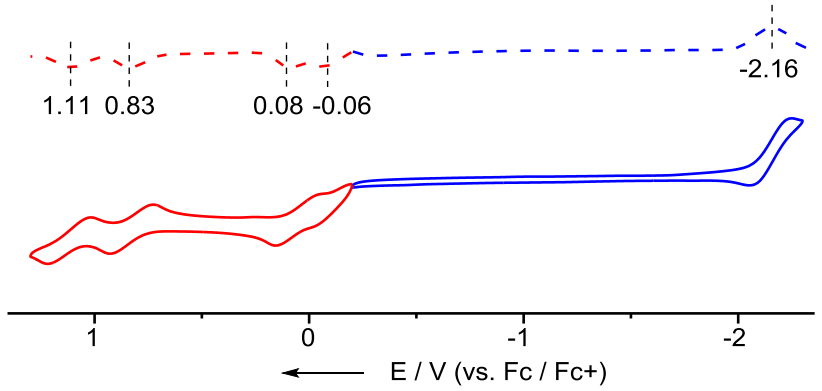


Fig. S79 Cyclic voltammogram and differential-pulse voltammogram of **1c**.

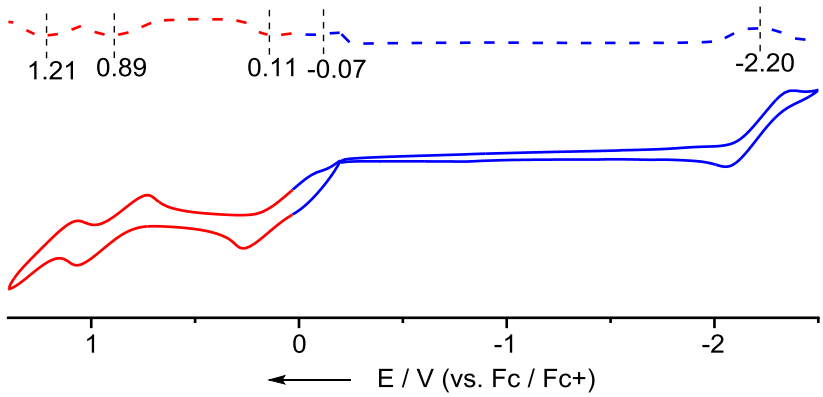


Fig. S80 Cyclic voltammogram and differential-pulse voltammogram of **4c**.

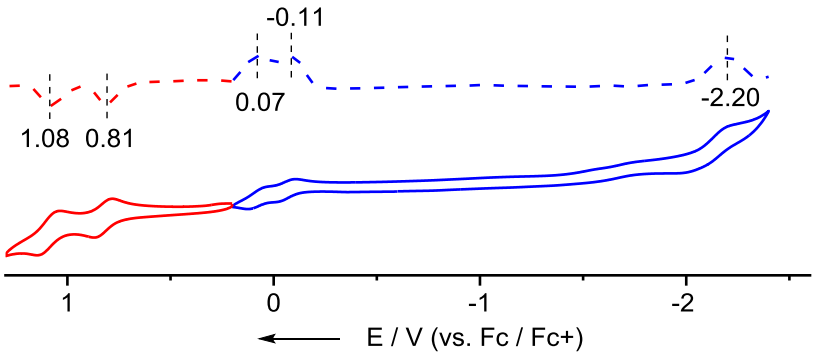


Fig. S81 Cyclic voltammogram and differential-pulse voltammogram of **7c**.

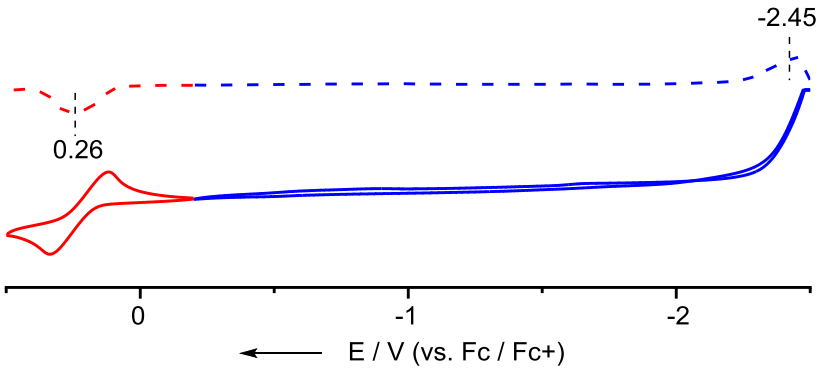


Fig. S82 Cyclic voltammogram and differential-pulse voltammogram of **1d-OH**.

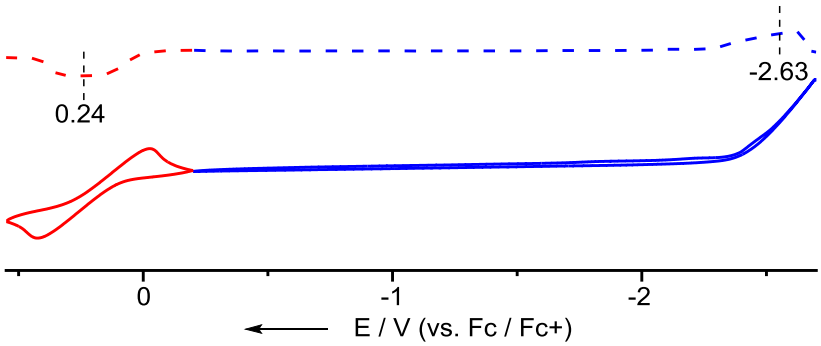


Fig. S83 Cyclic voltammogram and differential-pulse voltammogram of **1d**.

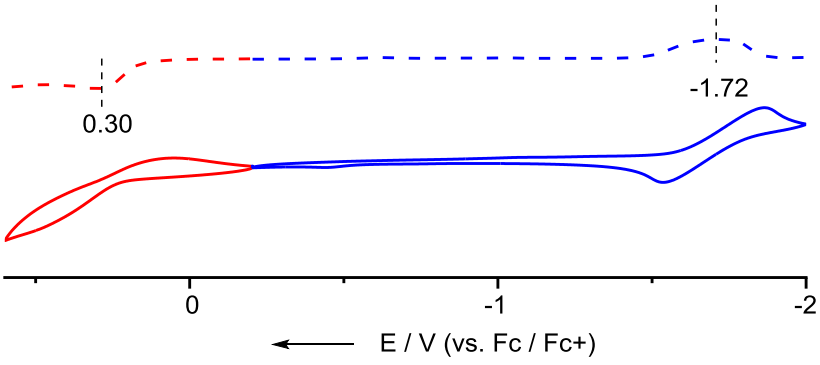


Fig. S84 Cyclic voltammogram and differential-pulse voltammogram of **2d-SbF_6**.

Table S16 Redox potentials and electrochemical HOMO–LUMO gaps

sample	E_{Ox3} [V]	E_{Ox2} [V]	E_{Ox1} [V]	E_{Red1} [V]	ΔE [eV][a]
1a	-	1.24	0.54	-2.04	2.58
2a-SbCl$_6$	-	1.30	0.74	-1.17	1.91
2a-BAr^F	-	-	0.74	-1.16	1.90
2a-SbF$_6$	-	-	0.75	-1.16	1.91
3a	-	-	0.78	-1.46	2.24
1b	-	0.97	0.44	-2.09	2.53
4b	-	-	0.88	0.43	0.45
2b-SbF$_6$	-	0.96	0.60	-1.20	1.80
1c	0.83	0.08	-0.06	-2.16	2.10
4c	1.21	0.89	0.11	-0.07	0.18
7c	-	1.08	0.81	0.07	0.74
1d-OH	-	-	0.26	-2.45	2.71
1d	-	-	0.24	-2.63	2.87
2d-SbF$_6$	-	-	0.30	-1.72	2.02

[a] $\Delta E = e(E_{ox1}-E_{red1})$, that is, electrochemical HOMO–LUMO gaps.

8. Copy of EPR Spectra

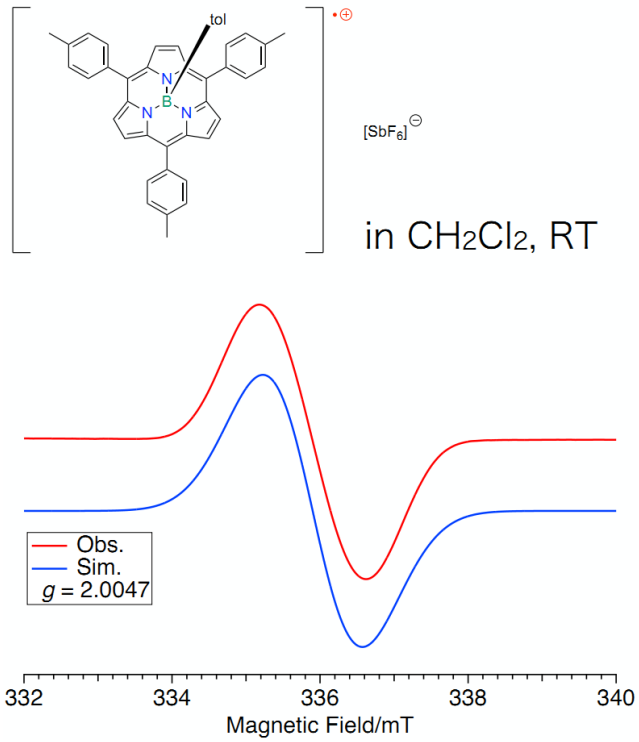


Fig. S85 EPR spectrum of **4a** (generated *in situ*) in DCM solution at room temperature.

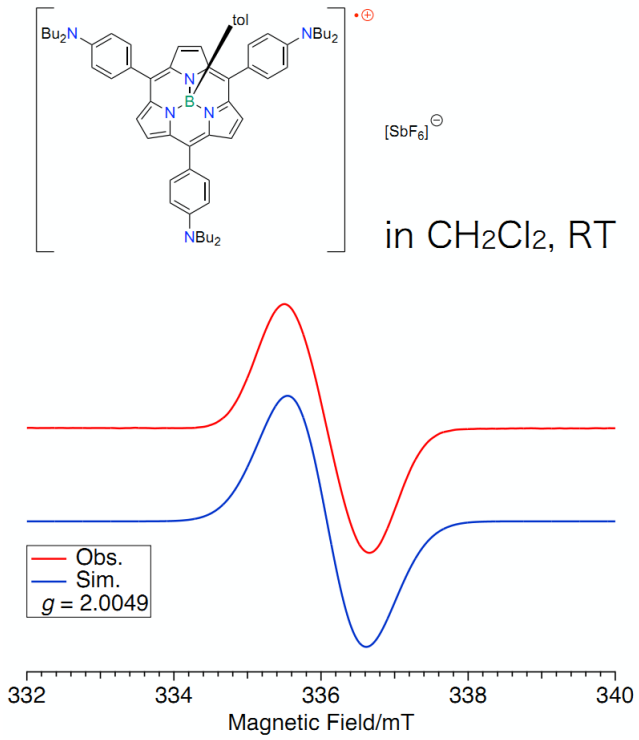


Fig. S86 EPR spectrum of **4c** in DCM solution at room temperature.

9. DFT Calculations

All calculations were carried out using the Gaussian 09 program (D.01 version).[5] Initial geometries of **1b**, **1c**, **2a**, **2b**, **2d**, **4b**, and **7c** were from corresponding X-ray structures. The optimization structure of all the minima and transition states were performed by the density functional theory (DFT) with B3LYP (Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional)[6] level using the 6-31G(d) basis set for all the atoms without any symmetry restriction. Harmonic frequency calculations were performed at the same level for every structure to confirm it as a local minimum or transition state and to derive the thermochemical corrections for enthalpies and free energies. The intrinsic reaction coordinate (IRC) analysis was carried out throughout the pathways to confirm that all stationary points are smoothly connected to each other. The effects of solvent CH_2Cl_2 were considered by performing solvation model based on density (SMD) for all the structures (including transition states) in optimization and harmonic frequency calculation. All enthalpies, zero-point Energies and the Gibbs free energies in the text below were given in Hartree. All distances were given in Å.

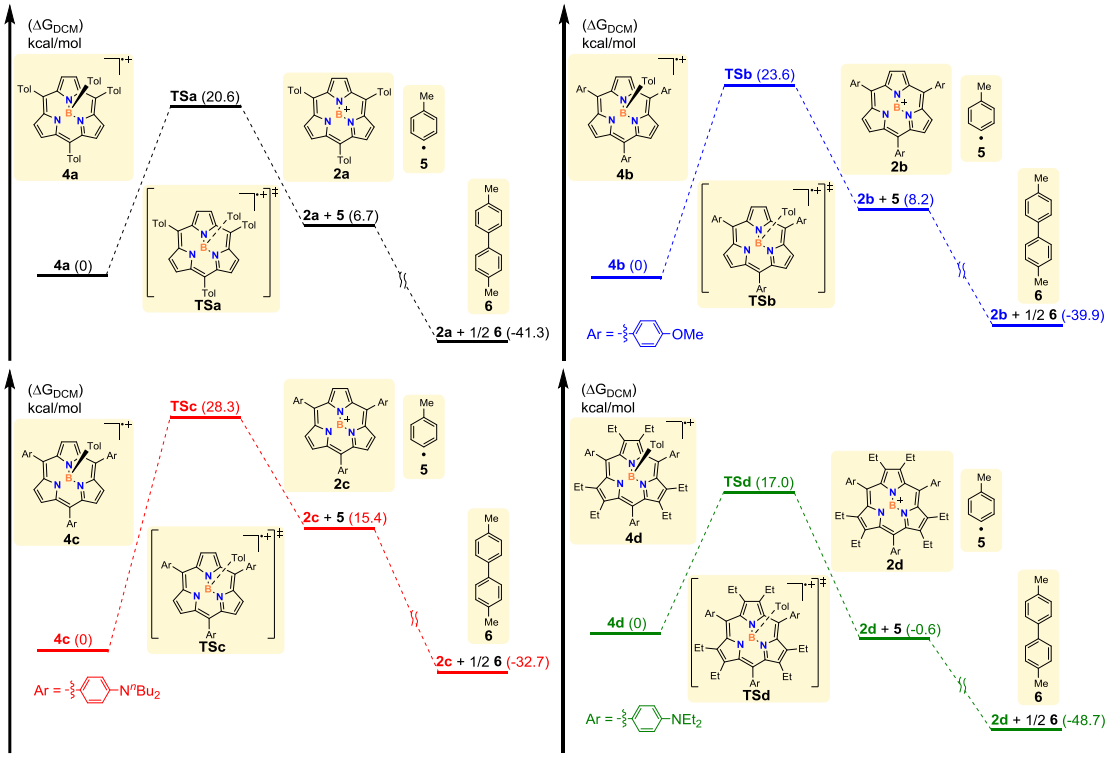


Fig. S87 DFT-calculated potential-energy surfaces of the transformation from **4a-d** to **2a-d**. SbF_6^- is not included in the calculations.

Calculated Total Energies and Geometrical Coordinates

1a

Zero-point correction= 0.656111 (Hartree/Particle)
Thermal correction to Energy= 0.694935
Thermal correction to Enthalpy= 0.695879
Thermal correction to Gibbs Free Energy= 0.578829
Sum of electronic and zero-point Energies= -1847.642773
Sum of electronic and thermal Energies= -1847.603949
Sum of electronic and thermal Enthalpies= -1847.603004
Sum of electronic and thermal Free Energies= -1847.720055

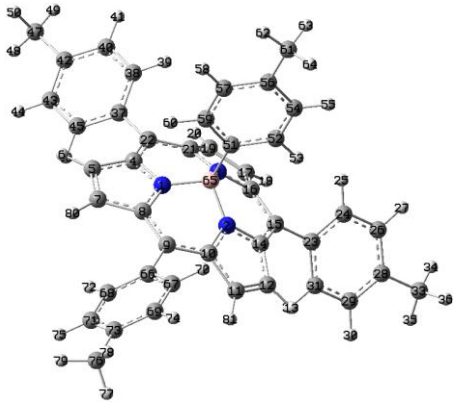


Fig. S88 Optimized structures of **1a**.

Table S17 Coordinates of atoms in **1a**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.394832	5.292740	3.880253
2	7	0	4.254266	6.766471	5.737379
3	7	0	6.374097	5.893955	5.062633
4	6	0	5.044522	4.301730	3.200598
5	6	0	4.011407	3.556856	2.523929
6	1	0	4.169427	2.708347	1.873661
7	6	0	2.789678	4.083806	2.899116
8	6	0	3.035448	5.167613	3.817890
9	6	0	2.230668	5.936354	4.709099
10	6	0	2.892440	6.661942	5.742630
11	6	0	2.466677	7.138490	7.034594
12	6	0	3.595852	7.435056	7.771194
13	1	0	3.621375	7.775585	8.796252
14	6	0	4.749170	7.128178	6.959286
15	6	0	6.136406	6.942671	7.230760
16	6	0	6.908830	6.216522	6.277883
17	6	0	8.117691	5.439042	6.397764
18	1	0	8.776147	5.442961	7.255398
19	6	0	8.207948	4.622646	5.289430
20	1	0	8.950652	3.858606	5.105680
21	6	0	7.056134	4.874703	4.459123
22	6	0	6.441863	4.119566	3.417374
23	6	0	6.749467	7.327191	8.522945

24	6	0	7.978517	8.009965	8.543323
25	1	0	8.454188	8.270902	7.602149
26	6	0	8.581293	8.370160	9.746462
27	1	0	9.530537	8.901368	9.727618
28	6	0	7.984807	8.068283	10.977258
29	6	0	6.766398	7.376329	10.957899
30	1	0	6.291195	7.105623	11.898407
31	6	0	6.159725	7.009503	9.759093
32	1	0	5.238070	6.436486	9.779901
33	6	0	8.622766	8.490591	12.279592
34	1	0	9.714556	8.525517	12.199276
35	1	0	8.364707	7.804858	13.093727
36	1	0	8.287601	9.492400	12.580702
37	6	0	7.219011	3.072229	2.717579
38	6	0	8.481713	3.373617	2.178247
39	1	0	8.864591	4.386609	2.262943
40	6	0	9.232613	2.401373	1.520732
41	1	0	10.203841	2.667323	1.109169
42	6	0	8.757092	1.092567	1.372436
43	6	0	7.504168	0.788075	1.922260
44	1	0	7.119156	-0.226565	1.844414
45	6	0	6.749139	1.753444	2.582934
46	1	0	5.801051	1.475712	3.032977
47	6	0	9.556435	0.048834	0.628708
48	1	0	9.414453	-0.948315	1.059734
49	1	0	10.627497	0.276166	0.646153
50	1	0	9.252888	-0.008404	-0.425405
51	6	0	5.291648	7.743837	3.510698
52	6	0	5.850711	8.951157	3.972286
53	1	0	6.146564	9.040904	5.016159
54	6	0	6.036961	10.047425	3.134193
55	1	0	6.471702	10.962984	3.533096
56	6	0	5.669997	9.992193	1.781045
57	6	0	5.112607	8.800828	1.308943
58	1	0	4.815712	8.727912	0.263932
59	6	0	4.928724	7.704601	2.157022
60	1	0	4.487698	6.798720	1.746263
61	6	0	5.872633	11.183660	0.873152
62	1	0	5.519356	10.976210	-0.142351
63	1	0	6.931886	11.463872	0.805789
64	1	0	5.332549	12.066175	1.239584
65	5	0	5.091332	6.479009	4.506991
66	6	0	0.751678	5.874431	4.691290
67	6	0	-0.003885	7.058785	4.751186
68	6	0	0.052987	4.656189	4.629716
69	6	0	-1.396264	7.023472	4.739289
70	1	0	0.512476	8.013970	4.781188
71	6	0	-1.339604	4.629147	4.615735
72	1	0	0.606625	3.722295	4.622196
73	6	0	-2.092260	5.809549	4.671201
74	1	0	-1.952464	7.957857	4.773986
75	1	0	-1.852445	3.670612	4.572079
76	6	0	-3.602335	5.773838	4.687768
77	1	0	-3.989149	5.755218	5.715725
78	1	0	-4.029542	6.655513	4.197926
79	1	0	-3.988494	4.883741	4.179848
80	1	0	1.817222	3.722526	2.596333

81	1	0	1.441829	7.181215	7.376681

1b

Zero-point correction= 0.672303 (Hartree/Particle)
Thermal correction to Energy= 0.712747
Thermal correction to Enthalpy= 0.713691
Thermal correction to Gibbs Free Energy= 0.598171
Sum of electronic and zero-point Energies= -2073.290872
Sum of electronic and thermal Energies= -2073.250429
Sum of electronic and thermal Enthalpies= -2073.249485
Sum of electronic and thermal Free Energies= -2073.365005

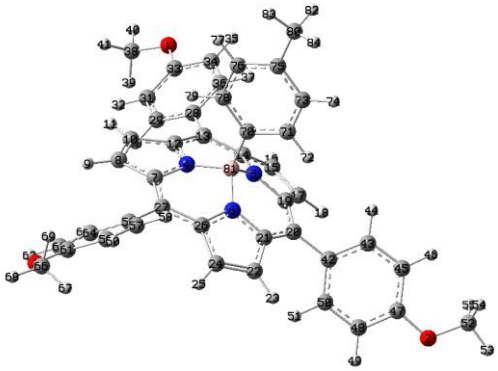


Fig. S89 Optimized structures of **1b**.

Table S18 Coordinates of atoms in **1b**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.678664	14.323976	5.549494
2	8	0	7.833547	1.323847	0.125915
3	8	0	-1.630013	3.430977	10.790261
4	7	0	4.558102	6.944344	7.413968
5	7	0	6.233436	6.523945	5.772708
6	7	0	4.864421	4.741069	6.583649
7	6	0	3.406457	6.590014	8.063004
8	6	0	2.807591	7.830986	8.487856
9	1	0	1.886636	7.932054	9.044815
10	6	0	3.581672	8.869060	8.001454
11	1	0	3.371726	9.923711	8.112010
12	6	0	4.680405	8.298676	7.261998
13	6	0	5.661913	8.806413	6.358445
14	6	0	6.348718	7.866037	5.532241
15	6	0	6.962195	7.982606	4.233221
16	1	0	7.181482	8.913160	3.727276
17	6	0	7.104490	6.710406	3.714793
18	1	0	7.456575	6.452754	2.725045
19	6	0	6.585559	5.776073	4.682309
20	6	0	6.165022	4.416419	4.577407
21	6	0	5.206625	3.944195	5.523863

22	6	0	4.276291	2.841905	5.551258
23	1	0	4.262576	2.010781	4.860549
24	6	0	3.357618	3.084245	6.554707
25	1	0	2.484463	2.488755	6.784865
26	6	0	3.708093	4.330608	7.187087
27	6	0	2.994285	5.223145	8.043033
28	6	0	5.875919	10.255625	6.147288
29	6	0	4.814546	11.163122	5.995952
30	1	0	3.792008	10.799226	6.001207
31	6	0	5.035970	12.526609	5.795637
32	1	0	4.186871	13.188889	5.670934
33	6	0	6.347300	13.017881	5.738035
34	6	0	7.422340	12.125036	5.875424
35	1	0	8.435264	12.514616	5.832451
36	6	0	7.187279	10.771677	6.074341
37	1	0	8.031112	10.098948	6.196951
38	6	0	5.626687	15.277534	5.409583
39	1	0	5.004527	15.063673	4.531981
40	1	0	6.117270	16.243854	5.276416
41	1	0	4.995188	15.312943	6.306039
42	6	0	6.606883	3.603367	3.420662
43	6	0	7.968862	3.536426	3.083466
44	1	0	8.694695	4.065352	3.694518
45	6	0	8.424321	2.788303	1.996065
46	1	0	9.486289	2.759426	1.780167
47	6	0	7.506855	2.082112	1.207498
48	6	0	6.139306	2.143454	1.522953
49	1	0	5.433542	1.607916	0.894576
50	6	0	5.700897	2.891530	2.606521
51	1	0	4.635939	2.951026	2.806256
52	6	0	9.208595	1.223159	-0.241375
53	1	0	9.233916	0.584721	-1.126758
54	1	0	9.803697	0.760837	0.555680
55	1	0	9.630334	2.204327	-0.491539
56	6	0	1.787358	4.748134	8.756481
57	6	0	1.833146	3.561814	9.507290
58	1	0	2.766543	3.010192	9.572285
59	6	0	0.719310	3.083895	10.200012
60	1	0	0.804859	2.168633	10.774715
61	6	0	-0.485493	3.796966	10.151738
62	6	0	-0.555365	4.978561	9.394909
63	1	0	-1.499406	5.513728	9.347509
64	6	0	0.559770	5.441275	8.710184
65	1	0	0.471286	6.339487	8.107258
66	6	0	-1.610297	2.251604	11.593371
67	1	0	-1.389813	1.360681	10.992574
68	1	0	-2.613540	2.161815	12.014802
69	1	0	-0.880319	2.333396	12.408136
70	6	0	6.721543	5.669298	8.228687
71	6	0	7.759138	4.731693	8.058720
72	1	0	7.833388	4.177328	7.124651
73	6	0	8.704056	4.482560	9.054152
74	1	0	9.488280	3.746955	8.881197
75	6	0	8.659721	5.163490	10.280839
76	6	0	7.630933	6.094682	10.466945
77	1	0	7.563902	6.634974	11.409947
78	6	0	6.687949	6.337789	9.463121

79	1	0	5.905100	7.068994	9.654180
80	6	0	9.699713	4.915559	11.348743
81	5	0	5.639182	5.957028	7.044434
82	1	0	10.617379	5.488705	11.155651
83	1	0	9.336020	5.210414	12.339218
84	1	0	9.987201	3.858574	11.392997

1c

Zero-point correction= 1.308583 (Hartree/Particle)
Thermal correction to Energy= 1.378308
Thermal correction to Enthalpy= 1.379252
Thermal correction to Gibbs Free Energy= 1.193058
Sum of electronic and zero-point Energies= -2838.667961
Sum of electronic and thermal Energies= -2838.598236
Sum of electronic and thermal Enthalpies= -2838.597292
Sum of electronic and thermal Free Energies= -2838.783486

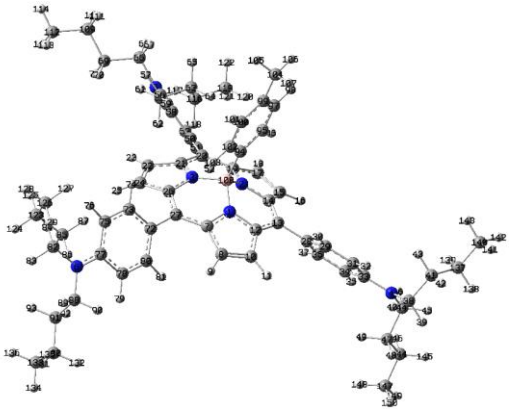


Fig. S90 Optimized structures of **1c**.

Table S19 Coordinates of atoms in **1c**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	23.526487	13.133367	5.112208
2	7	0	24.625465	14.842939	6.336428
3	7	0	22.246825	14.697808	6.389414
4	7	0	30.831723	11.722068	2.436926
5	7	0	22.909067	21.725935	9.949906
6	7	0	16.282086	11.813482	2.077181
7	6	0	22.421877	12.752986	4.397026
8	6	0	22.926971	11.989185	3.283742
9	1	0	22.328106	11.521098	2.515473
10	6	0	24.308486	12.036705	3.324773
11	1	0	24.987397	11.629762	2.587559
12	6	0	24.693921	12.810403	4.475975
13	6	0	25.919708	13.435584	4.865375
14	6	0	25.833493	14.544886	5.764176
15	6	0	26.713629	15.617789	6.150307
16	1	0	27.759186	15.705254	5.890542

17	6	0	25.973038	16.547092	6.860999
18	1	0	26.340537	17.484839	7.253165
19	6	0	24.614148	16.073895	6.935436
20	6	0	23.361653	16.644335	7.323833
21	6	0	22.173456	15.959737	6.916368
22	6	0	20.836027	16.420221	6.646096
23	1	0	20.445666	17.393850	6.909899
24	6	0	20.194944	15.452583	5.895717
25	1	0	19.207622	15.523755	5.459749
26	6	0	21.120418	14.369980	5.683385
27	6	0	21.146124	13.301084	4.734879
28	6	0	27.187322	13.017063	4.235183
29	6	0	27.514703	11.652739	4.115019
30	1	0	26.834865	10.906748	4.517814
31	6	0	28.698882	11.222302	3.529946
32	1	0	28.893268	10.157330	3.498439
33	6	0	29.645817	12.142500	3.009985
34	6	0	29.305731	13.517069	3.113437
35	1	0	29.959857	14.276205	2.702175
36	6	0	28.120581	13.930362	3.708034
37	1	0	27.897446	14.992904	3.722903
38	6	0	31.102104	10.298771	2.209127
39	1	0	31.800339	10.233374	1.367804
40	1	0	30.183227	9.799589	1.879495
41	6	0	31.694257	9.546908	3.415514
42	1	0	31.762159	8.484698	3.138090
43	1	0	30.996835	9.601420	4.261553
44	6	0	31.778166	12.675927	1.852969
45	1	0	32.763339	12.199764	1.859068
46	1	0	31.864155	13.550772	2.506698
47	6	0	31.435186	13.113501	0.419253
48	1	0	31.366684	12.220572	-0.218011
49	1	0	30.442696	13.582870	0.406258
50	6	0	23.257678	17.959532	7.984319
51	6	0	24.034537	19.071464	7.605014
52	1	0	24.725010	18.984035	6.771898
53	6	0	23.926129	20.301186	8.240444
54	1	0	24.561274	21.109740	7.898939
55	6	0	23.015214	20.507515	9.309623
56	6	0	22.219255	19.392401	9.680136
57	1	0	21.489154	19.478865	10.476248
58	6	0	22.343943	18.167952	9.036233
59	1	0	21.724555	17.340574	9.372326
60	6	0	23.646162	22.905702	9.494834
61	1	0	23.054599	23.785660	9.772664
62	1	0	23.692560	22.908209	8.400398
63	6	0	25.058142	23.032706	10.088699
64	1	0	25.645823	22.143472	9.824913
65	1	0	24.982514	23.042420	11.185152
66	6	0	22.072315	21.905098	11.136931
67	1	0	22.103966	20.995244	11.746133
68	1	0	22.533988	22.691226	11.745608
69	6	0	20.616708	22.290483	10.828937
70	1	0	20.153251	21.504802	10.217786
71	1	0	20.613234	23.204039	10.217661
72	6	0	19.904127	12.921612	4.030884
73	6	0	18.714472	12.687986	4.747497

74	1	0	18.724664	12.764410	5.831632
75	6	0	17.529549	12.323477	4.120425
76	1	0	16.663511	12.123835	4.740112
77	6	0	17.452760	12.179198	2.710835
78	6	0	18.646519	12.436693	1.986900
79	1	0	18.650583	12.389251	0.904543
80	6	0	19.825383	12.788575	2.631251
81	1	0	20.697074	13.007652	2.022179
82	6	0	15.024415	11.654318	2.808384
83	1	0	14.210438	11.886013	2.111840
84	1	0	14.965596	12.407350	3.601813
85	6	0	14.809622	10.248326	3.391579
86	1	0	14.870949	9.512388	2.577581
87	1	0	15.627017	10.013004	4.085994
88	6	0	16.233388	11.537333	0.640099
89	1	0	15.448178	10.790846	0.483911
90	1	0	17.169475	11.062142	0.326081
91	6	0	15.956530	12.781476	-0.221534
92	1	0	16.719212	13.539150	-0.001626
93	1	0	14.991810	13.214444	0.078699
94	6	0	23.588318	12.862939	7.743394
95	6	0	24.554019	13.018516	8.749922
96	1	0	25.291214	13.814711	8.667114
97	6	0	24.604805	12.179360	9.868888
98	1	0	25.371431	12.338243	10.625601
99	6	0	23.684693	11.138260	10.033900
100	6	0	22.714060	10.966299	9.033353
101	1	0	21.983899	10.163822	9.129938
102	6	0	22.672083	11.806602	7.921775
103	1	0	21.902230	11.632779	7.171838
104	6	0	23.731035	10.223867	11.235977
105	1	0	22.763881	10.189580	11.753489
106	1	0	24.485840	10.551773	11.958727
107	1	0	23.973367	9.191991	10.948149
108	5	0	23.497140	13.846683	6.445362
109	6	0	19.787222	22.517181	12.098894
110	1	0	20.262328	23.299524	12.708100
111	1	0	19.799882	21.603311	12.710053
112	6	0	18.336819	22.911637	11.806369
113	1	0	17.822543	22.134663	11.226588
114	1	0	17.770416	23.064239	12.732997
115	1	0	18.286327	23.843540	11.228801
116	6	0	25.788105	24.294838	9.611597
117	1	0	25.187732	25.180628	9.864931
118	1	0	25.863144	24.279439	8.514708
119	6	0	27.188487	24.440391	10.214224
120	1	0	27.825943	23.586904	9.950383
121	1	0	27.684922	25.349592	9.854305
122	1	0	27.146339	24.495565	11.309470
123	6	0	13.463005	10.107132	4.111927
124	1	0	12.648912	10.349519	3.413730
125	1	0	13.403388	10.849325	4.920880
126	6	0	13.237985	8.706673	4.689185
127	1	0	14.018615	8.446227	5.415099
128	1	0	12.270874	8.636208	5.201541
129	1	0	13.252487	7.944324	3.899748
130	6	0	15.946385	12.500986	-1.733416

131	1	0	15.864724	13.460476	-2.261215
132	1	0	16.915264	12.073079	-2.029313
133	6	0	14.816556	11.578266	-2.205535
134	1	0	14.822801	11.479493	-3.297787
135	1	0	14.904636	10.568826	-1.786742
136	1	0	13.834793	11.973979	-1.914296
137	6	0	33.073429	10.043408	3.866078
138	1	0	33.779513	9.973163	3.025908
139	1	0	33.009114	11.106860	4.131488
140	6	0	33.625468	9.258451	5.060186
141	1	0	33.729246	8.191679	4.823416
142	1	0	34.613111	9.629772	5.359807
143	1	0	32.961864	9.341230	5.930334
144	6	0	32.473067	14.081913	-0.162428
145	1	0	33.465443	13.609252	-0.137004
146	1	0	32.541303	14.971321	0.480257
147	6	0	32.153566	14.514831	-1.596069
148	1	0	31.182197	15.022306	-1.651966
149	1	0	32.911955	15.206750	-1.982112
150	1	0	32.115478	13.652269	-2.273521

1d

Zero-point correction= 1.304947 (Hartree/Particle)
Thermal correction to Energy= 1.376812
Thermal correction to Enthalpy= 1.377756
Thermal correction to Gibbs Free Energy= 1.190071
Sum of electronic and zero-point Energies= -2838.653205
Sum of electronic and thermal Energies= -2838.581339
Sum of electronic and thermal Enthalpies= -2838.580395
Sum of electronic and thermal Free Energies= -2838.768080

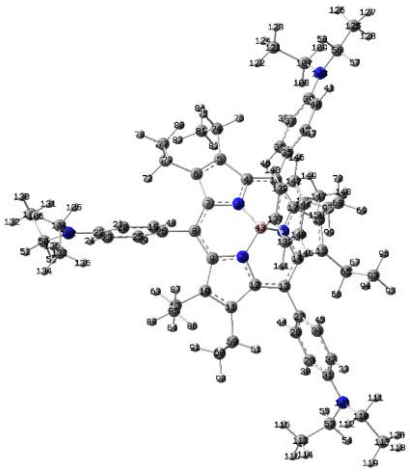


Fig. S91 Optimized structures of **1d**.

Table S20 Coordinates of atoms in **1d**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	4.441854	9.437153	3.935343
2	7	0	2.492121	10.431013	4.866249
3	7	0	3.432690	11.299418	2.862000
4	6	0	4.194041	11.120697	1.741849
5	6	0	3.628598	12.013853	0.740346
6	6	0	2.509143	12.628404	1.302376
7	6	0	2.353748	12.113421	2.655058
8	6	0	1.316749	12.136954	3.637905
9	6	0	1.367758	11.194466	4.712537
10	6	0	0.396194	10.650009	5.649312
11	6	0	0.967240	9.526308	6.247222
12	6	0	2.307372	9.366161	5.702376
13	6	0	3.305256	8.342254	5.749593
14	6	0	4.352643	8.363867	4.779371
15	6	0	5.314997	7.391498	4.277799
16	6	0	5.851240	7.898161	3.095139
17	6	0	5.244334	9.199545	2.854217
18	6	0	5.199202	10.104123	1.750148
19	6	0	0.067067	14.289728	4.067536
20	6	0	-1.037657	15.126070	3.923378
21	1	0	-1.025469	16.082470	4.432260
22	6	0	-2.161574	14.737436	3.152003
23	6	0	-2.097871	13.456879	2.543334
24	1	0	-2.914363	13.102293	1.925332
25	6	0	-0.986737	12.633868	2.703658
26	6	0	0.125245	13.024468	3.466089
27	6	0	3.176437	7.211154	6.720251
28	6	0	2.558850	5.998085	6.376880
29	6	0	2.425574	4.954793	7.287434
30	1	0	1.940054	4.046709	6.950734
31	6	0	2.918552	5.059388	8.612467
32	6	0	3.521300	6.292681	8.960381
33	1	0	3.888019	6.465122	9.964277
34	6	0	3.650008	7.327077	8.033518
35	6	0	6.135626	9.950523	0.593265
36	6	0	5.828314	9.173727	-0.533479
37	6	0	6.702204	9.057331	-1.610406
38	1	0	6.394094	8.444866	-2.449027
39	6	0	7.959207	9.712420	-1.619736
40	6	0	8.260307	10.504661	-0.483785
41	1	0	9.187123	11.060900	-0.426955
42	6	0	7.373312	10.608551	0.586376
43	5	0	3.806839	10.777105	4.222262
44	1	0	2.172855	5.862210	5.369687
45	1	0	4.120773	8.254030	8.352205
46	1	0	4.879030	8.646973	-0.576173
47	1	0	7.652312	11.229418	1.434313
48	1	0	0.903679	14.631318	4.672462
49	1	0	-0.983648	11.661340	2.216695
50	6	0	-4.474620	15.111979	2.316995
51	1	0	-5.317548	15.658402	2.753989
52	1	0	-4.650477	14.055373	2.544906
53	6	0	1.773485	2.997383	9.343244
54	1	0	2.040972	2.117822	9.931497
55	1	0	1.762918	2.657713	8.304880
56	6	0	10.092626	10.366518	-2.640651

57	1	0	10.552910	10.213330	-1.659282
58	1	0	9.866638	11.443611	-2.715061
59	6	0	0.252859	8.620047	7.219986
60	1	0	-0.358939	9.235564	7.890843
61	1	0	0.978560	8.106708	7.855112
62	6	0	-0.979577	11.181865	5.961799
63	1	0	-1.433960	11.607909	5.064383
64	1	0	-1.626038	10.353995	6.272347
65	6	0	5.717889	6.086847	4.915806
66	1	0	4.842820	5.571373	5.319321
67	1	0	6.141858	5.424854	4.153441
68	6	0	6.825524	7.163256	2.207884
69	1	0	7.565701	6.654804	2.837906
70	1	0	7.383338	7.876532	1.596707
71	6	0	1.664624	13.670314	0.614479
72	1	0	0.613400	13.549707	0.886344
73	1	0	1.722614	13.528440	-0.469861
74	6	0	4.094084	12.216628	-0.680874
75	1	0	3.993083	13.278761	-0.936305
76	1	0	5.158669	11.983996	-0.760908
77	6	0	2.103959	15.109288	0.947121
78	1	0	1.469269	15.835492	0.424587
79	1	0	2.030507	15.308259	2.021650
80	1	0	3.142593	15.287141	0.644129
81	6	0	3.317085	11.387373	-1.720636
82	1	0	3.390767	10.315646	-1.510790
83	1	0	2.253391	11.651174	-1.728595
84	1	0	3.716128	11.562388	-2.727356
85	6	0	-0.977833	12.248529	7.073985
86	1	0	-0.572663	11.847451	8.010615
87	1	0	-0.371727	13.116029	6.791913
88	1	0	-1.998478	12.599360	7.270059
89	6	0	-0.657439	7.573956	6.549386
90	1	0	-1.143091	6.946302	7.306857
91	1	0	-1.443281	8.051478	5.952906
92	1	0	-0.086793	6.917451	5.884685
93	6	0	6.753337	6.267493	6.042146
94	1	0	6.358658	6.896503	6.847032
95	1	0	7.025085	5.296349	6.473727
96	1	0	7.668624	6.739481	5.665855
97	6	0	6.163560	6.120257	1.288380
98	1	0	6.915066	5.631435	0.656345
99	1	0	5.653449	5.343520	1.869365
100	1	0	5.421153	6.584626	0.631464
101	7	0	2.841333	3.991237	9.510163
102	7	0	-3.262135	15.561746	3.001058
103	7	0	8.859185	9.565079	-2.676546
104	6	0	-3.276056	16.931248	3.515591
105	1	0	-2.280622	17.373127	3.401682
106	1	0	-3.940359	17.515484	2.869500
107	6	0	8.355849	9.135621	-3.986132
108	1	0	7.747558	8.236796	-3.853323
109	1	0	9.210824	8.818111	-4.584915
110	6	0	3.369214	4.196330	10.867051
111	1	0	4.354959	4.659631	10.763183
112	1	0	2.746832	4.907036	11.436982
113	6	0	0.378802	3.487904	9.750313

114	1	0	0.351845	3.777664	10.807340
115	1	0	0.070414	4.353791	9.153586
116	1	0	-0.361062	2.691906	9.600980
117	6	0	3.550179	2.917000	11.683314
118	1	0	4.095728	3.166487	12.600575
119	1	0	2.602067	2.459698	11.983628
120	1	0	4.138642	2.172410	11.134876
121	6	0	7.561482	10.204227	-4.746684
122	1	0	6.680187	10.526092	-4.180878
123	1	0	8.177641	11.088826	-4.946156
124	1	0	7.219417	9.807855	-5.710694
125	6	0	11.134901	9.997525	-3.694736
126	1	0	10.826633	10.256440	-4.712696
127	1	0	12.052538	10.557001	-3.480344
128	1	0	11.379048	8.929571	-3.664086
129	6	0	-4.454629	15.334096	0.800464
130	1	0	-4.332375	16.397270	0.561947
131	1	0	-3.634066	14.785337	0.325611
132	1	0	-5.396862	14.993439	0.353686
133	6	0	-3.747115	17.048160	4.969719
134	1	0	-4.765168	16.657626	5.085110
135	1	0	-3.092671	16.491080	5.648845
136	1	0	-3.750422	18.099107	5.284279
137	6	0	4.730186	11.805544	5.102210
138	6	0	4.695641	11.823491	6.508531
139	6	0	5.617637	12.716979	4.499535
140	6	0	5.502938	12.677469	7.265036
141	1	0	4.010656	11.162202	7.035500
142	6	0	6.428654	13.574570	5.246090
143	1	0	5.670839	12.773450	3.414280
144	6	0	6.391937	13.567203	6.647566
145	1	0	5.436787	12.657569	8.351903
146	1	0	7.095606	14.266326	4.733264
147	6	0	7.290297	14.472476	7.458149
148	1	0	8.292350	14.037762	7.580157
149	1	0	7.421959	15.447399	6.974302
150	1	0	6.887314	14.643786	8.462525

2a

Zero-point correction= 0.539251 (Hartree/Particle)
Thermal correction to Energy= 0.570574
Thermal correction to Enthalpy= 0.571519
Thermal correction to Gibbs Free Energy= 0.475296
Sum of electronic and zero-point Energies= -1576.706517
Sum of electronic and thermal Energies= -1576.675194
Sum of electronic and thermal Enthalpies= -1576.674249
Sum of electronic and thermal Free Energies= -1576.770472

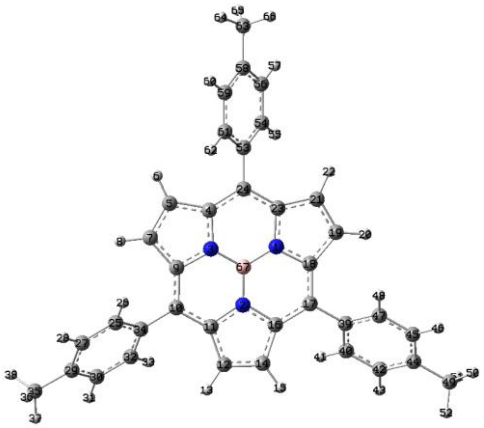


Fig. S92 Optimized structures of **2a**.

Table S21 Coordinates of atoms in **2a**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.149979	9.787943	4.218163
2	7	0	2.137381	9.713552	5.485353
3	7	0	3.151949	7.692031	4.741403
4	6	0	4.198969	6.996036	4.178470
5	6	0	3.883751	5.625755	4.479322
6	1	0	4.484381	4.768852	4.207553
7	6	0	2.691223	5.582190	5.197813
8	1	0	2.217261	4.686616	5.574366
9	6	0	2.204551	6.922665	5.380091
10	6	0	1.121188	7.597155	6.041851
11	6	0	1.087165	9.034121	6.062034
12	6	0	0.212197	10.088952	6.496849
13	1	0	-0.739087	9.951594	6.991751
14	6	0	0.777994	11.316336	6.159516
15	1	0	0.335264	12.284011	6.349994
16	6	0	2.034701	11.087308	5.499575
17	6	0	3.075315	11.848558	4.864065
18	6	0	4.163334	11.164922	4.220819
19	6	0	5.377347	11.483015	3.518761
20	1	0	5.746730	12.479942	3.323577
21	6	0	6.002340	10.299373	3.133137
22	1	0	6.928762	10.230501	2.580410
23	6	0	5.217592	9.184713	3.591437
24	6	0	5.259541	7.748666	3.566713
25	6	0	-0.502198	5.681834	6.086884
26	1	0	-0.177658	5.396559	5.090835
27	6	0	-1.498588	4.944449	6.719953
28	1	0	-1.923348	4.080559	6.214377
29	6	0	-1.972398	5.300394	7.991919
30	6	0	-1.416974	6.432962	8.604628
31	1	0	-1.762141	6.730778	9.591877
32	6	0	-0.421695	7.179315	7.978493
33	1	0	0.007718	8.033316	8.493365
34	6	0	0.057043	6.815420	6.706328
35	6	0	-3.025830	4.473713	8.685853

36	1	0	−3.750517	4.067699	7.971642
37	1	0	−3.568946	5.060787	9.433493
38	1	0	−2.572759	3.619186	9.207049
39	6	0	3.020318	13.326148	4.863454
40	6	0	2.692154	14.037942	6.033536
41	1	0	2.506533	13.499159	6.957891
42	6	0	2.638773	15.427945	6.028207
43	1	0	2.394278	15.954117	6.948137
44	6	0	2.906398	16.163424	4.862313
45	6	0	3.230907	15.452257	3.699366
46	1	0	3.431889	15.995654	2.779324
47	6	0	3.290296	14.059693	3.694836
48	1	0	3.516314	13.537799	2.769782
49	6	0	2.844098	17.670295	4.870425
50	1	0	3.071596	18.084973	3.883684
51	1	0	3.559083	18.092853	5.587719
52	1	0	1.849082	18.025469	5.166515
53	6	0	6.387396	7.044807	2.919790
54	6	0	7.718367	7.446450	3.140486
55	1	0	7.928491	8.266245	3.820798
56	6	0	8.773383	6.775101	2.529637
57	1	0	9.793535	7.095447	2.728162
58	6	0	8.546752	5.684550	1.675169
59	6	0	7.220109	5.287751	1.457569
60	1	0	7.013732	4.449518	0.796626
61	6	0	6.156994	5.951025	2.066865
62	1	0	5.139145	5.635670	1.857996
63	6	0	9.696244	4.975067	1.003749
64	1	0	9.392990	3.995422	0.620828
65	1	0	10.533796	4.829761	1.695438
66	1	0	10.078203	5.558191	0.155003
67	5	0	3.143609	9.064487	4.810978

2b

Zero-point correction= 0.554449 (Hartree/Particle)
Thermal correction to Energy= 0.588340
Thermal correction to Enthalpy= 0.589284
Thermal correction to Gibbs Free Energy= 0.486792
Sum of electronic and zero-point Energies= -1802.309264
Sum of electronic and thermal Energies= -1802.275374
Sum of electronic and thermal Enthalpies= -1802.274430
Sum of electronic and thermal Free Energies= -1802.376921

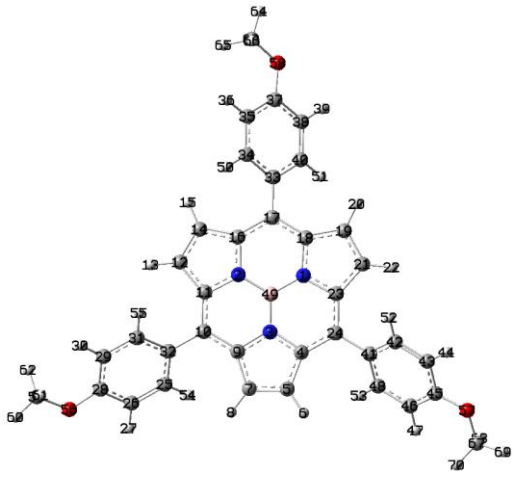


Fig. S93 Optimized structures of **2b**.

Table S22 Coordinates of atoms in **2b**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.350582	9.838028	4.109260
2	7	0	2.379939	9.690436	5.434559
3	7	0	3.374114	7.712610	4.552929
4	6	0	4.419050	7.050749	3.945021
5	6	0	4.134227	5.667956	4.212200
6	1	0	4.742826	4.829969	3.901889
7	6	0	2.962385	5.582437	4.961650
8	1	0	2.516423	4.667478	5.325780
9	6	0	2.460286	6.907498	5.198280
10	6	0	1.393795	7.541835	5.925768
11	6	0	1.350706	8.977494	6.009394
12	6	0	0.479513	10.003572	6.511425
13	1	0	-0.458287	9.837293	7.023021
14	6	0	1.026701	11.250189	6.212818
15	1	0	0.579138	12.203846	6.455394
16	6	0	2.267222	11.061708	5.512603
17	6	0	3.284164	11.861273	4.882536
18	6	0	4.358840	11.213798	4.179340
19	6	0	5.552792	11.571561	3.463037
20	1	0	5.914063	12.578063	3.305414
21	6	0	6.172926	10.410935	3.004698
22	1	0	7.085504	10.374824	2.426366
23	6	0	5.406511	9.271659	3.429341
24	6	0	5.461951	7.837330	3.343421
25	6	0	-0.197375	5.594700	5.963623
26	6	0	-1.160982	4.825857	6.597042
27	1	0	-1.599953	3.964530	6.102752
28	6	0	-1.597532	5.158215	7.891983
29	6	0	-1.050861	6.277836	8.536496
30	1	0	-1.357101	6.549275	9.539835
31	6	0	-0.086446	7.045660	7.887517
32	6	0	0.363248	6.726326	6.594372
33	6	0	3.216967	13.333818	4.943569

34	6	0	2.882250	14.000442	6.134664
35	6	0	2.811068	15.390939	6.198498
36	1	0	2.561396	15.866719	7.139620
37	6	0	3.075417	16.154390	5.051749
38	6	0	3.411959	15.503305	3.851821
39	1	0	3.602211	16.103023	2.966873
40	6	0	3.482980	14.120334	3.801895
41	6	0	6.588365	7.171835	2.660272
42	6	0	7.920310	7.587170	2.872874
43	6	0	8.976270	6.962066	2.228533
44	1	0	10.000862	7.275242	2.405217
45	6	0	8.737183	5.898748	1.339960
46	6	0	7.420320	5.470329	1.116698
47	1	0	7.206032	4.659207	0.430371
48	6	0	6.367154	6.103629	1.774593
49	5	0	3.363086	9.080481	4.691870
50	1	0	2.702022	13.428166	7.039640
51	1	0	3.713889	13.637839	2.857242
52	1	0	8.130325	8.386696	3.576714
53	1	0	5.351959	5.778511	1.567990
54	1	0	0.104998	5.335528	4.953622
55	1	0	0.347441	7.889794	8.414299
56	8	0	-2.537940	4.343008	8.427684
57	8	0	9.834136	5.358996	0.754996
58	8	0	3.031857	17.507698	4.997515
59	6	0	-3.033205	4.636377	9.736337
60	1	0	-3.766104	3.858020	9.955567
61	1	0	-2.231578	4.601458	10.483451
62	1	0	-3.522989	5.616725	9.766545
63	6	0	2.672164	18.229791	6.177538
64	1	0	2.689202	19.283969	5.895291
65	1	0	1.665056	17.960383	6.516791
66	1	0	3.392230	18.058562	6.986420
67	6	0	9.657958	4.274327	-0.158748
68	1	0	9.054228	4.575304	-1.023248
69	1	0	10.660936	4.004399	-0.493980
70	1	0	9.194664	3.410673	0.332652

2c

Zero-point correction= 1.192341 (Hartree/Particle)
Thermal correction to Energy= 1.254843
Thermal correction to Enthalpy= 1.255788
Thermal correction to Gibbs Free Energy= 1.087021
Sum of electronic and zero-point Energies= -2567.692200
Sum of electronic and thermal Energies= -2567.629698
Sum of electronic and thermal Enthalpies= -2567.628754
Sum of electronic and thermal Free Energies= -2567.797521

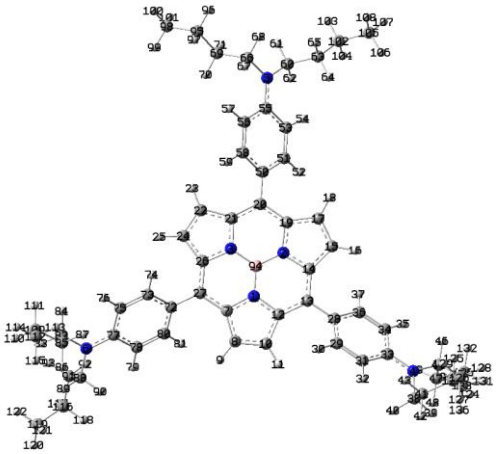


Fig. S94 Optimized structures of **2c**.

Table S23 Coordinates of atoms in **2c**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	23.360740	13.958357	4.042399
2	7	0	24.500477	15.611770	5.324268
3	7	0	22.121491	15.469827	5.403658
4	7	0	30.811432	11.738456	2.521565
5	7	0	23.028525	21.672114	10.215835
6	7	0	16.074502	11.549823	2.120510
7	6	0	22.212757	13.356995	3.570211
8	6	0	22.714088	12.302783	2.736386
9	1	0	22.112106	11.590522	2.189821
10	6	0	24.108972	12.339323	2.745094
11	1	0	24.753128	11.669287	2.193591
12	6	0	24.544590	13.401702	3.605402
13	6	0	25.779721	13.961910	4.093770
14	6	0	25.733555	15.085704	4.996610
15	6	0	26.641167	15.845245	5.805917
16	1	0	27.713209	15.712780	5.843703
17	6	0	25.914567	16.762753	6.566457
18	1	0	26.336984	17.451075	7.284850
19	6	0	24.519752	16.618093	6.268166
20	6	0	23.258466	17.157762	6.716087
21	6	0	22.032826	16.574187	6.225885
22	6	0	20.622576	16.826595	6.286315
23	1	0	20.149267	17.634765	6.825851
24	6	0	19.955729	15.876896	5.510279
25	1	0	18.886703	15.835222	5.355741
26	6	0	20.918718	14.988283	4.929237
27	6	0	20.942651	13.882031	4.004546
28	6	0	27.070274	13.389462	3.692360
29	6	0	27.261788	11.997774	3.568589
30	1	0	26.448873	11.321640	3.814942
31	6	0	28.478939	11.452818	3.193285
32	1	0	28.562177	10.374262	3.152017
33	6	0	29.602630	12.273788	2.898656
34	6	0	29.405018	13.677225	3.019270
35	1	0	30.205862	14.365873	2.781176

36	6	0	28.185200	14.205674	3.409300
37	1	0	28.081216	15.285868	3.451684
38	6	0	30.965388	10.300632	2.264770
39	1	0	31.794654	10.189726	1.558559
40	1	0	30.074619	9.926561	1.747816
41	6	0	31.242294	9.439803	3.510243
42	1	0	31.264815	8.391463	3.178902
43	1	0	30.402553	9.523696	4.212494
44	6	0	31.958461	12.591721	2.191479
45	1	0	32.861562	11.997172	2.356966
46	1	0	32.009527	13.422769	2.902628
47	6	0	31.952327	13.118952	0.747731
48	1	0	31.906285	12.264761	0.057805
49	1	0	31.041643	13.707783	0.576004
50	6	0	23.220524	18.294645	7.639990
51	6	0	24.152197	19.351452	7.551922
52	1	0	24.913910	19.331032	6.778425
53	6	0	24.104078	20.448639	8.395021
54	1	0	24.850700	21.222691	8.268720
55	6	0	23.101195	20.573572	9.396142
56	6	0	22.176496	19.497050	9.498489
57	1	0	21.396382	19.515442	10.249426
58	6	0	22.238645	18.406314	8.647659
59	1	0	21.522584	17.602753	8.790428
60	6	0	23.918297	22.825983	10.051877
61	1	0	23.364822	23.709911	10.386941
62	1	0	24.123034	22.983166	8.987947
63	6	0	25.231557	22.715604	10.840528
64	1	0	25.777748	21.819663	10.516582
65	1	0	24.996129	22.570817	11.904062
66	6	0	22.034598	21.775891	11.289073
67	1	0	21.905278	20.798538	11.765646
68	1	0	22.457590	22.432861	12.056331
69	6	0	20.677772	22.331800	10.829739
70	1	0	20.261283	21.678867	10.051307
71	1	0	20.834738	23.314060	10.362819
72	6	0	19.687368	13.304661	3.511588
73	6	0	18.576559	13.120329	4.361615
74	1	0	18.656740	13.386995	5.411435
75	6	0	17.395634	12.549955	3.915876
76	1	0	16.598492	12.399428	4.633263
77	6	0	17.236648	12.129329	2.566563
78	6	0	18.349348	12.339246	1.705217
79	1	0	18.283815	12.085755	0.654252
80	6	0	19.529345	12.895557	2.171029
81	1	0	20.336806	13.056885	1.463121
82	6	0	14.896114	11.407991	2.981300
83	1	0	14.017684	11.408048	2.326723
84	1	0	14.799885	12.294329	3.617081
85	6	0	14.896665	10.131264	3.836932
86	1	0	15.008995	9.259717	3.177027
87	1	0	15.771969	10.135338	4.499814
88	6	0	15.952126	10.998793	0.767033
89	1	0	15.238752	10.171437	0.823765
90	1	0	16.907107	10.556119	0.464804
91	6	0	15.485622	12.027075	-0.276670
92	1	0	16.186915	12.871009	-0.279050

93	1	0	14.511817	12.431329	0.033659
94	5	0	23.327322	15.017820	4.918779
95	6	0	19.676434	22.462879	11.984046
96	1	0	20.097398	23.120362	12.758045
97	1	0	19.537569	21.480777	12.458499
98	6	0	18.317393	23.008521	11.536636
99	1	0	17.854624	22.355596	10.785796
100	1	0	17.622612	23.088142	12.381319
101	1	0	18.416471	24.006776	11.091821
102	6	0	26.120758	23.954254	10.673136
103	1	0	25.555985	24.849728	10.969644
104	1	0	26.365630	24.085194	9.609446
105	6	0	27.415349	23.878399	11.487251
106	1	0	28.018809	23.008666	11.197695
107	1	0	28.030227	24.774144	11.338866
108	1	0	27.205439	23.793080	12.560930
109	6	0	13.617978	9.983281	4.671360
110	1	0	12.747379	9.960760	4.000584
111	1	0	13.492356	10.871401	5.307172
112	6	0	13.618483	8.727697	5.548022
113	1	0	14.450094	8.742506	6.263969
114	1	0	12.687896	8.642659	6.121901
115	1	0	13.719054	7.818372	4.941979
116	6	0	15.376389	11.456390	-1.700366
117	1	0	15.168595	12.286467	-2.388560
118	1	0	16.350995	11.046795	-2.003148
119	6	0	14.295368	10.383885	-1.876695
120	1	0	14.224792	10.069387	-2.924864
121	1	0	14.501263	9.486541	-1.281354
122	1	0	13.309617	10.762815	-1.577205
123	6	0	32.548514	9.767774	4.244151
124	1	0	33.390681	9.692829	3.541399
125	1	0	32.523125	10.809632	4.590116
126	6	0	32.801660	8.844104	5.439641
127	1	0	32.871157	7.795060	5.124635
128	1	0	33.737435	9.100342	5.950760
129	1	0	31.991171	8.914824	6.176381
130	6	0	33.188308	13.970905	0.432313
131	1	0	34.095081	13.376266	0.613406
132	1	0	33.234143	14.818407	1.131159
133	6	0	33.204511	14.497512	-1.005633
134	1	0	32.328361	15.126050	-1.209608
135	1	0	34.099014	15.102207	-1.197297
136	1	0	33.198005	13.674665	-1.731715

2d

Zero-point correction= 1.187995 (Hartree/Particle)
Thermal correction to Energy= 1.252827
Thermal correction to Enthalpy= 1.253771
Thermal correction to Gibbs Free Energy= 1.082339
Sum of electronic and zero-point Energies= -2567.686803
Sum of electronic and thermal Energies= -2567.621971
Sum of electronic and thermal Enthalpies= -2567.621027

Sum of electronic and thermal Free Energies= -2567.792459

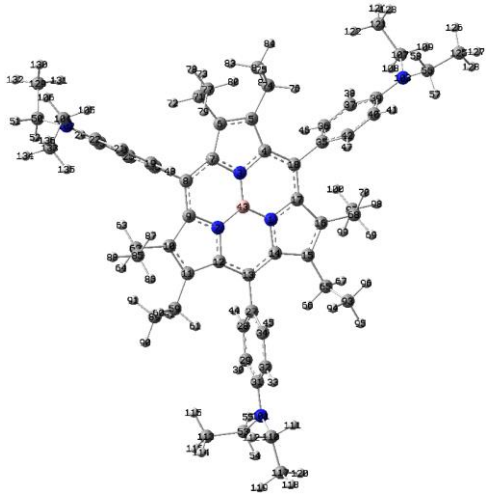


Fig. S95 Optimized structures of **2d**.

Table S24 Coordinates of atoms in **2d**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.934214	8.945429	3.493681
2	7	0	2.021571	9.982361	4.464114
3	7	0	2.946779	10.842184	2.444230
4	6	0	3.886542	10.842063	1.436968
5	6	0	3.507424	11.974243	0.615775
6	6	0	2.370679	12.578947	1.183415
7	6	0	2.002708	11.842801	2.375731
8	6	0	1.004773	11.888350	3.405001
9	6	0	1.023044	10.931633	4.473131
10	6	0	0.243512	10.595650	5.647088
11	6	0	0.816915	9.465504	6.258608
12	6	0	1.979325	9.064944	5.491061
13	6	0	2.998907	8.055797	5.523209
14	6	0	4.001463	8.005318	4.498579
15	6	0	5.166369	7.216237	4.150067
16	6	0	5.719629	7.732838	2.964061
17	6	0	4.921112	8.863679	2.535958
18	6	0	4.906395	9.834627	1.480725
19	6	0	0.035970	14.156348	3.982417
20	6	0	-0.973908	15.111397	3.913165
21	1	0	-0.833164	16.044243	4.445938
22	6	0	-2.169192	14.872019	3.186679
23	6	0	-2.277633	13.610851	2.543334
24	1	0	-3.155992	13.367559	1.957862
25	6	0	-1.259647	12.667126	2.624514
26	6	0	-0.078847	12.914635	3.341395
27	6	0	3.012545	7.049984	6.627553
28	6	0	2.413103	5.790354	6.474901
29	6	0	2.408896	4.854339	7.502882
30	1	0	1.919366	3.905943	7.320865
31	6	0	3.027570	5.119449	8.752710
32	6	0	3.612880	6.403214	8.902794

33	1	0	4.072937	6.695932	9.837575
34	6	0	3.607155	7.331544	7.864279
35	6	0	5.981634	9.823519	0.443793
36	6	0	5.835098	9.136220	-0.769849
37	6	0	6.835245	9.139769	-1.736595
38	1	0	6.652587	8.592702	-2.653092
39	6	0	8.058942	9.830520	-1.537980
40	6	0	8.188939	10.536410	-0.313694
41	1	0	9.077369	11.116240	-0.100769
42	6	0	7.179695	10.522078	0.645167
43	5	0	2.966935	9.922710	3.466976
44	1	0	1.934160	5.534075	5.533058
45	1	0	4.067384	8.302509	8.030378
46	1	0	4.918546	8.587004	-0.970171
47	1	0	7.328876	11.078594	1.567355
48	1	0	0.931961	14.385421	4.553829
49	1	0	-1.386199	11.717820	2.109616
50	6	0	-4.468406	15.513657	2.491212
51	1	0	-5.217133	16.139366	2.989077
52	1	0	-4.745220	14.477993	2.713603
53	6	0	2.142402	3.036120	9.739484
54	1	0	2.527055	2.270228	10.414174
55	1	0	2.162301	2.581284	8.745568
56	6	0	10.270401	10.636152	-2.230717
57	1	0	10.616535	10.418518	-1.215209
58	1	0	10.006822	11.706483	-2.250099
59	6	0	0.249286	8.775539	7.470754
60	1	0	-0.206553	9.524709	8.127121
61	1	0	1.053430	8.306092	8.042685
62	6	0	-0.955883	11.336318	6.177210
63	1	0	-1.489369	11.814796	5.351916
64	1	0	-1.650398	10.617325	6.625631
65	6	0	5.743417	6.062365	4.927033
66	1	0	4.942832	5.525113	5.441679
67	1	0	6.195864	5.352475	4.226134
68	6	0	6.914857	7.152965	2.255007
69	1	0	7.613169	6.754045	2.998814
70	1	0	7.446565	7.943909	1.720135
71	6	0	1.708989	13.822413	0.651290
72	1	0	0.647264	13.816435	0.910582
73	1	0	1.764397	13.817473	-0.442753
74	6	0	4.171791	12.431044	-0.656504
75	1	0	4.125135	13.524451	-0.710063
76	1	0	5.231542	12.164045	-0.635834
77	6	0	2.351410	15.119313	1.179193
78	1	0	1.841784	15.993194	0.757238
79	1	0	2.280630	15.181363	2.270239
80	1	0	3.410890	15.178994	0.905919
81	6	0	3.526257	11.842411	-1.925296
82	1	0	3.579481	10.748646	-1.927614
83	1	0	2.471576	12.128517	-2.005583
84	1	0	4.046032	12.208198	-2.818387
85	6	0	-0.591700	12.399921	7.230452
86	1	0	-0.084005	11.950195	8.091333
87	1	0	0.070772	13.164220	6.810870
88	1	0	-1.497275	12.899823	7.592926
89	6	0	-0.808182	7.711883	7.117791

90	1	0	−1.204332	7.254359	8.031739
91	1	0	−1.647507	8.150966	6.566614
92	1	0	−0.379486	6.915379	6.500790
93	6	0	6.805331	6.493154	5.956347
94	1	0	6.379923	7.166865	6.707644
95	1	0	7.204097	5.615335	6.477720
96	1	0	7.642156	7.010674	5.473431
97	6	0	6.545569	6.033117	1.263648
98	1	0	7.448539	5.642112	0.780798
99	1	0	6.043851	5.201084	1.770647
100	1	0	5.876660	6.402604	0.479245
101	7	0	3.077049	4.167206	9.764007
102	7	0	−3.174590	15.813394	3.107793
103	7	0	9.081949	9.802558	−2.478970
104	6	0	−3.010721	17.167353	3.639830
105	1	0	−1.975956	17.492240	3.492070
106	1	0	−3.626771	17.834009	3.026725
107	6	0	8.782770	9.407679	−3.859812
108	1	0	8.217631	8.471854	−3.845536
109	1	0	9.726206	9.164946	−4.350385
110	6	0	3.665458	4.561191	11.054809
111	1	0	4.633856	5.026125	10.843793
112	1	0	3.048620	5.330951	11.547200
113	6	0	0.703808	3.393400	10.130945
114	1	0	0.658753	3.792341	11.151109
115	1	0	0.278615	4.143214	9.454596
116	1	0	0.067879	2.500686	10.089970
117	6	0	3.912626	3.414407	12.032283
118	1	0	4.463280	3.812031	12.892202
119	1	0	2.988110	2.970324	12.414424
120	1	0	4.521857	2.622688	11.581936
121	6	0	8.034158	10.467131	−4.676953
122	1	0	7.066672	10.712349	−4.225147
123	1	0	8.616367	11.392939	−4.753892
124	1	0	7.850055	10.099049	−5.693665
125	6	0	11.445291	10.390947	−3.174843
126	1	0	11.243930	10.709309	−4.202449
127	1	0	12.300219	10.973684	−2.813853
128	1	0	11.741312	9.335974	−3.186874
129	6	0	−4.514780	15.768079	0.980572
130	1	0	−4.279339	16.814157	0.752332
131	1	0	−3.799638	15.135671	0.443330
132	1	0	−5.517849	15.554590	0.591674
133	6	0	−3.412265	17.309522	5.111740
134	1	0	−4.461856	17.029547	5.259489
135	1	0	−2.798199	16.672315	5.757427
136	1	0	−3.290022	18.348764	5.440504

4a

Zero-point correction= 0.656775 (Hartree/Particle)

Thermal correction to Energy= 0.694925

Thermal correction to Enthalpy= 0.695869

Thermal correction to Gibbs Free Energy= 0.584527

Sum of electronic and zero-point Energies= -1847.513411

Sum of electronic and thermal Energies= -1847.475260
Sum of electronic and thermal Enthalpies= -1847.474316
Sum of electronic and thermal Free Energies= -1847.585658

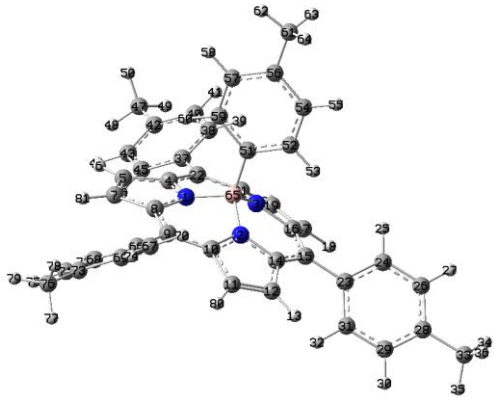


Fig. S96 Optimized structures of **4a**.

Table S25 Coordinates of atoms in **4a**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.392731	5.188799	3.953921
2	7	0	4.257026	6.671446	5.798936
3	7	0	6.383949	5.832974	5.096477
4	6	0	5.040338	4.229911	3.232413
5	6	0	4.016267	3.518506	2.517313
6	1	0	4.169522	2.702554	1.826484
7	6	0	2.791461	4.041009	2.898825
8	6	0	3.036532	5.083705	3.857740
9	6	0	2.227997	5.872043	4.753305
10	6	0	2.896135	6.601485	5.799453
11	6	0	2.472964	7.101274	7.078652
12	6	0	3.607471	7.404803	7.810588
13	1	0	3.629454	7.778930	8.823305
14	6	0	4.751123	7.068601	7.005937
15	6	0	6.157983	6.902328	7.259567
16	6	0	6.940430	6.178504	6.293065
17	6	0	8.153496	5.416512	6.407174
18	1	0	8.828266	5.431310	7.251426
19	6	0	8.238503	4.591541	5.300261
20	1	0	8.991887	3.839040	5.115823
21	6	0	7.079772	4.831744	4.485248
22	6	0	6.454031	4.062845	3.440041
23	6	0	6.779035	7.317243	8.521570
24	6	0	8.054525	7.922732	8.509392
25	1	0	8.556665	8.094914	7.562397
26	6	0	8.653871	8.341834	9.691519
27	1	0	9.627108	8.824519	9.652905
28	6	0	8.024088	8.156063	10.932643
29	6	0	6.768115	7.526914	10.946153
30	1	0	6.272214	7.345133	11.896368
31	6	0	6.149829	7.122149	9.769593

32	1	0	5.199003	6.603577	9.820437
33	6	0	8.663743	8.638650	12.207838
34	1	0	9.756382	8.632921	12.136388
35	1	0	8.366940	8.023640	13.063758
36	1	0	8.357580	9.670971	12.427168
37	6	0	7.234947	3.046220	2.730961
38	6	0	8.553474	3.337427	2.313886
39	1	0	8.966902	4.324025	2.497586
40	6	0	9.307885	2.392732	1.630300
41	1	0	10.312676	2.648355	1.303139
42	6	0	8.794438	1.115233	1.350178
43	6	0	7.492826	0.818540	1.785054
44	1	0	7.083079	-0.171837	1.604599
45	6	0	6.721948	1.761340	2.455281
46	1	0	5.737715	1.483542	2.815356
47	6	0	9.614698	0.104187	0.593058
48	1	0	9.212695	-0.907143	0.708161
49	1	0	10.657657	0.104292	0.929116
50	1	0	9.624320	0.336854	-0.480577
51	6	0	5.242025	7.650793	3.566346
52	6	0	5.785559	8.863307	4.029570
53	1	0	6.098166	8.953499	5.068264
54	6	0	5.933283	9.967991	3.192988
55	1	0	6.354792	10.889889	3.589878
56	6	0	5.541939	9.912306	1.845348
57	6	0	5.000458	8.710715	1.375607
58	1	0	4.684941	8.637106	0.336703
59	6	0	4.853595	7.604590	2.219462
60	1	0	4.422480	6.694478	1.808652
61	6	0	5.711154	11.108628	0.939216
62	1	0	5.229576	10.946521	-0.030705
63	1	0	6.772063	11.321368	0.751850
64	1	0	5.279371	12.013497	1.384377
65	5	0	5.082291	6.379386	4.570714
66	6	0	0.763692	5.858156	4.708016
67	6	0	0.046658	7.057048	4.918189
68	6	0	0.025898	4.681492	4.457620
69	6	0	-1.341188	7.076610	4.853534
70	1	0	0.587843	7.982949	5.085488
71	6	0	-1.362469	4.710871	4.410021
72	1	0	0.540187	3.733575	4.346658
73	6	0	-2.074925	5.906299	4.601063
74	1	0	-1.866928	8.017768	4.992933
75	1	0	-1.907711	3.787978	4.229279
76	6	0	-3.580395	5.928983	4.564631
77	1	0	-3.996145	5.792664	5.572602
78	1	0	-3.956153	6.885711	4.186972
79	1	0	-3.978776	5.125372	3.936846
80	1	0	1.451145	7.167689	7.424203
81	1	0	1.825341	3.701400	2.555605

3b

Zero-point correction= 0.672800 (Hartree/Particle)

Thermal correction to Energy= 0.713659

Thermal correction to Enthalpy= 0.714603

Thermal correction to Gibbs Free Energy= 0.595335
Sum of electronic and zero-point Energies= -2073.033228
Sum of electronic and thermal Energies= -2072.992369
Sum of electronic and thermal Enthalpies= -2072.991425
Sum of electronic and thermal Free Energies= -2073.110693

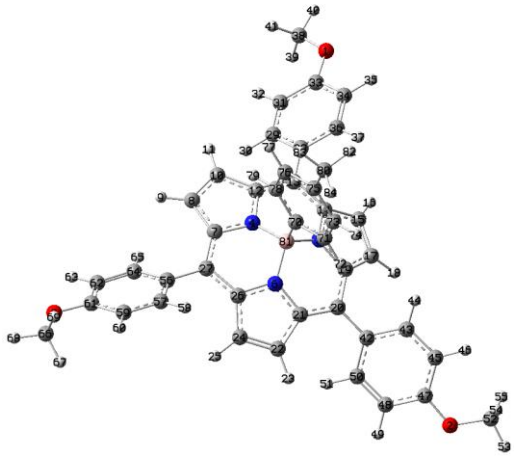


Fig. S97 Optimized structures of **4b**.

Table S26 Coordinates of atoms in **4b**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.765872	14.280087	5.518817
2	8	0	7.959129	1.248791	0.245202
3	8	0	-1.496759	3.427214	10.932269
4	7	0	4.473656	6.971939	7.299037
5	7	0	6.186543	6.532143	5.703703
6	7	0	4.796271	4.761424	6.509522
7	6	0	3.361001	6.626572	8.007001
8	6	0	2.810041	7.860903	8.493357
9	1	0	1.937595	7.968978	9.120274
10	6	0	3.585464	8.897378	7.997491
11	1	0	3.420016	9.949769	8.173625
12	6	0	4.629589	8.322166	7.195646
13	6	0	5.632317	8.821160	6.290576
14	6	0	6.321468	7.866410	5.459642
15	6	0	6.928277	7.977166	4.162025
16	1	0	7.145888	8.902288	3.647723
17	6	0	7.070710	6.699031	3.653165
18	1	0	7.420272	6.434866	2.665522
19	6	0	6.555933	5.778835	4.629740
20	6	0	6.131223	4.406089	4.535864
21	6	0	5.149733	3.938957	5.481545
22	6	0	4.246440	2.821304	5.544165
23	1	0	4.253314	1.958644	4.895445
24	6	0	3.329443	3.074660	6.549160
25	1	0	2.470447	2.469196	6.800551
26	6	0	3.670618	4.334935	7.147958
27	6	0	2.961331	5.241669	8.012812

28	6	0	5.874629	10.245896	6.092780
29	6	0	4.836279	11.200978	6.102323
30	1	0	3.807753	10.873071	6.204142
31	6	0	5.086831	12.552686	5.907127
32	1	0	4.258015	13.250369	5.894287
33	6	0	6.406312	12.996756	5.707227
34	6	0	7.457346	12.058425	5.689983
35	1	0	8.470088	12.420105	5.546197
36	6	0	7.193737	10.714726	5.868101
37	1	0	8.017504	10.008219	5.882037
38	6	0	5.763563	15.297851	5.536986
39	1	0	5.035732	15.149659	4.730777
40	1	0	6.296422	16.235517	5.379345
41	1	0	5.247837	15.326236	6.503732
42	6	0	6.603361	3.591206	3.419528
43	6	0	7.959335	3.651566	3.032342
44	1	0	8.642749	4.282430	3.592173
45	6	0	8.457637	2.881617	1.988576
46	1	0	9.511567	2.936675	1.743409
47	6	0	7.593018	2.033648	1.275873
48	6	0	6.230068	1.977121	1.631990
49	1	0	5.571911	1.340091	1.050412
50	6	0	5.750647	2.732183	2.683734
51	1	0	4.689875	2.708862	2.905590
52	6	0	9.319660	1.257652	-0.190322
53	1	0	9.363461	0.559997	-1.026607
54	1	0	9.991140	0.917916	0.606636
55	1	0	9.618935	2.256333	-0.528694
56	6	0	1.803120	4.764017	8.761036
57	6	0	1.847934	3.506274	9.400188
58	1	0	2.760418	2.920421	9.352448
59	6	0	0.776937	3.024994	10.142767
60	1	0	0.863934	2.068117	10.643390
61	6	0	-0.396153	3.791700	10.248210
62	6	0	-0.468494	5.041042	9.598479
63	1	0	-1.393104	5.604477	9.667960
64	6	0	0.609313	5.517422	8.879420
65	1	0	0.513624	6.458661	8.349730
66	6	0	-1.513684	2.170327	11.611057
67	1	0	-1.380966	1.340297	10.907615
68	1	0	-2.497477	2.102087	12.075306
69	1	0	-0.738876	2.129882	12.385311
70	6	0	6.610227	5.703795	8.167161
71	6	0	7.620403	4.736368	8.025833
72	1	0	7.693986	4.157067	7.106681
73	6	0	8.540132	4.484036	9.040918
74	1	0	9.305166	3.723864	8.895823
75	6	0	8.493476	5.191979	10.250917
76	6	0	7.488389	6.152805	10.402842
77	1	0	7.421160	6.713520	11.332844
78	6	0	6.568079	6.402772	9.382208
79	1	0	5.803302	7.157721	9.549588
80	6	0	9.507931	4.937160	11.340669
81	5	0	5.563793	5.981272	6.961761
82	1	0	10.444307	5.476312	11.144949
83	1	0	9.139517	5.267810	12.316976
84	1	0	9.758871	3.873411	11.415306

4c

Zero-point correction= 1.311516 (Hartree/Particle)
Thermal correction to Energy= 1.380669
Thermal correction to Enthalpy= 1.381613
Thermal correction to Gibbs Free Energy= 1.198098
Sum of electronic and zero-point Energies= -2838.513132
Sum of electronic and thermal Energies= -2838.443979
Sum of electronic and thermal Enthalpies= -2838.443034
Sum of electronic and thermal Free Energies= -2838.626550

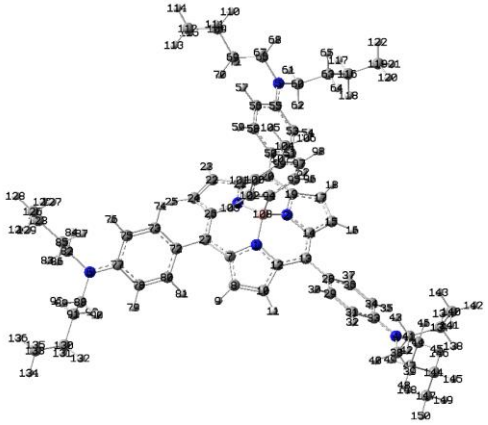


Fig. S98 Optimized structures of **4c**.

Table S27 Coordinates of atoms in **4c**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	23.562868	13.290203	4.785119
2	7	0	24.646739	15.034600	5.970710
3	7	0	22.276624	14.826865	6.090525
4	7	0	30.902884	11.779581	2.356979
5	7	0	22.861381	21.629177	9.995015
6	7	0	16.201344	11.690101	2.244018
7	6	0	22.461813	12.862598	4.098438
8	6	0	22.967096	12.079535	3.005205
9	1	0	22.381341	11.565248	2.258486
10	6	0	24.350713	12.153654	3.031257
11	1	0	25.024860	11.740342	2.294230
12	6	0	24.728827	12.951797	4.160593
13	6	0	25.960362	13.594770	4.547928
14	6	0	25.865479	14.730566	5.432230
15	6	0	26.749419	15.773497	5.866674
16	1	0	27.805234	15.851620	5.653738
17	6	0	26.003741	16.693336	6.589962
18	1	0	26.387808	17.601153	7.030670
19	6	0	24.642854	16.237552	6.618021
20	6	0	23.375407	16.778154	7.047758
21	6	0	22.183515	16.077948	6.629210

22	6	0	20.844860	16.522527	6.367453
23	1	0	20.441605	17.491762	6.625529
24	6	0	20.208036	15.539959	5.627330
25	1	0	19.216593	15.600574	5.200957
26	6	0	21.142866	14.471350	5.418872
27	6	0	21.167415	13.376214	4.480022
28	6	0	27.218621	13.156215	3.965131
29	6	0	27.468879	11.780365	3.737633
30	1	0	26.719881	11.050676	4.028204
31	6	0	28.664786	11.323379	3.219283
32	1	0	28.801449	10.254786	3.114967
33	6	0	29.710491	12.222778	2.860629
34	6	0	29.444642	13.610816	3.052671
35	1	0	30.171036	14.353174	2.747795
36	6	0	28.252650	14.049546	3.593209
37	1	0	28.090723	15.118713	3.672065
38	6	0	31.133807	10.355916	2.067691
39	1	0	31.919969	10.310296	1.308043
40	1	0	30.235777	9.932890	1.605494
41	6	0	31.546647	9.505837	3.282307
42	1	0	31.594887	8.462080	2.940274
43	1	0	30.758495	9.545205	4.045153
44	6	0	31.971418	12.710915	1.968582
45	1	0	32.914924	12.163475	2.039056
46	1	0	32.032364	13.520486	2.702612
47	6	0	31.812732	13.276953	0.548622
48	1	0	31.758235	12.442057	-0.163586
49	1	0	30.859191	13.815817	0.472911
50	6	0	23.251685	18.033306	7.767582
51	6	0	24.136081	19.125904	7.587812
52	1	0	24.909285	19.072608	6.830350
53	6	0	24.008538	20.301113	8.299273
54	1	0	24.714609	21.097323	8.100271
55	6	0	22.979753	20.476465	9.271602
56	6	0	22.078849	19.385229	9.443784
57	1	0	21.269696	19.451610	10.160137
58	6	0	22.213914	18.220260	8.716053
59	1	0	21.522771	17.406912	8.912336
60	6	0	23.740500	22.785437	9.777472
61	1	0	23.168207	23.676670	10.054433
62	1	0	23.959596	22.883062	8.710141
63	6	0	25.038910	22.730803	10.595603
64	1	0	25.602504	21.828291	10.324840
65	1	0	24.784702	22.634411	11.660082
66	6	0	21.861027	21.783032	11.058958
67	1	0	21.741455	20.832336	11.587197
68	1	0	22.276339	22.487573	11.786676
69	6	0	20.502275	22.297645	10.560322
70	1	0	20.093600	21.592369	9.824575
71	1	0	20.651965	23.249940	10.033406
72	6	0	19.918690	12.930448	3.883428
73	6	0	18.733035	12.883505	4.660385
74	1	0	18.781978	13.134556	5.715214
75	6	0	17.524439	12.464203	4.141546
76	1	0	16.673498	12.403296	4.808286
77	6	0	17.397638	12.081840	2.774313
78	6	0	18.586280	12.137388	1.987915

79	1	0	18.553356	11.901365	0.931729
80	6	0	19.791335	12.538400	2.527975
81	1	0	20.642419	12.618684	1.862363
82	6	0	14.951618	11.753832	3.011658
83	1	0	14.143381	11.924622	2.292685
84	1	0	14.971872	12.631445	3.664707
85	6	0	14.660722	10.482468	3.822965
86	1	0	14.635864	9.621770	3.140562
87	1	0	15.485532	10.302649	4.524902
88	6	0	16.080406	11.185141	0.870204
89	1	0	15.241185	10.483846	0.866051
90	1	0	16.970553	10.600725	0.618108
91	6	0	15.852851	12.294517	-0.170104
92	1	0	16.685592	13.006578	-0.114429
93	1	0	14.945082	12.853506	0.096238
94	6	0	23.690796	13.036126	7.407695
95	6	0	24.664958	13.224916	8.399945
96	1	0	25.375963	14.043456	8.310736
97	6	0	24.757481	12.384000	9.514322
98	1	0	25.530159	12.563997	10.259555
99	6	0	23.874152	11.312739	9.687877
100	6	0	22.896508	11.111004	8.700297
101	1	0	22.196748	10.283020	8.801996
102	6	0	22.810779	11.952268	7.592122
103	1	0	22.038303	11.753084	6.851391
104	6	0	23.953413	10.410999	10.897285
105	1	0	23.114181	10.588225	11.583383
106	1	0	24.878720	10.575765	11.459629
107	1	0	23.914387	9.352358	10.612985
108	5	0	23.544791	14.010903	6.111847
109	6	0	19.499871	22.491672	11.704967
110	1	0	19.916019	23.198535	12.436822
111	1	0	19.368107	21.539401	12.238095
112	6	0	18.137460	22.998793	11.223857
113	1	0	17.679226	22.296489	10.516125
114	1	0	17.442682	23.127152	12.062426
115	1	0	18.230323	23.967468	10.716778
116	6	0	25.915176	23.972056	10.384947
117	1	0	25.339092	24.872445	10.641840
118	1	0	26.167806	24.062467	9.318942
119	6	0	27.203529	23.939190	11.211711
120	1	0	27.816937	23.065018	10.959162
121	1	0	27.811066	24.834667	11.034440
122	1	0	26.985809	23.892209	12.286176
123	6	0	13.336122	10.572702	4.591174
124	1	0	12.516174	10.757371	3.882743
125	1	0	13.364056	11.442987	5.262185
126	6	0	13.031503	9.312495	5.405894
127	1	0	13.818779	9.115999	6.144637
128	1	0	12.083498	9.410279	5.948203
129	1	0	12.955268	8.428977	4.759582
130	6	0	15.731456	11.767715	-1.609661
131	1	0	15.735505	12.628790	-2.290539
132	1	0	16.626840	11.179631	-1.857511
133	6	0	14.477108	10.928618	-1.878744
134	1	0	14.423203	10.635811	-2.934101
135	1	0	14.458874	10.007327	-1.284434

136	1	0	13.565945	11.494268	-1.644753
137	6	0	32.887003	9.894449	3.919483
138	1	0	33.680902	9.844473	3.160535
139	1	0	32.844476	10.937884	4.258956
140	6	0	33.257292	8.995546	5.102852
141	1	0	33.344109	7.945978	4.794226
142	1	0	34.216277	9.293395	5.543198
143	1	0	32.497702	9.046548	5.893249
144	6	0	32.967102	14.210431	0.162161
145	1	0	33.918303	13.665568	0.243989
146	1	0	33.023833	15.037182	0.884486
147	6	0	32.825694	14.779611	-1.252426
148	1	0	31.897455	15.355132	-1.358686
149	1	0	33.660634	15.446874	-1.497467
150	1	0	32.807934	13.979805	-2.003573

4d

Zero-point correction= 1.307179 (Hartree/Particle)
Thermal correction to Energy= 1.378203
Thermal correction to Enthalpy= 1.379147
Thermal correction to Gibbs Free Energy= 1.196512
Sum of electronic and zero-point Energies= -2838.485297
Sum of electronic and thermal Energies= -2838.414274
Sum of electronic and thermal Enthalpies= -2838.413329
Sum of electronic and thermal Free Energies= -2838.595964

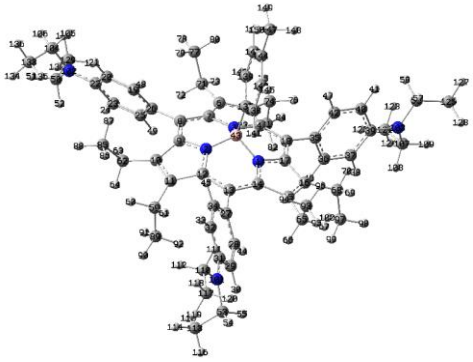


Fig. S99 Optimized structures of **4d**.

Table S28 Coordinates of atoms in **4d**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.267285	9.325695	3.818973
2	7	0	2.433105	10.455723	4.852008
3	7	0	3.281431	11.187111	2.739640
4	6	0	4.086471	11.037260	1.645341
5	6	0	3.571850	11.952770	0.646074
6	6	0	2.448831	12.587202	1.190117
7	6	0	2.240115	12.035609	2.521917
8	6	0	1.235039	12.118624	3.556601

9	6	0	1.302237	11.199546	4.667432
10	6	0	0.291528	10.610363	5.523918
11	6	0	0.859108	9.486411	6.133898
12	6	0	2.229890	9.385014	5.674359
13	6	0	3.219192	8.333240	5.725016
14	6	0	4.247501	8.297998	4.712958
15	6	0	5.298208	7.381990	4.290356
16	6	0	5.823374	7.875429	3.090542
17	6	0	5.130430	9.110495	2.782150
18	6	0	5.095112	10.021079	1.676840
19	6	0	-0.125893	13.986592	4.497879
20	6	0	-1.169898	14.892159	4.445210
21	1	0	-1.275588	15.602733	5.255365
22	6	0	-2.097261	14.887207	3.363701
23	6	0	-1.897070	13.901406	2.353174
24	1	0	-2.583104	13.823603	1.519101
25	6	0	-0.824857	13.029544	2.403394
26	6	0	0.100442	13.045613	3.468981
27	6	0	3.101681	7.291985	6.752499
28	6	0	2.968990	5.922661	6.442278
29	6	0	2.840148	4.957276	7.424241
30	1	0	2.690260	3.932401	7.110865
31	6	0	2.885352	5.294732	8.808974
32	6	0	2.992202	6.682179	9.118529
33	1	0	3.003294	7.018919	10.146476
34	6	0	3.079213	7.638019	8.120772
35	6	0	6.046860	9.877504	0.537883
36	6	0	5.823802	8.981040	-0.517526
37	6	0	6.712655	8.868759	-1.580954
38	1	0	6.472090	8.165587	-2.368504
39	6	0	7.901734	9.640695	-1.640162
40	6	0	8.105160	10.561715	-0.580492
41	1	0	8.968333	11.214721	-0.572642
42	6	0	7.202365	10.668623	0.474270
43	5	0	3.708516	10.700180	4.097427
44	1	0	2.908090	5.617557	5.402174
45	1	0	3.158664	8.683883	8.404873
46	1	0	4.929094	8.364559	-0.518527
47	1	0	7.402849	11.389521	1.262836
48	1	0	0.559439	14.024582	5.339602
49	1	0	-0.727712	12.279282	1.624531
50	6	0	-4.157684	15.716898	2.252169
51	1	0	-5.073802	16.137457	2.677695
52	1	0	-4.378173	14.671142	2.021514
53	6	0	2.537430	2.939151	9.457268
54	1	0	2.927347	2.313388	10.259624
55	1	0	3.107501	2.666413	8.565987
56	6	0	10.002265	10.371945	-2.678128
57	1	0	10.436252	10.345083	-1.673651
58	1	0	9.708333	11.418031	-2.865191
59	6	0	0.069272	8.492954	6.950315
60	1	0	-0.741306	9.022232	7.461670
61	1	0	0.685898	8.055257	7.736613
62	6	0	-1.148990	11.024360	5.691634
63	1	0	-1.475968	11.600222	4.823322
64	1	0	-1.776244	10.125534	5.716378
65	6	0	5.848452	6.179966	5.016403

66	1	0	5.058832	5.469497	5.268691
67	1	0	6.527908	5.645173	4.346568
68	6	0	6.896947	7.203079	2.272702
69	1	0	7.681298	6.840351	2.947878
70	1	0	7.374822	7.934196	1.617674
71	6	0	1.699140	13.699357	0.500180
72	1	0	0.622983	13.518202	0.507634
73	1	0	1.991452	13.718711	-0.553859
74	6	0	4.085249	12.158577	-0.756656
75	1	0	4.027614	13.224994	-1.004166
76	1	0	5.141909	11.891193	-0.810401
77	6	0	1.979168	15.082824	1.115769
78	1	0	1.427730	15.859879	0.572984
79	1	0	1.673618	15.123860	2.166439
80	1	0	3.046460	15.327978	1.065695
81	6	0	3.306945	11.358508	-1.817446
82	1	0	3.360818	10.282511	-1.620016
83	1	0	2.248755	11.643285	-1.835160
84	1	0	3.724493	11.539818	-2.814947
85	6	0	-1.414793	11.842278	6.969596
86	1	0	-1.163164	11.269438	7.869260
87	1	0	-0.824032	12.763687	6.986086
88	1	0	-2.474401	12.117716	7.030888
89	6	0	-0.538937	7.362177	6.098702
90	1	0	-1.112282	6.673937	6.731243
91	1	0	-1.214582	7.760749	5.333106
92	1	0	0.239719	6.783829	5.590416
93	6	0	6.616670	6.553609	6.297503
94	1	0	5.968846	7.056229	7.023239
95	1	0	7.020479	5.652288	6.774009
96	1	0	7.455275	7.222951	6.072871
97	6	0	6.386071	6.021712	1.427749
98	1	0	7.208754	5.580136	0.853153
99	1	0	5.954730	5.237007	2.059636
100	1	0	5.614463	6.343027	0.720326
101	7	0	2.830967	4.338275	9.792915
102	7	0	-3.132628	15.779135	3.302098
103	7	0	8.825272	9.488549	-2.669360
104	6	0	-3.280210	16.870169	4.273930
105	1	0	-2.290589	17.244391	4.550002
106	1	0	-3.785851	17.691111	3.756319
107	6	0	8.399613	8.885200	-3.937619
108	1	0	7.872134	7.951180	-3.726176
109	1	0	9.296258	8.592193	-4.485164
110	6	0	2.788168	4.769583	11.205641
111	1	0	3.598789	5.489431	11.356645
112	1	0	1.846995	5.305773	11.396860
113	6	0	1.046258	2.651687	9.252224
114	1	0	0.473006	2.877611	10.158411
115	1	0	0.631696	3.245611	8.430573
116	1	0	0.900459	1.591357	9.014322
117	6	0	2.955384	3.659439	12.238771
118	1	0	2.971129	4.126123	13.229756
119	1	0	2.132718	2.937588	12.228963
120	1	0	3.900110	3.119987	12.111260
121	6	0	7.533819	9.796343	-4.815851
122	1	0	6.615353	10.095833	-4.299031

123	1	0	8.075713	10.706302	-5.099411
124	1	0	7.248862	9.273101	-5.736752
125	6	0	11.101723	9.975470	-3.661549
126	1	0	10.813387	10.115563	-4.708103
127	1	0	11.973010	10.613574	-3.475689
128	1	0	11.413381	8.934493	-3.519899
129	6	0	-3.775902	16.485686	0.984202
130	1	0	-3.591116	17.542498	1.207665
131	1	0	-2.873326	16.072949	0.521245
132	1	0	-4.591946	16.430849	0.254179
133	6	0	-4.077553	16.474222	5.520102
134	1	0	-5.086982	16.142663	5.251505
135	1	0	-3.586549	15.663506	6.068767
136	1	0	-4.170561	17.336126	6.191182
137	6	0	4.753390	11.704924	4.855950
138	6	0	5.432120	11.311760	6.025375
139	6	0	5.000110	13.010506	4.402520
140	6	0	6.299952	12.169328	6.700472
141	1	0	5.285677	10.309917	6.423582
142	6	0	5.868069	13.877069	5.075629
143	1	0	4.508403	13.371922	3.502278
144	6	0	6.536074	13.473151	6.236661
145	1	0	6.805460	11.823833	7.600972
146	1	0	6.029265	14.881930	4.689208
147	6	0	7.489202	14.393247	6.961974
148	1	0	8.526182	14.041165	6.879033
149	1	0	7.451159	15.409663	6.556253
150	1	0	7.257768	14.448216	8.032996

5

Zero-point correction= 0.115204 (Hartree/Particle)
Thermal correction to Energy= 0.121358
Thermal correction to Enthalpy= 0.122303
Thermal correction to Gibbs Free Energy= 0.084168
Sum of electronic and zero-point Energies= -270.773424
Sum of electronic and thermal Energies= -270.767270
Sum of electronic and thermal Enthalpies= -270.766325
Sum of electronic and thermal Free Energies= -270.804460

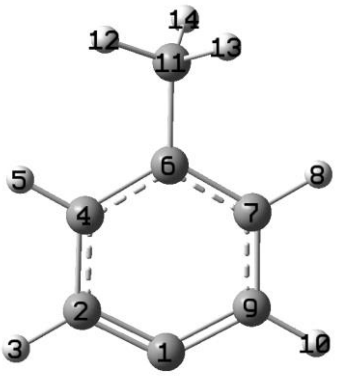


Fig. S100 Optimized structures of **5**.

Table S29 Coordinates of atoms in **5**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.196084	-0.057996	2.522310
2	6	0	-0.349855	-1.139962	3.175905
3	1	0	-0.828287	-1.962942	2.650771
4	6	0	-0.260835	-1.141130	4.578923
5	1	0	-0.678076	-1.977194	5.136862
6	6	0	0.354240	-0.087009	5.269592
7	6	0	0.891277	0.982603	4.534043
8	1	0	1.374392	1.805660	5.057726
9	6	0	0.817035	1.011291	3.132997
10	1	0	1.236688	1.842848	2.572243
11	6	0	0.426416	-0.087974	6.779929
12	1	0	0.144347	-1.062228	7.191913
13	1	0	1.436476	0.149991	7.133885
14	1	0	-0.249425	0.661982	7.211827

6

Zero-point correction= 0.237054 (Hartree/Particle)
Thermal correction to Energy= 0.249551
Thermal correction to Enthalpy= 0.250496
Thermal correction to Gibbs Free Energy= 0.197560
Sum of electronic and zero-point Energies= -541.722657
Sum of electronic and thermal Energies= -541.710160
Sum of electronic and thermal Enthalpies= -541.709215
Sum of electronic and thermal Free Energies= -541.762151

Fig. S101 Optimized structures of **6**.

Table S30 Coordinates of atoms in **6**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.850955	8.417454	7.794477

2	6	0	7.903368	9.292317	7.472370
3	1	0	8.211033	9.403893	6.436203
4	6	0	8.547535	10.038895	8.457944
5	1	0	9.356643	10.708910	8.174770
6	6	0	8.168064	9.948935	9.804556
7	6	0	7.118677	9.076563	10.127377
8	1	0	6.808603	8.974552	11.165368
9	6	0	6.472284	8.327179	9.145736
10	1	0	5.680351	7.642183	9.436312
11	6	0	8.847458	10.780260	10.865821
12	1	0	9.880894	11.016952	10.590023
13	1	0	8.861838	10.263136	11.831684
14	1	0	8.325379	11.735296	11.017611
15	6	0	6.168072	7.613028	6.748097
16	6	0	4.789458	7.345550	6.817497
17	6	0	6.876073	7.092147	5.650488
18	6	0	4.151332	6.591099	5.834075
19	1	0	4.203639	7.754116	7.636641
20	6	0	6.233210	6.338623	4.669560
21	1	0	7.946686	7.261761	5.572742
22	6	0	4.859061	6.069269	4.741971
23	1	0	3.081034	6.411836	5.911440
24	1	0	6.811717	5.946409	3.835684
25	6	0	4.171306	5.225559	3.695628
26	1	0	4.205410	4.159111	3.958588
27	1	0	3.115423	5.498282	3.591060
28	1	0	4.650092	5.331702	2.715879

7c

Zero-point correction= 1.314356 (Hartree/Particle)
Thermal correction to Energy= 1.383238
Thermal correction to Enthalpy= 1.384182
Thermal correction to Gibbs Free Energy= 1.201078
Sum of electronic and zero-point Energies= -2838.339255
Sum of electronic and thermal Energies= -2838.270373
Sum of electronic and thermal Enthalpies= -2838.269429
Sum of electronic and thermal Free Energies= -2838.452533

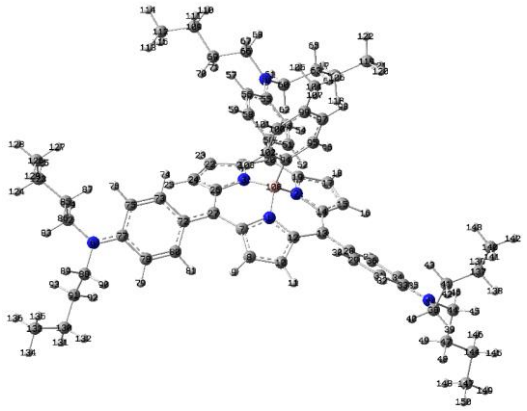


Fig. S102 Optimized structures of **7c**.

Table S31 Coordinates of atoms in **7c**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	23.572375	13.396644	4.606553
2	7	0	24.641779	15.191490	5.731214
3	7	0	22.285615	14.891258	5.965183
4	7	0	30.896243	11.756144	2.366099
5	7	0	22.794430	21.557149	10.023903
6	7	0	16.180653	11.671309	2.332617
7	6	0	22.469517	12.929501	3.953263
8	6	0	22.962967	12.143985	2.863591
9	1	0	22.380503	11.594804	2.140482
10	6	0	24.347732	12.247717	2.858736
11	1	0	25.010439	11.840204	2.108947
12	6	0	24.728736	13.060294	3.970186
13	6	0	25.967262	13.731399	4.333070
14	6	0	25.859258	14.909283	5.182644
15	6	0	26.728194	15.965016	5.598271
16	1	0	27.778399	16.071076	5.375385
17	6	0	25.977601	16.869640	6.340154
18	1	0	26.362182	17.777761	6.778343
19	6	0	24.634038	16.384541	6.393927
20	6	0	23.360794	16.873842	6.897871
21	6	0	22.168312	16.133444	6.511512
22	6	0	20.819857	16.548300	6.283567
23	1	0	20.398129	17.507729	6.547252
24	6	0	20.187457	15.546740	5.559924
25	1	0	19.185000	15.586467	5.158445
26	6	0	21.140079	14.503963	5.336588
27	6	0	21.163865	13.402953	4.388715
28	6	0	27.208720	13.266848	3.792252
29	6	0	27.405885	11.877127	3.528717
30	1	0	26.613441	11.176868	3.766843
31	6	0	28.598994	11.377766	3.071921
32	1	0	28.694145	10.307136	2.951047
33	6	0	29.711203	12.239864	2.800052
34	6	0	29.499605	13.643619	3.009717
35	1	0	30.273651	14.354561	2.753398
36	6	0	28.312739	14.122524	3.501638
37	1	0	28.196737	15.195140	3.589427
38	6	0	31.095006	10.322009	2.077457
39	1	0	31.927241	10.260681	1.371261
40	1	0	30.214463	9.939307	1.554712
41	6	0	31.397524	9.457405	3.313966
42	1	0	31.459891	8.419278	2.959356
43	1	0	30.548707	9.497315	4.008391
44	6	0	32.044306	12.636200	2.080677
45	1	0	32.945384	12.035309	2.223809
46	1	0	32.080912	13.436391	2.824188
47	6	0	32.021420	13.207006	0.655089
48	1	0	31.969572	12.375390	-0.060536
49	1	0	31.108477	13.800518	0.514755
50	6	0	23.223104	18.079796	7.653821
51	6	0	24.122114	19.182098	7.546010
52	1	0	24.907742	19.160954	6.802421

53	6	0	23.976011	20.320648	8.294895
54	1	0	24.677977	21.129866	8.144171
55	6	0	22.923820	20.449697	9.261392
56	6	0	22.017025	19.345617	9.374422
57	1	0	21.205046	19.378119	10.088906
58	6	0	22.156027	18.227819	8.592038
59	1	0	21.465590	17.405421	8.741166
60	6	0	23.674065	22.729100	9.870264
61	1	0	23.086300	23.602186	10.168271
62	1	0	23.917763	22.864536	8.813749
63	6	0	24.949212	22.642062	10.720874
64	1	0	25.518111	21.748197	10.433246
65	1	0	24.668136	22.512163	11.774428
66	6	0	21.772183	21.674261	11.078664
67	1	0	21.639958	20.703985	11.564380
68	1	0	22.182214	22.348806	11.835748
69	6	0	20.430333	22.218246	10.566742
70	1	0	20.027591	21.535330	9.807301
71	1	0	20.600031	23.181694	10.067691
72	6	0	19.924688	12.927616	3.851000
73	6	0	18.743483	12.928068	4.654451
74	1	0	18.815450	13.218722	5.696649
75	6	0	17.532744	12.488575	4.182537
76	1	0	16.696426	12.449272	4.868122
77	6	0	17.379002	12.051601	2.826099
78	6	0	18.561996	12.048660	2.015357
79	1	0	18.504945	11.768199	0.971906
80	6	0	19.773160	12.453730	2.514446
81	1	0	20.609913	12.498812	1.829977
82	6	0	14.938030	11.775550	3.116506
83	1	0	14.129879	11.948615	2.399580
84	1	0	14.985357	12.661873	3.753965
85	6	0	14.642773	10.516527	3.944114
86	1	0	14.610666	9.648201	3.272344
87	1	0	15.468766	10.342714	4.646281
88	6	0	16.016559	11.140238	0.967832
89	1	0	15.161967	10.459931	1.002795
90	1	0	16.887671	10.534649	0.705638
91	6	0	15.783708	12.245263	-0.075322
92	1	0	16.641369	12.929193	-0.061841
93	1	0	14.905257	12.835057	0.219590
94	6	0	23.822654	13.167294	7.216509
95	6	0	24.860202	13.371363	8.138067
96	1	0	25.558549	14.193224	7.996672
97	6	0	25.031308	12.536996	9.247956
98	1	0	25.849499	12.727026	9.939998
99	6	0	24.168659	11.460985	9.484329
100	6	0	23.128441	11.246249	8.565159
101	1	0	22.442727	10.414752	8.718502
102	6	0	22.962257	12.080665	7.461427
103	1	0	22.143841	11.875104	6.773545
104	6	0	24.338663	10.561760	10.685520
105	1	0	23.498498	10.665338	11.384791
106	1	0	25.257119	10.795655	11.233967
107	1	0	24.379737	9.505107	10.393161
108	5	0	23.581659	14.127306	5.927538
109	6	0	19.413615	22.393275	11.701907

110	1	0	19.822873	23.083710	12.452528
111	1	0	19.270368	21.431103	12.213435
112	6	0	18.061165	22.916389	11.210325
113	1	0	17.609694	22.230049	10.482957
114	1	0	17.355843	23.031321	12.041762
115	1	0	18.165865	23.894410	10.724174
116	6	0	25.827516	23.890642	10.568829
117	1	0	25.244488	24.781209	10.842266
118	1	0	26.103039	24.015171	9.512141
119	6	0	27.096924	23.831058	11.422842
120	1	0	27.718298	22.967190	11.155029
121	1	0	27.704799	24.733384	11.288253
122	1	0	26.855269	23.748412	12.489846
123	6	0	13.319827	10.628958	4.712220
124	1	0	12.500865	10.806359	4.001300
125	1	0	13.354368	11.509723	5.368783
126	6	0	13.010885	9.382708	5.546284
127	1	0	13.796917	9.194759	6.288450
128	1	0	12.063139	9.493585	6.086085
129	1	0	12.931052	8.489878	4.913515
130	6	0	15.588138	11.702339	-1.500510
131	1	0	15.586973	12.556479	-2.189834
132	1	0	16.456846	11.088393	-1.777604
133	6	0	14.301561	10.895375	-1.706342
134	1	0	14.194158	10.597004	-2.755807
135	1	0	14.285095	9.978590	-1.104955
136	1	0	13.416793	11.486853	-1.437889
137	6	0	32.685069	9.816607	4.066142
138	1	0	33.536292	9.782494	3.371878
139	1	0	32.622646	10.848717	4.436100
140	6	0	32.952129	8.874836	5.244323
141	1	0	33.056519	7.835867	4.907135
142	1	0	33.874441	9.148545	5.770016
143	1	0	32.132331	8.906435	5.973199
144	6	0	33.255783	14.068610	0.360369
145	1	0	34.163205	13.468774	0.516366
146	1	0	33.304977	14.894620	1.083759
147	6	0	33.258371	14.635869	-1.061991
148	1	0	32.379792	15.268374	-1.241001
149	1	0	34.150545	15.247117	-1.241635
150	1	0	33.248483	13.833808	-1.810703

TSa

Zero-point correction= 0.655019 (Hartree/Particle)
Thermal correction to Energy= 0.693526
Thermal correction to Enthalpy= 0.694471
Thermal correction to Gibbs Free Energy= 0.581032
Sum of electronic and zero-point Energies= -1847.478844
Sum of electronic and thermal Energies= -1847.440337
Sum of electronic and thermal Enthalpies= -1847.439393
Sum of electronic and thermal Free Energies= -1847.552832

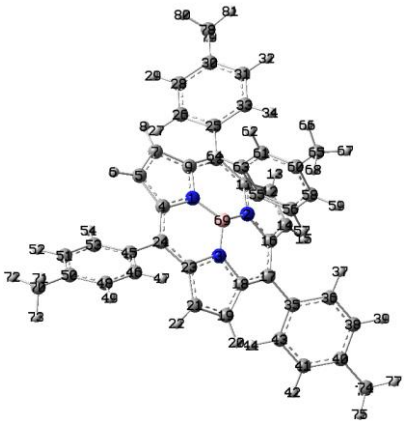


Fig. S103 Optimized structures of **TSa**.

Table S32 Coordinates of atoms in **TSa**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.628794	4.232655	7.204803
2	7	0	6.445048	3.677448	5.758261
3	7	0	4.898112	1.989423	6.454095
4	6	0	3.441460	3.934595	7.837001
5	6	0	2.979056	5.206990	8.319628
6	1	0	2.079724	5.372817	8.895581
7	6	0	3.859742	6.194472	7.893008
8	1	0	3.756587	7.253538	8.082237
9	6	0	4.909841	5.579172	7.129368
10	6	0	6.002532	5.996392	6.302720
11	6	0	6.729294	5.012235	5.557402
12	6	0	7.605998	5.018121	4.419709
13	1	0	8.032850	5.900991	3.964782
14	6	0	7.746667	3.716490	3.957464
15	1	0	8.301416	3.411682	3.080920
16	6	0	6.962854	2.845551	4.788118
17	6	0	6.478666	1.500675	4.697215
18	6	0	5.388439	1.091125	5.530302
19	6	0	4.474400	-0.015599	5.601004
20	1	0	4.547942	-0.929718	5.029363
21	6	0	3.450752	0.307950	6.481939
22	1	0	2.587825	-0.305377	6.699739
23	6	0	3.695512	1.619145	7.015357
24	6	0	2.961532	2.585572	7.776717
25	6	0	6.331180	7.427849	6.135126
26	6	0	5.327928	8.398175	5.952472
27	1	0	4.286830	8.096045	5.898602
28	6	0	5.657902	9.741453	5.798542
29	1	0	4.863607	10.469440	5.651538
30	6	0	6.993620	10.171787	5.818079
31	6	0	7.990805	9.203026	5.999406
32	1	0	9.033922	9.508255	6.030778
33	6	0	7.671071	7.855692	6.152592
34	1	0	8.464223	7.132735	6.318216
35	6	0	7.050799	0.593376	3.677929

36	6	0	8.445340	0.472980	3.544478
37	1	0	9.099231	1.032635	4.207324
38	6	0	8.998461	-0.382897	2.593935
39	1	0	10.079904	-0.468374	2.521123
40	6	0	8.187589	-1.140857	1.738270
41	6	0	6.795685	-1.011858	1.868776
42	1	0	6.142279	-1.579586	1.210394
43	6	0	6.233325	-0.163802	2.818277
44	1	0	5.153607	-0.064966	2.873867
45	6	0	1.684877	2.196846	8.412358
46	6	0	1.580971	0.976967	9.109323
47	1	0	2.453534	0.337563	9.204556
48	6	0	0.383220	0.597179	9.706068
49	1	0	0.333790	-0.345991	10.245271
50	6	0	-0.757444	1.412624	9.633620
51	6	0	-0.651439	2.625216	8.939274
52	1	0	-1.521878	3.271436	8.857330
53	6	0	0.543570	3.014345	8.336777
54	1	0	0.577631	3.942574	7.775512
55	6	0	6.861430	2.795157	8.607566
56	6	0	7.867349	1.865172	8.449243
57	1	0	8.061022	1.363864	7.505308
58	6	0	8.649612	1.584249	9.579695
59	1	0	9.454018	0.855978	9.497523
60	6	0	8.415250	2.225746	10.806390
61	6	0	7.377658	3.165053	10.888959
62	1	0	7.187440	3.676460	11.830244
63	6	0	6.576287	3.468588	9.775774
64	1	0	5.778645	4.201794	9.853857
65	6	0	9.251224	1.889356	12.019532
66	1	0	9.210940	2.688498	12.766712
67	1	0	10.300527	1.725524	11.750448
68	1	0	8.894444	0.970084	12.502897
69	5	0	5.457824	3.254165	6.652622
70	6	0	-2.054445	0.983251	10.272449
71	1	0	-1.915120	0.742388	11.333477
72	1	0	-2.815469	1.766343	10.199075
73	1	0	-2.452248	0.080880	9.790205
74	6	0	8.786619	-2.048845	0.693324
75	1	0	8.251709	-3.003887	0.639032
76	1	0	8.728908	-1.592972	-0.304259
77	1	0	9.841080	-2.256886	0.900749
78	6	0	7.342727	11.625968	5.621719
79	1	0	7.354523	11.885867	4.554356
80	1	0	6.610522	12.282795	6.104175
81	1	0	8.333348	11.857689	6.026048

TSb

Zero-point correction= 0.671175 (Hartree/Particle)

Thermal correction to Energy= 0.711942

Thermal correction to Enthalpy= 0.712886

Thermal correction to Gibbs Free Energy= 0.595053

Sum of electronic and zero-point Energies= -2073.080710

Sum of electronic and thermal Energies= -2073.039943

Sum of electronic and thermal Enthalpies= -2073.038999

Sum of electronic and thermal Free Energies= -2073.156832

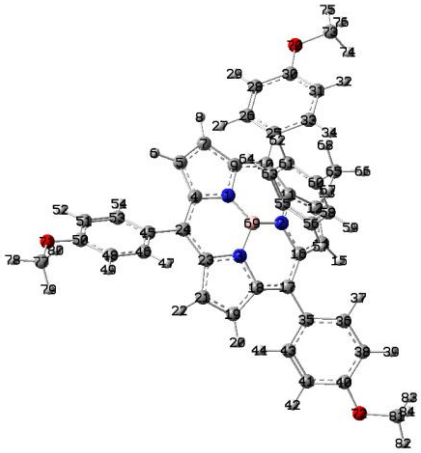


Fig. S104 Optimized structures of **TSb**.

Table S33 Coordinates of atoms in **TSb**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.565867	4.292915	7.342683
2	7	0	6.369733	3.659571	5.911008
3	7	0	4.778191	2.027518	6.642977
4	6	0	3.375670	4.038566	7.989204
5	6	0	2.952942	5.331001	8.452757
6	1	0	2.064169	5.533166	9.033352
7	6	0	3.858404	6.286476	8.003641
8	1	0	3.786944	7.350773	8.178029
9	6	0	4.885143	5.629538	7.244551
10	6	0	5.987634	6.002472	6.407706
11	6	0	6.686173	4.982951	5.681032
12	6	0	7.554049	4.944000	4.538203
13	1	0	7.998897	5.806419	4.061794
14	6	0	7.658352	3.629826	4.100766
15	1	0	8.198389	3.294257	3.226324
16	6	0	6.859216	2.795654	4.953079
17	6	0	6.337697	1.461963	4.887484
18	6	0	5.242180	1.097415	5.736628
19	6	0	4.301501	0.016298	5.835482
20	1	0	4.349578	-0.912569	5.285513
21	6	0	3.288948	0.384999	6.712369
22	1	0	2.411693	-0.201746	6.945554
23	6	0	3.568472	1.699827	7.216430
24	6	0	2.861141	2.699745	7.961737
25	6	0	6.350948	7.418289	6.210187
26	6	0	5.368762	8.415161	6.025744
27	1	0	4.319345	8.141098	5.993036
28	6	0	5.722095	9.741415	5.836187
29	1	0	4.964163	10.502616	5.678158
30	6	0	7.075621	10.122761	5.826077
31	6	0	8.067115	9.147244	6.007158

32	1	0	9.118034	9.412477	6.015548
33	6	0	7.699096	7.815557	6.192801
34	1	0	8.478004	7.076769	6.355756
35	6	0	6.871089	0.525450	3.877746
36	6	0	8.258199	0.379811	3.706523
37	1	0	8.938186	0.944593	4.337741
38	6	0	8.790647	-0.499839	2.765000
39	1	0	9.866779	-0.594636	2.676664
40	6	0	7.929183	-1.256205	1.956980
41	6	0	6.538375	-1.112115	2.106613
42	1	0	5.881155	-1.687889	1.461992
43	6	0	6.021187	-0.239387	3.050947
44	1	0	4.944881	-0.121142	3.125745
45	6	0	1.582896	2.357331	8.613618
46	6	0	1.442807	1.152217	9.324133
47	1	0	2.292947	0.483409	9.417858
48	6	0	0.246522	0.806070	9.949701
49	1	0	0.184882	-0.125669	10.499520
50	6	0	-0.854259	1.671505	9.871055
51	6	0	-0.733308	2.878841	9.160284
52	1	0	-1.596860	3.533415	9.091242
53	6	0	0.462035	3.212698	8.543902
54	1	0	0.517720	4.131911	7.970135
55	6	0	6.771866	2.834018	8.783906
56	6	0	7.783771	1.907003	8.641041
57	1	0	7.986898	1.399920	7.702079
58	6	0	8.557680	1.636134	9.778996
59	1	0	9.365198	0.909880	9.708489
60	6	0	8.310719	2.284899	10.999991
61	6	0	7.267851	3.218588	11.068307
62	1	0	7.066389	3.733096	12.005530
63	6	0	6.474806	3.512384	9.945923
64	1	0	5.672361	4.241388	10.013861
65	6	0	9.144248	1.964364	12.219120
66	1	0	10.214992	1.965125	11.984392
67	1	0	8.902626	0.968838	12.613821
68	1	0	8.971982	2.689071	13.021121
69	5	0	5.368406	3.282388	6.810198
70	8	0	7.314319	11.442423	5.632420
71	8	0	-2.062981	1.436358	10.436578
72	8	0	8.332803	-2.139956	1.011819
73	6	0	8.669039	11.891163	5.556604
74	1	0	9.203659	11.405800	4.731640
75	1	0	8.614019	12.965342	5.370571
76	1	0	9.202975	11.712540	6.497519
77	6	0	-2.264848	0.204129	11.132498
78	1	0	-3.299813	0.226293	11.478016
79	1	0	-2.120121	-0.655931	10.468223
80	1	0	-1.594898	0.118740	11.996199
81	6	0	9.734065	-2.328147	0.804308
82	1	0	9.816931	-3.071158	0.009038
83	1	0	10.219143	-1.398004	0.485003
84	1	0	10.223511	-2.707892	1.709021

TSc

Zero-point correction= 1.307789 (Hartree/Particle)
Thermal correction to Energy= 1.377776
Thermal correction to Enthalpy= 1.378720
Thermal correction to Gibbs Free Energy= 1.190634
Sum of electronic and zero-point Energies= -2838.464309
Sum of electronic and thermal Energies= -2838.394322
Sum of electronic and thermal Enthalpies= -2838.393378
Sum of electronic and thermal Free Energies= -2838.581464

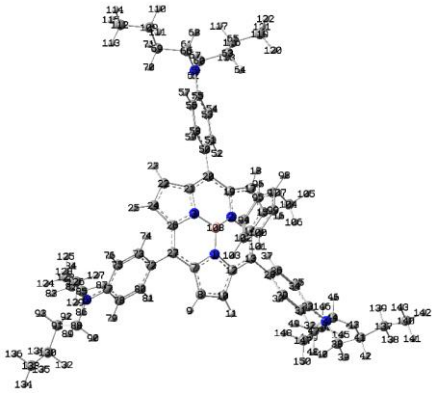


Fig. S105 Optimized structures of **TSc**.

Table S34 Coordinates of atoms in **TSc**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	23.519271	13.327659	4.770280
2	7	0	24.620467	15.042620	6.002002
3	7	0	22.237943	14.882346	6.065420
4	7	0	30.923195	11.799124	2.442449
5	7	0	22.978206	21.648771	10.080696
6	7	0	16.204772	11.589162	2.193720
7	6	0	22.390841	12.830855	4.150071
8	6	0	22.912588	11.934400	3.157643
9	1	0	22.326731	11.330566	2.479734
10	6	0	24.302485	12.005744	3.173858
11	1	0	24.966926	11.484010	2.499369
12	6	0	24.707305	12.925576	4.195621
13	6	0	25.928119	13.561895	4.606716
14	6	0	25.857487	14.669983	5.518589
15	6	0	26.751694	15.636772	6.084645
16	1	0	27.824202	15.657649	5.953290
17	6	0	26.010051	16.562435	6.814314
18	1	0	26.418589	17.413046	7.340653
19	6	0	24.620964	16.212096	6.732983
20	6	0	23.351967	16.773717	7.114658
21	6	0	22.146983	16.111826	6.686409
22	6	0	20.770027	16.477790	6.535382
23	1	0	20.323830	17.397954	6.885396
24	6	0	20.123686	15.495785	5.791139
25	1	0	19.092237	15.525426	5.469269
26	6	0	21.071857	14.478021	5.447475

27	6	0	21.113030	13.380271	4.517897
28	6	0	27.210946	13.118518	4.045543
29	6	0	27.508444	11.748712	3.893596
30	1	0	26.790408	11.006198	4.229500
31	6	0	28.717337	11.310844	3.376178
32	1	0	28.891226	10.243679	3.320450
33	6	0	29.719880	12.226526	2.953654
34	6	0	29.408838	13.607637	3.090756
35	1	0	30.107237	14.362873	2.752941
36	6	0	28.201798	14.029075	3.624658
37	1	0	28.005149	15.095816	3.671074
38	6	0	31.184808	10.375703	2.192999
39	1	0	31.949719	10.323162	1.411623
40	1	0	30.286794	9.909690	1.770976
41	6	0	31.658792	9.574759	3.419110
42	1	0	31.728276	8.521592	3.110212
43	1	0	30.894168	9.615722	4.205736
44	6	0	31.934769	12.750262	1.968024
45	1	0	32.901943	12.242189	2.015605
46	1	0	32.000810	13.591043	2.666906
47	6	0	31.697108	13.258114	0.536793
48	1	0	31.651725	12.396330	-0.143578
49	1	0	30.718649	13.752862	0.480017
50	6	0	23.261480	18.032646	7.860069
51	6	0	24.153424	19.106003	7.650550
52	1	0	24.912585	19.032248	6.878589
53	6	0	24.067046	20.286916	8.368119
54	1	0	24.785692	21.067684	8.151861
55	6	0	23.067577	20.482966	9.361725
56	6	0	22.163917	19.403747	9.566199
57	1	0	21.374756	19.482424	10.303720
58	6	0	22.265242	18.228322	8.841219
59	1	0	21.569046	17.424942	9.063353
60	6	0	23.858056	22.793032	9.822268
61	1	0	23.304099	23.694783	10.104405
62	1	0	24.043928	22.877508	8.746610
63	6	0	25.183578	22.742609	10.596431
64	1	0	25.731891	21.831603	10.321935
65	1	0	24.964162	22.663632	11.670283
66	6	0	22.003925	21.820003	11.163011
67	1	0	21.893795	20.877158	11.708827
68	1	0	22.434566	22.533235	11.873983
69	6	0	20.632885	22.329596	10.692925
70	1	0	20.208847	21.620050	9.969864
71	1	0	20.770230	23.278628	10.156417
72	6	0	19.864182	12.910476	3.907539
73	6	0	18.683597	12.795211	4.672146
74	1	0	18.713698	13.014686	5.735433
75	6	0	17.489996	12.354981	4.124408
76	1	0	16.634190	12.249841	4.779693
77	6	0	17.387819	12.010778	2.748303
78	6	0	18.577689	12.132084	1.977867
79	1	0	18.565416	11.921734	0.915492
80	6	0	19.765808	12.563931	2.543580
81	1	0	20.626594	12.687203	1.894516
82	6	0	14.946886	11.608356	2.945851
83	1	0	14.139988	11.766809	2.221567

84	1	0	14.934667	12.479375	3.609293
85	6	0	14.672640	10.324409	3.743934
86	1	0	14.668072	9.469284	3.053784
87	1	0	15.494960	10.151431	4.450714
88	6	0	16.121858	11.101201	0.813546
89	1	0	15.304109	10.374976	0.782597
90	1	0	17.032654	10.543809	0.569902
91	6	0	15.882930	12.211088	-0.224092
92	1	0	16.692776	12.947272	-0.147205
93	1	0	14.954296	12.742263	0.027880
94	6	0	23.615886	12.747498	7.757786
95	6	0	24.118447	13.264982	8.933889
96	1	0	24.493196	14.281616	9.012968
97	6	0	24.135703	12.411406	10.048006
98	1	0	24.527659	12.783048	10.992769
99	6	0	23.663743	11.092654	9.963491
100	6	0	23.171537	10.631094	8.733596
101	1	0	22.809045	9.608557	8.648679
102	6	0	23.141476	11.461872	7.601923
103	1	0	22.762740	11.088118	6.654737
104	6	0	23.664170	10.196504	11.180807
105	1	0	24.511703	10.416748	11.838839
106	1	0	23.714902	9.139390	10.899639
107	1	0	22.749053	10.332885	11.772832
108	5	0	23.468595	14.287960	5.780616
109	6	0	19.652631	22.530890	11.855310
110	1	0	20.083153	23.241175	12.575679
111	1	0	19.530209	21.581653	12.396372
112	6	0	18.281307	23.036879	11.398834
113	1	0	17.808594	22.331459	10.703759
114	1	0	17.602801	23.170814	12.249832
115	1	0	18.365211	24.002652	10.884651
116	6	0	26.063144	23.972971	10.340758
117	1	0	25.500545	24.882123	10.597217
118	1	0	26.287259	24.043649	9.266825
119	6	0	27.373408	23.945863	11.132632
120	1	0	27.974608	23.063643	10.878343
121	1	0	27.982032	24.834191	10.924969
122	1	0	27.184509	23.917524	12.213272
123	6	0	13.341300	10.383016	4.503579
124	1	0	12.523212	10.562209	3.791393
125	1	0	13.349778	11.246637	5.183897
126	6	0	13.050011	9.110149	5.303421
127	1	0	13.835565	8.917507	6.045118
128	1	0	12.097382	9.187967	5.841039
129	1	0	12.990848	8.232192	4.647779
130	6	0	15.804975	11.693629	-1.670183
131	1	0	15.805707	12.558546	-2.346326
132	1	0	16.717828	11.125819	-1.901903
133	6	0	14.575274	10.829690	-1.973059
134	1	0	14.551614	10.541381	-3.030871
135	1	0	14.562649	9.905289	-1.383536
136	1	0	13.647052	11.374644	-1.757524
137	6	0	33.004796	10.023588	4.001483
138	1	0	33.777430	9.968707	3.221030
139	1	0	32.939862	11.077499	4.302839
140	6	0	33.437011	9.180833	5.205364

141	1	0	33.546855	8.123242	4.933245
142	1	0	34.399045	9.522078	5.606323
143	1	0	32.699516	9.238880	6.016107
144	6	0	32.793386	14.224996	0.071585
145	1	0	33.769991	13.724185	0.135317
146	1	0	32.841612	15.079075	0.762183
147	6	0	32.576103	14.736791	-1.355182
148	1	0	31.622394	15.272143	-1.445272
149	1	0	33.373889	15.426412	-1.656134
150	1	0	32.561499	13.910408	-2.077135

TSd

Zero-point correction= 1.304255 (Hartree/Particle)
Thermal correction to Energy= 1.376096
Thermal correction to Enthalpy= 1.377040
Thermal correction to Gibbs Free Energy= 1.190274
Sum of electronic and zero-point Energies= -2838.454942
Sum of electronic and thermal Energies= -2838.383100
Sum of electronic and thermal Enthalpies= -2838.382156
Sum of electronic and thermal Free Energies= -2838.568923

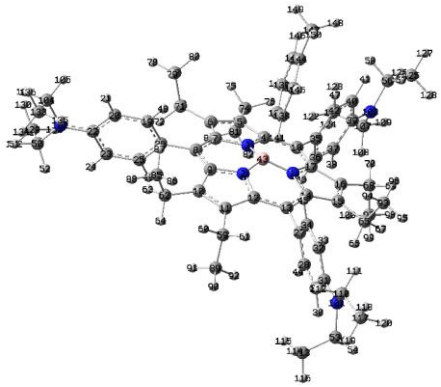


Fig. S106 Optimized structures of **TSd**.

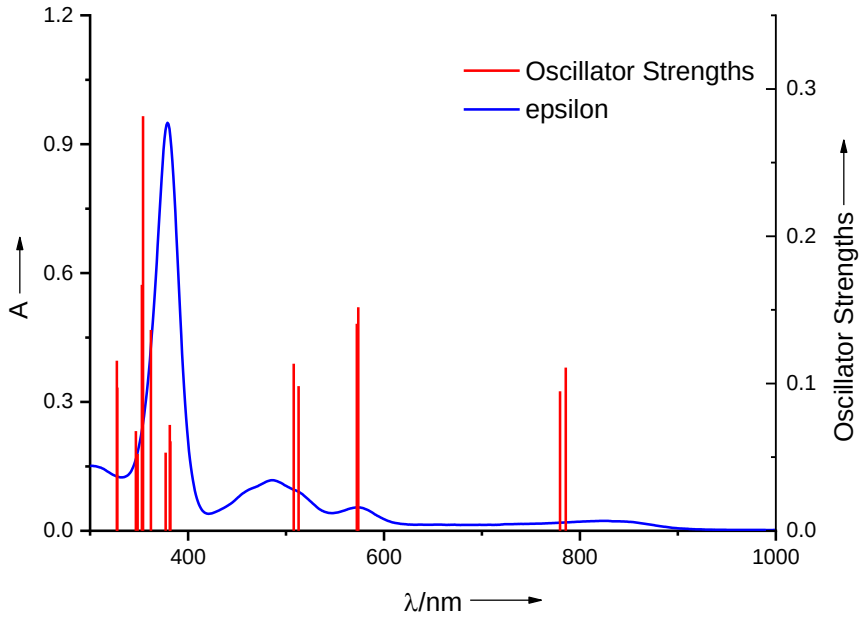
Table S35 Coordinates of atoms in **TSd**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.303876	9.332946	3.832810
2	7	0	2.383966	10.380258	4.798539
3	7	0	3.278343	11.178425	2.730090
4	6	0	4.113633	11.056255	1.643852
5	6	0	3.621533	12.041555	0.701425
6	6	0	2.492894	12.662543	1.259852
7	6	0	2.240243	12.066719	2.558431
8	6	0	1.219928	12.099074	3.562990
9	6	0	1.272756	11.185379	4.667902
10	6	0	0.354340	10.694426	5.673604
11	6	0	0.936714	9.581162	6.299918
12	6	0	2.239900	9.355707	5.708980

13	6	0	3.247097	8.332963	5.745604
14	6	0	4.291849	8.321634	4.766511
15	6	0	5.364422	7.436968	4.348798
16	6	0	5.895813	7.926921	3.146327
17	6	0	5.183688	9.138534	2.792543
18	6	0	5.122330	10.040068	1.683771
19	6	0	-0.051180	14.155830	4.259380
20	6	0	-1.127426	15.030781	4.164213
21	1	0	-1.157957	15.878185	4.838406
22	6	0	-2.170373	14.819229	3.225104
23	6	0	-2.055163	13.669082	2.399272
24	1	0	-2.811450	13.451864	1.654805
25	6	0	-0.970289	12.805976	2.506087
26	6	0	0.059591	13.025499	3.434633
27	6	0	3.150030	7.241782	6.757523
28	6	0	2.712626	5.952403	6.415834
29	6	0	2.605010	4.939665	7.361859
30	1	0	2.242811	3.975197	7.028908
31	6	0	2.954371	5.152455	8.722023
32	6	0	3.373210	6.465515	9.062171
33	1	0	3.627563	6.717424	10.083327
34	6	0	3.469290	7.470164	8.103436
35	6	0	6.088345	9.903725	0.552472
36	6	0	5.800265	9.136900	-0.585567
37	6	0	6.698285	9.031263	-1.642327
38	1	0	6.408328	8.427658	-2.493276
39	6	0	7.956412	9.686563	-1.616585
40	6	0	8.233228	10.468148	-0.465060
41	1	0	9.159158	11.022133	-0.383038
42	6	0	7.324716	10.562799	0.585913
43	5	0	3.472152	10.458681	3.917633
44	1	0	2.436506	5.734427	5.387167
45	1	0	3.798728	8.457487	8.417622
46	1	0	4.851663	8.611128	-0.653227
47	1	0	7.584142	11.174343	1.446580
48	1	0	0.723984	14.360916	4.993115
49	1	0	-0.929371	11.936575	1.854571
50	6	0	-4.372410	15.411447	2.233691
51	1	0	-5.252493	15.889805	2.676460
52	1	0	-4.583699	14.337338	2.228862
53	6	0	2.190760	2.891327	9.357431
54	1	0	2.548542	2.121350	10.042201
55	1	0	2.484868	2.550572	8.361115
56	6	0	10.111941	10.352497	-2.580106
57	1	0	10.554865	10.184708	-1.592905
58	1	0	9.884835	11.429582	-2.642576
59	6	0	0.238449	8.731311	7.330852
60	1	0	-0.388851	9.377853	7.954394
61	1	0	0.971827	8.274559	7.998653
62	6	0	-1.008595	11.240964	6.009891
63	1	0	-1.438302	11.731596	5.133637
64	1	0	-1.674980	10.408331	6.259437
65	6	0	5.888334	6.233652	5.086764
66	1	0	5.061855	5.654536	5.505265
67	1	0	6.404065	5.574888	4.381665
68	6	0	6.983068	7.252820	2.349495
69	1	0	7.728478	6.844644	3.041550

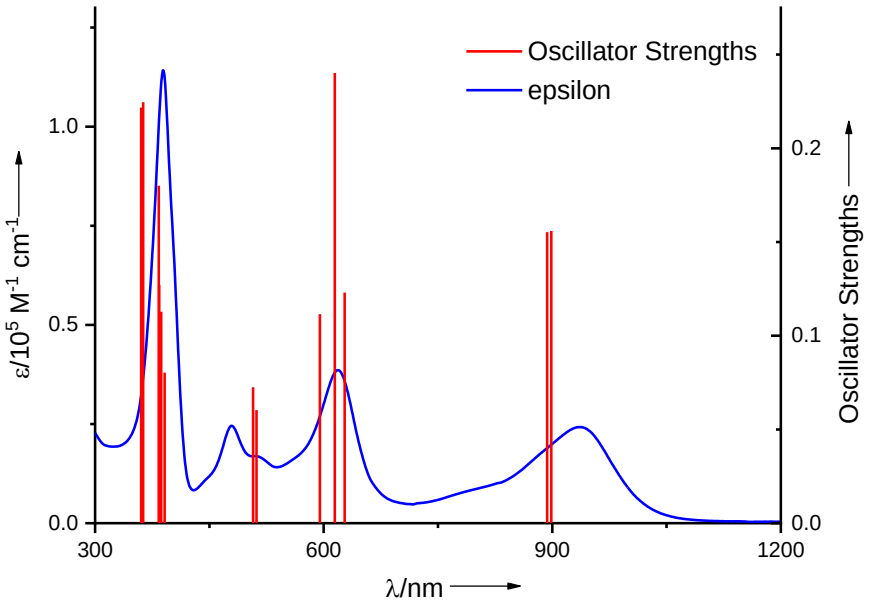
70	1	0	7.503526	7.992055	1.736233
71	6	0	1.739020	13.797841	0.619783
72	1	0	0.663795	13.666058	0.761694
73	1	0	1.914758	13.783694	-0.460057
74	6	0	4.173978	12.337468	-0.669460
75	1	0	4.117564	13.417405	-0.848392
76	1	0	5.233488	12.073648	-0.705574
77	6	0	2.152069	15.173773	1.176338
78	1	0	1.588299	15.969390	0.675426
79	1	0	1.952779	15.243747	2.250842
80	1	0	3.219959	15.362820	1.016805
81	6	0	3.430445	11.607196	-1.803466
82	1	0	3.484510	10.520753	-1.679501
83	1	0	2.372021	11.889342	-1.831960
84	1	0	3.875607	11.859758	-2.772902
85	6	0	-0.990097	12.233298	7.188022
86	1	0	-0.604803	11.762338	8.099467
87	1	0	-0.361580	13.102037	6.966937
88	1	0	-2.004435	12.593506	7.395488
89	6	0	-0.643060	7.625362	6.719058
90	1	0	-1.125253	7.044390	7.513908
91	1	0	-1.429982	8.046742	6.083245
92	1	0	-0.050522	6.935583	6.109234
93	6	0	6.859989	6.611164	6.221419
94	1	0	6.368053	7.235888	6.974627
95	1	0	7.228183	5.707342	6.720628
96	1	0	7.725158	7.163469	5.837032
97	6	0	6.467900	6.117316	1.445360
98	1	0	7.300800	5.662568	0.896732
99	1	0	5.977699	5.331420	2.030980
100	1	0	5.744704	6.490493	0.712623
101	7	0	2.909341	4.132909	9.662141
102	7	0	-3.240091	15.682845	3.121747
103	7	0	8.876720	9.553817	-2.650702
104	6	0	-3.307317	16.926258	3.892318
105	1	0	-2.305294	17.359333	3.974413
106	1	0	-3.896702	17.638767	3.305686
107	6	0	8.418835	9.095052	-3.967514
108	1	0	7.820941	8.188889	-3.837651
109	1	0	9.295922	8.782695	-4.535409
110	6	0	3.154113	4.478611	11.072983
111	1	0	4.089214	5.046283	11.116680
112	1	0	2.362610	5.147339	11.448967
113	6	0	0.664559	2.998933	9.454709
114	1	0	0.352489	3.277666	10.467984
115	1	0	0.268520	3.747990	8.760112
116	1	0	0.202219	2.034121	9.212905
117	6	0	3.298760	3.289431	12.019765
118	1	0	3.583668	3.672670	13.006046
119	1	0	2.368718	2.725672	12.144152
120	1	0	4.084851	2.600830	11.690090
121	6	0	7.632054	10.140783	-4.766193
122	1	0	6.732055	10.460920	-4.229576
123	1	0	8.242908	11.029283	-4.964159
124	1	0	7.320940	9.723823	-5.731819
125	6	0	11.172332	10.001025	-3.621396
126	1	0	10.877630	10.268548	-4.641050

127	1	0	12.081843	10.565294	-3.386332
128	1	0	11.424879	8.935000	-3.597888
129	6	0	-4.174217	15.925843	0.804063
130	1	0	-4.010638	17.009826	0.797881
131	1	0	-3.311636	15.450936	0.323900
132	1	0	-5.062932	15.713629	0.197233
133	6	0	-3.935931	16.762407	5.280204
134	1	0	-4.957291	16.371370	5.203197
135	1	0	-3.356231	16.073611	5.904402
136	1	0	-3.982126	17.731059	5.792629
137	6	0	4.815129	11.942470	5.067695
138	6	0	4.833436	11.839181	6.442829
139	6	0	5.605450	12.811313	4.339201
140	6	0	5.738481	12.659806	7.135924
141	1	0	4.183293	11.160723	6.986266
142	6	0	6.498143	13.618782	5.057739
143	1	0	5.552310	12.882634	3.257254
144	6	0	6.579232	13.552269	6.457810
145	1	0	5.780301	12.599358	8.221391
146	1	0	7.137157	14.311703	4.513498
147	6	0	7.555299	14.427444	7.209918
148	1	0	8.592093	14.189999	6.939854
149	1	0	7.399324	15.488605	6.980495
150	1	0	7.454708	14.298623	8.292094



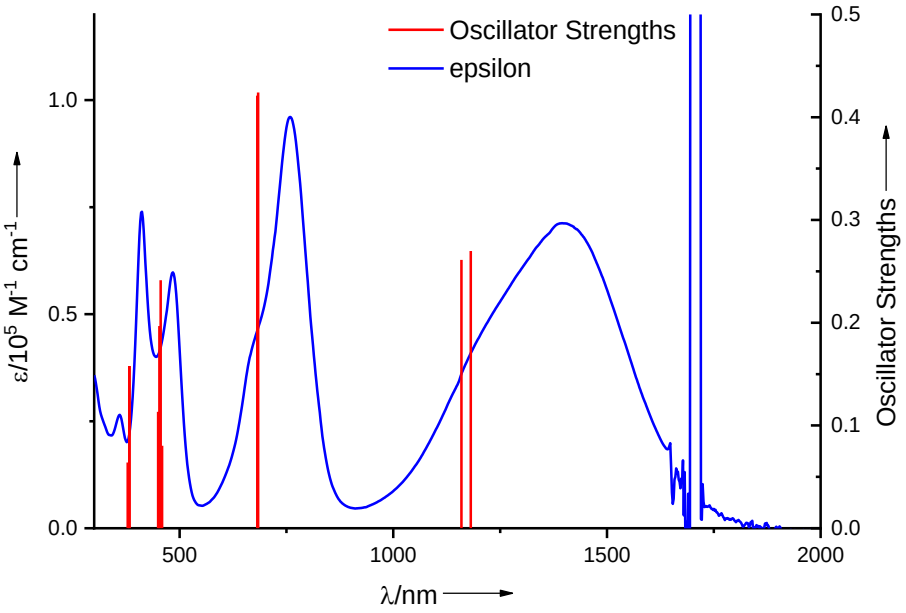
Wavelength (nm)	Oscillator Strengths	Major Transitions
785.51	0.1108	H_b-3→L_b (84.0%), H_a→L_a (10.5%)
779.68	0.09470	Hb-4→Lb 81.2%, Ha→La+1 11.0%
573.71	0.1518	H_a→L_a (62.9%), H_a-3→L_a+1 (15.2%), H_b-3→L_b (6.3%), H_b-10→L_b (5.9%)
572.23	0.1406	H_a→L_a+1 (61.5%), H_a-3→L_a (16.4%), H_b-4→L_b (6.8%)
512.86	0.09820	H_a-3→L_a 26.4%, H_b-2→L_b+1 21.6%, H_a-1→L_a 21.0%, H_a→L_a+1 15.4%, H_a-2→L_a 6.4%
507.94	0.1134	H_a-3→L_a+1 (35.3%), H_b-2→L_b+2 (24.3%), H_a→L_a (13.6%), H_a-1→L_a+1 (10.2%), H_a-2→L_a+1 (7.4%)
381.97	0.06080	H_b-2→L_b+1 32.3%, H_b-13→L_b 21.9%, H_b-12→L_b 12.3%, H_b-15→L_b 6.6%, H_a-3→L_a 6.5%
381.37	0.07190	H_a-4→L_a+1 19.4%, H_a-10→L_a 18.5%, H_a-5→L_a 7.8%, H_b-9→L_b+1 7.4%, H_a-9→L_a 5.0%
377.17	0.05310	H_b-2→L_b+2 16.9%, H_b-14→L_b 14.0%, H_a-11→L_a+1 9.3%
362.09	0.1364	H_b-13→L_b (41.4%), H_b-2→L_b+1 (15.2%), H_b-15→L_b (8.8%), H_a-3→L_a (6.2%)
354.12	0.2815	H_b-14→L_b (34.0%), H_b-2→L_b+2 (16.6%), H_a-3→L_a+1 (7.6%), H_a-12→L_a (7.3%), H_b-3→L_b+2 (5.1%)
352.92	0.167	H_b-15→L_b (51.8%), H_b-4→L_b+2 (7.6%), H_b-2→L_b+1 (6.0%), H_a-12→L_a+1 (5.5%)
348.48	0.05220	H_b-3→L_b+1 51.6%, H_a-4→L_a 35.7%
346.69	0.06770	H_b-4→L_b+1 30.9%, H_b-3→L_b+2 19.2%, H_a-5→L_a 18.4%, H_a-4→L_a+1 15.0%
327.72	0.09730	H_b-5→L_b+1 42.6%, H_a-10→L_a+1 9.3%, H_b-5→L_b+2 9.0%, H_a-9→L_a 6.5%, H_b-16→L_b 5.1%
327.38	0.1155	H_b-5→L_b+2 (43.9%), H_b-5→L_b+1 (14.0%), H_a-9→L_a+1 (5.3%), H_a-10→L_a+1 (5.2%)

Fig. S107 Calculated vertical transitions and major transitions of **4a**.



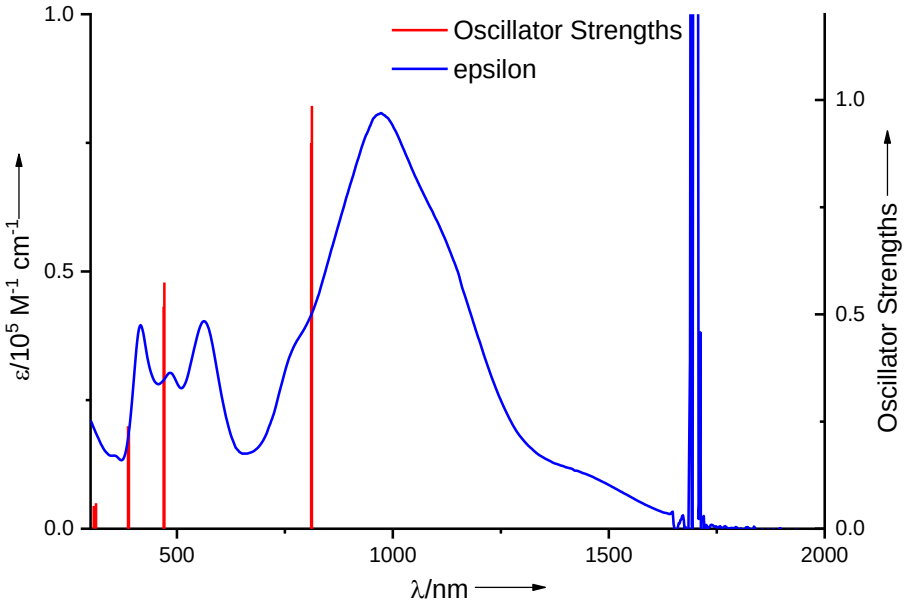
Wavelength (nm)	Oscillator Strengths	Major Transitions
898.70	0.1559	H_b-3→L_b (69.7%), H_b-1→L_b (18.4%), H_a→L_a (7.4%)
893.26	0.1553	H_b-2→L_b (82.3%), H_a→L_a+1 (8.2%), H_b-4→L_b (5.0%)
627.55	0.1230	H_b-6→L_b (33.0%), H_b-7→L_b (28.8%), H_a→L_a+1 (24.6%)
614.60	0.2402	H_a→L_a (60.3%), H_b-8→L_b (13.0%), H_a-2→L_a+1 (5.1%)
595.11	0.1115	H_a→L_a+1 (46.1%), H_b-6→L_b (37.5%)
511.93	0.06030	Ha-2→La 35.1%, Hb-4→Lb+1 23.5%, Ha-3→La 13.5%, Ha-1→La 9.1%, Ha→La+1 6.2%
507.28	0.07250	Ha-2 → La+1 36.8%, Hb-4 → Lb+2 26.8%, Ha-3 → La+1 17.9%, Ha→La 5.8%
391.24	0.08030	Hb-1→Lb+2 74.1%, Ha-4→La+1 8.7%, Hb-3→Lb+2 8.6%
386.79	0.1128	H_b-12→L_b (27.8%), H_b-4→L_b+1 (14.6%), H_b-2→L_b+2 (9.6%), H_b-2→L_b+1 (5.9%)
384.22	0.1271	H_b-3→L_b+1 (11.7%), H_b-2→L_b+1 (9.2%), H_a-4→L_a (6.8%), H_b-12→L_b (6.7%), H_a-6→L_a (6.6%), H_a-6→ L_a+1 (5.2%)
383.51	0.1800	H_b-3→L_b+1 (12.9%), H_b-2→L_b+1 (12.3%), H_a-5→L_a (10.4%), H_b-3→L_b+2 (8.6%), H_a-8→L_a (7.1%), H_b-7→L_b+1 (6.2%)
363.06	0.2246	H_b-4→L_b+1 (36.2%), H_b-12→L_b (15.6%), H_a-2→L_a (11.3%), H_a-7→L_a+1 (9.8%), H_a-3→L_a (6.0%)
360.44	0.2217	H_b-4→L_b+2 (38.5%), H_b-13→L_b (11.8%), H_a-2→L_a+1 (8.9%), H_a-7→La (7.9%), H_a-3→L_a+1 (6.8%)

Fig. S108 Calculated vertical transitions and major transitions of **4b**.



Wavelength (nm)	Oscillator Strengths	Major Transitions
1181.14	0.26980	$H_b \rightarrow L_b$ (89.6%), $H_a \rightarrow L_a$ (6.5%)
1159.49	0.26120	H_b-1$\rightarrow L_b$ (89.2%), $H_a \rightarrow L_a$+1 (6.9%)
683.71	0.42400	$H_a \rightarrow L_a$ (53.1%), $H_a \rightarrow L_a$+1 (31.3%)
681.64	0.42100	$H_a \rightarrow L_a$+1 (52.2%), $H_a \rightarrow L_a$ (31.6%)
458.76	0.08020	$H_b \rightarrow L_b$+2 (37.6%), H_a-1 $\rightarrow L_a$+1 (37.1%), H_a-3 $\rightarrow L_a$+1 (8.2%), H_b-1$\rightarrow L_b$+1 (5.5%)
455.62	0.24130	H_a-1$\rightarrow L_a$ (32.8%), $H_b \rightarrow L_b$+1 (19.0%), H_a-3$\rightarrow L_a$ (14.6%), H_a-2$\rightarrow L_a$+1 (10.7%), H_b-1$\rightarrow L_b$+2 (8.0%)
452.53	0.19680	H_a-2 $\rightarrow L_a$ (57.1%), H_b-1 $\rightarrow L_b$+1 (19.6%), H_a-3 $\rightarrow L_a$+1 (11.1%)
450.74	0.10230	H_a-3$\rightarrow L_a$+1 (40.7%), H_a-3$\rightarrow L_a$ (27.3%), H_a-1$\rightarrow L_a$+1 (6.3%)
449.64	0.11330	H_a-3$\rightarrow L_a$ (35.9%), H_a-3$\rightarrow L_a$+1 (24.6%), H_a-2$\rightarrow L_a$+1 (6.7%), H_b-1$\rightarrow L_b$+1 (5.8%), H_b-1$\rightarrow L_b$+2 (5.7%), H_a-1$\rightarrow L_a$+1 (5.1%)
382.92	0.15790	H_b-3 $\rightarrow L_b$+1 (22.1%), H_a-8 $\rightarrow L_a$ (14.2%), H_a-6 $\rightarrow L_a$+1 (14.0%), H_a-4$\rightarrow L_a$ (9.3%), H_b-7$\rightarrow L_b$+1 (7.6%), H_a-7$\rightarrow L_a$+1 (5.8%), H_b-6$\rightarrow L_b$+2 (5.5%)
382.17	0.15790	H_b-3 $\rightarrow L_b$+2 (26.0%), H_a-6 $\rightarrow L_a$ (14.9%), H_a-4 $\rightarrow L_a$+1 (12.4%), H_b-3$\rightarrow L_b$+1 (6.2%)
378.40	0.06400	H_a-8 $\rightarrow L_a$ (16.2%), H_b-3 $\rightarrow L_b$+1 (16.2%), H_b-5 $\rightarrow L_b$+1 (15.5%), H_a-7$\rightarrow L_a$+1 (9.5%), H_b-7$\rightarrow L_b$+1 (8.9%), H_a-6$\rightarrow L_a$+1 (6.4%)

Fig. S109 Calculated vertical transitions and major transitions of **4c**.



Wavelength (nm)	Oscillator Strengths	Major Transitions
812.64	0.98630	H→L (50.7%), H-1→L (26.4%), H-2→L (22.8%)
810.94	0.89980	H-1→L (74.8%), H→L (12.7%), H-2→L (12.2%)
470.72	0.57410	H-1→L+2 (36.5%), H→L+1 (23.1%), H-2→L+1 (20.6%), H-1→L+1 (9.3%), H-2→L+2 (5.0%)
469.05	0.51810	H-1→L+1 (35.9%), H-2→L+2 (22.5%), H→L+2 (22.4%), H-1→L+2 (8.1%), H-2→L+1 (5.1%)
388.87	0.22230	H-4→L+1 (70.2%), H-13→L (12.4%), H-12→L (8.0%)
386.86	0.23920	H-4→L+2 (64.4%), H-12→L (18.9%), H-13→L (6.7%)
312.60	0.05960	H-6→L+1 (38.7%), H-30→L (17.5%), H-7→L+1 (9.1%), H-5→L+1 (5.4%)
307.33	0.05320	H-6→L+2 (22.2%), H-25→L (15.9%), H-8→L+2 (15.6%), H-26→L (10.9%), H-8→L+1 (9.2%)

Fig. S110 Calculated vertical transitions and major transitions of **7c**.

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