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Control of dual emission behaviour of *μ*-oxo-bridged Si(IV) corrole dimers by substituent bulkiness

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1. Experimental Section

Instrumental

The chemicals used for synthesis were of reagent grade quality unless otherwise mentioned. Thin-layer chromatography (TLC) was carried out on aluminum sheets coated with silica gel 60 F_{254} (Merck 5554). ^{1}H, ^{19}F and ^{29}Si NMR spectra were recorded on a JEOL ECA-600 spectrometer (operating as 600.17 MHz for ^{1}H, 564.73 MHz for ^{19}F, and 119.24 MHz for ^{29}Si) using the residual solvent as the internal reference for ^{1}H (δ = 7.26 ppm in $CDCl_3$ and 6.00 ppm in $C_2D_2Cl_4$) and hexafluorobenzene and tetramethylsilane as an external reference for ^{19}F (δ = –162.9 ppm) and ^{29}Si (δ = 0.00 ppm). Coupling constant (J) are given in Hz. High-Resolution Atmospheric-Pressure-Chemical-Ionization Time-Of-Flight (HR-APCI-TOF) mass spectra were recorded on a BRUKER Daltonics micrOTOF LC instrument. UV/Vis/NIR absorption spectra were recorded on a Shimadzu UV-3600PC spectrometer. Absolute fluorescence quantum yields were determined on a HAMAMATSU C9920–02S. Fluorescence lifetime was recorded on Hamamatsu Photonics Quantaurus-Tau C11367. Redox potentials were measured by cyclic voltammetry on ALS electrochemical analyzer model 612E.

X-Ray Crystallographic Details

Single-crystal X-ray diffraction analysis data were collected at –180 °C with a Rigaku XtaLAB P200 by using graphite monochromated Cu-$K\alpha$ radiation (λ = 1.54187 Å). The structures were solved by dual space methods (SHELXT-2014/5) and refined with full-matrix least-square technique (SHELXL-2014/7).[S1-3]

Synthesis of Freebase Corroles 1b, 1c and 1d

Freebase corroles **1b** was synthesized according to the previous report.[S4]

Freebase corroles **1c** and **1d** were synthesized from the respective 5-aryldipyrromethanes and arylaldehydes in a MeOH/H_2O co-solvent according to Gryko's acid-catalyzed condensation method.[S5] The details are shown below.

Synthesis of 5,15-Bis(pentafluorophenyl)-10-substituted corrole 1c and 1d

Dipyrromethane (3 mmol) and aldehyde (1.5 mmol) were dissolved in MeOH (150 mL). Subsequently, a solution of aqueous HCl (36%, 7.5 mL) in H_2O (150 mL) was added, and the reaction was stirred at room temperature for 1 h. The mixture was extracted with $CHCl_3$, and the organic layer was washed twice with H_2O, dried with anhydrous Na_2SO_4, filtered, and diluted to 750 mL with $CHCl_3$. Then, DDQ (1.02 g, 4.5 mmol) was added, and the mixture was stirred overnight at room temperature. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-

hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded freebase corroles. Yield: **1c** (637 μmol, 450 mg, 42%) and **1d** (817 μmol, 650 mg, 54%).
1c: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.11 (2H, d, J = 4.1 Hz, β-H), 8.71 (4H, m, , β-H), 8.52 (2H, s, β-H), 8.20 (2H, m, Ph-H), 7.75 (3H, m, Ph-H); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –137.73 (4F, d, J = 19.5 Hz, *o*-F), –152.69 (2F, s, *p*-F), –161.62 (4F, t, J = 18.4 Hz, *m*-H); HRMS m/z = 706.1189 (calcd. for $[C_{37}H_{16}N_4F_{10}]^+$; $[M]^+$, m/z = 706.1210).
1d : ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.03 (2H, d, J = 4.1 Hz, β-H), 8.62 (4H, s, β-H), 8.49 (2H, s, β-H), 6.58 (2H, d, J = 8.3 Hz, *m*-H), 4.11 (3H, m, *p* -C<u>H</u>$_3$), 3.53 (6H, d, J = 11.5 Hz, *o* -C<u>H</u>$_3$); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –137.61 (4F, d, J = 19.5 Hz, *o*-F), –153.11 (2F, s, *p*-F), –161.90 (4F, s, *m*-H); HRMS m/z = 796.1490 (calcd. for $[C_{40}H_{22}N_4O_3F_{10}]^+$; $[M]^+$, m/z = 796.1527).

Synthesis of 5,15-Bis(pentafluorophenyl)corrole Si(IV) Complex (2b)
5,15-Bis(pentafluorophenyl)corrole **1b** (60 μmol, 38 mg) was dissolved in dry 1,2-dichloroethane (9.0 mL, 6.7 mM) and dry diisopropylethylamine (1.5 mL, 9.0 mmol, 150 eq.), to which tetrachlorosilane (0.36 mL, 3.0 mmol, 50 eq.) was slowly added. The reaction mixture was stirred at 60 °C for 40 h. Then, the reaction mixture was washed twice with NaOH aq. (2 × 50 mL, 1 M) and extracted with dichloromethane. The organic extract was neutralized with saturated NH_4Cl aq. and washed with brine. The organic extract was dried over anhydrous Na_2SO_4. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **2b** (50 μmol, 30 mg, 84%).
2b: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 10.20 (1H, s, *meso*-H), 9.52 (2H, d, J = 4.1 Hz, β-H), 9.41 (2H, d, J = 4.1 Hz, β-H), 9.13 (2H, d, J = 4.1 Hz, β-H), 9.04 (2H, d, J = 4.1 Hz, β-H), –4.50 (1H, s, Si-O<u>H</u>); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –136.26 (2F, m, *o*-F), –137.15 (2F, m, *o*-F), –152.28 (2F, t, J = 20.6 Hz, *p*-F), –161.37 (4F, m, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = –148.89 ppm; HRMS m/z = 672.0429 (calcd. for $[C_{31}H_{10}N_4OF_{10}Si]^+$; $[M]^+$, m/z = 672.0459); UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 377 (5.26×10^4), 400 (3.29×10^5), 559 (5.36×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm) λ_{max} / nm = 565, 615, Φ_F = 0.16, τ = 4.1 ns.

Synthesis of 5,15-Bis(pentafluorophenyl)-10-phenylcorrole Si(IV) Complex (2c)
5,10,15-Triphenylcorrole **2c** (480 μmol, 340 mg) was dissolved in dry 1,2-dichloroethane (72.0 mL, 6.7 mM) and dry diisopropylethylamine (12 mL, 72.0 mmol, 150 eq.), to which tetrachlorosilane (1.44 mL, 12.0 mmol, 50 eq.) was slowly added. The reaction mixture was stirred at 60 °C for 12 h. Then, the reaction mixture was washed twice with NaOH aq. (2 × 50 mL, 1 M) and extracted with dichloromethane. The organic extract was neutralized with

saturated NH_4Cl aq. and washed with brine. The organic extract was dried over anhydrous Na_2SO_4. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **2c** (326 μmol, 245 mg, 68%).

2c: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.51 (2H, d, J = 4.6 Hz, β-H), 9.02 (6H, m, β-H), 8.30 (1H, d, J = 7.1 Hz, *o*-H), 8.05 (1H, d, J = 7.1 Hz, *o*-H), 7.80 (3H, m, *m*-H, *p*-H), –4.47 (1H, s, Si-O<u>H</u>) ; ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –136.31 (2F, dd, J = 23.8, 6.5 Hz, *o*-F), –137.20 (2F, dd, J = 23.8, 6.5 Hz, *o*-F), –152.29 (2F, t, J = 20.6 Hz, *p*-H), –161.38 (4F, m, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = –148.18 ppm; HRMS *m*/*z* = 749.0835 (calcd. for $[C_{37}H_{15}N_4OF_{10}Si]^+$; $[M+H]^+$, *m*/*z* = 749.0850) ; UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 380 (5.80×10^4), 405 (3.66×10^5), 564 (3.80×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 573, 625, Φ_F = 0.20, τ = 4.1 ns.

Synthesis of 5,15-Bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole Si(IV) Complex (2d)

5,15-Bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole **2d** (480 μmol, 340 mg) was dissolved in dry 1,2-dichloroethane (72.0 mL, 6.7 mM) and dry diisopropylethylamine (12 mL, 72.0 mmol, 150 eq.), to which tetrachlorosilane (1.44 mL, 12.0 mmol, 50 eq.) was slowly added. The reaction mixture was stirred at 60 °C for 40 h. Then, the reaction mixture was washed twice with NaOH aq. (2 × 50 mL, 1 M) and extracted with dichloromethane. The organic extract was neutralized with saturated NH_4Cl aq. and washed with brine. The organic extract was dried over anhydrous Na_2SO_4. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **2d** (417 μmol, 350 mg, 87%).

2d: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.45 (2H, d, J = 4.1 Hz, β-H), 8.95 (6H, m, β-H), 6.62 (1H, d, J = 2.1 Hz, *m*-H), 6.56 (1H, d, J = 2.1 Hz, *m*-H), 4.10 (3H, s, -OC<u>H</u>$_3$), 3.61 (3H, s, -OC<u>H</u>$_3$), 3.44 (3H, s, -OC<u>H</u>$_3$), –4.29 (1H, s, -Si-O<u>H</u>); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –136.25 (2F, dd, J = 23.8, 6.5 Hz, *o*-F), –137.05 (2F, dd, J = 23.8, 6.5 Hz, *o*-F), –152.69 (2F, t, J = 21.7 Hz, *p*-F), –161.66 (4F, dtd, J = 95.4, 22.8, 7.9 Hz, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = –148.99 ppm ; HRMS *m*/*z* = 839.1149 (calcd. for $[C_{40}H_{20}N_4OF_{10}Si]^+$; $[M+H]^+$, *m*/*z* = 839.1167); UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 381 (4.82×10^4), 405 (2.84×10^5), 565 (3.86×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 570, 616, Φ_F = 0.20, τ = 4.2 ns.

Synthesis of μ-Oxo Silicon(IV) 5,15-Bis(pentafluorophenyl)corrole Dimer (3b)

Silicon complex **2b** (156 μmol, 105 mg) was dissolved in dry pyridine (1 mL).

Methanesulfonyl chloride (49 μL, 624 μmol, 4 eq.) was slowly added to the solution. The reaction mixture was stirred at 100 °C for 5 h. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **3b** (15.0 mg, 15%).

3b: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.08 (2H, s, *meso*-H), 8.89 (4H, d, J = 3.7 Hz, β-H), 8.71 (4H, d, J = 4.1 Hz, β-H), 8.42 (4H, d, J = 4.1 Hz, β-H), 8.35 (4H, d, J = 4.1 Hz, β-H); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –134.34 (4F, d, J = 21.7 Hz, *o*-F), –137.08 (4F, t, J = 13.0 Hz, *o*-F), –153.12 (4F, t, J = 21.7 Hz, *m*-F), –161.96 (8F, m, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = –164.58 ppm; HRMS m/z = 1327.0888 (calcd. for $[C_{62}H_{19}N_8OF_{20}Si_2]^+$; $[M+H]^+$, m/z = 1327.0896); UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 384 (5.33×10^5), 565 (5.90×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 565 nm): λ_{max} / nm = 594, 645, Φ_F = 0.06, τ_1 = 3.1 ns, τ_2 = 6.5 ns.

Synthesis of *μ*-Oxo Silicon(IV) 5,15-Bis(pentafluorophenyl)-10-phenylcorrole Dimer (3c)

Silicon complex **2c** (190 μmol, 140 mg) was dissolved in dry pyridine (1 mL). Methanesulfonyl chloride (59 μL, 760 μmol, 4 eq.) was slowly added to the solution. The reaction mixture was stirred at 100 °C for 5 h. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **3c** (59.0 mg, 43%).

3c: ^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 25 °C) δ / ppm = 9.03 (4H, d, J = 4.1 Hz, β-H), 8.45 (4H, d, J = 4.2 Hz, β-H), 8.41 (8H, m, β-H), 7.90 (2H, br-s, Ph-H), 7.86 (2H, br-s, Ph-H), 7.81 (2H, t, J = 7.8 Hz, *p*-H), 7.72 (2H, br-s, Ph-H), 7.67 (2H, br-s, Ph-H); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –133.99 (4F, d, J = 21.7 Hz, *o*-F), –137.30 (4F, d, J = 17.3 Hz, *o*-F), –153.11 (4F, t, J = 20.6 Hz, *p*-F), –161.77 (4F, t, J = 18.4 Hz, *m*-F), –163.00 (4F, t, J = 18.4 Hz, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = –166.39 ppm ; HRMS m/z = 1479.1458 (calcd. for $[C_{74}H_{27}N_8OF_{20}Si_2]^+$; $[M+H]^+$, m/z = 1479.1522); UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 391 (4.80×10^5), 565 (4.65×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 592, 653, Φ_F = 0.08, τ_1 = 2.0 ns, τ_2 = 5.7 ns.

Synthesis of *μ*-Oxo Silicon(IV) 5,15-Bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole Dimer (3d)

Silicon complex **2d** (200 μmol, 168 mg) was dissolved in dry pyridine (1 mL). Methanesulfonyl chloride (62 μL, 800 μmol, 4 eq.) was slowly added to the solution. The reaction mixture was stirred at 100 °C for 5 h. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-

hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **3d** (12.0 mg, 7%).

3d: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.07 (4H, s, β-H), 8.60 (4H, s, β-H), 8.16 (8H, d, J = 14.2 Hz, β-H), 6.54 (2H, d, J = 2.3 Hz, Ph-H), 6.19 (2H, d, J = 2.3 Hz, Ph-H), 4.01 (6H, s, -OC$\underline{H}_3$), 3.43 (6H, s, -OC$\underline{H}_3$), 2.84 (6H, s, -OC$\underline{H}_3$) ;^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –133.17 (4F, s, *o*-F), –137.05 (4F, s, *o*-F), –153.92 (4F, s, *p*-F), –162.32 (4F, s, *m*-F), –163.11 (4F, s, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = –165.03 ppm. HRMS m/z = 1658.2085 (calcd. for $[C_{80}H_{38}N_8O_7F_{20}Si_2]^+$; $[M]^+$, m/z = 1658.2088); UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 390 (3.35×10^5), 567 (2.30×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 673, Φ_F = 0.13, τ = 8.5 ns.

Synthesis of Trimethylsiloxosilicon(IV) 5,10,15-Tris(pentafluorophenyl)corrole (4a)

Silicon complex **2a** (72 μmol, 60 mg) dissolved in dry THF (40 mM) was added trimethylchlorosilane (1.5 mL, 12 mmol, 167 eq.). The reaction mixture was stirred at room temperature for 30 min. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **4a** (42.0 mg, 64%).

4a: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) (δ / ppm) = (2H, d, J = 4.1 Hz, β-H), 9.08 (2H, d, J = 4.6 Hz, β-H), 9.04 (2H, d, J = 4.1 Hz, β-H), 8.88 (2H, d, J = 4.6 Hz, β-H), –2.57 (9H, m, Si(C$\underline{H}_3$)$_3$); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) (δ / ppm) = –136.35 (1F, dd, J = 23.8, 6.5 Hz, *o*-F), –136.5(1F, dd, J = 23.8, 6.5 Hz, *o*-F), –137.12 (2F, dd, J = 23.8, 6.5 Hz, *o*-F), –152.00 (2F, m, *p*-F), –161.24 (4F, m, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25°C) (δ / ppm) = 3.83 (Si(CH$_3$)$_3$), –158.28 (corrole-Si).; HRMS m/z = 910.0715 (calcd. for $[C_{40}H_{17}N_4OF_{15}Si_2]^+$;$[M]^+$, m/z = 910.0696) ; UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) =379 (4.72×10^4) 405 (3.19×10^5), 558 (2.73×10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 569, 621, Φ_F = 0.10, τ = 4.4 ns.

Synthesis of Trimethylsiloxosilicon(IV) 5,15-Bis(pentafluorophenyl)corrole (4b).

Silicon complex **2b** (80 μmol, 60 mg) was dissolved in dry THF (40 mM). TMSCl (1.5 mL, 12 mmol, 150 eq.) was added to the solution. The reaction mixture was stirred at room temperature for 30 min. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **4b** (42.0 mg, 64%).

4b: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 10.14 (1H, s, *meso*-H), 9.48 (2H, d, J = 4.1 Hz, β-H), 9.36 (2H, d, J = 4.6 Hz, β-H), 9.09 (2H, d, J = 4.6 Hz, β-H), 9.02 (2H, d, J = 4.1 Hz, β–H), –2.62 (9H, s, Si(C$\underline{H}_3$)$_3$); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –136.58 (2F, dd, J = 24.9, 7.6 Hz, *o*-F), –137.19 (2F, dd, J = 10.8 Hz, *o*-F), –152.62 (2F, t, J = 21.1 Hz, *p*-F), –161.60(4F, m,

m-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = 2.82 (Si(CH_3)$_3$), –158.08 (corrole-Si); HRMS *m*/*z* = 745.0932 (calcd. for $[C_{34}H_{19}N_4OF_{10}Si_2]^+$; [*M*+H]$^+$, *m*/*z* = 745.0932; UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 377 (5.31 × 10^4), 400 (3.31 × 10^5), 559 (5.88 × 10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 563, 615, Φ_F = 0.16, τ = 4.0 ns.

Synthesis of Trimethylsiloxosilicon(IV) 5,15-Bis(pentafluorophenyl)-10-phenylcorrole (4c)

Silicon complex **2c** (60 μmol, 40 mg) was dissolved in dry THF (40 mM). TMSCl (1.5 mL, 12 mmol, 200 eq.) was added to the solution. The reaction mixture was stirred at room temperature for 30 min. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **4c** (25.0 mg, 56%).

4c: ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) δ / ppm = 9.48 (2H, d, *J* = 4.1 Hz, *β*-H), 9.00 (6H, m, *β*-H), 8.31 (1H, d, *J* = 7.3 Hz, Ph-H), 8.04 (1H, d, *J* = 6.9 Hz, Ph-H), 7.80 (3H, m, Ph-H), –2.54 (9H, s, Si(C$\underline{H}_3$)$_3$); ^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) δ / ppm = –136.68 (2F, dd, *J* = 23.8, 6.5 Hz, *o*-F), –137.32 (2F, dd, *J* = 23.8, 6.5 Hz, *o*-F), –152.67 (2F, t, *J* = 20.6 Hz, *m*-F), –161.63 (4F, m, *p*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) δ / ppm = 2.44 (Si(CH_3)$_3$), –157.98 (corrole-Si); HRMS *m*/*z* = 821.1218 (calcd. for $[C_{40}H_{23}N_4OF_{10}Si_2]^+$; [*M*+H]$^+$, *m*/*z* = 821.1245; UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 382 (6.10 × 10^4), 405 (3.53 × 10^5), 565 (4.11 × 10^4). Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 573, 624, Φ_F = 0.16, τ = 4.0 ns.

Synthesis of Trimethylsiloxosilicon(IV) 5,15-Bis(pentafluorophenyl)-10-2,4,6-trimethoxyphenylcorrole (4d)

Silicon complex **2d** (72 μmol, 60 mg) was dissolved in dry THF (40 mM). TMSCl (1.5 mL, 12 mmol, 167 eq.) was added to the solution. The reaction mixture was stirred at room temperature for 30 min. After the solvent was removed under reduced pressure, the residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane as an eluent. Recrystallization from dichloromethane/*n*-hexane afforded **4d** (14.5 mg, 22%).

4d : ^{1}H NMR (600 MHz, $CDCl_3$, 25 °C) (δ / ppm) = 9.41 (2H, d, *J* = 4.1 Hz, *β*-H), 8.93 (6H, m, *β*-H), 6.62 (1H, d, *J* = 2.3 Hz, Ph-H), 6.56 (1H, d, *J* = 2.3 Hz, Ph-H), 4.11 (3H, s, -OC$\underline{H}_3$), 3.55 (3H, s, -OC$\underline{H}_3$), 3.46 (3H, s, -OC$\underline{H}_3$), –2.51 (9H, s, Si(C$\underline{H}_3$)$_3$);^{19}F NMR (565 MHz, $CDCl_3$, 25 °C) (δ/ ppm) = –136.60 (2F, dd, *J* = 24.9, 7.6 Hz, *o*-F), –137.16 (2F, dd, *J* = 23.8, 6.5 Hz, *p*-F), –152.96 (2F, t, *J* = 20.6 Hz), –161.85 (4F, m, *m*-F); ^{29}Si NMR (119 MHz, $CDCl_3$, 25 °C) (δ / ppm) = 2.35 (Si(CH_3)$_3$), –157.86 (corrole-Si); HRMS *m*/*z* = 910.1445 (calcd. for $[C_{43}H_{28}N_4O_4F_{10}Si_2]^+$; [*M*]$^+$, *m*/*z* = 910.1484); UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 384 (6.19×10^4), 406 (3.26×10^5), 565 (5.04×10^4). Fluorescence (CH_2Cl_2, λ_{ex}= 400 nm): λ_{max} / nm = 571, 624, Φ_F = 0.15, τ = 4.3 ns.

2. NMR Spectra

5,15-Bis(pentafluorophenyl)-10-phenylcorrole **1c**

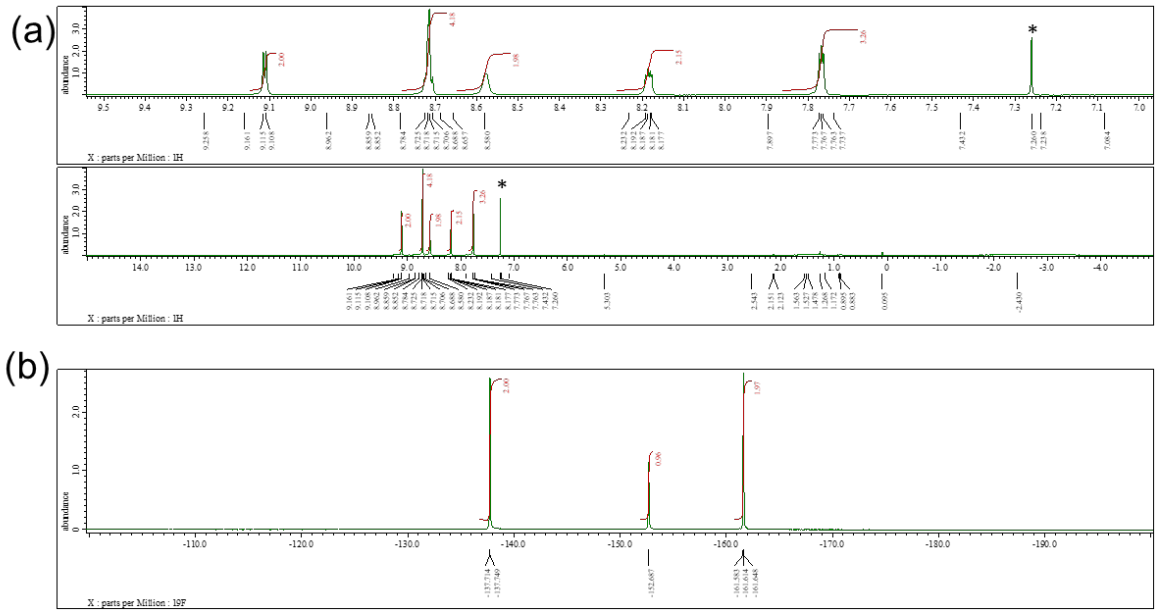


Figure S2-1. (a) ^{1}H and (b) ^{19}F NMR spectra of **1c** in $CDCl_3$ at room temperature. A peak marked with * is due to residual solvents and impurities.

5,15-Bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole **1d**

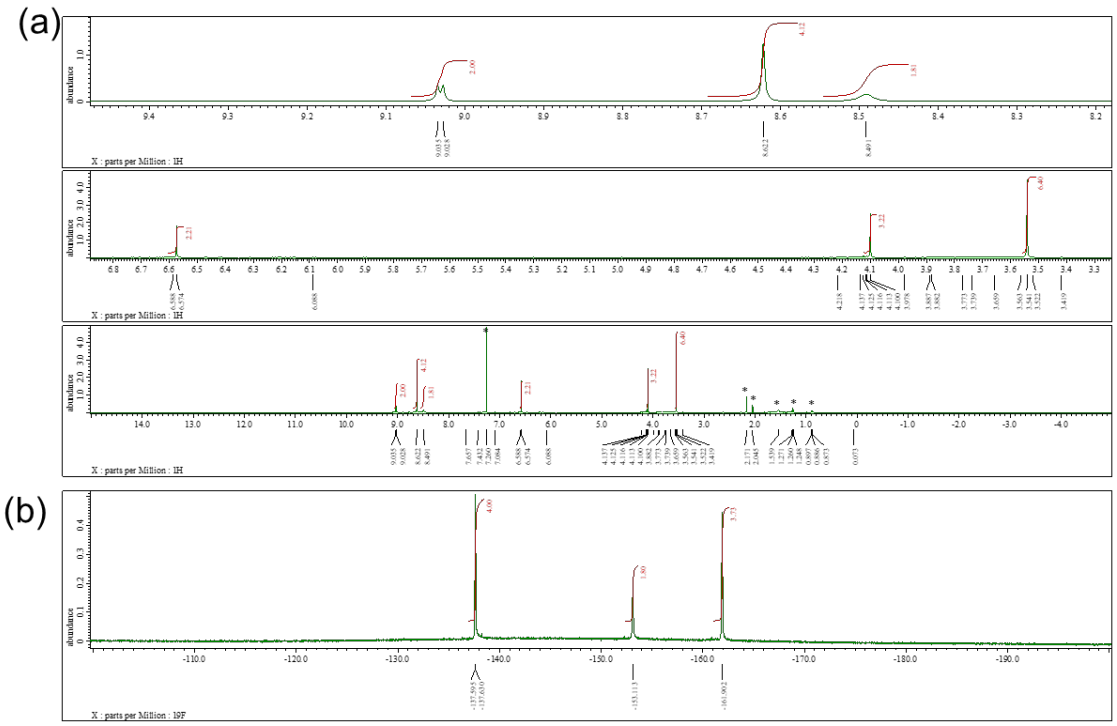


Figure S2-2. (a) ^{1}H and (b) ^{19}F NMR spectra of **1c** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

5,15-Bis(pentafluorophenyl)corrole Si(IV) complex **2b**

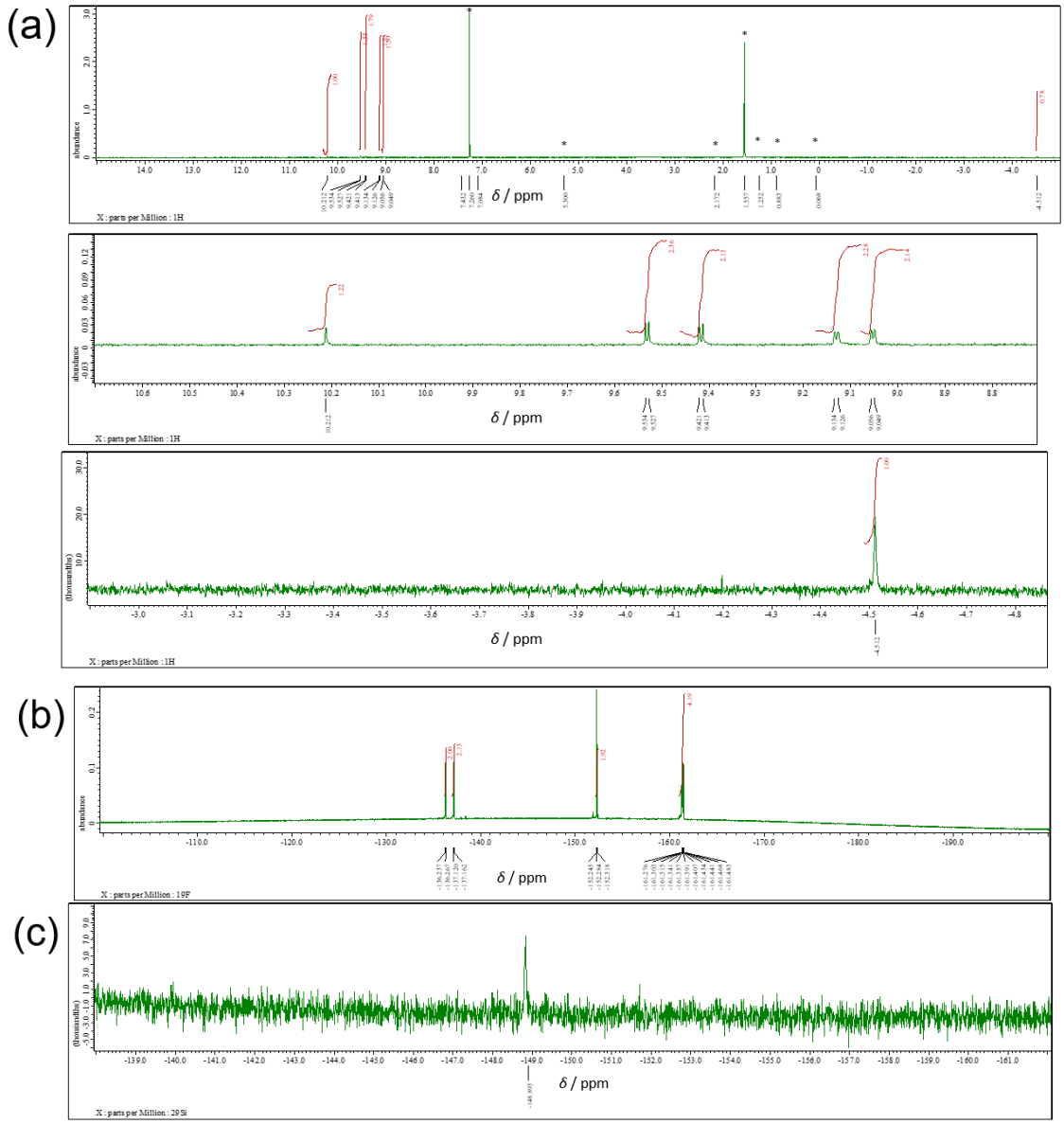


Figure S2-3. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **2b** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

5,15-Bis(pentafluorophenyl)-10-phenylcorrole Si(IV) complex **2c**

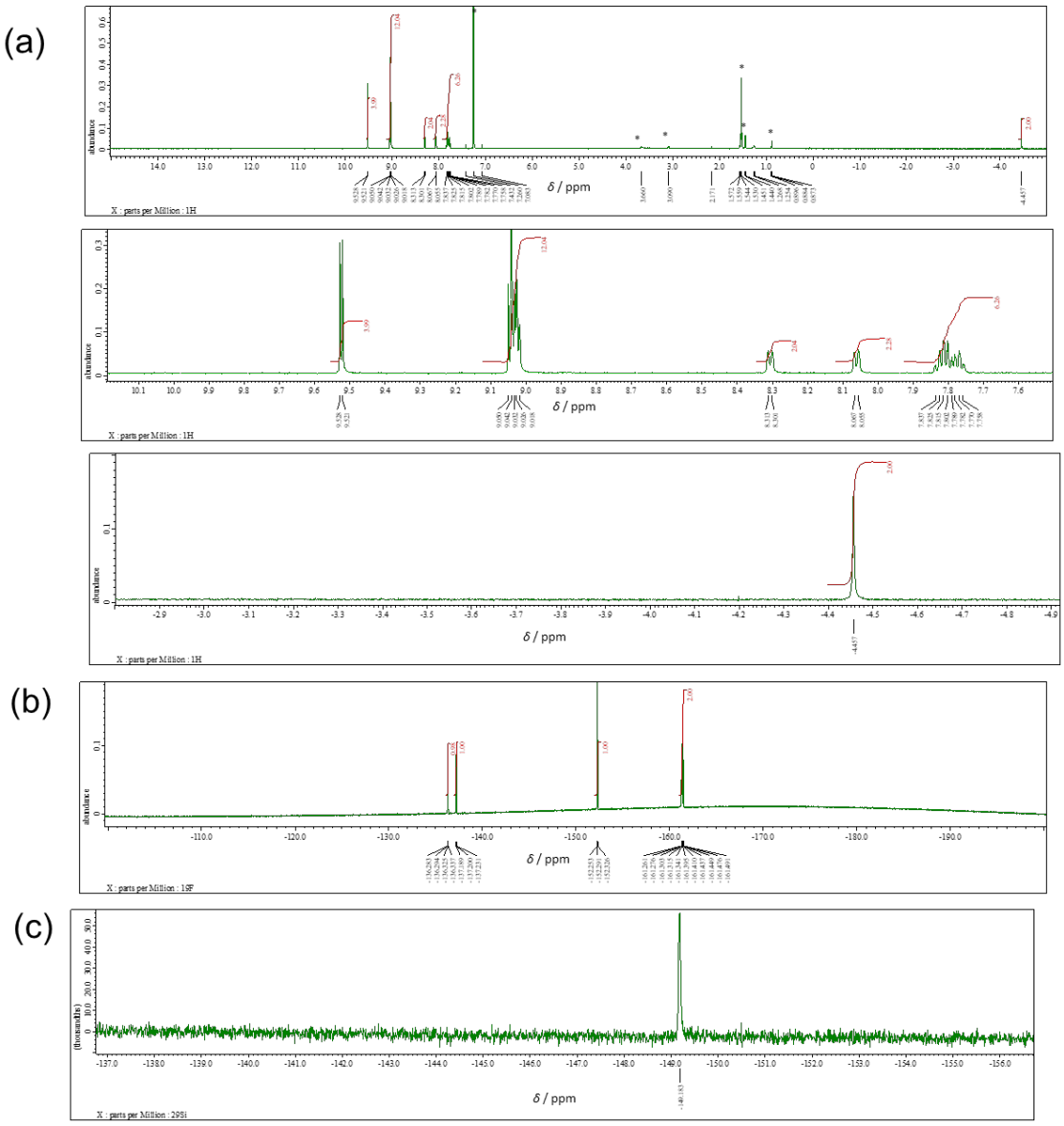


Figure S2-4. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **2c** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

5,15-Bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole Si(IV) complex **2d**

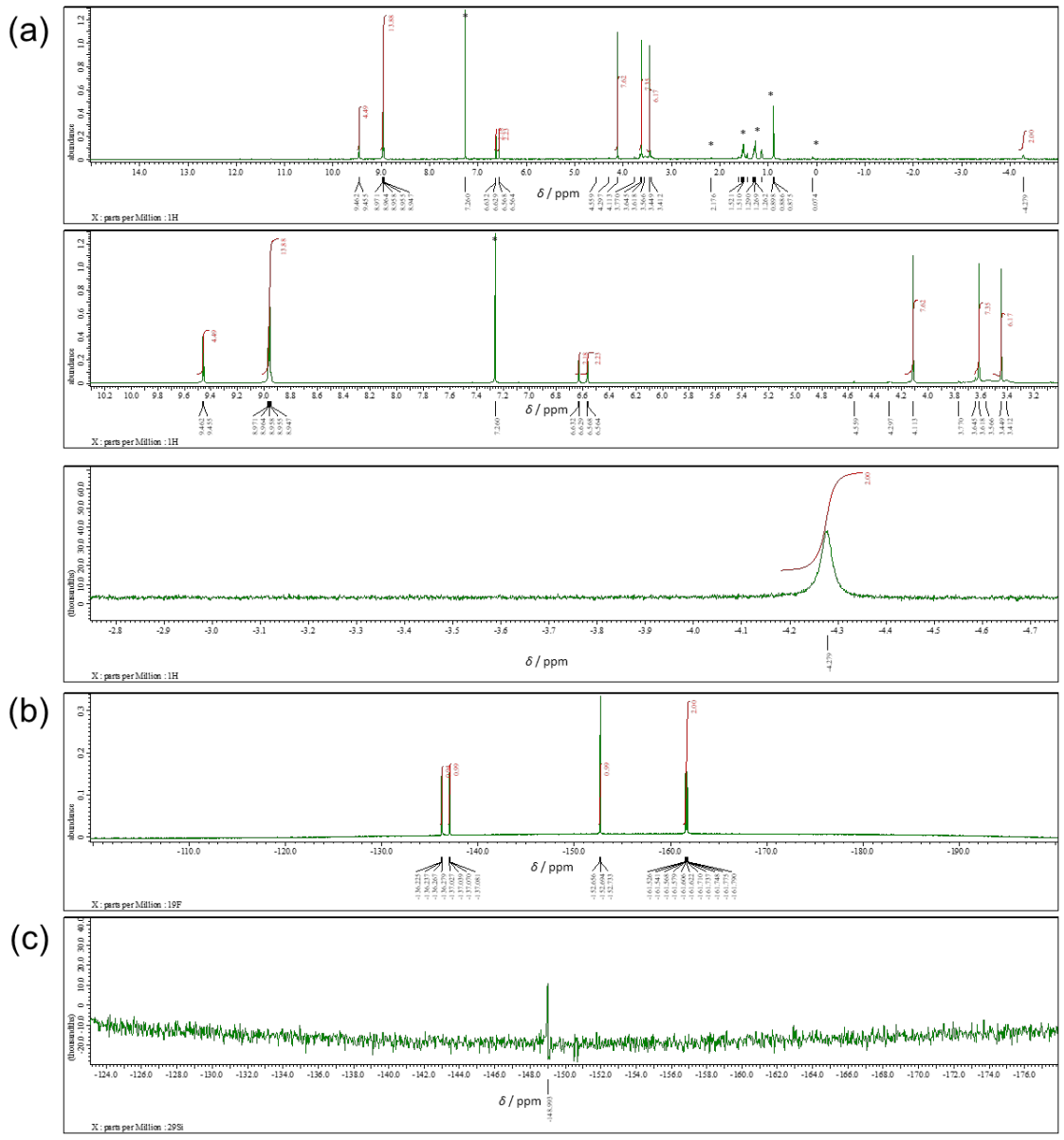


Figure S2-5. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **2d** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

μ-Oxo Si(IV) 5,15-bis(pentafluorophenyl)corrole dimer **3b**

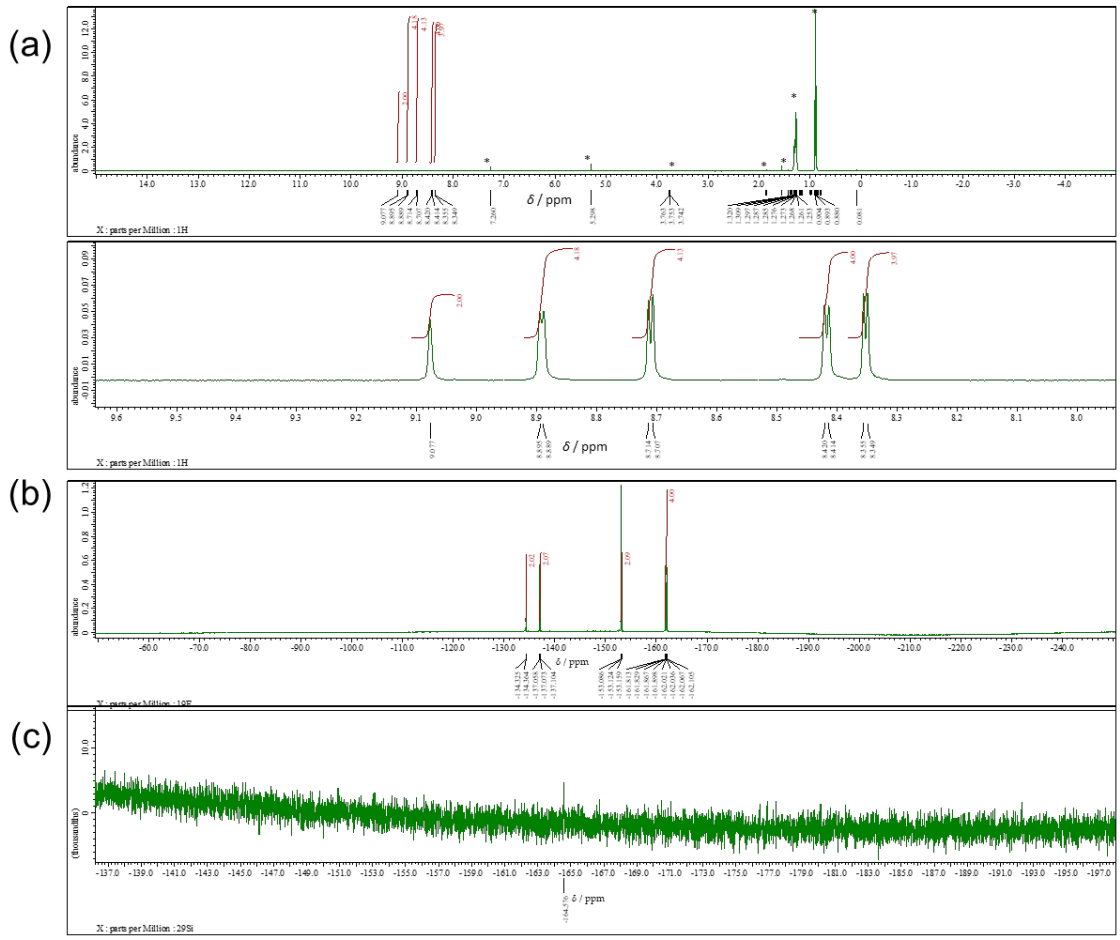


Figure S2-6. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **3b** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

μ-Oxo Si(IV) 5,15-bis(pentafluorophenyl)-10-phenylcorrole dimer **3c**

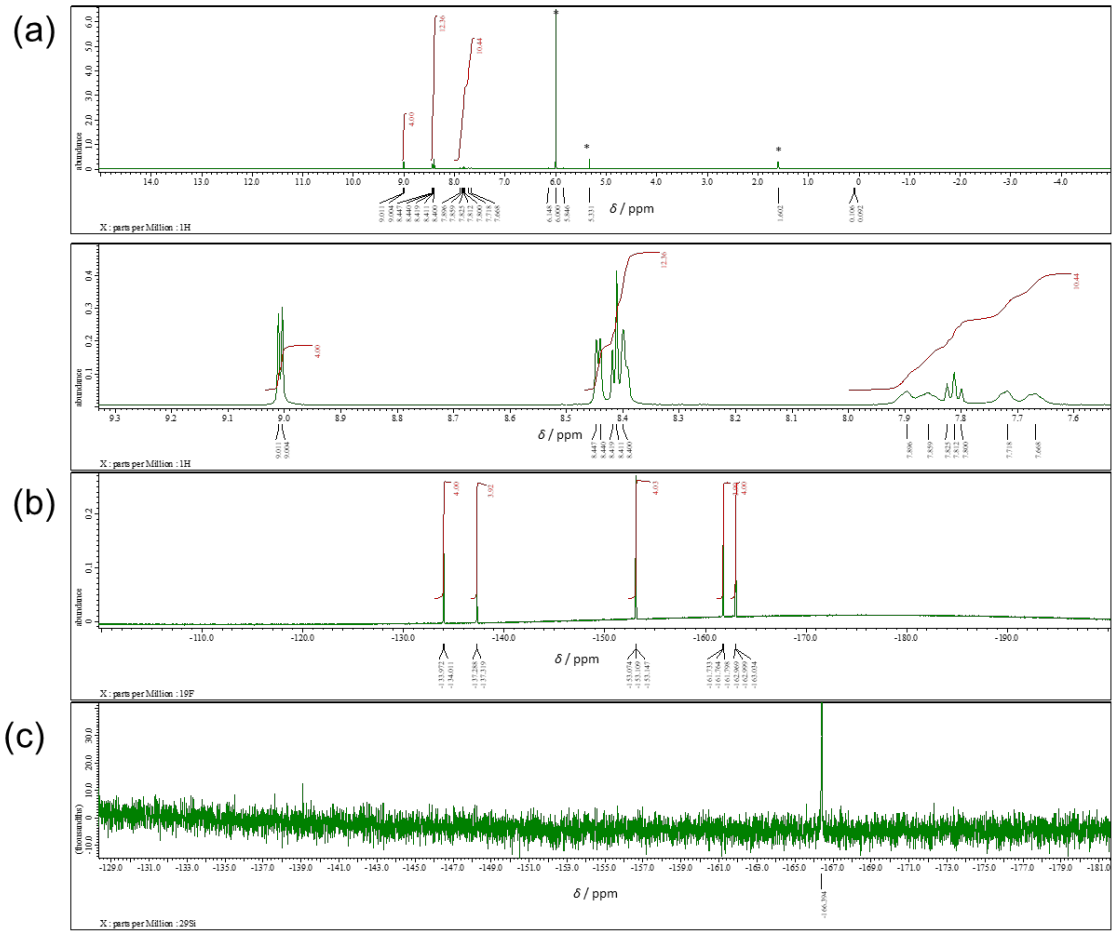


Figure S2-7. (a) ^{1}H NMR spectra of **3c** in $C_2D_2Cl_4$ and (b) ^{19}F and (c) ^{29}Si NMR spectra of **3c** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

μ-Oxo Si(IV) 5,15-bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole dimer **3d**

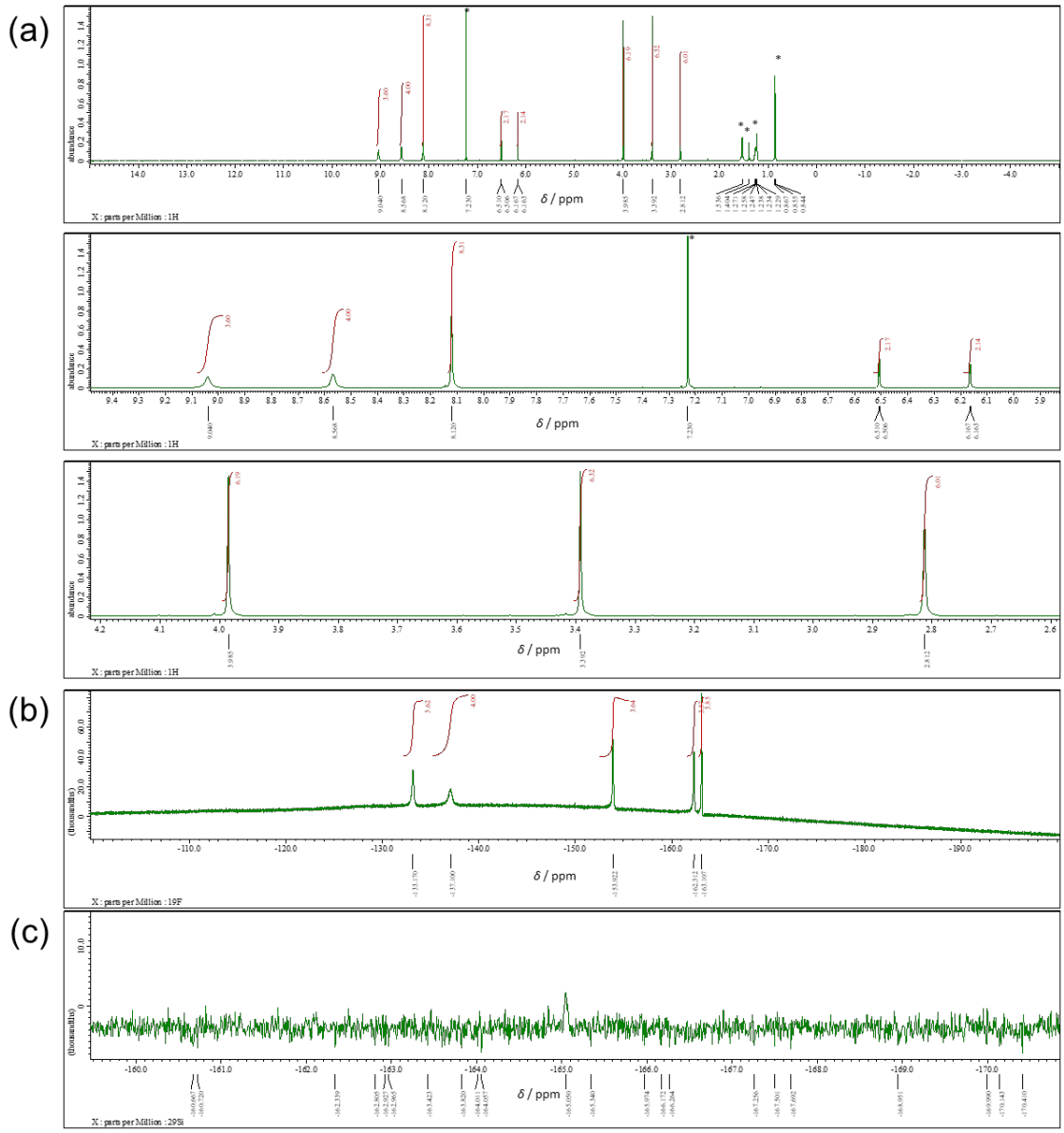


Figure S2-8. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **3d** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

Trimethylsiloxy-substituted Si(IV) 5,10,15-tris(pentafluorophenyl)corrole **4a**

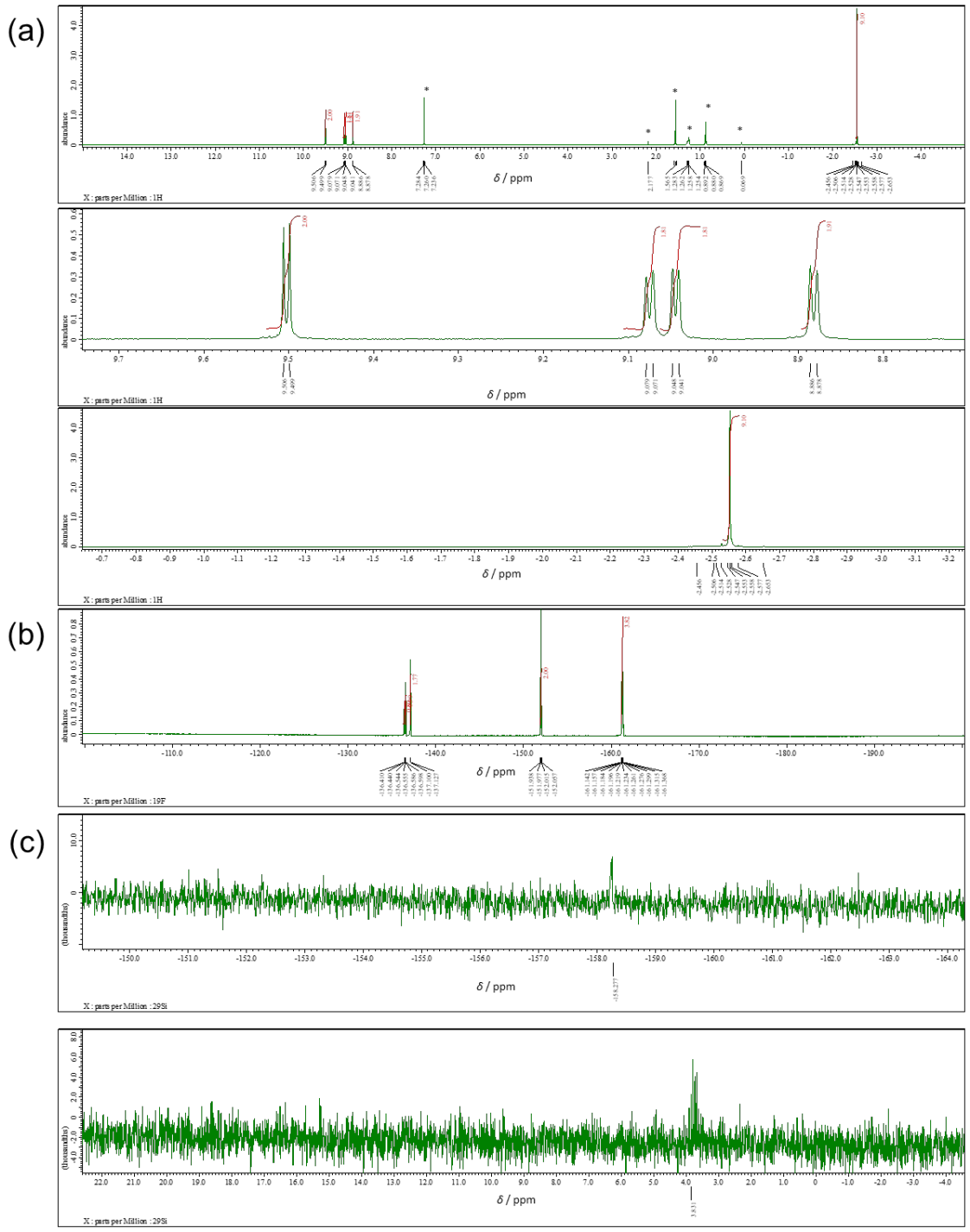


Figure S2-9. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **4a** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

Trimethylsiloxy-substituted Si(IV) 5,15-bis(pentafluorophenyl)corrole **4b**

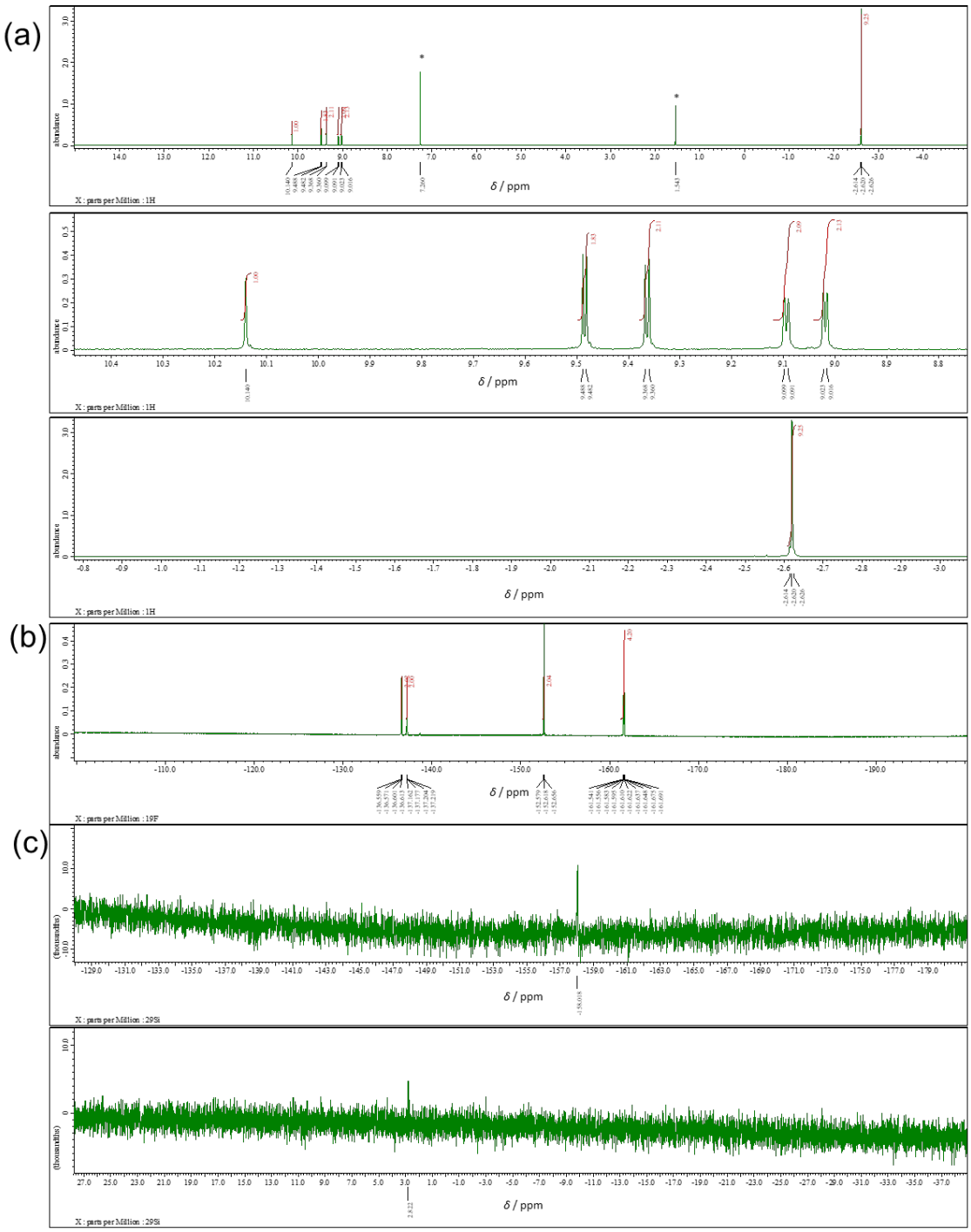


Figure S2-10. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **4b** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

Trimethylsiloxy-substituted Si(IV) 5,15-bis(pentafluorophenyl)-10-phenylcorrole **4c**

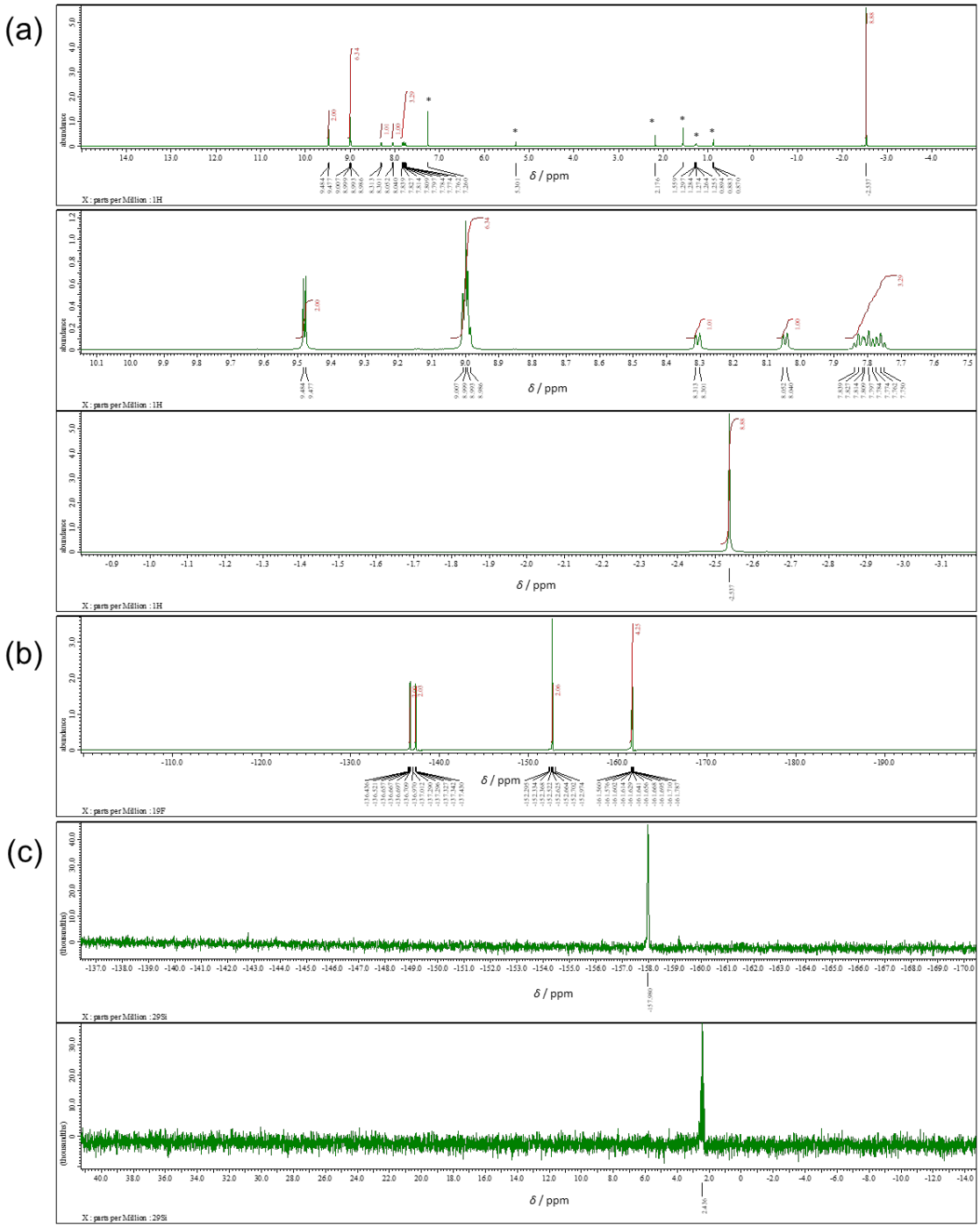


Figure S2-11. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **4c** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

Trimethylsiloxy-substituted Si(IV) 5,15-bis(pentafluorophenyl)-10-(2,4,6-trimethoxyphenyl)corrole dimer **4d**

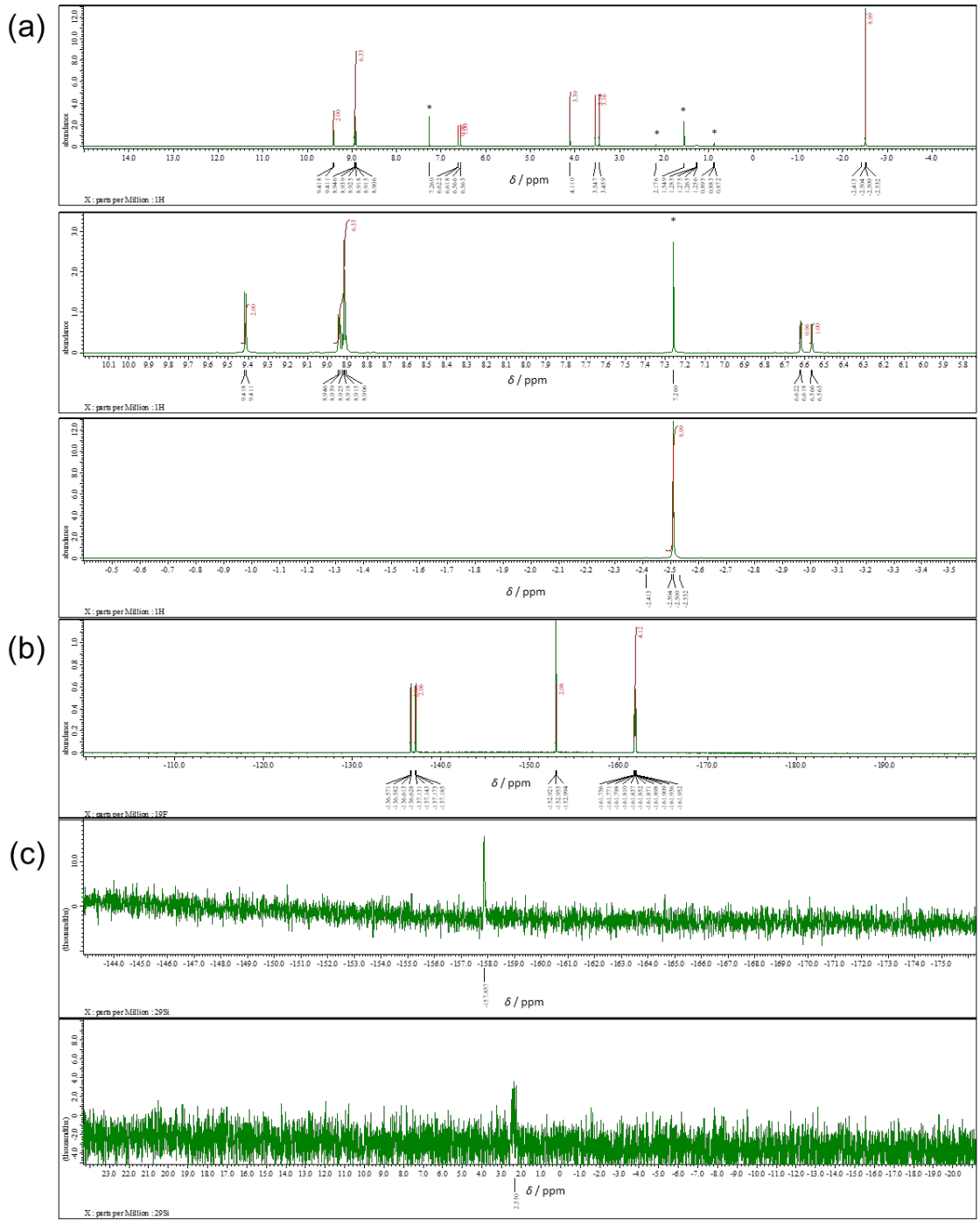


Figure S2-12. (a) ^{1}H, (b) ^{19}F and (c) ^{29}Si NMR spectra of **4d** in $CDCl_3$ at room temperature. Peaks marked with * are due to residual solvents and impurities.

3. Mass Spectra

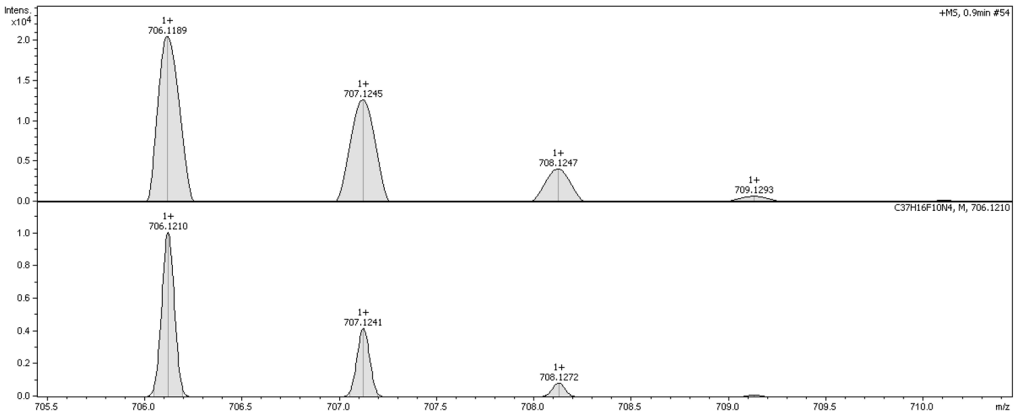


Figure S3-1. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **1c**. *m*/*z* = 706.1189 (calcd. for $[C_{37}H_{16}N_4F_{10}]^+$;$[M]^+$, *m*/*z* = 706.1210)

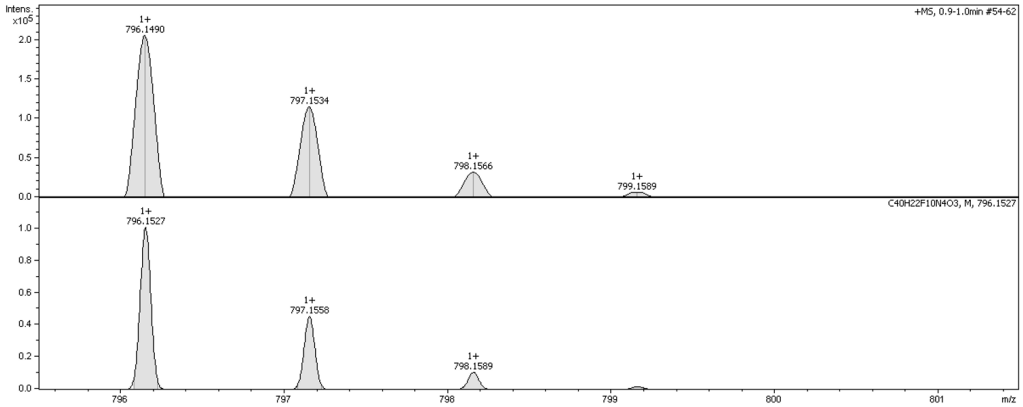


Figure S3-2. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **1d**. *m*/*z* = 796.1490 (calcd. for $[C_{40}H_{22}N_4O_3F_{10}]^+$;$[M]^+$, *m*/*z* = 796.1527)

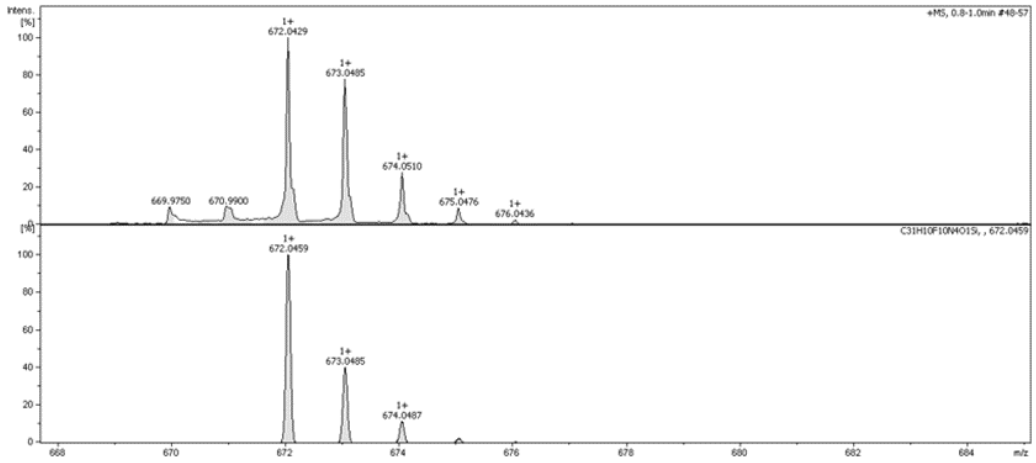


Figure S3-3. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **2b**. m/z = 672.0429 (calcd. for $[C_{31}H_{10}N_4OF_{10}Si]^+$;$[M]^+$, m/z = 672.0459)

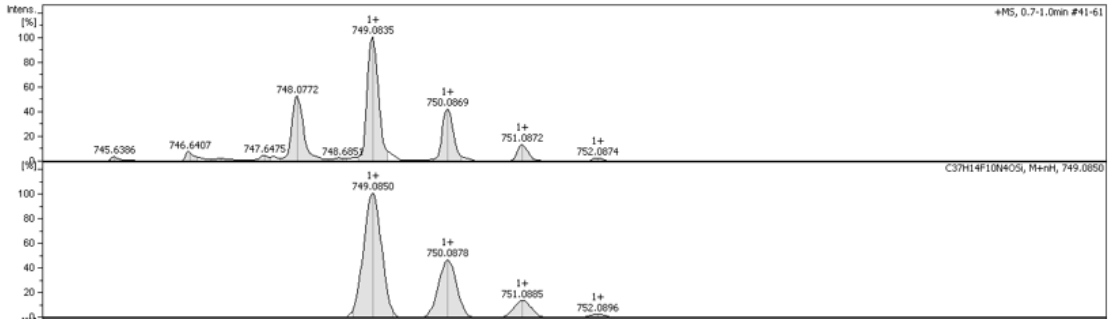


Figure S3-4. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **2c**. m/z = 749.0835 (calcd. for $[C_{37}H_{15}N_4OF_{10}Si]^+$;$[M+H]^+$, m/z = 749.0850)

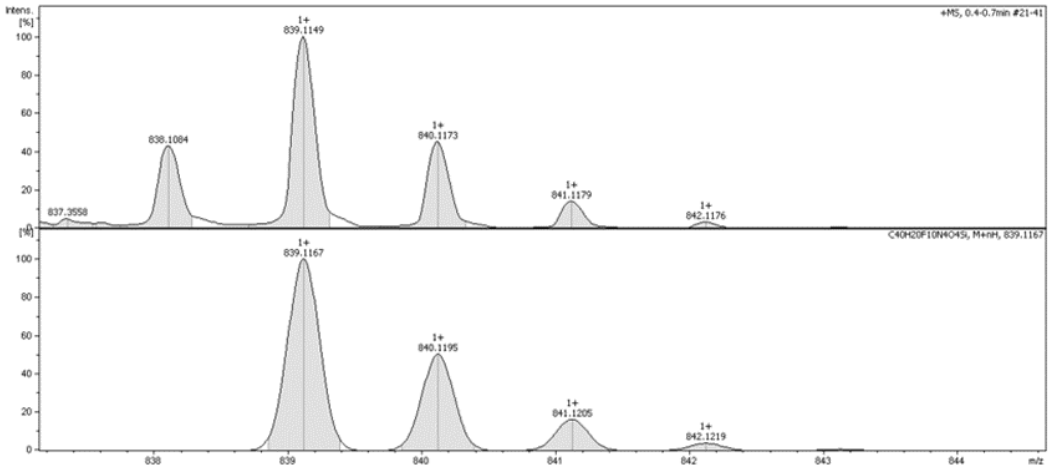


Figure S3-5. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **2d**. m/z = 839.1149 (calcd. for $[C_{40}H_{21}N_4OF_{10}Si]^+$;$[M+H]^+$, m/z = 839.1167)

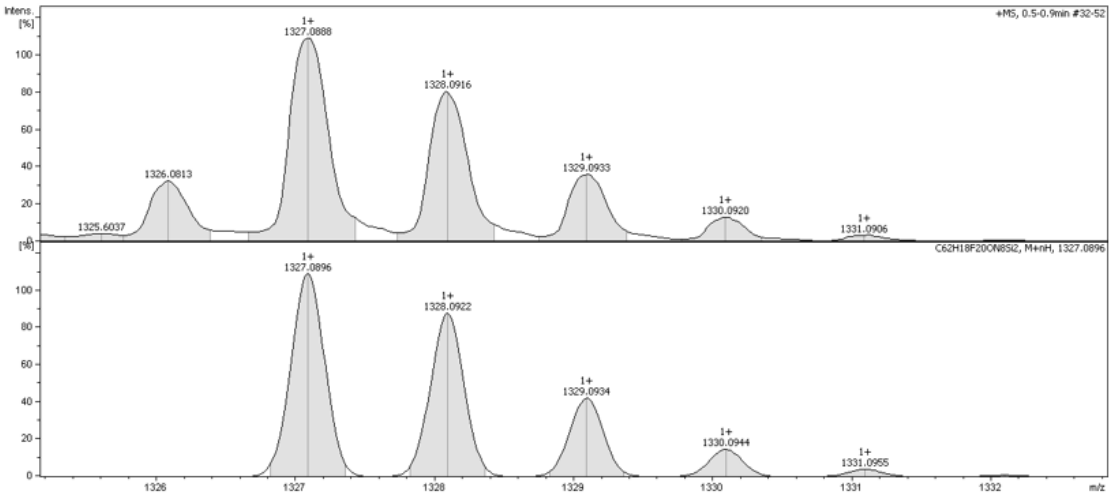


Figure S3-6. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **3b**.
m/*z* = 1327.0888 (calcd. for $[C_{62}H_{19}N_8OF_{20}Si_2]^+$;$[M+H]^+$, *m*/*z* = 1327.0896)

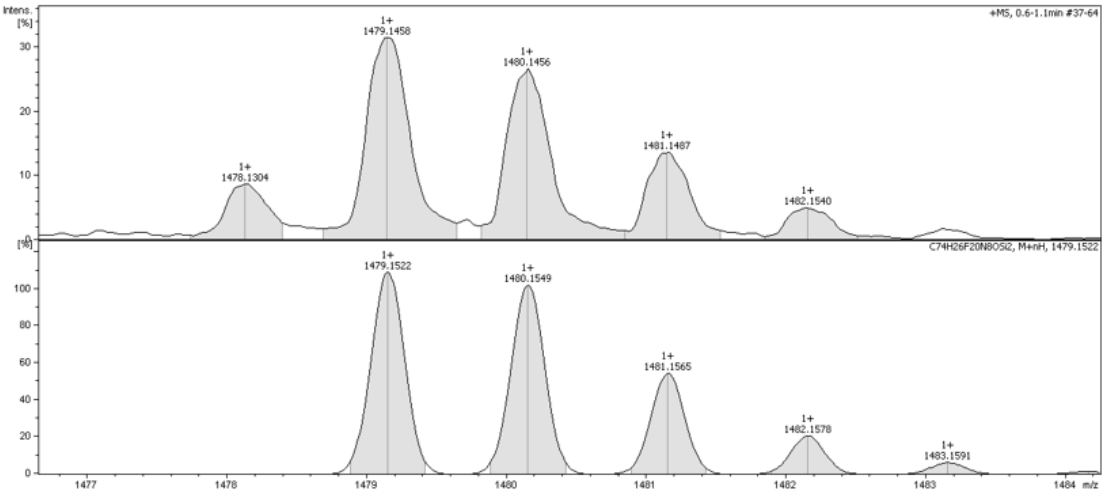


Figure S3-7. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **3c**.
m/*z* = 1479.1458 (calcd. for $[C_{74}H_{27}N_8OF_{20}Si_2]^+$;$[M+H]^+$, *m*/*z* = 1479.1522)

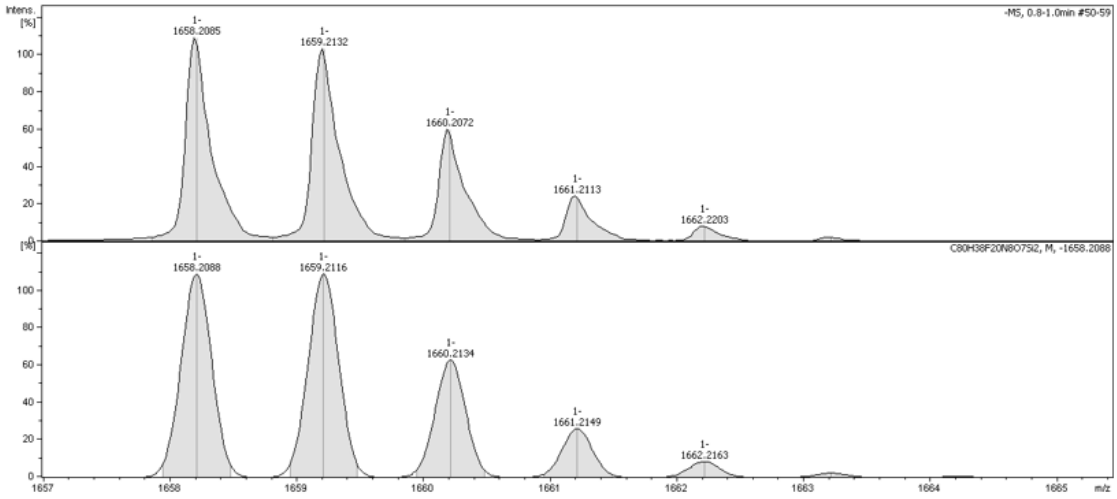


Figure S3-8. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **3d**.
m/*z* = 1658.2085 (calcd. for $[C_{80}H_{38}N_8O_7F_{20}Si_2]^+$;$[M]^+$, *m*/*z* = 1658.2088)

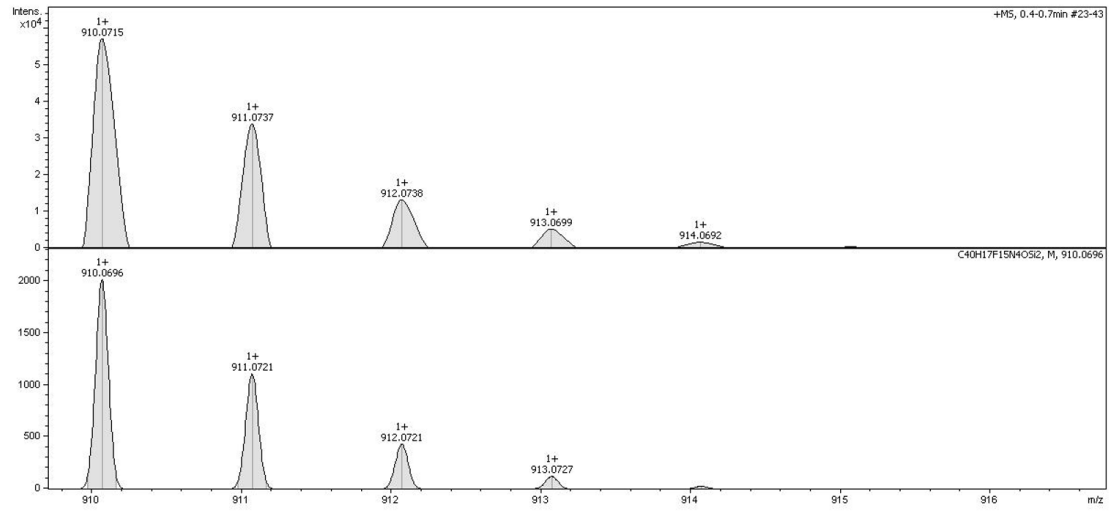


Figure S3-9. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **4a**.
m/*z* = 910.0715 (calcd. for $[C_{40}H_{17}N_4OF_{15}Si_2]^+$;$[M]^+$, *m*/*z* = 910.0696)

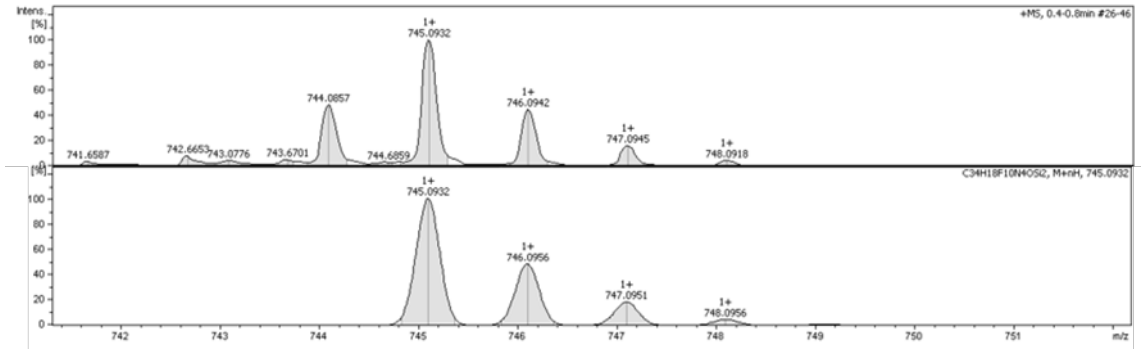


Figure S3-10. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **4b**.
m/*z* = 745.0932 (calcd. for $[C_{34}H_{19}N_4OF_{10}Si_2]^+$;$[M+H]^+$, *m*/*z* = 745.0932)

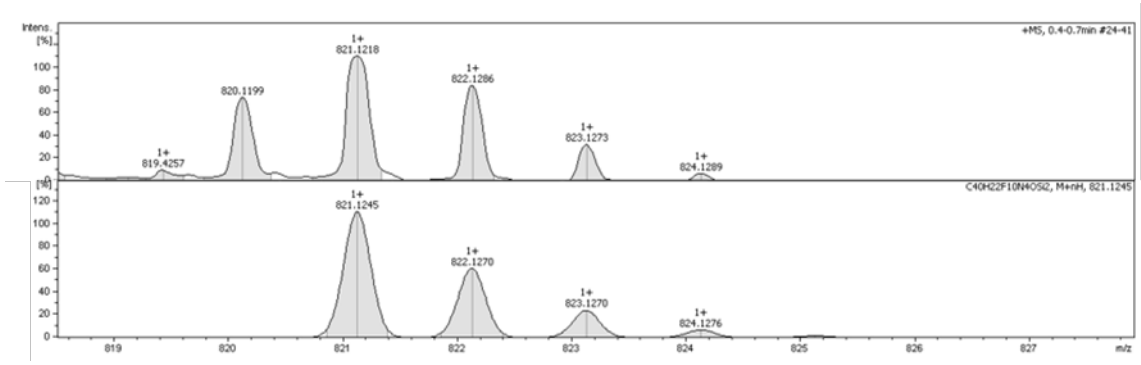


Figure S3-11. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **4c**.
m/*z* = 821.1218 (calcd. for $[C_{40}H_{23}N_4OF_{10}Si_2]^+$;$[M+H]^+$, *m*/*z* = 821.1245)

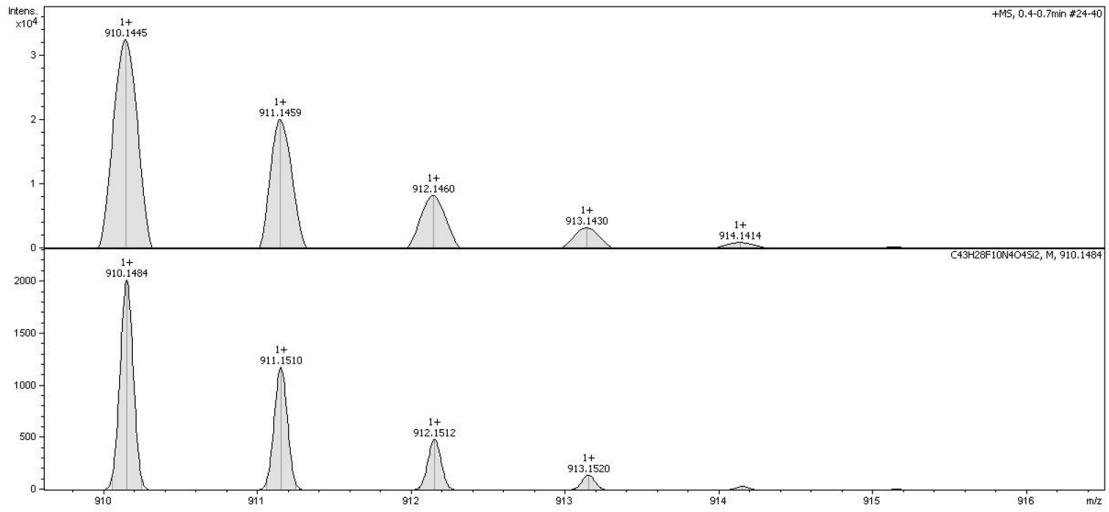


Figure S3-12. Observed (top) and simulated (bottom) HR-APCI-TOF-MS of **4d**.
m/*z* = 910.1445 (calcd. for $[C_{43}H_{28}N_4O4F_{10}Si_2]^+$;$[M]^+$, *m*/*z* = 910.1484)

4. Electrochemical Properties

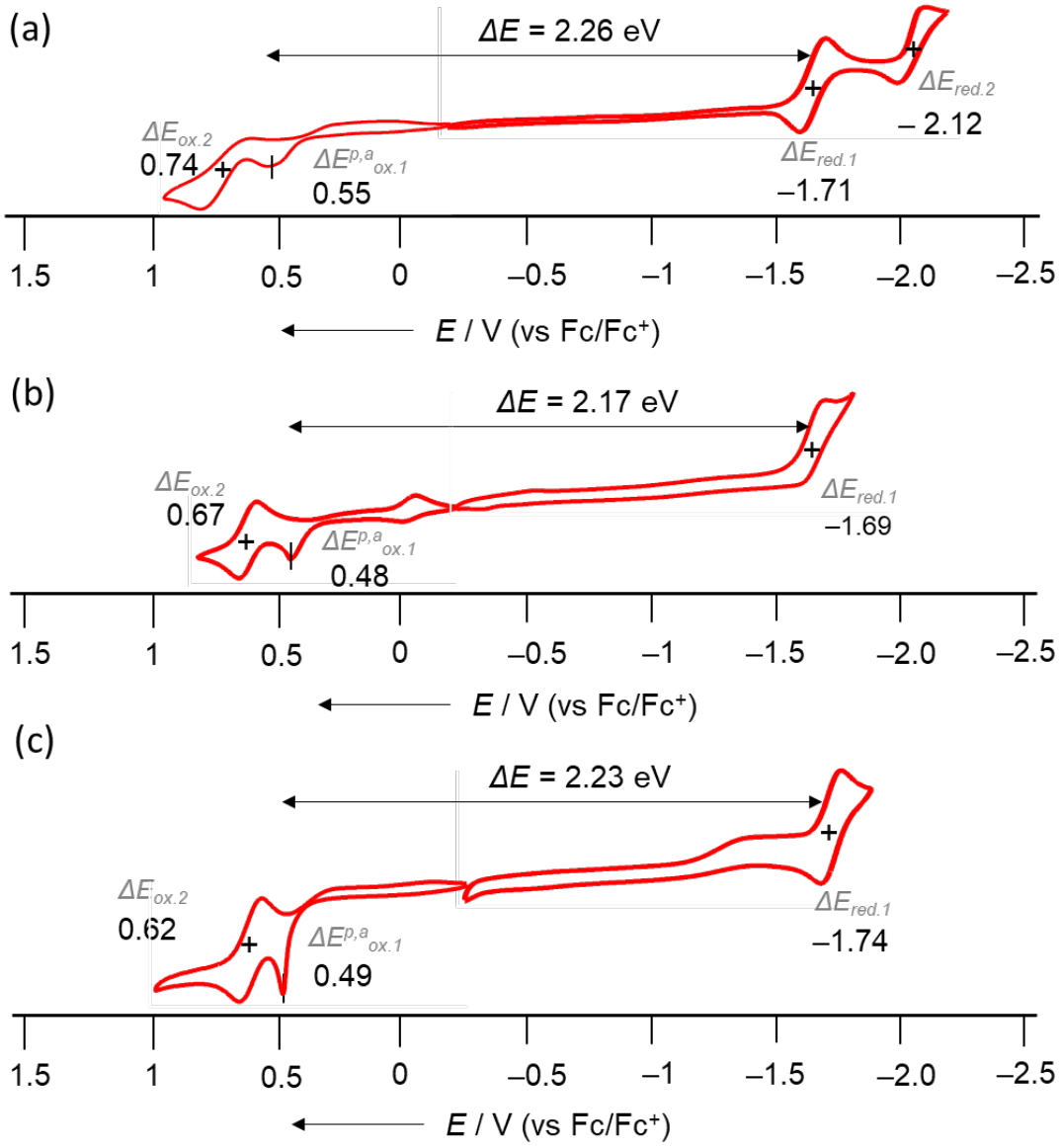


Figure S4-1. Cyclic voltammograms of (a) **2b**, (b) **2c** and (c) **2d**. Measurement conditions: solvent: CH_2Cl_2; scan rate: 0.05 V/s; working electrode: glassy carbon; reference electrode: $Ag/AgNO_3$; counter electrode: Pt; supporting electrolyte: 0.1 M *n*-Bu_4NPF_6.

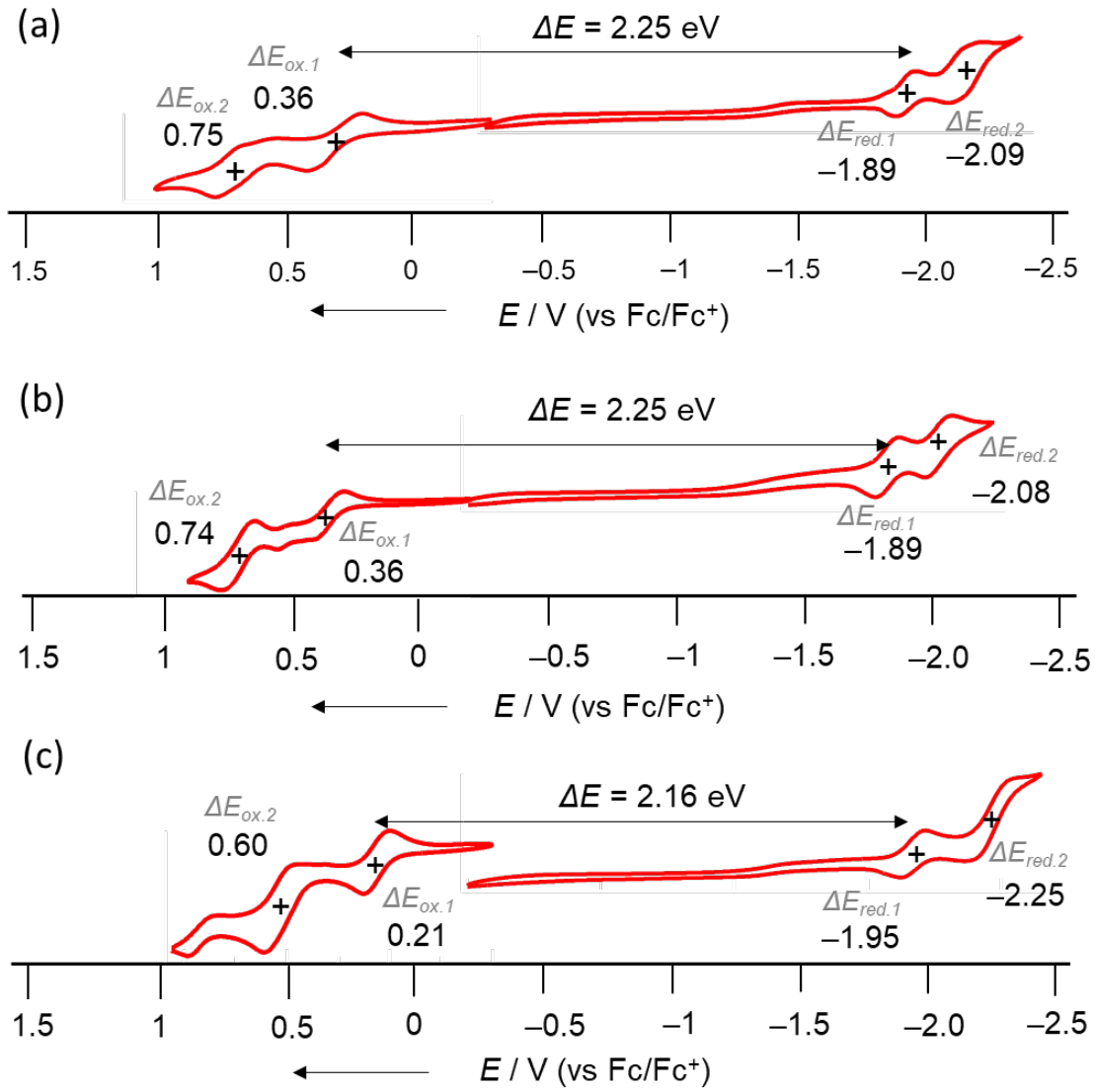


Figure S4-2. Cyclic voltammograms of (a) **3b**, (b) **3c** and (c) **3d**. Measurement conditions: solvent: CH_2Cl_2; scan rate: 0.05 V/s; working electrode: glassy carbon; reference electrode: $Ag/AgNO_3$; counter electrode: Pt; supporting electrolyte: 0.1 M *n*-Bu_4NPF_6.

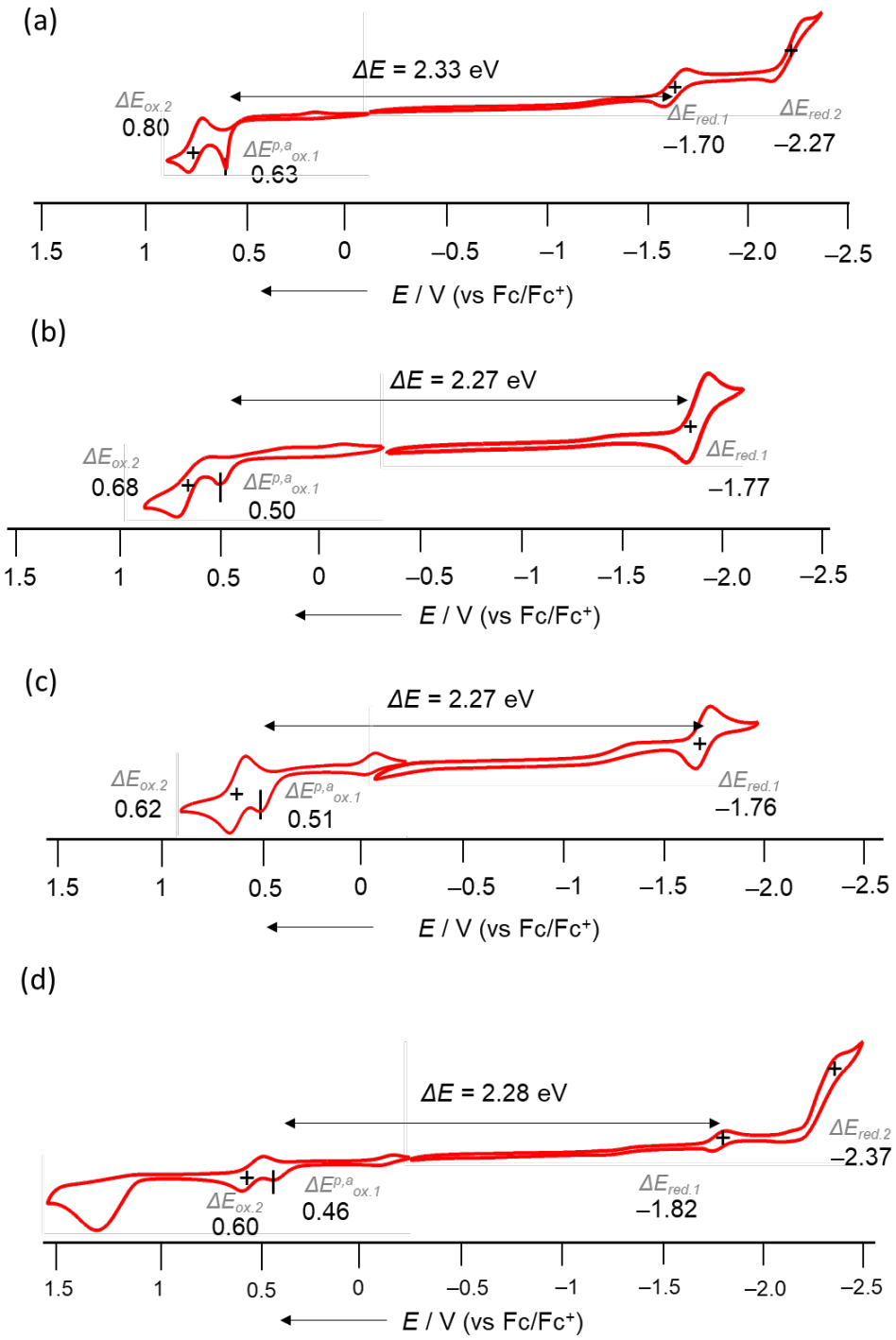


Figure S4-3. Cyclic voltammograms of (a) **4a**, (b) **4b**, (c) **4c** and (d) **4d**. Measurement conditions: solvent: CH_2Cl_2; scan rate: 0.05 V/s; working electrode: glassy carbon; reference electrode: $Ag/AgNO_3$; counter electrode: Pt; supporting electrolyte: 0.1 M *n*-Bu_4NPF_6.

5. Crystallographic Data

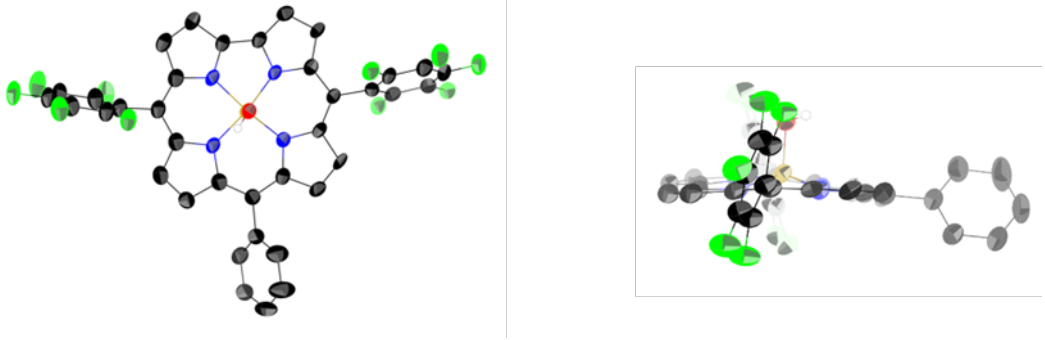


Figure S5-1. X-Ray crystal structure of **2c** (left) top view, (right) side view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms except for OHs are omitted for clarity.

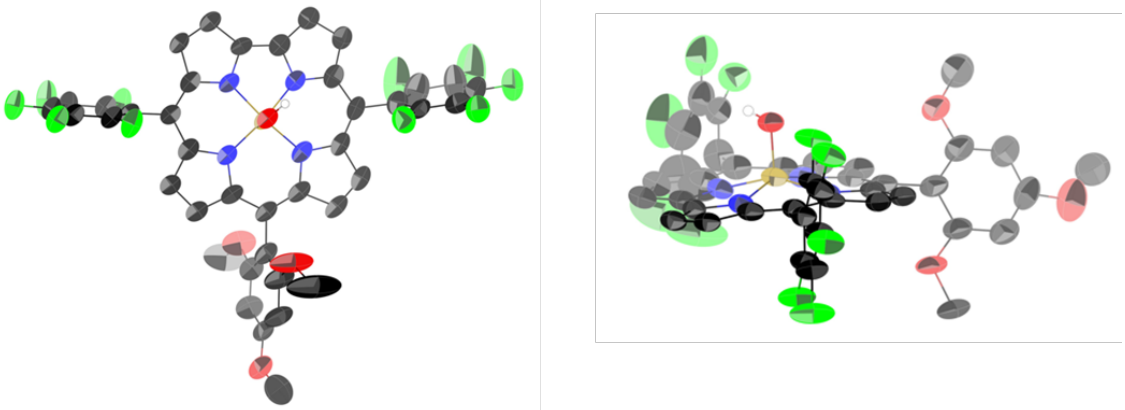


Figure S5-2. X-Ray crystal structure of **2d** (left) top view, (right) side view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms except for OHs are omitted for clarity.

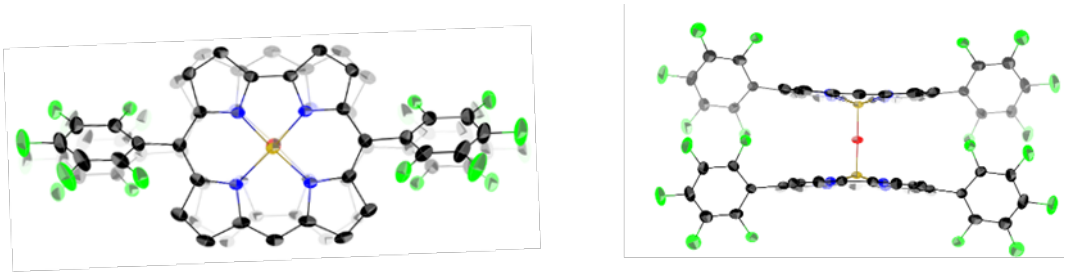


Figure S5-3. X-Ray crystal structure of **3b** (left) top view, (right) side view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms are omitted for clarity.

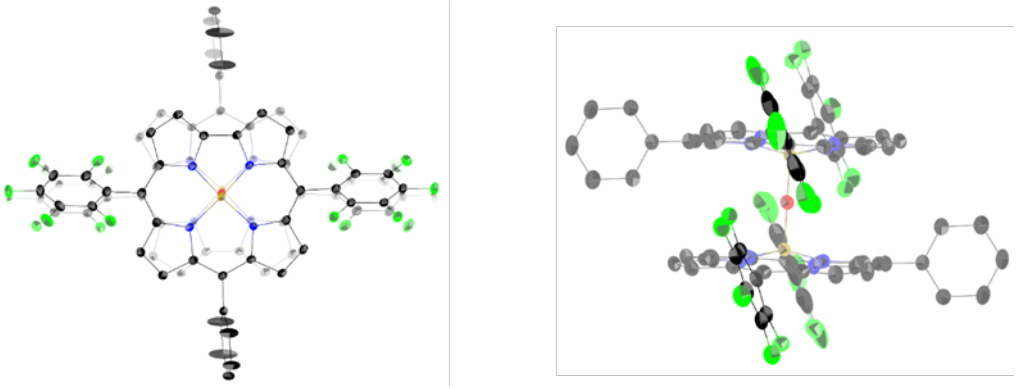


Figure S5-4. X-Ray crystal structure of **3c** (left) top view, (right) side view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms are omitted for clarity.

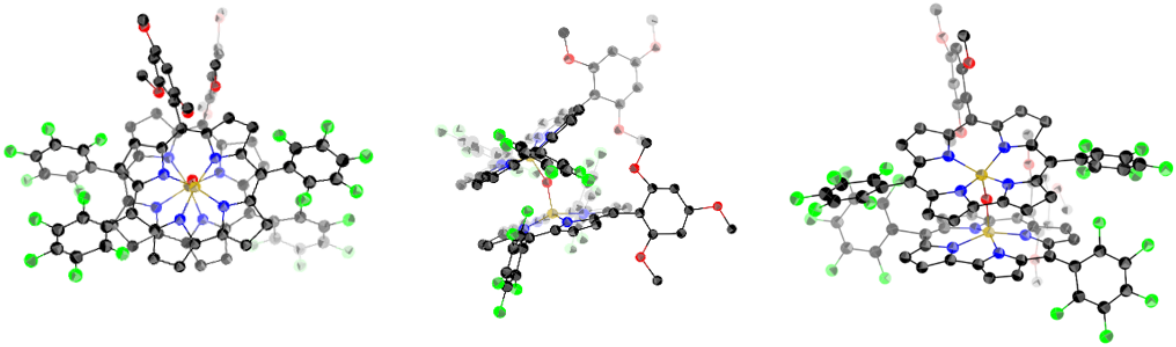


Figure S5-5. X-Ray crystal structure of **3d** (left) top view, (middle) side view and (right) perspective view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms are omitted for clarity.

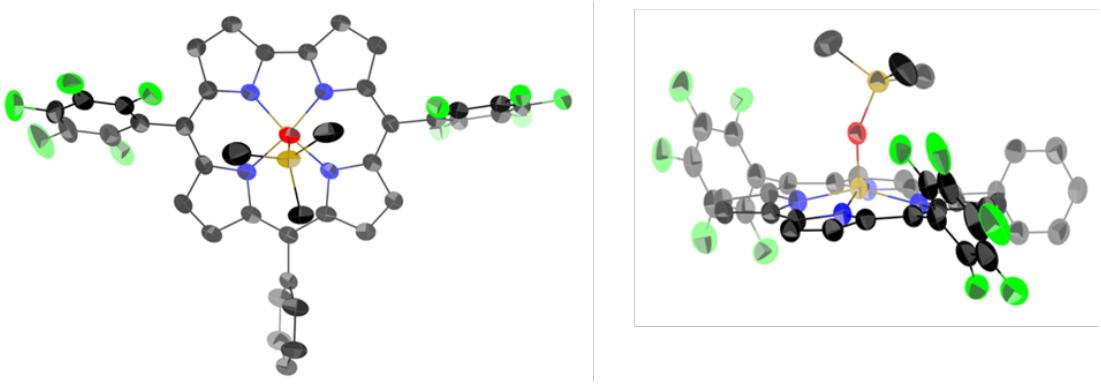


Figure S5-6. X-Ray crystal structure of **4b** (left) top view, (right) side view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms are omitted for clarity.

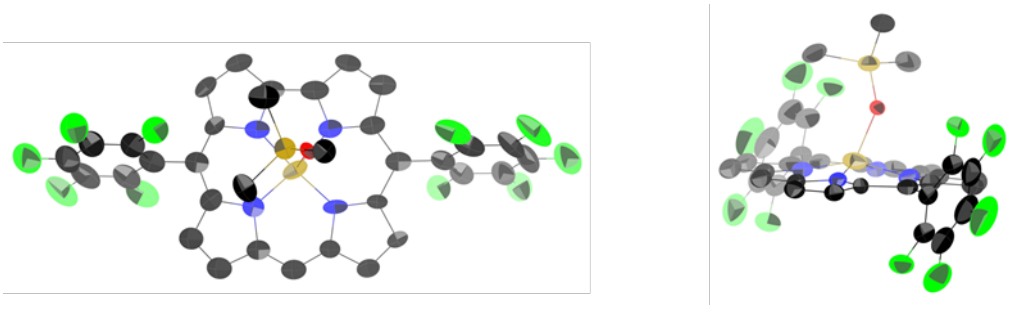


Figure S5-7. X-Ray crystal structure of **4c** (left) top view, (right) side view. The thermal ellipsoids are 50% probability. Solvent molecules and hydrogen atoms are omitted for clarity.

Table S5. Crystallographic data for **2c**, **2d**, **3b-3d**, **4b** and **4c**.

Compound	**2c**	**2d**	**3b**	**3c**	**3d**[a]	**4b**	**4c**
Empirical formula	$2(C_{37}H_{14}F_{10}N_4OSi)\cdot 2(CH_2Cl_2)$	$6(C_{40}H_{20}F_{10}N_4O_4Si)\cdot 3.5(C_6H_{14})\cdot 4(H_2O)$	$C_{15.5}H_{4.5}F_5N_2O_{0.25}Si_{0.5}\cdot 0.5(CH_2Cl_2)$	$C_{74}H_{26}F_{20}N_8OSi_2\cdot CH_2Cl_2$	$4(C_{80}H_{34}F_{20}N_8O_7Si_2)$	$C_{34}H_{18}F_{10}N_4OSi_2\cdot 0.5(C_6H_{14})$	$2(C_{40}H_{22}F_{10}N_4OSi_2)\cdot 0.5(C_6H_{14})\cdot CH_2Cl_2$
Molecular weight	1667.07	5405.80	374.22	1564.13	6637.45	389.43	1769.60
Crystal system	Triclinic	Monoclinic	Orthorhombic	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	*P*-1	*C*2/*c*	*Cmca*	*P*-1	$P2_1/n$	*P*-1	*P*-1
a [Å]	10.9143(4)	68.084(4)	37.2939(5)	10.2905(1)	26.9658(2)	8.2034(3)	15.8132(3)
b [Å]	18.2103(7)	17.3582(4)	11.9947(1)	11.1256(1)	15.3385(1)	13.6311(5)	15.8561(4)
c [Å]	18.9895(7)	50.3185(19)	13.4180(1)	15.3136(2)	82.2466(5)	15.9823(6)	18.1911(3)
α [°]	64.960(4)	90	90	108.192(1)	90	96.950(3)	72.484(2)
β [°]	80.933(3)	120.753(4)	90	104.216(1)	98.4360(10)	103.794(3)	89.3890(10)
γ [°]	82.291(3)	90	90	97.506(1)	90	100.029(3)	62.843(2)
Volume [Å^3]	3367.2(2)	51105(4)	6002.26(10)	1573.15(3)	33650.3(4)	1684.24(11)	3826.76(15)
Z	2	8	16	1	4	2	2
Density [g·cm^{-3}]	1.644	1.405	1.656	1.651	1.310	1.553	1.536
Completeness	0.963	0.994	1.000	0.963	0.999	0.969	0.971
Goodness-of-Fit	1.012	1.047	1.119	1.081	1.135	1.043	1.031
R_1 [$I>2\sigma(I)$]	0.0949	0.1020	0.0750	0.0460	0.1644	0.0564	0.0704
wR_2 (all data)	0.3091	0.3301	0.2196	0.1318	0.3831	0.1663	0.2191
Solvent system	CH_2Cl_2 /*n*-hexane	CH_2Cl_2 /*n*-hexane	CH_2Cl_2 /*n*-hexane	CH_2Cl_2 /*n*-hexane	CH_2Cl_2 /*n*-hexane	CH_2Cl_2 /*n*-hexane	CH_2Cl_2 /*n*-hexane
CCDC	2165329	2165326	2165327	2165330	2165311	2165328	2165331

[a] The contributions to the scattering arising from the presence of the disordered solvents in the crystal were removed by use of the utility SQUEEZE in the PLATON software package.

A. L. Spek, PLATON, A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, 2005; P. van der Sluis and A. L. Spek, *Acta Crystallogr. Sect. A*, 1990, **46**, 194.

6. UV/Vis Absorption and Fluorescence Spectra

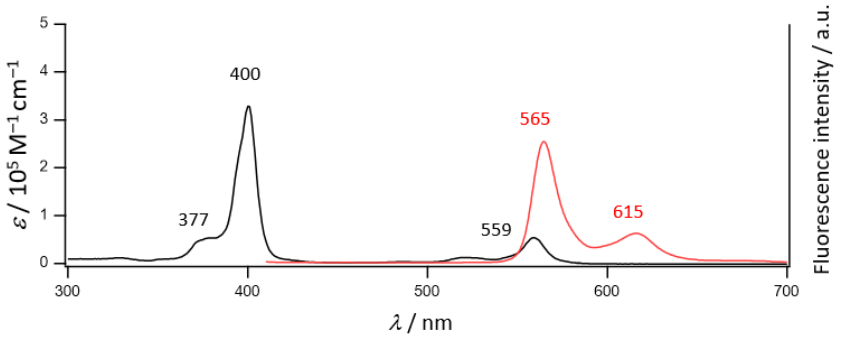


Figure S6-1. UV/Vis absorption (black) and fluorescence (red) spectra of **2b**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 377 (5.26×10^4), 400 (3.29×10^5), 559 (5.36×10^4).

Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 565, 615, Φ_F = 0.16. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.1 ns.

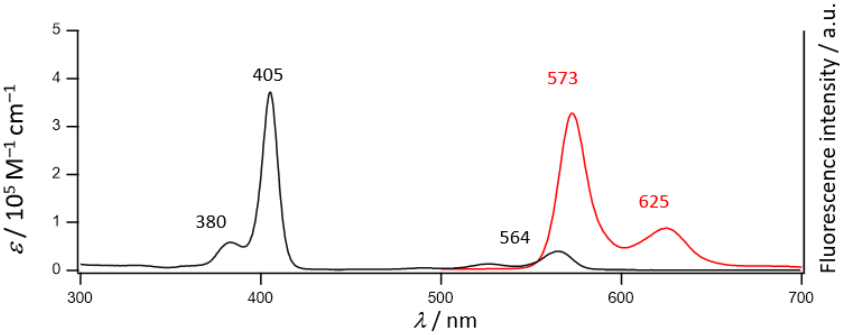


Figure S6-2. UV/Vis absorption (black) and fluorescence (red) spectra of **2c**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 380 (5.80×10^4), 405 (3.66×10^5), 564 (3.80×10^4).

Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 573, 625, Φ_F = 0.20. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.1 ns.

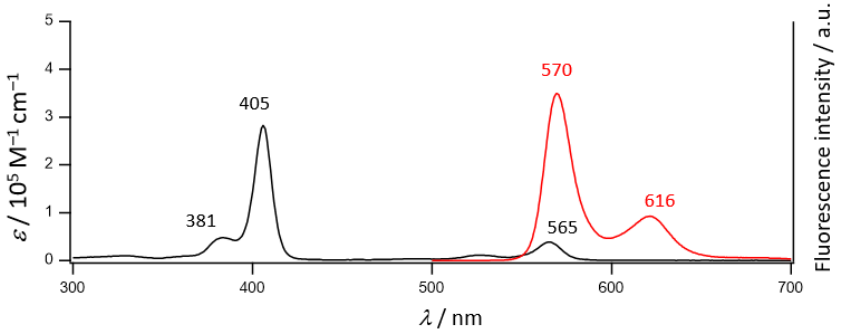


Figure S6-3. UV/Vis absorption (black) and fluorescence (red) spectra of **2d.**

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 381 (4.82×10^4), 405 (2.84×10^5), 565 (3.86×10^4).

Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 570, 616, Φ_F = 0.20. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.2 ns.

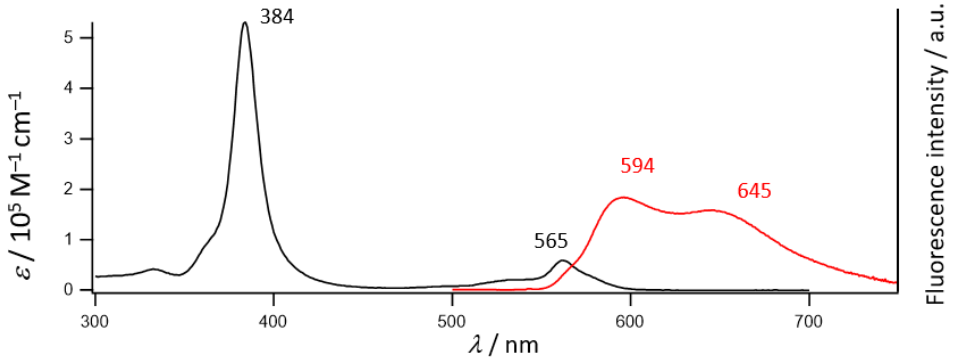


Figure S6-4. UV/Vis absorption (black) and fluorescence (red) spectra of **3b**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 384 (5.33×10^5), 565 (5.90×10^4).

Fluorescence (CH_2Cl_2, λ_{ex}= 565 nm): λ_{max} / nm = 594, 645, Φ_F = 0.06. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ_1 = 3.1 ns, τ_2 = 6.5 ns.

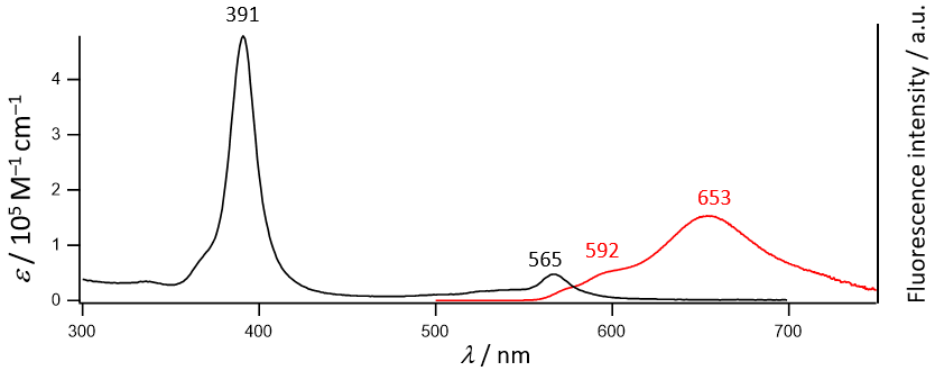


Figure S6-5. UV/Vis absorption (black) and fluorescence (red) spectra of **3c**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 391 (4.80×10^5), 565 (4.65×10^4).

Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 592, 653, Φ_F = 0.08. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ_1 = 2.0 ns, τ_2 = 5.7 ns.

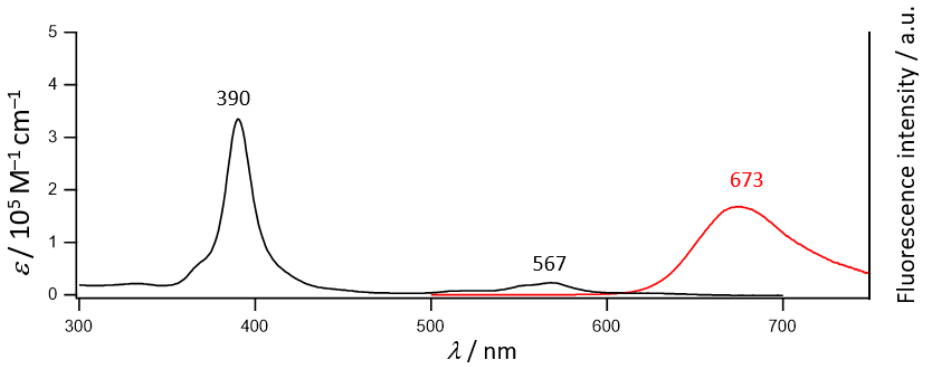


Figure S6-6. UV/Vis absorption (black) and fluorescence (red) spectra of **3d**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) = 390 (3.35×10^5), 567 (2.30×10^4).

Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 673, Φ_F = 0.13. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 8.5 ns.

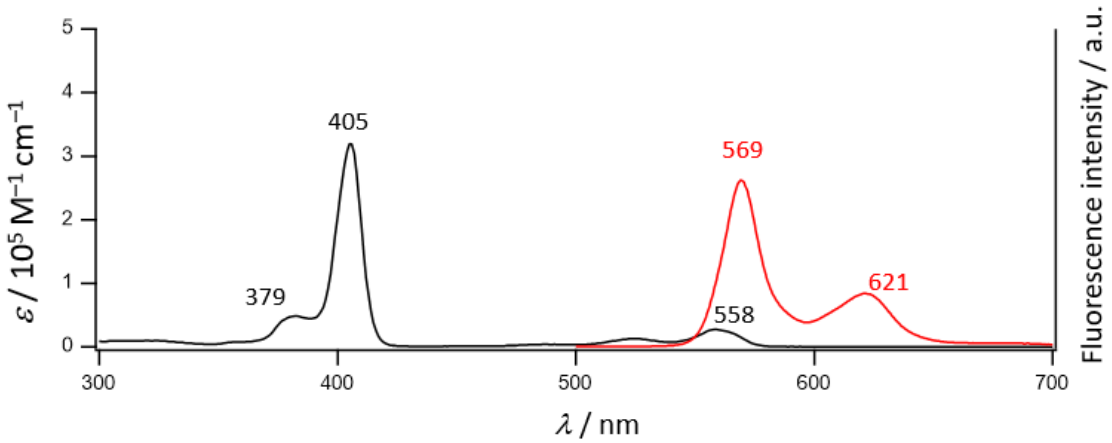


Figure S6-7. UV/Vis absorption (black) and fluorescence (red) spectra of **4a**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) =379 (4.72×10^4), 405 (3.19×10^5), 558 (2.73×10^4).

Fluorescence (CH_2Cl_2, λ_{ex} = 400 nm): λ_{max} / nm = 569, 621, Φ_F = 0.10. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.4 ns.

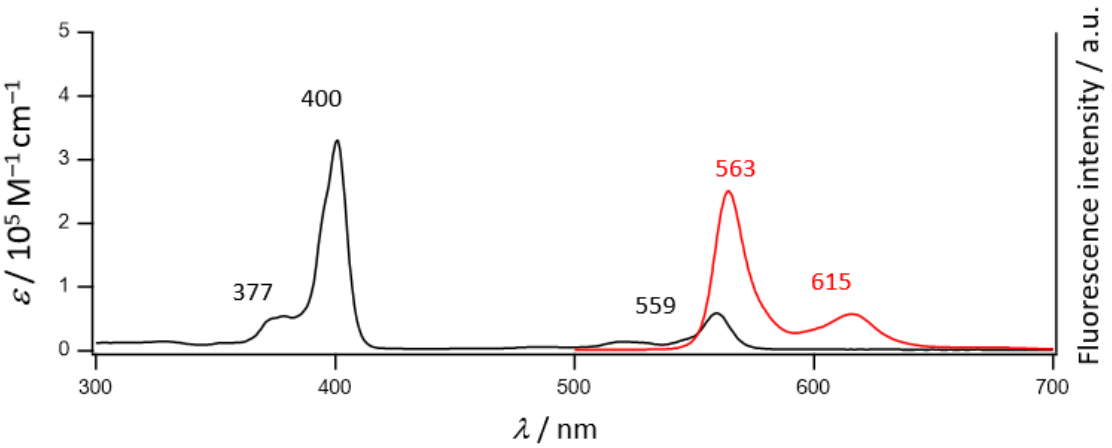


Figure S6-8. UV/Vis absorption (black) and fluorescence (red) spectra of **4b**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) =377 (5.31×10^4) 400 (3.31×10^5), 559 (5.88×10^4).

Fluorescence (CH_2Cl_2, λ_{ex}= 400 nm): λ_{max} / nm = 563, 615, Φ_F = 0.16. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.0 ns.

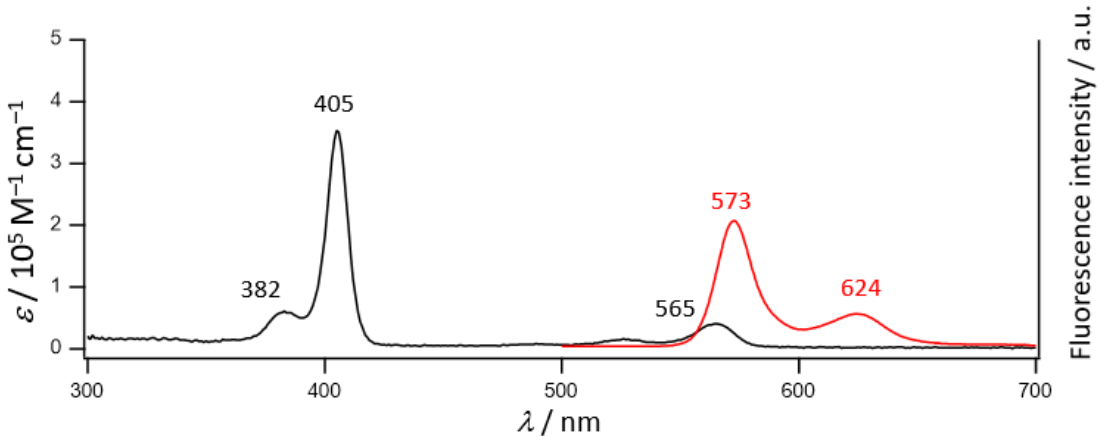


Figure S6-9. UV/Vis absorption (black) and fluorescence (red) spectra of **4c**.

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) =382 (6.10×10^4), 405 (3.53×10^5), 565 (4.11×10^4).

Fluorescence (CH_2Cl_2, λ_{ex}= 400 nm) : λ_{max} / nm = 573, 624, Φ_F = 0.16, Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.0 ns.

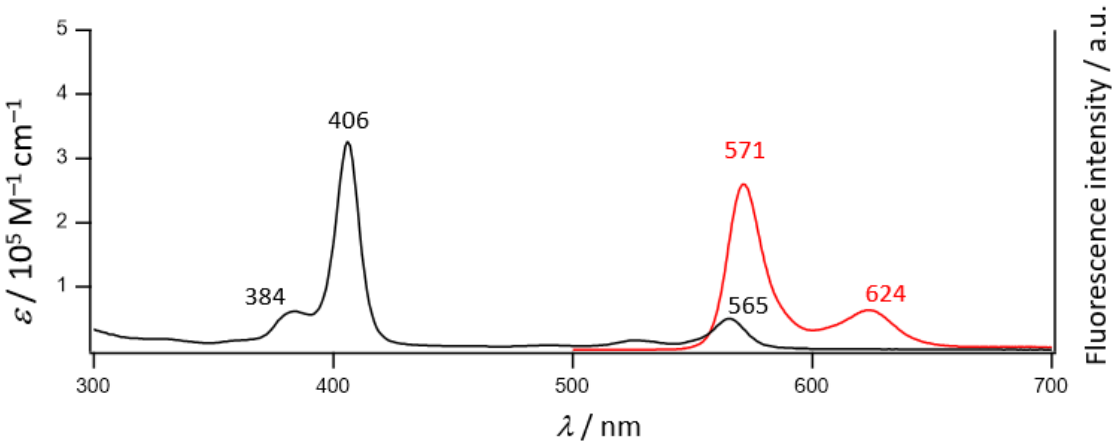


Figure S6-10. UV/Vis absorption (black) and fluorescence (red) spectra of **4d.**

UV/Vis (CH_2Cl_2): λ_{max} / nm (ε / $M^{-1}cm^{-1}$) =384 (6.19×10^4), 405 (3.26×10^5), 565 (5.04×10^4).

Fluorescence (CH_2Cl_2, λ_{ex}= 400 nm): λ_{max} / nm = 571, 624, Φ_F = 0.15. Fluorescence lifetime (CH_2Cl_2, λ_{ex}= 405 nm): τ = 4.3 ns.

Table S6-1. Summary of optical properties in CH_2Cl_2 (fluorescence quantum yield Φ_F, fluorescence lifetime τ_F, χ value) at room temperature.

Compound	Φ_F	τ_{F1} [ns]	τ_{F2} [ns]	χ
2b	0.151	4.1		1.37
2c	0.197	4.1		1.50
2d	0.146	4.2		1.70
3a	0.070	3.1	5.9	1.12
3b	0.060	3.1	6.5	1.42
3c	0.080	2.0	5.7	1.27
3d	0.132	8.5		1.03
4a	0.104	4.4		1.26
4b	0.155	4.0		1.23
4c	0.158	4.0		1.55
4d	0.146	4.3		1.12

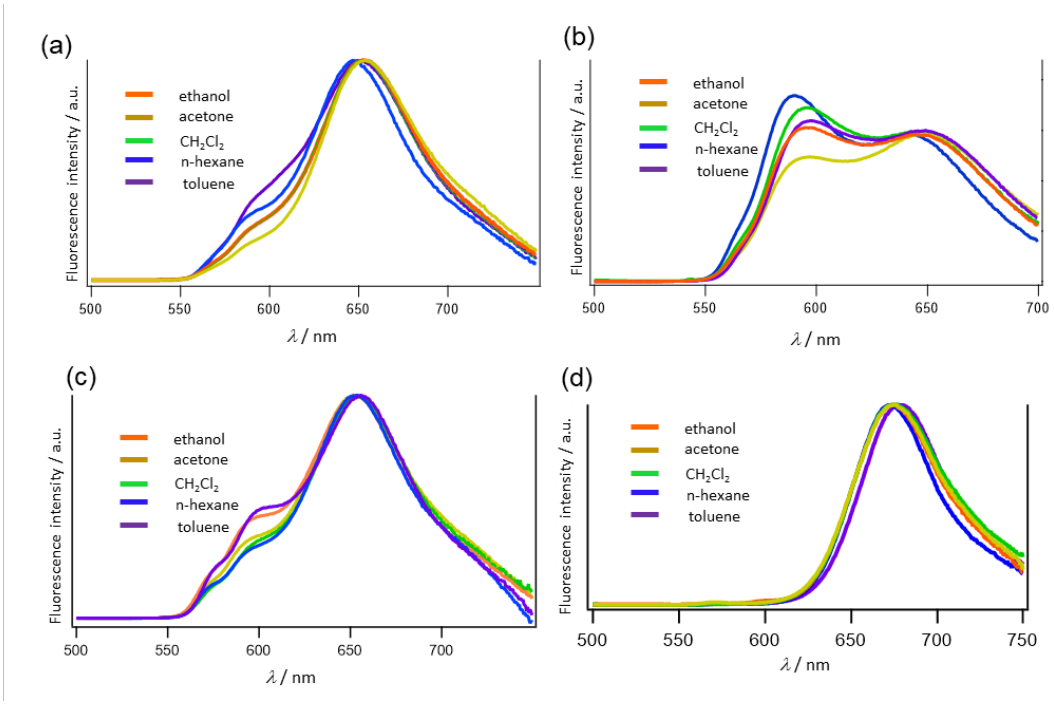


Figure S6-11. Fluorescence spectra of (a) **3a,** (b) **3b**, (c) **3c** and (d) **3d** in various polarity solvents. Solvent viscosities are 1.08 cP (ethanol), 0.30 cP (acetone), 0.41 cP (CH_2Cl_2), 0.30 cP (*n*-hexane), and 0.55 cP (toluene).

7. DFT Calculations

All calculations were carried out using the Gaussian 16 program.[S6] All structures were fully optimized without any symmetry restriction. The calculations were performed by the density functional theory (DFT) method with restricted B3LYP level,[S7] employing basis sets 6-311G(d,p) for S_0 conformers and 6-31G(d) for S_1 conformers. The D3 version of Grimme's dispersion with Becke–Johnson damping was implemented for all calculations.[S8]

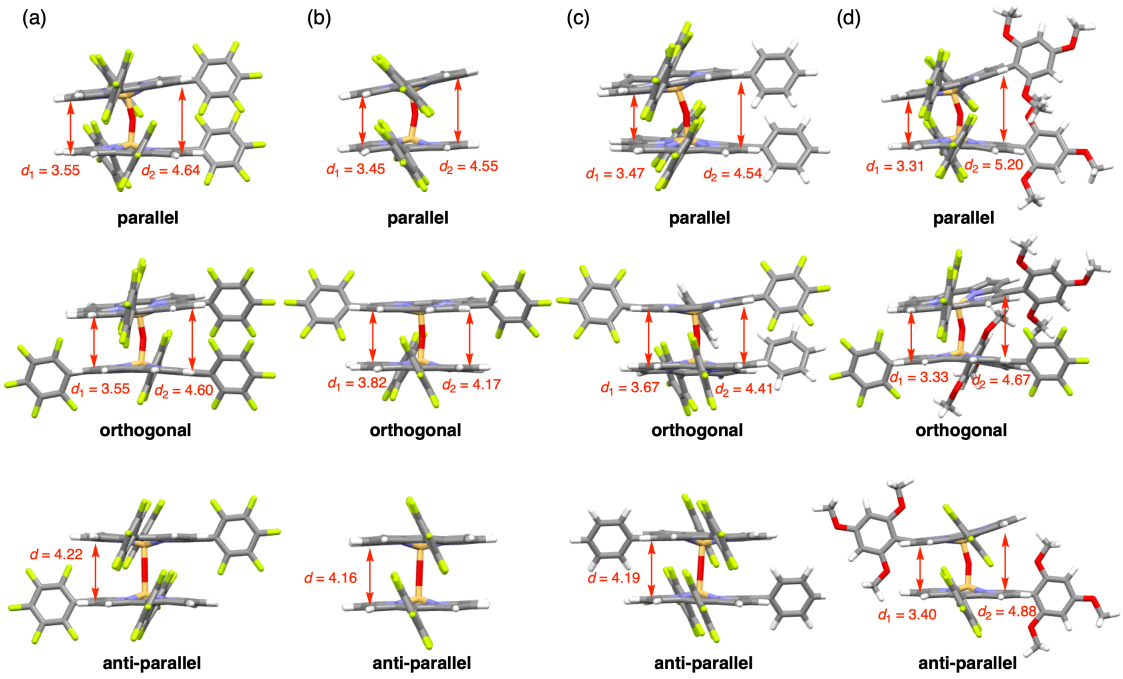


Figure S7-1. Optimized structures of (a) **3a**, (b) **3b**, (c) **3c** and (d) **3d** in the S_0-state.

*The distances (***d***, d_1, and d_2) are defined as follows;

d: the distance between two mean-planes in Å

d_1: the closest distance between the mean-plane of one corrole unit and the β-carbon (2 or 22-positions) (for parallel conformer) or the *meso*-carbon (for orthogonal and anti-parallel conformers) of the opposite corrole unit in Å.

d_2: the longest distance between the mean-plane of one corrole unit and the *meso*-carbon of the opposite corrole unit in Å.

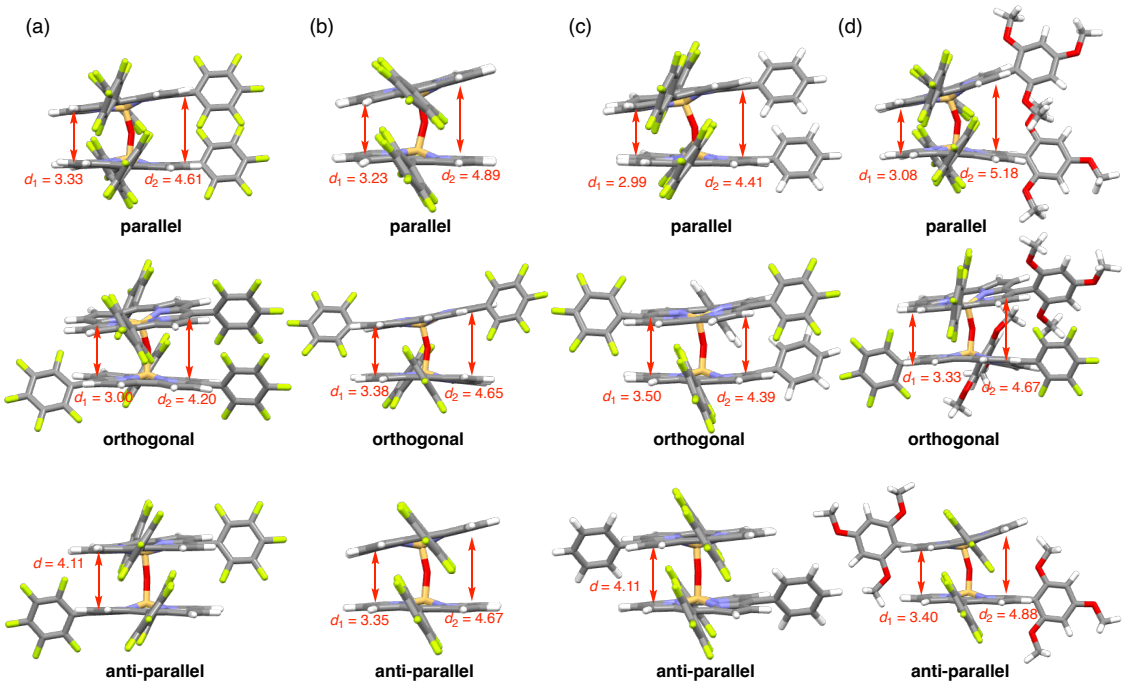


Figure S7-2. Optimized structures of (a) **3a**, (b) **3b**, (c) **3c** and (d) **3d** in the S_1-state.

*The distances (***d***, d_1, and d_2) are defined as follows;

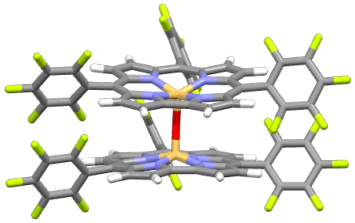
d: the distance between two mean-planes in Å

d_1: the closest distance between the mean-plane of one corrole unit and the β-carbon (2 or 22-positions) (for parallel conformer) or the *meso*-carbon (for orthogonal and anti-parallel conformers) of the opposite corrole unit in Å.

d_2: the longest distance between the mean-plane of one corrole unit and the *meso*-carbon of the opposite corrole unit in Å.

Cartesian coordinates for the stationary points

3a-*P* (S_0)



Si	-0.12007085	-0.97577712	-1.61002514
Si	0.12024483	-0.97517550	1.61213226
F	5.01028111	-2.91728450	-0.03540143
F	-4.63997151	-2.26854029	4.40303665
F	1.46939587	3.73140411	0.11721616
F	5.00592686	-0.93106495	4.26691423
F	-7.32454614	-2.44457733	4.46112140
F	0.23470510	3.86332893	-4.52968955
F	-1.46890897	3.73195332	-0.11638355
F	-5.01096618	-2.92025540	0.03679834
F	-0.23406297	3.86525774	4.53047833
F	-4.91427798	0.23020287	0.39165024
O	0.00059305	-0.71929427	0.00093822
F	-8.81773405	-1.30341356	2.48820036
F	7.66339818	-3.22901205	0.11631077
F	1.62536333	6.41444531	0.09671794
F	-5.00573073	-0.92981850	-4.26375546
F	4.91702082	0.22340354	-0.39116256
F	7.66448230	-1.26572466	4.40727190
F	0.85142711	7.84587532	2.28581916
F	9.02152889	-2.40354351	2.33714190
F	-7.58906873	0.04234488	0.45842533
F	-7.66387894	-3.23144391	-0.11574458
F	4.63599427	-2.26631232	-4.40749350
F	-0.06850110	6.55347054	4.50003742
F	8.81721541	-1.30343478	-2.49893751
F	7.59197735	0.03720968	-0.46363014
F	0.06898807	6.55148364	-4.50084467
F	-1.62526240	6.41501243	-0.09760352
F	-0.85127213	7.84516855	-2.28747703
F	7.32074120	-2.44112052	-4.47122555

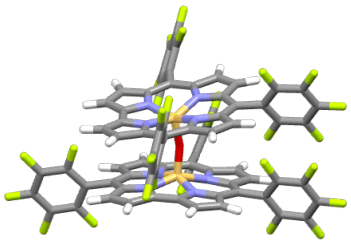
F	-9.02167605	-2.40357564	-2.33585165
F	-7.66410823	-1.26394097	-4.40474724
N	1.08734413	0.30829908	-2.23102541
N	1.59884392	0.05780334	2.07618790
N	1.21640598	-2.48206888	1.75859034
N	-1.08711324	0.30921045	2.23233439
N	-1.21648750	-2.48258394	-1.75568023
N	-1.59861449	0.05721448	-2.07402832
N	-1.17392392	-2.26677057	1.95154972
N	1.17378799	-2.26769606	-1.94983194
C	-1.59212194	1.44676333	-2.19438995
C	-0.82716255	1.67482255	2.32550919
C	0.59515699	-3.71144669	1.73741844
C	2.57368480	-2.69872277	1.81724065
C	0.82763577	1.67393633	-2.32403906
C	1.59257828	1.44735936	2.19614257
C	-2.54186974	-2.23559411	2.09822077
C	0.44725466	2.22769559	2.27757676
C	-2.48372972	0.17037547	2.34484598
C	2.54161137	-2.23676604	-2.09746556
C	2.48385866	0.16916755	-2.34414966
C	-3.19958567	-1.02158440	2.28066915
C	-0.79213231	-3.58525609	1.83460448
C	2.95689483	-0.32632799	2.07943630
C	0.79189731	-3.58608368	-1.83234145
C	3.44817000	-1.62637774	1.97620653
C	-0.44673028	2.22697524	-2.27602538
C	3.19941883	-1.02299386	-2.28062187
C	-0.59479269	3.70408853	-2.31713888
C	-0.59536860	-3.71205942	-1.73447120
C	0.59541225	3.70481645	2.31802171
C	5.63354521	-2.49041948	1.07395409
C	2.80225907	-4.10421838	1.79496853
H	3.77023583	-4.57671439	1.83818294
C	1.57059007	-4.73161496	1.74163226
H	1.37547219	-5.79222182	1.73168337
C	4.90639186	-1.86985204	2.08971977
C	-3.05697983	1.46259664	2.52883897
H	-4.10881917	1.64993733	2.66791748
C	-2.05123431	2.38166353	2.50041547
H	-2.13838978	3.45090245	2.58842476
C	-5.33961091	-1.68349713	3.42316249
C	3.75900620	0.84573586	2.20068382
H	4.83526129	0.84989111	2.20701736
C	-2.95674275	-0.32674033	-2.07722120
C	-3.02266987	-3.57641311	2.06048954
H	-4.05591152	-3.86767643	2.14213764
C	4.67814920	-1.01527212	-2.39595322
C	2.93170904	1.92519092	2.26718140
H	3.21073854	2.95998372	2.37615165
C	-4.67846340	-1.01352145	2.39383320
C	2.05180726	2.38057410	-2.49914651
H	2.13914896	3.44981263	-2.58698226
C	-6.72500594	-1.78566220	3.46576415
C	3.05736903	1.46129152	-2.52800115
H	4.10922563	1.64837945	-2.66734387
C	-2.57379823	-2.69911843	-1.81426166
C	-3.44821374	-1.62671478	-1.97345192
C	1.09133229	4.40060102	1.21608362
C	3.02230797	-3.57762241	-2.05969102
H	4.05552017	-3.86890148	-2.14190081
C	-1.93425989	-4.41193746	1.89842414
H	-1.94008149	-5.48803285	1.83220910
C	-1.09082995	4.40051870	-1.21564052
C	-4.90644507	-1.87012893	-2.08714071
C	-7.49013645	-1.19820513	2.46684660
C	0.22596826	4.46569973	3.42611483
C	-0.22535673	4.46436010	-3.42565289
C	-2.80250510	-4.10457879	-1.79187175
H	-3.77051280	-4.57699798	-1.83508698
C	7.00640319	-2.67077547	1.14026302
C	-5.47930873	-0.41203007	1.42406721
C	-3.75863052	0.84542634	-2.19902163
H	-4.83487194	0.84982657	-2.20545253
C	-2.93118882	1.92472949	-2.26573295
H	-3.21010781	2.95952038	-2.37499356
C	-1.57090299	-4.73210569	-1.73858875
H	-1.37590083	-5.79273284	-1.72855335
C	5.48054478	-0.41585406	-1.42626705
C	5.63071676	-1.48692198	3.22232902
C	1.18318467	5.78287083	1.19214049
C	1.93388955	-4.41296417	-1.89672166
H	1.93957915	-5.48904374	-1.83023719
C	0.78047351	6.51559537	2.30090181
C	7.00650061	-1.65680482	3.31298806
C	-5.63386246	-2.49177983	-1.07214880
C	7.70117471	-2.24405051	2.26329139
C	0.30536896	5.85348345	3.42552435
C	6.86293118	-0.50440657	-1.44866251
C	5.33743689	-1.68304225	-3.42787172
C	-7.00672631	-2.67208331	-1.13898038
C	-6.86170401	-0.50120195	1.44365461
C	-1.18283912	5.78279257	-1.19255633
C	-5.63064876	-1.48632028	-3.21957883
C	7.48960341	-1.19888909	-2.47464902
C	6.72279266	-1.78457162	-3.47334771
C	-0.30487622	5.85214188	-3.42591108
C	-0.78013974	6.51488982	-2.30174364
C	-7.70133564	-2.24420147	-2.26165305
C	-7.00641854	-1.65602567	-3.31065202

3a-*P* (S_1)

Si	-0.16068043	-1.00912660	-1.62642710
Si	0.15221856	-0.94508159	1.57203447
F	5.07620178	-3.00412062	-0.00073516
F	-4.60086911	-2.53840247	4.21218963
F	1.52861519	3.74394718	0.10408752
F	5.06716994	-0.65134544	4.12238649
F	-7.28238791	-2.77307397	4.22182521
F	0.36243171	3.86348532	-4.51253126
F	-1.43490066	3.71237404	-0.12416393
F	-5.11332860	-2.95143395	0.10129804
F	-0.38150319	3.92168861	4.43810792
F	-4.89236654	0.35235725	0.46428200
O	-0.00184454	-0.67496210	-0.00339863
F	-8.78247577	-1.46845722	2.35168311
F	7.73863374	-3.23734926	0.14760991
F	1.65202869	6.43244146	0.05100166
F	-5.11573162	-0.71766187	-4.09808055
F	4.90727904	0.23626803	-0.43155967
F	7.73550451	-0.90674885	4.25732829
F	0.75410842	7.88616508	2.17847662
F	9.10044250	-2.18554764	2.26904262
F	-7.56445839	0.10887316	0.48766379
F	-7.75941670	-3.22105701	-0.05122798
F	4.62100369	-2.59169067	-4.23424920
F	-0.25173418	6.61436916	4.37277446
F	8.80451457	-1.52391583	-2.36953015
F	7.57302804	0.01341442	-0.47018468
F	0.23483607	6.55189862	-4.45854330
F	-1.56835307	6.39408188	-0.08932252
F	-0.72579741	7.84147664	-2.25104713
F	7.29781497	-2.81932179	-4.24707619
F	-9.13974206	-2.23480206	-2.20565279
F	-7.77410471	-0.98646034	-4.21899827
N	1.08204027	0.23900565	-2.24809214
N	1.62393751	0.10674682	2.05481118
N	1.28352304	-2.43998757	1.72438470
N	-1.07553567	0.31352836	2.23958482
N	-1.30256437	-2.48671571	-1.65736703
N	-1.62151981	0.05570957	-2.06222748
N	-1.11018408	-2.26844280	1.95079392
N	1.10260495	-2.33966674	-1.90303294
C	-1.57665409	1.45733228	-2.19310278
C	-0.84254624	1.68722926	2.31478550
C	0.69304193	-3.66851478	1.68820354
C	2.65281472	-2.63606270	1.75906812
C	0.85508423	1.62286837	-2.34605206
C	1.59333739	1.50123482	2.15013463
C	-2.49094692	-2.26022835	2.04381652
C	0.42979553	2.26237876	2.24646229
C	-2.46157187	0.15466847	2.33484337
C	2.47920737	-2.34962541	-2.04640069
C	2.47885152	0.06928909	-2.33648730
C	-3.16890257	-1.06727773	2.23732989
C	-0.71626958	-3.56646772	1.78777950
C	2.98008803	-0.24322961	2.01319183
C	0.69122963	-3.65288082	-1.73675547
C	3.50573477	-1.55605704	1.91278134
C	-0.40793495	2.20300122	-2.29123297
C	3.17222368	-1.13799075	-2.24027666
C	-0.52334323	3.68308050	-2.31911771
C	-0.71488024	-3.74011599	-1.61271111
C	0.55531127	3.74120612	2.26610908
C	5.69894036	-2.46155754	1.05294408
C	2.89996297	-4.04590890	1.72115103
H	3.87575749	-4.50696431	1.73651608
C	1.67734502	-4.68604120	1.66970742
H	1.48862320	-5.74900624	1.63389754
C	4.96803485	-1.76423405	2.02305958
C	-3.06664001	1.42757690	2.51471395
H	-4.12431635	1.59506425	2.64525614
C	-2.07432041	2.37353578	2.47856708
H	-2.18569598	3.44410615	2.54347035
C	-5.30504261	-1.87105283	3.28658881

C	3.76891908	0.93634561	2.08569501
H	4.84524386	0.95898375	2.03620139
C	-2.99297342	-0.28397920	-2.02203344
C	-2.94923191	-3.61316313	1.93496809
H	-3.98123971	-3.92283519	1.95439448
C	4.64617629	-1.16012303	-2.33928952
C	2.91999109	2.00696464	2.17215501
H	3.18455674	3.04976080	2.25642484
C	-4.64672571	-1.08059495	2.33776855
C	2.09410704	2.29464035	-2.51501378
H	2.20867401	3.36300608	-2.61775234
C	-6.68962806	-2.00449907	3.30377088
C	3.08276184	1.34880471	-2.53006318
H	4.14070690	1.51039490	-2.67232343
C	-2.67432657	-2.67341227	-1.68952290
C	-3.52937519	-1.56787382	-1.86340437
C	1.09515307	4.42532303	1.17129921
C	2.92500886	-3.68766131	-1.96307055
H	3.95059667	-4.01183825	-2.04874546
C	-1.83991417	-4.42280273	1.78621599
H	-1.81969703	-5.49454258	1.65757144
C	-1.03484090	4.38116171	-1.22104420
C	-4.98681848	-1.77307385	-1.96720104
C	-7.45871850	-1.33337241	2.35686023
C	0.11855198	4.51447262	3.34527833
C	-0.11552188	4.45462136	-3.41103515
C	-2.93763598	-4.06024755	-1.62918389
H	-3.91858281	-4.51146566	-1.65754357
C	7.07966069	-2.60455087	1.12266761
C	-5.45197312	-0.39671670	1.42040779
C	-3.76022495	0.91329014	-2.13771067
H	-4.83755188	0.95291073	-2.11125680
C	-2.89764667	1.96957588	-2.23832076
H	-3.14973799	3.01314810	-2.35760491
C	-1.70465132	-4.72648179	-1.58016694
H	-1.53599692	-5.79461555	-1.56319965
C	5.46201326	-0.48871788	-1.42137036
C	5.69727964	-1.27025120	3.11456705
C	1.16918628	5.81168670	1.13252232
C	1.79803163	-4.50178859	-1.77633935
H	1.77638387	-5.57893661	-1.68507395
C	0.69977715	6.55645373	2.21099328
C	7.07910331	-1.40018118	3.20404196
C	-5.72810686	-2.45207568	-0.99055967
C	7.77721129	-2.06154514	2.19684416
C	0.17970472	5.90514766	3.32637899
C	6.84603126	-0.59318567	-1.42527346
C	5.31558779	-1.93260175	-3.29823976
C	-7.10583888	-2.61466003	-1.05632897
C	-6.83583455	-0.51440378	1.41995309
C	-1.11349521	5.76690788	-1.18704774
C	-5.73095976	-1.31493790	-3.06909804
C	7.47477623	-1.39523239	-2.37209071
C	6.70223301	-2.06260629	-3.31746618
C	-0.17507730	5.84720079	-3.39817500
C	-0.67174745	6.50780154	-2.27882271
C	-7.81182695	-2.10198905	-2.13856765
C	-7.11322238	-1.45263684	-3.15258536

3a-*O* (S_0)



Si	-0.29665160	0.75525726	1.58612986
F	2.49307869	-2.59330030	5.18296523
F	4.52236859	-4.28280090	5.70596391
F	4.50489840	-1.49568154	1.04149175
O	0.00009966	0.49395602	0.00001072
F	-4.32239774	3.68941548	3.73755445
F	6.53506692	-4.61159589	3.90132819
F	6.50681410	-3.20521111	1.56073831
F	-3.30327974	4.88244214	-0.72798480
F	-6.25405539	5.57086766	3.78815736
F	-5.22093829	6.75953052	-0.65996843
N	1.41253234	1.06490673	2.24970400
N	-2.16134518	0.74838346	1.68222467
N	-0.36249854	2.61164787	1.75049071
F	-6.71243846	7.11743167	1.59543158
N	-0.17141556	-0.98901218	2.23397510
C	-2.96624876	-0.39060477	1.64024953
C	2.46708274	0.24835444	2.58099006
C	-3.03433986	1.84235179	1.52167460
C	0.83232129	3.26610279	1.96310255
C	1.86782339	2.36475899	2.23347320
C	3.61989410	1.06530065	2.76572816
H	4.59660701	0.70516908	3.04742166
C	-1.34732565	3.56523401	1.62754247
C	3.24507506	2.37961568	2.55065933
H	3.86495428	3.25882360	2.60744785
C	1.00683480	-1.68209752	2.57322794
C	-1.16980200	-1.95520482	2.13025802
C	-2.67826890	3.18530216	1.51085511
C	-4.32282004	-0.00878536	1.43606072
H	-5.14686345	-0.69446388	1.34204788
C	2.27055008	-1.12061256	2.74062918
C	-4.36372901	1.35197020	1.37651932
H	-5.23046234	1.97646408	1.23387325
C	-2.49450840	-1.68448540	1.81810692
C	3.46848314	-2.72086240	4.27585610
C	3.41584233	-1.99772036	3.08344145
C	0.61032601	4.66168207	1.94648163
H	1.36445239	5.41866665	2.07792692
C	4.50777679	-3.59872838	4.55891924
C	5.53974924	-3.76427679	3.64352467
C	-0.62352827	-3.23863415	2.41623145
H	-1.18589205	-4.15782814	2.42216774
C	5.52856084	-3.03917926	2.45967749
C	-3.74456086	4.21957903	1.50473742
C	0.70090841	-3.07040281	2.68899710
H	1.41982661	-3.83622222	2.92535863
C	-0.74366984	4.84918994	1.73950258
H	-1.27210118	5.78809852	1.68943054
C	4.48350708	-2.16571552	2.20331038
C	-4.52574678	4.42967634	2.64351418
C	-4.00640693	5.03162757	0.40545914
C	-5.52387984	5.39426931	2.68437679
C	-4.99586358	6.00570139	0.42099405
C	-5.75822583	6.18725337	1.56717328
C	-3.44803898	-2.81404810	1.66657076
C	-3.37490780	-3.65817239	0.56080942
C	-4.30685807	-4.65696711	0.32911877
C	-5.34478690	-4.84699217	1.23196360
C	-5.43082265	-4.04153940	2.36063430
C	-4.48542219	-3.04357087	2.56797721
Si	0.29668670	0.75516765	-1.58617394
F	4.32233040	3.68947552	-3.73759534
F	6.25380128	5.57111378	-3.78818877
F	3.30272022	4.88277184	0.72776465
F	-2.49281065	-2.59369720	-5.18279816
F	6.71184626	7.11790523	-1.59555583
F	5.22018615	6.76004049	0.65975022
F	-4.50498158	-1.49604039	-1.04150012
F	-4.52205660	-4.28316755	-5.70596698
F	-6.50687950	-3.20552178	-1.56093424
N	0.36236401	2.61146205	-1.75094426
N	0.17153303	-0.98906273	-2.23401683
N	-1.41276284	1.06460537	-2.24936630
F	-6.53494045	-4.61192540	-3.90151134
N	2.16137475	0.74841317	-1.68223387
C	1.17001825	-1.95518355	-2.13035076
C	1.34708112	3.56515330	-1.62778569
C	-1.00669839	-1.68226993	-2.57316625
C	-1.86809661	2.36442153	-2.23325060
C	-0.83257300	3.26583968	-1.96324636
C	0.74326821	4.84904869	-1.73945720
H	1.27158324	5.78801369	-1.68922680
C	-2.46721345	0.24798682	-2.58069624
C	-0.61073528	4.66142736	-1.94632547
H	-1.36495874	5.41835957	-2.07751375
C	3.03428043	1.84245837	-1.52175618
C	2.96636351	-0.39050022	-1.64023455
C	-2.27050684	-1.12094487	-2.74045793
C	0.62383034	-3.23865614	-2.41626246
H	1.18627472	-4.15780064	-2.42223809
C	2.67806453	3.18536860	-1.51102019
C	-0.70064673	-3.07054345	-2.68891378
H	-1.41951401	-3.83644118	-2.92517483
C	2.49469836	-1.68439477	-1.81815684
C	4.52550951	4.42984568	-2.64359694
C	3.74424780	4.21975797	-1.50486889
C	-3.24537268	2.37918670	-2.55041123
H	-3.86530018	3.25835854	-2.60725254
C	5.52354937	5.39453464	-2.68445498
C	5.75772380	6.18763486	-1.56729871

C	4.32290562	-0.00857212	-1.43604399
H	5.14700038	-0.69418590	-1.34200923
C	4.99528221	6.00609970	-0.42117043
C	-3.41571468	-1.99812572	-3.08332974
C	4.36370676	1.35218985	-1.37656014
H	5.23038543	1.97676300	-1.23392424
C	-3.62009978	1.06485006	-2.76545631
H	-4.59678212	0.70464914	-3.04716975
C	4.00592504	5.03192447	-0.40563465
C	-3.46827276	-2.72126842	-4.27574793
C	-4.48347519	-2.16609532	-2.20330214
C	-4.50755555	-3.59911714	-4.55890832
C	-5.52852475	-3.03952994	-2.45977351
C	-5.53961863	-3.76464227	-3.64361455
F	-2.40452106	-3.48517214	-0.34682319
F	-4.23046632	-5.41354348	-0.77407190
F	-6.25295676	-5.79771425	1.01655691
F	-6.42133054	-4.22995278	3.23701013
F	-4.60766414	-2.27772486	3.65850693
C	3.44830737	-2.81389060	-1.66657690
C	3.37524086	-3.65795167	-0.56077035
C	4.48573848	-3.04333435	-2.56794784
F	2.40479189	-3.48502002	0.34680872
C	4.30730727	-4.65662060	-0.32898970
F	4.60791986	-2.27752148	-3.65850439
C	5.43125414	-4.04117488	-2.36051619
F	4.23097536	-5.41314347	0.77423946
C	5.34528781	-4.84656057	-1.23179023
F	6.42182103	-4.22951847	-3.23684013
F	6.25357183	-5.79715851	-1.01630091

3a-*O* (S_1)

Si	-0.63063960	0.15852321	1.65044774
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F	6.18815102	2.93569149	5.07707175
F	3.02482037	4.06684704	0.79298455
O	-0.33623156	0.08253374	0.01516997
F	-5.52044570	-0.73623629	3.86120925
F	6.90496849	4.89265470	3.30701714
F	5.28133261	5.43904977	1.16918293
F	-5.01574068	-2.71940118	-0.42607228
F	-8.03683475	-1.66504632	3.97906568
F	-7.50869750	-3.67572174	-0.26789842
N	-0.22760841	1.92925187	2.06248388
N	-1.32352546	-1.56555411	1.84976124
N	-2.35880698	0.82104771	1.80353764
F	-9.05838958	-3.15396983	1.93014182
N	1.06863315	-0.31157405	2.24496173
C	-0.54966929	-2.74012698	1.79635512
C	0.93479664	2.62583835	2.33413268
C	-2.66400561	-1.97496169	1.68933825
C	-2.51467597	2.19884938	1.89400680
C	-1.26696647	2.84393041	2.05740538
C	0.61401383	3.99197273	2.48580349
H	1.31551508	4.77517363	2.73399350
C	-3.62378894	0.26452641	1.73309297
C	-0.76953687	4.12502517	2.31495352
H	-1.35342259	5.02972562	2.39035043
C	2.17924891	0.54118189	2.44392508
C	1.58978130	-1.61741498	2.19239800
C	-3.78176538	-1.13099001	1.66413740
C	-1.40075983	-3.85483878	1.59901485
H	-1.06799718	-4.87829064	1.51204687
C	2.15190754	1.93653802	2.49196696
C	-2.69341825	-3.39358651	1.55530408
H	-3.59262816	-3.97954190	1.43849077
C	0.83699805	-2.75829406	1.94948618
C	4.23024995	2.48675329	3.82312271
C	3.38417587	2.71242910	2.72545432
C	-3.87086858	2.52226106	1.85896915
H	-4.28438069	3.51796632	1.92694008
C	5.41032523	3.19857425	4.02005582
C	5.77165159	4.20666350	3.13143106
C	2.99589869	-1.57132910	2.39437746
H	3.64150679	-2.43638468	2.43258949
C	4.93576407	4.49160819	2.05701137
C	-5.15245459	-1.68609855	1.71430112
C	3.35653476	-0.26219142	2.53966145
H	4.35306665	0.12698187	2.67705423
C	-4.57335470	1.30967876	1.75020612
H	-5.64528602	1.17753757	1.71380282
C	3.77164627	3.75780005	1.87352509
C	-5.98032337	-1.44309865	2.82296204
C	-5.72092693	-2.45439540	0.69461959
C	-7.28607411	-1.91888429	2.90067006
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F	-4.43314504	7.17449365	0.23924306
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F	3.47614104	-5.75054974	-5.26469270
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N	-1.27609890	-1.46742307	-2.09603765
F	3.08578525	-7.77274271	-3.47493151
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C	-4.59886548	1.36062602	-1.60654975
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C	-0.68817745	-2.66769627	-2.40784861
C	-4.66135279	-0.00391531	-1.74967424
H	-5.53754828	-0.63269974	-1.77465829
C	-1.19594430	3.09376899	-1.59610856
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C	3.31858841	-0.27252579	-2.45562148
H	4.32728564	0.10717923	-2.49862516
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C	2.71242364	-5.55311879	-4.18721937
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C	2.50615101	-6.59029048	-3.28136971
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F	3.50729741	-7.70069676	1.36155051
F	1.76540974	-7.33444102	3.43427278
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C	4.99423554	4.36268921	-2.44671786
F	6.46285031	2.48554334	0.28926098
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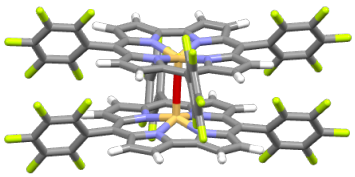
3a-*A* (S_0)



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F	7.71643269	-1.25275359	-1.02060395
F	-4.94264909	-1.31243328	-0.79571417
F	-7.50910708	2.30778087	-3.93028023
F	-7.62185835	-1.33603938	-0.93202161
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C	-0.62607110	-1.52202451	-3.02580126
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H	-3.85762292	-1.99549885	-3.45977107
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C	-3.31183048	-0.59718637	2.11117126
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H	4.48171462	-3.05903199	0.86210143
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C	-5.48446921	-1.43503121	3.07337854
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F	-5.06319262	-1.35835970	-0.95139496
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F	-7.74759023	-1.26507132	-1.02219096
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C	-2.45587064	-3.82473351	0.40113180
H	-2.59639819	-4.79810345	-0.04724789
C	-7.10643087	0.26751018	1.64195863
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C	-3.42432844	-2.96230508	0.84530373
H	-4.49261254	-3.09483095	0.78336701
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C	0.42473362	-7.60531717	0.15590557
F	-0.26253704	-6.86736335	-3.33481063
C	0.20676774	-7.79567646	-1.20607567
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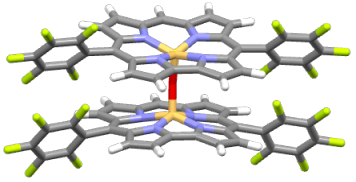
F	0.25884848	-9.02331185	-1.73072750

3b-*P* (S_0)



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F	7.69011359	-0.20207734	1.28757781
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C	3.34957342	-2.17736786	0.27019102
C	2.73669775	-2.27372000	1.51868818
F	7.51585689	-4.03152812	-1.46336296
F	8.96034415	-2.07360868	-0.23435254
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C	2.93683364	-1.99377082	-2.26645145
H	3.94399649	-1.93482470	-2.64350805
C	0.69942220	-2.06276808	-2.08885038
C	2.49146983	-2.48762540	3.75591400
H	2.65591714	-2.62113610	4.81392196
C	4.82793722	-2.18680954	0.18316197
C	3.42052421	-2.45499590	2.75783135
H	4.48786620	-2.56261161	2.85535553
C	5.60803744	-1.22043881	0.82072939
C	1.76991614	-1.97849271	-3.00738418
H	1.67901393	-1.91040770	-4.07955513
C	-0.00007030	-2.37477578	3.80960476
H	-0.00011112	-2.47238611	4.88668873
C	5.51480874	-3.13826395	-0.57305772
C	6.98697900	-1.17749005	0.69584485
C	7.63685142	-2.12000633	-0.08911016
C	6.89602581	-3.10843007	-0.72219823
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C	-2.74390915	2.08010060	0.97728596
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F	-8.90401677	2.79817501	-0.81818969
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C	-2.90694786	1.75632151	-2.79559517
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C	-2.73660122	-2.27397409	1.51838579
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3b-*P* (S_1)

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C	1.52523856	-2.79882933	2.92225195
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H	2.47530382	4.25045327	2.66176656
C	2.10689797	-0.44847665	4.81498706
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C	-2.14740188	0.28415533	-3.35496397
C	-2.32218906	1.54703427	-2.73356795
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C	-1.90768791	-2.24746474	-2.93683015
H	-1.78433403	-2.62480145	-3.93876922
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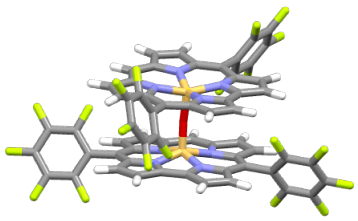
3b-*O* (S_0)



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C	3.06188603	-0.56950463	-1.85685948
C	3.01038542	-1.95692398	-1.95272908
C	1.78895722	-2.61435686	-2.07852103
F	7.25586534	-3.12820219	-4.03812470
F	7.88482372	-4.78250883	-1.96836183
C	-0.40510868	-3.04128000	-2.18900267
C	4.16334660	0.33275656	-1.78692111
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C	1.61821595	-4.02496752	-2.21284286
H	2.42856340	-4.73402125	-2.26259845
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C	3.65591317	1.61924006	-1.78061464
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C	-1.77276011	-2.86022929	-2.19204220
H	-2.40498148	-3.73530570	-2.23030291
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C	-1.78889667	-2.61419724	2.07861029
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H	2.40508507	-3.73495817	2.23054836
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C	-5.83370037	-4.28237745	0.91491903
C	-6.72519909	-4.12362377	1.96801679
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F	6.69978424	5.59773240	2.55647228
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C	0.58409854	3.78167342	2.00456458
H	1.17620912	4.67993200	2.07583934
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C	3.77646706	-1.36290458	2.16253517
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H	-4.87700719	0.53369519	-2.12922125
C	-3.82501259	3.86461603	-1.20214987
C	0.79364070	3.69779209	-1.92428618
H	1.50030960	4.51079078	-1.90062892
C	-4.34865550	2.95352738	-3.33122042
C	-4.88061216	4.75925031	-1.30888271
C	-5.68110322	4.74441427	-2.44310315
C	-5.41260398	3.83665540	-3.45990358

3b-*O* (S_1)

Si	0.11635074	-0.03514133	-1.75048475
F	3.67324469	-3.94709316	-0.44906765
O	-0.15249543	-0.50698792	-0.18240744
F	5.26995778	-0.95559047	-3.78255142
N	0.61988327	-1.68775442	-2.45169186
N	1.91089962	0.44903492	-1.75162932
F	6.01744373	-5.23445154	-0.49824565
C	3.09828552	-0.26055541	-1.77243475
C	3.09129655	-1.63735139	-2.06689594
C	1.89741886	-2.27870394	-2.41334848
F	7.62632138	-2.23684532	-3.78181867
F	8.02933748	-4.39499811	-2.15524699
C	-0.26617645	-2.70808552	-2.84679952
C	4.15684358	0.63955535	-1.51091557
H	5.20532787	0.38079317	-1.48371642
C	2.21773554	1.77989797	-1.50681813
C	0.46204670	-3.90189627	-3.08202242
H	0.01860028	-4.82896121	-3.42135896
C	4.36947837	-2.37685421	-2.10197055
C	1.78237737	-3.64442440	-2.82192226
H	2.61687240	-4.32229022	-2.92398187
C	4.61995698	-3.49636339	-1.29843140
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H	4.12951533	2.84576982	-1.19632599
C	-1.63197855	-2.54719594	-2.94928730
H	-2.22776730	-3.40792510	-3.23384777
C	5.42342687	-1.98857254	-2.94456877
C	5.82987527	-4.18033600	-1.30648607
C	6.85707620	-3.75136766	-2.14146110
C	6.65082381	-2.64531509	-2.96075715
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N	-0.56214201	-2.22984650	1.82364196
N	-1.92243744	-0.03542687	1.83016166
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C	-3.06012797	-2.14801957	1.83137348
C	-1.81979677	-2.82491803	1.81368284
F	-6.07885036	-5.35694257	3.93636404
F	-7.89607138	-5.04130557	1.92591570
C	0.36317575	-3.27998769	1.72016695
C	-4.19224990	0.16292361	1.91342227
H	-5.23427917	-0.11969186	1.94714893
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C	-0.33753744	-4.52849074	1.68240185
H	0.14326033	-5.49429317	1.61013503
C	-4.32680166	-2.91521116	1.85186358
C	-1.66979906	-4.25113326	1.74114029
H	-2.49099866	-4.95091424	1.71795816

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C	-4.63322542	-3.79749393	2.89466226
C	-6.48405434	-3.47803421	0.85720347
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F	4.23460748	1.28298143	4.16249034
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H	1.20396032	4.41774209	2.32436798
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C	3.74646546	-1.62856959	1.61208320
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C	3.93554664	-0.27669602	1.71910632
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C	-0.78181415	3.46893489	2.12843405
H	-1.48280545	4.28727303	2.18813236
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C	4.87980584	4.62179318	1.86212930
C	5.73486477	4.31832290	2.91753026
C	5.50700914	3.17496298	3.67812523
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F	-4.23312340	2.54953006	-4.10938826
N	-1.63830503	-0.15487071	-2.36986014
N	-0.08730802	1.80903480	-1.68410420
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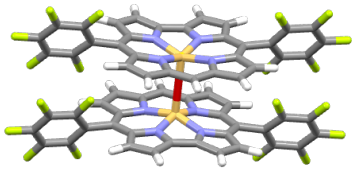
C	-1.17739661	2.66020864	-1.66425035
C	-2.47515220	2.15188334	-1.88055619
C	-2.65967041	0.80425275	-2.20598098
F	-6.31868116	4.23016902	-4.07632122
F	-6.84490629	5.74687900	-1.86474981
C	-2.28750384	-1.35369668	-2.71248636
C	-0.71118326	3.97566441	-1.45710264
H	-1.33098648	4.86016716	-1.42296299
C	1.04981643	2.57908317	-1.48646025
C	-3.68697999	-1.14101755	-2.75541715
H	-4.41410230	-1.90544884	-2.99425829
C	-3.62243700	3.07940904	-1.87060980
C	-3.92000208	0.17006664	-2.43114993
H	-4.87609762	0.66540480	-2.35216997
C	-3.91872641	3.89915123	-0.77311195
C	0.68703980	3.92050786	-1.34762807
H	1.36370039	4.74767251	-1.19310575
C	-4.46266921	3.24140742	-2.98599576
C	-4.98508703	4.78975526	-0.75506210
C	-5.80984316	4.89979303	-1.86982194
C	-5.54603438	4.11477387	-2.98889214

3b-*A* (S_0)



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F	4.38934881	-0.76818226	4.82650932
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N	2.04670375	1.35351252	1.20382636
F	0.38654806	1.55416559	7.68649655
C	2.14858477	1.42890563	2.57347774
C	2.17771860	0.26740702	3.34289152
C	2.09768163	-0.98515566	2.73744294
F	4.52124867	-0.71553853	7.51193061
F	2.52270485	0.43286800	8.96396970
C	1.89367731	-2.61184496	1.21389147
C	2.27649024	2.80087515	2.93326436
H	2.38985026	3.17049970	3.93988957
C	2.12679930	2.63299348	0.69961938
C	1.92571397	-3.22675675	2.49644005
H	1.86198233	-4.29043935	2.66470996
C	2.30340320	0.35834199	4.81703573
C	2.06159657	-2.23696213	3.42367475
H	2.10258764	-2.34594303	4.49359591
C	1.32203842	0.97071283	5.59517050
C	2.26044778	3.54728516	1.76717047
H	2.35110912	4.61806036	1.67491053
C	1.80907405	-3.26147032	-0.00000000
H	1.72261243	-4.33939101	-0.00000000
C	3.38946078	-0.18942326	5.50219792
C	1.37999106	0.99988858	6.97951173
C	2.45855913	0.41979043	7.63294937
C	3.47167699	-0.17146166	6.88918816
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F	-0.24810734	-1.52042352	5.00834466
F	-4.38902347	0.76877788	4.82728108
N	-2.00137427	1.22935184	1.35490133
N	-2.04808434	-1.35351183	1.20382027
F	-0.38588078	-1.55470712	7.68587377
C	-2.14973702	-1.42887099	2.57348400
C	-2.17811881	-0.26736800	3.34291177
C	-2.09762592	0.98516484	2.73746319
F	-4.52002381	0.71612475	7.51275269
F	-2.52129221	-0.43285008	8.96408601
C	-1.89316347	2.61178522	1.21389152
C	-2.27821829	-2.80078251	2.93328447
H	-2.39157477	-3.17036073	3.93992667
C	-2.12882103	-2.63294872	0.69961840
C	-1.92482818	3.22670362	2.49644339
H	-1.86066784	4.29036227	2.66470921
C	-2.30337963	-0.35829785	4.81709159
C	-2.06098435	2.23695727	3.42368942
H	-2.10182215	2.34595422	4.49361295
C	-1.32191413	-0.97095680	5.59487098
C	-2.26272732	-3.54718819	1.76718159
H	-2.35389962	-4.61791888	1.67492740
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C	-1.37940939	-1.00014511	6.97922994
C	-2.45759591	-0.41976021	7.63304410
C	-3.47080832	0.17178055	6.88964193
F	-0.24810734	-1.52042352	-5.00834466
F	-4.38902347	0.76877788	-4.82728108
N	-2.00137427	1.22935184	-1.35490133
N	-2.04808434	-1.35351183	-1.20382027
F	-0.38588078	-1.55470712	-7.68587377
C	-2.14973702	-1.42887099	-2.57348400
C	-2.17811881	-0.26736800	-3.34291177
C	-2.09762592	0.98516484	-2.73746319
F	-4.52002381	0.71612475	-7.51275269
F	-2.52129221	-0.43285008	-8.96408601
C	-1.89316347	2.61178522	-1.21389152
C	-2.27821829	-2.80078251	-2.93328447
H	-2.39157477	-3.17036073	-3.93992667
C	-2.12882103	-2.63294872	-0.69961840
C	-1.92482818	3.22670362	-2.49644339
H	-1.86066784	4.29036227	-2.66470921
C	-2.30337963	-0.35829785	-4.81709159
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C	-1.32191413	-0.97095680	-5.59487098
C	-2.26272732	-3.54718819	-1.76718159
H	-2.35389962	-4.61791888	-1.67492740
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F	4.52124867	-0.71553853	-7.51193061
F	2.52270485	0.43286800	-8.96396970
C	1.89367731	-2.61184496	-1.21389147
C	2.27649024	2.80087515	-2.93326436
H	2.38985026	3.17049970	-3.93988957
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C	1.92571397	-3.22675675	-2.49644005
H	1.86198233	-4.29043935	-2.66470996

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C	2.06159657	-2.23696213	-3.42367475
H	2.10258764	-2.34594303	-4.49359591
C	1.32203842	0.97071283	-5.59517050
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H	2.35110912	4.61806036	-1.67491053
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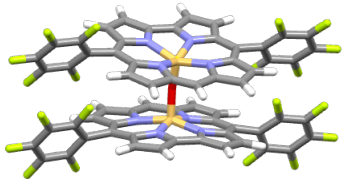
3b-*A* (S_1)



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H	-4.49041499	2.31220515	2.25668499
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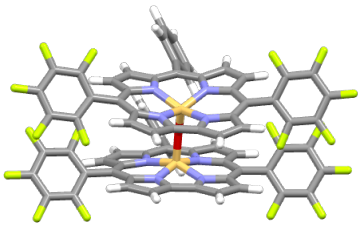

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F	-5.12812502	-2.29231854	0.38993871
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F	-5.19348056	-2.33252223	0.14928966
F	-7.45841523	-0.82769911	-4.56557541
F	-7.81603549	-2.61006630	-0.20081103
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C	-0.72594605	-2.60083807	2.25673265
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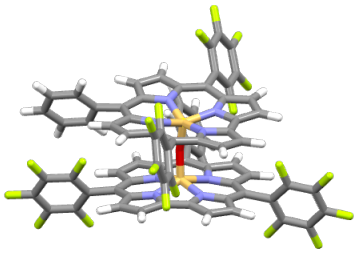

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F	-6.46545466	6.57529704	-2.58158904
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F	4.79328412	-1.85086603	-0.48772101
F	5.25793630	-4.72359413	-5.07588995
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N	0.21703458	-1.44095554	-2.16962706
N	1.76371813	0.63367974	-2.01888507
F	7.11717110	-4.97467078	-3.10129696
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C	6.08592038	-4.14210994	-2.94489052
C	-3.05280721	-3.31590456	-1.70287821
C	-2.86672243	-4.10803237	-0.56425502
H	-2.03937687	-3.88867724	0.09756670
C	-3.75225806	-5.13687352	-0.26283929
H	-3.60144955	-5.73073232	0.63181076
C	-4.83776885	-5.39209354	-1.09783353
H	-5.53938797	-6.18125547	-0.85569800
C	-5.01460534	-4.62754506	-2.24866121
H	-5.84745226	-4.83107711	-2.91144585
C	-4.12567044	-3.60024576	-2.55320916
H	-4.26226395	-3.01247772	-3.45289781
Si	0.02444210	0.32012014	1.61709826
F	-3.16551022	-3.05854637	4.76584501
F	-5.25684191	-4.72333211	5.07720072
F	-4.79401558	-1.85343664	0.48706885
F	3.80756627	3.14887015	4.38636015
F	-7.11663536	-4.97593256	3.10331236
F	-6.86990547	-3.52277742	0.80936880
F	3.29362149	4.43884361	-0.13911044
F	5.75004200	4.99622795	4.68121660
F	5.22072421	6.28319400	0.17194383
N	-1.76391051	0.63249561	2.01680222
N	1.85035852	0.27871255	1.98908186
N	0.07997715	2.16735685	1.83913041
F	6.46497004	6.57501986	2.58170702
N	-0.21709894	-1.44187058	2.16860123
C	2.64018710	-0.87474189	1.94033935
C	-2.86236299	-0.17385279	2.20451127
C	2.74530157	1.36285376	2.00147471
C	-1.12837420	2.83166505	1.85253672
C	-2.19987235	1.93835849	1.94363793
C	-4.02144270	0.65673989	2.22872508
H	-5.03139205	0.30753944	2.37273073
C	1.08066605	3.10974741	1.88623081
C	-3.60804818	1.96600251	2.06370160
H	-4.22128246	2.85160077	2.03368647
C	-1.43238485	-2.12025291	2.36918121
C	0.77451001	-2.42190257	2.10454752
C	2.40847874	2.71282846	1.97532818
C	4.01544284	-0.50140966	1.92182540
H	4.83566569	-1.19309529	1.85773455

C	-2.70417876	-1.54406005	2.39132411
C	4.07715047	0.85900453	1.98341927
H	4.96162300	1.47493650	1.98510189
C	2.13309494	-2.17045278	1.93374179
C	-4.05835380	-3.15429404	3.77249029
C	-3.88911895	-2.41038561	2.60204293
C	-0.89316387	4.22553965	1.87874871
H	-1.65155635	4.99001425	1.88275233
C	-5.13102194	-4.01822729	3.94834229
C	-6.08554657	-4.14333344	2.94607333
C	0.18275514	-3.70276919	2.29685168
H	0.73078258	-4.62965907	2.32189349
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C	-1.15848879	-3.51620455	2.47176994
H	-1.90182286	-4.27433750	2.65369190
C	0.47792698	4.40030513	1.90192504
H	1.01546017	5.33438089	1.94547030
C	-4.87999621	-2.54341647	1.62916158
C	4.13707378	3.90624578	3.33488050
C	3.87095037	4.55796671	1.06623713
C	5.13969521	4.85252182	3.50166568
C	4.86743096	5.51435545	1.20767521
C	5.50478385	5.66178317	2.43245957
C	3.05285887	-3.31656879	1.70179196
C	4.12559674	-3.60164669	2.55204133
H	4.26208479	-3.01463953	3.45223850
C	5.01444981	-4.62882346	2.24683584
H	5.84715645	-4.83298779	2.90959928
C	4.83769724	-5.39245984	1.09539382
H	5.53926980	-6.18150503	0.85274200
C	3.75239220	-5.13642556	0.26038180
H	3.60171087	-5.72953395	-0.63478770
C	2.86692546	-4.10771931	0.56245433
H	2.03976088	-3.88768971	-0.09936978

3c-*O* (S_1)

Si	-0.06151433	0.31321964	-1.66512625
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F	-6.08173660	4.73693074	-4.50960683
F	-3.28871102	4.53273052	0.16232115
O	0.01501044	0.06585570	-0.01741851
F	3.12958473	-3.13207533	-4.73051148
F	-6.64048189	6.48821870	-2.49101691
F	-5.21297576	6.36964717	-0.15762749
F	4.82642686	-1.77100464	-0.51139688
F	5.22016075	-4.79517707	-5.01778507
F	6.90412201	-3.43131227	-0.81433252
N	-0.15818984	2.16469849	-1.80879615
N	0.19610342	-1.45200807	-2.19005802
N	1.72004644	0.65373433	-2.03433671
F	7.13062438	-4.96665596	-3.07084294
N	-1.90034249	0.24040065	-1.95710376
C	-0.78766390	-2.45941223	-2.09703527
C	-1.17846919	3.09883496	-1.83868056
C	1.42246248	-2.11720196	-2.38973107
C	2.14506366	1.97080048	-1.92190158
C	1.04452659	2.85923191	-1.83136729
C	-0.60934691	4.38616146	-1.86258610
H	-1.16464808	5.31260858	-1.91109587
C	2.84067608	-0.14092719	-2.19210787
C	0.78840865	4.23190731	-1.85754364
H	1.53074761	5.01476526	-1.89647242
C	-2.82062466	1.31011677	-1.94038057
C	-2.67935897	-0.93835903	-1.90942573
C	2.69298623	-1.52937850	-2.39452086
C	-0.17799788	-3.72452503	-2.28403438
H	-0.71248192	-4.66304419	-2.30107097
C	-2.51801747	2.66633069	-1.89438772
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H	1.91843585	-4.27139346	-2.66169530
C	-2.14855158	-2.22384763	-1.91048049
C	-4.36474470	3.74873383	-3.20695394
C	-3.60628563	3.65800484	-2.02968917
C	3.53929060	2.01507619	-1.98861252
H	4.14516232	2.90863041	-1.93800968
C	-5.38456266	4.68233526	-3.36804501
C	-5.66751099	5.58256915	-2.34411541
C	-4.05556646	-0.58523625	-1.87005396
H	-4.86840934	-1.29054931	-1.81845208
C	-4.93536264	5.52564756	-1.16258326
C	3.87886596	-2.38342064	-2.60132765
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C	3.98071309	0.69130799	-2.16224939
H	5.00063812	0.35603969	-2.28597500
C	-3.93194600	4.57315523	-1.02554038
C	4.03898591	-3.17849352	-3.74724032
C	4.90016928	-2.48261589	-1.64910017
C	5.11330764	-4.04826936	-3.91019316
C	5.98833956	-3.33406964	-1.79074419
C	6.09579355	-4.12889175	-2.92686362
C	-3.05212709	-3.37839306	-1.65044057
C	-2.82053937	-4.18694199	-0.52688411
H	-1.95021910	-3.98505987	0.08725518
C	-3.69693924	-5.21715128	-0.19139565
H	-3.50414088	-5.82502954	0.68956734
C	-4.82598428	-5.46027147	-0.97632567
H	-5.51864866	-6.25379694	-0.71091126
C	-5.04887892	-4.68459673	-2.11499126
H	-5.91213529	-4.88036391	-2.74489583
C	-4.16554492	-3.65962079	-2.45433899
H	-4.33822108	-3.06455048	-3.34544721
Si	0.06415060	0.34261722	1.55415692
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F	-4.79859697	-1.86266952	0.53915047
F	3.98666988	3.03339385	4.22094636
F	-6.96779564	-5.03839178	3.23171141
F	-6.80914216	-3.60854020	0.91190463
F	3.18186546	4.64190085	-0.16171108
F	5.95970218	4.85400569	4.51794690
F	5.14134190	6.46030862	0.15008978
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N	0.11394736	2.20386458	1.75545848
F	6.54456412	6.57837029	2.48702006
N	-0.16917433	-1.40365554	2.19702676
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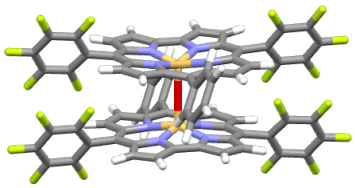
C	-2.83252951	-0.14215732	2.15288962
C	2.78087888	1.39763006	1.93408926
C	-1.08065910	2.86143702	1.73290420
C	-2.16849140	1.95399998	1.83820560
C	-3.99966190	0.68467252	2.09379812
H	-5.01564924	0.33217962	2.19426179
C	1.11758409	3.15594405	1.77391766
C	-3.58327191	1.98856225	1.89277351
H	-4.19206047	2.87209336	1.77993790
C	-1.37501574	-2.07944034	2.39799876
C	0.81658862	-2.38480482	2.12141354
C	2.43599906	2.77024292	1.88703111
C	4.05883740	-0.45493035	1.83875222
H	4.88081414	-1.14261689	1.73909694
C	-2.66717430	-1.49772493	2.39548970
C	4.11311670	0.91427210	1.87931205
H	4.99172527	1.53852410	1.82454752
C	2.18274315	-2.12792067	1.92043533
C	-3.95341237	-3.11714568	3.82211621
C	-3.83572479	-2.37684695	2.63863557
C	-0.86314593	4.26491267	1.71472221
H	-1.62999596	5.02058885	1.67086175
C	-4.99750273	-4.01098224	4.03047575
C	-5.96714760	-4.17820948	3.04310461
C	0.23577748	-3.66228031	2.32263537
H	0.78417729	-4.59155666	2.33777786
C	-5.89027392	-3.44292604	1.86455473
C	3.51379562	3.77978243	2.02119814
C	-1.11398715	-3.47229050	2.50367884
H	-1.86384478	-4.23058373	2.66696253
C	0.50272985	4.44950952	1.74407227
H	1.03661422	5.38857679	1.74574039
C	-4.83980588	-2.54972684	1.68072582
C	4.25558484	3.86464134	3.20590753
C	3.83806763	4.67830180	1.00167305
C	5.27468408	4.79581742	3.37277833
C	4.85266124	5.62079760	1.14716447
C	5.57206916	5.67987040	2.33760958
C	3.09556057	-3.26695434	1.66108801
C	4.22087337	-3.51655274	2.45942959
H	4.39278958	-2.91494984	3.34668398
C	5.11059708	-4.53289766	2.11827786
H	5.98208389	-4.71628224	2.73948790
C	4.88635713	-5.30909691	0.97967901
H	5.59269411	-6.08630900	0.70429183
C	3.75273937	-5.08260443	0.19768442
H	3.57461284	-5.67752842	-0.69316709
C	2.85592769	-4.07271687	0.53729470
H	1.99809941	-3.87030037	-0.09509711

3c-*A* (S_0)



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F	-4.81328044	2.76552305	-3.50549507
F	8.94415630	0.82204269	-2.39012307
F	7.64041262	-1.20130868	-1.10376884
F	-5.05013805	-1.19073051	-0.91608001
F	-7.49676058	2.80067813	-3.67304844
F	-7.72624359	-1.13563061	-1.07856195
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N	-1.36646315	2.04296688	-1.15254486
N	-1.22179953	-0.20068145	-2.44096443
F	-8.97565414	0.86322059	-2.45663949
N	1.33366006	2.05451655	-1.16744865
C	-1.22835211	3.21768465	-0.41065321
C	2.55168826	-0.17977944	-2.62396790
C	-2.74882083	1.87345063	-1.36119827
C	-0.71852396	-1.26588780	-3.15525589
C	0.67892596	-1.24192739	-3.19062506
C	2.90928717	-1.28092952	-3.45190059
H	3.91318234	-1.52489241	-3.76093970
C	-2.59260627	-0.22912033	-2.54957370
C	1.74279218	-1.93742999	-3.80667726
H	1.64757234	-2.79590407	-4.45260319
C	2.71714753	1.87530391	-1.36008534
C	1.19869311	3.20941189	-0.39360102
C	-3.35784416	0.80673330	-2.02065539
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H	-2.68739840	4.70182804	0.35911784
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C	5.49449707	1.81841445	-2.86689479
C	4.79626994	0.80792500	-2.20408547
C	-1.78670506	-2.01228300	-3.69890773
H	-1.69317259	-2.90499524	-4.29658409
C	6.88232568	1.83338095	-2.93388762
C	7.61246778	0.81114222	-2.34128754
C	2.48984977	3.73123691	-0.09174403
H	2.66923639	4.60783291	0.50695280
C	6.94544658	-0.22335350	-1.69940298
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C	3.41056257	2.92892995	-0.69525225
H	4.48156920	3.02742448	-0.66174781
C	-2.95368747	-1.36828617	-3.32511745
H	-3.96202112	-1.64746461	-3.58593814
C	5.56060845	-0.21707535	-1.64818830
C	-5.50220781	1.79311060	-2.89658489
C	-5.62292119	-0.19634154	-1.61045249
C	-6.88802137	1.82562367	-2.99182389
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C	-0.52881825	4.96000033	2.12614159
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C	-0.53509160	6.10486683	2.91726848
H	-0.93110336	6.06088590	3.92566932
C	-0.03306028	7.30411075	2.41654183
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F	5.04966129	1.19075637	0.91576037
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C	-1.74313549	1.93714268	3.80685047
H	-1.64799207	2.79553572	4.45289592
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C	-1.19850235	-3.20949589	0.39356176
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C	1.78638248	2.01233775	3.69908187
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H	0.93195623	-6.06165130	-3.92495230
C	0.03359555	-7.30461558	-2.41580169
H	0.03802264	-8.19677651	-3.03100294
C	-0.46983266	-7.35269319	-1.11775102
H	-0.85291076	-8.28437244	-0.71783657
C	-0.47503853	-6.20753113	-0.32601512
H	-0.85610163	-6.24711163	0.68751608

3c-*A* (S_1)

Si	-0.03674057	0.73890009	-1.44609475
F	4.89711740	2.67922058	-3.46859791
F	7.59447364	2.63607559	-3.42386167
F	4.81162843	-1.38239958	-1.03204424
O	0.03850703	-0.04187466	-0.06047871
F	-4.85768984	2.79819748	-3.29248399
F	8.91078045	0.60978354	-2.15825436
F	7.50115947	-1.40335730	-0.97277555
F	-5.10608058	-1.31484648	-0.95129909
F	-7.54659177	2.90720983	-3.36305740
F	-7.78724000	-1.18423096	-1.01093422
N	1.12804421	-0.24213951	-2.54718240
N	-1.38505397	2.01362428	-1.18182523
N	-1.27945048	-0.25179597	-2.44453058
F	-9.03224902	0.93102349	-2.20806733
N	1.32041362	2.02886154	-1.29775784
C	-1.22504907	3.20154408	-0.46090318
C	2.50019256	-0.29001830	-2.67922702
C	-2.76340686	1.83450159	-1.32019697
C	-0.80740730	-1.33940843	-3.11597274
C	0.60989749	-1.32669033	-3.19175758
C	2.83509060	-1.44536404	-3.44591157
H	3.83696363	-1.73602859	-3.72678010
C	-2.66119823	-0.29790870	-2.48486874
C	1.65071009	-2.09018991	-3.76954018
H	1.52799766	-2.99206133	-4.35160872
C	2.69562321	1.81527090	-1.47687901
C	1.21689979	3.19421320	-0.54176838
C	-3.40619492	0.74235327	-1.96020550
C	-2.49988532	3.76084730	-0.17561474
H	-2.66074497	4.68524471	0.35624438
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C	-3.44308166	2.91816161	-0.70049288
H	-4.51361376	3.01630320	-0.63461710
C	0.00499035	3.76707922	-0.12969812
C	5.51487769	1.66106391	-2.85337654
C	4.76282001	0.65292842	-2.24174045
C	-1.88624845	-2.13195504	-3.58313379
H	-1.79936559	-3.06000169	-4.12933236
C	6.90573876	1.65485629	-2.83400257
C	7.58072180	0.61746637	-2.19461106
C	2.50980304	3.69840427	-0.24832517
H	2.71018851	4.57040627	0.35302697
C	6.85940659	-0.41633722	-1.60485245
C	-4.88315138	0.75359791	-2.08482035
C	3.41779975	2.85879034	-0.83915697
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C	-3.04265825	-1.48235896	-3.19705565
H	-4.05963952	-1.79007298	-3.38973686
C	5.47057095	-0.39357535	-1.64135162
C	-5.55385964	1.80928312	-2.71448349
C	-5.67792011	-0.26376804	-1.54783366
C	-6.94230522	1.87990539	-2.75965203
C	-7.06626462	-0.21381532	-1.57933463
C	-7.70316876	0.86862075	-2.17818124
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C	-0.52711337	5.06054701	1.93971443
H	-0.97134611	4.15836599	2.34405233
C	-0.49076638	6.23588386	2.68671779
H	-0.91937880	6.25023727	3.68455912
C	0.09751806	7.38697345	2.15947380
H	0.12283201	8.30244734	2.74321547
C	0.65272286	7.35942136	0.87880854
H	1.10307538	8.25422786	0.45945502
C	0.62697184	6.18389691	0.13095252
H	1.04916918	6.16307876	-0.86910903
Si	0.02949073	-0.75463452	1.44567227
F	-4.81753148	-2.86000415	3.30782732
F	-7.49775199	-2.92237707	3.41380871
F	-5.03384781	1.27260986	0.97504800
F	4.86070649	-2.51910601	3.61387156
F	-8.97659740	-0.90228111	2.31488841
F	-7.70314458	1.19718125	1.09777848
F	5.08130514	1.27336498	0.76729401
F	7.53977904	-2.53833301	3.77186591
F	7.75084763	1.23648611	0.92728256
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N	1.21942799	0.35166319	2.34345215
F	9.02125393	-0.67091132	2.43459356
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C	2.77959326	-1.80416589	1.46926430
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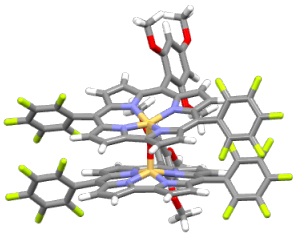
C	-0.71998479	1.43100618	2.99174390
C	-2.95763701	1.41971832	3.24541284
H	-3.96721484	1.66205127	3.54516496
C	2.59767269	0.43471207	2.41698482
C	-1.78632567	2.13859950	3.55059244
H	-1.70952509	3.03251208	4.15496339
C	-2.69830297	-1.85718849	1.34719165
C	-1.14482993	-3.21775354	0.44479393
C	3.38243364	-0.66166023	2.00103251
C	2.57270565	-3.80900726	0.43083621
H	2.76450789	-4.77163592	-0.01903738
C	-3.33342777	-0.78928321	1.98594651
C	3.48114868	-2.95107898	0.98675063
H	4.55187370	-3.07495252	1.02782152
C	0.08678190	-3.78566742	0.13346874
C	-5.49277301	-1.84480111	2.75342277
C	-4.80090419	-0.79527927	2.12853215
C	1.73760147	2.31928863	3.35608145
H	1.62927332	3.27362267	3.85310485
C	-6.88301335	-1.89368622	2.81543879
C	-7.64059482	-0.86131643	2.27036994
C	-2.42129585	-3.74495886	0.12322117
H	-2.58690865	-4.64256160	-0.45296634
C	-6.98923562	0.21374314	1.67513457
C	4.84927063	-0.63287841	2.16714501
C	-3.36650760	-2.93482072	0.69261127
H	-4.43738683	-3.04864684	0.64181153
C	2.93704287	1.65947489	3.02913519
H	3.94261470	1.99257802	3.24400647
C	-5.60239975	0.23355789	1.61885050
C	5.53773662	-1.58097521	2.93976717
C	5.65094451	0.32501296	1.53775835
C	6.92716006	-1.60686225	3.03000592
C	7.03728947	0.32670764	1.61466344
C	7.68612407	-0.65047215	2.36145486
C	0.12626650	-5.04992809	-0.65200761
C	0.80161951	-5.09585300	-1.88061138
H	1.30226513	-4.19988161	-2.23090087
C	0.84175860	-6.26882340	-2.63263944
H	1.37138960	-6.28498590	-3.58205619
C	0.20425167	-7.42085979	-2.16865698
H	0.23371443	-8.33617842	-2.75316226
C	-0.46333628	-7.39085962	-0.94331518
H	-0.95002881	-8.28628431	-0.56656005
C	-0.49871169	-6.21749495	-0.19022801
H	-1.00546476	-6.19927252	0.76941058

3d-*P* (S_0)



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F	5.08844468	-2.96940297	-0.25570081
F	4.77516312	0.33356389	-0.60248604
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F	5.15972581	-1.00172396	4.05774876
F	-4.77632232	0.33167624	0.60426110
F	-7.81570396	-1.32272530	-4.14681345
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F	7.45122853	0.16453871	-0.63768757
F	7.73821389	-3.28531249	-0.14772920
F	-4.54876985	-2.49924933	4.39446576
F	-8.70440185	-1.34016108	2.54057619
F	-7.45223645	0.16167065	0.64038755
F	-7.23282544	-2.65597531	4.42034943
F	9.13798683	-2.46235748	2.04918937
F	7.81542551	-1.33109473	4.14624975
N	-0.96731862	0.22497588	2.35729877
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N	-1.31709251	-2.52222395	-1.64721743
N	0.96729858	0.22945855	-2.35728484
N	1.31741933	-2.52545456	1.64225097
N	1.70485690	0.00045403	2.05209055
N	1.06771031	-2.32509705	-1.93984178
N	-1.06740498	-2.32885251	1.93534017
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C	-0.70086079	-3.75574147	-1.64838555
C	-2.67689780	-2.73567040	-1.65336113
C	-0.68929395	1.56364440	2.63204596
C	-1.70371506	1.37632525	-2.32225198
C	2.43286355	-2.30444712	-2.11683281
C	-0.57708705	2.13749150	-2.59161184
C	2.35777368	0.08112349	-2.50906241
C	-2.43250455	-2.30868599	2.11297136
C	-2.35775356	0.07627980	2.50890636
C	3.08369956	-1.09944453	-2.36801029
C	0.68136165	-3.63879274	-1.79477688
C	-3.06228586	-0.36878092	-1.95542834
C	-0.68102686	-3.64226993	1.78753265
C	-3.55481933	-1.66217477	-1.79023921
C	0.57696060	2.13270258	2.59484048
C	-3.08348702	-1.10421731	2.36634234
C	0.73874472	3.57901497	2.90631087
C	0.70117496	-3.75892867	1.64078692
C	-0.73901573	3.58415626	-2.90136913
C	-5.72670660	-2.53225648	-0.84439938
C	-2.90957304	-4.13963629	-1.62432500
H	-3.88030296	-4.60848364	-1.62810772
C	-1.67886295	-4.77159456	-1.61844828
H	-1.48672828	-5.83288274	-1.61551634
C	-5.01567749	-1.90626387	-1.86913907
C	2.91293940	1.33562534	-2.89503534
H	3.95617120	1.49859844	-3.11150700
C	1.89566839	2.24095103	-2.97391444

H	1.94939905	3.27322533	-3.27476898
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H	-4.94199958	0.80811799	-2.05943528
C	3.06242299	-0.37268604	1.95596060
C	2.90664070	-3.64799275	-2.06567230
H	3.93464916	-3.94930826	-2.16791716
C	-4.55986944	-1.08464614	2.49150258
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H	-3.31677825	2.87935466	-2.54273274
C	4.56013330	-1.07926570	-2.49247891
C	-1.89596904	2.23562436	2.97626092
H	-1.94990553	3.26753189	3.27832098
C	6.62172377	-1.91308103	-3.48757821
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H	-3.93410060	-3.95377102	2.16161449
C	1.81645821	-4.47375424	-1.87374535
H	1.81703132	-5.54874096	-1.79142011
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H	4.94213158	0.80392739	2.06328857
C	3.04394964	1.85077049	2.35618610
H	3.31676761	2.87435950	2.54922877
C	1.67918709	-4.77475735	1.60907181
H	1.48702333	-5.83603060	1.60380114
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C	-1.81602282	-4.47745477	1.86530965
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F	7.18662500	-3.08963300	-4.09550200
F	5.15854300	-3.05590200	-0.22014500
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F	8.65589000	-1.56650500	-2.37016800
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F	5.26832500	-0.66530400	3.89336800
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C	0.58763300	-3.69995400	-1.61412400
C	-3.09607600	-0.36845900	-1.89942700
C	-0.60533100	-3.64150600	1.84846100
C	-3.62479400	-1.66555900	-1.68444200
C	0.56505200	2.19097000	2.54135300
C	-3.06313800	-1.10950700	2.35113300
C	0.70182100	3.65200600	2.79821000
C	0.79459800	-3.73525300	1.68552000
C	-0.69926900	3.51237300	-2.93619900
C	-5.80994900	-2.53278400	-0.74967100
C	-3.02380300	-4.14553400	-1.40079600
H	-4.00233400	-4.59958500	-1.36432000
C	-1.80419700	-4.79131700	-1.37029900
H	-1.61908400	-5.85339300	-1.30247300
C	-5.09012000	-1.87746100	-1.75718300
C	2.90952300	1.16731700	-2.94517600
H	3.95873200	1.30163400	-3.16023700
C	1.90827800	2.10151700	-3.04503300
H	1.99095300	3.13080200	-3.35582100
C	5.18905700	-2.12590000	-3.26862400
C	-3.88528200	0.80171300	-2.07442500
H	-4.95749700	0.83739000	-1.96818800
C	3.09395300	-0.27937500	1.88774200
C	2.81517100	-3.77252200	-1.81875600
H	3.84181600	-4.09611600	-1.85581300
C	-4.53553600	-1.08904000	2.43198800
C	-3.04155400	1.84077300	-2.35357400
H	-3.29987300	2.86620100	-2.56665300
C	4.51197900	-1.25364000	-2.40948000
C	-1.90649900	2.25724800	2.94925200
H	-1.97677900	3.29323000	3.24510200
C	6.57542400	-2.23697600	-3.26646000
C	-2.91678700	1.33264600	2.87679700
H	-3.96318300	1.48079200	3.10008200
C	2.75593800	-2.67339200	1.62557400

C	3.62109900	-1.56580400	1.71799500
C	-1.14108800	4.41127100	-1.93652200
C	-2.83597400	-3.66825300	2.10232600
H	-3.85762100	-3.99178000	2.22199400
C	1.70226600	-4.56452300	-1.60294600
H	1.67784300	-5.62806900	-1.41914000
C	1.08984200	4.54062600	1.77470200
C	5.07997000	-1.77790800	1.79237000
C	7.32877400	-1.45390600	-2.39666500
C	-0.39959400	4.03338000	-4.20635200
C	0.47919900	4.19192500	4.07536800
C	3.01493300	-4.06236700	1.63127600
H	3.99594000	-4.51445800	1.64299500
C	-7.19064800	-2.69267400	-0.80113400
C	5.30172900	-0.45540200	-1.57392600
C	3.87325400	0.91276200	1.99320700
H	4.94538900	0.95055700	1.88009400
C	3.02832800	1.95833500	2.23208300
H	3.28546200	2.99441300	2.39337300
C	1.78090100	-4.72553100	1.67155500
H	1.60922900	-5.79241900	1.71711000
C	-5.30370300	-0.33384600	1.53558900
C	-5.83625800	-1.45167400	-2.86791300
C	-1.23635400	5.77895000	-2.19048000
C	-1.71185600	-4.48797500	1.93557500
H	-1.69182900	-5.56755100	1.87787400
C	-0.90045200	6.26612400	-3.45815600
C	-7.21800400	-1.59099300	-2.93551800
C	5.79636100	-2.50862000	0.83364400
C	-7.90331100	-2.20533700	-1.89081000
C	-0.48479000	5.40491400	-4.47839900
C	-6.68906400	-0.40277700	1.48707500
C	-5.25937700	-1.88841100	3.32802100
C	7.17371900	-2.68579700	0.88030200
C	6.68752200	-0.55115800	-1.55435000
C	1.21916100	5.91128400	2.00588200
C	5.85333800	-1.29259200	2.86453700
C	-7.37071400	-1.23917700	2.36545900
C	-6.64814800	-1.98115500	3.29389300
C	0.59099300	5.56766800	4.32986600
C	0.96119200	6.41504200	3.28429700
C	7.90783900	-2.13527000	1.92378800
C	7.23529100	-1.43959300	2.92456300
H	-0.25533600	5.78312700	-5.46266900
H	-1.55397600	6.48332500	-1.43407900
H	1.51005500	6.60462500	1.22834200
H	0.41250100	5.95654700	5.32075300
O	-1.01717600	7.61254700	-3.60860000
O	-0.04483300	3.11484600	-5.14699400
O	-1.44529900	3.85049700	-0.74835300
O	1.31868400	3.97426900	0.56009400
O	1.10271300	7.76651500	3.41519600
O	0.15819300	3.29104600	5.04414900
C	-0.69273500	8.18210100	-4.86747900
H	-0.84797500	9.25617900	-4.75734800
H	0.35407500	7.99063800	-5.13588100
H	-1.34684900	7.79924700	-5.66122800
C	0.31041200	3.56503300	-6.44403800
H	-0.52992100	4.06886600	-6.93796700
H	1.17268000	4.24330500	-6.41162900
H	0.57543800	2.66796000	-7.00499000
C	-1.99146200	4.66766200	0.28050400
H	-1.26785700	5.41609200	0.62010100
H	-2.90962300	5.16231900	-0.06025000
H	-2.21486700	3.98108200	1.09426800
C	0.86969300	8.34127500	4.68952600
H	1.03571200	9.41322700	4.56990000
H	-0.16079100	8.16852600	5.02707700
H	1.56527900	7.94761500	5.44217500
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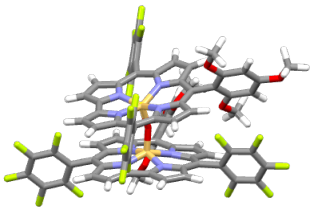
H	-0.95259600	4.44991200	6.37686300
H	-0.34127000	2.87015900	6.94192800
H	0.77863400	4.25294700	6.78867400
C	1.94123300	4.76051700	-0.44123800
H	1.28215600	5.56076500	-0.79912800
H	2.88089200	5.19494100	-0.07695200
H	2.14735900	4.07215300	-1.25965900

3d-*O* (S_0)



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F	4.03029909	-4.20095711	6.11210957
F	4.19614931	-1.57129023	1.36234445
O	0.00005027	0.47774736	0.00003089
F	-4.61509755	3.74391019	3.25693169
F	6.09429133	-4.61512575	4.38403006
F	6.16975983	-3.27480326	2.00897278
F	-3.24577388	4.98385329	-1.10286350
F	-6.54071504	5.62762875	3.17581513
F	-5.15616599	6.86491607	-1.16246322
N	1.17050187	1.09478459	2.34944365
N	-2.33926980	0.81665241	1.41550375
N	-0.53004652	2.65461859	1.66617930
F	-6.82132059	7.20164335	0.97168120
N	-0.46503335	-0.91480146	2.27662125
C	-3.15836684	-0.31210888	1.32956575
C	2.18245594	0.26341439	2.76131528
C	-3.16854328	1.91626315	1.13034383
C	0.64684721	3.29818132	1.99406441
C	1.64560678	2.38675696	2.35533133
C	3.33670306	1.06131888	3.01161535
H	4.28557588	0.68731709	3.36248286
C	-1.48876340	3.61940952	1.44869177
C	2.99852524	2.38072326	2.76677237
H	3.62749706	3.24984242	2.86263226
C	0.64969627	-1.61011864	2.78405806
C	-1.49983785	-1.84763834	2.19262125
C	-2.80055936	3.25470891	1.17245444
C	-4.46985995	0.08283475	0.93771468
H	-5.28239302	-0.60253051	0.77191410
C	1.93000544	-1.09000607	2.97017396
C	-4.47921165	1.44042911	0.83186324
H	-5.30897393	2.07517449	0.56578075
C	-2.76801596	-1.59451307	1.68728878
C	3.04575349	-2.66859859	4.59944834
C	3.03496430	-1.98973606	3.38025711
C	0.43750189	4.69479325	1.96616106
H	1.18044877	5.44503651	2.17487671
C	4.05814772	-3.55705793	4.93987079
C	5.11387317	-3.76809579	4.06167008
C	-1.05123777	-3.09799904	2.70032286
H	-1.67296114	-3.97412582	2.78268089
C	5.15045792	-3.08462314	2.85310447
C	-3.85648120	4.29637794	1.08288416
C	0.25684904	-2.95360586	3.05778544
H	0.89816400	-3.70058038	3.49253427
C	-0.88923092	4.89584373	1.63109714
H	-1.40128350	5.83999541	1.53151576
C	4.12218055	-2.20957404	2.53216512
C	-4.72692651	4.49658868	2.15752450
C	-4.03097449	5.12143196	-0.02381913
C	-5.72375623	5.46251174	2.13063392
C	-5.01749042	6.09813506	-0.07520492
C	-5.86791972	6.26903936	1.00827075
C	-3.74531981	-2.70983861	1.57409312
C	-3.56317156	-3.73911315	0.63238840
C	-4.50294654	-4.75154686	0.47187249
C	-5.65010719	-4.75088257	1.26621213
C	-5.85172219	-3.76764107	2.23363989
C	-4.88804447	-2.76169176	2.38218241
Si	0.47624996	0.79329175	-1.53431854
F	4.61503972	3.74393506	-3.25696833
F	6.54061381	5.62770188	-3.17582785
F	3.24556084	4.98392648	1.10276583
F	-2.05458222	-2.48676350	-5.48218988
F	6.82110575	7.20177316	-0.97172635
F	5.15590108	6.86505360	1.16237527
F	-4.19612183	-1.57149788	-1.36229076
F	-4.03027548	-4.20109411	-6.11209528
F	-6.16971131	-3.27503993	-2.00892431
N	0.52997508	2.65455751	-1.66628152
N	0.46504310	-0.91486439	-2.27658311
N	-1.17057657	1.09465107	-2.34935528
F	-6.09422745	-4.61534163	-4.38399483
N	2.33924595	0.81665113	-1.41548945

C	1.49987729	-1.84766730	-2.19256907
C	1.48866154	3.61937917	-1.44878851
C	-0.64967036	-1.61022380	-2.78399445
C	-1.64570854	2.38661849	-2.35530699
C	-0.64694770	3.29808150	-1.99414062
C	0.88908580	4.89579338	-1.63119484
H	1.40110654	5.83996255	-1.53161471
C	-2.18249745	0.26325199	-2.76125547
C	-0.43764538	4.69469903	-1.96623691
H	-1.18061579	5.44492078	-2.17494725
C	3.16848824	1.91628967	-1.13035540
C	3.15837224	-0.31208232	-1.32953607
C	-1.93000054	-1.09015752	-2.97012286
C	1.05130820	-3.09805680	-2.70023357
H	1.67305371	-3.97416928	-2.78256728
C	2.80046287	3.25472228	-1.17251782
C	-0.25678912	-2.95371195	-3.05767358
H	-0.89810391	-3.70073209	-3.49234229
C	2.76805182	-1.59450006	-1.68724587
C	4.72682303	4.49663239	-2.15757194
C	3.85635343	4.29642396	-1.08294567
C	-2.99860828	2.38054419	-2.76679922
H	-3.62759590	3.24964557	-2.86270543
C	5.72362759	5.46257905	-2.13067031
C	5.86773134	6.26914001	-1.00832090
C	4.46985343	0.08290266	-0.93768285
H	5.28239386	-0.60244561	-0.77184941
C	5.01727564	6.09824195	0.07513232
C	-3.03493317	-1.98992169	-3.38020479
C	4.47916816	1.44049739	-0.83185128
H	5.30890730	2.07527072	-0.56576434
C	-3.33675170	1.06112438	-3.01160945
H	-4.28560939	0.68708925	-3.36248176
C	4.03078748	5.12150891	0.02373985
C	-3.04572876	-2.66875452	-4.59941390
C	-4.12214312	-2.20978488	-2.53211082
C	-4.05811268	-3.55722455	-4.93983912
C	-5.15040834	-3.08484612	-2.85305250
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C	3.74540979	-2.70978980	-1.57407794
C	3.56334942	-3.73908837	-0.63238125
C	4.88811389	-2.76156316	-2.38220342
C	4.50319256	-4.75146199	-0.47189972
C	5.85186110	-3.76745667	-2.23369813
C	5.65033162	-4.75071475	-1.26627462
O	4.99037967	-1.77682474	-3.31457549
O	6.52166191	-5.76777748	-1.02574054
O	2.42550402	-3.66748980	0.10871933
O	-2.42534025	-3.66741019	-0.10872436
O	-6.52136700	-5.76799598	1.02565186
O	-4.99039059	-1.77696969	3.31456728
H	6.72512617	-3.78322095	-2.86397443
H	4.39653096	-5.52990289	0.26748943
H	-4.39619220	-5.52996808	-0.26752570
H	-6.72500208	-3.78346948	2.86389488
C	6.15959772	-1.70212362	-4.11372267
H	6.02860757	-0.82418328	-4.74303126
H	7.05712578	-1.57704091	-3.49827036
H	6.27129805	-2.58889326	-4.74711207
C	7.73086251	-5.81067809	-1.76810506
H	8.33087871	-4.90884802	-1.60549849
H	8.27525969	-6.67775174	-1.39905565
H	7.53918223	-5.93310690	-2.83985211
C	2.05077644	-4.80575372	0.87068644
H	2.06462260	-5.71253328	0.25776763
H	2.71034270	-4.94322193	1.73512794
H	1.04116408	-4.60284965	1.21562258
C	-2.05022703	-4.80583448	-0.87026891
H	-2.06416040	-5.71244866	-0.25711012
H	-2.70950893	-4.94361927	-1.73487962
H	-1.04053538	-4.60290150	-1.21495677
C	-6.15960423	-1.70240119	4.11373577
H	-6.02867128	-0.82448546	4.74309009
H	-7.05715018	-1.57735286	3.49830213
H	-6.27122878	-2.58921502	4.74707603
C	-7.73067301	-5.81086897	1.76784508
H	-8.33062931	-4.90901100	1.60517765
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H	-7.53914969	-5.93333534	2.83961679

3d-*O* (S_1)

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F	4.21373200	-1.63771900	1.29128000
O	-0.00932800	0.43841100	-0.03654300
F	-4.77693900	3.54556400	3.12885800
F	6.06529800	-4.61639800	4.41640100
F	6.13456000	-3.40278200	1.96984000
F	-3.11028500	5.18597100	-0.99364400
F	-6.75031500	5.38247300	3.05132100
F	-5.06857400	7.02332000	-1.04870100
N	1.20443700	1.13870100	2.27160200
N	-2.33453700	0.83620200	1.45303800
N	-0.51665300	2.67671600	1.58572900
F	-6.90676000	7.13601200	0.96619400
N	-0.43283500	-0.88249200	2.28646700
C	-3.15106900	-0.30402000	1.37874600
C	2.24195000	0.31421300	2.64378000
C	-3.16330700	1.90926600	1.14381400
C	0.65628200	3.32577600	1.85041600
C	1.68626600	2.41693400	2.20114300
C	3.41374800	1.11411400	2.79521600
H	4.38567000	0.74438000	3.08853700
C	-1.48865100	3.63915500	1.37024500
C	3.06217200	2.42862800	2.52522800
H	3.69627000	3.30097800	2.53237500
C	0.69390800	-1.56088300	2.78206800
C	-1.45289100	-1.82112200	2.23899100
C	-2.79790900	3.27644100	1.15476200
C	-4.46287300	0.07816000	0.97415700
H	-5.26929700	-0.61377400	0.79651700
C	1.98817800	-1.02932500	2.91419400
C	-4.47270500	1.43768500	0.84570800
H	-5.29583500	2.06913600	0.54794200
C	-2.74969400	-1.57724900	1.74204900
C	3.09178200	-2.55104900	4.59881800
C	3.08725300	-1.92751400	3.34703000
C	0.45544300	4.73410300	1.79442700
H	1.21447000	5.48338800	1.94249900
C	4.08245900	-3.45688300	4.96438600
C	5.11172900	-3.74970100	4.07171800
C	-1.00006800	-3.05639200	2.76173200
H	-1.61545000	-3.93747300	2.86212000
C	5.14654800	-3.13081500	2.82491700
C	-3.87026500	4.29930500	1.07037400
C	0.32313500	-2.89814800	3.09147200
H	0.98753700	-3.64240400	3.50073500
C	-0.87338200	4.92953600	1.50088500
H	-1.38655400	5.87225100	1.37886000
C	4.14721200	-2.22388400	2.48428400
C	-4.83018000	4.38661600	2.08743800
C	-3.97975000	5.21414400	0.02093200
C	-5.85343700	5.32748000	2.06150700
C	-4.99278300	6.16915800	-0.02457200
C	-5.93234100	6.22637900	1.00020300
C	-3.70331900	-2.70426400	1.61707700
C	-3.46284400	-3.73105500	0.67503300
C	-4.39456500	-4.74126000	0.45848900
C	-5.59027400	-4.73618600	1.18432300
C	-5.84817500	-3.75713500	2.14878700
C	-4.89614400	-2.75167000	2.35694300
Si	0.48960100	0.81744700	-1.59233600
F	4.88435300	3.48863500	-3.10953400
F	6.84220900	5.32865000	-3.03469600
F	3.21942600	5.12791300	1.02734600
F	-2.23229900	-2.48065800	-5.46434000
F	6.98691900	7.10563800	-0.96670900
F	5.14347700	6.98788300	1.05414500
F	-4.15359000	-1.50020200	-1.23905000
F	-4.23783000	-4.19926300	-5.95947300
F	-6.17120400	-3.18748000	-1.76087300
N	0.56912900	2.67995000	-1.63726700
N	0.44659900	-0.87676200	-2.35365900
N	-1.17524700	1.15388700	-2.33649500
F	-6.22806300	-4.57402100	-4.12577000
N	2.34846200	0.80118500	-1.42699200
C	1.47518900	-1.83940900	-2.28347800
C	1.55516700	3.63194000	-1.43064800
C	-0.68192100	-1.55057300	-2.86834100
C	-1.64555500	2.45664600	-2.28551700
C	-0.60417100	3.35939800	-1.95131400
C	0.99476400	4.90894100	-1.61425600
H	1.53372600	5.84303200	-1.53463700
C	-2.22185500	0.33471900	-2.70554800
C	-0.36225300	4.73454600	-1.93867700
H	-1.08042800	5.50666200	-2.16813000
C	3.20559700	1.87866000	-1.12209400
C	3.15133500	-0.35638700	-1.35034200
C	-1.97595800	-1.02976800	-2.97034000
C	1.01087700	-3.06195300	-2.82373600
H	1.62220300	-3.94691400	-2.92931700
C	2.87256100	3.22724400	-1.13543600
C	-0.29932300	-2.88947300	-3.18943300

H	-0.94601800	-3.61810200	-3.65214600
C	2.73447300	-1.62011900	-1.74097400
C	4.92111200	4.32814400	-2.06898900
C	3.95314400	4.23557600	-1.05569300
C	-3.00715400	2.46741100	-2.60321900
H	-3.63624000	3.34402900	-2.65671600
C	5.94156600	5.27408600	-2.04467600
C	6.01426300	6.18767400	-0.99645900
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C	-3.37546000	1.13419100	-2.86172200
H	-4.34359700	0.77550300	-3.18316300
C	4.07181100	5.16537300	-0.02046500
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C	-4.15188000	-2.13359300	-2.42199000
C	-4.20782600	-3.53226500	-4.79686500
C	-5.20086300	-3.00942500	-2.67216700
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C	3.67407700	-2.76592800	-1.59145000
C	3.44362300	-3.76736200	-0.62932100
C	4.83773100	-2.87300700	-2.36937000
C	4.34527700	-4.81027000	-0.42354700
C	5.76707800	-3.90684400	-2.17531400
C	5.51119000	-4.86404100	-1.19225700
O	4.99417700	-1.91379300	-3.32244000
O	6.34529100	-5.90696300	-0.90969300
O	2.29586400	-3.64088400	0.10252700
O	-2.29326900	-3.63659400	-0.00010000
O	-6.44716200	-5.74682500	0.88769600
O	-5.04753000	-1.77077800	3.29042800
H	6.65581600	-3.96424700	-2.78530000
H	4.18940800	-5.57229200	0.32841000
H	-4.24846900	-5.51361500	-0.28341400
H	-6.75736500	-3.77933400	2.72970300
C	6.18162300	-1.90076600	-4.09216500
H	6.09887400	-1.03252800	-4.74742000
H	7.07167600	-1.79426200	-3.45786100
H	6.27939700	-2.80871300	-4.70223900
C	7.55861600	-6.00483200	-1.63484300
H	8.18792700	-5.11737700	-1.48715100
H	8.07339700	-6.88302700	-1.24138100
H	7.37675300	-6.14194100	-2.70902900
C	1.80480100	-4.79883100	0.75389300
H	1.80914500	-5.66512100	0.08103500
H	2.39316500	-5.04297900	1.65021600
H	0.78294000	-4.56130100	1.04829700
C	-1.93999900	-4.68560100	-0.89407600
H	-1.92148000	-5.65241300	-0.37558300
H	-2.63931800	-4.73484600	-1.73698200
H	-0.95005500	-4.42627400	-1.26349100
C	-6.26824400	-1.69419800	4.00843600
H	-6.17921100	-0.81555800	4.64864400
H	-7.12346600	-1.56883500	3.33229300
H	-6.42488800	-2.58399500	4.63124700
C	-7.71154400	-5.77203700	1.53206000
H	-8.28126300	-4.85710200	1.32706100
H	-8.24051000	-6.63043600	1.11603600
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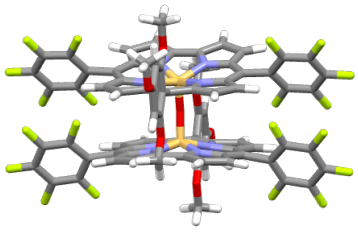
3d-*A* (S_0)



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F	4.79828900	-1.30307400	-1.07440600
O	0.00008400	-0.18563700	-0.27988600
F	-5.04105800	2.97620300	-3.08444400
F	8.96604200	0.63326600	-2.01153100
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F	-7.72642200	2.82880400	-3.04475100
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N	-1.34924500	2.11035700	-1.03831600
N	-1.20187000	0.11842200	-2.68878300
F	-8.96692600	0.63385300	-2.01082500
N	1.34865200	2.11043100	-1.03878400
C	-1.20839000	3.28967300	-0.30405300
C	2.57124000	0.06522400	-2.74774100
C	-2.73881200	1.91592700	-1.19603200
C	-0.70074400	-0.77240800	-3.61055700
C	0.69945800	-0.77244600	-3.61070500
C	2.93907500	-0.89170300	-3.73462900
H	3.95091000	-1.13567200	-4.01706000
C	-2.57230500	0.06545700	-2.74730600
C	1.77228200	-1.40567100	-4.27584600
H	1.68907000	-2.13583900	-5.06461800
C	2.73817400	1.91597100	-1.19684400
C	1.20800300	3.28975100	-0.30451600
C	-3.34298000	0.93678500	-1.98107100
C	-2.49414000	3.80950500	0.01324500
H	-2.65666600	4.71529100	0.57356600
C	3.34212200	0.93663300	-1.98181400
C	-3.42416300	2.96190400	-0.50770800
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C	-0.00014700	3.88248600	0.02783400
C	5.61023300	1.87702500	-2.57335600
C	4.82010000	0.84885900	-2.06018900
C	-1.77373900	-1.40511100	-4.27592100
H	-1.69072300	-2.13492000	-5.06504900
C	6.99852700	1.81617600	-2.56011900
C	7.63450900	0.69552400	-2.04298600
C	2.49383500	3.80962000	0.01238000
H	2.65651000	4.71542200	0.57263400
C	6.87444100	-0.36076500	-1.55975100
C	-4.82098300	0.84918700	-2.05936400
C	3.42371700	2.96199900	-0.50879900
H	4.49394700	3.04507000	-0.43856200
C	-2.94039700	-0.89105400	-3.73449900
H	-3.95230000	-1.13464200	-4.01701000
C	5.49142700	-0.27782400	-1.58671400
C	-5.61103700	1.87764500	-2.57207500
C	-5.49238400	-0.27768200	-1.58641600
C	-6.99933600	1.81686800	-2.55888100
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F	-7.30111500	-2.94571000	3.82908400
F	-5.16699300	1.11537900	0.92083100
F	4.64423800	-2.82871900	3.49630300
F	-8.91643400	-1.05891700	2.70770100
F	-7.81534400	0.97519000	1.25305900
F	5.16684200	1.11606100	0.92021700
F	7.30171800	-2.94363900	3.82985700
F	7.81521500	0.97635400	1.25230000
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N	1.34932300	-2.12855700	1.07675700
N	1.20470000	0.22588400	2.14423900
F	8.91671000	-1.05704800	2.70763100
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C	-0.69971400	1.37881400	2.70882100
C	-2.92886200	1.43563200	2.98064000
H	-3.93213600	1.72307900	3.25022500
C	2.57069200	0.23317600	2.30903500
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H	-1.68491300	3.11360100	3.68332500
C	-2.72962700	-1.95586200	1.29040500
C	-1.20919900	-3.37179800	0.45637900
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C	-3.33573500	-0.85678200	1.89879900
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C	0.00043100	-3.96753000	0.14008100
C	-5.39409500	-1.88635800	2.91465200
C	-4.79639100	-0.87909800	2.15037700

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H	1.68424900	3.11418800	3.68309600
C	-6.76862000	-1.95817200	3.10189900
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C	0.00008800	-6.88507300	-2.30803000
C	0.00160800	-7.76261800	-0.04122900
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H	-0.89359300	5.74897100	4.38789600
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H	0.89560400	10.31363300	-0.05547200
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H	-0.89163600	-7.82735500	2.61805700
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F	-8.88274512	-1.32638620	-2.68808471
F	-7.88060718	0.80949385	-1.30857909
F	5.19120146	1.29402281	-0.87625694
F	7.32603075	-2.76098216	-3.80578682
F	7.84457704	1.14014927	-1.19004508
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C	-5.32620431	-2.01046959	-2.84473374
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H	1.59086035	3.33058740	-3.36195214
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H	3.89937200	1.99705586	-2.99492643
C	-5.68157879	0.00973221	-1.63895944
C	5.42075902	-1.70558762	-2.88192144
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C	6.79704988	-1.78124003	-3.06611329
C	7.06166681	0.21318791	-1.75051854
C	7.62508908	-0.82286211	-2.48742436
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H	0.47618053	-8.63658043	-0.62032447
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F	7.34559814	-1.51265109	0.91696451
F	-4.76320981	-1.44754584	1.05719948
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F	-7.42921412	-1.67866893	0.90866505
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F	-9.04010370	0.37527700	1.73397011
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C	-2.80831942	1.88377427	1.16324288
C	-0.77267800	-0.73042887	3.69180093
C	0.64472462	-0.72524423	3.70207303
C	2.88942681	-0.87280612	3.77147264
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C	-2.64353315	0.03872310	2.74478641
C	1.70532349	-1.36890272	4.34544885
H	1.62158378	-2.09649305	5.14120226
C	2.68485295	1.95553306	1.25103231
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H	-2.72694241	4.71053362	-0.57978482
C	3.29550329	0.95094467	2.00469967
C	-3.49335449	2.92674678	0.46673103
H	-4.56524598	3.00985332	0.39083333
C	-0.06899647	3.89979131	-0.01340807
C	5.61037043	1.85997849	2.50012630
C	4.76762916	0.83841723	2.04419918
C	-1.83854990	-1.35653486	4.34451756
H	-1.76358889	-2.04671338	5.17367270
C	6.99858762	1.77562252	2.41620864
C	7.59409501	0.63158798	1.89535647
C	2.42267347	3.86885921	0.06200675
H	2.58337520	4.79032766	-0.47919493
C	6.78844149	-0.42276732	1.47666254
C	-4.88696979	0.74871581	1.95269914
C	3.36343122	3.02230781	0.58440685
H	4.43431535	3.13541249	0.54291544
C	-3.01798476	-0.88482350	3.74227371
H	-4.03475910	-1.13029809	4.01553578
C	5.40806797	-0.31180879	1.56952482
C	-5.74572063	1.76799242	2.38368264
C	-5.50952258	-0.42554254	1.51330039

C	-7.13260567	1.65694880	2.30973094
C	-6.88820362	-0.56344829	1.43242467
C	-7.71035938	0.48786254	1.82608666
C	-0.07994628	5.32891888	-0.45969182
C	-0.10611973	5.78833205	-1.78665553
C	-0.11747137	7.15092642	-2.09279402
H	-0.13758772	7.52162937	-3.10779605
C	-0.10264424	8.08823305	-1.05777582
C	-0.07765271	7.68046817	0.27567624
H	-0.06799033	8.40297556	1.07752567
C	-0.06825752	6.30749684	0.55578344
O	-0.11469801	9.39344292	-1.45628683
O	0.27117108	-9.15692312	2.03583539
O	-0.11500428	-4.43187084	2.44071396
O	0.40951501	-6.21114144	-1.82859786
O	-0.04828960	5.82056635	1.82347444
O	-0.11923072	4.83114886	-2.77336446
C	0.59722314	-7.28913953	-2.73105815
H	-0.24965423	-7.98659176	-2.70460152
H	0.66369113	-6.83767598	-3.72185417
H	1.52467953	-7.83501909	-2.51616406
C	0.43648327	-10.31899737	1.23940008
H	0.43626669	-11.15965977	1.93470104
H	-0.38885038	-10.43726065	0.52541984
H	1.38819775	-10.29910723	0.69282681
C	-0.17373506	-4.52996427	3.85720041
H	-0.26723940	-3.50586994	4.20678770
H	-1.04534489	-5.11445670	4.17671931
H	0.74064118	-4.98444543	4.25740257
C	-0.02683101	6.72915120	2.90932531
H	-0.00926773	6.11184249	3.80834227
H	0.86892338	7.36354116	2.88568463
H	-0.92244384	7.36412913	2.92104072
C	-0.10211074	10.39582507	-0.45377202
H	0.80324364	10.33553617	0.16424694
H	-0.11502836	11.34967674	-0.98374508
H	-0.98567332	10.32798666	0.19425446
C	-0.14020691	5.27401305	-4.12209075
H	-1.04112644	5.86090585	-4.33949758
H	0.74609334	5.87376994	-4.36337004
H	-0.14166468	4.37036855	-4.73541825

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