Electronic Supporting Information

Mono- and bis-Pd(II) complexes of N-confused dithiahexaphyrin (1.1.1.1.1.0) with the absorption and aromaticity modulated by Pd(II) coordination, macrocycle contraction and ancillary ligands

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CONTENTS

Experimental

General

Commercially available solvents and reagents were used without further purification unless otherwise mentioned. Intermediate **a** was synthesized by a procedure modified from a reported one,[1] and **b** was synthesized by a reported method.[2] Thin-layer chromatography (TLC) was carried out on glass sheets coated with silica gel 60 F254 (Qingdao Haiyang Chemical Co., Ltd). ^{1}H NMR spectra were obtained using Bruker AM 400 or Bruker Ascend 600 spectrometers, and the chemical shifts were reported relative to tetramethylsilane (TMS, δ = 0) in ppm. ^{13}C NMR spectra were recorded at 101 MHz (Bruker AM 400) or 151 MHz (Bruker Ascend 600), and the chemical shifts were reported relative to $CDCl_3$ (δ = 77.00) or DMSO-d_6 (δ = 39.52) in ppm. HRMS were performed using a Waters LCT Premier XE spectrometer or a JEOL-JMS-T100L AccuTOF spectrometer. UV-Vis-NIR absorption spectra were recorded on a Shimadzu UV2600 spectrophotometer and all absorption spectra were recorded at room temperature.

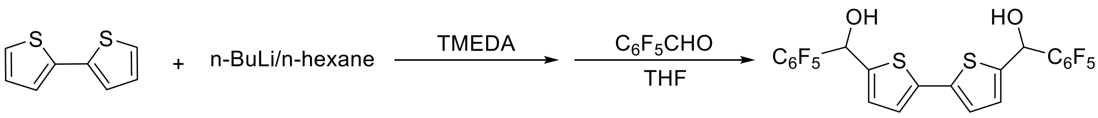
Crystallography

Single crystals of **1, 2** and **3** were obtained by the slow recrystallization from the dichloromethane/n-hexane solutions, and crystals of **4-Ph** and **5** were obtained by the slow recrystallization from the dichloromethane/methanol solutions. X-ray analyses were performed on a SMART APEX equipped with CCD detector (Bruker) using MoKα (graphite, monochromated, λ = 0.71073 Å). The structures were solved by the direct method of SHELXS-2013/2014 and refined using the SHELXS-2013/2014 program.[3-6] The positional parameters and thermal parameters of non-hydrogen atoms were refined anisotropically on F^2 by the full-matrix least-squares method. Hydrogen atoms were placed at calculated positions and refined riding on their corresponding carbon atoms. CCDC 2277039 (**1**), 2277040 (**2**), 2277041 (**3**), 2277042 (**4-Ph**) and 2277043 (**5**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Details for Theoretical Calculations.

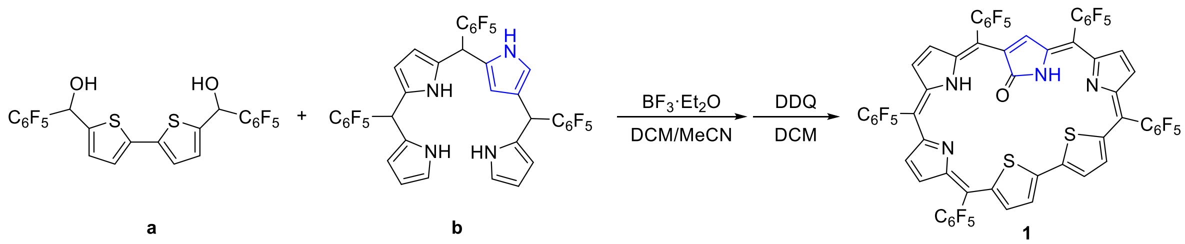
Density functional theory (DFT) calculations were carried out using Gaussian 16 program. The optimized structures and molecular orbitals were all calculated at the level of B3LYP.[7, 8] The nucleus-independent chemical shift (NICS) calculations were obtained using the GIAO method at the B3LYP/6-31G* level.[9] The local ring center chosen for determination of the NICS values[10] represent the nonweighted means of the carbon and nitrogen coordinates on the peripheral positions of the macrocycles. ACID contours with the associated vectors were obtained in accord with the continuous set of gauge transformation (CSGT) methods[11]. At the optimized geometries, time-dependent (TD) DFT calculations with the hybrid PBE0 functional[12] were carried out to simulate the absorption spectra. Solvent effects arising from CH_2Cl_2 were accounted for using the polarizable continuum model (PCM).[13]

Synthetic Details



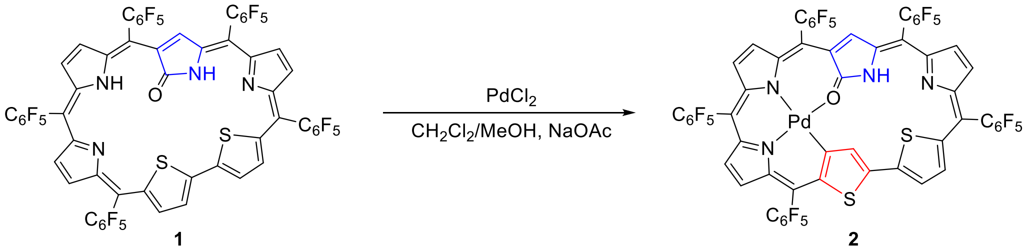
a: (5,5'-bis-[(pentafluorophenyl)hydroxymethyl]-2,2'-bithiophene diol): n-Butylithium (n-BuLi, 2.5 M solution in hexane 18.0 mL, 45.0 mmol) was added to a solution of N,N,N',N'-tetramethylethylenediamine (TMEDA, 6.80 mL, 45.4 mmol) in dry n-hexane (68 mL), followed by addition of bithiophene (3.00 g, 18.0 mmol) in dry THF (10.0 mL) under argon. The reaction mixture was heated under reflux for 1 h. As the reaction proceeded, a white suspension formed indicating the generation of the 5,5'-dilithiated salt of bithiophene. The reaction mixture was cooled to 0 °C in an ice bath and a solution of pentafluorobenzaldehyde (C_6F_5CHO, 5.10 mL, 41.8 mmol) in tetrahydrofuran (THF, 10 mL) was added. The reaction mixture was stirred at 0 °C for 15 min and then warmed to room temperature. An ice-cold saturated NH_4Cl solution (80.0 mL) was added and the reaction mixture was extracted with dichloromethane (40.0 × 4 mL). The organic layers were combined and washed with brine and dried over anhydrous Na_2SO_4. After removing the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel columns using petroleum ether (PE)/dichloromethane (DCM) = 1/3 (v/v) as the eluent, **a** was collected as a pale yellow solid (4.53 g, 45%).

a: ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.11 (d, J = 3.7 Hz, 2H), 6.94 (d, J = 5.1 Hz, 2H, OH), 6.82 (d, J = 3.6 Hz, 2H), 6.28 (d, J = 4.9 Hz, 2H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 145.8 (s), 144.6 (d, $^1J_{CF}$ = 248 Hz*), 140.7 (d, $^1J_{CF}$ = 252 Hz*), 137.7 (d, $^1J_{CF}$ = 249 Hz*), 137.6 (d, $^1J_{CF}$ = 248 Hz*), 137.5 (d, $^1J_{CF}$ = 248 Hz*), 136.3 (s), 125.3 (s), 123.9 – 123.7 (m), 117.9, 117.8, 117.7, 62.7 (s). HRMS: m/z; $[M]^+$: calcd for $C_{22}H_8F_{10}O_2S_2$): 557.9801; Found: 557.9796.



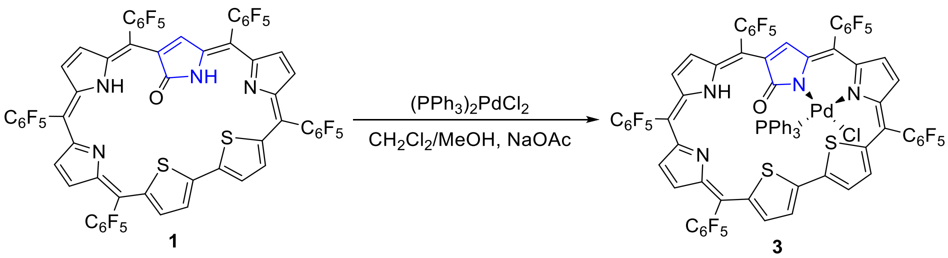
1: Boron trifluoride etherate **(**$BF_3{\cdot}Et_2O$, 1.90 mL, 15.0 mmol) in DCM (20 mL) was added into the solution of **a** (3.41 g, 6.11 mmol) and **b** (4.81 g, 5.99 mmol) in DCM/MeCN (300/80 mL) under nitrogen atmosphere. After stirring for 2 h, DCM (400 mL) was added to dilute the solution. Then 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 5.44g, 24.0 mmol) was added to the reaction mixture under air, and the solution was stirred for 1 h. Then the reaction mixture was quenched with triethylamine (TEA, 2.08 mL, 15.0 mmol), and the mixture was passed through a basic alumina column to remove tar and residual solids. After the solvent was removed in vacuo, the raw products were purified on silica gel columns using PE/DCM = 2/1(v/v) as the eluent. Finally, **1** was obtained as a violet solid (921 mg, 12%)

1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.69 (d, *J* = 4.6 Hz, 1H), 10.04 (s, 1H), 9.78 (d, *J* = 4.5 Hz, 1H), 9.71 (s, 1H), 9.09 (s, 1H), 8.75 (d, *J* = 5.3 Hz, 1H), 8.70 (t, *J* = 4.6 Hz, 2H), 8.57 (d, *J* = 4.7 Hz, 1H), 8.53 (d, *J* = 4.6 Hz, 1H), 8.34 (d, *J* = 4.8 Hz, 1H), 1.50 (s, 1H, NH), 1.28 (s, 1H, NH). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.1, 160.6, 159.0, 154.5, 151.42, 146.8 (d, $^{1}J_{CF}$ = 245 Hz*), 146.5 (d, $^{1}J_{CF}$ = 248 Hz*), 144.7, 143.9, 142.6 (d, $^{1}J_{CF}$ = 258 Hz*), 141.5, 140.3, 139.0, 137.7 (d, $^{1}J_{CF}$ = 252 Hz*), 137.6, 136.7, 136.4, 135.8, 135.4, 135.3, 134.8, 132.5, 132.2, 131.1, 130.4, 129.5, 128.3, 122.0, 119.1, 118.9, 118.1, 117.8 (d, $^{1}J_{CF}$ = 266 Hz*), 113.9 (d, $^{1}J_{CF}$ = 211 Hz*), 102.6, 101.6, 99.6. UV/Vis/NIR [(CH_2Cl_2): λ_{max} (nm) (ε ×10^5 $mol^{-1}dm^3cm^{-1}$)]: 552 (3.39), 679 (0.35), 835 (0.07). HRMS: m/z; $[M]^+$: calcd for $C_{59}H_{13}F_{25}N_4OS_2$): 1332.0126; Found: 1332.0127.



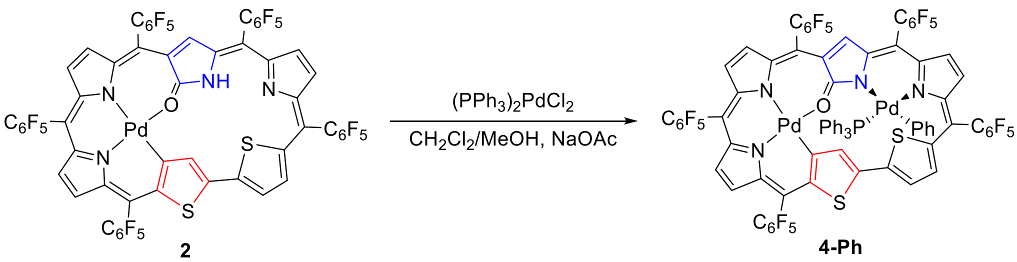
2: Palladium(II) dichloride ($PdCl_2$, 102 mg, 0.573 mmol) was added slowly to the solution of **1** (382 mg, 0.287 mmol) in DCM/MeOH (320/80 mL) with sodium acetate (NaOAc, 47.0 mg, 0.573 mmol), and the mixture was stirred for 8 h. The reaction mixture was passed through a basic alumina column to remove insoluble solids. After the solvent was removed in vacuo, the raw products were purified on silica gel columns using PE/DCM = 2/1(v/v) as the eluent. Finally, **2** was obtained as a blue solid (185 mg, 45%).

2: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.49 (d, *J* = 4.6 Hz, 1H), 10.16 (d, *J* = 4.5 Hz, 1H), 10.12 (s, 1H), 9.25 (t, *J* = 4.6 Hz, 2H), 9.12 (d, *J* = 5.0 Hz, 1H), 9.08 (d, *J* = 4.5 Hz, 1H), 9.01 (d, *J* = 5.0 Hz, 1H), 8.94 (d, *J* = 4.5 Hz, 1H), -0.93 (s, 1H, NH), -2.85 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.1, 156.7, 153.0, 151.7, 148.4, 147.7, 147.0 (d, $^{1}J_{CF}$ = 247 Hz*), 146.6 (d, $^{1}J_{CF}$ = 248 Hz*), 146.3 (d, $^{1}J_{CF}$ = 245 Hz*), 146.0 (d, $^{1}J_{CF}$ = 255 Hz*), 146.1, 145.2, 144.5, 142.8 (d, $^{1}J_{CF}$ = 244 Hz*), 142.4, 140.5, 139.1, 138.8, 138.3 (d, $^{1}J_{CF}$ = 254 Hz*), 137.7, 137.3, 136.8, 134.8, 133.3, 132.9, 132.4, 131.7, 130.9, 127.0, 123.7, 122.5, 116.3, 114.8 (t, $^{2}J_{CF}$ = 163 Hz*), 112.2, 111.5, 105.4, 102.8. UV/Vis/NIR [(CH_2Cl_2): λmax (nm) (ε ×10^5 $mol^{-1}dm^3cm^{-1}$)]: 588 (2.40), 622 (1.41), 737 (0.27), 858 (0.12). HRMS: m/z; $[M]^+$: calcd for $C_{59}H_{11}F_{25}N_4OPdS_2$: 1435.9023; Found: 1435.9018.



3: Bis(triphenylphosphine) palladium(II) dichloride (($(PPh_3)_2PdCl_2$, 219 mg, 0.312 mmol) was added slowly to the solution of **1** (208 mg, 0.156 mmol) in DCM/MeOH (160/20 mL) with sodium acetate (NaOAc, 26.0 mg, 312 mmol), and the mixture was stirred for 36 h. The reaction mixture was passed through a basic alumina column to remove insoluble solids. After the solvent was removed in vacuo, the raw products were purified on silica gel columns using PE/DCM = 1/1(v/v) as the eluent. Finally, **3** was obtained as a blue solid (65.0 mg, 24%)

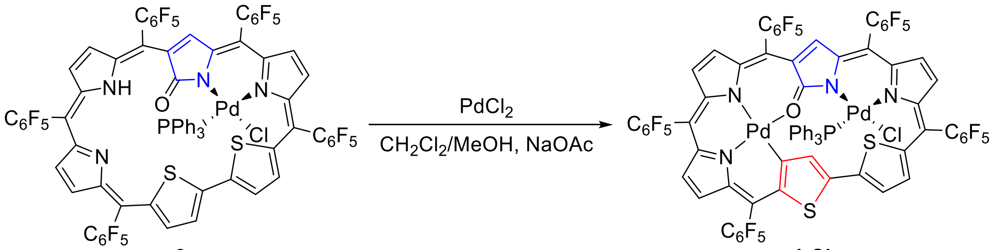
3: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.27 (d, J = 4.7 Hz, 2H), 10.14 (d, J = 4.4 Hz, 2H), 9.62 (s, 1H), 9.18 (d, J = 2.3 Hz, 1H), 9.12 (d, J = 4.6 Hz, 1H), 8.81 (d, J = 4.8 Hz, 1H), 8.67 (d, J = 4.6 Hz, 1H), 8.60 (d, J = 5.0 Hz, 1H), 8.47 (d, J = 4.6 Hz, 1H), 6.22 (s, 3H, Ph-H), 5.41 (s, 6H, Ph-H), 4.29 (s, 6H, Ph-H), 0.28 (s, 1H, NH). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.2, 158.3, 156.9, 154.3, 152.9, 151.6,143.9, 142.5 (d, $^1J_{CF}$ = 258 H$_Z$*), 141.8, 139.0, 138.6, 137.8, 137.6 (d, $^1J_{CF}$ = 240 H$_Z$*), 136.1, 135.8, 135.7, 135.4, 135.0, 133.9, 131.4, 131.2, 130.3, 130.0, 129.9, 128.6, 126.4 (d, $^1J_{CF}$ = 240 H$_Z$*),125.9, 125.9, 121.2, 117.2, 115.5, 106.3, 102.7, 99.3. UV/Vis/NIR [(CH_2Cl_2): λmax (nm) (ε ×10^5 mol^{-1}dm^{3}cm^{-1})]: 589 (1.32), 628 (1.38), 746 (0.33), 882 (0.11). HRMS: m/z; $[M]^+$: calcd for $C_{77}H_{27}ClF_{25}N_4OPPdS_2$: 1733.9784; Found: 1733.9787.



4-Ph: Bis(triphenylphosphine) palladium(II) dichloride (($(PPh_3)_2PdCl_2$, 89.0 mg, 0.127 mmol) was added slowly to the solution of **2** (91.0 mg, 63.0 μmol) in DCM/MeOH (80/20 mL) with sodium acetate (NaOAc, 10.0 mg, 0.127 mmol), and the mixture was stirred for 24 h. The reaction mixture was passed through a basic alumina column to remove insoluble solids. After the solvent was removed in vacuo, the raw products were purified on silica gel columns using PE/DCM = 2/1(v/v) as the eluent. Finally, **4-Ph** was obtained as a green solid (36.0 mg, 31%).

4-Ph: ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.75 (d, J = 4.3 Hz, 1H), 9.96 – 9.92 (m, 1H), 9.69 (s, 1H), 9.36 (d, J = 4.7 Hz, 1H), 9.09 (t, J = 5.0 Hz, 2H), 9.01 (d, J = 4.8 Hz, 1H), 9.00 – 8.98 (m, 1H), 8.93 (d, J = 3.2 Hz, 1H), 6.37 (t,

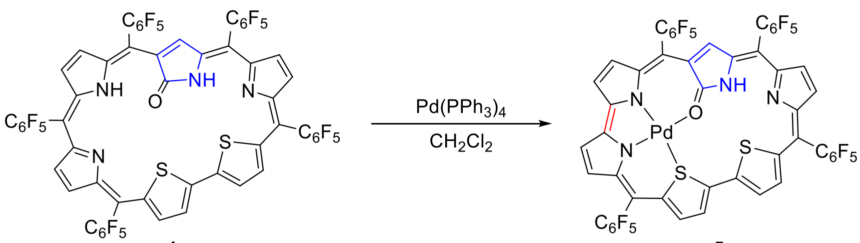
J = 7.3 Hz, 3H, Ph-H), 6.09 (t, J = 6.8 Hz, 1H, Ph-H), 5.88 (t, J = 7.1 Hz, 1H, Ph-H), 5.80 (t, J = 6.8 Hz, 6H, Ph-H), 5.47 (t, J = 7.3 Hz, 1H, Ph-H), 4.52 (d, J = 6.4 Hz, 1H, Ph-H), 4.06 (dd, J = 11.0, 8.0 Hz, 6H, Ph-H), 2.30 – 2.25 (m, 1H, Ph-H), -3.78 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 156.4, 155.8, 149.7, 149.4, 147.2, 146.3 (d, $^{1}J_{CF}$ = 240 Hz*), 145.9, 145.3, 144.0 (t, $^{2}J_{CF}$ = 60 Hz*), 143.6, 143.1, 142.6, 142.6, 138.4 (d, $^{1}J_{CF}$ = 258 Hz*), 138.0, 137.5 (d, $^{1}J_{CF}$ = 253 Hz*), 137.4, 136.1, 136.0, 134.5, 133.8, 132.8, 132.3, 132.2, 131.3, 131.2, 131.1, 130.8, 130.3, 128.3, 127.5, 127.3, 126.9, 126.6, 126.3, 126.0, 125.9, 124.5, 124.1, 121.9, 116.4, 114.4, 112.9, 109.3, 108.8, 102.8. UV/Vis/NIR [(CH_2Cl_2): λ_{max} (nm) (ε ×10^5 mol^{-1}dm^{3}cm^{-1})]: 622 (3.70), 760 (0.46), 870 (0.30). 984 (0.61). HRMS: m/z; $[M]^+$: calcd for $C_{83}H_{30}F_{25}N_4OPPd_2S_2$: 1879.9297; Found: 1879.9299.



3 → 4-Cl

4-Cl: Palladium(II) dichloride ($PdCl_2$, 6.10 mg, 35.0 μmol) was added slowly to the solution of **3** (30.0 mg, 17.0 μmol) in DCM/MeOH (24/6 mL) with sodium acetate (NaOAc, 2.80 mg, 35.0 μmol), and the mixture was stirred for 10 h. The reaction mixture was passed through a basic alumina column to remove insoluble solids. After the solvent was removed in vacuo, the raw products were purified on silica gel columns using PE/DCM = 1.5/1(v/v) as the eluent. Finally, **4-Cl** was obtained as a green solid (11.0 mg, 37%).

4-Cl: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (d, J = 2.8 Hz, 1H), 10.15 (s, 1H), 9.78 (s, 1H), 9.42 (s, 1H), 9.34 (s, 1H), 9.16 (s, 3H), 9.10 (s, 1H), 6.25 (s, 3H, Ph-H), 5.76 (s, 6H, Ph-H), 4.22 (s, 6H, Ph-H), -4.08 (s, 1H). UV/Vis/NIR [(CH_2Cl_2): λ_{max} (nm) (ε ×10^5 mol^{-1}dm^{3}cm^{-1})]: 622 (3.52), 768 (0.30), 862 (0.28), 974 (0.52). HRMS: m/z; $[M]^+$: calcd for $C_{77}H_{25}ClF_{25}N_4OPPd_2S_2$: 1837.8588; Found: 1837.8573.



1 → 5

5: Tetrakis(triphenylphosphine) palladium(0) ($Pd(PPh_3)_4$, 260 mg, 0.225 mmol) was added slowly to the solution of **1** (150 mg, 0.113 mmol) in DCM (150 mL), and the mixture was stirred for 24 h. The reaction mixture was passed through a basic alumina column to remove insoluble solids. After the solvent was removed in vacuo, the raw products were purified on silica gel columns using PE/DCM = 2/1(v/v) as the eluent. Finally, **5** was obtained as a violet solid (21.0 mg, 15%).

5: ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.13 (dd, *J* = 10.6, 4.9 Hz, 2H), 11.19 (s, 1H), 10.91 (d, *J* = 4.7 Hz, 1H), 10.78 (dd, *J* = 8.6, 4.7 Hz, 2H), 10.66 (d, *J* = 2.8 Hz, 1H), 9.94 (d, *J* = 4.4 Hz, 1H), 9.87 (d, *J* = 3.8 Hz, 1H), 9.62 (d, *J* = 4.3 Hz, 1H), 9.57 (d, *J* = 4.4 Hz, 1H), -2.10 (s, 1H, NH). δ 11.46 (d, *J* = 5.1 Hz, 1H), 11.38 (d, *J* = 5.4 Hz, 1H), 10.45 (s, 1H), 10.38 (d, *J* = 4.9 Hz, 1H), 10.00 (d, *J* = 5.3 Hz, 1H), 9.75 (d, *J* = 4.8 Hz, 1H), 9.57 (d, *J* = 4.4 Hz, 1H), 9.45 (d, *J* = 4.7 Hz, 1H), 9.28 (d, *J* = 4.2 Hz, 1H), 9.16 (d, *J* = 4.2 Hz, 1H), 8.90 (t, *J* = 12.6 Hz, 1H), 1.11 (s, 1H, NH). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.0, 154.3, 149.9, 148.3, 148.2, 146.4 (d, $^1J_{CF}$ = 255 H_Z*), 142.6, 142.3 (d, $^1J_{CF}$ = 253 H_Z*), 138.8, 138.1 (d, $^1J_{CF}$ = 252 H_Z*), 137.4, 136.6, 136.1, 136.1, 135.2, 135.1, 133.8, 132.9, 132.6, 132.5, 131.9, 131.2, 131.1, 130.1, 129.9, 129.8, 129.7, 126.2, 125.5, 125.3, 125.2, 124.8, 123.9, 122.1, 121.3, 120.5, 119.9, 118.9, 116.5, 113.7, 112.9, 108.2, 106.2, 104.0. UV/Vis/NIR [(CH_2Cl_2): λ_{max} (nm) (ε ×10^5 $mol^{-1}dm^3cm^{-1}$)]: 568 (1.22), 602 (1.24), 840 (0.27). HRMS: m/z; $[M]^+$: calcd for $C_{52}H_{12}F_{20}N_4OPdS_2$: 1257.9179; Found: 1257.9174.

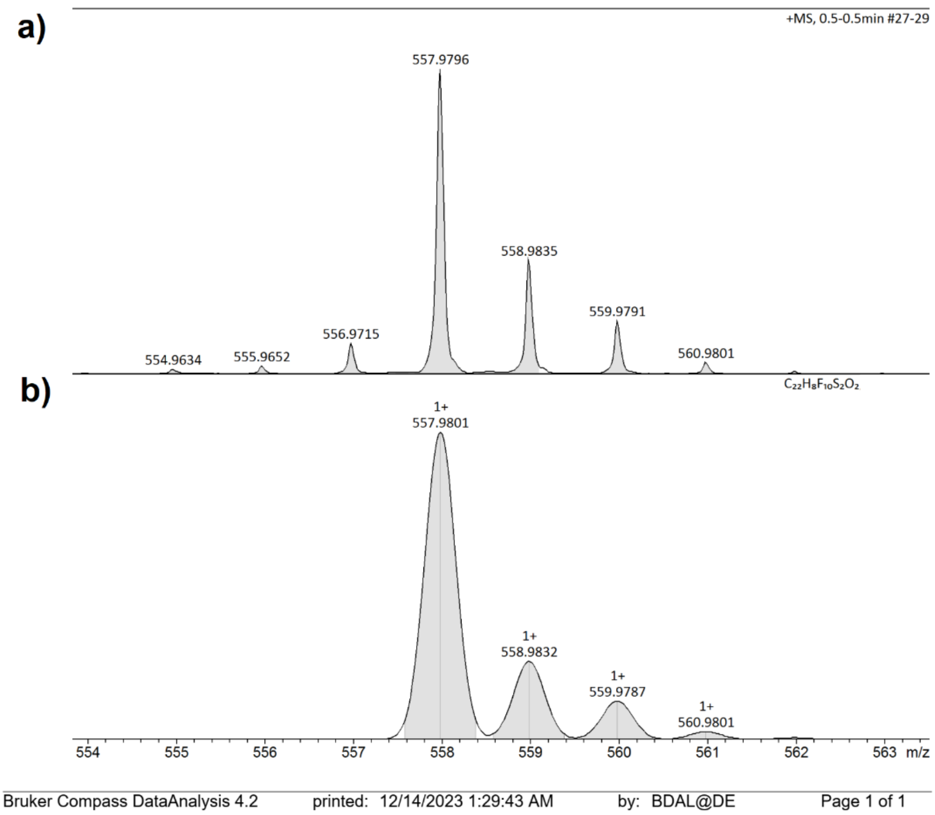


Figure S1. a) Experimental HR-ESI-MS and b) simulated HRMS of **a**.

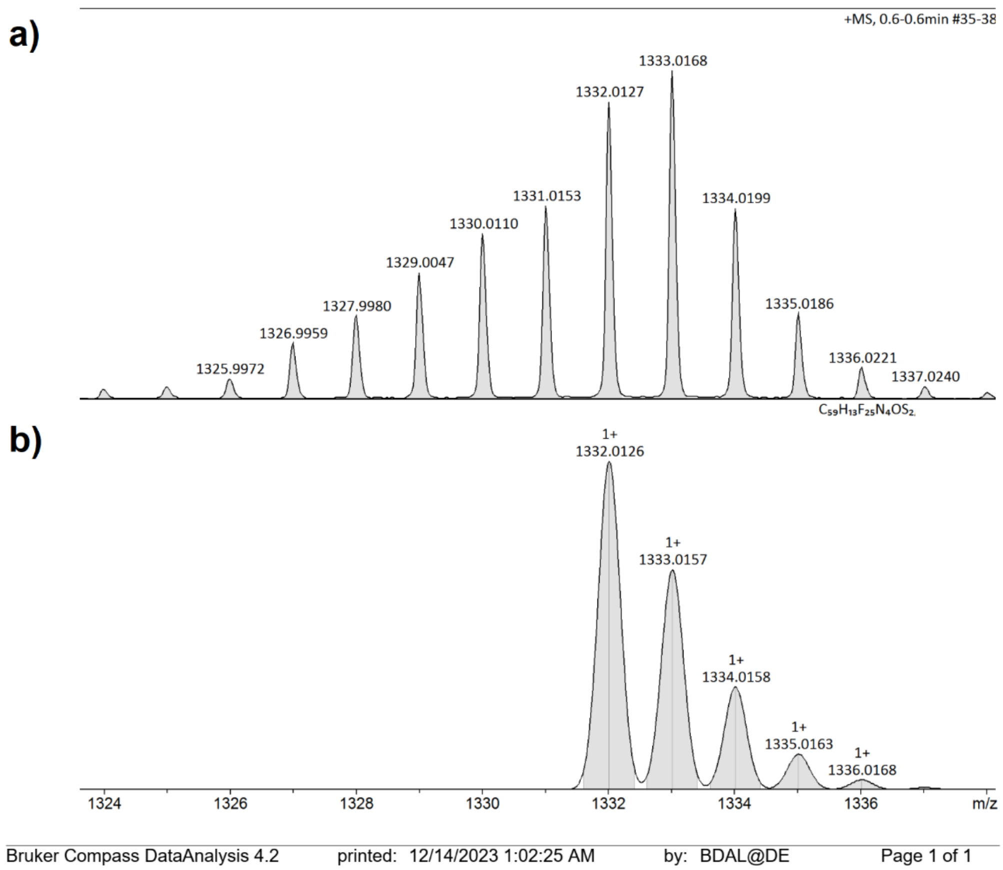


Figure S2. a) Experimental HR-ESI-MS and b) simulated HRMS of **1**.

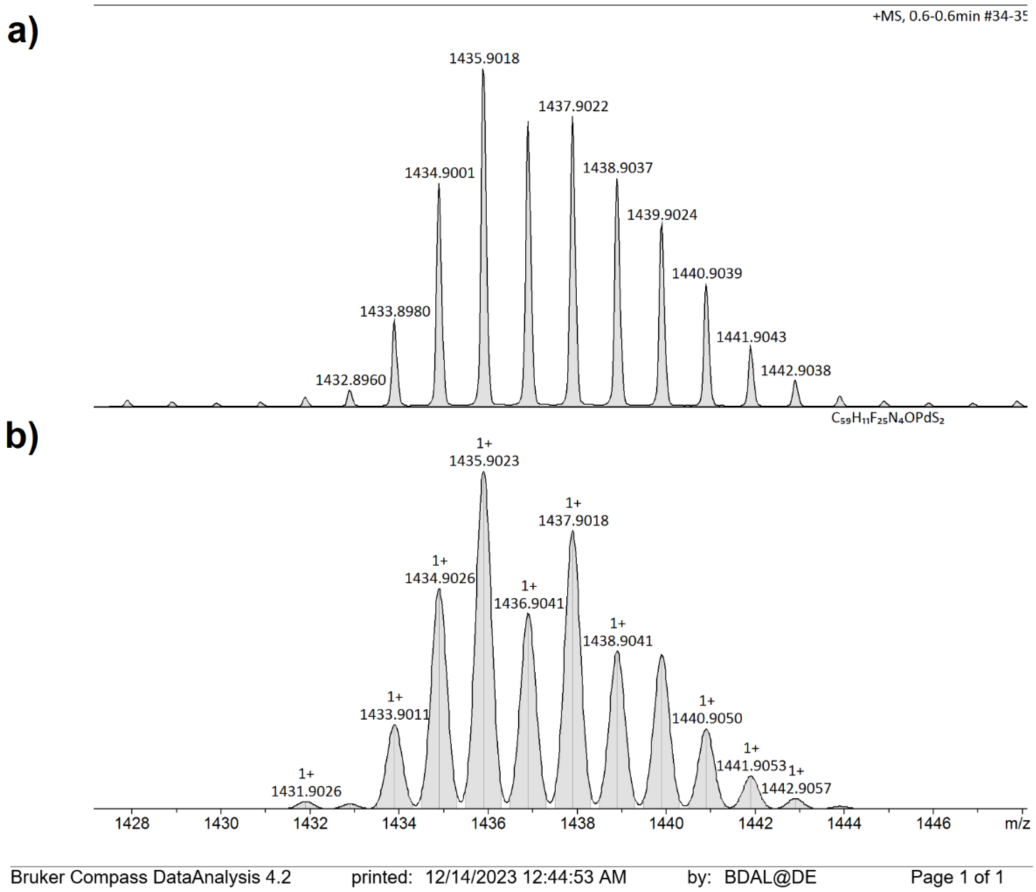


Figure S3. a) Experimental HR-ESI-MS and b) simulated HRMS of **2**.

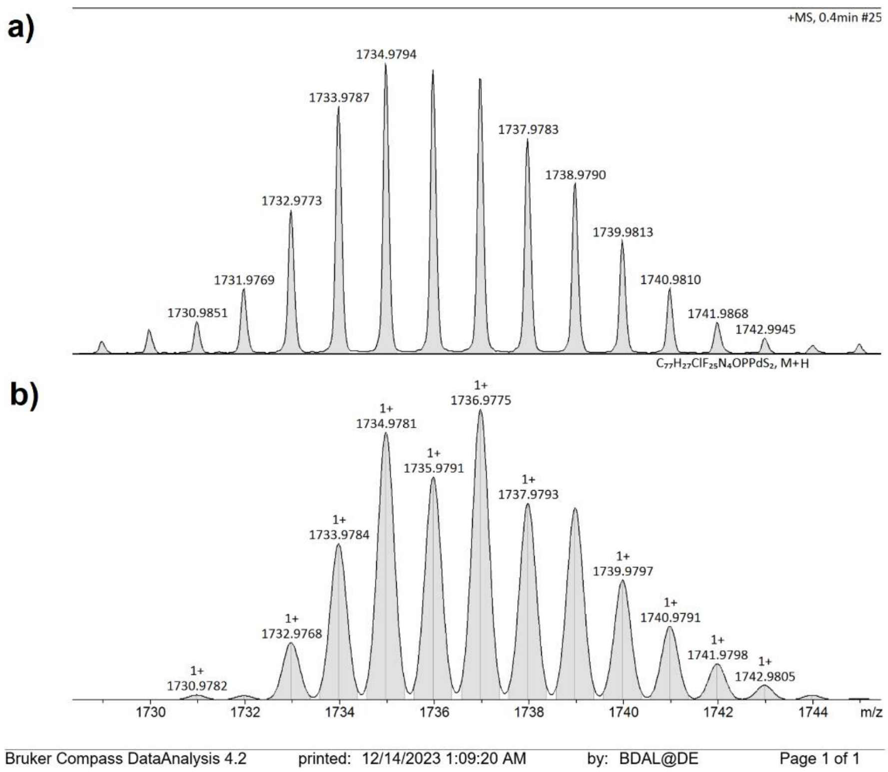


Figure S4. a) Experimental HR-ESI-MS and b) simulated HRMS of **3**.

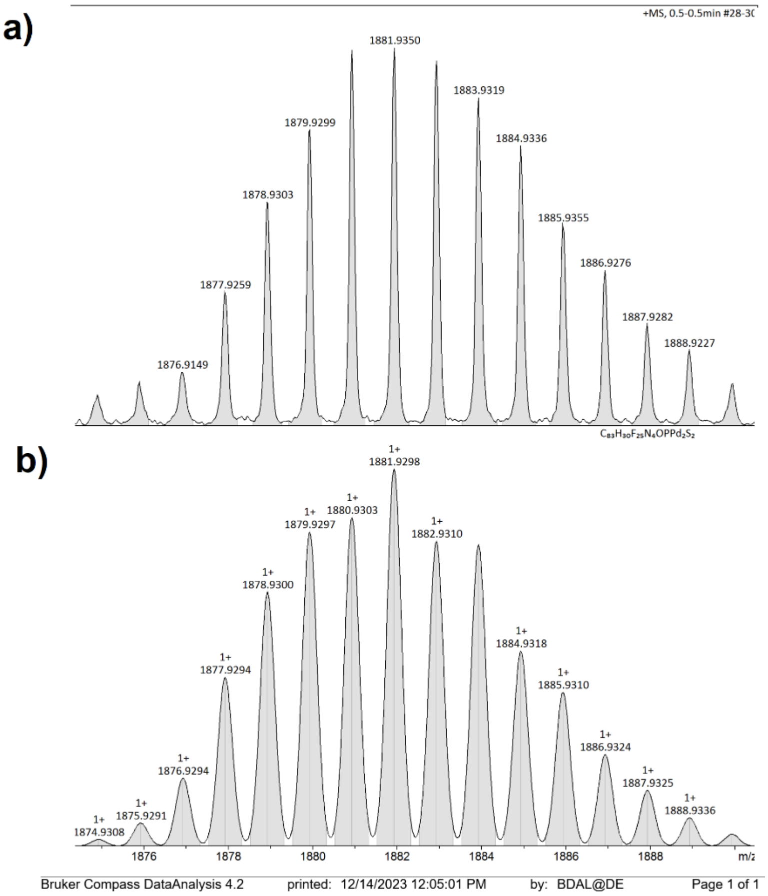


Figure S5. a) Experimental HR-ESI-MS and b) simulated HRMS of **4-Ph**.

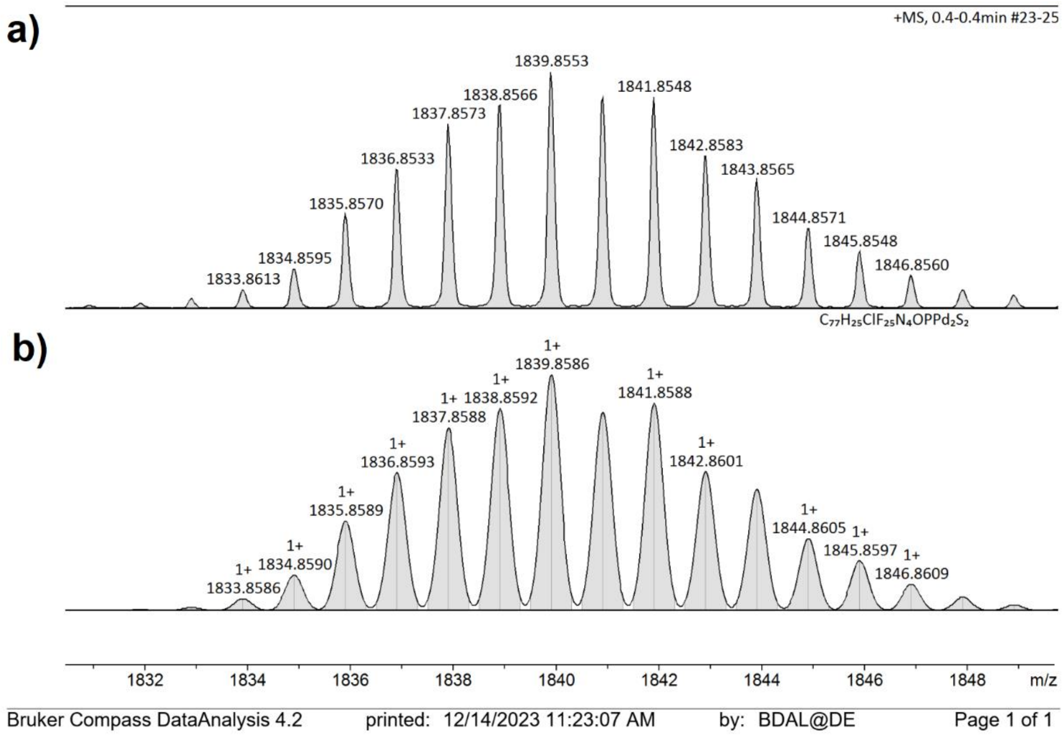


Figure S6. a) Experimental HR-ESI-MS and b) simulated HRMS of **4-Cl**.

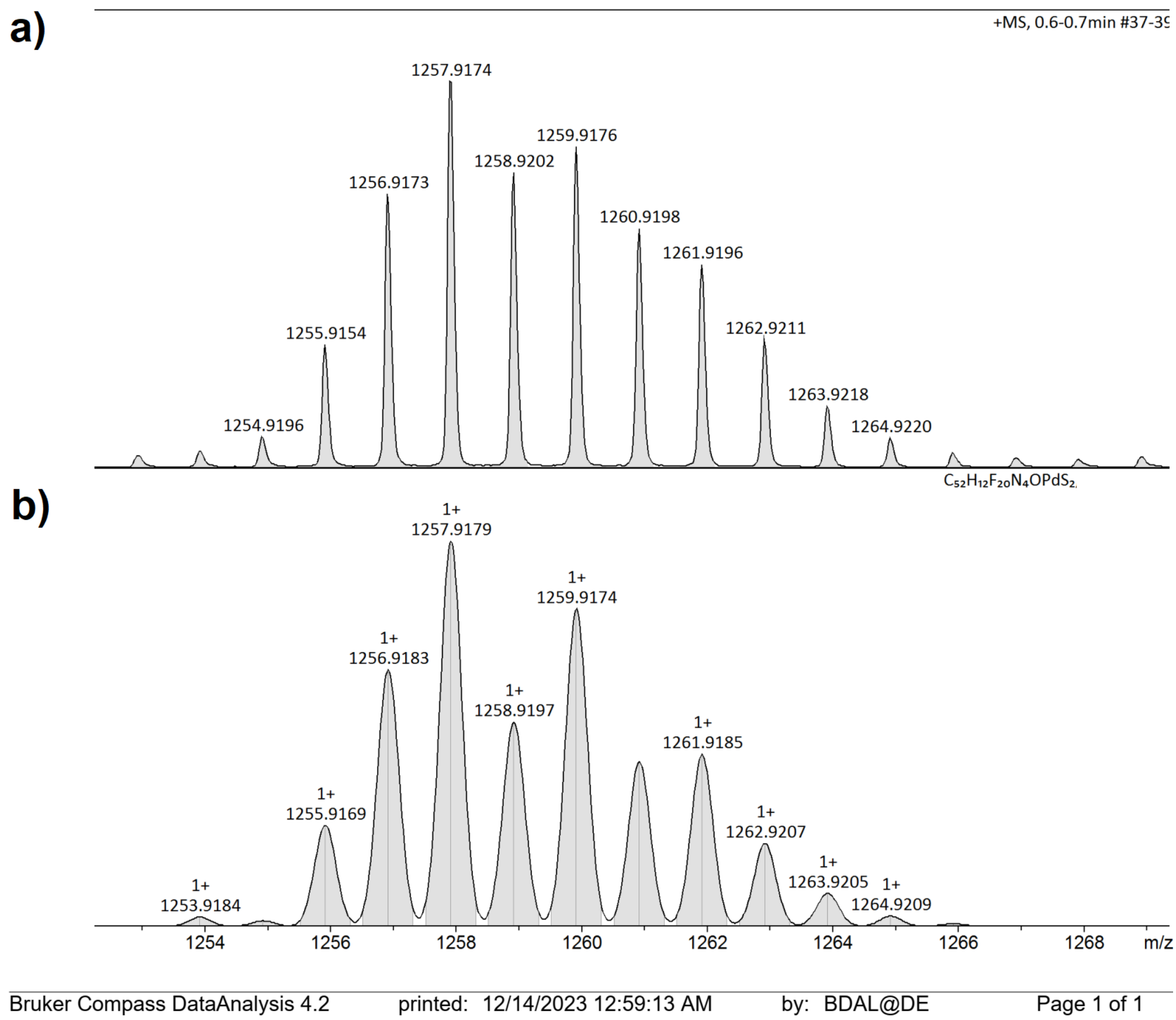


Figure S7. a) Experimental HR-ESI-MS and b) simulated HRMS of **5**.

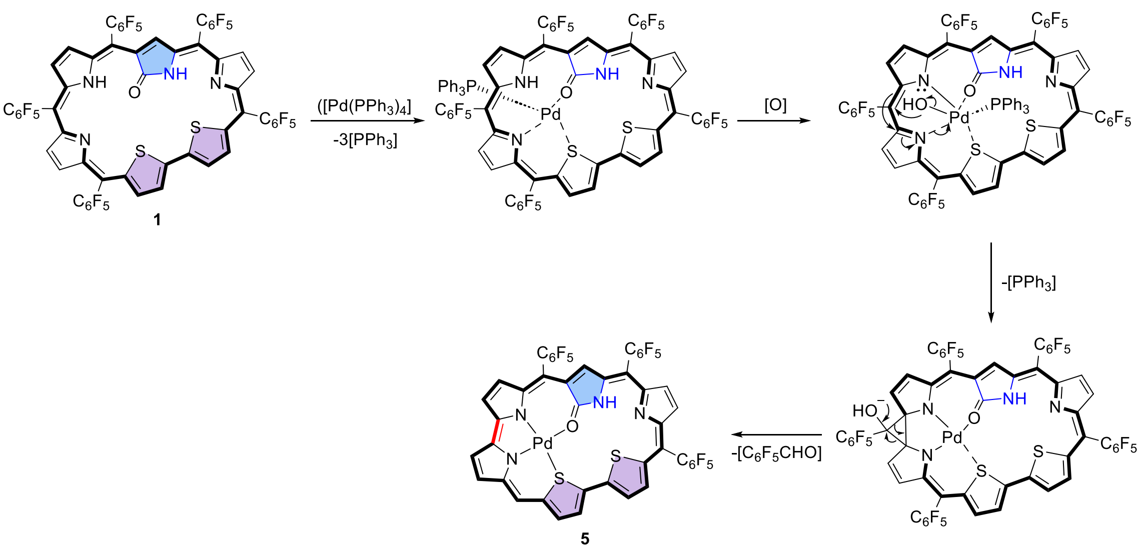


Figure S8. The plausible mechanism for generating **5** from **1**.

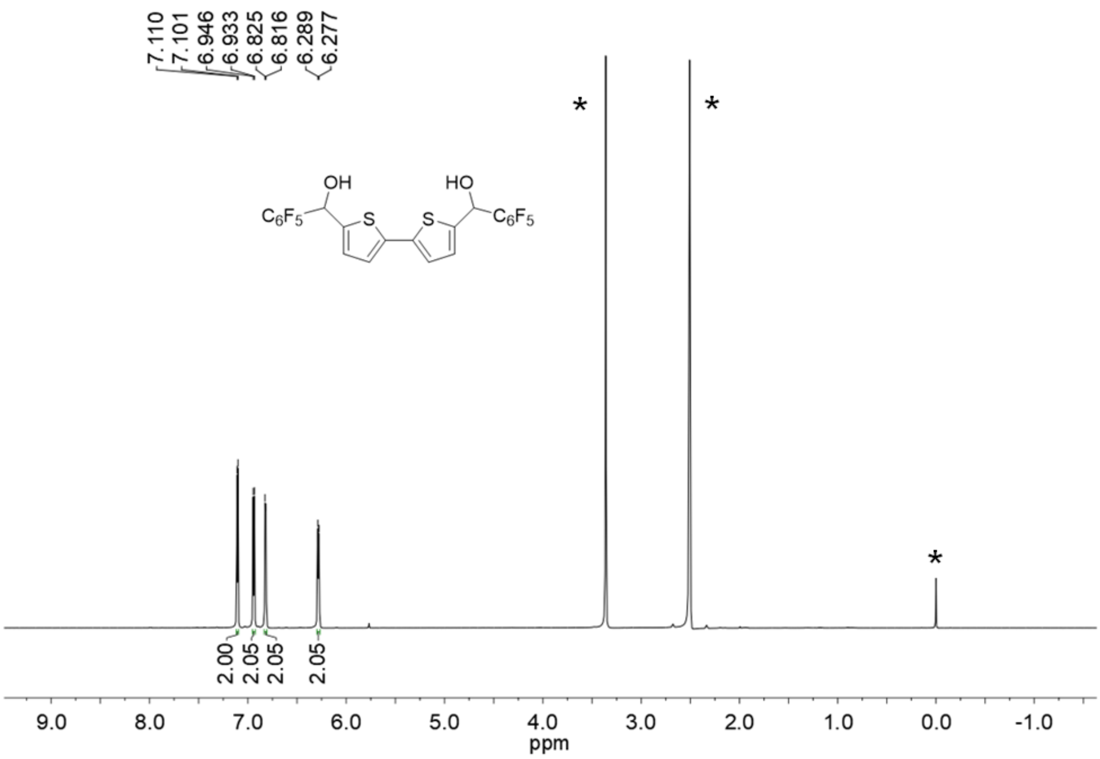


Figure S9. ^{1}H NMR (400 MHz) spectrum of **a** in DMSO-d_6.

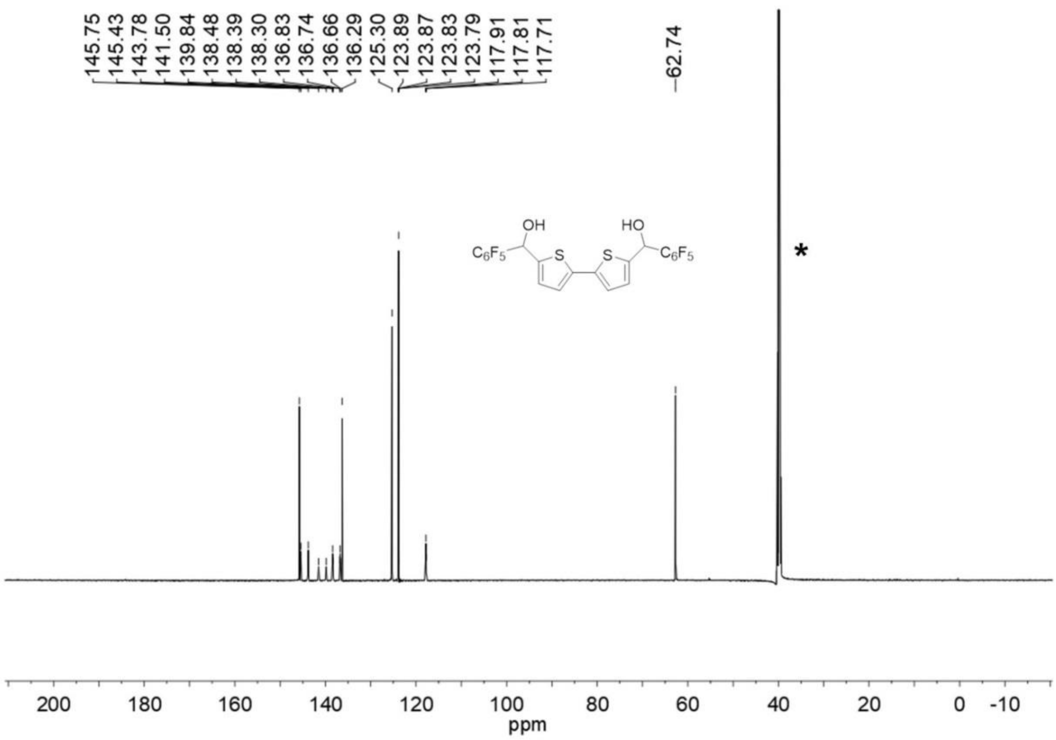


Figure S10. ^{13}C NMR (151 MHz) spectrum of **a** in DMSO-d_6.

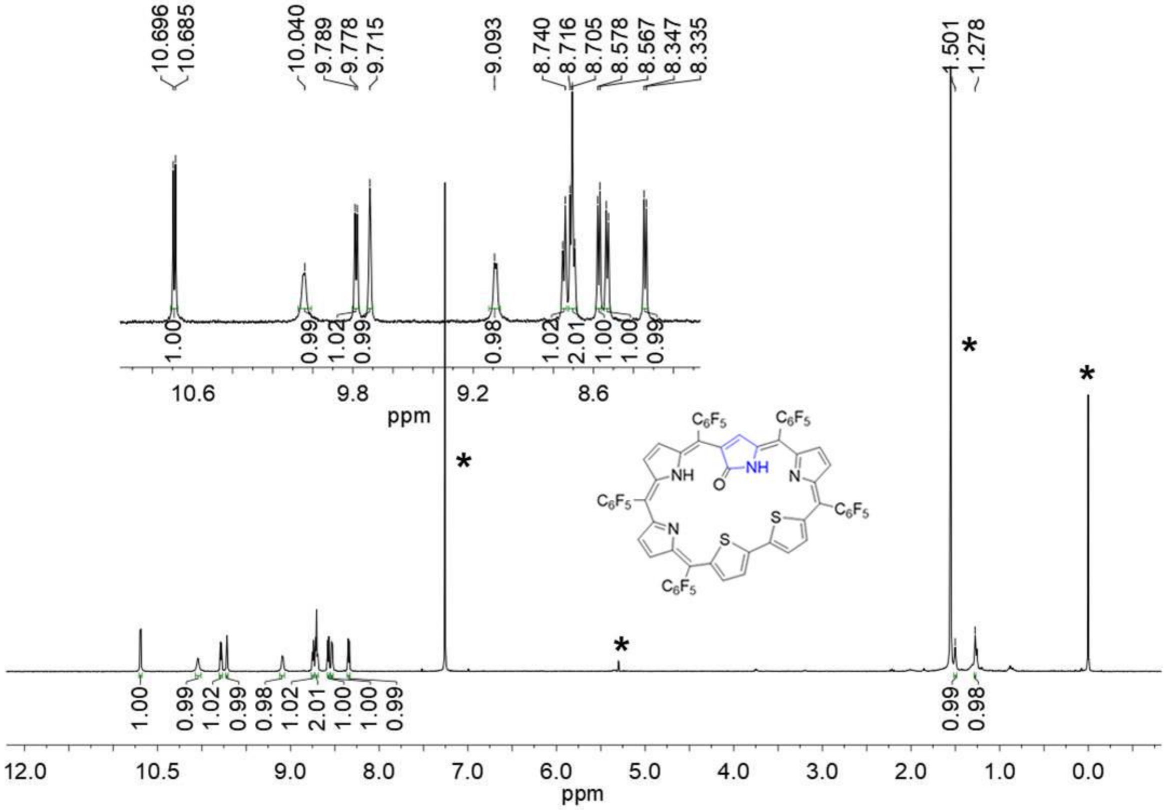


Figure S11. ^{1}H NMR (400 MHz) spectrum of **1** in $CDCl_3$.

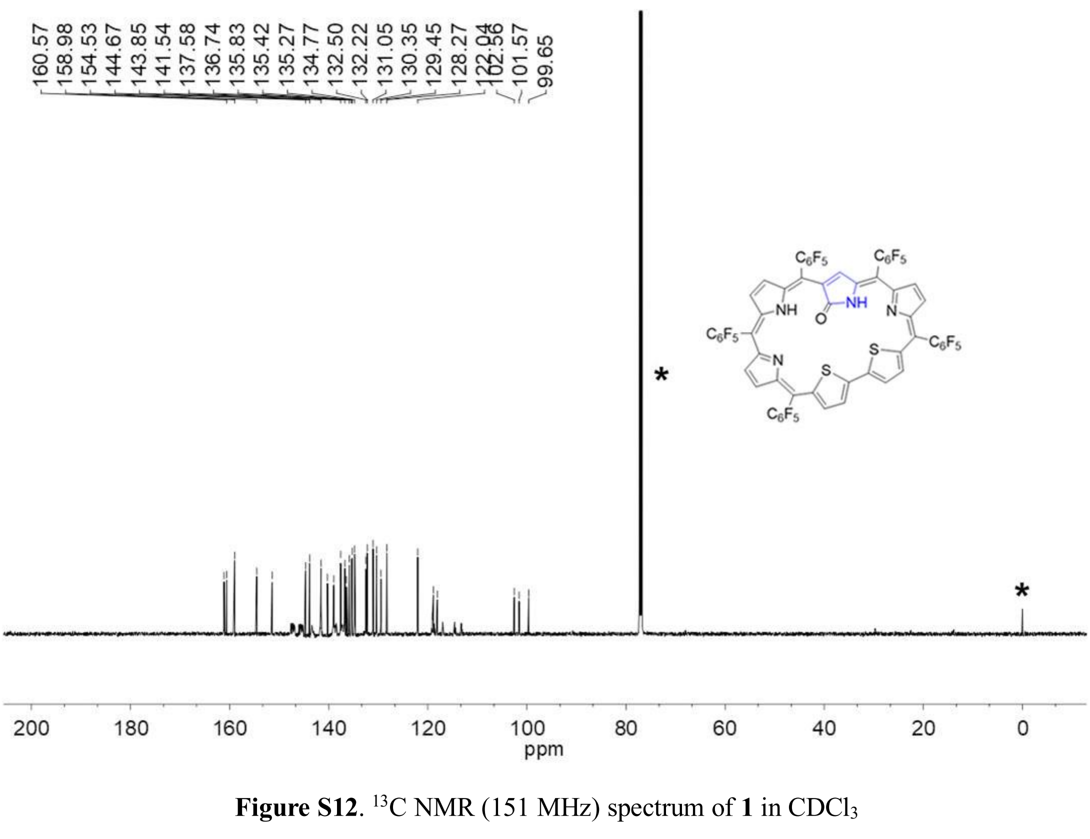


Figure S12. ^{13}C NMR (151 MHz) spectrum of **1** in $CDCl_3$

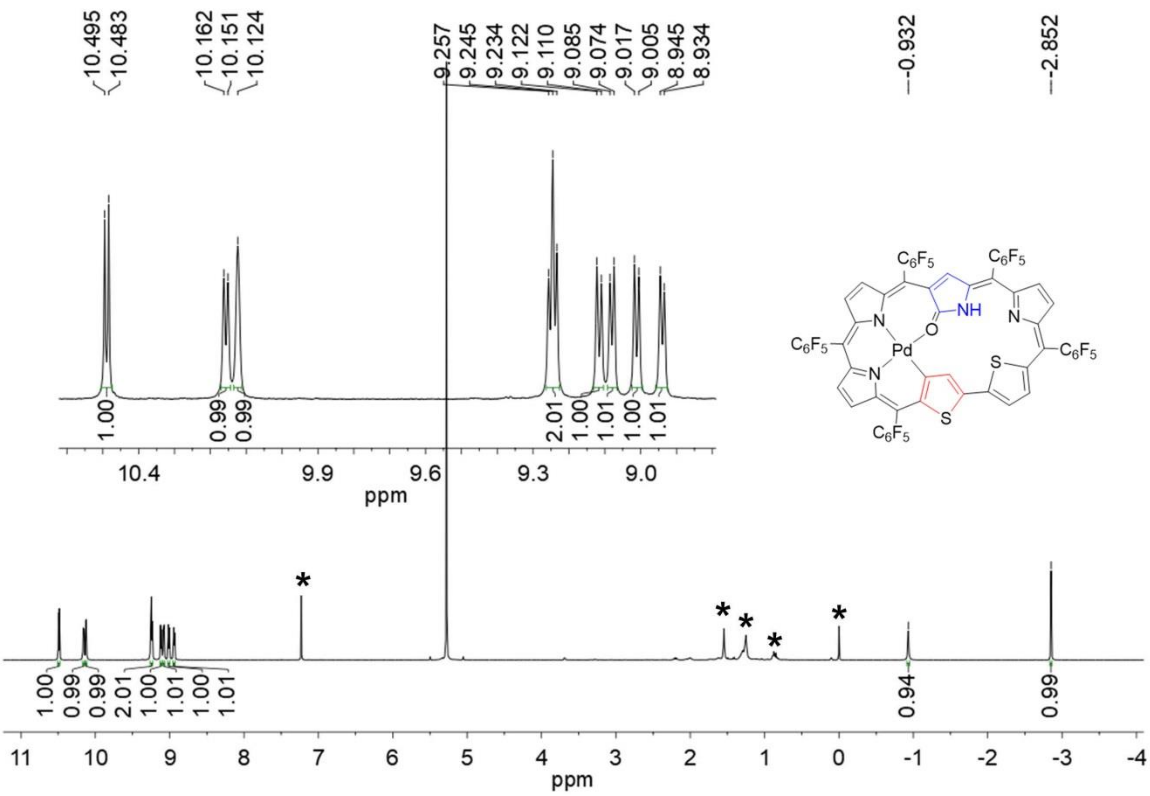


Figure S13. ^{1}H NMR (400 MHz) spectrum of **2** in $CDCl_3$.

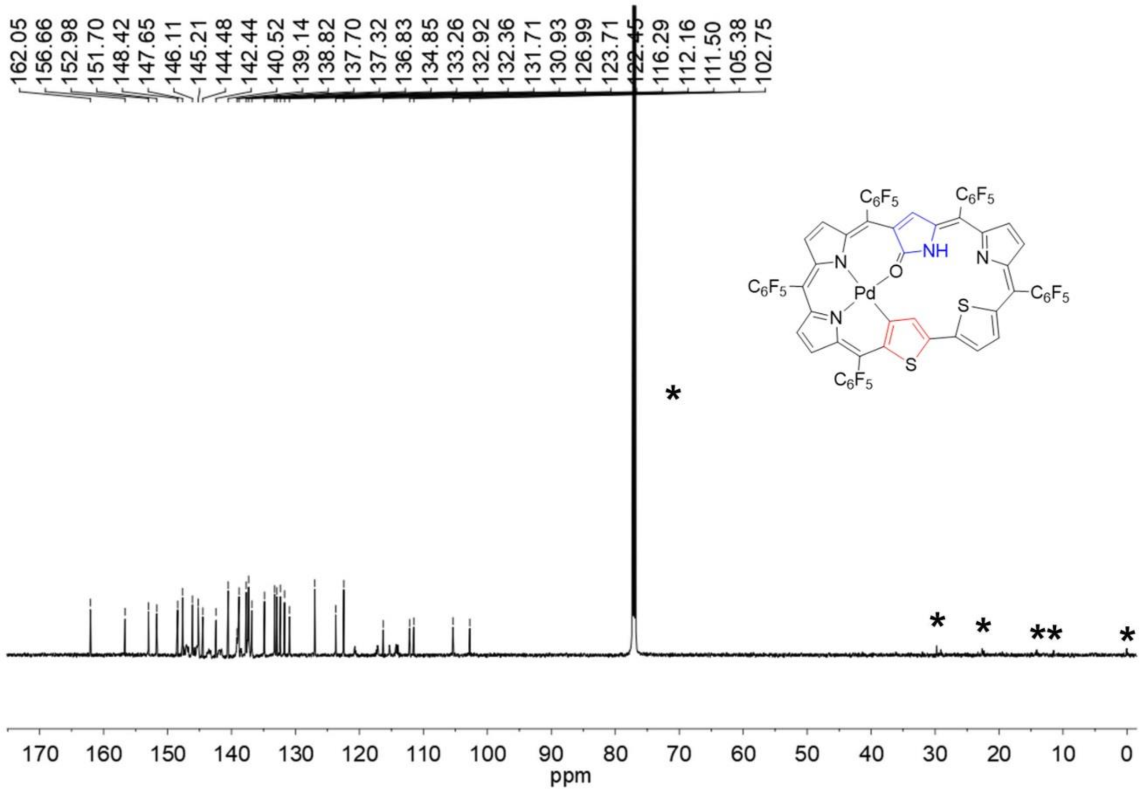


Figure S14. ^{13}C NMR (151 MHz) spectrum of **2** in $CDCl_3$.

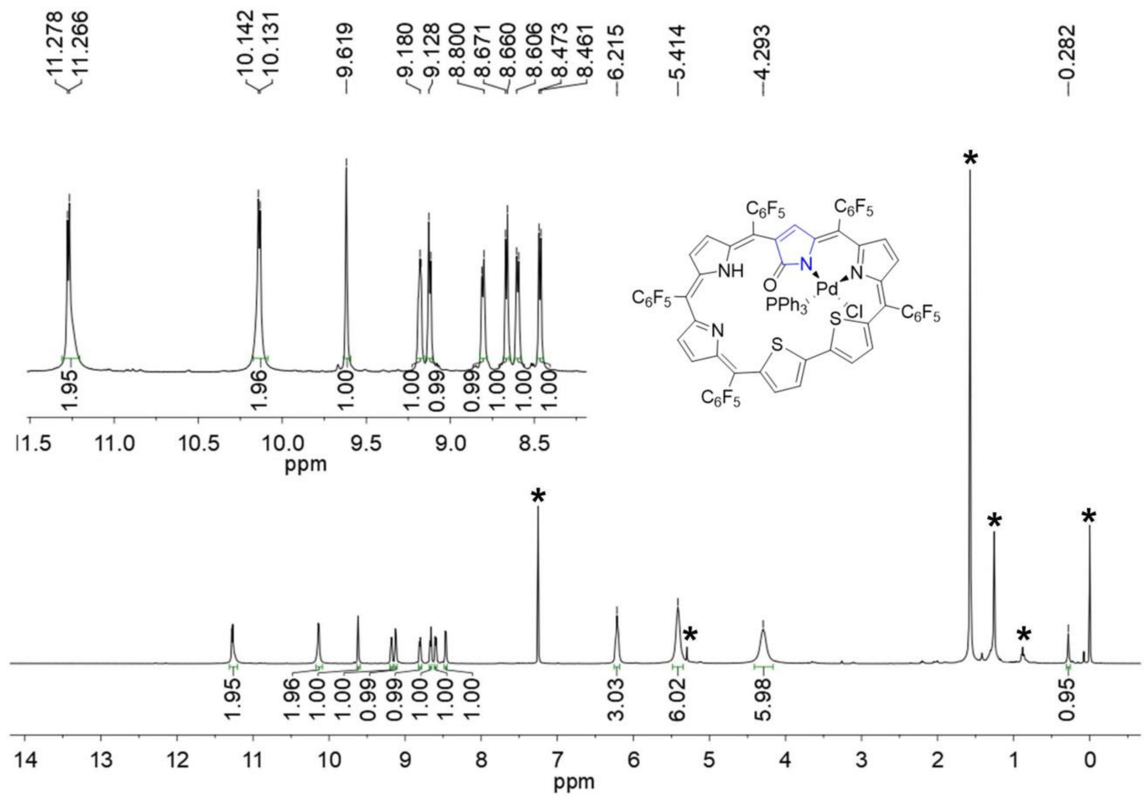


Figure S15. ^{1}H NMR (400 MHz) spectrum of **3** in $CDCl_3$.

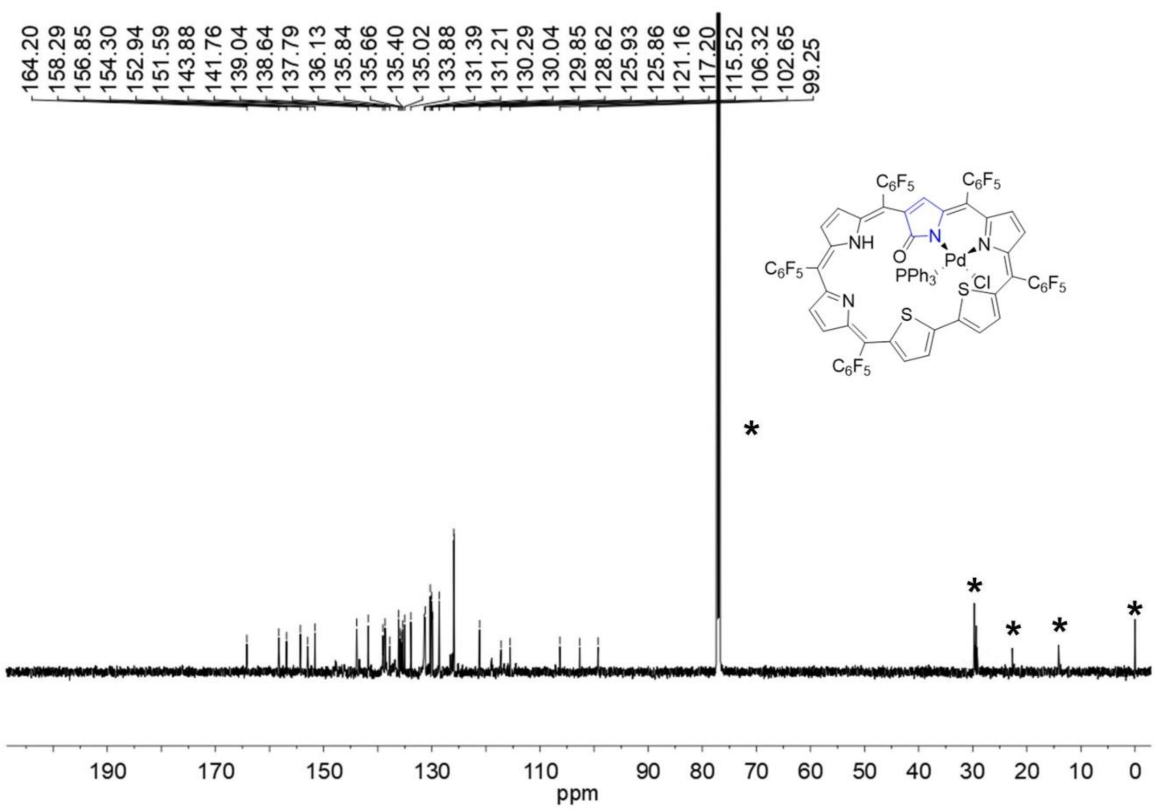


Figure S16. ^{13}C NMR (151 MHz) spectrum of **3** in $CDCl_3$.

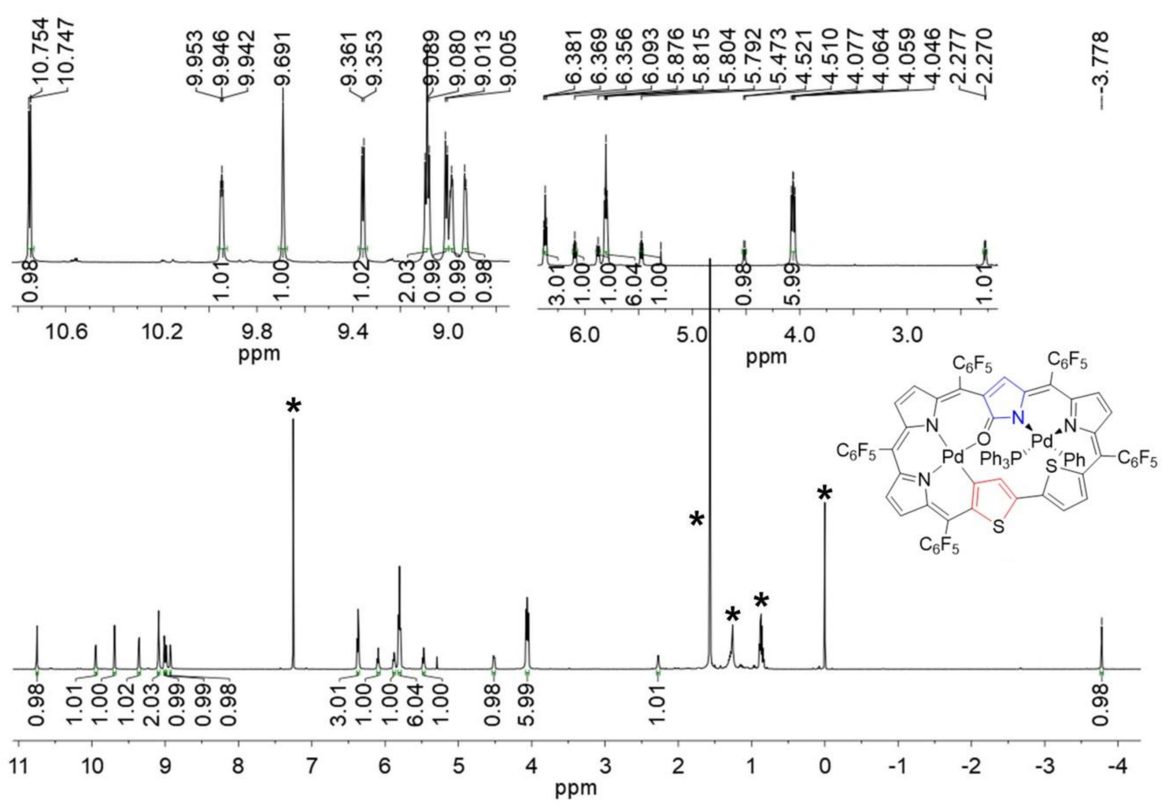


Figure S17. ^{1}H NMR (600 MHz) spectrum of **4-Ph** in $CDCl_3$.

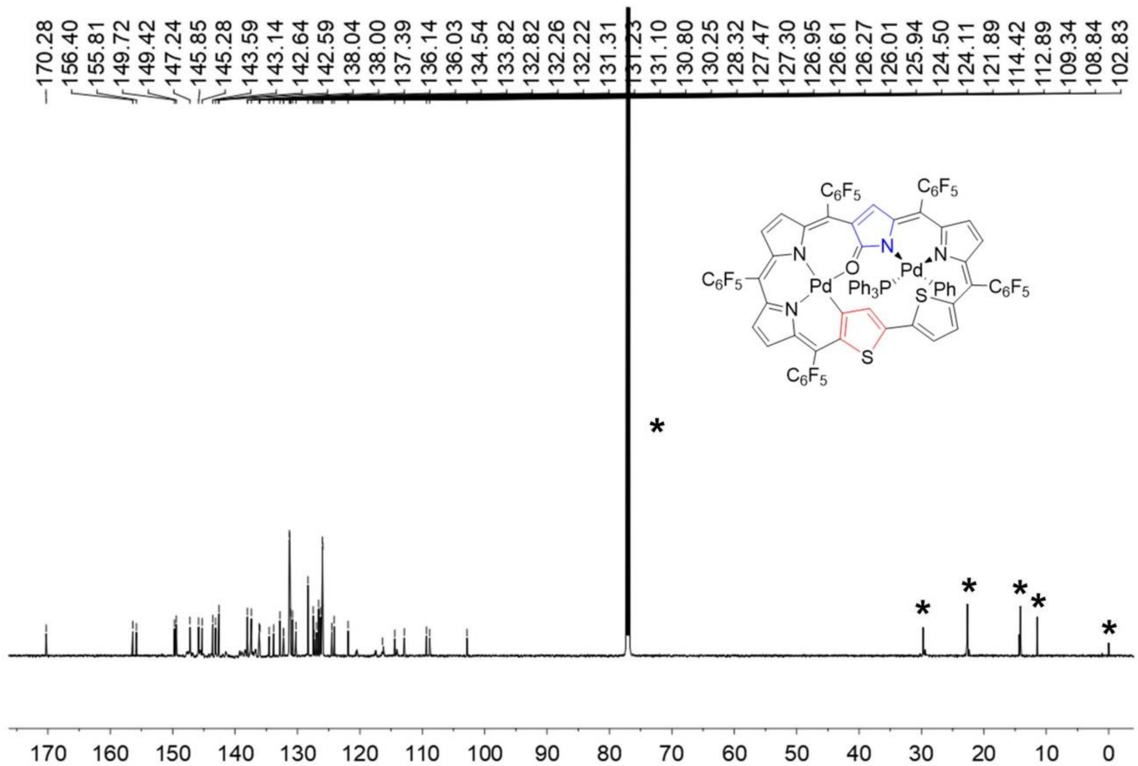


Figure S18. ^{13}C NMR (151 MHz) spectrum of **4-Ph** in $CDCl_3$.

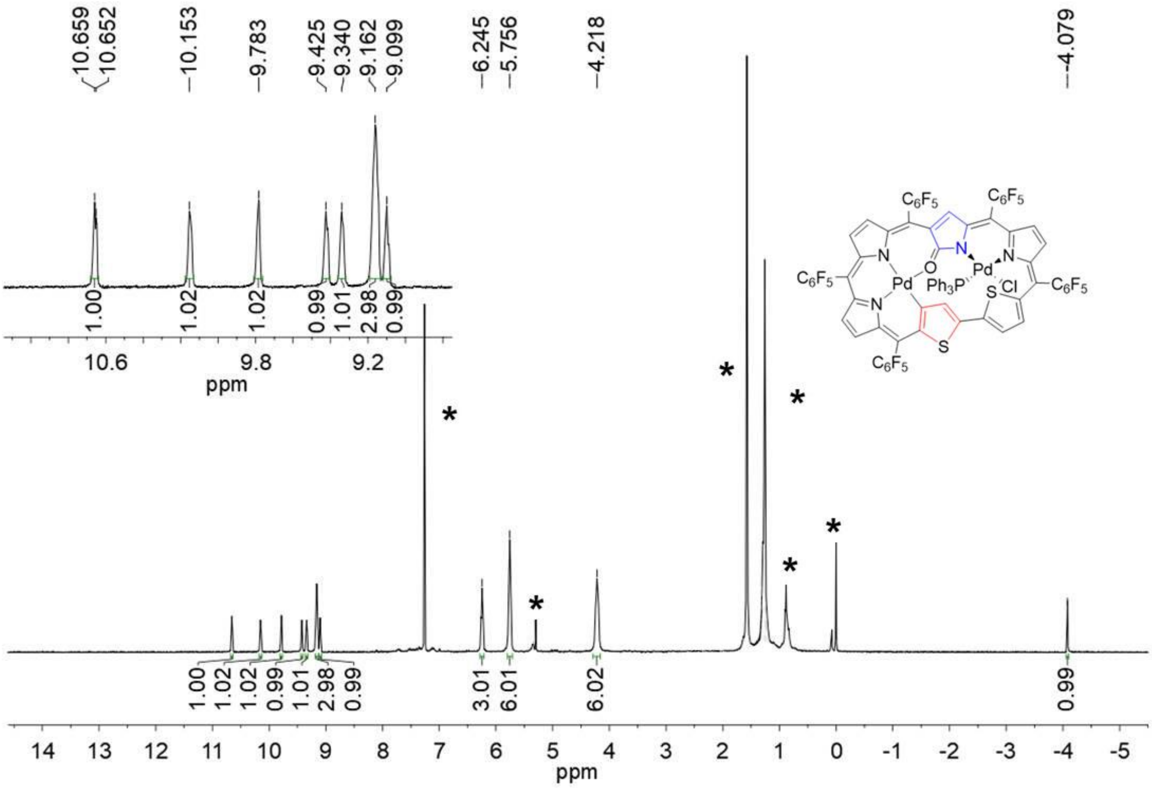


Figure S19. ^{1}H NMR (400 MHz) spectrum of **4-Cl** in $CDCl_3$.

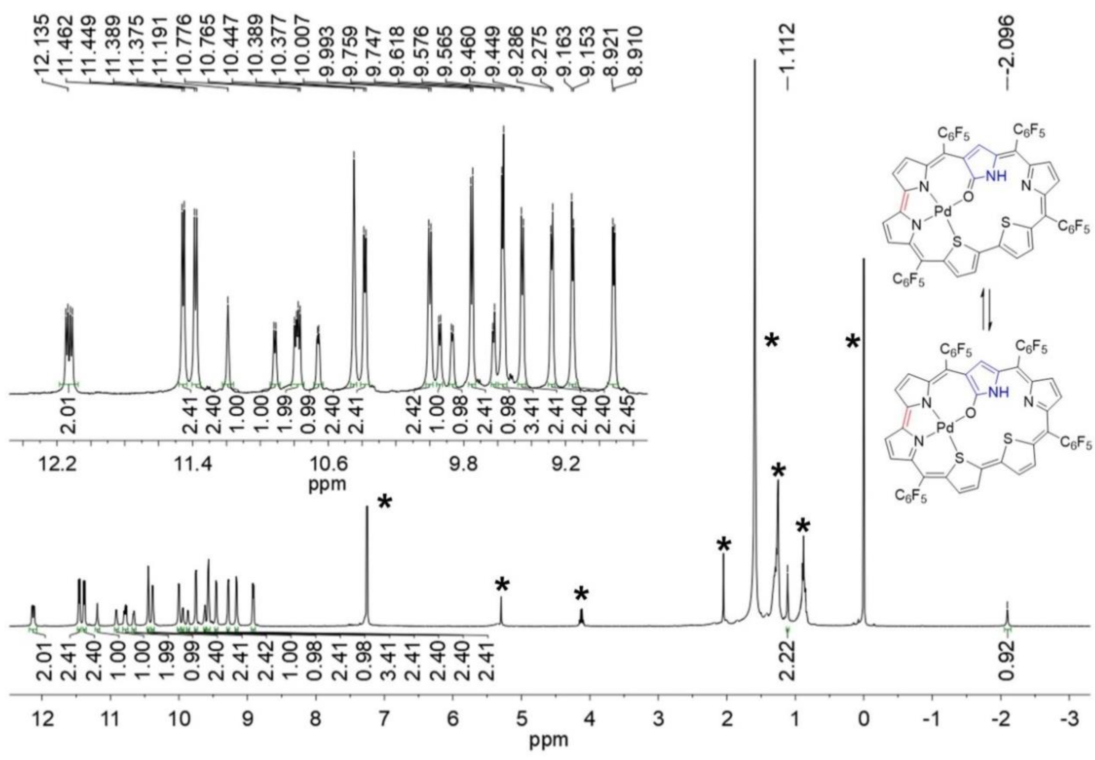


Figure S20. ^{1}H NMR (400 MHz) spectrum of **5** in $CDCl_3$. Two sets of peaks are observed with the molar ratio of 1:2.4, indicating the coexistence of two isomers.

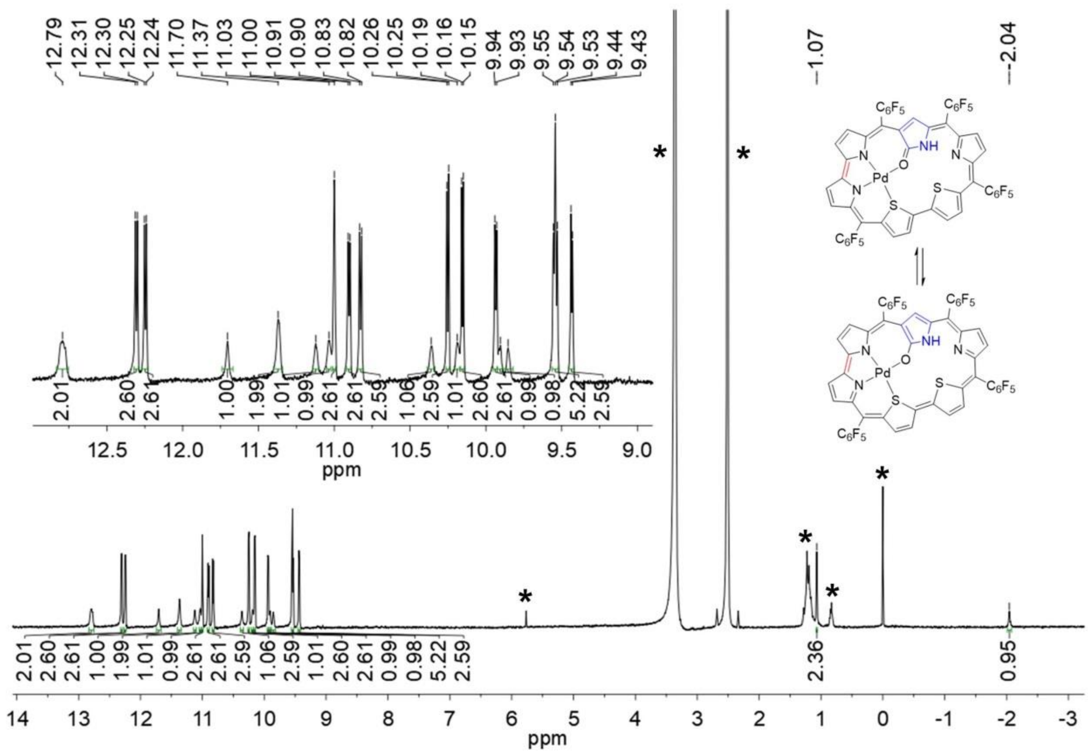


Figure S21. ^{1}H NMR (400 MHz) spectrum of **5** in DMSO-d_6. Two sets of peaks are observed with the molar ratio of 1:2.6, indicating the coexistence of two isomers.

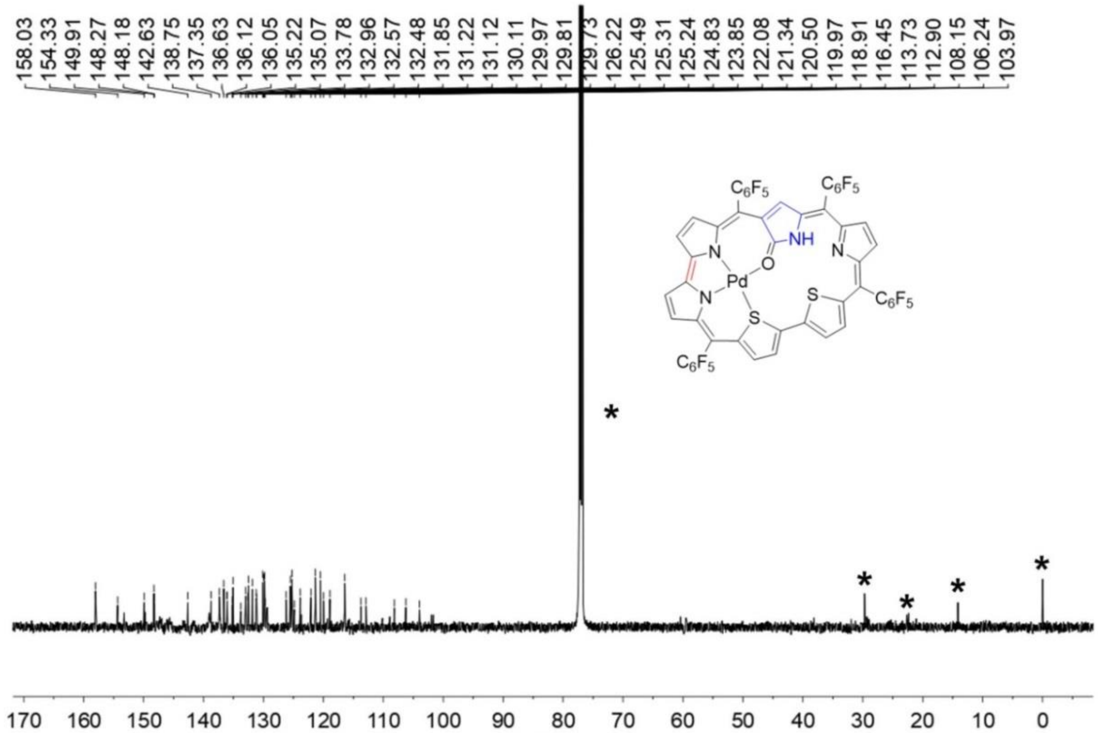


Figure S22. ^{13}C NMR (151 MHz) spectrum of **5** in $CDCl_3$.

Table S1. Crystal data and structure refinements of **1**, **2**, **3**, **4-Ph** and **5**.

Compounds	**1**	**2**	**3**	**4-Ph**	**5**
Formula	$C_{59}H_{13}F_{25}N_4OS_2$	$C_{59}H_{11}F_{25}N_4OPdS_2$	$C_{77}H_{27}ClF_{25}N_4OPPdS_2$	$C_{87}H_{36}F_{25}N_6OPPd_2S_2$	$C_{52}H_{12}F_{20}N_4OPdS_2$
Formula weight (g/mol)	1332.85	1437.24	1735.96	1964.11	1259.18
Crystal system	triclinic	triclinic	triclinic	triclinic	triclinic
Temperature (K)	213(2)	213(2)	213(2)	213(2)	213(2)
Crystal size (mm^3)	0.18 × 0.14 × 0.07	0.12 × 0.1 × 0.06	0.16 × 0.13 × 0.11	0.19 × 0.16 × 0.12	0.19 × 0.16 × 0.12
Theta range for data collection (°)	2.10 to 25.00	1.86 to 25.00	2.49 to 27.52	1.89 to 26.00	2.05 to 26.00
Space group	*P-1*	*P-1*	*P-1*	*P-1*	*P-1*
a (Å)	9.774(10)	12.633(2)	16.915(6)	14.976(2)	17.633(3)
b (Å)	14.769(14)	16.870(3)	17.3251(16)	16.782(2)	18.145(3)
c (Å)	18.881(19)	18.510(3)	19.0029(17)	16.991(2)	19.027(3)
α (°)	95.08(3)	113.418(4)	70.416(9)	106.814(4)	104.695(4)
β (°)	95.96(4)	96.893(4)	65.162(8)	90.699(5)	103.672(5)
γ (°)	92.17(3)	108.505(4)	76.985(9)	107.905(4)	112.112(4)
Volume (Å^3)	2697(5)	3292.4(10)	4738.3(7)	3866.0(9)	5067.6(14)
Z	2	2	2	2	4
ρ_{calc} (g/cm^3)	1.641	1.450	1.217	1.687	1.650
F (000)	1320	1408	1720	1944	2472
μ (mm^{-1})	0.233	0.456	0.372	0.655	0.566
Index ranges	$-11 \leq h \leq 11$, $-17 \leq k \leq 17$, $-22 \leq l \leq 22$	$-15 \leq h \leq 15$, $-20 \leq k \leq 20$, $-22 \leq l \leq 21$	$-21 \leq h \leq 21$, $-22 \leq k \leq 22$, $-24 \leq l \leq 24$	$0 \leq h \leq 19$, $21 \leq k \leq 21$, $-22 \leq l \leq 22$	$-21 \leq h \leq 21$, $-22 \leq k \leq 22$, $-23 \leq l \leq 23$
R_1 [I>2σ(I)]	0.1215	0.0708	0.0471	0.0650	0.0685
wR_2 (all data)	0.3407	0.2058	0.1539	0.1725	0.2321
GOF	1.086	0.977	1.028	1.043	1.031
CCDC number	2277039	2277040	2277041	2277042	2277043

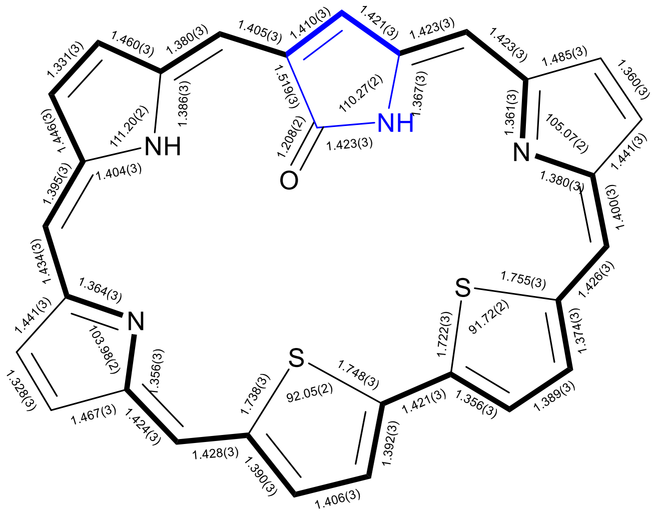


Figure S23. Selected bond lengths (Å) in the crystal structure of **1** (the HOMA value was calculated to be 0.60).

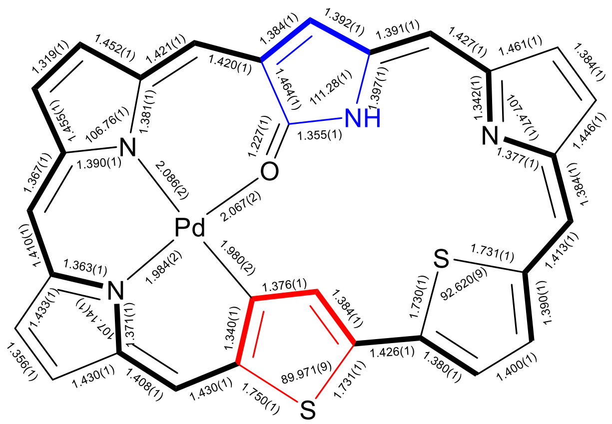


Figure S24. Selected bond lengths (Å) in the crystal structure of **2** (the HOMA value was calculated to be 0.62).

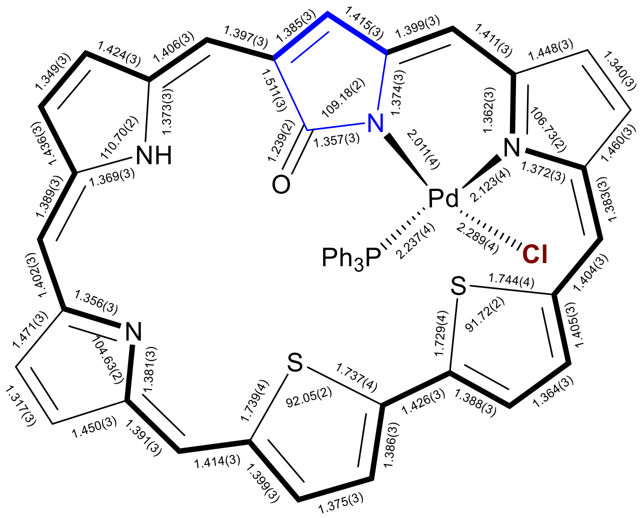


Figure S25. Selected bond lengths (Å) in the crystal structure of **3** (the HOMA value was calculated to be 0.77).

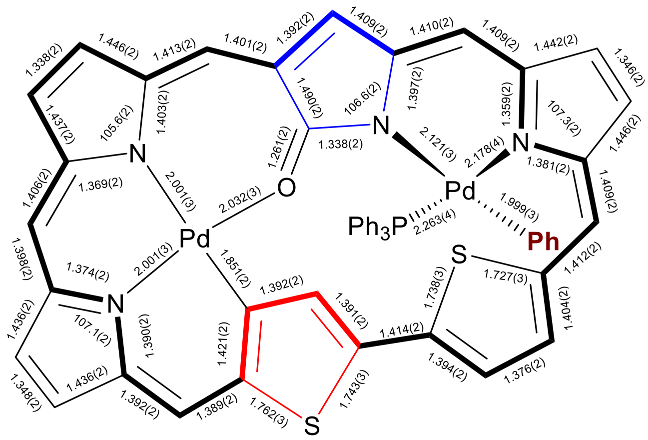


Figure S26. Selected bond lengths (Å) in the crystal structure of **4-Ph** (the HOMA value was calculated to be 0.65).

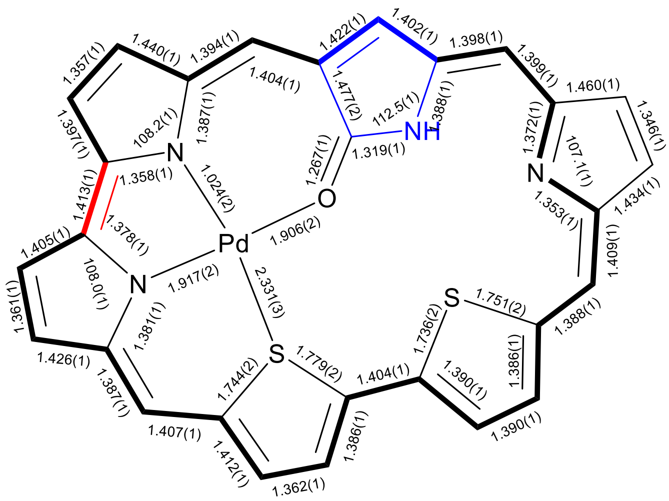


Figure S27. Selected bond lengths (Å) in the crystal structure of **5** (the HOMA value was calculated to be 0.84).

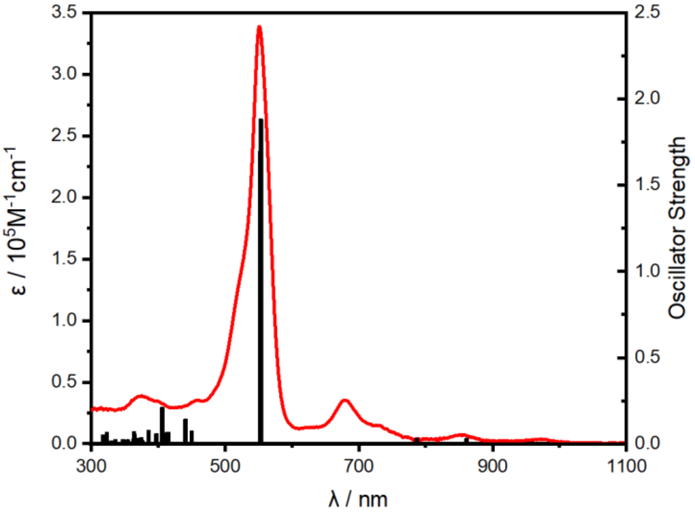


Figure S28. TD-DFT-computed vertical energies of **1** along with the experimental spectrum.

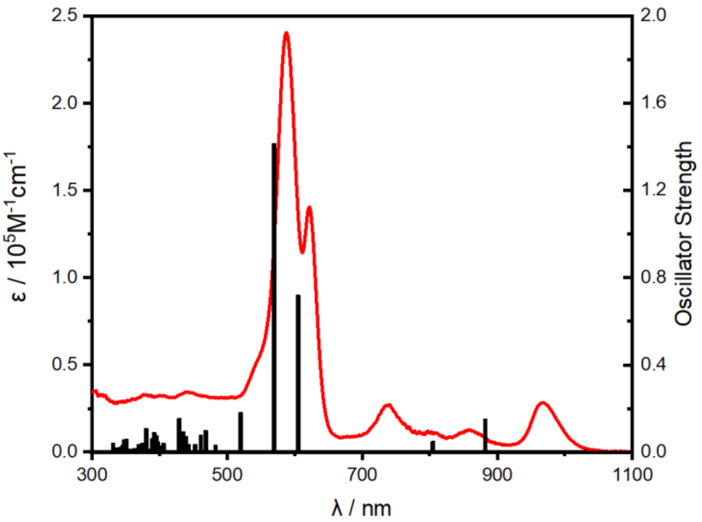


Figure S29. TD-DFT-computed vertical energies of **2** along with the experimental spectrum.

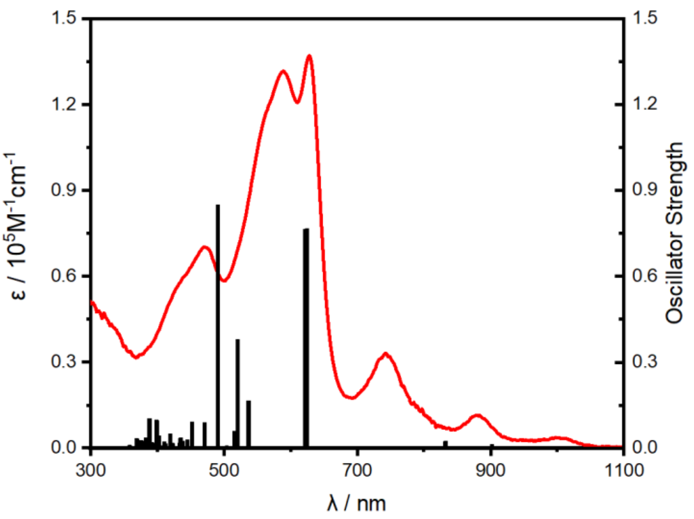


Figure S30. TD-DFT-computed vertical energies of **3** along with the experimental spectrum.

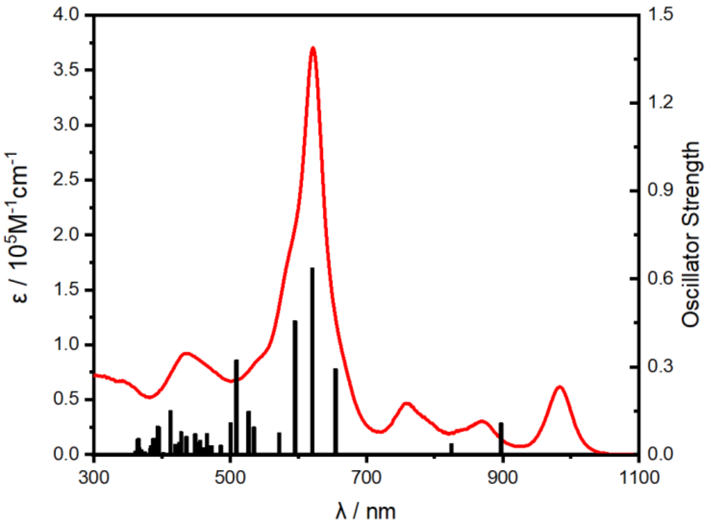


Figure S31. TD-DFT-computed vertical energies of **4-Ph** along with the experimental spectrum.

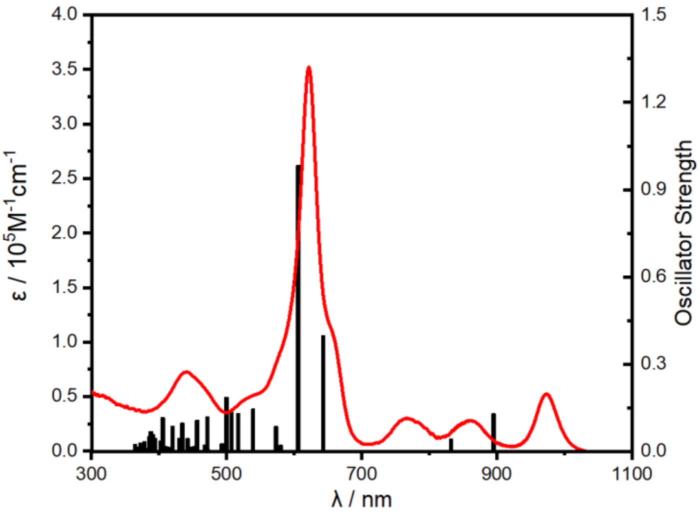


Figure S32. TD-DFT-computed vertical energies of **4-Cl** along with the experimental spectrum.

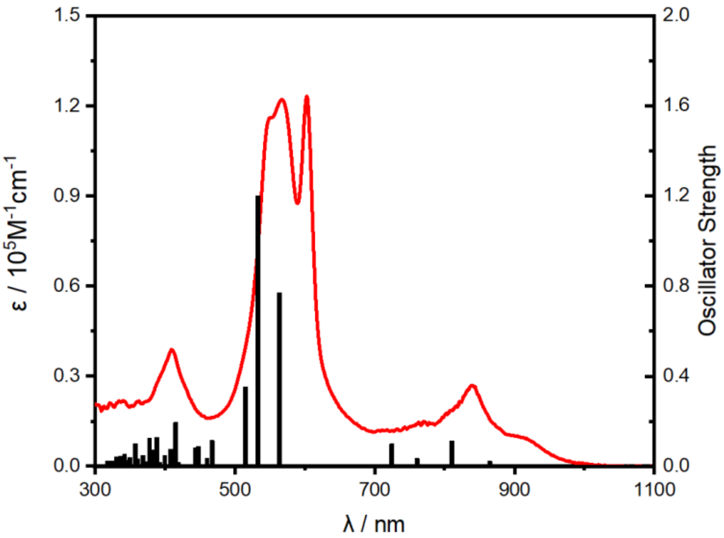


Figure S33. TD-DFT-computed vertical energies of **5** along with the experimental spectrum.

Table S2. Selected computed excitation energies, oscillator strengths and molecular orbital compositions for low-lying excited states of **1**.

Excited State	Wavelength	Oscillator strength	MO compositions
S1	872.6	0.0005	H→L+1 (62%), H-1→L (36%)
S2	652.5	0.6137	H-1→L+1(60%), H-2→L (21%)
S3	612.1	0.8754	H-1→L (51%), H→L+1(34%)
S4	506.1	0.6844	H-2→L (56%), H-3→L (11%)
S5	494.6	0.4432	H-2→L+1(53%), H-3→L+1(30%)
S6	489.1	0.2104	H-3→L (76%), H-2→L (9%)
S7	482.5	0.1869	H-3→L+1(63%), H-2→L+1(18%)
S8	463.1	0.4612	H→L+2(77%), H-2→L (6%)
S9	435.8	0.3107	H-4→L (81%), H-4→L+1(9%)
S10	426.8	0.3765	H-1→L+2(43%), H-4→L+1(29%)

Table S3. Selected computed excitation energies, oscillator strengths and molecular orbital compositions for low-lying excited states of **2**.

Excited State	Wavelength	Oscillator strength	MO compositions
S1	883.1	0.1515	H→L (67%), H-1→L+1 (18%)
S2	805.6	0.0481	H→L+1 (42%), H-1→L (42%)
S3	605.9	0.7188	H-1→L (46%), H→L+1(45%)
S4	570.3	1.4149	H-1→L+1(68%), H→L (18%)
S5	521	0.1809	H-2→L (87%)
S6	483.7	0.0302	H-4→L (47%), H-3→L (25%)
S7	469.4	0.0990	H-2→L+1(55%), H-3→L (26%)
S8	462.3	0.0772	H-3→L (34%), H-5→L (17%)
S9	453.7	0.0359	H→L+2 (34%), H→L+3 (19%)
S10	444	0.0349	H-5→L (30%), H→L+3 (14%)

Table S4. Selected computed excitation energies, oscillator strengths and molecular orbital compositions for low-lying excited states of **3**.

Excited State	Wavelength	Oscillator strength	MO compositions
S1	902.7	0.0111	H→L (36%), H→L+1(22%)
S2	833.4	0.0239	H→L+1(29%), H-1→L (26%)
S3	625.6	0.7662	H-1→L (42%), H→L+1(38%)
S4	623.1	0.7646	H-1→L+1(49%), H→L (31%)
S5	537.8	0.1645	H →L+2(42%), H-1→L+2(37%)
S6	521.6	0.3791	H-2→L(58%), H →L+2(10%)
S7	516.4	0.0569	H-1→L+2(36%), H →L+2(31%)
S8	505	0.0065	H-3→L (77%), H-3→L+1(5%)
S9	491.7	0.8481	H-2→L+1(61%), H-1→L+2(6%)
S10	472.2	0.0870	H-3→L+1(87%), H-3→L (5%)

Table S5. Selected computed excitation energies, oscillator strengths and molecular orbital compositions for low-lying excited states of **4-Ph**.

Excited State	Wavelength	Oscillator strength	MO compositions
S1	898.4	0.0818	H→L (68%), H-1→L+1(22%)
S2	812.5	0.0190	H-1→L (46%), H→L+1(43%)
S3	644.8	0.2845	H-1→L+1(33%), H-2→L (22%)
S4	618.7	0.5489	H-2→L (26%), H-1→L+1(26%)
S5	596.9	0.4859	H-2→L (36%), H→L+1(22%)
S6	568.6	0.1064	H-3→L (65%), H-2→L (13%)
S7	537.2	0.1817	H-2→L+1(64%), H-3→L+1(16%)
S8	527.9	0.0184	H-4→L (74%), H-3→L+1(11%)
S9	509.5	0.3951	H-3→L+1(56%), H-2→L+1(14%)
S10	500.7	0.1104	H-5→L (48%), H-7→L (15%)

Table S6. Selected computed excitation energies, oscillator strengths and molecular orbital compositions for low-lying excited states of **4-Cl**.

Excited State	Wavelength	Oscillator strength	MO compositions
S1	895.4	0.1294	H-1→L+1 (18%), H→L (64%)
S2	832.7	0.0429	H-1→L (40%), H→L+1 (42%)
S3	643.0	0.3980	H-1→L (34%), H→L+1 (32%)
S4	606.2	0.9834	H-1→L+1 (53%), H→L (14%)
S5	580.4	0.0220	H-2→L (35%), H→L+2 (58%)
S6	573.4	0.0851	H-2→L (48%), H→L+2 (37%)
S7	539.5	0.1453	H-1→L+2 (75%)
S8	517.2	0.1300	H-3→L (75%), H-2→L+1 (11%)
S9	507.8	0.1359	H-4→L (27%), H-2→L+1 (49%)
S10	500.0	0.1868	H-4→L (53%), H-2→L+1 (20%)

Table S7. Selected computed excitation energies, oscillator strengths and molecular orbital compositions for low-lying excited states of **5**.

Excited State	Wavelength	Oscillator strength	MO compositions
S1	832.8	0.0988	H→L (73%), H-1→L+1(21%)
S2	799.4	0.0410	H→L+1(62%), H-1→L (26%)
S3	741.4	0.0059	H→L+2 (76%), H-1→L (19%)
S4	673.9	0.1178	H-1→L+2 (68%), H-1→L (9%)
S5	566.4	0.6701	H-1→L+1 (56%), H→L (16%)
S6	554.5	1.0250	H-1→L (39%), H→L+1(21%)
S7	535	0.1413	H-2→L (39%), H-2→L+2 (25%)
S8	489.7	0.1794	H-2→L (54%), H-2→L+2 (26%)
S9	467	0.5857	H-2→L+1 (64%)
S10	459	0.0140	H→L+3 (27%), H-10→L+2 (15%)

Table S8. Contour plots of the frontier molecular orbitals for compounds **1**, **2**, **3**, **4-Ph**, **4-Cl** and **5**.

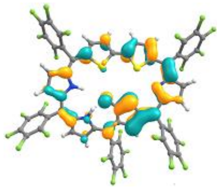
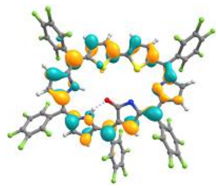
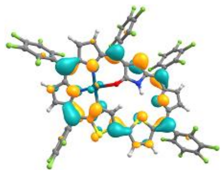
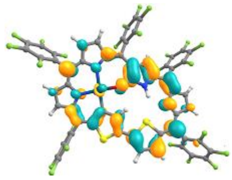
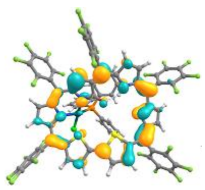
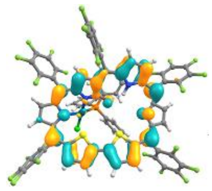
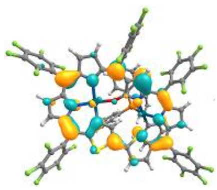
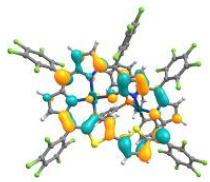
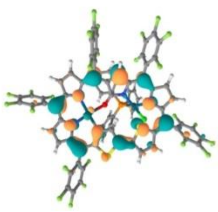
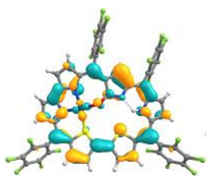
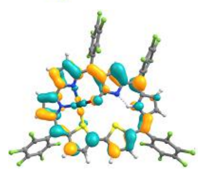
Compounds	HOMO	LUMO
1		
2		
3		
4-Ph		
4-Cl		
5		

Table S9. Calculated energy levels of the frontier molecular orbitals of compounds **1**, **2**, **3**, **4-Ph**, **4-Cl** and **5**.

Compounds	E_{HOMO} (eV)	E_{LUMO}(eV)	H-L gap(eV)
1	–5.28	–3.36	1.92
2	–5.26	–3.52	1.74
3	–5.20	–3.36	1.84
4-Ph	–5.11	–3.34	1.77
4-Cl	–5.18	–3.43	1.75
5	–4.92	–3.10	1.82

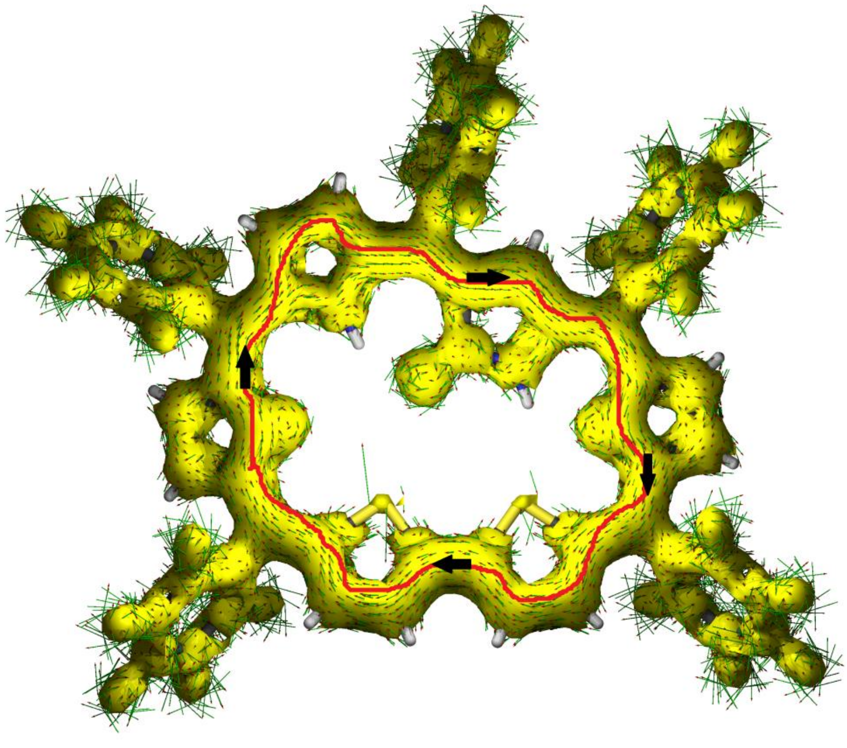


Figure S34. ACID plots of **1**. Direction of the applied magnetic field is perpendicular to the paper and pointing outward. The current density vectors indicate clockwise current.

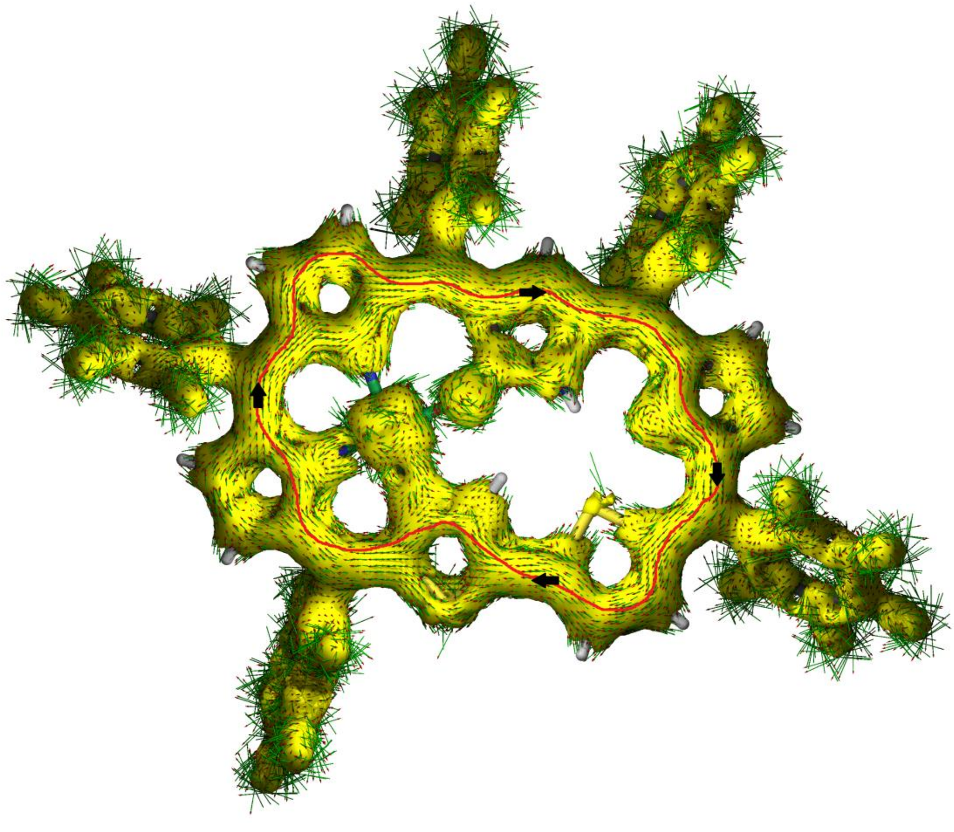


Figure S35. ACID plots of **2**. Direction of the applied magnetic field is perpendicular to the paper and pointing outward. The current density vectors indicate clockwise current.

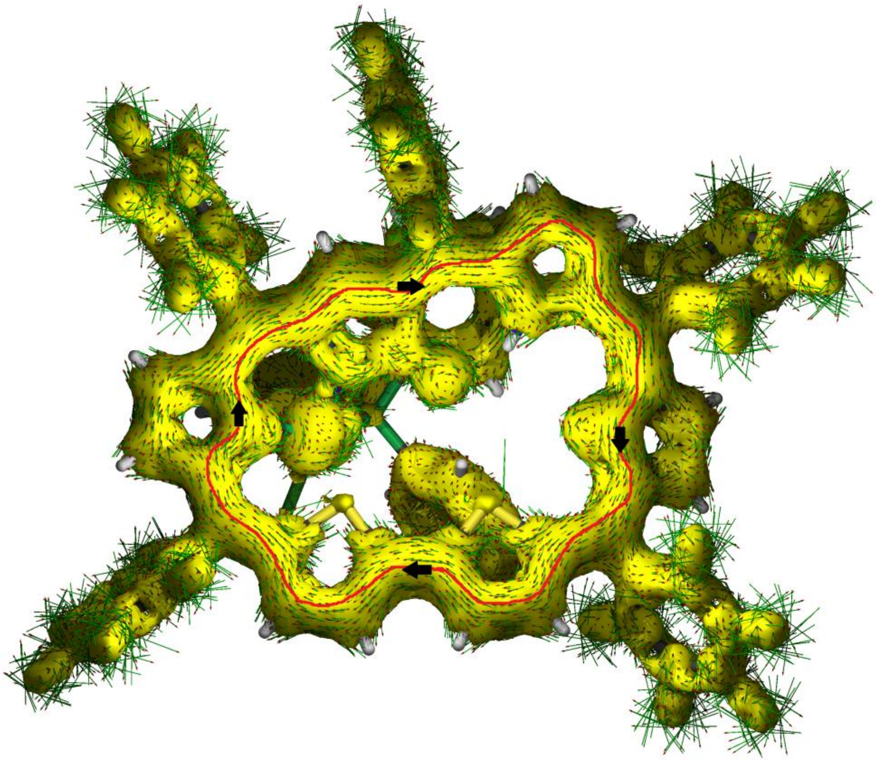


Figure S36. ACID plots of **3**. Direction of the applied magnetic field is perpendicular to the paper and pointing outward. The current density vectors indicate clockwise current.

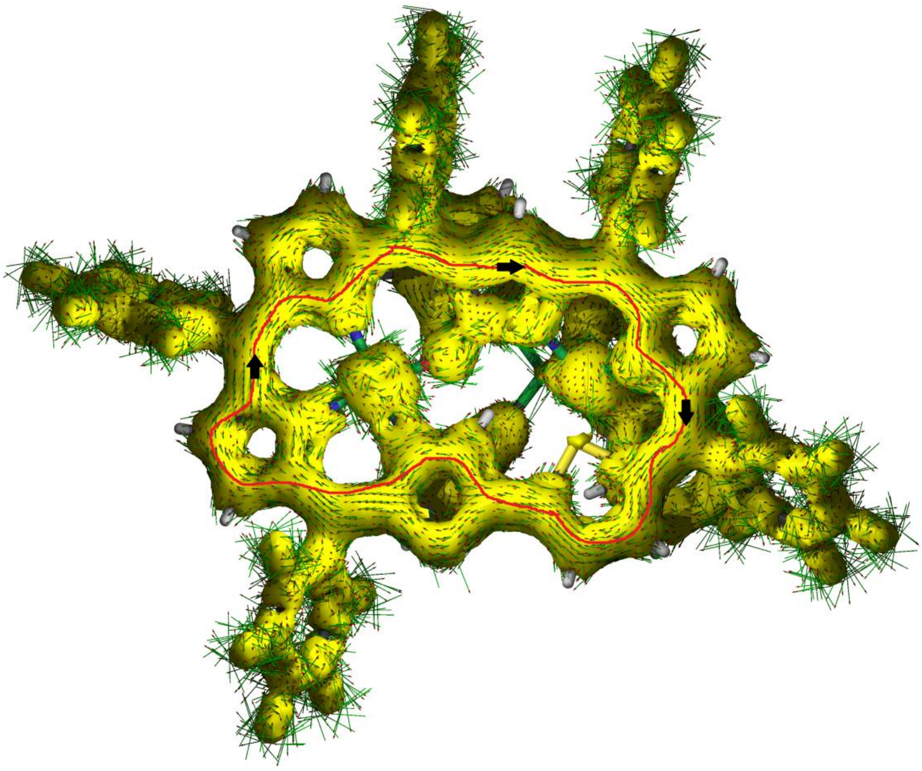


Figure S37. ACID plots of **4-Ph**. Direction of the applied magnetic field is perpendicular to the paper and pointing outward. The current density vectors indicate clockwise current.

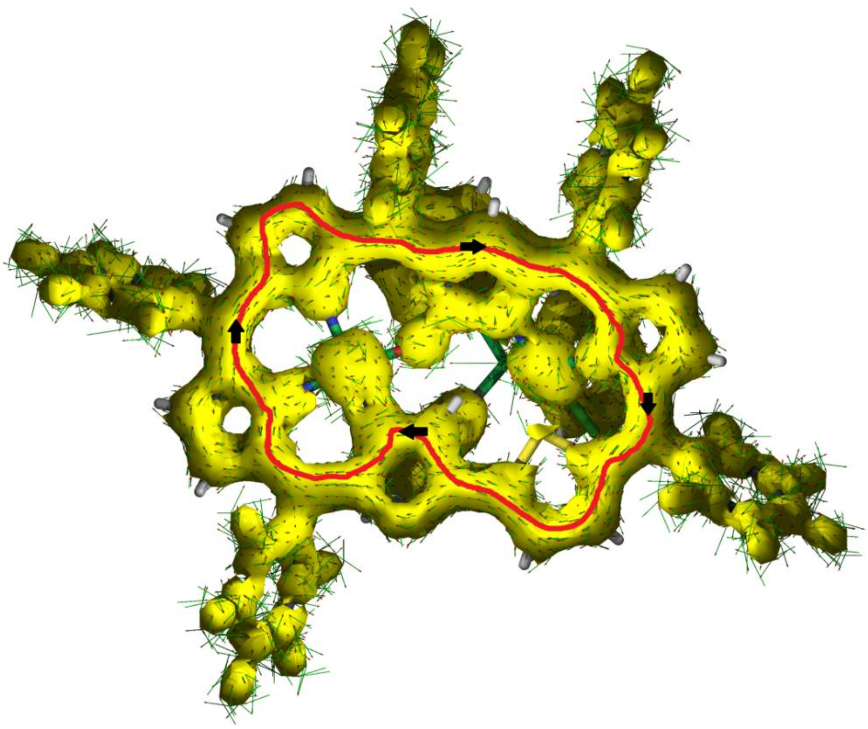


Figure S38. ACID plots of **4-Cl**. Direction of the applied magnetic field is perpendicular to the paper and pointing outward. The current density vectors indicate clockwise current.

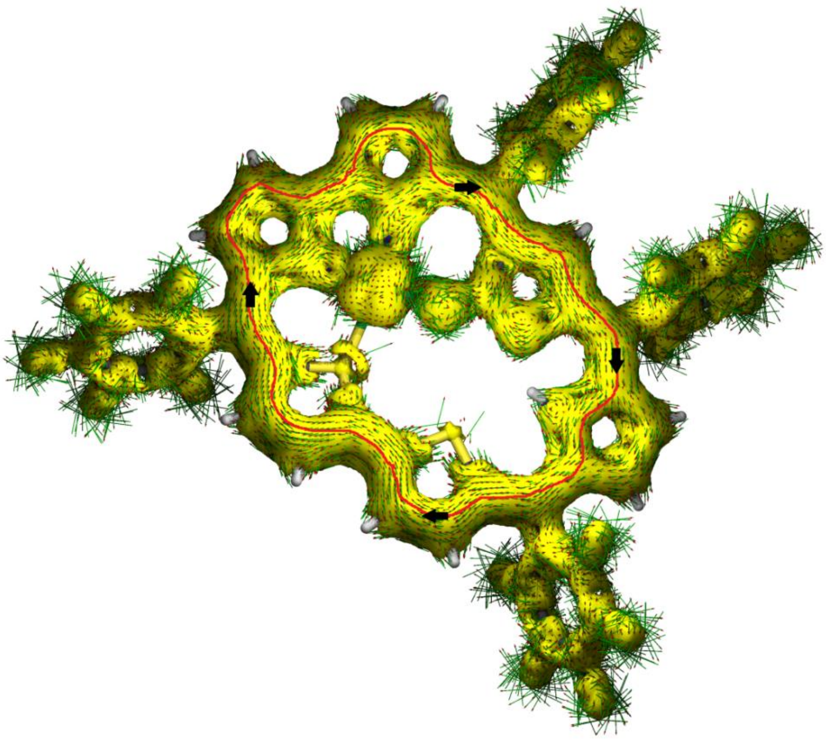


Figure S39. ACID plots of **5**. Direction of the applied magnetic field is perpendicular to the paper and pointing outward. The current density vectors indicate clockwise current.

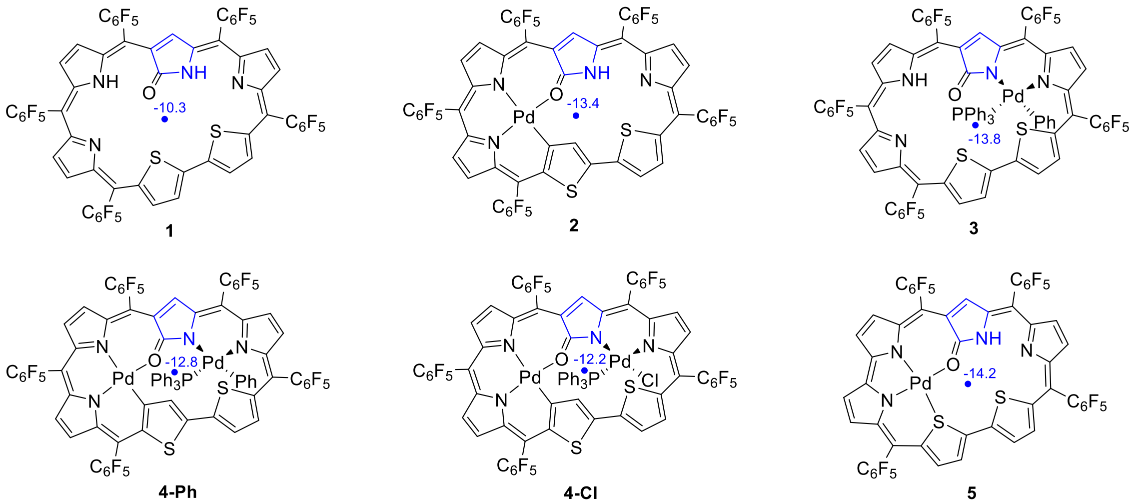


Figure S40. NICS(0) values of **1, 2, 3, 4-Ph, 4-Cl** and **5**.

Table S10. Cartesian coordinates of the optimized structures for compounds **1, 2, 3, 4-Ph, 4-Cl and 5.**

1

Row	Symbol	X	Y	Z
1	S	1.336769	-2.77626	-0.18517
2	C	2.795093	-3.75084	-0.34884
3	C	2.451731	-5.07055	-0.71716
4	H	3.197536	-5.83273	-0.90021
5	C	1.095163	-5.29822	-0.81938
6	H	0.670698	-6.25894	-1.08364
7	C	0.310448	-4.16776	-0.53178
8	C	-1.10708	-4.1833	-0.48208
9	S	-2.10452	-2.78417	-0.13755
10	C	-3.58746	-3.73494	-0.19873
11	C	-3.26949	-5.07452	-0.50049
12	C	-1.91694	-5.32094	-0.66004
13	H	-1.51685	-6.30172	-0.88594
14	H	-4.03003	-5.83841	-0.60451
15	C	-4.88487	-3.2147	0.021388
16	C	-5.1784	-1.85934	0.222972
17	N	-4.22948	-0.88161	0.195534
18	C	-4.88322	0.291136	0.366015
19	C	-6.31596	0.060737	0.539756
20	C	-6.49902	-1.28087	0.453389
21	H	-7.42874	-1.82577	0.542211
22	H	-7.0673	0.818775	0.713204
23	C	-4.24074	1.560197	0.346982
24	C	-2.8559	1.708004	0.236832
25	N	-1.96186	0.646651	0.250142
26	C	-0.6632	1.072196	0.109924
27	O	0.323255	0.338517	0.099181
28	C	-0.74788	2.569855	-0.02307
29	C	-2.09839	2.894194	0.077995
30	H	-2.52693	3.883062	0.024458

31	C	0.313722	3.477008	-0.251
32	C	1.695398	3.249065	-0.30764
33	N	2.41709	2.083231	-0.1084
34	H	1.965603	1.174165	0.036184
35	C	3.769729	2.344102	-0.15178
36	C	3.903426	3.751027	-0.44224
37	C	2.661384	4.291153	-0.54255
38	H	2.416713	5.319542	-0.75948
39	H	4.84338	4.264888	-0.56998
40	C	4.863536	1.500807	0.092171
41	C	4.94245	0.091102	0.26738
42	N	3.99468	-0.84422	0.009055
43	C	4.624598	-2.04907	0.190591
44	C	6.004966	-1.85996	0.642869
45	C	6.203143	-0.52871	0.695902
46	H	7.098074	-0.01066	1.007664
47	H	6.705335	-2.63976	0.904129
48	C	4.116531	-3.33502	-0.06282
49	C	5.123879	-4.44974	-0.0237
50	C	5.159559	-5.36798	1.031165
51	F	4.279888	-5.26719	2.035931
52	C	6.093622	-6.39976	1.080739
53	F	6.105254	-7.2575	2.106815
54	C	7.02348	-6.53428	0.051876
55	F	7.922406	-7.52008	0.088312
56	C	7.012313	-5.63865	-1.01478
57	F	7.901477	-5.76976	-2.00479
58	C	6.06926	-4.61332	-1.04157
59	F	6.085523	-3.77253	-2.08245
60	C	6.181392	2.22043	0.169015
61	C	6.524394	3.008687	1.272524
62	F	5.663549	3.146932	2.289614
63	C	7.748248	3.668507	1.358854

64	F	8.045778	4.412277	2.429903
65	C	8.667953	3.54742	0.319633
66	F	9.843543	4.175663	0.390435
67	C	8.357497	2.770663	-0.79438
68	F	9.238092	2.65769	-1.79452
69	C	7.127178	2.120451	-0.857
70	F	6.86123	1.382521	-1.94153
71	C	-0.11195	4.90472	-0.43715
72	C	-0.66921	5.345035	-1.64184
73	C	-0.80419	4.49292	-2.66601
74	C	-1.09571	6.659014	-1.82081
75	F	-1.61936	7.05056	-2.98711
76	C	-0.97023	7.570218	-0.77425
77	F	-1.37345	8.832064	-0.93515
78	C	-0.42144	7.162308	0.439396
79	F	-0.30051	8.035797	1.444145
80	C	-0.00472	5.841867	0.594975
81	F	0.520197	5.48135	1.772928
82	C	-5.07341	2.792938	0.422057
83	C	-5.9936	3.119422	-0.58261
84	F	-6.13001	2.32214	-1.64991
85	C	-6.78581	4.262755	-0.51886
86	F	-7.65134	4.544128	-1.49838
87	C	-6.66458	5.123719	0.56952
88	F	-7.41567	6.224492	0.638943
89	C	-5.75658	4.832436	1.584564
90	F	-5.64225	5.654052	2.633515
91	C	-4.98004	3.679069	1.502999
92	F	-4.12792	3.427984	2.505924
93	C	-6.01999	-4.18733	0.017313
94	C	-6.18142	-5.12787	1.041436
95	F	-5.30277	-5.17475	2.05123
96	C	-7.23977	-6.03277	1.053647

97	F	-7.36642	-6.91579	2.049671
98	C	-8.17526	-6.00998	0.021581
99	F	-9.1944	-6.8712	0.024062
100	C	-8.04375	-5.08674	-1.01293
101	F	-8.93722	-5.06756	-2.00727
102	C	-6.97436	-4.19393	-1.00644
103	F	-6.87564	-3.32653	-2.02132
104	H	-2.28325	-0.31611	0.287316

2

Row	Symbol	X	Y	Z
1	Pd	2.104627	-0.452205	-0.60046
2	O	0.214774	0.273904	-1.177868
3	C	-0.562137	1.129374	-0.701904
4	N	-1.902557	0.921429	-0.573446
5	H	-2.406051	0.057192	-0.755386
6	C	-2.551175	2.067233	-0.105061
7	C	-1.551585	3.05503	0.055766
8	C	-0.299595	2.523215	-0.28367
9	C	0.930267	3.23142	-0.3632
10	C	2.264461	2.809408	-0.542983
11	N	2.858743	1.553174	-0.476813
12	C	4.210645	1.749573	-0.549515
13	C	5.221678	0.780382	-0.379604
14	C	5.055878	-0.593573	-0.129746
15	N	3.878534	-1.296243	-0.147324
16	C	4.163212	-2.606578	0.153698
17	C	3.243316	-3.672705	0.182225
18	C	1.901564	-3.489379	-0.168148
19	S	0.693891	-4.802565	-0.066149
20	C	-0.56337	-3.717718	-0.633494
21	C	-1.974918	-3.87878	-0.579794
22	S	-2.839186	-2.360469	-0.420607
23	C	-4.397884	-3.136751	-0.468606

24	C	-4.214137	-4.537218	-0.566176
25	H	-5.047688	-5.227734	-0.621023
26	C	-2.880689	-4.950072	-0.601114
27	H	-2.577174	-5.988077	-0.684743
28	C	-5.592518	-2.383383	-0.359617
29	C	-5.603226	-0.976815	-0.243483
30	N	-4.470558	-0.215616	-0.285127
31	C	-4.841156	1.056585	-0.001773
32	C	-3.930192	2.145198	0.125727
33	C	-4.472317	3.4693	0.554241
34	C	-4.207997	3.995877	1.823618
35	F	-3.448397	3.311287	2.688833
36	C	-4.713514	5.228731	2.230791
37	F	-4.441835	5.703787	3.450464
38	C	-5.513115	5.96564	1.360008
39	F	-6.004839	7.145874	1.740815
40	C	-5.797829	5.467685	0.090177
41	F	-6.561931	6.175279	-0.747693
42	C	-5.275549	4.236125	-0.29756
43	F	-5.565004	3.787295	-1.525675
44	C	-6.285745	1.126593	0.210467
45	H	-6.853423	2.012915	0.457552
46	C	-6.75995	-0.136465	0.048043
47	H	-7.783332	-0.470986	0.149012
48	C	-6.889649	-3.116698	-0.328077
49	C	-7.846165	-2.941744	-1.336766
50	F	-7.600291	-2.111671	-2.357905
51	C	-9.065071	-3.615453	-1.323471
52	F	-9.953577	-3.428277	-2.304244
53	C	-9.353735	-4.496195	-0.283368
54	F	-10.517377	-5.147909	-0.262108
55	C	-8.42357	-4.69438	0.734699
56	F	-8.70114	-5.533539	1.73759

57	C	-7.212652	-4.007187	0.703903
58	F	-6.349526	-4.214015	1.707409
59	C	-0.011618	-2.468144	-0.946661
60	H	-0.608969	-1.684174	-1.381817
61	C	1.32322	-2.284032	-0.62577
62	C	3.728757	-5.023827	0.586601
63	C	3.8291	-6.070639	-0.337838
64	F	3.508034	-5.863193	-1.620725
65	C	4.264068	-7.340504	0.033245
66	F	4.353553	-8.319125	-0.872615
67	C	4.6168	-7.585751	1.358669
68	F	5.037429	-8.797776	1.723985
69	C	4.531136	-6.563977	2.302174
70	F	4.867307	-6.800873	3.573913
71	C	4.089908	-5.302595	1.90997
72	F	4.01365	-4.342877	2.840064
73	C	5.580943	-2.730585	0.392005
74	H	6.090277	-3.647949	0.650282
75	C	6.1321	-1.50128	0.205588
76	H	7.171281	-1.225165	0.307008
77	C	6.63706	1.2677	-0.426113
78	C	7.463985	0.984201	-1.518521
79	F	6.989091	0.274803	-2.550279
80	C	8.786066	1.4199	-1.576277
81	F	9.550099	1.134976	-2.635798
82	C	9.311003	2.162125	-0.52048
83	F	10.575484	2.586146	-0.565345
84	C	8.51357	2.461363	0.582323
85	F	9.018321	3.170485	1.59721
86	C	7.195529	2.011636	0.618848
87	F	6.456563	2.312801	1.694291
88	C	4.498827	3.155754	-0.755518
89	H	5.480242	3.585271	-0.891383

90	C	3.313358	3.803378	-0.742265
91	H	3.152336	4.862849	-0.869603
92	C	0.75272	4.715158	-0.194114
93	C	1.118108	5.363553	0.990083
94	F	1.668672	4.667472	1.991944
95	C	0.929932	6.732768	1.169029
96	F	1.290763	7.324231	2.311947
97	C	0.359191	7.487062	0.146191
98	F	0.175796	8.798997	0.305239
99	C	-0.019641	6.869251	-1.044454
100	F	-0.564029	7.593538	-2.02759
101	C	0.175836	5.498953	-1.199097
102	F	-0.198789	4.934264	-2.354331
103	H	-1.744427	4.061131	0.393587

3

Row	Symbol	X	Y	Z
1	Pd	2.296358	-0.749349	1.150257
2	Cl	3.086605	-2.7234	2.191234
3	P	0.985524	-0.401071	3.040858
4	C	-0.169143	-1.784292	3.362905
5	C	-1.086806	-2.129446	2.355698
6	H	-1.110952	-1.566674	1.426867
7	C	-1.966713	-3.194214	2.548507
8	H	-2.676535	-3.456706	1.76988
9	C	-1.926668	-3.931542	3.73484
10	H	-2.608001	-4.766129	3.877486
11	C	-1.005971	-3.60113	4.729638
12	H	-0.963496	-4.178506	5.649222
13	C	-0.127473	-2.531374	4.547534
14	H	0.592549	-2.289796	5.321596
15	C	1.9704	-0.133662	4.576251
16	C	1.32035	0.361889	5.721717
17	H	0.255195	0.571973	5.696163

18	C	2.036779	0.596994	6.89387
19	H	1.521603	0.97579	7.772432
20	C	3.412674	0.35581	6.933603
21	H	3.972075	0.54586	7.845789
22	C	4.065012	-0.125591	5.7989
23	H	5.134521	-0.315395	5.822323
24	C	3.35046	-0.37308	4.623994
25	H	3.8579	-0.77206	3.753971
26	C	-0.031665	1.135254	2.998445
27	C	0.641627	2.3606	2.857251
28	H	1.724552	2.38399	2.774539
29	C	-0.072753	3.555926	2.803462
30	C	-1.467939	3.543153	2.887142
31	H	-2.025374	4.47397	2.829946
32	C	-2.142937	2.331538	3.036434
33	C	-1.429457	1.131327	3.093264
34	H	-1.967165	0.195597	3.197902
35	H	-3.227557	2.31554	3.090619
36	H	0.458725	4.494122	2.676779
37	N	3.864792	-0.698128	-0.393752
38	C	4.787678	-1.662513	-0.698301
39	C	6.110351	-1.069451	-0.747946
40	H	7.025385	-1.591405	-0.990758
41	C	5.956281	0.265346	-0.530528
42	H	6.725674	1.024272	-0.537226
43	C	4.539148	0.497758	-0.339724
44	C	3.902229	1.755169	-0.282534
45	C	2.497302	1.884757	-0.276375
46	N	1.632568	0.884682	0.111492
47	C	0.355014	1.243149	-0.223662
48	O	-0.650829	0.538106	-0.066205
49	C	0.425022	2.639212	-0.823316
50	C	1.775261	2.982683	-0.802991

51	H	2.224459	3.881011	-1.199716
52	C	-0.619922	3.460437	-1.291038
53	C	-2.008311	3.252681	-1.25779
54	N	-2.71053	2.134855	-0.852757
55	H	-2.232755	1.280235	-0.539757
56	C	-4.053639	2.41899	-0.782187
57	C	-4.211816	3.780586	-1.218139
58	C	-2.981694	4.272732	-1.539367
59	H	-2.752088	5.259698	-1.911359
60	H	-5.159599	4.290039	-1.306834
61	C	-5.117087	1.604489	-0.349841
62	C	-5.191569	0.194641	-0.249933
63	N	-4.304657	-0.709839	-0.747064
64	C	-4.917783	-1.920403	-0.611376
65	C	-6.213267	-1.78904	0.058447
66	C	-6.37827	-0.470812	0.29712
67	H	-7.208829	0.00912	0.79466
68	H	-6.881924	-2.595533	0.323628
69	C	-4.446275	-3.162319	-1.083087
70	C	-3.162504	-3.49989	-1.556443
71	S	-1.717198	-2.497172	-1.426205
72	C	-0.683264	-3.84062	-1.915143
73	C	-1.466008	-4.960071	-2.263988
74	C	-2.816508	-4.774112	-2.067294
75	H	-3.558205	-5.537968	-2.261824
76	H	-1.037562	-5.886146	-2.626884
77	C	0.729731	-3.854019	-1.853842
78	S	1.724361	-2.471636	-1.441945
79	C	3.184763	-3.458807	-1.383362
80	C	2.863179	-4.795717	-1.710883
81	C	1.527216	-5.012769	-1.9762
82	H	1.117757	-5.989556	-2.202076
83	H	3.606364	-5.58271	-1.713743

84	C	4.478883	-2.976438	-1.089145
85	F	6.190229	-3.809495	1.04162
86	C	6.433148	-4.290716	-0.179169
87	C	5.622304	-3.921518	-1.261812
88	C	5.950057	-4.463097	-2.51226
89	F	5.230231	-4.138136	-3.595083
90	C	7.019143	-5.338096	-2.68353
91	C	7.803119	-5.688235	-1.58634
92	C	7.510734	-5.162027	-0.330665
93	F	8.262692	-5.497824	0.722505
94	F	8.832522	-6.523692	-1.739669
95	F	7.303997	-5.833765	-3.893011
96	C	-5.429458	-4.295052	-1.038443
97	C	-6.494852	-4.372913	-1.941446
98	C	-7.421917	-5.412737	-1.899247
99	C	-7.295145	-6.408331	-0.93313
100	C	-6.24503	-6.358831	-0.018146
101	C	-5.330263	-5.310969	-0.081855
102	F	-4.334317	-5.292067	0.817899
103	F	-6.125643	-7.311236	0.913025
104	F	-8.177473	-7.408183	-0.883084
105	F	-8.42748	-5.462349	-2.778631
106	F	-6.644533	-3.434588	-2.882886
107	C	-6.361746	2.362187	0.001223
108	C	-7.52601	2.282418	-0.772772
109	C	-8.682607	2.985479	-0.442442
110	C	-8.694677	3.79899	0.688677
111	C	-7.552532	3.903563	1.479532
112	C	-6.408396	3.191934	1.128035
113	F	-5.329736	3.317348	1.91762
114	F	-7.562839	4.680949	2.567775
115	F	-9.797157	4.477007	1.013427
116	F	-9.77617	2.891048	-1.205861

117	F	-7.549496	1.519825	-1.871636
118	C	-0.18949	4.796764	-1.824763
119	C	0.057329	5.880457	-0.977198
120	C	0.479559	7.115819	-1.463148
121	C	0.665393	7.286762	-2.83368
122	C	0.428445	6.225395	-3.704414
123	C	0.007532	4.9987	-3.19369
124	F	-0.210897	3.997702	-4.055028
125	F	0.605701	6.389456	-5.019095
126	F	1.068336	8.466207	-3.31085
127	F	0.703149	8.135421	-0.627014
128	F	-0.117637	5.75044	0.346531
129	C	4.708372	3.002343	-0.361645
130	C	4.693248	3.919818	0.697919
131	C	5.422888	5.105115	0.663999
132	C	6.195002	5.40322	-0.456775
133	C	6.229907	4.516161	-1.530662
134	C	5.488551	3.338154	-1.475593
135	F	5.530465	2.523031	-2.538044
136	F	6.961314	4.807576	-2.611486
137	F	6.899164	6.535695	-0.501917
138	F	5.392506	5.952619	1.697603
139	F	3.975661	3.660229	1.801786

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Row	Symbol	X	Y	Z
1	Pd	2.698486	-0.397278	-0.421667
2	N	4.471836	-1.346849	-0.634645
3	C	4.70436	-2.691845	-0.78651
4	C	3.733068	-3.683007	-1.059391
5	C	2.375358	-3.370489	-1.148772
6	S	1.116014	-4.5553	-1.625938
7	C	-0.129229	-3.320633	-1.497949

8	C	-1.532066	-3.423413	-1.658335
9	S	-2.378614	-1.899762	-1.447549
10	C	-3.943933	-2.65269	-1.545196
11	C	-5.116917	-1.869697	-1.415494
12	C	-5.081513	-0.504857	-1.054955
13	N	-3.93171	0.155498	-0.682032
14	Pd	-2.606421	-0.229352	1.134218
15	P	-1.56216	-0.146507	3.232508
16	C	-2.645199	0.003564	4.728976
17	C	-3.357181	-1.116067	5.194531
18	H	-3.276784	-2.067519	4.681453
19	C	-4.177271	-1.017909	6.317483
20	H	-4.71758	-1.896041	6.659959
21	C	-4.312674	0.198918	6.989192
22	H	-4.956013	0.273777	7.861852
23	C	-3.615177	1.316518	6.532646
24	H	-3.707255	2.268412	7.048723
25	C	-2.783809	1.220498	5.414176
26	H	-2.23861	2.098473	5.088089
27	C	-0.473159	-1.580018	3.609733
28	C	-0.198856	-1.984967	4.926617
29	H	-0.666461	-1.476318	5.763108
30	C	0.672288	-3.048279	5.167836
31	H	0.87433	-3.355013	6.190608
32	C	1.28063	-3.714165	4.101589
33	H	1.956827	-4.54322	4.292206
34	C	1.019946	-3.31283	2.789876
35	H	1.498108	-3.822466	1.958405
36	C	0.145587	-2.252157	2.544744
37	H	-0.04215	-1.93251	1.525954
38	C	-0.478106	1.33547	3.352597
39	C	0.820059	1.277766	3.877226
40	H	1.237216	0.330578	4.201655

41	C	1.588902	2.439986	3.975968
42	H	2.597297	2.381851	4.376501
43	C	1.070279	3.665924	3.557261
44	H	1.674232	4.566209	3.624461
45	C	-0.223767	3.730687	3.034439
46	H	-0.631754	4.673867	2.686254
47	C	-0.989002	2.571385	2.924225
48	H	-1.983391	2.628896	2.493139
49	N	-1.277592	1.126847	0.027748
50	C	0.065666	1.23981	-0.050266
51	O	0.846357	0.306821	0.287198
52	C	0.43624	2.600194	-0.572979
53	C	1.70239	3.219323	-0.703595
54	C	3.030396	2.787069	-0.466209
55	N	3.567342	1.525496	-0.281506
56	C	4.921933	1.669469	-0.171619
57	C	5.881546	0.634995	-0.126589
58	C	5.668581	-0.739751	-0.340744
59	C	6.702958	-1.750103	-0.313036
60	C	6.11151	-2.943576	-0.594414
61	H	6.584964	-3.913308	-0.652876
62	H	7.747643	-1.570207	-0.106015
63	C	7.295152	1.057385	0.126259
64	C	8.262395	1.048019	-0.884668
65	C	9.57766	1.444194	-0.651628
66	C	9.951849	1.870024	0.62112
67	C	9.011719	1.894608	1.648921
68	C	7.703542	1.490308	1.392487
69	F	6.825675	1.522813	2.404057
70	F	9.370933	2.299928	2.871921
71	F	11.2088	2.253587	0.855297
72	F	10.478594	1.425354	-1.639717
73	F	7.934881	0.651889	-2.12131

74	C	5.270508	3.075086	-0.21498
75	H	6.268005	3.481784	-0.13384
76	C	4.119056	3.755914	-0.42503
77	H	4.009647	4.825027	-0.524782
78	C	1.609387	4.639379	-1.204108
79	C	1.322355	5.721108	-0.368897
80	C	1.216283	7.022931	-0.854086
81	C	1.394657	7.266037	-2.214261
82	C	1.680004	6.208416	-3.07485
83	C	1.783825	4.916152	-2.563611
84	F	2.059903	3.92242	-3.41722
85	F	1.852305	6.439118	-4.380257
86	F	1.294308	8.509175	-2.690372
87	F	0.948527	8.037296	-0.023709
88	F	1.156077	5.529248	0.949109
89	C	-0.797947	3.215901	-0.815526
90	H	-0.957996	4.194519	-1.24185
91	C	-1.826806	2.303257	-0.469615
92	C	-3.211214	2.516725	-0.666627
93	C	-4.19678	1.498471	-0.737878
94	C	-5.604973	1.695663	-1.037878
95	H	-6.10648	2.649548	-1.125197
96	C	-6.153028	0.460785	-1.216691
97	H	-7.173671	0.236921	-1.493494
98	C	-3.639894	3.92118	-0.933305
99	C	-3.555788	4.902191	0.062612
100	C	-3.937718	6.222575	-0.159227
101	C	-4.419771	6.595431	-1.412009
102	C	-4.51466	5.64685	-2.428027
103	C	-4.123259	4.332562	-2.18203
104	F	-4.212691	3.454775	-3.18904
105	F	-4.968483	6.005683	-3.633293
106	F	-4.790217	7.857331	-1.637746

107	F	-3.851154	7.12925	0.820014
108	F	-3.11224	4.582269	1.290611
109	C	-3.949724	-1.46484	1.991553
110	C	-5.198751	-0.980121	2.403388
111	H	-5.432463	0.077782	2.311117
112	C	-6.155902	-1.845348	2.943329
113	H	-7.119928	-1.451384	3.258012
114	C	-5.874137	-3.205518	3.089942
115	H	-6.616362	-3.876443	3.514975
116	C	-4.63422	-3.697654	2.678705
117	H	-4.405661	-4.756259	2.781554
118	C	-3.677282	-2.833072	2.132573
119	H	-2.712711	-3.234151	1.831702
120	C	-6.422865	-2.492666	-1.790057
121	C	-7.10032	-2.111666	-2.955678
122	C	-8.314104	-2.683516	-3.329104
123	C	-8.87635	-3.682361	-2.537848
124	C	-8.220466	-4.09799	-1.382244
125	C	-7.010786	-3.505837	-1.024529
126	F	-6.406089	-3.945607	0.085023
127	F	-8.75323	-5.061378	-0.622368
128	F	-10.036806	-4.241228	-2.888288
129	F	-8.93485	-2.288401	-4.44592
130	F	-6.584873	-1.167284	-3.755082
131	C	-3.783799	-4.0393	-1.797399
132	H	-4.626517	-4.711591	-1.907087
133	C	-2.457856	-4.46604	-1.854376
134	H	-2.168372	-5.500475	-2.007225
135	C	0.452626	-2.097296	-1.126041
136	H	-0.141342	-1.210528	-0.9765
137	C	1.814275	-2.098213	-0.903066
138	C	4.17952	-5.09352	-1.239849
139	C	4.914567	-5.498152	-2.360162

140	C	5.317845	-6.81955	-2.537966
141	C	4.982598	-7.775416	-1.581325
142	C	4.250895	-7.405185	-0.454861
143	C	3.861534	-6.078002	-0.296346
144	F	3.170786	-5.753709	0.807338
145	F	3.936815	-8.320737	0.467562
146	F	5.363334	-9.043994	-1.74266
147	F	6.016943	-7.176672	-3.619782
148	F	5.246765	-4.605376	-3.30012

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Row	Symbol	X	Y	Z
1	H	1.230837	-3.02192	6.140528
2	C	0.92003	-2.85082	5.113468
3	C	0.005492	-1.83743	4.828985
4	H	-0.39272	-1.23142	5.636825
5	C	-0.40505	-1.60803	3.503651
6	C	0.107572	-2.41029	2.476607
7	C	1.024085	-3.42381	2.765602
8	C	1.430381	-3.64392	4.082348
9	H	2.141416	-4.43468	4.305942
10	H	1.422528	-4.03703	1.963329
11	H	-0.20668	-2.23852	1.454398
12	P	-1.55837	-0.24463	3.09729
13	C	-2.72924	-0.19891	4.527704
14	C	-3.13356	1.010526	5.112782
15	C	-4.03154	1.015792	6.18197
16	C	-4.53226	-0.18427	6.685558
17	H	-5.22928	-0.17897	7.51926
18	C	-4.12962	-1.39314	6.114368
19	H	-4.51331	-2.33417	6.498581
20	C	-3.24048	-1.4042	5.041186

21	H	-2.94954	-2.34905	4.599683
22	H	-4.33116	1.962744	6.622681
23	H	-2.7431	1.954851	4.752522
24	C	-0.60331	1.31836	3.262342
25		0.702604	1.349486	3.770442
26	H	1.203288	0.42935	4.050114
27	C	1.373105	2.567104	3.909473
28	H	2.387368	2.576792	4.298977
29	C	0.750802	3.760978	3.54375
30	H	1.278456	4.705096	3.643477
31	C	-0.54797	3.737247	3.029824
32	C	-1.21657	2.523892	2.881219
33	H	-2.21398	2.518563	2.453209
34	H	-1.03507	4.655297	2.717423
35	Pd	-2.64212	-0.38139	1.017307
36	N	-1.49642	1.05425	0.053685
37	C	-0.15028	1.194871	-0.02971
38	O	0.648819	0.282463	0.307428
39	Pd	2.536944	-0.34962	-0.39292
40	N	4.34839	-1.23351	-0.56398
41	C	4.630887	-2.57144	-0.6987
42	C	6.043277	-2.77117	-0.48051
43	H	6.551357	-3.72411	-0.52179
44	C	6.586485	-1.55572	-0.19969
45	C	5.517083	-0.58232	-0.25403
46	C	5.679147	0.799945	-0.04633
47		4.682025	1.797505	-0.11381
48	N	3.33619	1.601554	-0.23597
49	C	2.754802	2.840502	-0.44639
50	C	3.806848	3.8496	-0.40771
51	C	4.979245	3.214891	-0.17295
52	H	5.960109	3.658962	-0.08532
53	H	3.659151	4.912458	-0.52378

54	C	1.416327	3.218719	-0.70138
55	C	0.169603	2.556902	-0.56568
56	C	-1.08169	3.13108	-0.82184
57	C	-2.08866	2.201275	-0.46977
58	C	-3.46945	2.346992	-0.70168
59	C	-4.39319	1.271455	-0.76994
60	N	-4.05308	-0.05002	-0.65194
61	C	-5.16581	-0.79078	-0.98179
62	C	-5.17244	-2.1876	-1.21554
63	C	-3.98329	-2.92556	-1.42195
64	S	-2.48743	-2.10561	-1.77476
65	C	-1.55549	-3.5781	-1.64235
66	C	-0.15791	-3.3864	-1.49992
67	S	1.131018	-4.57786	-1.55324
68	C	2.332972	-3.33265	-1.09185
69	C	3.700506	-3.59749	-0.97043
70	C	4.199613	-4.99358	-1.12846
71	C	3.918696	-5.97897	-0.17458
72	F	3.214974	-5.66982	0.925614
73	C	4.358372	-7.29215	-0.31781
74	F	4.07831	-8.20811	0.614806
75	C	5.105109	-7.64691	-1.43936
76	F	5.534368	-8.9015	-1.58588
77	C	5.40473	-6.68965	-2.40638
78	C	4.950875	-5.3828	-2.24368
79	F	5.249985	-4.48848	-3.19321
80	F	6.118556	-7.03152	-3.48328
81	C	1.721542	-2.07652	-0.8999
82	C	0.364081	-2.12752	-1.16494
83	H	-0.2797	-1.27364	-1.02931
84	C	-2.41276	-4.68251	-1.4698
85	H	-2.05188	-5.69822	-1.34923
86	C	-3.75112	-4.31947	-1.34729

87	H	-4.5412	-5.02633	-1.12259
88	C	-6.47246	-2.89989	-1.26518
89	C	-7.41861	-2.7843	-0.23181
90	F	-7.1715	-2.02097	0.834341
91	C	-8.63527	-3.46197	-0.26705
92	F	-9.50793	-3.33569	0.737649
93	C	-8.94191	-4.28081	-1.35093
94	C	-8.02983	-4.41474	-2.39528
95	C	-6.82012	-3.72903	-2.34483
96	F	-5.98857	-3.86787	-3.3865
97	F	-8.32699	-5.18795	-3.44538
98	F	-10.1054	-4.93201	-1.39109
99	C	-6.27423	0.103833	-1.22916
100	C	-5.79552	1.37612	-1.11495
101	H	-6.34032	2.29565	-1.27619
102	H	-7.26693	-0.19702	-1.53506
103	C	-3.95857	3.723484	-0.99897
104	C	-3.92606	4.723131	-0.01804
105	F	-3.47479	4.443937	1.216581
106	C	-4.36665	6.020611	-0.26461
107	F	-4.3279	6.946241	0.699322
108	C	-4.85673	6.350293	-1.52646
109	C	-4.9003	5.382184	-2.52757
110	C	-4.45041	4.09168	-2.2577
111	F	-4.49053	3.194535	-3.25116
112	F	-5.36062	5.700168	-3.74159
113	F	-5.28265	7.589705	-1.77553
114	H	-1.26898	4.094456	-1.27085
115	C	1.275082	4.62495	-1.22827
116	C	0.92763	5.708315	-0.41827
117	F	0.7389	5.531398	0.898452
118	C	0.781481	6.996642	-0.92846
119	F	0.45626	8.013228	-0.12194

120	C	0.979614	7.223767	-2.28872
121	C	1.32405	6.163897	-3.12465
122	C	1.46702	4.88543	-2.58878
123	F	1.799037	3.889108	-3.41904
124	F	1.514809	6.379145	-4.42994
125	F	0.841144	8.453614	-2.78846
126	C	7.072077	1.27574	0.223401
127	C	7.442626	1.74328	1.489104
128	F	6.546254	1.760591	2.484898
129	C	8.730759	2.198273	1.7613
130	F	9.053415	2.635628	2.983374
131	C	9.689373	2.19082	0.750396
132	F	10.92744	2.622732	0.999714
133	C	9.353162	1.731524	-0.52134
134	C	8.057076	1.285139	-0.77044
135	F	7.765871	0.858286	-2.00598
136	F	10.27147	1.729217	-1.49334
137	H	7.62001	-1.33671	0.024779
138	Cl	-3.9178	-2.13632	1.935169

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Row	Symbol	X	Y	Z
1	C	-2.941147	2.534897	-0.422536
2	C	-1.751607	3.283875	-0.452037
3	C	0.619674	4.222112	-0.309481
4	C	1.999922	4.472137	-0.158638
5	C	3.00448	3.497426	0.038245
6	N	2.811218	2.146315	-0.043034
7	C	3.975709	1.455886	0.194283
8	C	4.03447	0.040502	0.155662
9	C	2.891463	-0.730066	-0.147037
10	N	1.697291	-0.113389	-0.479931
11	C	0.767736	-1.046988	-0.595654

12	C	1.366076	-2.41044	-0.331157
13	C	0.780702	-3.703728	-0.316882
14	C	-0.566211	-4.072917	-0.184432
15	N	-1.660118	-3.252774	0.022709
16	C	-2.749597	-4.036063	0.2626
17	C	-3.97988	-3.380508	0.49521
18	N	-3.992076	-2.027256	0.298281
19	C	-5.270132	-1.569716	0.485822
20	C	-6.089194	-2.698767	0.845581
21	C	-5.28923	-3.818916	0.847882
22	C	-5.698832	-0.240468	0.260685
23	C	-4.874588	0.860239	-0.009518
24	C	-5.260089	2.108368	-0.548678
25	C	-4.227261	2.993601	-0.780915
26	C	-7.170702	0.00679	0.238828
27	C	-7.785752	0.832833	1.188991
28	C	-9.158368	1.067782	1.185251
29	C	-9.955945	0.468992	0.212258
30	C	-9.375946	-0.355889	-0.749068
31	C	-8.000358	-0.574678	-0.72911
32	C	-2.376348	-5.415589	0.204575
33	C	-1.038442	-5.44129	-0.081823
34	C	1.763854	-4.835973	-0.368944
35	C	2.436152	-5.146443	-1.55625
36	C	3.371759	-6.175911	-1.625064
37	C	3.660789	-6.919599	-0.482505
38	C	3.012271	-6.631054	0.716042
39	C	2.078017	-5.598109	0.760555
40	C	2.716783	-2.140838	-0.086695
41	C	5.321712	-0.634844	0.463485
42	C	5.955877	-1.464474	-0.471935
43	C	7.158209	-2.110293	-0.193874
44	C	7.766607	-1.931533	1.046211

45	C	7.165651	-1.111749	1.998494
46	C	5.959702	-0.481839	1.702133
47	C	4.982023	2.44095	0.454874
48	C	4.392874	3.681221	0.357433
49	C	2.450875	5.892598	-0.230129
50	C	3.304309	6.34148	-1.247203
51	C	3.742082	7.662077	-1.315904
52	C	3.320937	8.577944	-0.354504
53	C	2.468518	8.166407	0.667843
54	C	2.04806	6.839893	0.721218
55	C	-0.362354	5.156469	-0.726465
56	C	-1.642051	4.649951	-0.810668
57	H	-6.291617	2.322555	-0.799744
58	Pd	-2.174145	-1.293167	-0.22594
59	S	-3.11776	0.911626	0.300218
60	S	-0.170219	2.665297	-0.012145
61	H	1.996965	1.581229	-0.349429
62	O	-0.411358	-0.738479	-0.993512
63	H	-7.141268	-2.650289	1.089654
64	H	-5.581883	-4.836295	1.0701
65	H	-4.380913	3.977686	-1.208019
66	F	3.989234	-6.457404	-2.776848
67	F	-7.052467	1.418443	2.143901
68	F	-9.714776	1.85588	2.110944
69	F	-11.272074	-0.686693	-0.200218
70	F	-10.139416	-0.922471	-1.688953
71	F	-7.477931	-1.35763	-1.680346
72	H	-3.036315	-6.258474	0.359473
73	H	-0.422568	-6.318757	-0.216043
74	F	2.177965	-4.453316	-2.671143
75	F	4.555786	-7.908424	-0.537024
76	F	3.291535	-7.342045	1.814191
77	F	1.476933	-5.34352	1.930851

78	H	3.476597	-2.862604	0.176958
79	F	5.414599	-1.651426	-1.682496
80	F	7.736093	-2.89107	-1.113066
81	F	8.920606	-2.543109	1.321026
82	F	7.742504	-0.943715	3.19343
83	F	5.407257	0.284728	2.652973
84	H	6.016242	2.232843	0.688289
85	H	4.870164	4.637597	0.516513
86	F	3.719114	5.495967	-2.198557
87	F	4.553452	8.057209	-2.30242
88	F	3.731854	9.845968	-0.412865
89	F	2.067948	9.042903	1.594843
90	F	1.238038	6.480879	1.724906
91	H	-0.110193	6.178935	-0.97996
92	H	-2.49606	5.242719	-1.116171

References

1. D. Wu, A. B. Descalzo, F. Weik, F. Emmerling, Z. Shen, X.-Z. You and K. Rurack, *Angew. Chem., Int. Ed.*, 2008, **47**, 193-197.
2. M. Toganoh, S. Gokulnath, Y. Kawabe and H. Furuta, *Chem. -Eur. J.*, 2012, **18**, 4380-4391.
3. G. Sheldrick, *SHELXTI93, Program for crystal structure refinement*, 1997.
4. H. Puschmann, L. Bourhis, R. Gildea and O. Dolomanov, *Acta Crystallogr., Sect. A: Found. Crystallogr*, 2009, **65**, 315-316.
5. G. Sheldrick, *Acta Crystallogr., Sect. A*, 2008, **64**, 112-122.
6. G. Sheldrick, *Acta Crystallogr., Sect. C*, 2015, **71**, 3-8.
7. I. Y. Zhang, J. Wu and X. Xu, *Chem. Commun.*, 2010, **46**, 3057-3070.
8. G. A. Petersson and M. A. Al‐Laham, *J. Chem. Phys.*, 1991, **94**, 6081-6090.
9. Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta and P. v. R. Schleyer, *Chem. Rev.*, 2005, **105**, 3842-3888.
10. P. v. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao and N. J. R. van Eikema Hommes, *J. Am. Chem. Soc.*, 1996, **118**, 6317-6318.
11. T. A. Keith and R. F. W. Bader, *Chem. Phys. Lett.*, 1992, **194**, 1-8.
12. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
13. F. J. Luque, J. M. López and M. Orozco, *Theor. Chem. Acc.*, 2000, **103**, 343-345.