Supporting Information

Structural, Optical, and Electronic Properties of a Series of 3,4-Propylenedioxythiophene Oligomers in Neutral and Various Oxidation States

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Contents

General

^{1}H and ^{13}C NMR spectra were recorded on JEOL JNM-270, LA-400, L-500, or Bruker AV500 instruments. Chemical shifts are reported in ppm with reference to tetramethylsilane, using the signal of internal tetramethylsilane or the solvents. Mass spectra were recorded on a SHIMADZU GC-MS QP2020 or an AXIMA-CFR instrument for EI or LDI-TOF method, respectively. Only the more intense or structurally diagnostic mass spectral fragment ion peaks are reported. Electronic absorption spectra were recorded on a SHIMADZU UV-Vis-NIR scanning spectrophotometer (Model UV-3101-PC). Variable-temperature measurements of electronic absorption spectra were performed using a Oxford Optistat DN liquid-nitrogen cryostat. Cyclic voltammetry (CV) was performed on a BAS-ALS620B electrochemical analyzer using a standard three-electrode cell consisting of Pt wire and glassy-carbon working electrodes, a Pt wire counter electrode, and a $Ag/AgNO_3$ reference electrode under nitrogen atmosphere. The potentials were calibrated with ferrocene as an external standard. ESR spectra were recorded on a JEOL JES-RE3X instrument. Preparative gel-permeation chromatography (GPC) was performed with a JAI LC-08 chromatograph equipped with JAIGEL 1H and 2H columns. Elemental analyses were performed at the microanalysis laboratory of Tokyo Metropolitan University.

Commercially available reagents were used as received. Solvents were distilled from relevant drying agents prior to use. ProDOT-Hex monomer **1** with dihexyl side chain were prepared according to the literature procedures.[1]

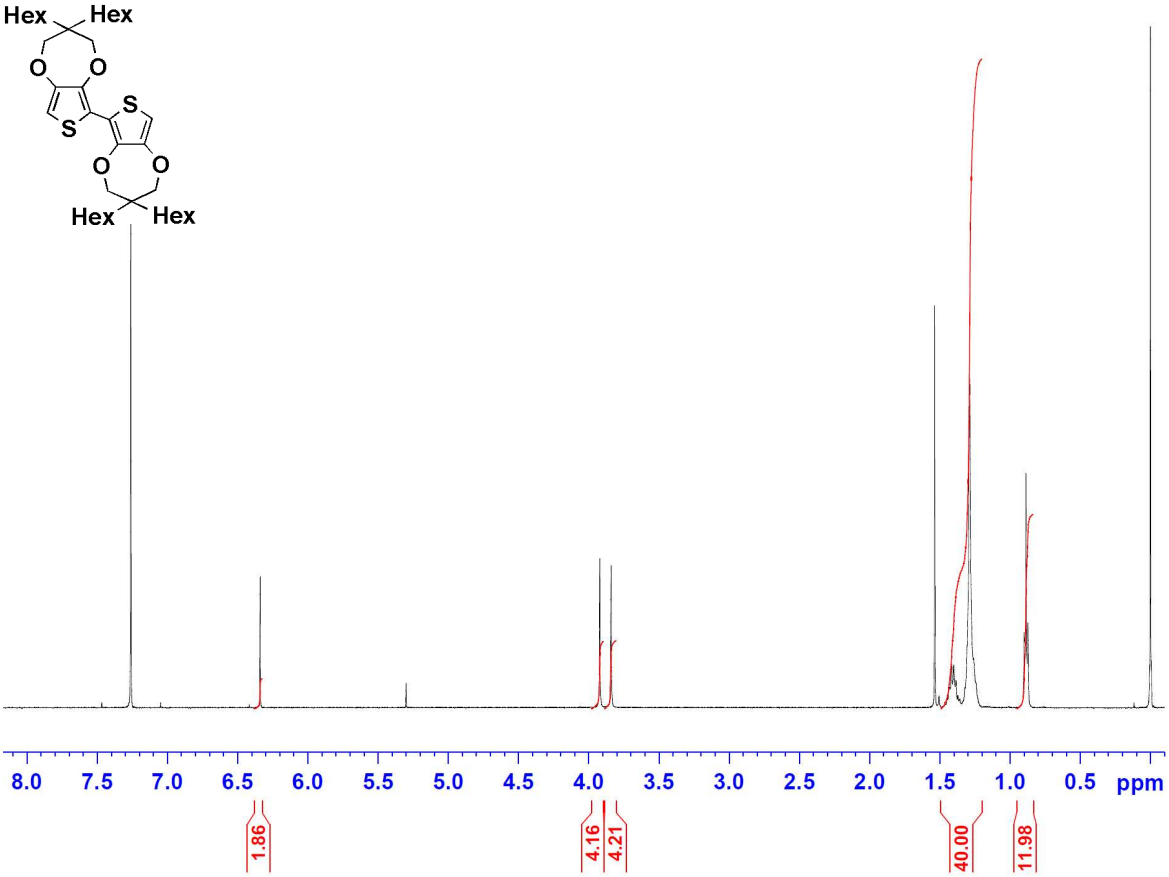
Computational methods

DFT calculations were performed with the Gaussian 03 program.[2] All geometry optimizations were carried out at the B3LYP/6–31G(d) basis set. For all compounds, C_i symmetry was applied for the geometry optimizations based on the X-ray structure of **11**. Singlet biradical character was estimated with the symmetry-broken UB3LYP/6–31G(d) method with a geometry optimization and the biradical index was determined on the basis of the LUMO occupation number in natural orbital analysis. Excitation energy was computed using time-dependent density functional theory (TD–B3LYP) with 6-31G(d) basis set in the B3LYP optimized geometry.

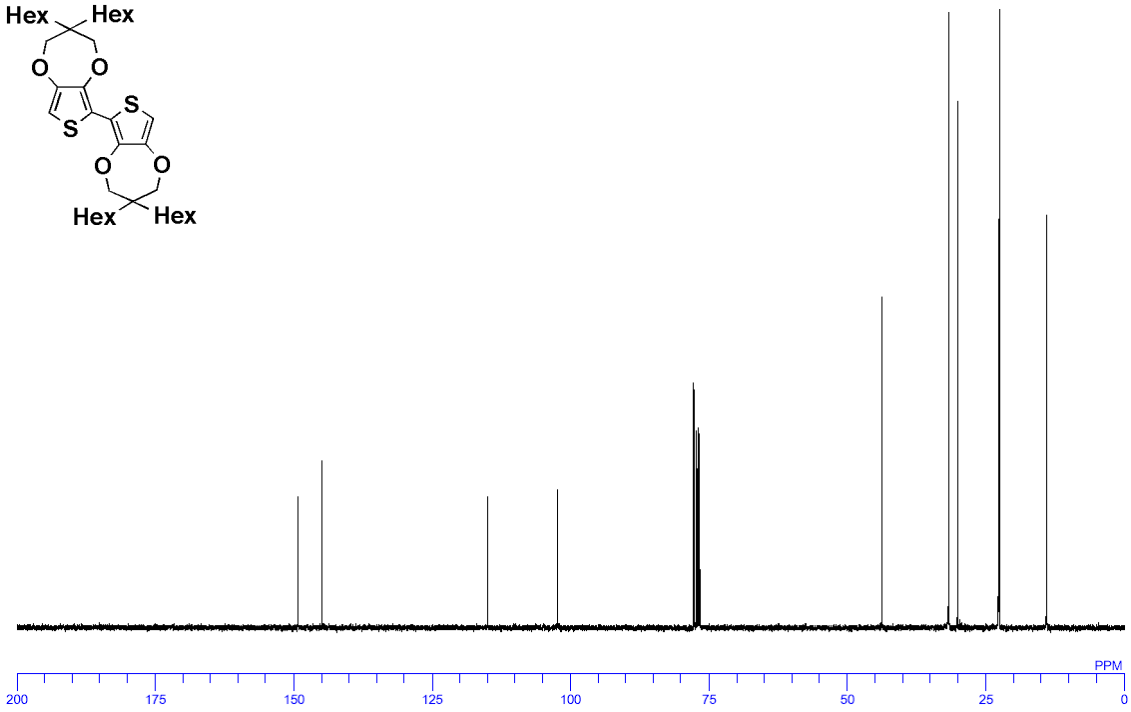
Synthesis

Synthesis of 2. To a THF solution (500 mL) of ProDOT-Hex monomer **1** (10.3 g, 31.7 mmol) and TMEDA (9.60 mL, 63.8 mmol) was added n-butyllithium (1.7 M, 34.5 mmol) in hexane at –10°C under N_2. After stirring for 30 min at –10°C, the solution was transferred into a refluxing THF solution (80 mL) of $Fe(acac)_3$ under N_2 via cannula and the reaction mixture was refluxed overnight. Volatiles were removed in vacuo, and the residue was purified by column chromatography (SiO_2 deactivated with 10% water) with hexane-CH_2Cl_2 (v/v = 10:1) as eluent to give **2** (8.62 g, 13.3 mmol, 84%) as white solid: mp 58.4-59.4°C; ^{1}H NMR($CDCl_3$) δ 6.34 (s, 2H), 3.92 (s, 4H), 3.84 (s, 4H), 1.45-1.36 (m, 8H), 1.33-1.20(m, 32H), 0.88 (m, 12H); ^{13}C NMR($CDCl_3$) δ 149.3, 145.0, 115.0, 102.5, 77.8, 43.8, 31.8, 30.1, 22.8, 22.6, 14.0. Anal. Calcd for $C_{38}H_{62}O_4S_2$: C, 70.54; H, 9.66. Found: C, 70.38; H, 9.76.

^{1}H-NMR spectrum of **2**

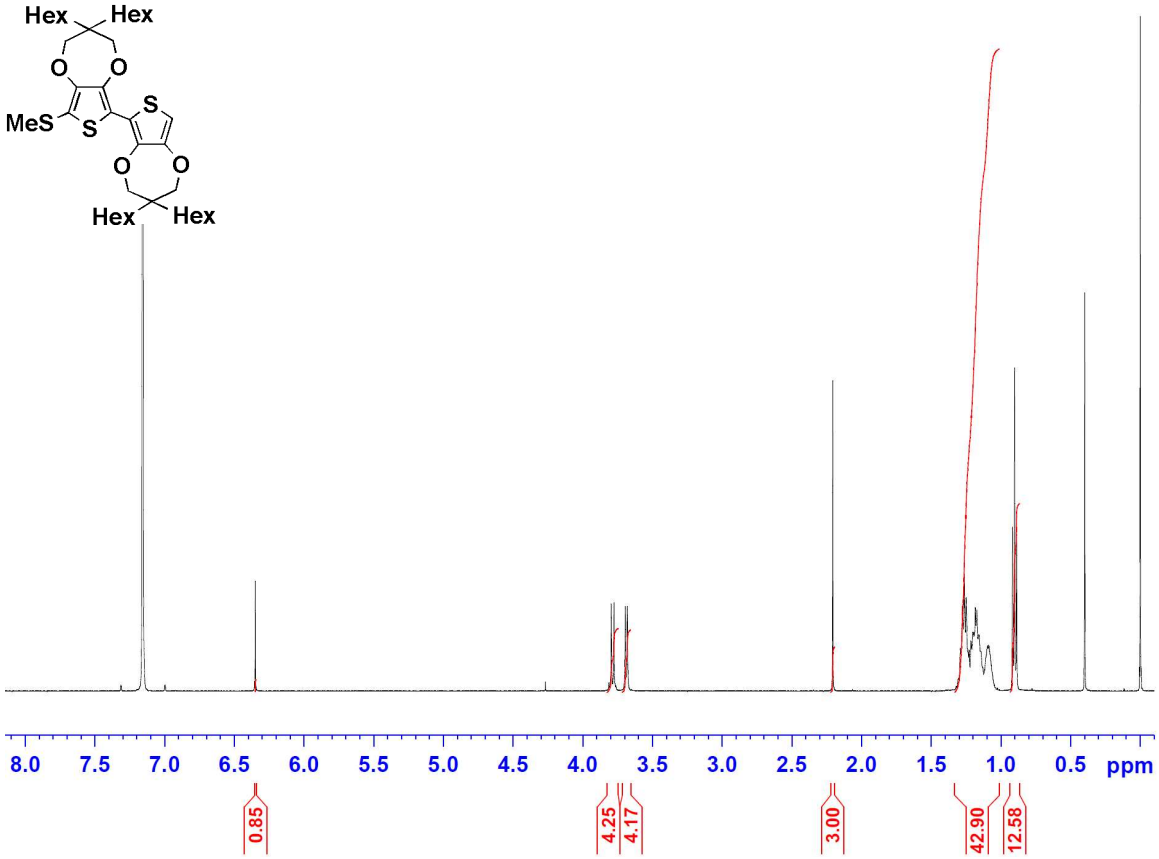


^{13}C-NMR spectrum of **2**

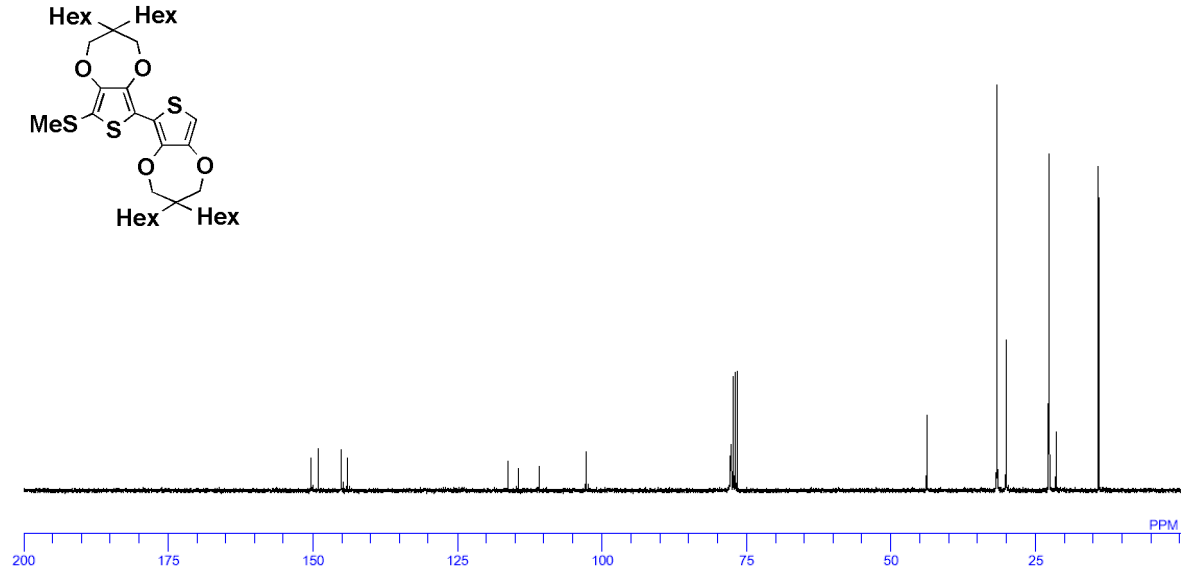


Synthesis of 3. To a THF solution (15 mL) of **2** (0.663 g, 1.02 mmol) was added n-butyllithium (1.7 M, 1.22 mmol) in hexane at 0°C under N_2. After stirring for 120 min at 0°C, dimethyldisulfide (0.92 mL, 10.2mmol) was added dropwise to the reaction mixture and then allowed to warm to room temperature. After stirring for 14 h, water was added and the mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) using hexane/acetyl acetate (v/v = 25:1) as eluent. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **3** (0.699 g, 1.01 mmol, 99%) as yellow-orange oil: ^{1}H NMR (C_6D_6) δ 6.35 (s, 1H), 3.80 (s, 2H), 3.78 (s, 2H), 3.69 (s, 2H), 3.68 (s, 2H), 2.38 (s, 3H), 1.45-1.20 (m, 40H), 0.90-0.86 (m, 12H); ^{13}C NMR ($CDCl_3$) δ 150.4, 149.0, 145.1, 144.1, 116.3, 114.5, 111.0, 102.8, 77.8, 77.8, 77.7, 43.8, 31.7, 30.1, 22.8, 22.7, 21.5, 14.2; MS (DI) *m/z* = 692 [M^+]. Anal. Calcd for $C_{39}H_{64}O_4S_3$: C, 67.58; H, 9.31. Found: C, 67.62.; H, 9.32.

^{1}H-NMR spectrum of **3**

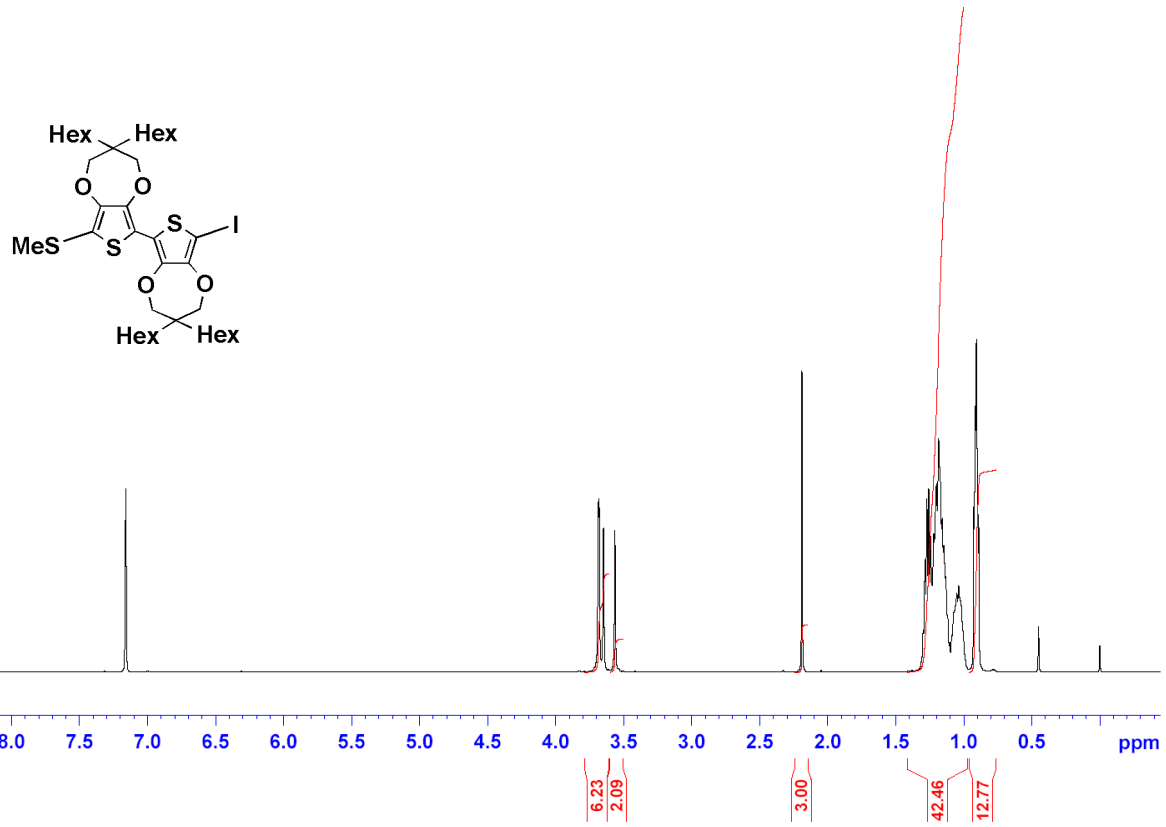


^{13}C-NMR spectrum of **3**

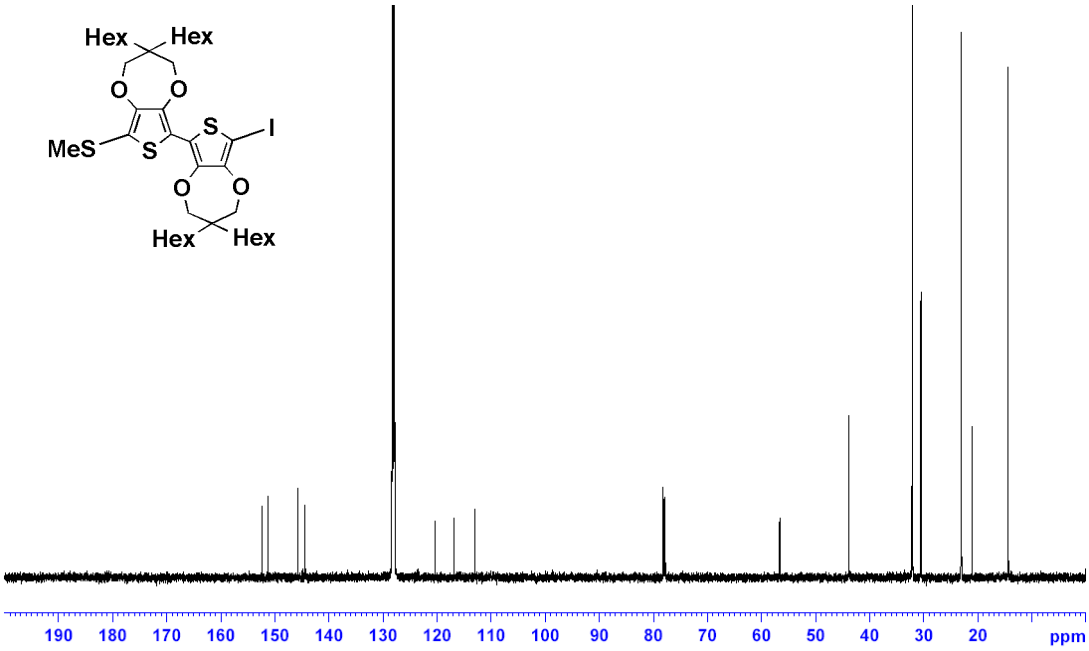


Synthesis of 4. To a THF solution (50 mL) of **3** (3.90 g, 5.62 mmol) was added *N*-iodosuccinimide (1.64 g, 7.29 mmol) under dark condition. After stirring for overnight at room temperature, the reaction was quenched with aqueous $Na_2S_2O_3$. The mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was recrystallized from a mixture of dichloromethane and methanol (ca. 1 : 2) at -30°C to give **4** (4.11 g, 5.02 mmol, 89%) as white crystals: mp 92.9-94.3 °C; ^{1}H NMR (C_6D_6) δ 3.69 (s, 2H), 3.68 (s, 2H), 3.64 (s, 2H), 3.56 (s, 2H), 2.18 (s, 3H), 1.30-1.04 (m, 40H), 0.93-0.90 (m, 12H); ^{13}C NMR (C_6D_6) δ 152.38, 151.21, 145.75, 144.39, 120.39, 116.82, 112.97, 78.18, 78.04, 77.87, 77.82, 56.63, 43.87, 43.78, 32.06, 30.52, 30.48, 23.09, 21.01, 14.36. Anal. Calcd for $C_{39}H_{63}IO_4S_3$: C, 57.19; H, 7.75. Found: C, 57.13.; H, 7.86.

^{1}H-NMR spectrum of **4**

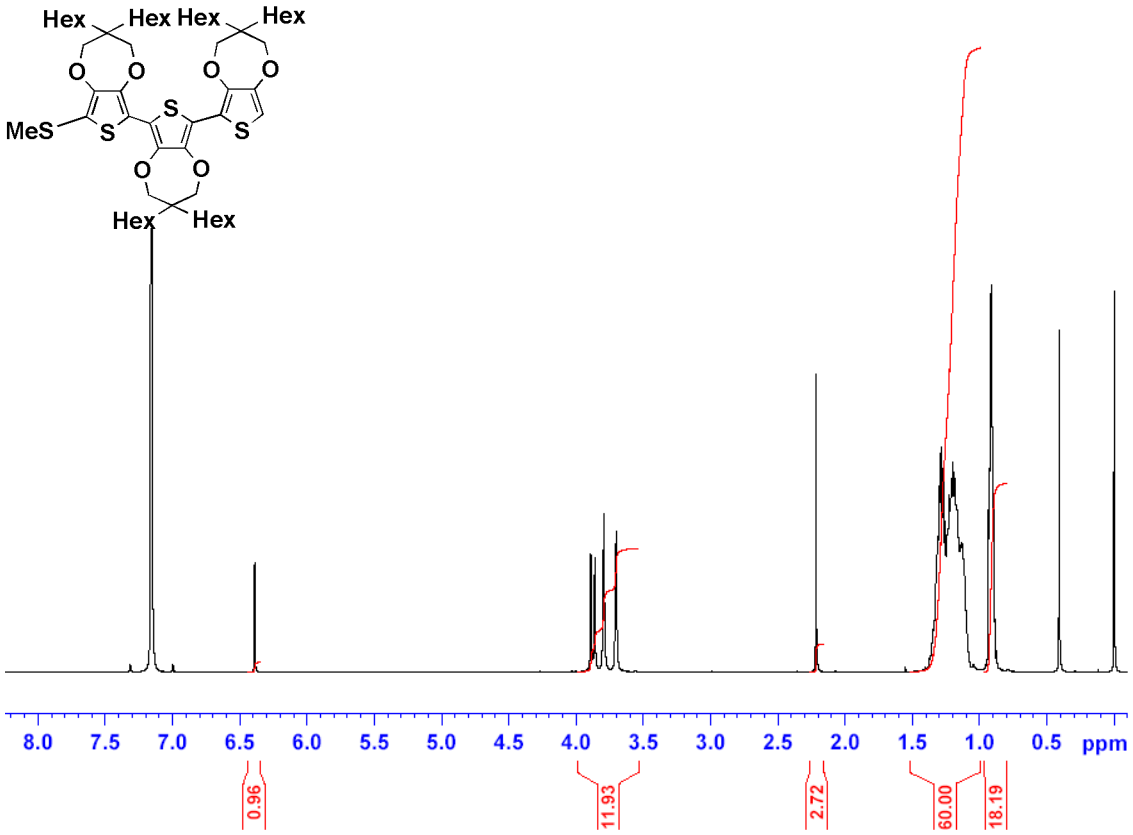


^{13}C-NMR spectrum of **4**

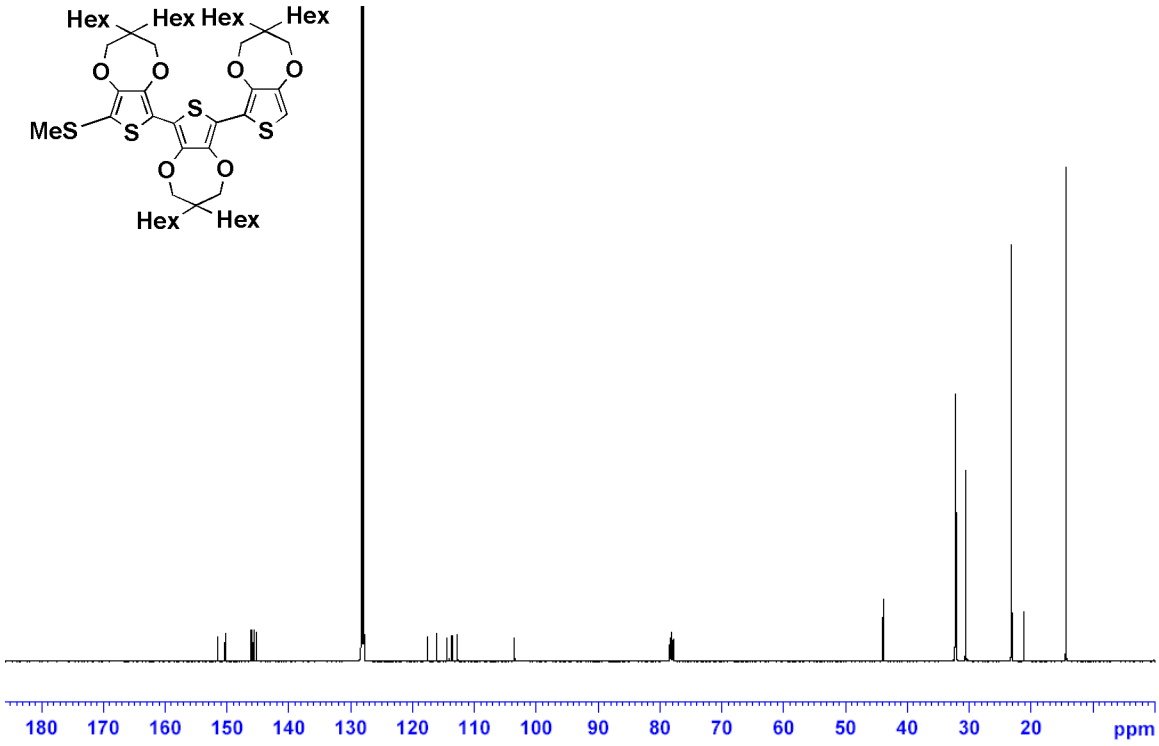


Synthesis of 5. To a THF solution (15 mL) of **1** (0.996 g, 3.07 mmol) was added n-butyllithium (1.6 M, 2.46 mmol) in hexane at -78°C under N_2. After stirring for 60 min at -78°C and 30 min at 0°C, trimethyltin chloride (1.0 M, 3.07 mmol) in dichloromethane was added to the solution at -78°C and then allowed to warm to room temperature. After stirring overnight, water was added to the reaction mixture and the mixture was extracted with ethyl acetate, and then the organic layer was washed with brine and dried over Na_2SO_4. After removal of the solvent in vacuo to give crude stannylated ProDOT-Hex monomer (65%, determined by NMR) as yellow-black oil. To this crude stannylated ProDOT-Hex monomer, **4** (1.27 g, 1.55 mmol), Pd $(PPh_3)_4$ (0.28 g, 0.24 mmol), and toluene (80 mL) were added under N_2. After refluxed overnight, the reaction mixture was quenched with water and the mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) using hexane/dichloromethane (v/v = 3:1) as eluent. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **5** (0.843 g, 0.830mmol, 54%) as yellow oil: ^{1}H NMR (C_6D_6) δ 6.39 (s, 1H), 3.89 (s, 2H), 3.86 (s, 2H), 3.79 (s, 4H), 3.70 (s, 4H), 2.21 (s, 3H), 1.29-1.20(m, 60H), 0.92-0.91(m, 18H); ^{13}C NMR (C_6D_6) δ151.55, 150.31, 146.12, 145.90, 145.70, 145.29, 117.55, 116.11, 114.43, 113.62, 112.73, 103.55, 78.39, 78.34, 78.15, 77.88, 77.80, 43.92, 43.89, 32.15, 32.11, 30.58, 23.12, 21.13, 14.38; MS(LDI-TOF) *m/z* = 1015 [M^+]. Anal. Calcd for $C_{58}H_{94}O_6S_4$: C, 68.59; H, 9.33. Found: C, 68.46; H, 9.52.

^{1}H-NMR spectrum of **5**

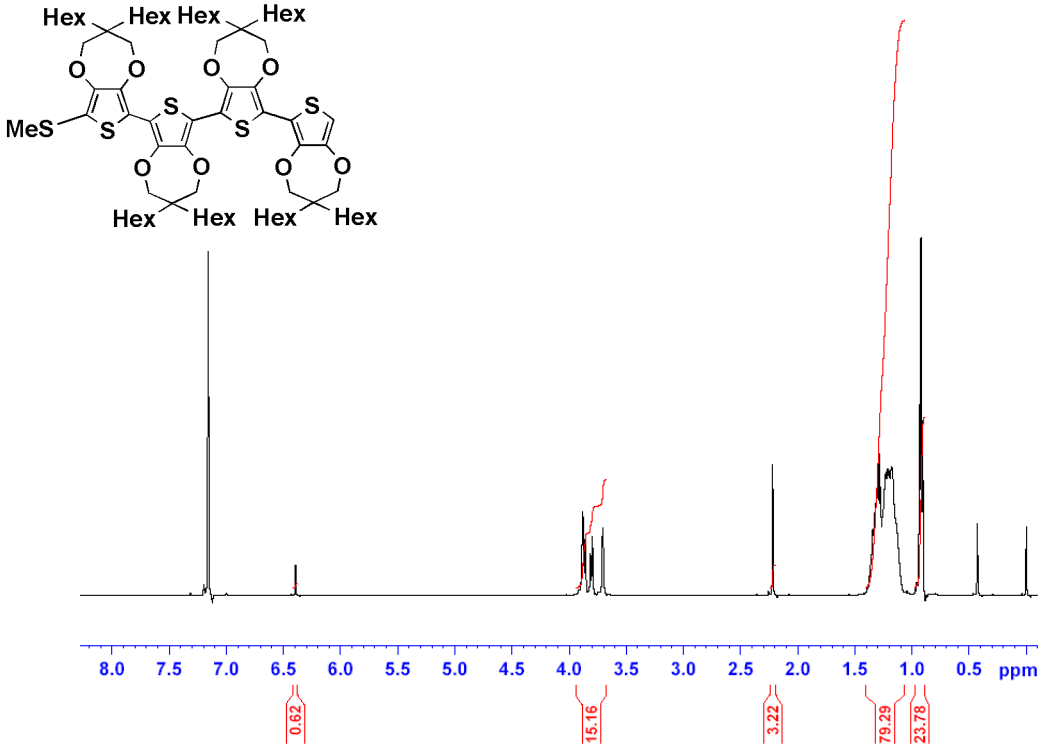


^{13}C-NMR spectrum of **5**

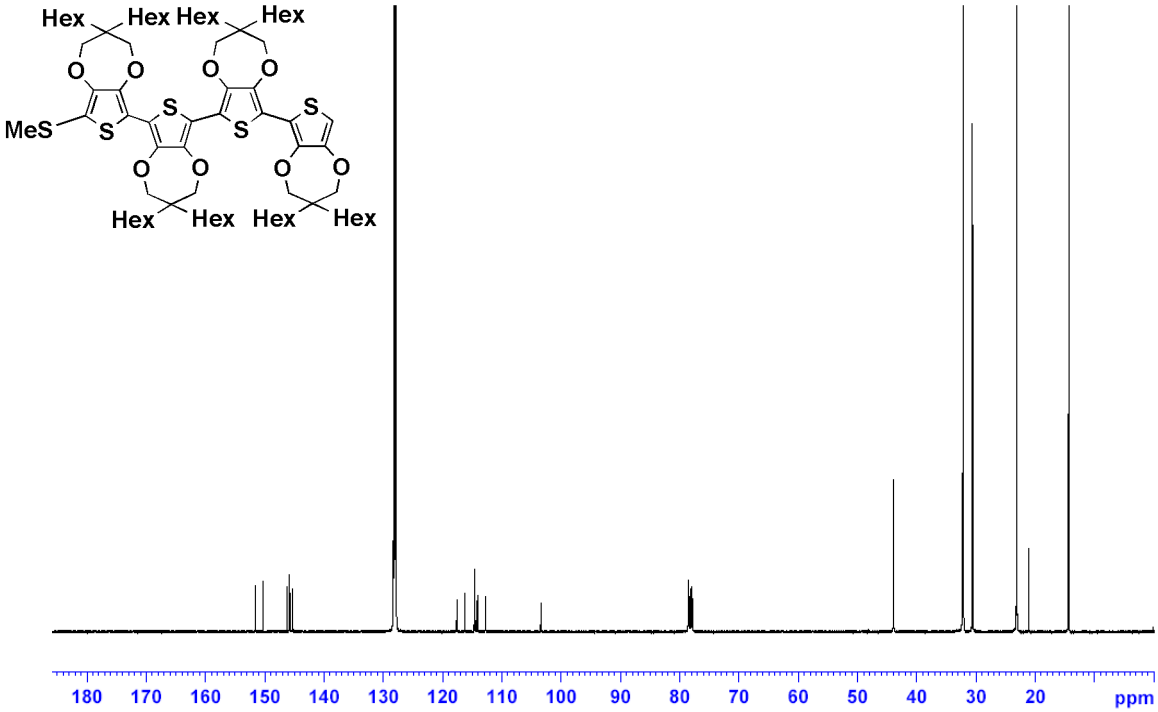


Synthesis of 6. To a THF solution (15 mL) of **2** (1.23 g, 1.9 mmol) was added n-butyllithium (1.7 M, 2.5 mmol) in hexane at 0°C under N_2. After stirring for 120 min at 0°C, trimethyltin chloride (1.0 M, 2.3 mmol) in dichloromethane was added and then allowed to warm to room temperature. After stirring overnight, the reaction mixture was quenched with NH_4Cl and the mixture was extracted with dichloromethane. The organic layer was washed with brine and dried over Na_2SO_4. Removal of the solvent in vacuo gave crude stannylated ProDOT-Hex dimer (59%, determined by NMR) as dark yellow oil. To the crude Stannylated ProDOT-Hex dimer, **4** (0.397 g, 0.484 mmol) Pd $(PPh_3)_4$ (92 mg, 0.082 mmol), and added toluene (30 mL) were under N_2. After refluxed overnight, the reaction mixture was quenched with water and the mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) using hexane/dichloromethane (v/v = 3:1) as eluent. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **6** (0.486 g, 0.363 mmol, 75%) as orange oil: ^{1}H NMR (C_6D_6) δ 6.39 (s, 1H), 3.88 (s, 6H), 3.85 (s, 2H), 3.81 (s, 2H), 3.80 (s, 2H), 3.70 (s, 4H), 2.22 (s, 3H), 1.34-1.18 (m, 80H), 0.93-0.91 (m, 24H); ^{13}C NMR (C_6D_6) δ 151.57, 150.34, 146.30, 145.88, 145.81, 145.71, 145.35, 145.29, 117.63, 117.56, 116.22, 114.67, 114.56, 114.24, 114.14, 114.05 78.55, 78.47, 78.41, 78.16, 78.09, 77.91, 77.84, 43.95, 43.92, 43.90, 32.31, 32.24, 32.21, 32.15, 30.60, 23.13, 21.12, 14.39; MS(LDI-TOF) *m/z* = 1334 [M^+-2]. Anal. Calcd for $C_{77}H_{124}O_8S_5$: C, 69.11; H9.34. Found: C, 68.88.; H, 9.54.

^{1}H-NMR spectrum of **6**

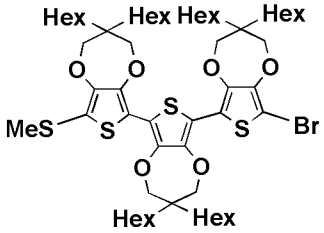


^{13}C-NMR spectrum of **6**

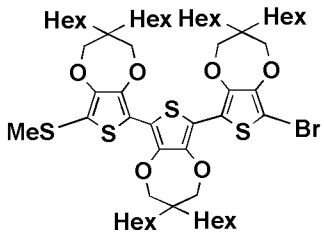


Synthesis of 7. To a THF solution (5 mL) of **5** (0.243 g, 0.239 mmol) was added *N*-brosuccinimide (0.0530 g, 0.298 mmol) at -78°C under dark condition. After allowing to warm to room temperature and stirring overnight, the reaction mixture was quenched with water. The mixture was extracted with ether and the organic layer was washed with K_2CO_3 aqueous, $Na_2S_2O_3$ aqueous, brine, dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) quickly using toluene as eluent under dark condition. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **7** (0.242g, 0.221mmol, 92%) as yellow oil: ^{1}H NMR (C_6D_6) δ 3.86 (s, 2H), 3.80 (s, 2H), 3.75 (s, 2H), 3.70 (s, 4H), 3.60 (s, 2H), 2.21 (s, 3H), 1.30-1.09 (m, 60H), 0.93-0.90 (m, 18H); ^{13}C NMR (C_6D_6) δ 151.52, 148.30, 145.91, 145.47, 144.57, 117.33, 116.09, 113.98, 113.71, 113.14, 92.63, 78.56, 78.44, 78.15, 77.85, 43.90, 43.84, 32.13, 32.12, 32.09, 30.55, 30.52, 23.11, 23.08, 21.05, 14.36; MS(LDI-TOF) m/z = 1093 [M^+]. Anal. Calcd for $C_{58}H_{93}BrO_6S_4$: C, 63.65; H, 8.56. Found: C, 63.71.; H, 8.69.

^{1}H-NMR spectrum of **7**

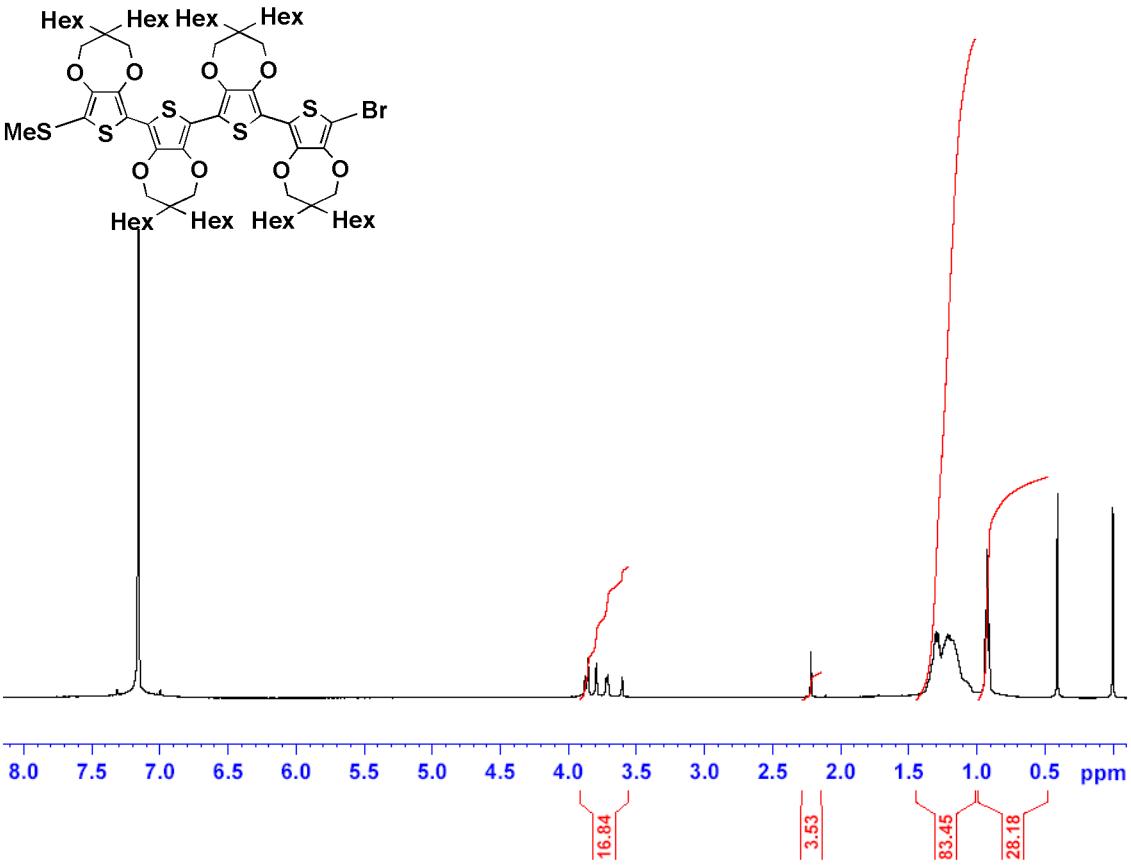


^{13}C-NMR spectrum of **7**

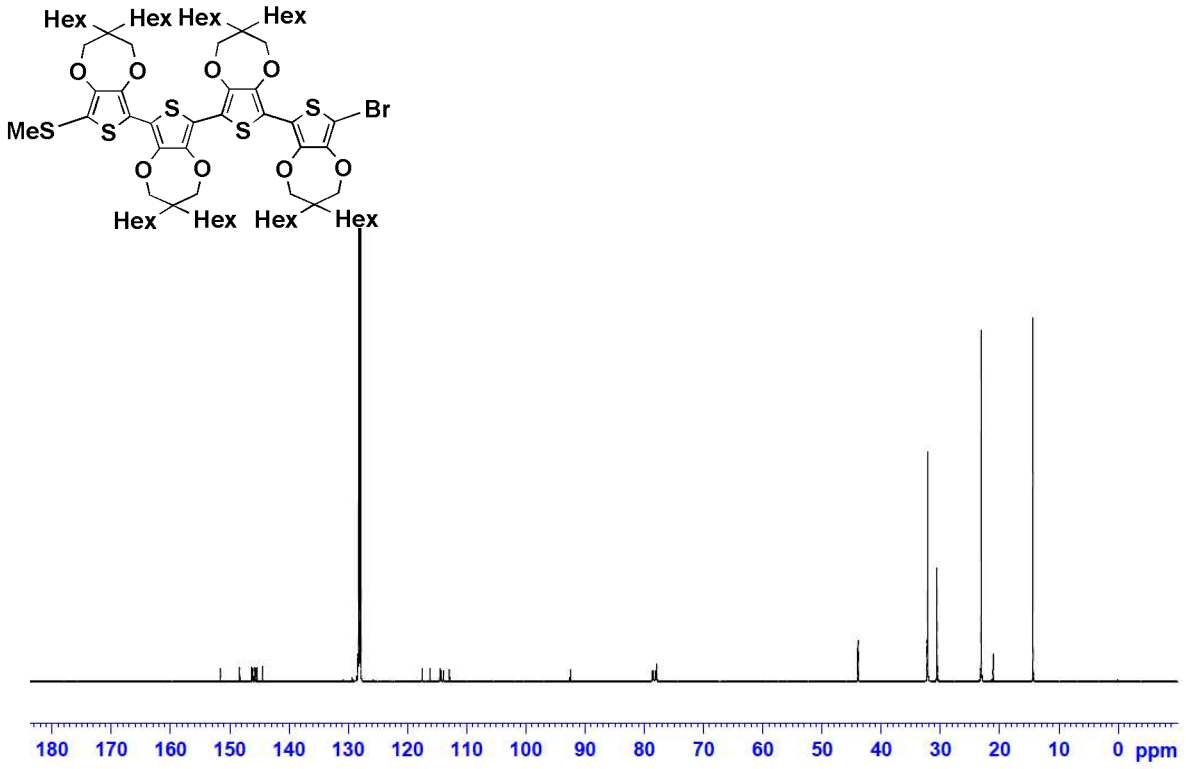


Synthesis of 8. To a THF solution (5 mL) of **6** (0.318 g, 0.238 mmol) was added N-bromosuccinimide (47.2 mg, 0.265 mmol) at -78°C under dark condition. After allowing to warm to room temperature and stirring overnight, the reaction was quenched with water. The reaction mixture was extracted with toluene and the organic layer was washed with K_2CO_3 aqueous, $Na_2S_2O_3$ aqueous, brine, dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) quickly using toluene as eluent under dark condition. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **8** (0.278 g, 0.196 mmol, 82 %) as orange oil: ^{1}H NMR (C_6D_6) δ 3.88 (s, 2H), 3.86 (s, 4H), 3.79 (s, 4H), 3.72 (s, 2H), 3.71 (s, 2H), 3.60 (s, 2H), 2.22 (s, 3H), 1.34-1.18 (m, 80H), 0.93-0.91 (m, 24H); ^{13}C NMR (C_6D_6) δ151.54, 148.31, 146.25, 146.06, 145.84, 145.65, 145.37, 144.48, 117.50, 116.19, 114.52, 114.41, 114.34, 113.88, 112.89, 92.50, 78.67, 78.62, 78.55, 78.46, 78.15, 78.10, 77.90, 43.94, 43.90, 43.88, 32.24, 32.21, 32.19, 32.14, 30.59, 30.54, 23.13, 23.08, 21.10, 14.39; MS(LDI-TOF) *m*/*z* = 1415 [M$^+$]. Anal. Calcd for $C_{77}H_{123}BrO_8S_5$: C,65.27; H,8.75. Found: C, 65.31; H, 8.99.

^{1}H-NMR spectrum of **8**

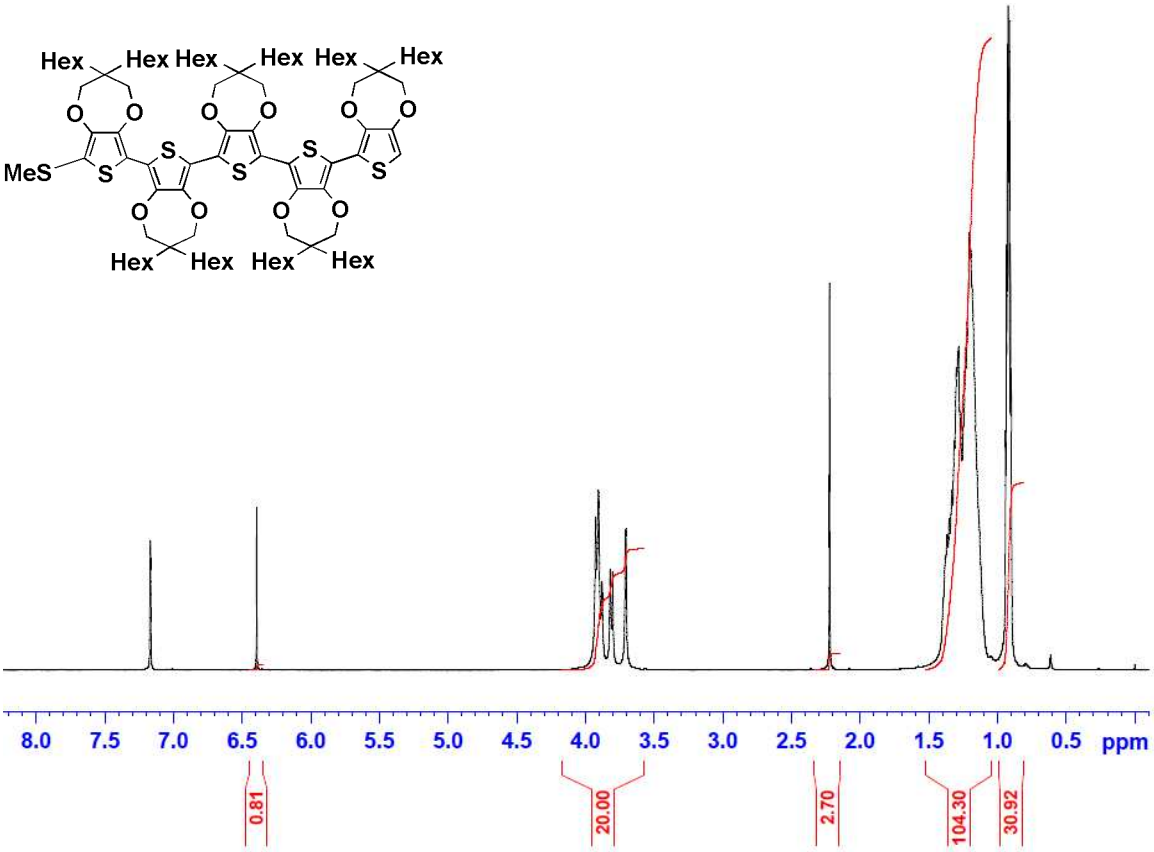


^{13}C-NMR spectrum of **8**

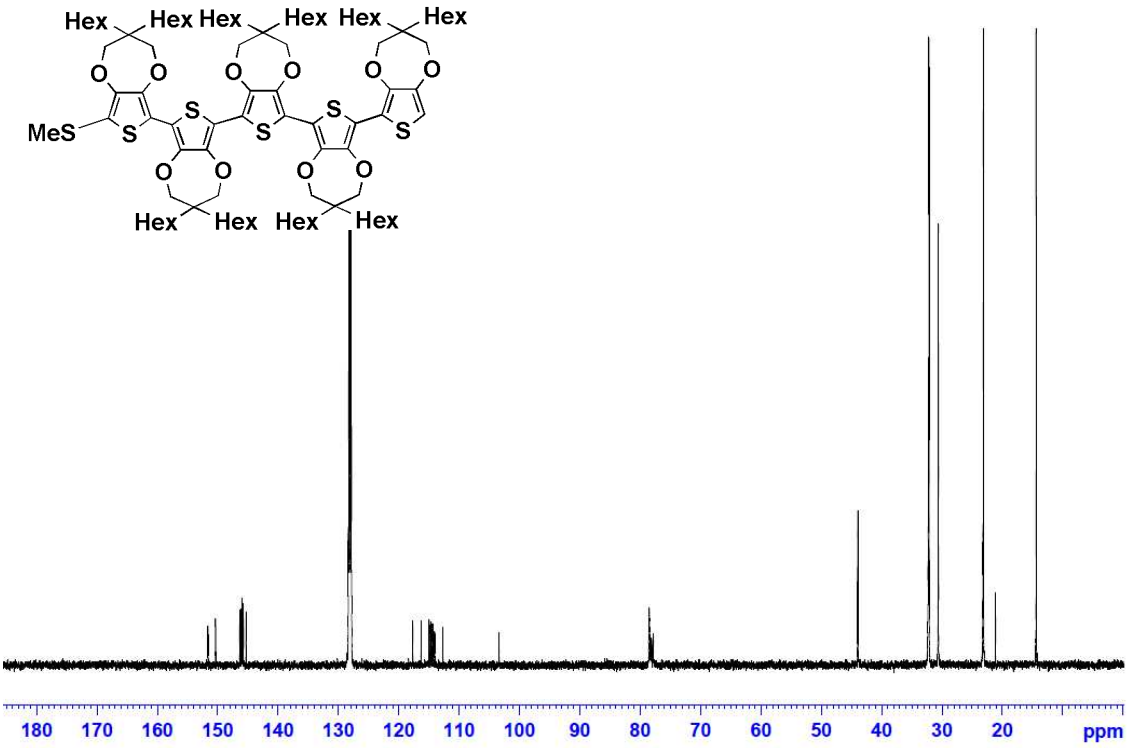


Synthesis of 9. To a mixture of crude stannylated ProDOT-Hex dimer (0.23 g, 0.28 mmol) prepared as described above, **7** (0.151 g, 0.138 mmol) and Pd $(PPh_3)_4$ (24 mg, 0.021 mmol) were added toluene (20 mL) under N_2. After refluxed overnight, the reaction mixture was quenched with water and the mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) using hexane/dichloromethane (v/v = 3:1) as eluent. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **9** (0.146 g, 0.0879 mmol, 64%) as orange oil: ^{1}H NMR (C_6D_6) δ 6.39 (s, 1H), 3.93 (s, 4H), 3.91 (s, 6H), 3.88 (s, 2H), 3.82 (s, 2H), 3.80 (s, 2H), 3.71 (s, 4H), 2.22 (s, 3H), 1.37-1.19 (m, 100H), 0.94-0.90 (m, 30H); ^{13}C NMR (C_6D_6) δ 151.60, 150.36, 146.35, 146.96, 145.87, 145.86, 145.75, 145.31, 117.69, 116.30, 114.95, 114.80, 114.63, 114.56, 114.32, 114.06, 112.71, 103.40, 78.50, 78.17, 78.11, 77.90, 77.82, 43.94, 43.92, 32.30, 32.23, 32.19, 32.15, 30.61, 30.58, 23.13, 21.13, 14.39, 14.38; MS(LDI-TOF) *m*/*z* = 1659 [M^+]. Anal. Calcd for $C_{96}H_{154}O_{10}S_6$: C, 69.43; H, 9.35. Found: C, 69.19; H, 9.47.

^{1}H-NMR spectrum of **9**

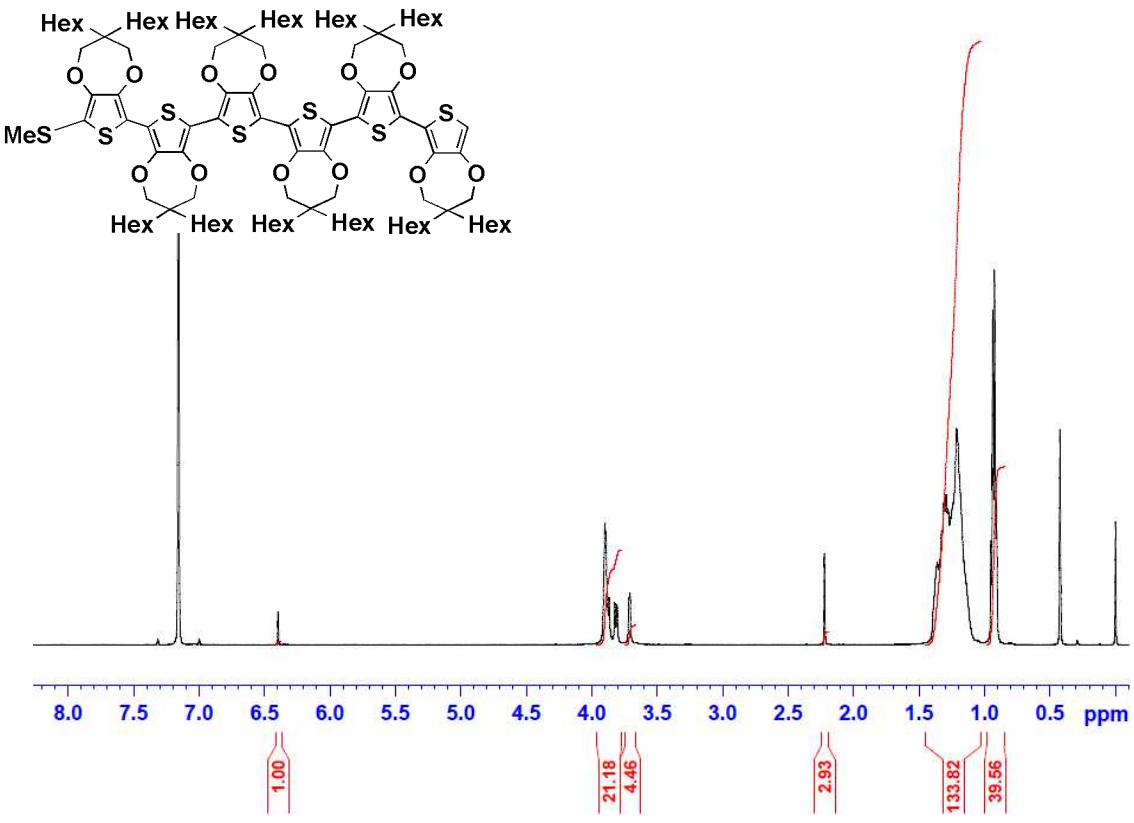


^{13}C-NMR spectrum of **9**

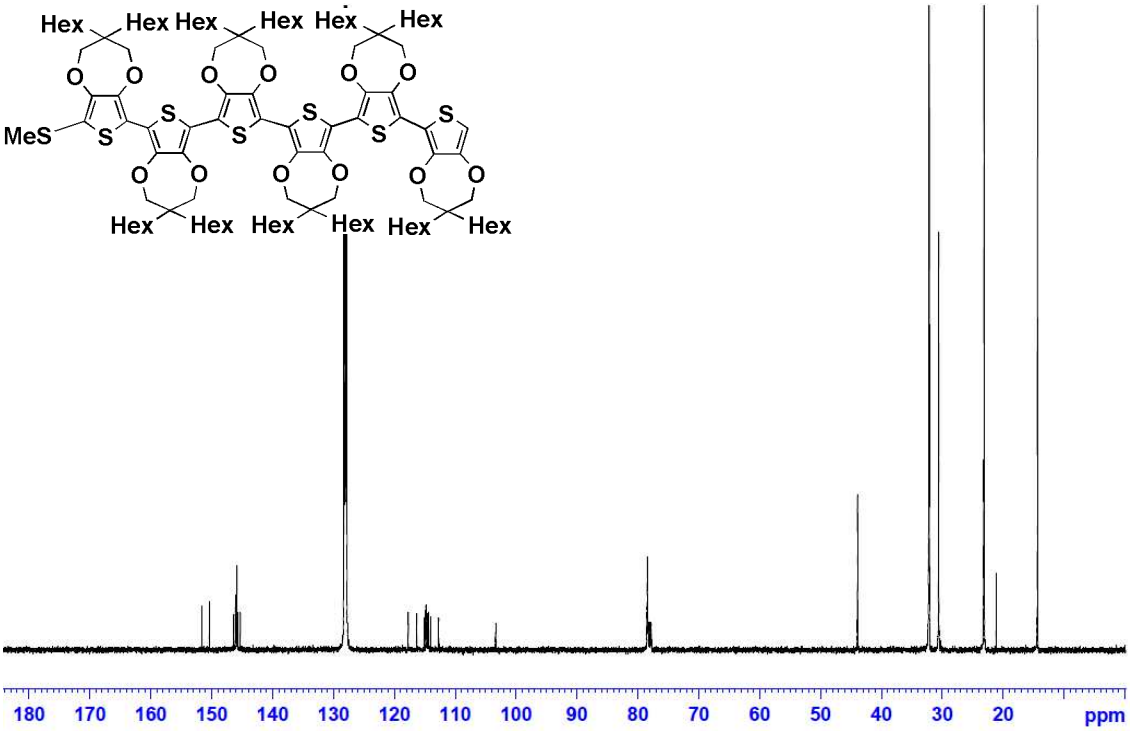


Synthesis of 10. To a mixture of crude stannylated ProDOT-Hex dimer (0.38 g, 0.46 mmol) prepared as described above, **8** (0.374 g, 0.264 mmol) and Pd $(PPh_3)_4$ (31 mg, 0.027 mmol) were added toluene (25 mL) under N_2. After refluxed overnight, the reaction mixture was quenched with water and the mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (SiO_2 deactivated with 10% water) using hexane/dichloromethane (v/v = 3:1) as eluent. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **10** (0.196 g, 0.0988 mmol, 38%) as orange powder: mp 64.4-65.1°C; ^{1}H NMR (C_6D_6) δ 6.40 (s, 1H) 3.90 (s, 14H), 3.87 (s,2H), 3.82 (s,2H), 3.81 (s,2H), 3.71 (m, 4H), 2.22 (s, 3H), 1.36-1.21(m, 120H), 0.95-0.91(m, 36H); ^{13}C NMR (C_6D_6) δ 151.62, 150.37, 146.38, 146.08, 146.03, 146.01, 146.00, 145.87, 145.78, 145.33, 117.72, 116.32, 115.08, 114.87, 114.82, 114.81, 114.64, 114.52, 114.41, 114.06, 112.71, 103.37, 78.47, 78.36, 78.17, 78.10, 78.89, 77.80, 43.94, 32.29, 32.20, 32.15, 30.63, 30.60, 23.21, 23.16, 23.14, 21.14, 14.37; MS(LDI-TOF) *m*/*z* = 1981 [M^+]. Anal. Calcd for $C_{115}H_{184}O_{12}S_7$: C, 69.65; H, 9.35. Found: C, 69.45; H, 9.24.

^{1}H-NMR spectrum of **10**

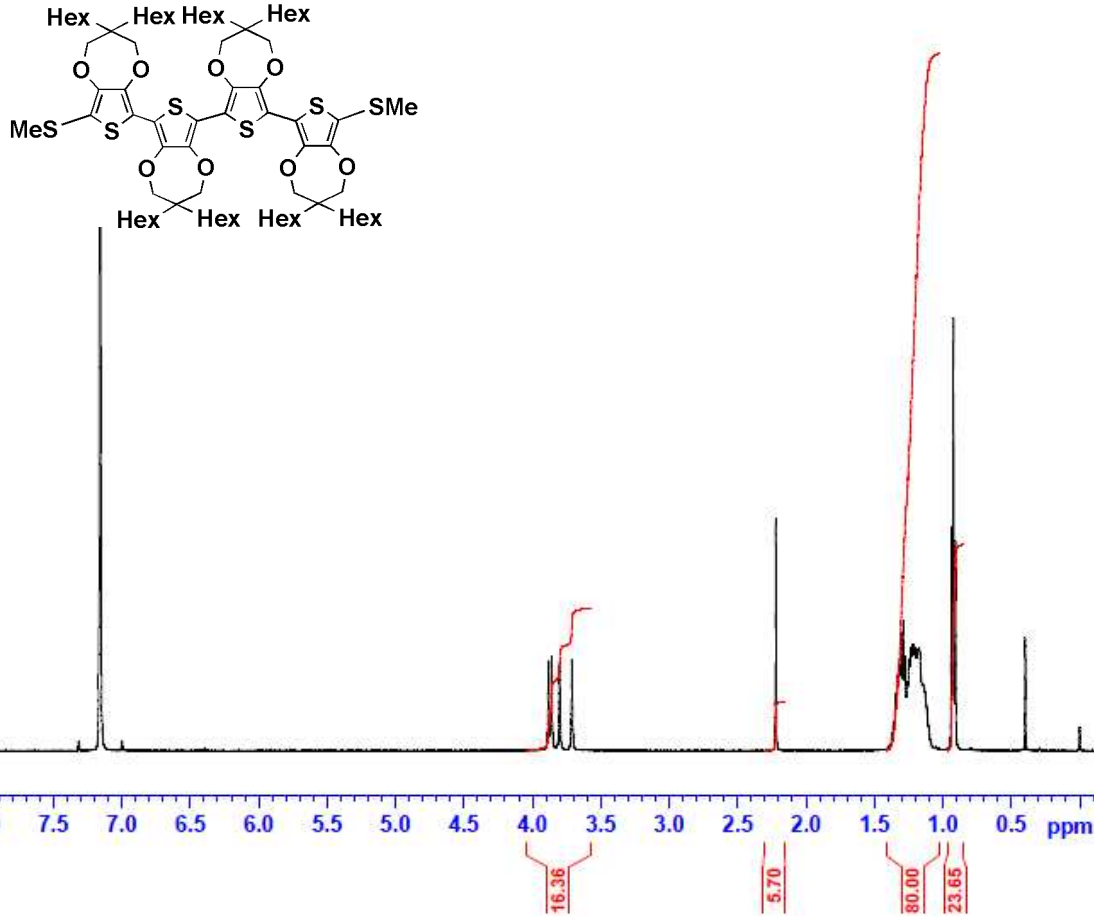


^{13}C-NMR spectrum of **10**

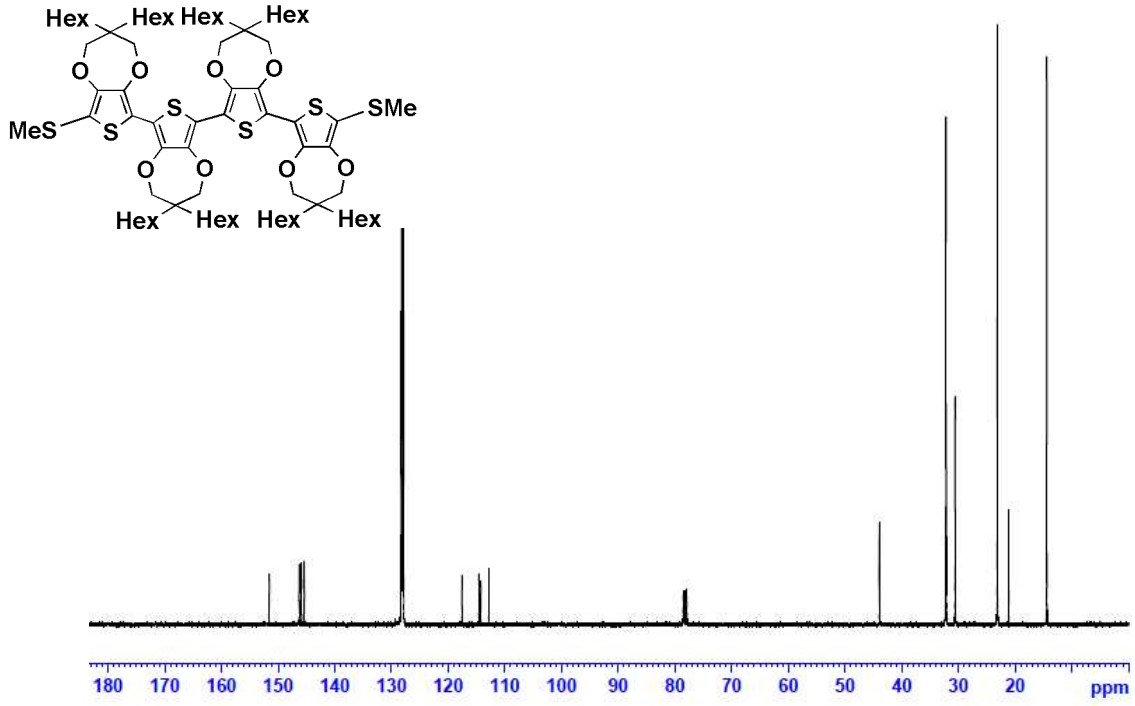


Synthesis of 4P$_{Hex}$. To a THF solution (20 mL) of **3** (0.428 g, 0.617 mmol) and TMEDA (0.19 mL, 1.26 mmol) was added n-butyllithium (1.6 M, 0.736 mmol) in hexane at 0°C under N_2. After stirring for 120min at 0°C, the solution was transferred into refluxing THF solution (10 mL) of $Fe(acac)_3$ (0.268g, 0.759mmol) under N_2 via cannula and the reaction mixture was refluxed overnight. The volatiles were removed in vacuo, and the residue was purified by column chromatography (SiO_2 deactivated with 10% water) with hexane-CH_2Cl_2 (v/v = 4:1) as eluent to give **4P$_{Hex}$** (0.198 g, 0.143 mmol, 46%) as orange oil: ^{1}H NMR (C_6D_6) δ 3.88 (s, 4H), 3.86 (s, 4H), 3.80 (s, 4H), 3.71 (s, 4H), 2.22 (s, 6H), 1.36-1.15 (m, 80H), 0.94-0.91(m, 24H); ^{13}C NMR (C_6D_6) δ 151.56, 146.27, 145.83, 145.36, 117.56, 114.56, 114.25, 112.82, 78.54, 78.45, 78.15, 77.90, 43.94, 43.90, 32.24, 32.21, 32.14, 30.59, 30.58, 23.13, 21.11, 14.38; MS(LDI-TOF) *m/z* = 1383 [M^+]. Anal. Calcd for $C_{78}H_{126}O_8S_6$: C, 67.68; H, 9.17. Found: C, 67.44; H, 9.24.

^{1}H-NMR spectrum of **4P$_{Hex}$**



^{13}C-NMR spectrum of **4P$_{Hex}$**



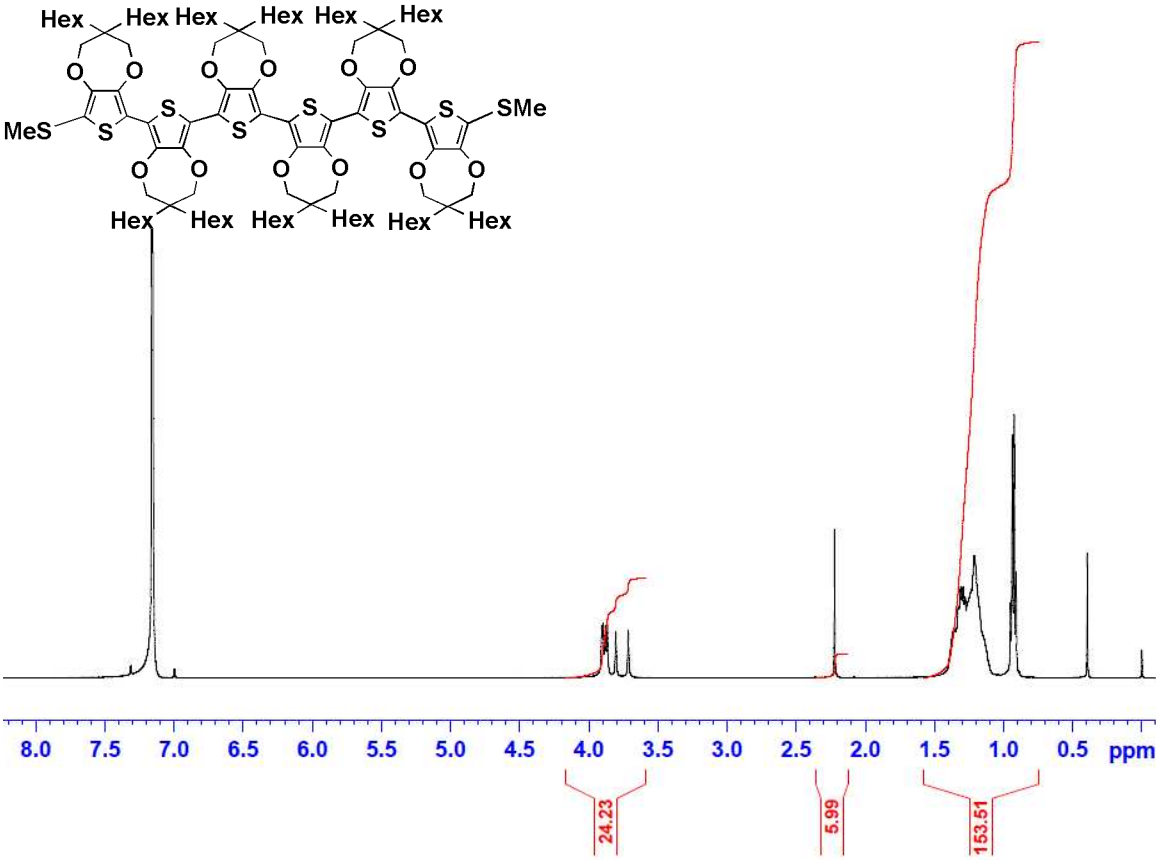
Synthesis of $n\mathbf{P}_{\mathbf{Hex}}$ (n = 6,8,10,12). A chloroform solution (10mL) of **5** (0.277 g, 0.273 mmol) was quickly transferred to an acetonitrile solution (5 mL) of iron(III) perchlorate hydrate (0.17 g, 0.38 mmol) via cannula at 0°C under N_2. After stirring overnight and allowing to warm to room temperature, the reaction was treated with saturated aqueous sodium hydrosulfite solution for 90min. Then the mixture was extracted with dichloromethane and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was passed through a short column chromatography (Al_2O_3) using hexane-dichloromethane (v/v = 5:1) as eluent. After evaporation, the residue was separated by preparative GPC eluted with toluene to give $\mathbf{6P}_{\mathbf{Hex}}$ (0.189mg, 0.0931 mmol, 68%) as orange powder: ^{1}H NMR(C_6D_6) δ 3.91 (s, 4H), 3.90 (s, 4H), 3.88 (s, 4H), 3.87 (s, 4H), 3.81 (s, 4H), 3.72 (s, 4H), 2.22 (s, 6H), 1.36-1.21(m, 120H), 0.95-0.91(m, 36H); ^{13}C NMR (C_6D_6) δ 151.63, 146.39, 146.14, 146.06, 145.82, 145.36, 117.71, 115.02, 114.85, 114.73, 114.11, 112.74, 78.44, 78.17, 77.88, 43.94, 43.93, 43.90, 32.20, 32.15, 30.62, 30.60, 30.57, 23.21, 23.15, 23.13, 21.14, 14.39, 14.37; MS (LDI-TOF) m/z = 2027 [M^+]. Anal. Calcd for $C_{116}H_{186}O_{12}S_8$: C, 68.66; H, 9.24. Found: C, 68.59; H, 9.42.

Similar homo-coupling of **6** gave $\mathbf{8P}_{\mathbf{Hex}}$ (45%) as red solid: ^{1}H NMR(C_6D_6) δ 3.91 (s, 16H), 3.88 (s, 4H), 3.87 (s, 4H), 3.81 (s, 4H), 3.72 (s, 4H), 2.22 (s, 6H), 1.33-1.22(m, 160H), 0.95-0.91(m, 48H); ^{13}C NMR (C_6D_6) δ 151.62, 146.39, 146.15, 146.10, 146.05, 145.99, 145.77, 145.33, 117.73, 115.12, 114.96, 114.88, 114.84, 114.65, 114.06, 112.71, 78.51, 78.18, 77.90, 43.95, 43.90, 32.21, 32.15, 30.64, 30.60, 30.58, 23.22, 23.17, 23.14, 21.14, 14.40, 14.39; MS (LDI-TOF) m/z = 2672 [M^+]. Anal. Calcd for $C_{154}H_{246}O_{16}S_{10}$: C,69.17; H, 9.27. Found: C, 69.17; H, 9.27.

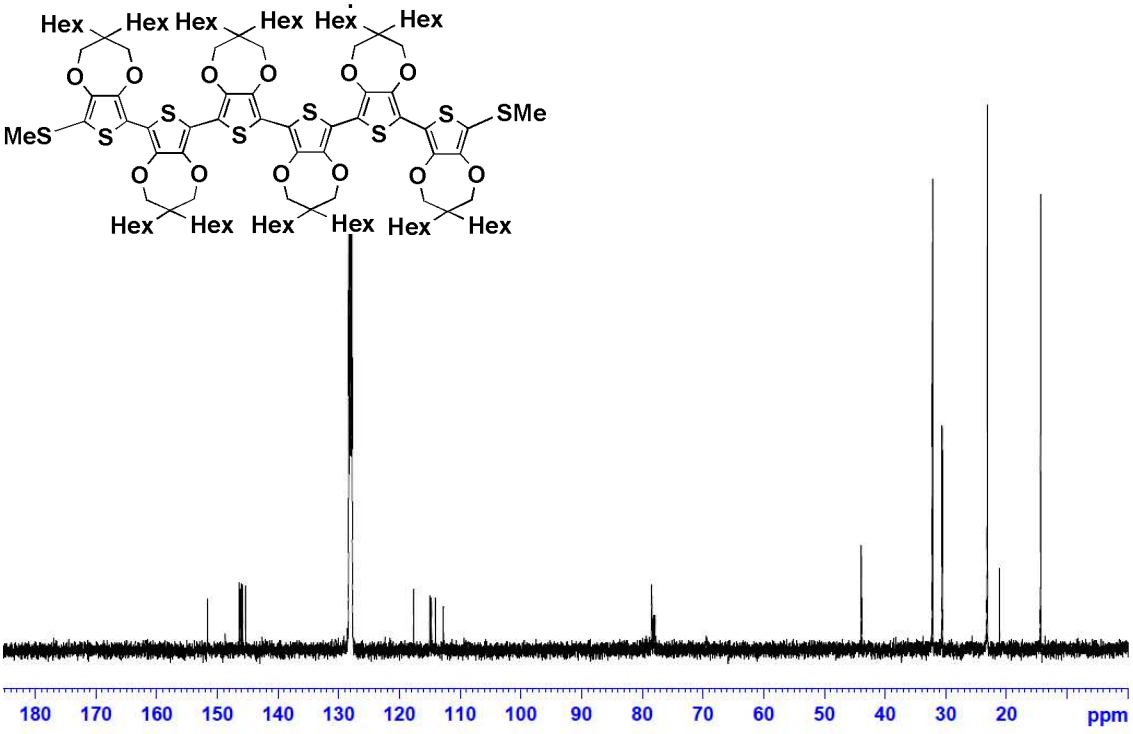
Similar homo-coupling of **9** gave $\mathbf{10P}_{\mathbf{Hex}}$ (56%) as madder solid: ^{1}H NMR (C_6D_6) δ3.91 (s, 24H), 3.88 (s, 4H), 3.87 (s, 4H), 3.81 (s, 4H), 3.72 (s, 4H), 2.22 (s, 6H), 1.38-1.22(m, 200H), 0.95-0.91(m, 60H); ^{13}C NMR (C_6D_6) δ151.63, 146.40, 146.17, 146.13, 146.09, 146.07, 146.04, 145.99, 145.78, 145.33, 117.74, 115.16, 115.01, 114.96, 114.90, 114.80, 114.63, 114.05, 112.70, 78.49, 78.18, 77.90, 43.94, 32.21, 32.15, 30.64, 30.61, 30.58, 23.22, 23.17, 23.14, 21.15, 14.40, 14.38; MS (LDI-TOF) m/z = 3316 [M^+]. Anal. Calcd for $C_{192}H_{306}O_{20}S_{12}$: C,69.48; H, 9.29. Found: C, 69.32; H, 9.47.

Similar homo-coupling of **10** gave $\mathbf{12P}_{\mathbf{Hex}}$ (53%) as madder solid: ^{1}H NMR (C_6D_6) δ3.91 (s, 36H), 3.87 (s, 4H), 3.81 (s, 4H), 3.72 (s, 4H), 2.22 (s, 6H), 1.37-0.91(m, 312H); ^{13}C NMR(C_6D_6) δ 151.62, 146.38, 146.14, 146.10, 146.05, 145.96, 145.74, 145.31, 117.73, 115.15, 115.02, 114.97, 114.92, 114.89, 114.85, 114.77, 114.60, 114.03, 112.69, 78.55, 78.52, 78.18, 77.91, 43.95, 43.91, 32.21, 32.15, 30.65, 30.61, 30.58, 23.23, 23.17, 23.14, 23.13, 21.13, 14.41, 14.39, 14.38; MS (LDI-TOF) m/z = 3960 [M^+]. Anal. Calcd for $C_{230}H_{366}O_{24}S_{14}$: C,69.68; H,9.31. Found: C, 69.41; H, 9.38.

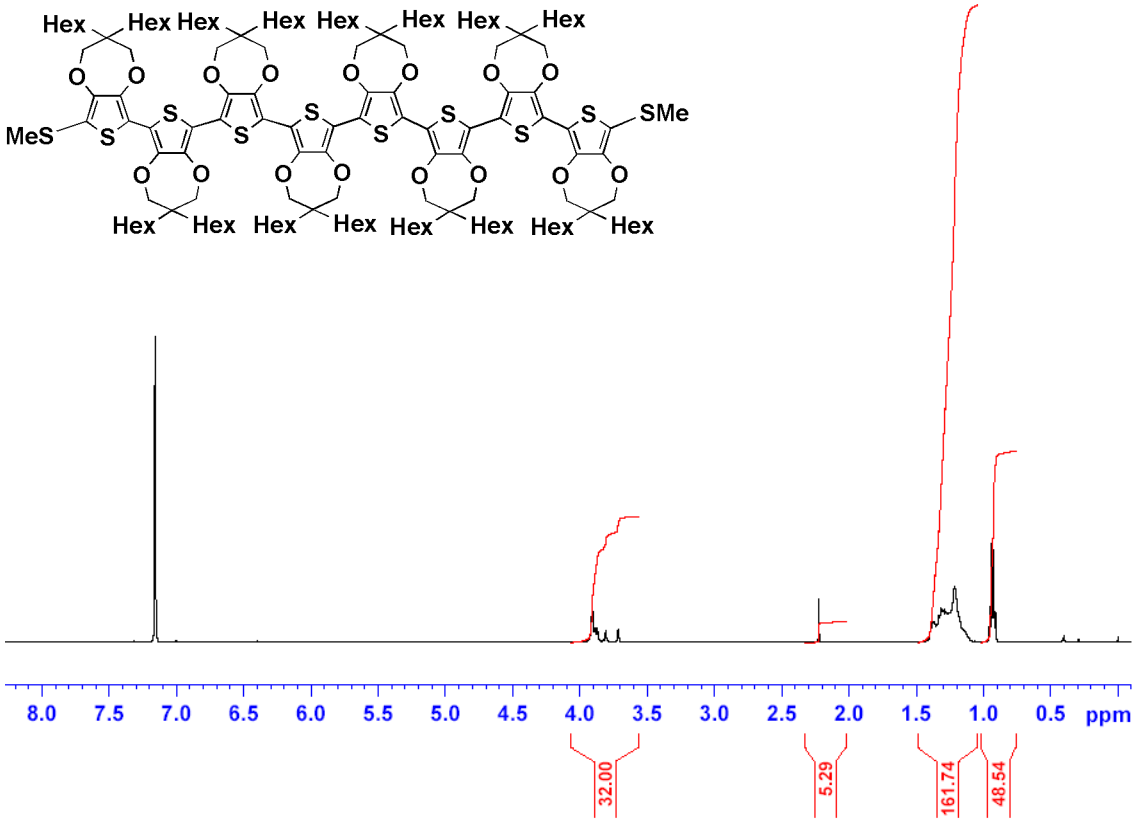
^{1}H-NMR spectrum of **6P$_{Hex}$**



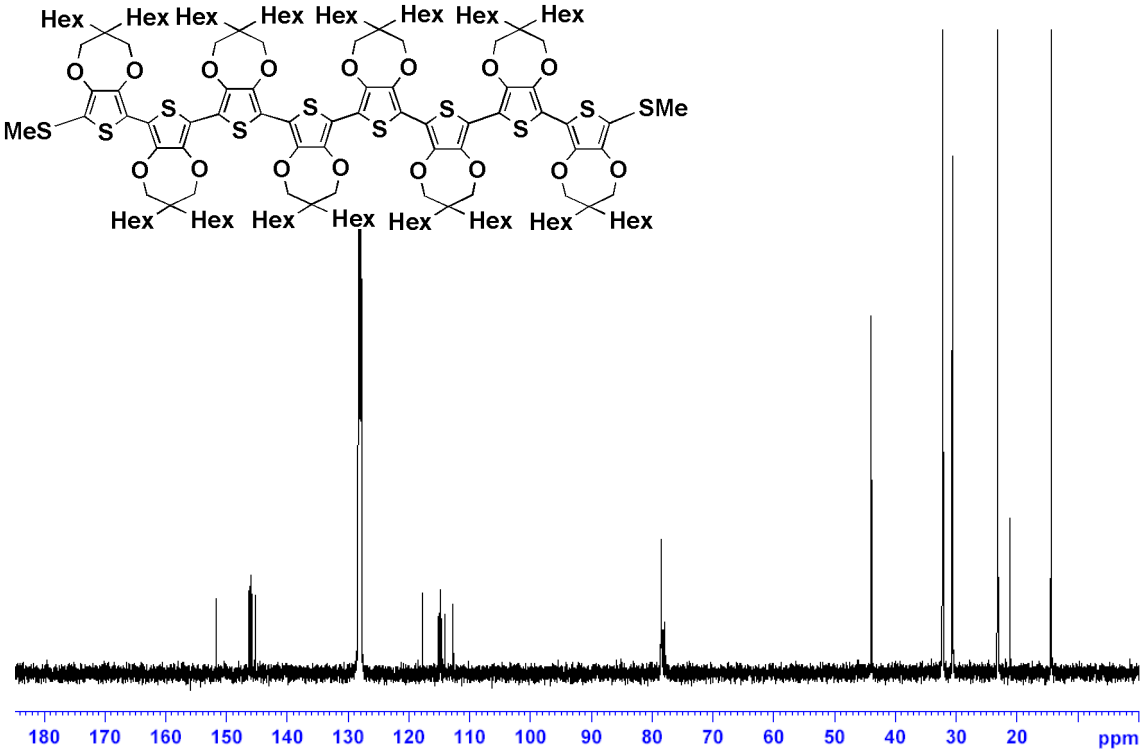
^{13}C-NMR spectrum of **6P$_{Hex}$**



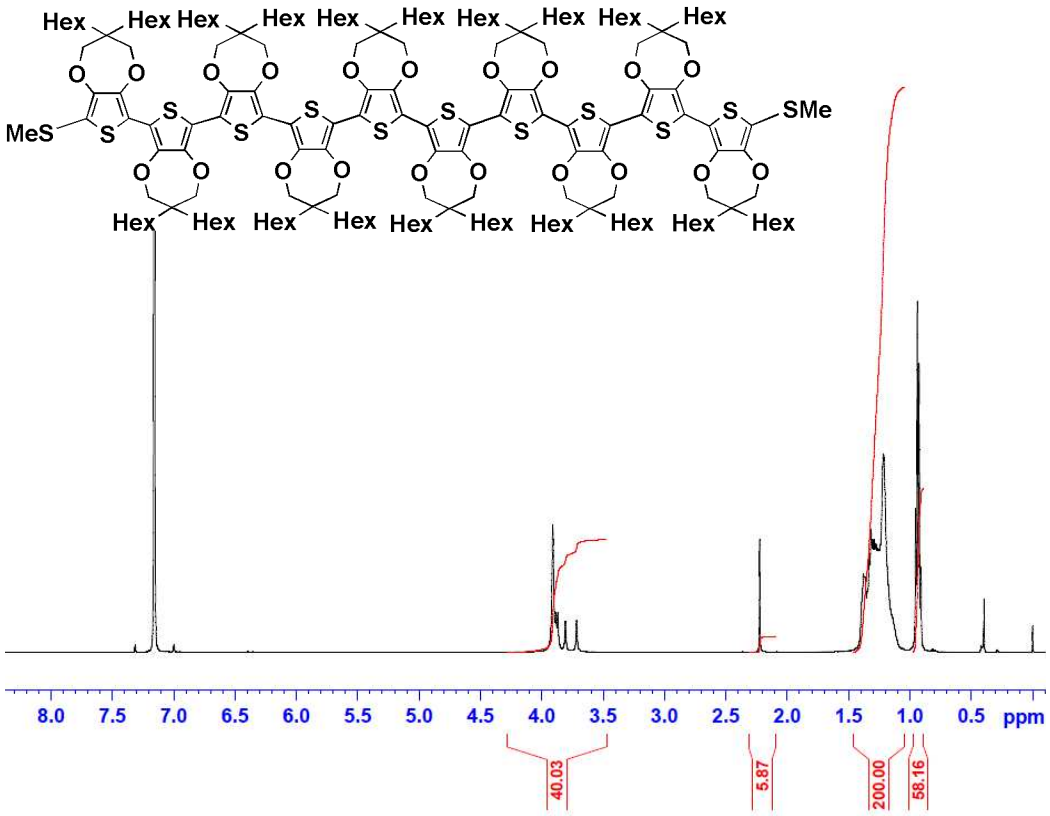
^{1}H-NMR spectrum of **8P$_{Hex}$**



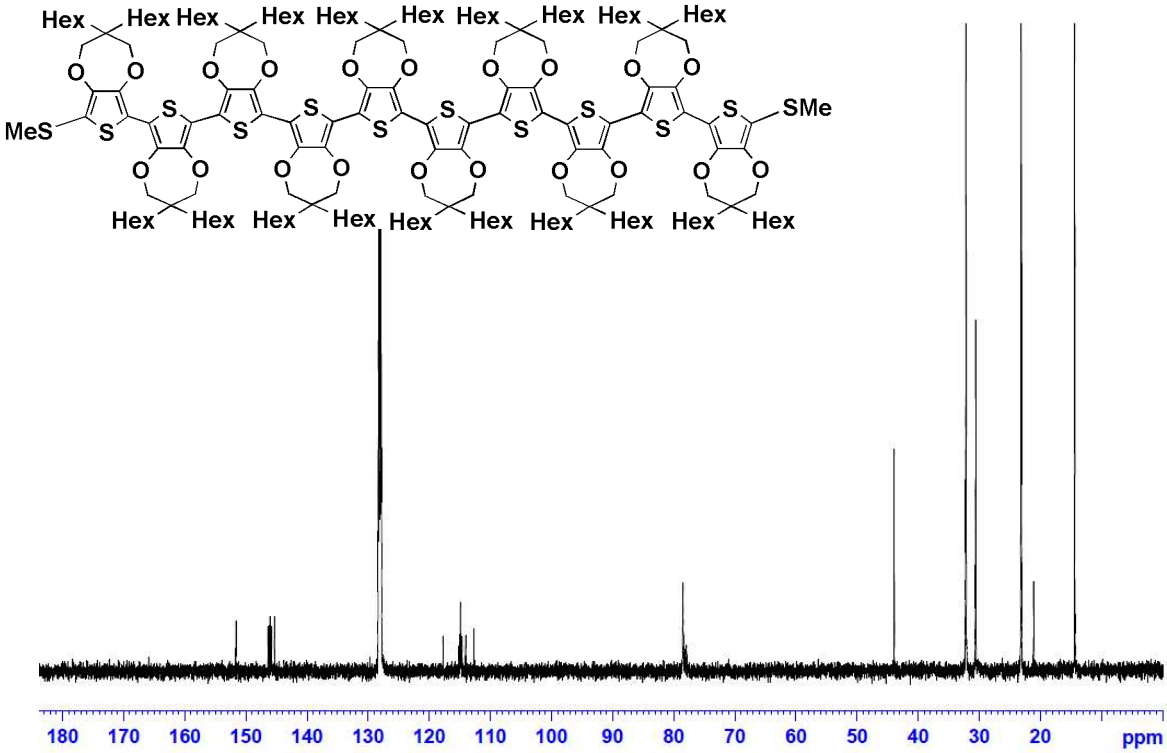
^{13}C-NMR spectrum of **8P$_{Hex}$**



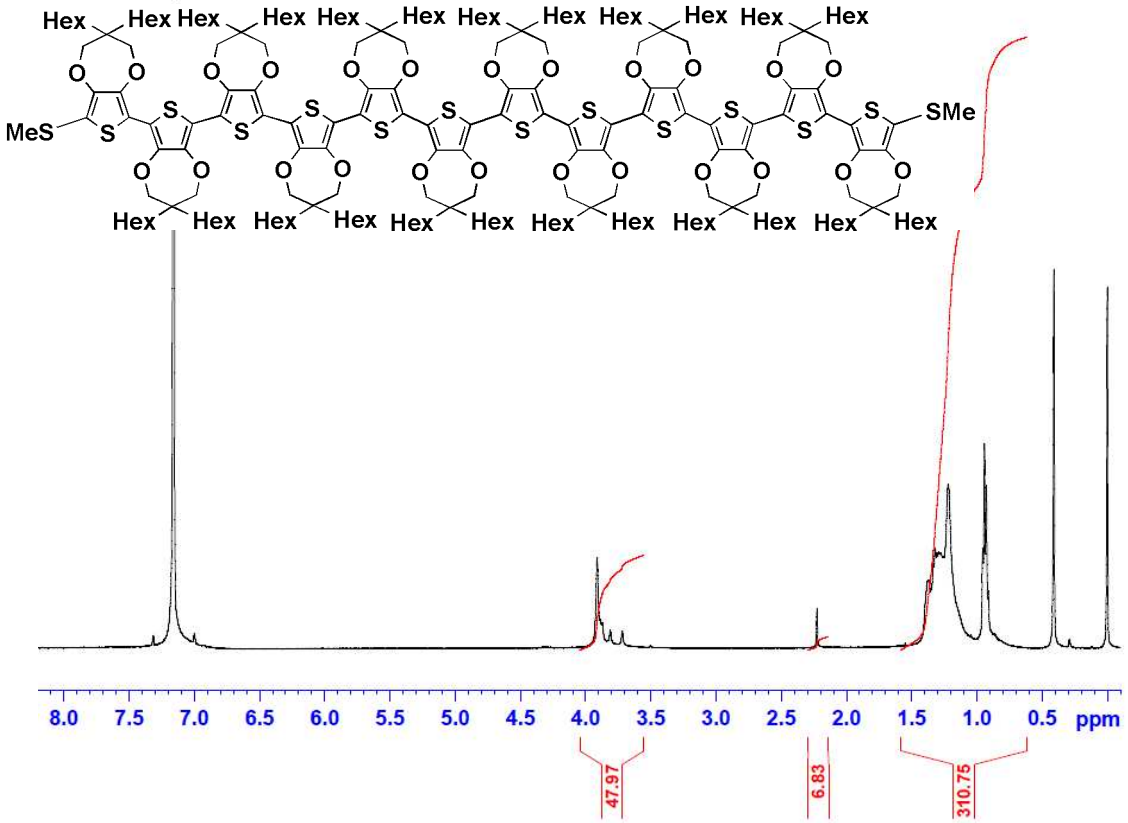
^{1}H-NMR spectrum of **10P$_{Hex}$**



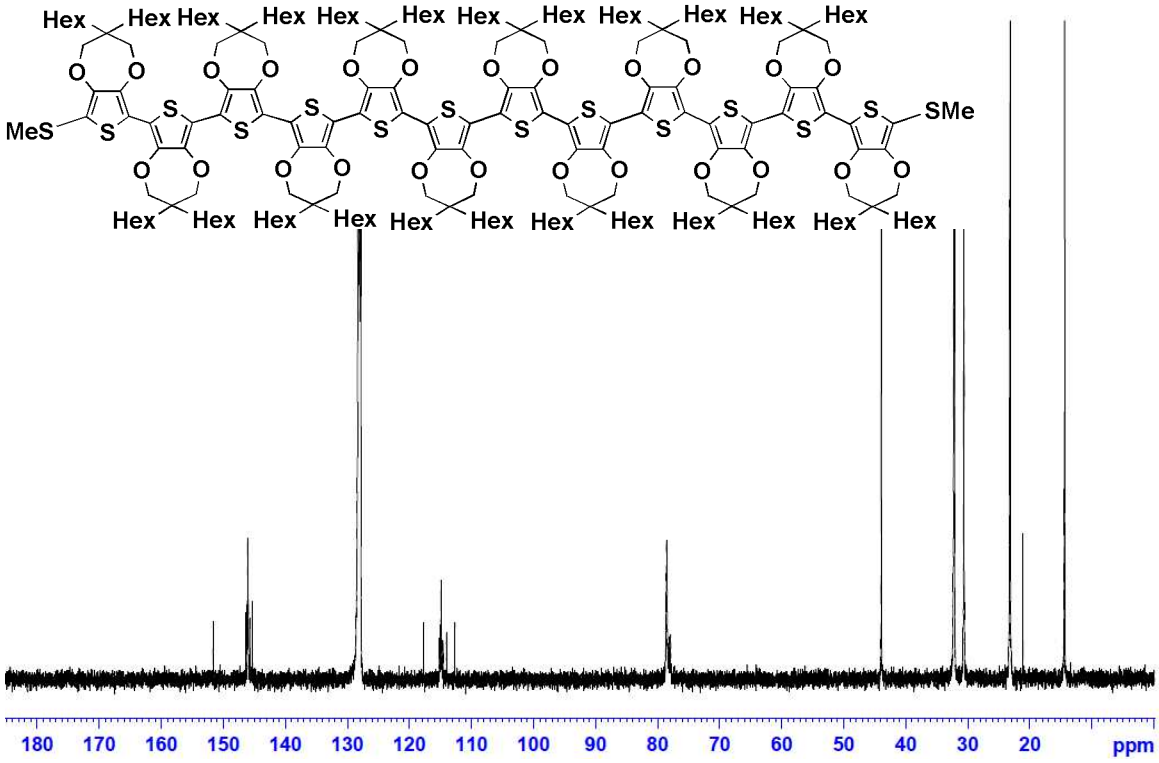
^{13}C-NMR spectrum of **10P$_{Hex}$**



^{1}H-NMR spectrum of **12P$_{Hex}$**



^{13}C-NMR spectrum of **12P$_{Hex}$**



Synthesis and X-ray crystallography of 11. To a THF solution (10 mL) of **2** (0.27 g, 0.42 mmol) was added n-butyllithium (1.7 M, 0.92 mmol) in hexane at 0°C under N_2. After stirring for 120 min at 0°C, iodine (0.25 g, 0.97 mmol) was added to the reaction mixture. After stirring for 20 min at room temperature, aqueous $Na_2S_2O_3$ was added and the mixture was extracted with ether and dried over Na_2SO_4. After removal of the solvent in vacuo, the reaction mixture was purified by column chromatography (SiO_2 deactivated with 10% water) using hexane/dichloromethane (v/v = 4:1) as eluent to give **11** (0.29 g, 0.32 mmol, 76%) as colorless crystals: ^{1}H NMR ($CDCl_3$) δ 3.91 (s, 4H), 3.89 (s,4H), 1.51-1.29 (m, 40H), 0.92-0.87(m, 12H); ^{13}C NMR (C_6D_6) δ 151.6, 143.8, 119.9, 78.3, 78.2, 56.2, 44.0, 31.9, 30.3, 22.8, 22.7, 14.3; MS(DI) *m/z* = 898 [M^+]. Anal. Calcd for $C_{38}H_{60}I_2O_4S_2$: C,50.78; H,6.73. Found: C, 50.86; H, 6.81.

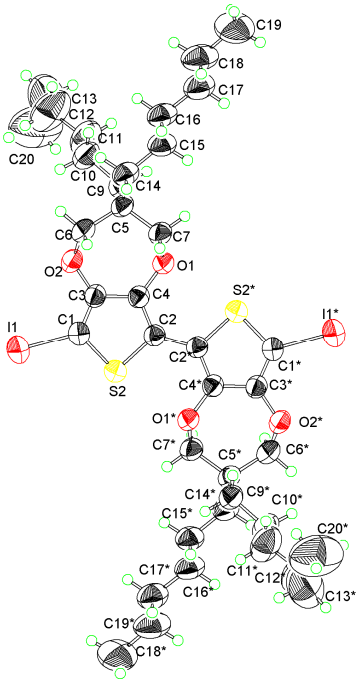
X-ray data were taken on a Bruker Smart APEX diffractometer equipped with a CCD area detector with graphite-monochromated $Mo_{k\alpha}$. radiation (λ = 0.71073 Å). The structure was solved by direct methods (SHELXTL) and refined by the full-matrix least-squares method on F^2 (SHELXL-97). Non-hydrogen atoms were refined anisotropically, and Hydrogen atoms were placed using AFIX instructions. Crystal data, structure refinement, bonde lengths, bond angles, and torsion angles for **11** are summarized in Table S1-S3.

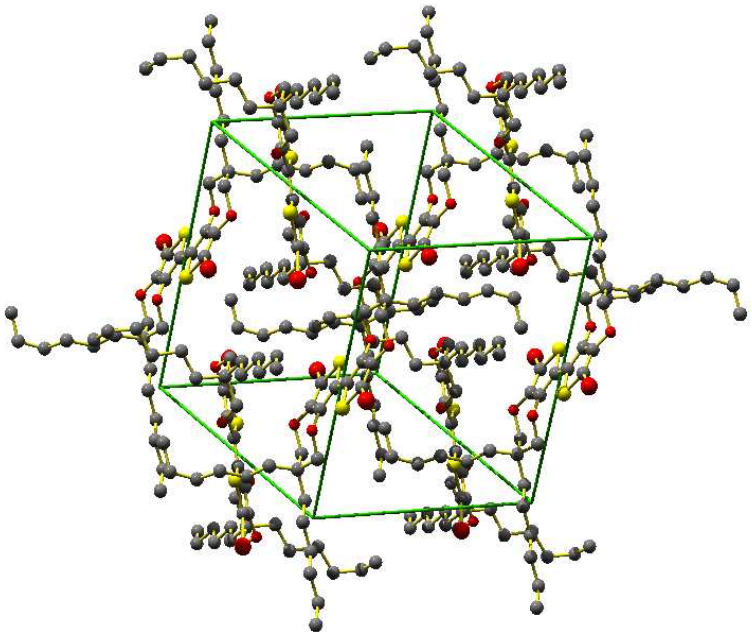
Table S1. Crystal data and structure refinement for **11**.

Identification code	**11**	
Empirical formula	C38 H60 I2 O4 S2	
Formula weight	898.78	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 12.2709(16) Å	α= 90°
	b = 15.242(2) Å	β= 109.757(2)°
	c = 12.2159(16) Å	γ = 90°
Volume	2150.3(5) Å^3	
Z	2	
Density (calculated)	1.388 Mg/m^3	
Absorption coefficient	1.593 mm^{-1}	
F(000)	916	
Theta range for data collection	2.21 to 23.23°.	
Index ranges	-13<=h<=9, -16<=k<=11, -13<=l<=13	
Reflections collected	7582	
Independent reflections	3061 [R(int) = 0.0252]	

Completeness to theta = 23.23°	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3061 / 0 / 210
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0893
R indices (all data)	R1 = 0.0469, wR2 = 0.0978
Largest diff. peak and hole	0.614 and -0.343 e.Å^{-3}

Table S2. Bond lengths [Å] and angles [°] for **11**.





S(2)-C(1)	1.721(4)
S(2)-C(2)	1.738(3)
O(1)-C(4)	1.363(4)
O(1)-C(7)	1.446(4)
C(3)-C(1)	1.344(5)
C(3)-O(2)	1.365(4)
C(3)-C(4)	1.421(5)
O(2)-C(6)	1.438(5)

C(1)-I(1)	2.067(4)
C(4)-C(2)	1.368(5)
C(5)-C(7)	1.522(5)
C(5)-C(6)	1.528(5)
C(5)-C(9)	1.536(5)
C(5)-C(14)	1.555(6)
C(2)-C(2)#1	1.446(7)
C(9)-C(10)	1.512(6)
C(14)-C(15)	1.519(6)
C(15)-C(16)	1.522(6)
C(10)-C(11)	1.513(7)
C(16)-C(17)	1.517(7)
C(17)-C(18)	1.512(7)
C(18)-C(19)	1.491(9)
C(11)-C(12)	1.498(9)
C(12)-C(13)	1.463(12)
C(13)-C(20)	1.408(15)
C(1)-S(2)-C(2)	91.14(17)
C(4)-O(1)-C(7)	115.1(3)
C(1)-C(3)-O(2)	123.3(3)
C(1)-C(3)-C(4)	111.8(3)
O(2)-C(3)-C(4)	124.8(3)
C(3)-O(2)-C(6)	115.8(3)
C(3)-C(1)-S(2)	113.0(3)
C(3)-C(1)-I(1)	127.8(3)
S(2)-C(1)-I(1)	119.2(2)
O(1)-C(4)-C(2)	121.1(3)
O(1)-C(4)-C(3)	125.1(3)
C(2)-C(4)-C(3)	113.8(3)
C(7)-C(5)-C(6)	110.5(3)
C(7)-C(5)-C(9)	109.4(3)
C(6)-C(5)-C(9)	112.0(3)
C(7)-C(5)-C(14)	106.9(3)
C(6)-C(5)-C(14)	105.1(3)
C(9)-C(5)-C(14)	112.7(3)
C(4)-C(2)-C(2)#1	128.0(4)

C(4)-C(2)-S(2)	110.3(3)
C(2)#1-C(2)-S(2)	121.7(4)
O(2)-C(6)-C(5)	115.7(3)
O(1)-C(7)-C(5)	113.8(3)
C(10)-C(9)-C(5)	117.1(3)
C(15)-C(14)-C(5)	117.6(3)
C(14)-C(15)-C(16)	112.5(4)
C(9)-C(10)-C(11)	113.4(4)
C(17)-C(16)-C(15)	113.6(4)
C(18)-C(17)-C(16)	113.9(5)
C(19)-C(18)-C(17)	114.2(6)
C(12)-C(11)-C(10)	115.6(5)
C(13)-C(12)-C(11)	117.7(8)
C(20)-C(13)-C(12)	117.2(10)

Table S3. Torsion angles [°] for **11**.

C(1)-C(3)-O(2)-C(6)	128.9(4)
C(4)-C(3)-O(2)-C(6)	-56.2(5)
O(2)-C(3)-C(1)-S(2)	174.0(3)
C(4)-C(3)-C(1)-S(2)	-1.5(4)
O(2)-C(3)-C(1)-I(1)	-7.7(6)
C(4)-C(3)-C(1)-I(1)	176.7(3)
C(2)-S(2)-C(1)-C(3)	1.6(3)
C(2)-S(2)-C(1)-I(1)	-176.8(2)
C(7)-O(1)-C(4)-C(2)	-127.7(4)
C(7)-O(1)-C(4)-C(3)	56.4(5)
C(1)-C(3)-C(4)-O(1)	176.7(4)
O(2)-C(3)-C(4)-O(1)	1.3(6)
C(1)-C(3)-C(4)-C(2)	0.6(5)
O(2)-C(3)-C(4)-C(2)	-174.9(3)
O(1)-C(4)-C(2)-C(2)#1	2.2(7)
C(3)-C(4)-C(2)-C(2)#1	178.5(5)
O(1)-C(4)-C(2)-S(2)	-175.7(3)

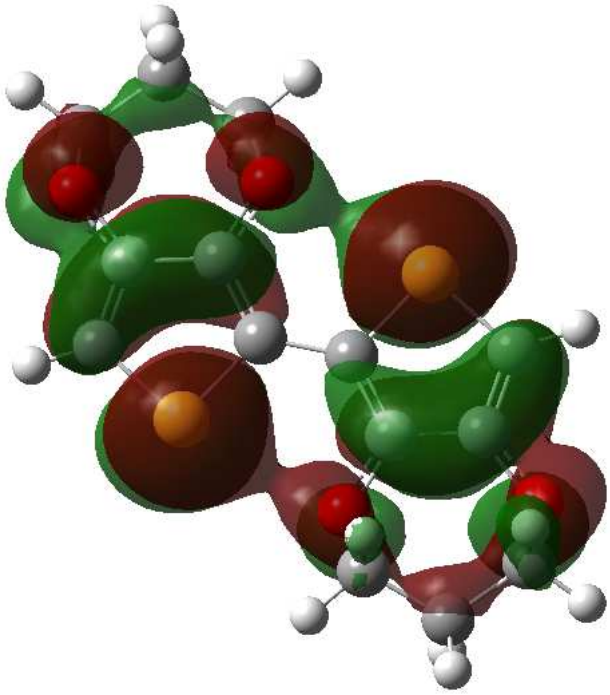
C(3)-C(4)-C(2)-S(2)	0.6(4)
C(1)-S(2)-C(2)-C(4)	-1.3(3)
C(1)-S(2)-C(2)-C(2)#1	-179.3(4)
C(3)-O(2)-C(6)-C(5)	74.7(4)
C(7)-C(5)-C(6)-O(2)	-68.8(4)
C(9)-C(5)-C(6)-O(2)	53.4(4)
C(14)-C(5)-C(6)-O(2)	176.2(3)
C(4)-O(1)-C(7)-C(5)	-78.3(4)
C(6)-C(5)-C(7)-O(1)	70.6(4)
C(9)-C(5)-C(7)-O(1)	-53.2(4)
C(14)-C(5)-C(7)-O(1)	-175.6(3)
C(7)-C(5)-C(9)-C(10)	-177.2(4)
C(6)-C(5)-C(9)-C(10)	59.9(5)
C(14)-C(5)-C(9)-C(10)	-58.5(5)
C(7)-C(5)-C(14)-C(15)	62.5(5)
C(6)-C(5)-C(14)-C(15)	-180.0(4)
C(9)-C(5)-C(14)-C(15)	-57.7(5)
C(5)-C(14)-C(15)-C(16)	-179.3(4)
C(5)-C(9)-C(10)-C(11)	-177.5(5)
C(14)-C(15)-C(16)-C(17)	177.3(4)
C(15)-C(16)-C(17)-C(18)	-179.4(4)
C(16)-C(17)-C(18)-C(19)	-175.9(5)
C(9)-C(10)-C(11)-C(12)	175.5(6)
C(10)-C(11)-C(12)-C(13)	-174.1(8)
C(11)-C(12)-C(13)-C(20)	69.7(14)

Ref.

1. B. D. Reeves, C. R. G. Grenier, A. A. Argun, A. Cirpan, T. D. McCarley, J. R. Reynolds, *Macromolecules* **2004**, *37*, 7559-7569.
2. Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G.

A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

(a)



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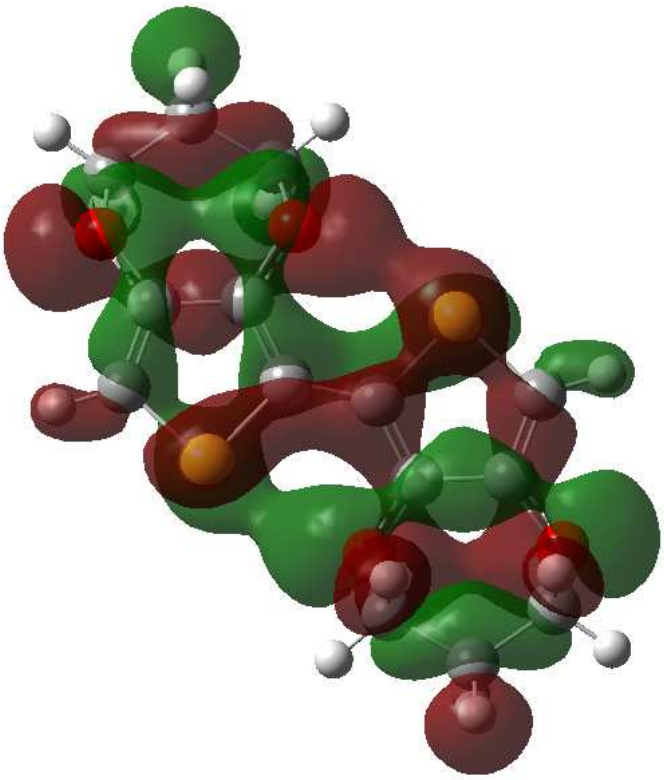


Figure S1. (a) HOMO-2 and (b) HOMO-5 of ProDOT dimer calculated at the B3LYP/6-31G(d,p) level.

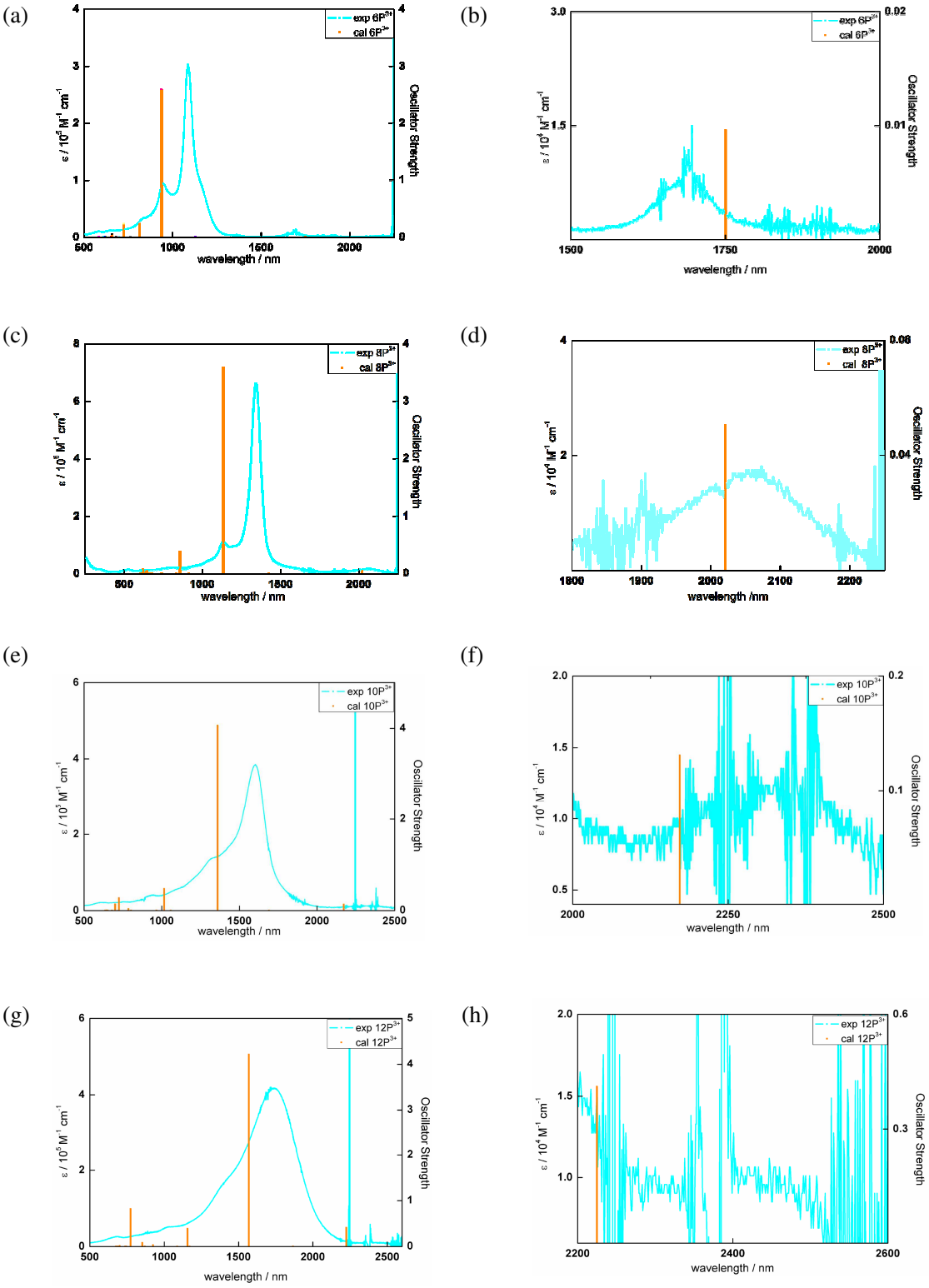


Figure S2. Observed UV-vis-NIR spectra of $n\mathbf{P}_{\mathbf{Hex}}^{3+}$ and calculated excitation energy of $n\mathbf{P}_{\mathbf{H}}^{3+}$ at the TD-B3LYP/6-31G(d) level ((a) (b) n = 6, (c) (d) n = 8, (e) (f) n = 10, and (g) (h) n = 12). The heights of the calculated spectra reflect the calculated oscillator strengths.

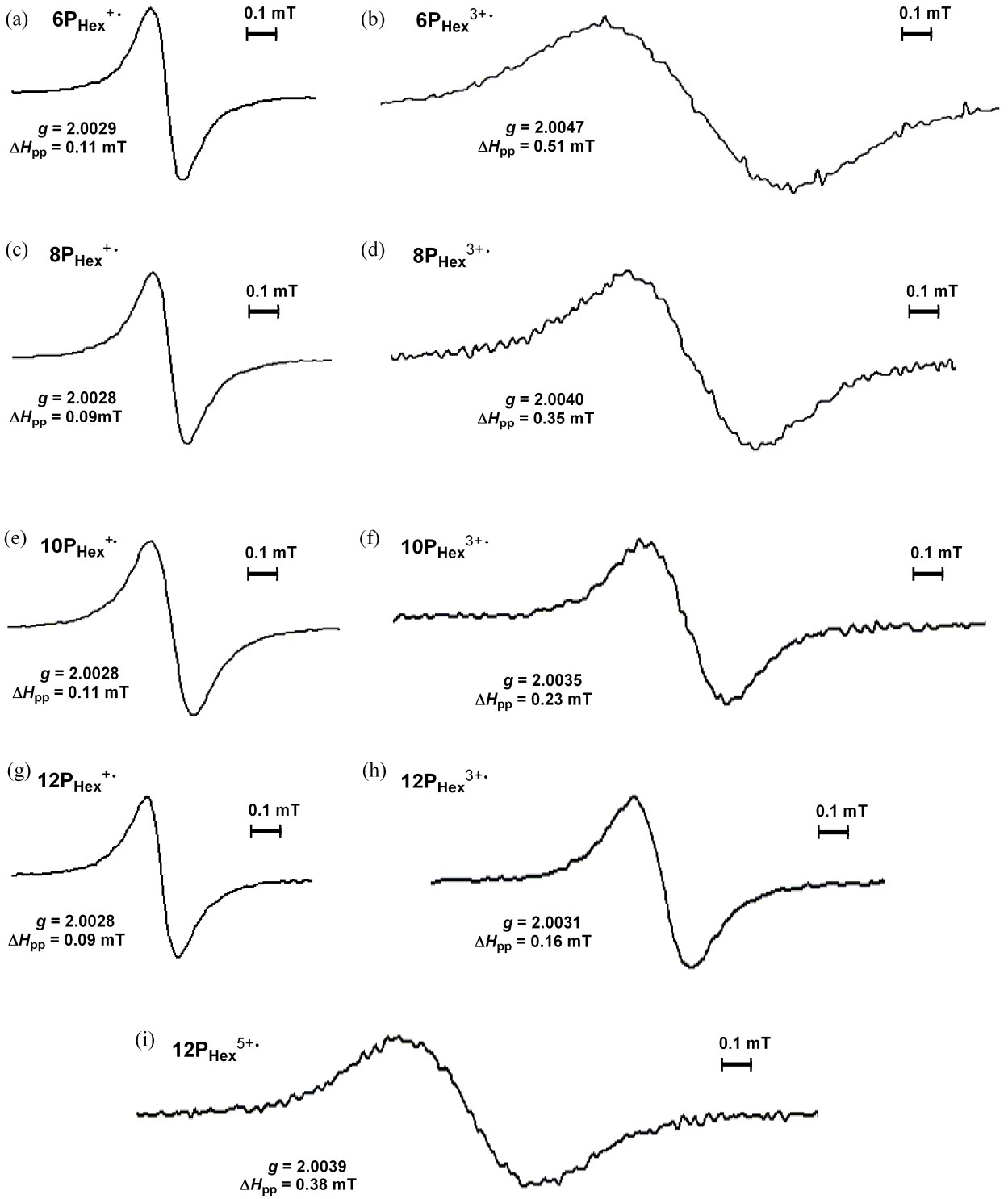
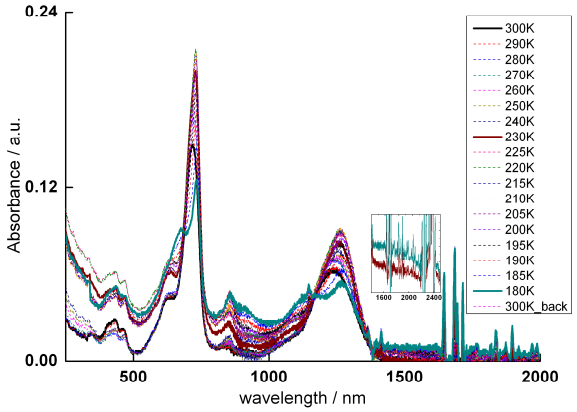
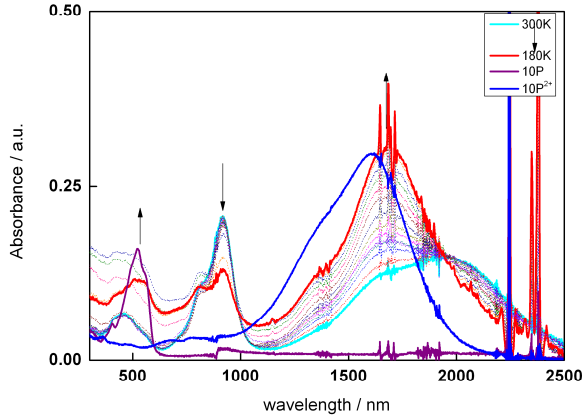


Figure S3. ESR spectra of (a) $\mathbf{6P_{Hex}^{+\cdot}}$, (b) $\mathbf{6P_{Hex}^{3+\cdot}}$, (c) $\mathbf{8P_{Hex}^{+\cdot}}$, (d) $\mathbf{8P_{Hex}^{3+\cdot}}$, (e) $\mathbf{10P_{Hex}^{+\cdot}}$, (f) $\mathbf{10P_{Hex}^{3+\cdot}}$, (g) $\mathbf{12P_{Hex}^{+\cdot}}$, (h) $\mathbf{12P_{Hex}^{3+\cdot}}$, and (i) $\mathbf{12P_{Hex}^{5+\cdot}}$, generated by the reaction of the corresponding neutral species with $SbCl_5$ in CH_2Cl_2 solutions at room temperature.

(a)



(b)



(c)

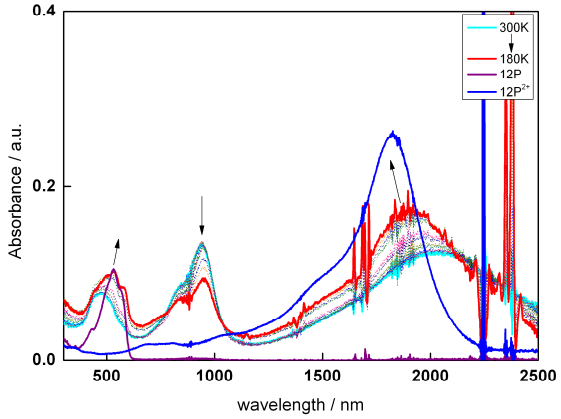


Figure S4. Change in absorption spectra upon cooling of CH_2Cl_2 solutions of (a) $\mathbf{4P_{Hex}}^{+\cdot}$ (33.2 μM), (b) $\mathbf{10P_{Hex}}^{+\cdot}$ (16.9 μM), and (c) $\mathbf{12P_{Hex}}^{+\cdot}$ (16.5 μM) generated by the reaction of the corresponding neutral species with 1.5 equivalents of $SbCl_5$.

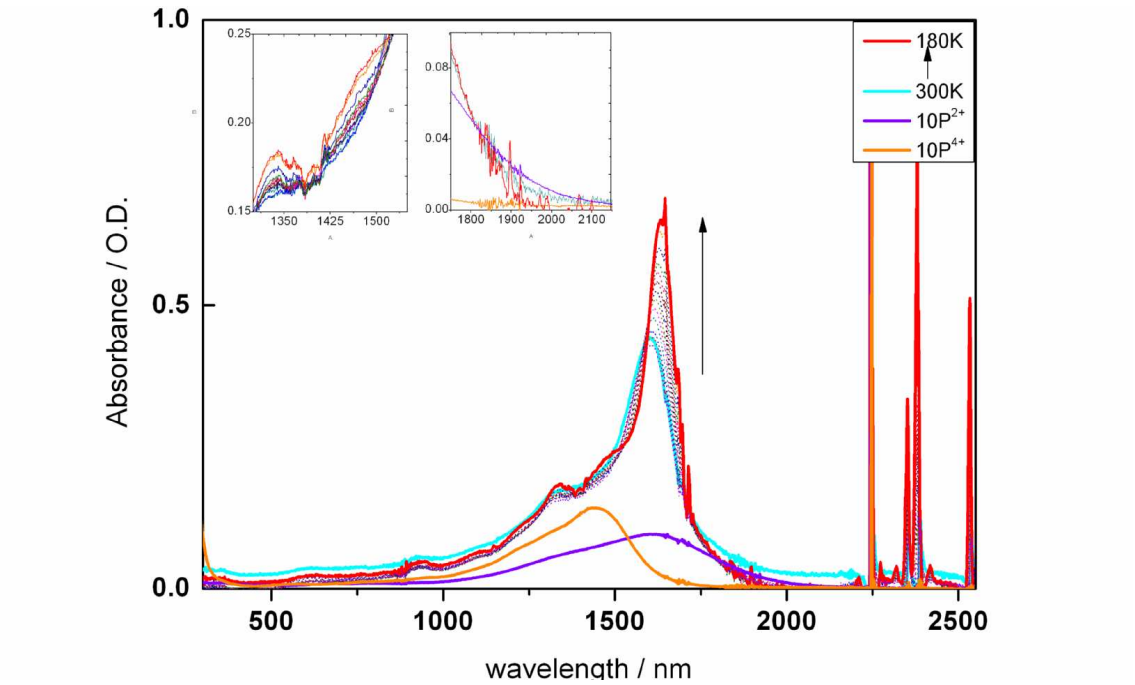
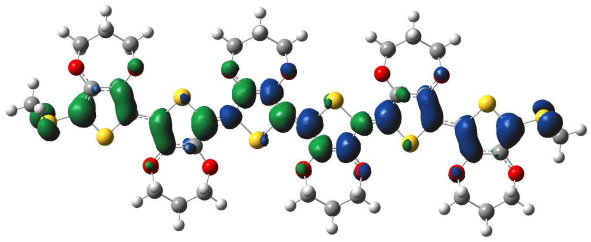
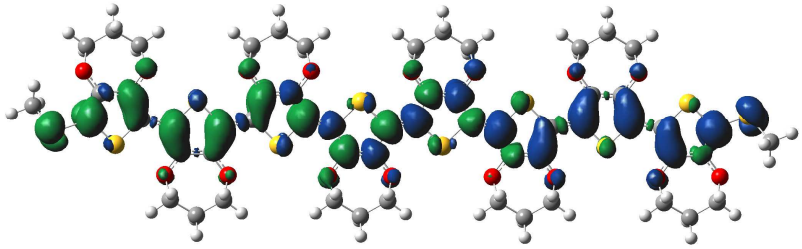


Figure S5. Change in absorption spectra upon cooling of CH_2Cl_2 solutions of (a) $\mathbf{10P_{Hex}}^{3+}$ generated by the reaction of $\mathbf{10P_{Hex}}$ with 4.5 equivalents of $SbCl_5$.

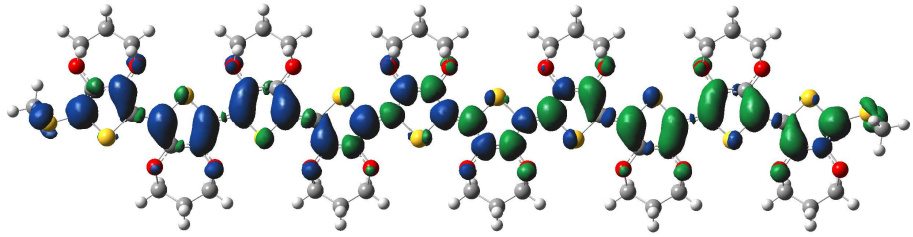
(a)



(b)



(c)



(d)

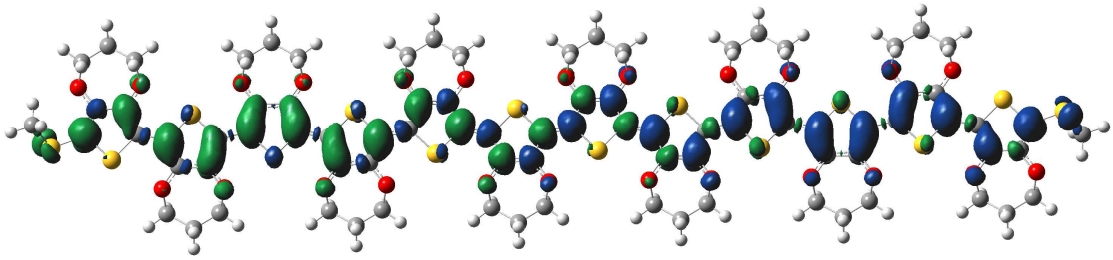
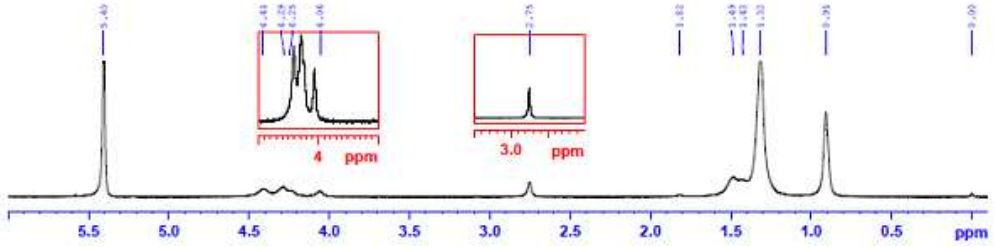


Figure S6. Spin distributions (isoval = 0.0008) of the singlet biradicals of (a) $\mathbf{6P_H}^{2+}$, (b) $\mathbf{8P_H}^{2+}$, (c) $\mathbf{10P_H}^{2+}$, and (d) $\mathbf{12P_H}^{2+}$ at the UB3LYP/6-31G(d,p) level.

(a)



(b)

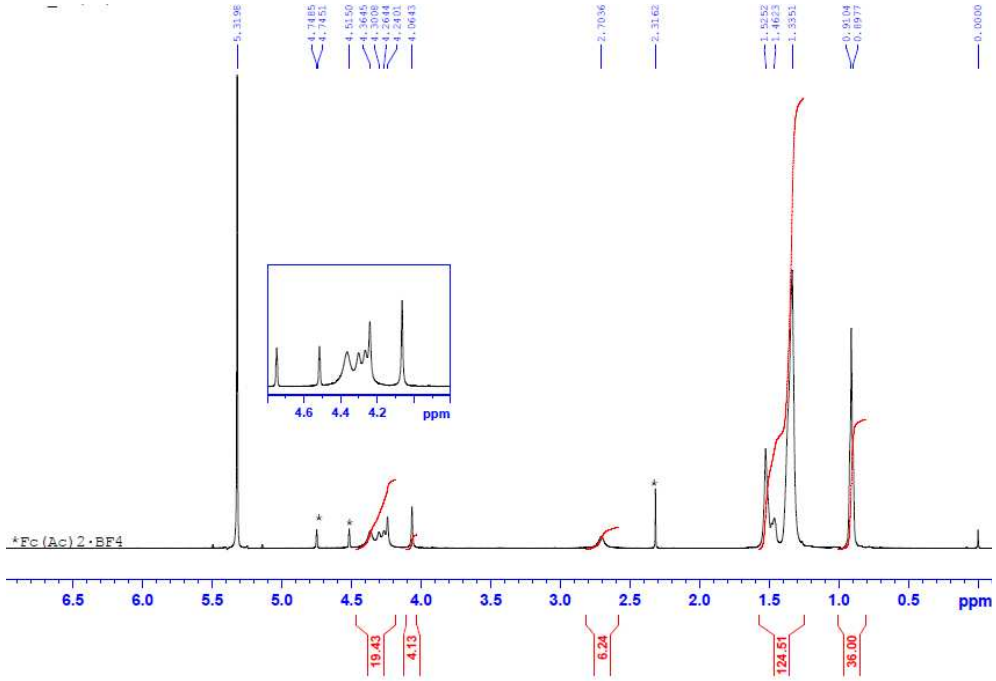
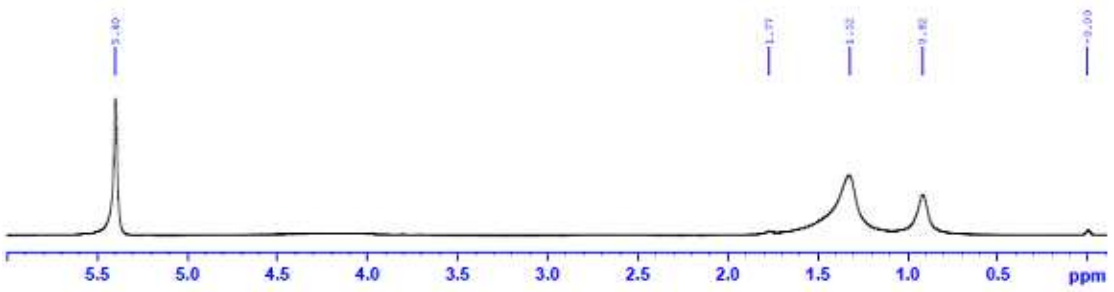
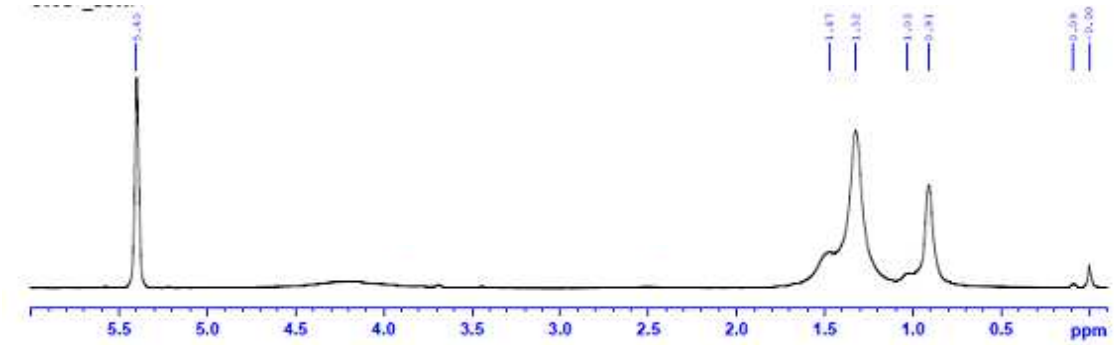


Figure S7. ^{1}H NMR spectra of (a) $\mathbf{6P_{Hex}}^{2+}$ at 210 K and (d) $\mathbf{6P_{Hex}}^{2+}$ at room temperature in the presence of $Fe(C_5H_4Ac)_2{\cdot}AgBF_4$ in CD_2Cl_2.

(a)



(b)



(c)

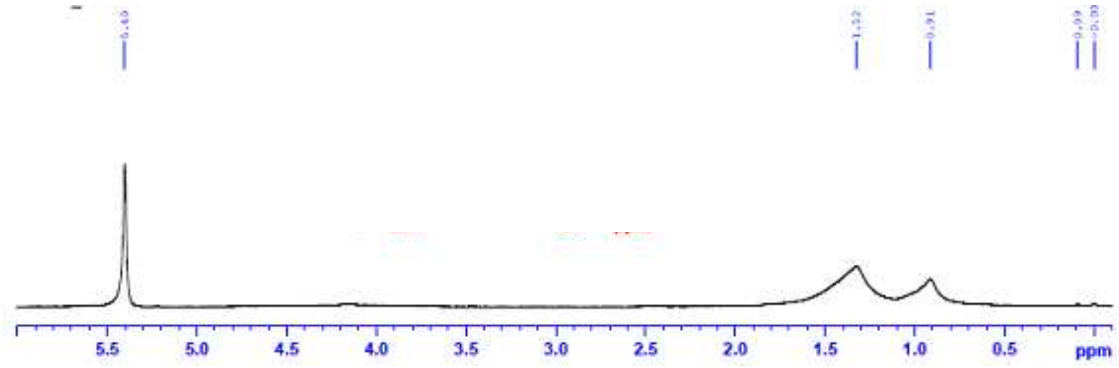


Figure S8. ^{1}H NMR spectra of (a) **8P$_{Hex}^{2+}$**, (b) **10P$_{Hex}^{2+}$**, and (c) **12P$_{Hex}^{2+}$** at 210 K and in CD_2Cl_2.

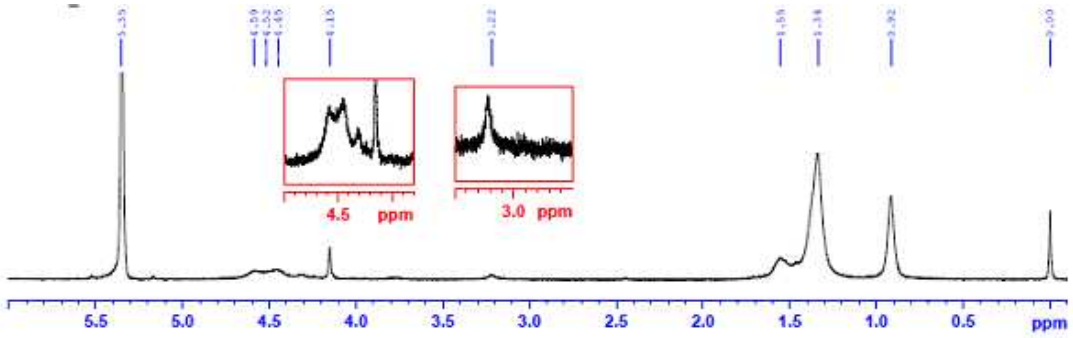


Figure S9. ^{1}H NMR spectra of $\mathbf{10P_{Hex}}^{4+}$ at 260 K and in CD_2Cl_2.

Table S4. Cartesian coordinate of optimized geometry of **11** at the RB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.179306	2.371770	0.000892
2	1	0	2.636523	3.350088	0.043926
3	6	0	2.810849	1.179896	-0.213810
4	6	0	1.898260	0.070002	-0.220672
5	6	0	0.580177	0.430797	-0.015390
6	16	0	0.464050	2.177807	0.178454
7	8	0	4.152783	1.088376	-0.470415
8	8	0	2.252309	-1.226586	-0.482877
9	6	0	4.896986	0.191822	0.362652
10	1	0	4.662600	0.390407	1.419125
11	1	0	5.943684	0.457811	0.189062
12	6	0	4.668889	-1.281032	0.026670
13	1	0	5.395140	-1.878981	0.596135
14	1	0	4.872481	-1.444169	-1.038329
15	6	0	3.269870	-1.795000	0.356030
16	1	0	3.020391	-1.608643	1.410618
17	1	0	3.207618	-2.871071	0.173351
18	6	0	-2.179306	-2.371770	-0.000892
19	1	0	-2.636523	-3.350088	-0.043926
20	6	0	-2.810849	-1.179896	0.213810
21	6	0	-1.898260	-0.070002	0.220672
22	6	0	-0.580177	-0.430797	0.015390
23	16	0	-0.464050	-2.177807	-0.178454
24	8	0	-4.152783	-1.088376	0.470415
25	8	0	-2.252309	1.226586	0.482877
26	6	0	-4.896986	-0.191822	-0.362652
27	1	0	-4.662600	-0.390407	-1.419125
28	1	0	-5.943684	-0.457811	-0.189062
29	6	0	-4.668889	1.281032	-0.026670
30	1	0	-5.395140	1.878981	-0.596135
31	1	0	-4.872481	1.444169	1.038329

32	6	0	-3.269870	1.795000	-0.356030
33	1	0	-3.020391	1.608643	-1.410618
34	1	0	-3.207618	2.871071	-0.173351

HF= -1639.1195802 hartree

Table S5. Cartesian coordinate of optimized geometry of **6P**$_{\mathbf{Hex}}^{2+}$ (S) at the RB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.687468	-0.106565	-0.008581
2	6	0	-1.342099	-1.367652	-0.164187
3	6	0	-2.729219	-1.282499	-0.161048
4	6	0	-3.220111	0.049504	-0.002994
5	16	0	-1.881671	1.194977	0.146271
6	8	0	-3.618329	-2.278239	-0.384255
7	6	0	-3.451316	-3.549006	0.280363
8	6	0	-2.223608	-4.316927	-0.187470
9	6	0	-0.911562	-3.706827	0.282706
10	8	0	-0.583703	-2.465053	-0.379323
11	1	0	-3.421648	-3.379901	1.365376
12	1	0	-4.365570	-4.092016	0.035082
13	1	0	-2.286342	-5.333684	0.223140
14	1	0	-2.228337	-4.405719	-1.279781
15	1	0	-0.069846	-4.357509	0.039899
16	1	0	-0.922447	-3.533863	1.367287
17	6	0	-4.561773	0.432666	0.021053
18	6	0	-5.054428	1.759993	0.171474
19	6	0	-6.448452	1.841707	0.181254
20	6	0	-7.087024	0.583207	0.037943
21	16	0	-5.910357	-0.714119	-0.111553
22	8	0	-4.172982	2.763666	0.362239
23	6	0	-4.368473	4.034962	-0.303347
24	6	0	-5.599200	4.795888	0.167239
25	6	0	-6.911301	4.169313	-0.281867

26	8	0	-7.209054	2.938555	0.410777
27	1	0	-4.404992	3.856928	-1.386302
28	1	0	-3.456818	4.587170	-0.069196
29	1	0	-5.544548	5.807853	-0.256148
30	1	0	-5.586507	4.898556	1.258269
31	1	0	-7.756041	4.816318	-0.040337
32	1	0	-6.911392	3.979228	-1.363718
33	6	0	-8.479531	0.365710	0.017155
34	6	0	-9.140972	-0.873302	-0.115188
35	6	0	-10.554092	-0.770459	-0.129620
36	6	0	-10.987173	0.551665	-0.017558
37	16	0	-9.663309	1.676586	0.085195
38	8	0	-11.438655	-1.784505	-0.302089
39	6	0	-11.294106	-2.969661	0.504826
40	6	0	-10.080871	-3.805927	0.118632
41	6	0	-8.751966	-3.177095	0.510308
42	8	0	-8.410113	-1.999624	-0.262479
43	1	0	-11.258561	-2.683218	1.564755
44	1	0	-12.216587	-3.525431	0.327163
45	1	0	-10.154284	-4.772255	0.635767
46	1	0	-10.097202	-4.010516	-0.957965
47	1	0	-7.924450	-3.860717	0.312525
48	1	0	-8.740211	-2.908072	1.574777
49	16	0	-12.607241	1.191959	0.108144
50	6	0	0.687468	0.106565	0.008581
51	6	0	1.342099	1.367652	0.164187
52	6	0	2.729219	1.282499	0.161048
53	6	0	3.220111	-0.049504	0.002994
54	16	0	1.881671	-1.194977	-0.146271
55	8	0	3.618329	2.278239	0.384255
56	6	0	3.451316	3.549006	-0.280363
57	6	0	2.223608	4.316927	0.187470
58	6	0	0.911562	3.706827	-0.282706
59	8	0	0.583703	2.465053	0.379323
60	1	0	3.421648	3.379901	-1.365376
61	1	0	4.365570	4.092016	-0.035082

62	1	0	2.286342	5.333684	-0.223140
63	1	0	2.228337	4.405719	1.279781
64	1	0	0.069846	4.357509	-0.039899
65	1	0	0.922447	3.533863	-1.367287
66	6	0	4.561773	-0.432666	-0.021053
67	6	0	5.054428	-1.759993	-0.171474
68	6	0	6.448452	-1.841707	-0.181254
69	6	0	7.087024	-0.583207	-0.037943
70	16	0	5.910357	0.714119	0.111553
71	8	0	4.172982	-2.763666	-0.362239
72	6	0	4.368473	-4.034962	0.303347
73	6	0	5.599200	-4.795888	-0.167239
74	6	0	6.911301	-4.169313	0.281867
75	8	0	7.209054	-2.938555	-0.410777
76	1	0	4.404992	-3.856928	1.386302
77	1	0	3.456818	-4.587170	0.069196
78	1	0	5.544548	-5.807853	0.256148
79	1	0	5.586507	-4.898556	-1.258269
80	1	0	7.756041	-4.816318	0.040337
81	1	0	6.911392	-3.979228	1.363718
82	6	0	8.479531	-0.365710	-0.017155
83	6	0	9.140972	0.873302	0.115188
84	6	0	10.554092	0.770459	0.129620
85	6	0	10.987173	-0.551665	0.017558
86	16	0	9.663309	-1.676586	-0.085195
87	8	0	11.438655	1.784505	0.302089
88	6	0	11.294106	2.969661	-0.504826
89	6	0	10.080871	3.805927	-0.118632
90	6	0	8.751966	3.177095	-0.510308
91	8	0	8.410113	1.999624	0.262479
92	1	0	11.258561	2.683218	-1.564755
93	1	0	12.216587	3.525431	-0.327163
94	1	0	10.154284	4.772255	-0.635767
95	1	0	10.097202	4.010516	0.957965
96	1	0	7.924450	3.860717	-0.312525
97	1	0	8.740211	2.908072	-1.574777

98	16	0	12.607241	-1.191959	-0.108144
99	6	0	-13.551053	0.272979	-1.172750
100	1	0	-13.551907	-0.796052	-0.969218
101	1	0	-13.140048	0.480028	-2.162495
102	1	0	-14.566216	0.671994	-1.107525
103	6	0	13.551053	-0.272979	1.172750
104	1	0	13.140048	-0.480028	2.162495
105	1	0	13.551907	0.796052	0.969218
106	1	0	14.566216	-0.671994	1.107525

HF= -5789.5554583 hartree

Table S6. Cartesian coordinate of optimized geometry of **6P**$_{\mathbf{Hex}}^{\mathbf{2+}}$ (U) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.689296	-0.107732	-0.007860
2	6	0	-1.341577	-1.366521	-0.162746
3	6	0	-2.731186	-1.281222	-0.159135
4	6	0	-3.220675	0.048627	-0.001272
5	16	0	-1.881921	1.193164	0.147417
6	8	0	-3.618175	-2.279032	-0.381411
7	6	0	-3.451304	-3.546413	0.290140
8	6	0	-2.223394	-4.317005	-0.172880
9	6	0	-0.910923	-3.703142	0.291606
10	8	0	-0.585636	-2.465957	-0.379719
11	1	0	-3.422425	-3.371464	1.374216
12	1	0	-4.365373	-4.090854	0.047276
13	1	0	-2.285770	-5.330973	0.244650
14	1	0	-2.228763	-4.413138	-1.264565
15	1	0	-0.069458	-4.355294	0.051719
16	1	0	-0.920058	-3.523361	1.375113
17	6	0	-4.564252	0.433751	0.022813
18	6	0	-5.055510	1.760026	0.174575
19	6	0	-6.450271	1.842072	0.184230

20	6	0	-7.089095	0.584274	0.039132
21	16	0	-5.911335	-0.712880	-0.110951
22	8	0	-4.174354	2.764081	0.368685
23	6	0	-4.368107	4.033934	-0.299307
24	6	0	-5.598421	4.796171	0.170534
25	6	0	-6.910966	4.170532	-0.278411
26	8	0	-7.210108	2.939072	0.413137
27	1	0	-4.404662	3.854748	-1.382114
28	1	0	-3.456248	4.586151	-0.065860
29	1	0	-5.543469	5.807943	-0.253271
30	1	0	-5.585629	4.899285	1.261523
31	1	0	-7.755342	4.817763	-0.036271
32	1	0	-6.911528	3.980921	-1.360307
33	6	0	-8.481495	0.366838	0.017081
34	6	0	-9.143260	-0.872101	-0.118187
35	6	0	-10.556038	-0.769047	-0.133690
36	6	0	-10.989232	0.553346	-0.019514
37	16	0	-9.664587	1.678025	0.087003
38	8	0	-11.440800	-1.782322	-0.308084
39	6	0	-11.296149	-2.970193	0.495158
40	6	0	-10.082693	-3.805197	0.107157
41	6	0	-8.754167	-3.177408	0.501712
42	8	0	-8.412156	-1.997973	-0.267802
43	1	0	-11.261145	-2.686855	1.555932
44	1	0	-12.218543	-3.525388	0.315306
45	1	0	-10.156635	-4.773091	0.621263
46	1	0	-10.098221	-4.006507	-0.970069
47	1	0	-7.926405	-3.860375	0.302745
48	1	0	-8.743304	-2.911220	1.566911
49	16	0	-12.607874	1.195504	0.106158
50	6	0	0.689296	0.107732	0.007860
51	6	0	1.341577	1.366521	0.162746
52	6	0	2.731186	1.281222	0.159135
53	6	0	3.220675	-0.048627	0.001272
54	16	0	1.881921	-1.193164	-0.147417
55	8	0	3.618175	2.279032	0.381411

56	6	0	3.451304	3.546413	-0.290140
57	6	0	2.223394	4.317005	0.172880
58	6	0	0.910923	3.703142	-0.291606
59	8	0	0.585636	2.465957	0.379719
60	1	0	3.422425	3.371464	-1.374216
61	1	0	4.365373	4.090854	-0.047276
62	1	0	2.285770	5.330973	-0.244650
63	1	0	2.228763	4.413138	1.264565
64	1	0	0.069458	4.355294	-0.051719
65	1	0	0.920058	3.523361	-1.375113
66	6	0	4.564252	-0.433751	-0.022813
67	6	0	5.055510	-1.760026	-0.174575
68	6	0	6.450271	-1.842072	-0.184230
69	6	0	7.089095	-0.584274	-0.039132
70	16	0	5.911335	0.712880	0.110951
71	8	0	4.174354	-2.764081	-0.368685
72	6	0	4.368107	-4.033934	0.299307
73	6	0	5.598421	-4.796171	-0.170534
74	6	0	6.910966	-4.170532	0.278411
75	8	0	7.210108	-2.939072	-0.413137
76	1	0	4.404662	-3.854748	1.382114
77	1	0	3.456248	-4.586151	0.065860
78	1	0	5.543469	-5.807943	0.253271
79	1	0	5.585629	-4.899285	-1.261523
80	1	0	7.755342	-4.817763	0.036271
81	1	0	6.911528	-3.980921	1.360307
82	6	0	8.481495	-0.366838	-0.017081
83	6	0	9.143260	0.872101	0.118187
84	6	0	10.556038	0.769047	0.133690
85	6	0	10.989232	-0.553346	0.019514
86	16	0	9.664587	-1.678025	-0.087003
87	8	0	11.440800	1.782322	0.308084
88	6	0	11.296149	2.970193	-0.495158
89	6	0	10.082693	3.805197	-0.107157
90	6	0	8.754167	3.177408	-0.501712
91	8	0	8.412156	1.997973	0.267802

92	1	0	11.261145	2.686855	-1.555932
93	1	0	12.218543	3.525388	-0.315306
94	1	0	10.156635	4.773091	-0.621263
95	1	0	10.098221	4.006507	0.970069
96	1	0	7.926405	3.860375	-0.302745
97	1	0	8.743304	2.911220	-1.566911
98	16	0	12.607874	-1.195504	-0.106158
99	6	0	-13.558797	0.268525	-1.163529
100	1	0	-13.565007	-0.798403	-0.949616
101	1	0	-13.148639	0.463575	-2.156041
102	1	0	-14.571562	0.673866	-1.100124
103	6	0	13.558797	-0.268525	1.163529
104	1	0	13.148639	-0.463575	2.156041
105	1	0	13.565007	0.798403	0.949616
106	1	0	14.571562	-0.673866	1.100124

HF= -5789.5555119 hartree

Table S7. Cartesian coordinate of optimized geometry of **6P**$_{\mathbf{Hex}}^{\mathbf{2+}}$ (T) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.706400	-0.118395	-0.002531
2	6	0	-1.339514	-1.356759	-0.145411
3	6	0	-2.752468	-1.267804	-0.140459
4	6	0	-3.227417	0.043799	0.007295
5	16	0	-1.884034	1.179458	0.145571
6	8	0	-3.621990	-2.285132	-0.349014
7	6	0	-3.456803	-3.513400	0.395126
8	6	0	-2.228076	-4.311630	-0.018037
9	6	0	-0.910333	-3.665750	0.388686
10	8	0	-0.606892	-2.477378	-0.370634
11	1	0	-3.433482	-3.276896	1.467380
12	1	0	-4.369679	-4.072087	0.180686
13	1	0	-2.288501	-5.294561	0.468698

14	1	0	-2.240002	-4.482105	-1.100541
15	1	0	-0.072816	-4.333729	0.178461
16	1	0	-0.902507	-3.419366	1.459221
17	6	0	-4.588549	0.450302	0.027161
18	6	0	-5.065147	1.767545	0.188270
19	6	0	-6.467288	1.854867	0.192242
20	6	0	-7.109881	0.605350	0.029778
21	16	0	-5.923258	-0.691951	-0.126023
22	8	0	-4.186317	2.773731	0.416317
23	6	0	-4.358413	4.030131	-0.274979
24	6	0	-5.585612	4.806950	0.181527
25	6	0	-6.901802	4.191375	-0.269370
26	8	0	-7.218482	2.955320	0.413224
27	1	0	-4.390345	3.839706	-1.356409
28	1	0	-3.444774	4.580790	-0.043752
29	1	0	-5.524840	5.815880	-0.248334
30	1	0	-5.575930	4.916720	1.271889
31	1	0	-7.742355	4.842915	-0.025824
32	1	0	-6.903202	4.004084	-1.351317
33	6	0	-8.501477	0.391302	-0.006607
34	6	0	-9.169942	-0.843031	-0.178608
35	6	0	-10.579083	-0.734535	-0.206240
36	6	0	-11.011112	0.590291	-0.060770
37	16	0	-9.673686	1.708529	0.094105
38	8	0	-11.465043	-1.736541	-0.422575
39	6	0	-11.328986	-2.961122	0.328386
40	6	0	-10.111973	-3.780851	-0.078277
41	6	0	-8.789350	-3.170394	0.360015
42	8	0	-8.439620	-1.964389	-0.361222
43	1	0	-11.307154	-2.723886	1.400830
44	1	0	-12.249950	-3.505454	0.111633
45	1	0	-10.195663	-4.768851	0.394300
46	1	0	-10.112679	-3.937595	-1.162958
47	1	0	-7.958690	-3.845392	0.147009
48	1	0	-8.793644	-2.944417	1.434614
49	16	0	-12.604296	1.274132	0.043850

50	6	0	0.706400	0.118395	0.002531
51	6	0	1.339514	1.356759	0.145411
52	6	0	2.752468	1.267804	0.140459
53	6	0	3.227417	-0.043799	-0.007295
54	16	0	1.884034	-1.179458	-0.145571
55	8	0	3.621990	2.285132	0.349014
56	6	0	3.456803	3.513400	-0.395126
57	6	0	2.228076	4.311630	0.018037
58	6	0	0.910333	3.665750	-0.388686
59	8	0	0.606892	2.477378	0.370634
60	1	0	3.433482	3.276896	-1.467380
61	1	0	4.369679	4.072087	-0.180686
62	1	0	2.288501	5.294561	-0.468698
63	1	0	2.240002	4.482105	1.100541
64	1	0	0.072816	4.333729	-0.178461
65	1	0	0.902507	3.419366	-1.459221
66	6	0	4.588549	-0.450302	-0.027161
67	6	0	5.065147	-1.767545	-0.188270
68	6	0	6.467288	-1.854867	-0.192242
69	6	0	7.109881	-0.605350	-0.029778
70	16	0	5.923258	0.691951	0.126023
71	8	0	4.186317	-2.773731	-0.416317
72	6	0	4.358413	-4.030131	0.274979
73	6	0	5.585612	-4.806950	-0.181527
74	6	0	6.901802	-4.191375	0.269370
75	8	0	7.218482	-2.955320	-0.413224
76	1	0	4.390345	-3.839706	1.356409
77	1	0	3.444774	-4.580790	0.043752
78	1	0	5.524840	-5.815880	0.248334
79	1	0	5.575930	-4.916720	-1.271889
80	1	0	7.742355	-4.842915	0.025824
81	1	0	6.903202	-4.004084	1.351317
82	6	0	8.501477	-0.391302	0.006607
83	6	0	9.169942	0.843031	0.178608
84	6	0	10.579083	0.734535	0.206240
85	6	0	11.011112	-0.590291	0.060770

86	16	0	9.673686	-1.708529	-0.094105
87	8	0	11.465043	1.736541	0.422575
88	6	0	11.328986	2.961122	-0.328386
89	6	0	10.111973	3.780851	0.078277
90	6	0	8.789350	3.170394	-0.360015
91	8	0	8.439620	1.964389	0.361222
92	1	0	11.307154	2.723886	-1.400830
93	1	0	12.249950	3.505454	-0.111633
94	1	0	10.195663	4.768851	-0.394300
95	1	0	10.112679	3.937595	1.162958
96	1	0	7.958690	3.845392	-0.147009
97	1	0	8.793644	2.944417	-1.434614
98	16	0	12.604296	-1.274132	-0.043850
99	6	0	-13.697958	0.147291	-0.905185
100	1	0	-13.843657	-0.797659	-0.385942
101	1	0	-13.297397	-0.019721	-1.905635
102	1	0	-14.643841	0.690370	-0.972727
103	6	0	13.697958	-0.147291	0.905185
104	1	0	13.297397	0.019721	1.905635
105	1	0	13.843657	0.797659	0.385942
106	1	0	14.643841	-0.690370	0.972727

HF= -5789.5465535 hartree

Table S8. Cartesian coordinate of optimized geometry of **8P$_{Hex}^{2+}$** (S) at the RB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.676878	0.174172	0.012942
2	6	0	-1.206120	1.483817	0.176425
3	6	0	-2.598632	1.530652	0.182886
4	6	0	-3.215324	0.259777	0.023473
5	16	0	-1.989908	-1.004897	-0.139205
6	8	0	-3.376884	2.617386	0.412497
7	6	0	-3.105369	3.836605	-0.307160

8	6	0	-1.807206	4.507980	0.120006
9	6	0	-0.558654	3.755306	-0.319174
10	8	0	-0.355035	2.516475	0.392227
11	1	0	-3.102765	3.621905	-1.384639
12	1	0	-3.963202	4.472232	-0.079587
13	1	0	-1.776189	5.506499	-0.336788
14	1	0	-1.798245	4.645068	1.207327
15	1	0	0.339900	4.334178	-0.097342
16	1	0	-0.584355	3.545072	-1.397148
17	6	0	-4.591552	0.003980	0.007458
18	6	0	-5.210308	-1.263186	-0.150847
19	6	0	-6.605679	-1.214156	-0.146862
20	6	0	-7.127543	0.094553	0.014438
21	16	0	-5.820740	1.270441	0.166903
22	8	0	-4.435801	-2.353401	-0.366210
23	6	0	-4.723224	-3.571963	0.351920
24	6	0	-6.022283	-4.238766	-0.079206
25	6	0	-7.270214	-3.477888	0.348521
26	8	0	-7.457457	-2.246330	-0.376029
27	1	0	-4.730398	-3.354248	1.428623
28	1	0	-3.867177	-4.212236	0.130571
29	1	0	-6.057651	-5.235039	0.382219
30	1	0	-6.026647	-4.381025	-1.165895
31	1	0	-8.169767	-4.054637	0.125134
32	1	0	-7.250385	-3.261018	1.425482
33	6	0	-8.486451	0.452460	0.038574
34	6	0	-9.007888	1.756115	0.198137
35	6	0	-10.409472	1.805337	0.205855
36	6	0	-11.016507	0.543527	0.045191
37	16	0	-9.806106	-0.721115	-0.112306
38	8	0	-11.181396	2.895361	0.452400
39	6	0	-10.930661	4.104283	-0.291518
40	6	0	-9.628865	4.782983	0.113552
41	6	0	-8.380961	4.027471	-0.323120
42	8	0	-8.162647	2.794373	0.399699
43	1	0	-10.941538	3.874806	-1.365766

44	1	0	-11.787525	4.740336	-0.062220
45	1	0	-9.600587	5.774447	-0.358591
46	1	0	-9.612253	4.937113	1.198504
47	1	0	-7.482749	4.611663	-0.113837
48	1	0	-8.412128	3.803389	-1.397911
49	6	0	-12.410231	0.287604	0.023452
50	6	0	-13.041272	-0.954174	-0.140677
51	6	0	-14.461145	-0.881499	-0.182658
52	6	0	-14.924294	0.421804	-0.030841
53	16	0	-13.622164	1.563601	0.169967
54	8	0	-12.288866	-2.061370	-0.347976
55	6	0	-12.632387	-3.279751	0.347547
56	6	0	-13.922218	-3.919367	-0.147182
57	6	0	-15.177653	-3.140257	0.224470
58	8	0	-15.307053	-1.900247	-0.493062
59	1	0	-12.682614	-3.069042	1.424462
60	1	0	-11.779094	-3.934697	0.160073
61	1	0	-13.995085	-4.918758	0.303258
62	1	0	-13.877647	-4.052899	-1.234086
63	1	0	-16.071442	-3.703853	-0.051307
64	1	0	-15.210847	-2.941262	1.305276
65	16	0	-16.545323	1.065859	-0.152332
66	6	0	0.676878	-0.174172	-0.012942
67	6	0	1.206120	-1.483817	-0.176425
68	6	0	2.598632	-1.530652	-0.182886
69	6	0	3.215324	-0.259777	-0.023473
70	16	0	1.989908	1.004897	0.139205
71	8	0	3.376884	-2.617386	-0.412497
72	6	0	3.105369	-3.836605	0.307160
73	6	0	1.807206	-4.507980	-0.120006
74	6	0	0.558654	-3.755306	0.319174
75	8	0	0.355035	-2.516475	-0.392227
76	1	0	3.102765	-3.621905	1.384639
77	1	0	3.963202	-4.472232	0.079587
78	1	0	1.776189	-5.506499	0.336788
79	1	0	1.798245	-4.645068	-1.207327

80	1	0	-0.339900	-4.334178	0.097342
81	1	0	0.584355	-3.545072	1.397148
82	6	0	4.591552	-0.003980	-0.007458
83	6	0	5.210308	1.263186	0.150847
84	6	0	6.605679	1.214156	0.146862
85	6	0	7.127543	-0.094553	-0.014438
86	16	0	5.820740	-1.270441	-0.166903
87	8	0	4.435801	2.353401	0.366210
88	6	0	4.723224	3.571963	-0.351920
89	6	0	6.022283	4.238766	0.079206
90	6	0	7.270214	3.477888	-0.348521
91	8	0	7.457457	2.246330	0.376029
92	1	0	4.730398	3.354248	-1.428623
93	1	0	3.867177	4.212236	-0.130571
94	1	0	6.057651	5.235039	-0.382219
95	1	0	6.026647	4.381025	1.165895
96	1	0	8.169767	4.054637	-0.125134
97	1	0	7.250385	3.261018	-1.425482
98	6	0	8.486451	-0.452460	-0.038574
99	6	0	9.007888	-1.756115	-0.198137
100	6	0	10.409472	-1.805337	-0.205855
101	6	0	11.016507	-0.543527	-0.045191
102	16	0	9.806106	0.721115	0.112306
103	8	0	11.181396	-2.895361	-0.452400
104	6	0	10.930661	-4.104283	0.291518
105	6	0	9.628865	-4.782983	-0.113552
106	6	0	8.380961	-4.027471	0.323120
107	8	0	8.162647	-2.794373	-0.399699
108	1	0	10.941538	-3.874806	1.365766
109	1	0	11.787525	-4.740336	0.062220
110	1	0	9.600587	-5.774447	0.358591
111	1	0	9.612253	-4.937113	-1.198504
112	1	0	7.482749	-4.611663	0.113837
113	1	0	8.412128	-3.803389	1.397911
114	6	0	12.410231	-0.287604	-0.023452
115	6	0	13.041272	0.954174	0.140677

116	6	0	14.461145	0.881499	0.182658
117	6	0	14.924294	-0.421804	0.030841
118	16	0	13.622164	-1.563601	-0.169967
119	8	0	12.288866	2.061370	0.347976
120	6	0	12.632387	3.279751	-0.347547
121	6	0	13.922218	3.919367	0.147182
122	6	0	15.177653	3.140257	-0.224470
123	8	0	15.307053	1.900247	0.493062
124	1	0	12.682614	3.069042	-1.424462
125	1	0	11.779094	3.934697	-0.160073
126	1	0	13.995085	4.918758	-0.303258
127	1	0	13.877647	4.052899	1.234086
128	1	0	16.071442	3.703853	0.051307
129	1	0	15.210847	2.941262	-1.305276
130	16	0	16.545323	-1.065859	0.152332
131	6	0	-17.574153	-0.172110	0.726300
132	1	0	-17.215774	-0.310806	1.748455
133	1	0	-17.591042	-1.117077	0.185624
134	1	0	-18.577002	0.261369	0.750654
135	6	0	17.574153	0.172110	-0.726300
136	1	0	17.591042	1.117077	-0.185624
137	1	0	17.215774	0.310806	-1.748455
138	1	0	18.577002	-0.261369	-0.750654

HF= -7427.5156681 hartree

Table S9. Cartesian coordinate of optimized geometry of **8P$_{Hex}^{2+}$** (U) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.683425	0.180375	0.012734
2	6	0	-1.203781	1.480323	0.174310
3	6	0	-2.606963	1.527802	0.182718
4	6	0	-3.217129	0.265722	0.026336
5	16	0	-1.992061	-0.996121	-0.135387

6	8	0	-3.375630	2.622698	0.410660
7	6	0	-3.107200	3.825952	-0.337269
8	6	0	-1.806515	4.506610	0.068000
9	6	0	-0.558162	3.741303	-0.351022
10	8	0	-0.360505	2.521863	0.393171
11	1	0	-3.111204	3.588200	-1.409850
12	1	0	-3.962988	4.467810	-0.119048
13	1	0	-1.776298	5.492792	-0.415092
14	1	0	-1.795343	4.672187	1.151330
15	1	0	0.340111	4.325660	-0.141868
16	1	0	-0.581503	3.505649	-1.423869
17	6	0	-4.603602	0.001709	0.013032
18	6	0	-5.216336	-1.260243	-0.145967
19	6	0	-6.617094	-1.210742	-0.140465
20	6	0	-7.136913	0.093745	0.023162
21	16	0	-5.826126	1.267170	0.175210
22	8	0	-4.446524	-2.354480	-0.372013
23	6	0	-4.724352	-3.562927	0.364080
24	6	0	-6.024279	-4.236923	-0.054491
25	6	0	-7.272810	-3.474161	0.368001
26	8	0	-7.464981	-2.246133	-0.363659
27	1	0	-4.726830	-3.333584	1.438538
28	1	0	-3.868809	-4.205311	0.146336
29	1	0	-6.058433	-5.228115	0.417919
30	1	0	-6.031113	-4.391037	-1.139553
31	1	0	-8.171729	-4.053646	0.149116
32	1	0	-7.253072	-3.249531	1.443245
33	6	0	-8.498009	0.454856	0.049882
34	6	0	-9.017487	1.758239	0.215653
35	6	0	-10.418904	1.807664	0.223976
36	6	0	-11.027615	0.546021	0.057450
37	16	0	-9.814361	-0.718581	-0.105510
38	8	0	-11.191455	2.895571	0.469814
39	6	0	-10.934630	4.112008	-0.261804
40	6	0	-9.632399	4.785028	0.150502
41	6	0	-8.385160	4.030671	-0.290400

42	8	0	-8.171154	2.794651	0.427049
43	1	0	-10.944381	3.891395	-1.337820
44	1	0	-11.791073	4.746923	-0.028136
45	1	0	-9.603369	5.780079	-0.313944
46	1	0	-9.616515	4.930878	1.236608
47	1	0	-7.486422	4.612667	-0.077323
48	1	0	-8.416029	3.812904	-1.366593
49	6	0	-12.419268	0.291732	0.032931
50	6	0	-13.052152	-0.950884	-0.137757
51	6	0	-14.470563	-0.877764	-0.176960
52	6	0	-14.933824	0.426121	-0.016099
53	16	0	-13.630168	1.567920	0.188400
54	8	0	-12.298911	-2.055190	-0.352132
55	6	0	-12.641906	-3.281375	0.330415
56	6	0	-13.931883	-3.915663	-0.170312
57	6	0	-15.186740	-3.141052	0.211798
58	8	0	-15.317956	-1.893003	-0.492355
59	1	0	-12.691382	-3.081908	1.409468
60	1	0	-11.788382	-3.933596	0.135182
61	1	0	-14.004181	-4.919894	0.269229
62	1	0	-13.888517	-4.037433	-1.258635
63	1	0	-16.081130	-3.701334	-0.068487
64	1	0	-15.218144	-2.953065	1.294569
65	16	0	-16.551344	1.075429	-0.128365
66	6	0	0.683425	-0.180375	-0.012734
67	6	0	1.203781	-1.480323	-0.174310
68	6	0	2.606963	-1.527802	-0.182718
69	6	0	3.217129	-0.265722	-0.026336
70	16	0	1.992061	0.996121	0.135387
71	8	0	3.375630	-2.622698	-0.410660
72	6	0	3.107200	-3.825952	0.337269
73	6	0	1.806515	-4.506610	-0.068000
74	6	0	0.558162	-3.741303	0.351022
75	8	0	0.360505	-2.521863	-0.393171
76	1	0	3.111204	-3.588200	1.409850
77	1	0	3.962988	-4.467810	0.119048

78	1	0	1.776298	-5.492792	0.415092
79	1	0	1.795343	-4.672187	-1.151330
80	1	0	-0.340111	-4.325660	0.141868
81	1	0	0.581503	-3.505649	1.423869
82	6	0	4.603602	-0.001709	-0.013032
83	6	0	5.216336	1.260243	0.145967
84	6	0	6.617094	1.210742	0.140465
85	6	0	7.136913	-0.093745	-0.023162
86	16	0	5.826126	-1.267170	-0.175210
87	8	0	4.446524	2.354480	0.372013
88	6	0	4.724352	3.562927	-0.364080
89	6	0	6.024279	4.236923	0.054491
90	6	0	7.272810	3.474161	-0.368001
91	8	0	7.464981	2.246133	0.363659
92	1	0	4.726830	3.333584	-1.438538
93	1	0	3.868809	4.205311	-0.146336
94	1	0	6.058433	5.228115	-0.417919
95	1	0	6.031113	4.391037	1.139553
96	1	0	8.171729	4.053646	-0.149116
97	1	0	7.253072	3.249531	-1.443245
98	6	0	8.498009	-0.454856	-0.049882
99	6	0	9.017487	-1.758239	-0.215653
100	6	0	10.418904	-1.807664	-0.223976
101	6	0	11.027615	-0.546021	-0.057450
102	16	0	9.814361	0.718581	0.105510
103	8	0	11.191455	-2.895571	-0.469814
104	6	0	10.934630	-4.112008	0.261804
105	6	0	9.632399	-4.785028	-0.150502
106	6	0	8.385160	-4.030671	0.290400
107	8	0	8.171154	-2.794651	-0.427049
108	1	0	10.944381	-3.891395	1.337820
109	1	0	11.791073	-4.746923	0.028136
110	1	0	9.603369	-5.780079	0.313944
111	1	0	9.616515	-4.930878	-1.236608
112	1	0	7.486422	-4.612667	0.077323
113	1	0	8.416029	-3.812904	1.366593

114	6	0	12.419268	-0.291732	-0.032931
115	6	0	13.052152	0.950884	0.137757
116	6	0	14.470563	0.877764	0.176960
117	6	0	14.933824	-0.426121	0.016099
118	16	0	13.630168	-1.567920	-0.188400
119	8	0	12.298911	2.055190	0.352132
120	6	0	12.641906	3.281375	-0.330415
121	6	0	13.931883	3.915663	0.170312
122	6	0	15.186740	3.141052	-0.211798
123	8	0	15.317956	1.893003	0.492355
124	1	0	12.691382	3.081908	-1.409468
125	1	0	11.788382	3.933596	-0.135182
126	1	0	14.004181	4.919894	-0.269229
127	1	0	13.888517	4.037433	1.258635
128	1	0	16.081130	3.701334	0.068487
129	1	0	15.218144	2.953065	-1.294569
130	16	0	16.551344	-1.075429	0.128365
131	6	0	-17.597091	-0.190712	0.687557
132	1	0	-17.248823	-0.375357	1.705885
133	1	0	-17.617036	-1.111681	0.107382
134	1	0	-18.595884	0.251306	0.721841
135	6	0	17.597091	0.190712	-0.687557
136	1	0	17.617036	1.111681	-0.107382
137	1	0	17.248823	0.375357	-1.705885
138	1	0	18.595884	-0.251306	-0.721841

HF= -7427.5171736 hartree

Table S10. Cartesian coordinate of optimized geometry of **8P$_{Hex}^{2+}$** (T) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.690825	0.187796	0.013598
2	6	0	-1.201022	1.477558	0.171925
3	6	0	-2.616539	1.525824	0.185012

4	6	0	-3.219484	0.273141	0.035253
5	16	0	-1.994913	-0.986030	-0.125826
6	8	0	-3.374440	2.630139	0.410364
7	6	0	-3.110121	3.813797	-0.370301
8	6	0	-1.806023	4.504289	0.007873
9	6	0	-0.558293	3.725498	-0.389562
10	8	0	-0.365883	2.529215	0.390742
11	1	0	-3.122749	3.549309	-1.436506
12	1	0	-3.963147	4.463058	-0.162545
13	1	0	-1.777531	5.475602	-0.504800
14	1	0	-1.790863	4.702240	1.085721
15	1	0	0.339812	4.316061	-0.196513
16	1	0	-0.580631	3.461012	-1.455806
17	6	0	-4.617770	-0.000931	0.027510
18	6	0	-5.223716	-1.257243	-0.130317
19	6	0	-6.631021	-1.207251	-0.121253
20	6	0	-7.148156	0.092222	0.044522
21	16	0	-5.832474	1.263153	0.193976
22	8	0	-4.459904	-2.356201	-0.368985
23	6	0	-4.725032	-3.552772	0.387993
24	6	0	-6.026762	-4.234965	-0.012954
25	6	0	-7.275191	-3.469653	0.405168
26	8	0	-7.474422	-2.246756	-0.335984
27	1	0	-4.719752	-3.309924	1.459632
28	1	0	-3.870521	-4.197552	0.172592
29	1	0	-6.058514	-5.219779	0.472893
30	1	0	-6.038630	-4.403602	-1.095809
31	1	0	-8.173790	-4.052581	0.194121
32	1	0	-7.253368	-3.234635	1.477996
33	6	0	-8.511989	0.457499	0.074699
34	6	0	-9.028844	1.760361	0.247981
35	6	0	-10.430429	1.810206	0.255583
36	6	0	-11.041063	0.549192	0.081009
37	16	0	-9.824226	-0.715567	-0.087114
38	8	0	-11.203780	2.895741	0.499759
39	6	0	-10.938180	4.121446	-0.215799

40	6	0	-9.635894	4.786968	0.207414
41	6	0	-8.388919	4.034231	-0.237408
42	8	0	-8.181250	2.794202	0.472823
43	1	0	-10.945036	3.912077	-1.293958
44	1	0	-11.794309	4.755041	0.022201
45	1	0	-9.605169	5.786601	-0.246937
46	1	0	-9.622414	4.922048	1.294941
47	1	0	-7.489829	4.613308	-0.018000
48	1	0	-8.417901	3.824989	-1.315468
49	6	0	-12.430208	0.296974	0.049818
50	6	0	-13.065317	-0.946320	-0.130250
51	6	0	-14.481713	-0.872225	-0.170971
52	6	0	-14.945565	0.432559	-0.001936
53	16	0	-13.639820	1.574185	0.210716
54	8	0	-12.311457	-2.048107	-0.349702
55	6	0	-12.654935	-3.281108	0.321047
56	6	0	-13.944293	-3.910605	-0.186859
57	6	0	-15.198982	-3.139037	0.201098
58	8	0	-15.329293	-1.884334	-0.492798
59	1	0	-12.705327	-3.091285	1.401742
60	1	0	-11.800894	-3.930786	0.120300
61	1	0	-14.017462	-4.918493	0.243971
62	1	0	-13.899908	-4.023200	-1.276110
63	1	0	-16.093791	-3.695780	-0.084519
64	1	0	-15.231020	-2.959387	1.285176
65	16	0	-16.556840	1.090680	-0.106632
66	6	0	0.690825	-0.187796	-0.013598
67	6	0	1.201022	-1.477558	-0.171925
68	6	0	2.616539	-1.525824	-0.185012
69	6	0	3.219484	-0.273141	-0.035253
70	16	0	1.994913	0.986030	0.125826
71	8	0	3.374440	-2.630139	-0.410364
72	6	0	3.110121	-3.813797	0.370301
73	6	0	1.806023	-4.504289	-0.007873
74	6	0	0.558293	-3.725498	0.389562
75	8	0	0.365883	-2.529215	-0.390742

76	1	0	3.122749	-3.549309	1.436506
77	1	0	3.963147	-4.463058	0.162545
78	1	0	1.777531	-5.475602	0.504800
79	1	0	1.790863	-4.702240	-1.085721
80	1	0	-0.339812	-4.316061	0.196513
81	1	0	0.580631	-3.461012	1.455806
82	6	0	4.617770	0.000931	-0.027510
83	6	0	5.223716	1.257243	0.130317
84	6	0	6.631021	1.207251	0.121253
85	6	0	7.148156	-0.092222	-0.044522
86	16	0	5.832474	-1.263153	-0.193976
87	8	0	4.459904	2.356201	0.368985
88	6	0	4.725032	3.552772	-0.387993
89	6	0	6.026762	4.234965	0.012954
90	6	0	7.275191	3.469653	-0.405168
91	8	0	7.474422	2.246756	0.335984
92	1	0	4.719752	3.309924	-1.459632
93	1	0	3.870521	4.197552	-0.172592
94	1	0	6.058514	5.219779	-0.472893
95	1	0	6.038630	4.403602	1.095809
96	1	0	8.173790	4.052581	-0.194121
97	1	0	7.253368	3.234635	-1.477996
98	6	0	8.511989	-0.457499	-0.074699
99	6	0	9.028844	-1.760361	-0.247981
100	6	0	10.430429	-1.810206	-0.255583
101	6	0	11.041063	-0.549192	-0.081009
102	16	0	9.824226	0.715567	0.087114
103	8	0	11.203780	-2.895741	-0.499759
104	6	0	10.938180	-4.121446	0.215799
105	6	0	9.635894	-4.786968	-0.207414
106	6	0	8.388919	-4.034231	0.237408
107	8	0	8.181250	-2.794202	-0.472823
108	1	0	10.945036	-3.912077	1.293958
109	1	0	11.794309	-4.755041	-0.022201
110	1	0	9.605169	-5.786601	0.246937
111	1	0	9.622414	-4.922048	-1.294941

112	1	0	7.489829	-4.613308	0.018000
113	1	0	8.417901	-3.824989	1.315468
114	6	0	12.430208	-0.296974	-0.049818
115	6	0	13.065317	0.946320	0.130250
116	6	0	14.481713	0.872225	0.170971
117	6	0	14.945565	-0.432559	0.001936
118	16	0	13.639820	-1.574185	-0.210716
119	8	0	12.311457	2.048107	0.349702
120	6	0	12.654935	3.281108	-0.321047
121	6	0	13.944293	3.910605	0.186859
122	6	0	15.198982	3.139037	-0.201098
123	8	0	15.329293	1.884334	0.492798
124	1	0	12.705327	3.091285	-1.401742
125	1	0	11.800894	3.930786	-0.120300
126	1	0	14.017462	4.918493	-0.243971
127	1	0	13.899908	4.023200	1.276110
128	1	0	16.093791	3.695780	0.084519
129	1	0	15.231020	2.959387	-1.285176
130	16	0	16.556840	-1.090680	0.106632
131	6	0	-17.634994	-0.218749	0.589100
132	1	0	-17.306537	-0.490111	1.594382
133	1	0	-17.661413	-1.090045	-0.062719
134	1	0	-18.625617	0.239262	0.644010
135	6	0	17.634994	0.218749	-0.589100
136	1	0	17.661413	1.090045	0.062719
137	1	0	17.306537	0.490111	-1.594382
138	1	0	18.625617	-0.239262	-0.644010

HF= -7427.5127471 hartree

Table S11. Cartesian coordinate of optimized geometry of **10P**$_{\mathbf{Hex}}^{2+}$ (S) at the RB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.688226	0.137686	-0.009967

2	6	0	1.289294	1.407725	-0.186106
3	6	0	2.686079	1.376824	-0.180953
4	6	0	3.227636	0.080645	-0.000865
5	16	0	1.930852	-1.109243	0.167873
6	8	0	3.519539	2.423160	-0.416252
7	6	0	3.312961	3.649320	0.312173
8	6	0	2.054884	4.395795	-0.112269
9	6	0	0.763386	3.705523	0.306538
10	8	0	0.504820	2.489976	-0.423451
11	1	0	3.295305	3.427796	1.388239
12	1	0	4.204423	4.240228	0.092385
13	1	0	2.075538	5.388583	0.357708
14	1	0	2.060586	4.546769	-1.197800
15	1	0	-0.100492	4.335114	0.083971
16	1	0	0.767031	3.482085	1.382301
17	6	0	4.590689	-0.257267	0.029235
18	6	0	5.132849	-1.551562	0.209944
19	6	0	6.531030	-1.582347	0.217659
20	6	0	7.129181	-0.312667	0.041074
21	16	0	5.890436	0.932865	-0.138468
22	8	0	4.300446	-2.599299	0.436649
23	6	0	4.517173	-3.826889	-0.288792
24	6	0	5.774672	-4.570962	0.141201
25	6	0	7.067119	-3.877474	-0.269918
26	8	0	7.314729	-2.664221	0.465510
27	1	0	4.539664	-3.605153	-1.364626
28	1	0	3.625824	-4.419641	-0.073432
29	1	0	5.756644	-5.563235	-0.329987
30	1	0	5.764271	-4.723212	1.226519
31	1	0	7.930913	-4.505719	-0.043343
32	1	0	7.069272	-3.652583	-1.345476
33	6	0	8.508549	-0.033835	0.020578
34	6	0	9.107463	1.231976	-0.156373
35	6	0	10.508883	1.200650	-0.154649
36	6	0	11.044900	-0.091941	0.025294
37	16	0	9.753743	-1.279900	0.196089

38	8	0	11.339111	2.248863	-0.401610
39	6	0	11.145271	3.467525	0.340329
40	6	0	9.885877	4.220159	-0.070209
41	6	0	8.594674	3.529782	0.349444
42	8	0	8.326417	2.317712	-0.385179
43	1	0	11.135018	3.238011	1.414922
44	1	0	12.036341	4.058434	0.118866
45	1	0	9.909369	5.209175	0.407626
46	1	0	9.886510	4.379822	-1.154519
47	1	0	7.731299	4.162852	0.134556
48	1	0	8.602317	3.299725	1.423700
49	6	0	12.414759	-0.438086	0.055165
50	6	0	12.950696	-1.725683	0.233102
51	6	0	14.358692	-1.755688	0.244043
52	6	0	14.945518	-0.493428	0.070938
53	16	0	13.716527	0.750049	-0.105284
54	8	0	12.124267	-2.779834	0.449209
55	6	0	12.352099	-3.999671	-0.289198
56	6	0	13.610930	-4.745039	0.135155
57	6	0	14.904611	-4.043526	-0.259128
58	8	0	15.138573	-2.840730	0.497483
59	1	0	12.376862	-3.764546	-1.362040
60	1	0	11.462294	-4.598587	-0.084092
61	1	0	13.596103	-5.730720	-0.349875
62	1	0	13.596540	-4.912851	1.218146
63	1	0	15.768562	-4.672422	-0.035691
64	1	0	14.914057	-3.804002	-1.331449
65	6	0	16.341250	-0.207816	0.042175
66	6	0	16.942519	1.042252	-0.131698
67	6	0	18.366159	1.000453	-0.135647
68	6	0	18.859232	-0.283530	0.030517
69	16	0	17.579280	-1.457874	0.166880
70	8	0	19.194835	2.056201	-0.359798
71	6	0	19.013560	3.231818	0.448326
72	6	0	17.758323	4.017085	0.083512
73	6	0	16.457248	3.320100	0.461707

74	8	0	16.178239	2.147696	-0.333509
75	1	0	19.007015	2.946353	1.509360
76	1	0	19.907156	3.830129	0.258242
77	1	0	17.789983	4.978012	0.615498
78	1	0	17.760703	4.237293	-0.990278
79	1	0	15.602573	3.973903	0.274287
80	1	0	16.455853	3.037668	1.523411
81	16	0	20.531640	-0.803321	0.165453
82	6	0	21.256301	-0.171079	-1.401352
83	1	0	21.126362	0.908861	-1.472771
84	1	0	20.805693	-0.673611	-2.259683
85	1	0	22.320515	-0.415569	-1.352573
86	6	0	-0.688226	-0.137686	0.009967
87	6	0	-1.289294	-1.407725	0.186106
88	6	0	-2.686079	-1.376824	0.180953
89	6	0	-3.227636	-0.080645	0.000865
90	16	0	-1.930852	1.109243	-0.167873
91	8	0	-3.519539	-2.423160	0.416252
92	6	0	-3.312961	-3.649320	-0.312173
93	6	0	-2.054884	-4.395795	0.112269
94	6	0	-0.763386	-3.705523	-0.306538
95	8	0	-0.504820	-2.489976	0.423451
96	1	0	-3.295305	-3.427796	-1.388239
97	1	0	-4.204423	-4.240228	-0.092385
98	1	0	-2.075538	-5.388583	-0.357708
99	1	0	-2.060586	-4.546769	1.197800
100	1	0	0.100492	-4.335114	-0.083971
101	1	0	-0.767031	-3.482085	-1.382301
102	6	0	-4.590689	0.257267	-0.029235
103	6	0	-5.132849	1.551562	-0.209944
104	6	0	-6.531030	1.582347	-0.217659
105	6	0	-7.129181	0.312667	-0.041074
106	16	0	-5.890436	-0.932865	0.138468
107	8	0	-4.300446	2.599299	-0.436649
108	6	0	-4.517173	3.826889	0.288792
109	6	0	-5.774672	4.570962	-0.141201

110	6	0	-7.067119	3.877474	0.269918
111	8	0	-7.314729	2.664221	-0.465510
112	1	0	-4.539664	3.605153	1.364626
113	1	0	-3.625824	4.419641	0.073432
114	1	0	-5.756644	5.563235	0.329987
115	1	0	-5.764271	4.723212	-1.226519
116	1	0	-7.930913	4.505719	0.043343
117	1	0	-7.069272	3.652583	1.345476
118	6	0	-8.508549	0.033835	-0.020578
119	6	0	-9.107463	-1.231976	0.156373
120	6	0	-10.508883	-1.200650	0.154649
121	6	0	-11.044900	0.091941	-0.025294
122	16	0	-9.753743	1.279900	-0.196089
123	8	0	-11.339111	-2.248863	0.401610
124	6	0	-11.145271	-3.467525	-0.340329
125	6	0	-9.885877	-4.220159	0.070209
126	6	0	-8.594674	-3.529782	-0.349444
127	8	0	-8.326417	-2.317712	0.385179
128	1	0	-11.135018	-3.238011	-1.414922
129	1	0	-12.036341	-4.058434	-0.118866
130	1	0	-9.909369	-5.209175	-0.407626
131	1	0	-9.886510	-4.379822	1.154519
132	1	0	-7.731299	-4.162852	-0.134556
133	1	0	-8.602317	-3.299725	-1.423700
134	6	0	-12.414759	0.438086	-0.055165
135	6	0	-12.950696	1.725683	-0.233102
136	6	0	-14.358692	1.755688	-0.244043
137	6	0	-14.945518	0.493428	-0.070938
138	16	0	-13.716527	-0.750049	0.105284
139	8	0	-12.124267	2.779834	-0.449209
140	6	0	-12.352099	3.999671	0.289198
141	6	0	-13.610930	4.745039	-0.135155
142	6	0	-14.904611	4.043526	0.259128
143	8	0	-15.138573	2.840730	-0.497483
144	1	0	-12.376862	3.764546	1.362040
145	1	0	-11.462294	4.598587	0.084092

146	1	0	-13.596103	5.730720	0.349875
147	1	0	-13.596540	4.912851	-1.218146
148	1	0	-15.768562	4.672422	0.035691
149	1	0	-14.914057	3.804002	1.331449
150	6	0	-16.341250	0.207816	-0.042175
151	6	0	-16.942519	-1.042252	0.131698
152	6	0	-18.366159	-1.000453	0.135647
153	6	0	-18.859232	0.283530	-0.030517
154	16	0	-17.579280	1.457874	-0.166880
155	8	0	-19.194835	-2.056201	0.359798
156	6	0	-19.013560	-3.231818	-0.448326
157	6	0	-17.758323	-4.017085	-0.083512
158	6	0	-16.457248	-3.320100	-0.461707
159	8	0	-16.178239	-2.147696	0.333509
160	1	0	-19.007015	-2.946353	-1.509360
161	1	0	-19.907156	-3.830129	-0.258242
162	1	0	-17.789983	-4.978012	-0.615498
163	1	0	-17.760703	-4.237293	0.990278
164	1	0	-15.602573	-3.973903	-0.274287
165	1	0	-16.455853	-3.037668	-1.523411
166	16	0	-20.531640	0.803321	-0.165453
167	6	0	-21.256301	0.171079	1.401352
168	1	0	-20.805693	0.673611	2.259683
169	1	0	-21.126362	-0.908861	1.472771
170	1	0	-22.320515	0.415569	1.352573

HF= -9065.4699531 hartree

Table S12. Cartesian coordinate of optimized geometry of **10P**$_{\mathbf{Hex}}^{2+}$ (U) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.695957	0.144366	-0.007931
2	6	0	1.287824	1.403964	-0.179268
3	6	0	2.696992	1.372270	-0.172059

4	6	0	3.230538	0.086277	0.004664
5	16	0	1.933596	-1.100107	0.167715
6	8	0	3.521212	2.428924	-0.402166
7	6	0	3.315445	3.634317	0.360652
8	6	0	2.056862	4.392950	-0.041566
9	6	0	0.762816	3.689124	0.347979
10	8	0	0.514358	2.496753	-0.420746
11	1	0	3.299730	3.383800	1.430369
12	1	0	4.206027	4.232496	0.156488
13	1	0	2.076146	5.370303	0.460055
14	1	0	2.065910	4.578427	-1.121733
15	1	0	-0.099034	4.325977	0.137315
16	1	0	0.757926	3.435915	1.417244
17	6	0	4.605153	-0.263217	0.034836
18	6	0	5.139953	-1.550603	0.215619
19	6	0	6.545649	-1.581354	0.223306
20	6	0	7.140412	-0.317567	0.046640
21	16	0	5.898332	0.925608	-0.132525
22	8	0	4.313186	-2.604125	0.452160
23	6	0	4.519802	-3.817478	-0.296734
24	6	0	5.777849	-4.570850	0.116835
25	6	0	7.071449	-3.873638	-0.284503
26	8	0	7.323439	-2.668291	0.464646
27	1	0	4.537715	-3.579412	-1.369336
28	1	0	3.628890	-4.413281	-0.087245
29	1	0	5.759207	-5.555431	-0.370356
30	1	0	5.768876	-4.740585	1.199578
31	1	0	7.934033	-4.506230	-0.065192
32	1	0	7.075017	-3.635632	-1.357119
33	6	0	8.524560	-0.034147	0.025338
34	6	0	9.120579	1.230270	-0.156002
35	6	0	10.523229	1.198539	-0.153908
36	6	0	11.059814	-0.093138	0.030553
37	16	0	9.764516	-1.279925	0.205208
38	8	0	11.353033	2.245868	-0.396895
39	6	0	11.152149	3.469811	0.337142

40	6	0	9.892576	4.218750	-0.078869
41	6	0	8.601212	3.527294	0.339205
42	8	0	8.340300	2.315602	-0.396447
43	1	0	11.140198	3.244835	1.412542
44	1	0	12.042989	4.060573	0.114621
45	1	0	9.915229	5.209128	0.396166
46	1	0	9.895197	4.375373	-1.163618
47	1	0	7.737703	4.159116	0.121127
48	1	0	8.606300	3.299099	1.413999
49	6	0	12.428276	-0.438669	0.061808
50	6	0	12.964920	-1.728059	0.246350
51	6	0	14.370832	-1.757816	0.254763
52	6	0	14.958990	-0.494256	0.073306
53	16	0	13.728109	0.749510	-0.107373
54	8	0	12.136488	-2.777919	0.472652
55	6	0	12.361300	-4.007331	-0.250301
56	6	0	13.620726	-4.747149	0.181630
57	6	0	14.913181	-4.052928	-0.228294
58	8	0	15.153999	-2.838466	0.509003
59	1	0	12.383871	-3.786392	-1.326219
60	1	0	11.471526	-4.602562	-0.035099
61	1	0	13.604351	-5.739982	-0.288425
62	1	0	13.609666	-4.898803	1.267034
63	1	0	15.777906	-4.678719	0.000337
64	1	0	14.917973	-3.828217	-1.303763
65	6	0	16.351879	-0.211072	0.039469
66	6	0	16.954166	1.040314	-0.142117
67	6	0	18.376264	0.998160	-0.150164
68	6	0	18.869565	-0.286924	0.019852
69	16	0	17.590357	-1.461353	0.166033
70	8	0	19.206208	2.051231	-0.378538
71	6	0	19.024759	3.234254	0.419513
72	6	0	17.769521	4.016105	0.048219
73	6	0	16.469314	3.323658	0.436610
74	8	0	16.187738	2.142557	-0.345740
75	1	0	19.018597	2.957629	1.482845

76	1	0	19.918492	3.830382	0.223736
77	1	0	17.802406	4.982401	0.570201
78	1	0	17.770141	4.225371	-1.027741
79	1	0	15.613981	3.974951	0.244221
80	1	0	16.470213	3.051571	1.500939
81	16	0	20.540060	-0.809422	0.154804
82	6	0	21.276712	-0.155754	-1.397589
83	1	0	21.146148	0.924660	-1.457196
84	1	0	20.834009	-0.648774	-2.265435
85	1	0	22.340513	-0.400332	-1.341969
86	6	0	-0.695957	-0.144366	0.007931
87	6	0	-1.287824	-1.403964	0.179268
88	6	0	-2.696992	-1.372270	0.172059
89	6	0	-3.230538	-0.086277	-0.004664
90	16	0	-1.933596	1.100107	-0.167715
91	8	0	-3.521212	-2.428924	0.402166
92	6	0	-3.315445	-3.634317	-0.360652
93	6	0	-2.056862	-4.392950	0.041566
94	6	0	-0.762816	-3.689124	-0.347979
95	8	0	-0.514358	-2.496753	0.420746
96	1	0	-3.299730	-3.383800	-1.430369
97	1	0	-4.206027	-4.232496	-0.156488
98	1	0	-2.076146	-5.370303	-0.460055
99	1	0	-2.065910	-4.578427	1.121733
100	1	0	0.099034	-4.325977	-0.137315
101	1	0	-0.757926	-3.435915	-1.417244
102	6	0	-4.605153	0.263217	-0.034836
103	6	0	-5.139953	1.550603	-0.215619
104	6	0	-6.545649	1.581354	-0.223306
105	6	0	-7.140412	0.317567	-0.046640
106	16	0	-5.898332	-0.925608	0.132525
107	8	0	-4.313186	2.604125	-0.452160
108	6	0	-4.519802	3.817478	0.296734
109	6	0	-5.777849	4.570850	-0.116835
110	6	0	-7.071449	3.873638	0.284503
111	8	0	-7.323439	2.668291	-0.464646

112	1	0	-4.537715	3.579412	1.369336
113	1	0	-3.628890	4.413281	0.087245
114	1	0	-5.759207	5.555431	0.370356
115	1	0	-5.768876	4.740585	-1.199578
116	1	0	-7.934033	4.506230	0.065192
117	1	0	-7.075017	3.635632	1.357119
118	6	0	-8.524560	0.034147	-0.025338
119	6	0	-9.120579	-1.230270	0.156002
120	6	0	-10.523229	-1.198539	0.153908
121	6	0	-11.059814	0.093138	-0.030553
122	16	0	-9.764516	1.279925	-0.205208
123	8	0	-11.353033	-2.245868	0.396895
124	6	0	-11.152149	-3.469811	-0.337142
125	6	0	-9.892576	-4.218750	0.078869
126	6	0	-8.601212	-3.527294	-0.339205
127	8	0	-8.340300	-2.315602	0.396447
128	1	0	-11.140198	-3.244835	-1.412542
129	1	0	-12.042989	-4.060573	-0.114621
130	1	0	-9.915229	-5.209128	-0.396166
131	1	0	-9.895197	-4.375373	1.163618
132	1	0	-7.737703	-4.159116	-0.121127
133	1	0	-8.606300	-3.299099	-1.413999
134	6	0	-12.428276	0.438669	-0.061808
135	6	0	-12.964920	1.728059	-0.246350
136	6	0	-14.370832	1.757816	-0.254763
137	6	0	-14.958990	0.494256	-0.073306
138	16	0	-13.728109	-0.749510	0.107373
139	8	0	-12.136488	2.777919	-0.472652
140	6	0	-12.361300	4.007331	0.250301
141	6	0	-13.620726	4.747149	-0.181630
142	6	0	-14.913181	4.052928	0.228294
143	8	0	-15.153999	2.838466	-0.509003
144	1	0	-12.383871	3.786392	1.326219
145	1	0	-11.471526	4.602562	0.035099
146	1	0	-13.604351	5.739982	0.288425
147	1	0	-13.609666	4.898803	-1.267034

148	1	0	-15.777906	4.678719	-0.000337
149	1	0	-14.917973	3.828217	1.303763
150	6	0	-16.351879	0.211072	-0.039469
151	6	0	-16.954166	-1.040314	0.142117
152	6	0	-18.376264	-0.998160	0.150164
153	6	0	-18.869565	0.286924	-0.019852
154	16	0	-17.590357	1.461353	-0.166033
155	8	0	-19.206208	-2.051231	0.378538
156	6	0	-19.024759	-3.234254	-0.419513
157	6	0	-17.769521	-4.016105	-0.048219
158	6	0	-16.469314	-3.323658	-0.436610
159	8	0	-16.187738	-2.142557	0.345740
160	1	0	-19.018597	-2.957629	-1.482845
161	1	0	-19.918492	-3.830382	-0.223736
162	1	0	-17.802406	-4.982401	-0.570201
163	1	0	-17.770141	-4.225371	1.027741
164	1	0	-15.613981	-3.974951	-0.244221
165	1	0	-16.470213	-3.051571	-1.500939
166	16	0	-20.540060	0.809422	-0.154804
167	6	0	-21.276712	0.155754	1.397589
168	1	0	-20.834009	0.648774	2.265435
169	1	0	-21.146148	-0.924660	1.457196
170	1	0	-22.340513	0.400332	1.341969

HF= -9065.4730902 hartree

Table S13. Cartesian coordinate of optimized geometry of **10P$_{Hex}^{2+}$** (T) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.700468	0.148447	-0.006664
2	6	0	1.287099	1.402340	-0.174328
3	6	0	2.703636	1.370092	-0.165936
4	6	0	3.232317	0.089715	0.007938
5	16	0	1.935177	-1.094744	0.166943

6	8	0	3.522875	2.432560	-0.392329
7	6	0	3.317263	3.625659	0.389637
8	6	0	2.058438	4.390843	-0.000159
9	6	0	0.762838	3.680081	0.372651
10	8	0	0.519907	2.501246	-0.417269
11	1	0	3.302318	3.358804	1.455420
12	1	0	4.207341	4.227906	0.194745
13	1	0	2.076934	5.359146	0.518924
14	1	0	2.069530	4.595542	-1.076845
15	1	0	-0.097715	4.321128	0.168721
16	1	0	0.753057	3.410340	1.437910
17	6	0	4.613755	-0.267170	0.037971
18	6	0	5.143967	-1.550675	0.218254
19	6	0	6.554398	-1.581692	0.225761
20	6	0	7.147074	-0.321585	0.049481
21	16	0	5.903171	0.920528	-0.129058
22	8	0	4.320525	-2.607544	0.460345
23	6	0	4.520779	-3.812430	-0.302101
24	6	0	5.779124	-4.571328	0.101369
25	6	0	7.073473	-3.872191	-0.294392
26	8	0	7.328527	-2.671826	0.462964
27	1	0	4.535746	-3.564790	-1.372679
28	1	0	3.630077	-4.409849	-0.095834
29	1	0	5.759836	-5.551216	-0.395272
30	1	0	5.771205	-4.751450	1.182446
31	1	0	7.935228	-4.507586	-0.079746
32	1	0	7.077649	-3.626297	-1.365165
33	6	0	8.534368	-0.035031	0.027620
34	6	0	9.128285	1.228350	-0.156295
35	6	0	10.532085	1.196511	-0.153985
36	6	0	11.068961	-0.094180	0.033163
37	16	0	9.771118	-1.280357	0.210141
38	8	0	11.361175	2.243704	-0.394581
39	6	0	11.155937	3.470353	0.335413
40	6	0	9.896111	4.217183	-0.083247
41	6	0	8.604695	3.524539	0.333162

42	8	0	8.348718	2.313597	-0.404097
43	1	0	11.143150	3.247450	1.411151
44	1	0	12.046510	4.061322	0.112503
45	1	0	9.918130	5.207989	0.390930
46	1	0	9.899936	4.372878	-1.168123
47	1	0	7.741061	4.155650	0.113447
48	1	0	8.608047	3.296684	1.408109
49	6	0	12.436865	-0.439683	0.065275
50	6	0	12.973807	-1.729870	0.254136
51	6	0	14.378661	-1.759405	0.261085
52	6	0	14.967645	-0.495225	0.074348
53	16	0	13.735281	0.748555	-0.109378
54	8	0	12.144373	-2.777300	0.487329
55	6	0	12.366997	-4.011946	-0.226953
56	6	0	13.626788	-4.748609	0.209180
57	6	0	14.918549	-4.058924	-0.209901
58	8	0	15.163675	-2.837490	0.515589
59	1	0	12.388171	-3.799150	-1.304559
60	1	0	11.477269	-4.605001	-0.005889
61	1	0	13.609552	-5.745501	-0.252111
62	1	0	13.617717	-4.890857	1.295868
63	1	0	15.783688	-4.682873	0.021903
64	1	0	14.920658	-3.843098	-1.287138
65	6	0	16.358674	-0.213459	0.037403
66	6	0	16.961823	1.038656	-0.149404
67	6	0	18.382840	0.996092	-0.160055
68	6	0	18.876244	-0.289857	0.012532
69	16	0	17.597267	-1.464117	0.165361
70	8	0	19.213717	2.047455	-0.390446
71	6	0	19.031715	3.235184	0.401113
72	6	0	17.776676	4.014902	0.025251
73	6	0	16.476875	3.325454	0.419647
74	8	0	16.194120	2.138886	-0.354544
75	1	0	19.025320	2.964086	1.465834
76	1	0	19.925649	3.829859	0.202141
77	1	0	17.810289	4.984545	0.540868

78	1	0	17.776567	4.217218	-1.052022
79	1	0	15.621196	3.975106	0.223733
80	1	0	16.478823	3.060022	1.485609
81	16	0	20.544862	-0.814871	0.148292
82	6	0	21.293227	-0.142203	-1.390310
83	1	0	21.162903	0.938657	-1.438787
84	1	0	20.857331	-0.625689	-2.266887
85	1	0	22.356408	-0.387819	-1.328581
86	6	0	-0.700468	-0.148447	0.006664
87	6	0	-1.287099	-1.402340	0.174328
88	6	0	-2.703636	-1.370092	0.165936
89	6	0	-3.232317	-0.089715	-0.007938
90	16	0	-1.935177	1.094744	-0.166943
91	8	0	-3.522875	-2.432560	0.392329
92	6	0	-3.317263	-3.625659	-0.389637
93	6	0	-2.058438	-4.390843	0.000159
94	6	0	-0.762838	-3.680081	-0.372651
95	8	0	-0.519907	-2.501246	0.417269
96	1	0	-3.302318	-3.358804	-1.455420
97	1	0	-4.207341	-4.227906	-0.194745
98	1	0	-2.076934	-5.359146	-0.518924
99	1	0	-2.069530	-4.595542	1.076845
100	1	0	0.097715	-4.321128	-0.168721
101	1	0	-0.753057	-3.410340	-1.437910
102	6	0	-4.613755	0.267170	-0.037971
103	6	0	-5.143967	1.550675	-0.218254
104	6	0	-6.554398	1.581692	-0.225761
105	6	0	-7.147074	0.321585	-0.049481
106	16	0	-5.903171	-0.920528	0.129058
107	8	0	-4.320525	2.607544	-0.460345
108	6	0	-4.520779	3.812430	0.302101
109	6	0	-5.779124	4.571328	-0.101369
110	6	0	-7.073473	3.872191	0.294392
111	8	0	-7.328527	2.671826	-0.462964
112	1	0	-4.535746	3.564790	1.372679
113	1	0	-3.630077	4.409849	0.095834

114	1	0	-5.759836	5.551216	0.395272
115	1	0	-5.771205	4.751450	-1.182446
116	1	0	-7.935228	4.507586	0.079746
117	1	0	-7.077649	3.626297	1.365165
118	6	0	-8.534368	0.035031	-0.027620
119	6	0	-9.128285	-1.228350	0.156295
120	6	0	-10.532085	-1.196511	0.153985
121	6	0	-11.068961	0.094180	-0.033163
122	16	0	-9.771118	1.280357	-0.210141
123	8	0	-11.361175	-2.243704	0.394581
124	6	0	-11.155937	-3.470353	-0.335413
125	6	0	-9.896111	-4.217183	0.083247
126	6	0	-8.604695	-3.524539	-0.333162
127	8	0	-8.348718	-2.313597	0.404097
128	1	0	-11.143150	-3.247450	-1.411151
129	1	0	-12.046510	-4.061322	-0.112503
130	1	0	-9.918130	-5.207989	-0.390930
131	1	0	-9.899936	-4.372878	1.168123
132	1	0	-7.741061	-4.155650	-0.113447
133	1	0	-8.608047	-3.296684	-1.408109
134	6	0	-12.436865	0.439683	-0.065275
135	6	0	-12.973807	1.729870	-0.254136
136	6	0	-14.378661	1.759405	-0.261085
137	6	0	-14.967645	0.495225	-0.074348
138	16	0	-13.735281	-0.748555	0.109378
139	8	0	-12.144373	2.777300	-0.487329
140	6	0	-12.366997	4.011946	0.226953
141	6	0	-13.626788	4.748609	-0.209180
142	6	0	-14.918549	4.058924	0.209901
143	8	0	-15.163675	2.837490	-0.515589
144	1	0	-12.388171	3.799150	1.304559
145	1	0	-11.477269	4.605001	0.005889
146	1	0	-13.609552	5.745501	0.252111
147	1	0	-13.617717	4.890857	-1.295868
148	1	0	-15.783688	4.682873	-0.021903
149	1	0	-14.920658	3.843098	1.287138

150	6	0	-16.358674	0.213459	-0.037403
151	6	0	-16.961823	-1.038656	0.149404
152	6	0	-18.382840	-0.996092	0.160055
153	6	0	-18.876244	0.289857	-0.012532
154	16	0	-17.597267	1.464117	-0.165361
155	8	0	-19.213717	-2.047455	0.390446
156	6	0	-19.031715	-3.235184	-0.401113
157	6	0	-17.776676	-4.014902	-0.025251
158	6	0	-16.476875	-3.325454	-0.419647
159	8	0	-16.194120	-2.138886	0.354544
160	1	0	-19.025320	-2.964086	-1.465834
161	1	0	-19.925649	-3.829859	-0.202141
162	1	0	-17.810289	-4.984545	-0.540868
163	1	0	-17.776567	-4.217218	1.052022
164	1	0	-15.621196	-3.975106	-0.223733
165	1	0	-16.478823	-3.060022	-1.485609
166	16	0	-20.544862	0.814871	-0.148292
167	6	0	-21.293227	0.142203	1.390310
168	1	0	-20.857331	0.625689	2.266887
169	1	0	-21.162903	-0.938657	1.438787
170	1	0	-22.356408	0.387819	1.328581

HF= -9065.4705179 hartree

Table S14. Cartesian coordinate of optimized geometry of **12P$_{Hex}^{2+}$** (S) at the RB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.684880	0.168503	-0.011000
2	6	0	1.231388	1.456172	-0.185691
3	6	0	2.633312	1.480782	-0.183973
4	6	0	3.224194	0.213186	-0.006880
5	16	0	1.976132	-1.026020	0.162013
6	8	0	3.417604	2.566605	-0.419314
7	6	0	3.169691	3.765135	0.339225

8	6	0	1.881868	4.472981	-0.063287
9	6	0	0.617796	3.722164	0.336553
10	8	0	0.410194	2.514356	-0.420504
11	1	0	3.165326	3.518600	1.410091
12	1	0	4.036600	4.395766	0.130738
13	1	0	1.864379	5.453637	0.431930
14	1	0	1.880209	4.651279	-1.144722
15	1	0	-0.269306	4.323185	0.125521
16	1	0	0.628114	3.477149	1.407706
17	6	0	4.605164	-0.075044	0.019865
18	6	0	5.196288	-1.342000	0.196306
19	6	0	6.598602	-1.317825	0.197551
20	6	0	7.144227	-0.029992	0.022597
21	16	0	5.854514	1.164413	-0.148718
22	8	0	4.412096	-2.428298	0.427462
23	6	0	4.664463	-3.627079	-0.330224
24	6	0	5.952121	-4.334243	0.073861
25	6	0	7.216422	-3.582277	-0.323411
26	8	0	7.419618	-2.375973	0.436024
27	1	0	4.670592	-3.380001	-1.400924
28	1	0	3.797662	-4.258538	-0.123642
29	1	0	5.970071	-5.314609	-0.421931
30	1	0	5.952477	-4.513189	1.155191
31	1	0	8.103527	-4.182868	-0.111249
32	1	0	7.207919	-3.336459	-1.394449
33	6	0	8.514581	0.308114	-0.002582
34	6	0	9.059953	1.594826	-0.175877
35	6	0	10.463263	1.619852	-0.180733
36	6	0	11.053156	0.352432	-0.009974
37	16	0	9.808192	-0.886668	0.161307
38	8	0	11.245078	2.706968	-0.421859
39	6	0	11.006800	3.900605	0.346277
40	6	0	9.716605	4.611750	-0.043052
41	6	0	8.454568	3.859834	0.361023
42	8	0	8.238774	2.654851	-0.399616
43	1	0	11.010437	3.648392	1.415863

44	1	0	11.872661	4.531574	0.134589
45	1	0	9.702252	5.589582	0.457851
46	1	0	9.707974	4.796220	-1.123421
47	1	0	7.566565	4.462621	0.158811
48	1	0	8.471675	3.609481	1.430798
49	6	0	12.436423	0.061615	0.010128
50	6	0	13.027397	-1.203019	0.177352
51	6	0	14.433221	-1.177815	0.174112
52	6	0	14.973419	0.108694	0.004342
53	16	0	13.686040	1.302076	-0.155665
54	8	0	12.247286	-2.293610	0.400454
55	6	0	12.503310	-3.484859	-0.369179
56	6	0	13.793243	-4.193838	0.024574
57	6	0	15.056101	-3.434696	-0.364545
58	8	0	15.253516	-2.238506	0.410374
59	1	0	12.506846	-3.226629	-1.437216
60	1	0	11.638307	-4.120556	-0.167736
61	1	0	13.811202	-5.168346	-0.482738
62	1	0	13.795571	-4.385435	1.103744
63	1	0	15.944318	-4.036161	-0.159489
64	1	0	15.047222	-3.176891	-1.432851
65	6	0	16.348203	0.455007	-0.024133
66	6	0	16.886474	1.738787	-0.187906
67	6	0	18.297047	1.765142	-0.199846
68	6	0	18.881110	0.503774	-0.040077
69	16	0	17.646345	-0.737074	0.123794
70	8	0	19.072769	2.857065	-0.445793
71	6	0	18.851603	4.036344	0.349752
72	6	0	17.556964	4.754844	-0.011165
73	6	0	16.296984	3.996765	0.388740
74	8	0	16.068958	2.805237	-0.392190
75	1	0	18.869748	3.764294	1.414156
76	1	0	19.715633	4.669746	0.138617
77	1	0	17.546975	5.722245	0.509774
78	1	0	17.538190	4.961835	-1.087348
79	1	0	15.408541	4.605245	0.205814

80	1	0	16.322404	3.725747	1.453190
81	6	0	20.278430	0.213025	-0.024561
82	6	0	20.880674	-1.035924	0.129728
83	6	0	22.306667	-0.992226	0.165179
84	6	0	22.797414	0.295537	0.022999
85	16	0	21.514416	1.462572	-0.161320
86	8	0	20.113647	-2.139642	0.340350
87	6	0	20.411047	-3.328324	-0.416683
88	6	0	21.696298	-4.017054	0.024924
89	6	0	22.963819	-3.246097	-0.326523
90	8	0	23.130419	-2.041886	0.438792
91	1	0	20.446901	-3.074006	-1.485243
92	1	0	19.548626	-3.975976	-0.242908
93	1	0	21.743866	-4.995877	-0.472304
94	1	0	21.663981	-4.199113	1.105308
95	1	0	23.847904	-3.841644	-0.087150
96	1	0	22.988080	-3.004099	-1.399203
97	16	0	24.449659	0.877393	0.138972
98	6	0	25.334870	-0.198112	-1.055380
99	1	0	24.910628	-0.091941	-2.056204
100	1	0	25.308010	-1.237774	-0.728759
101	1	0	26.368575	0.157280	-1.060288
102	6	0	-0.684880	-0.168503	0.011000
103	6	0	-1.231388	-1.456172	0.185691
104	6	0	-2.633312	-1.480782	0.183973
105	6	0	-3.224194	-0.213186	0.006880
106	16	0	-1.976132	1.026020	-0.162013
107	8	0	-3.417604	-2.566605	0.419314
108	6	0	-3.169691	-3.765135	-0.339225
109	6	0	-1.881868	-4.472981	0.063287
110	6	0	-0.617796	-3.722164	-0.336553
111	8	0	-0.410194	-2.514356	0.420504
112	1	0	-3.165326	-3.518600	-1.410091
113	1	0	-4.036600	-4.395766	-0.130738
114	1	0	-1.864379	-5.453637	-0.431930
115	1	0	-1.880209	-4.651279	1.144722

116	1	0	0.269306	-4.323185	-0.125521
117	1	0	-0.628114	-3.477149	-1.407706
118	6	0	-4.605164	0.075044	-0.019865
119	6	0	-5.196288	1.342000	-0.196306
120	6	0	-6.598602	1.317825	-0.197551
121	6	0	-7.144227	0.029992	-0.022597
122	16	0	-5.854514	-1.164413	0.148718
123	8	0	-4.412096	2.428298	-0.427462
124	6	0	-4.664463	3.627079	0.330224
125	6	0	-5.952121	4.334243	-0.073861
126	6	0	-7.216422	3.582277	0.323411
127	8	0	-7.419618	2.375973	-0.436024
128	1	0	-4.670592	3.380001	1.400924
129	1	0	-3.797662	4.258538	0.123642
130	1	0	-5.970071	5.314609	0.421931
131	1	0	-5.952477	4.513189	-1.155191
132	1	0	-8.103527	4.182868	0.111249
133	1	0	-7.207919	3.336459	1.394449
134	6	0	-8.514581	-0.308114	0.002582
135	6	0	-9.059953	-1.594826	0.175877
136	6	0	-10.463263	-1.619852	0.180733
137	6	0	-11.053156	-0.352432	0.009974
138	16	0	-9.808192	0.886668	-0.161307
139	8	0	-11.245078	-2.706968	0.421859
140	6	0	-11.006800	-3.900605	-0.346277
141	6	0	-9.716605	-4.611750	0.043052
142	6	0	-8.454568	-3.859834	-0.361023
143	8	0	-8.238774	-2.654851	0.399616
144	1	0	-11.010437	-3.648392	-1.415863
145	1	0	-11.872661	-4.531574	-0.134589
146	1	0	-9.702252	-5.589582	-0.457851
147	1	0	-9.707974	-4.796220	1.123421
148	1	0	-7.566565	-4.462621	-0.158811
149	1	0	-8.471675	-3.609481	-1.430798
150	6	0	-12.436423	-0.061615	-0.010128
151	6	0	-13.027397	1.203019	-0.177352

152	6	0	-14.433221	1.177815	-0.174112
153	6	0	-14.973419	-0.108694	-0.004342
154	16	0	-13.686040	-1.302076	0.155665
155	8	0	-12.247286	2.293610	-0.400454
156	6	0	-12.503310	3.484859	0.369179
157	6	0	-13.793243	4.193838	-0.024574
158	6	0	-15.056101	3.434696	0.364545
159	8	0	-15.253516	2.238506	-0.410374
160	1	0	-12.506846	3.226629	1.437216
161	1	0	-11.638307	4.120556	0.167736
162	1	0	-13.811202	5.168346	0.482738
163	1	0	-13.795571	4.385435	-1.103744
164	1	0	-15.944318	4.036161	0.159489
165	1	0	-15.047222	3.176891	1.432851
166	6	0	-16.348203	-0.455007	0.024133
167	6	0	-16.886474	-1.738787	0.187906
168	6	0	-18.297047	-1.765142	0.199846
169	6	0	-18.881110	-0.503774	0.040077
170	16	0	-17.646345	0.737074	-0.123794
171	8	0	-19.072769	-2.857065	0.445793
172	6	0	-18.851603	-4.036344	-0.349752
173	6	0	-17.556964	-4.754844	0.011165
174	6	0	-16.296984	-3.996765	-0.388740
175	8	0	-16.068958	-2.805237	0.392190
176	1	0	-18.869748	-3.764294	-1.414156
177	1	0	-19.715633	-4.669746	-0.138617
178	1	0	-17.546975	-5.722245	-0.509774
179	1	0	-17.538190	-4.961835	1.087348
180	1	0	-15.408541	-4.605245	-0.205814
181	1	0	-16.322404	-3.725747	-1.453190
182	6	0	-20.278430	-0.213025	0.024561
183	6	0	-20.880674	1.035924	-0.129728
184	6	0	-22.306667	0.992226	-0.165179
185	6	0	-22.797414	-0.295537	-0.022999
186	16	0	-21.514416	-1.462572	0.161320
187	8	0	-20.113647	2.139642	-0.340350

188	6	0	-20.411047	3.328324	0.416683
189	6	0	-21.696298	4.017054	-0.024924
190	6	0	-22.963819	3.246097	0.326523
191	8	0	-23.130419	2.041886	-0.438792
192	1	0	-20.446901	3.074006	1.485243
193	1	0	-19.548626	3.975976	0.242908
194	1	0	-21.743866	4.995877	0.472304
195	1	0	-21.663981	4.199113	-1.105308
196	1	0	-23.847904	3.841644	0.087150
197	1	0	-22.988080	3.004099	1.399203
198	16	0	-24.449659	-0.877393	-0.138972
199	6	0	-25.334870	0.198112	1.055380
200	1	0	-25.308010	1.237774	0.728759
201	1	0	-24.910628	0.091941	2.056204
202	1	0	-26.368575	-0.157280	1.060288

HF= -10703.4158526 hartree

Table S15. Cartesian coordinate of optimized geometry of **12P$_{Hex}^{2+}$** (U) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.691474	0.175475	-0.010906
2	6	0	1.229692	1.452941	-0.185505
3	6	0	2.643192	1.478009	-0.183713
4	6	0	3.227274	0.220407	-0.007062
5	16	0	1.979670	-1.015917	0.161470
6	8	0	3.417505	2.573501	-0.417991
7	6	0	3.172026	3.752617	0.370798
8	6	0	1.882198	4.470165	-0.009411
9	6	0	0.617061	3.707054	0.365417
10	8	0	0.417872	2.520929	-0.425176
11	1	0	3.172373	3.480987	1.435635
12	1	0	4.037017	4.390295	0.174830
13	1	0	1.864394	5.436345	0.513807

14	1	0	1.880693	4.679271	-1.085348
15	1	0	-0.269008	4.314064	0.166077
16	1	0	0.622027	3.435722	1.430391
17	6	0	4.619839	-0.078267	0.018890
18	6	0	5.204903	-1.337870	0.196242
19	6	0	6.615097	-1.312347	0.195740
20	6	0	7.156145	-0.030956	0.019411
21	16	0	5.863072	1.160058	-0.151713
22	8	0	4.428553	-2.430789	0.438333
23	6	0	4.669527	-3.614757	-0.342994
24	6	0	5.959458	-4.330025	0.041107
25	6	0	7.223591	-3.572589	-0.346868
26	8	0	7.430982	-2.375986	0.428130
27	1	0	4.667927	-3.351190	-1.409942
28	1	0	3.804274	-4.250072	-0.140819
29	1	0	5.976321	-5.301572	-0.471999
30	1	0	5.963890	-4.527933	1.119138
31	1	0	8.110354	-4.177300	-0.144510
32	1	0	7.214177	-3.312109	-1.414368
33	6	0	8.532094	0.313532	-0.006996
34	6	0	9.073928	1.597779	-0.183012
35	6	0	10.479871	1.622409	-0.186715
36	6	0	11.069277	0.356983	-0.013416
37	16	0	9.820573	-0.880979	0.159498
38	8	0	11.260430	2.710247	-0.421497
39	6	0	11.014135	3.905232	0.344462
40	6	0	9.724089	4.614720	-0.047921
41	6	0	8.461349	3.859721	0.349143
42	8	0	8.254941	2.658998	-0.418326
43	1	0	11.015193	3.652570	1.413827
44	1	0	11.879737	4.537423	0.135418
45	1	0	9.708434	5.591487	0.455053
46	1	0	9.718678	4.801559	-1.127906
47	1	0	7.573568	4.462234	0.144928
48	1	0	8.473960	3.606537	1.418445
49	6	0	12.452660	0.065664	0.007916

50	6	0	13.043497	-1.200560	0.178127
51	6	0	14.447777	-1.175085	0.173299
52	6	0	14.989378	0.112968	0.000349
53	16	0	13.699244	1.306635	-0.161215
54	8	0	12.261981	-2.288453	0.409740
55	6	0	12.513031	-3.484733	-0.352683
56	6	0	13.803211	-4.191517	0.044052
57	6	0	15.065320	-3.437613	-0.356480
58	8	0	15.270361	-2.232855	0.405240
59	1	0	12.514422	-3.234347	-1.422631
60	1	0	11.647809	-4.117804	-0.144467
61	1	0	13.820046	-5.170558	-0.454393
62	1	0	13.808274	-4.373410	1.124878
63	1	0	15.953899	-4.037608	-0.149210
64	1	0	15.052567	-3.189066	-1.426823
65	6	0	16.361294	0.456604	-0.030096
66	6	0	16.901027	1.743378	-0.196005
67	6	0	18.308958	1.769239	-0.207788
68	6	0	18.894108	0.505300	-0.046540
69	16	0	17.658821	-0.736421	0.119274
70	8	0	19.088174	2.857272	-0.453351
71	6	0	18.863055	4.045662	0.328688
72	6	0	17.569250	4.759500	-0.043211
73	6	0	16.309310	4.006290	0.365149
74	8	0	16.081030	2.806101	-0.402893
75	1	0	18.878412	3.784335	1.395746
76	1	0	19.727756	4.676402	0.112958
77	1	0	17.558896	5.732989	0.466105
78	1	0	17.551654	4.953805	-1.121754
79	1	0	15.420628	4.612113	0.175539
80	1	0	16.334824	3.746272	1.432285
81	6	0	20.288826	0.216684	-0.031176
82	6	0	20.892155	-1.034109	0.123598
83	6	0	22.316930	-0.990758	0.156704
84	6	0	22.807513	0.298178	0.012012
85	16	0	21.525280	1.466223	-0.172305

86	8	0	20.123592	-2.134930	0.335642
87	6	0	20.422509	-3.331101	-0.410323
88	6	0	21.707098	-4.015894	0.038434
89	6	0	22.974562	-3.248797	-0.320691
90	8	0	23.141771	-2.037904	0.434673
91	1	0	20.459182	-3.085625	-1.480814
92	1	0	19.559514	-3.976359	-0.231381
93	1	0	21.754076	-4.999261	-0.449662
94	1	0	21.674721	-4.188050	1.120413
95	1	0	23.858746	-3.842118	-0.076615
96	1	0	22.998326	-3.015459	-1.395212
97	16	0	24.457090	0.884584	0.127676
98	6	0	25.360906	-0.225085	-1.020352
99	1	0	24.948096	-0.152846	-2.028917
100	1	0	25.335465	-1.253571	-0.660705
101	1	0	26.392252	0.136911	-1.024261
102	6	0	-0.691474	-0.175475	0.010906
103	6	0	-1.229692	-1.452941	0.185505
104	6	0	-2.643192	-1.478009	0.183713
105	6	0	-3.227274	-0.220407	0.007062
106	16	0	-1.979670	1.015917	-0.161470
107	8	0	-3.417505	-2.573501	0.417991
108	6	0	-3.172026	-3.752617	-0.370798
109	6	0	-1.882198	-4.470165	0.009411
110	6	0	-0.617061	-3.707054	-0.365417
111	8	0	-0.417872	-2.520929	0.425176
112	1	0	-3.172373	-3.480987	-1.435635
113	1	0	-4.037017	-4.390295	-0.174830
114	1	0	-1.864394	-5.436345	-0.513807
115	1	0	-1.880693	-4.679271	1.085348
116	1	0	0.269008	-4.314064	-0.166077
117	1	0	-0.622027	-3.435722	-1.430391
118	6	0	-4.619839	0.078267	-0.018890
119	6	0	-5.204903	1.337870	-0.196242
120	6	0	-6.615097	1.312347	-0.195740
121	6	0	-7.156145	0.030956	-0.019411

122	16	0	-5.863072	-1.160058	0.151713
123	8	0	-4.428553	2.430789	-0.438333
124	6	0	-4.669527	3.614757	0.342994
125	6	0	-5.959458	4.330025	-0.041107
126	6	0	-7.223591	3.572589	0.346868
127	8	0	-7.430982	2.375986	-0.428130
128	1	0	-4.667927	3.351190	1.409942
129	1	0	-3.804274	4.250072	0.140819
130	1	0	-5.976321	5.301572	0.471999
131	1	0	-5.963890	4.527933	-1.119138
132	1	0	-8.110354	4.177300	0.144510
133	1	0	-7.214177	3.312109	1.414368
134	6	0	-8.532094	-0.313532	0.006996
135	6	0	-9.073928	-1.597779	0.183012
136	6	0	-10.479871	-1.622409	0.186715
137	6	0	-11.069277	-0.356983	0.013416
138	16	0	-9.820573	0.880979	-0.159498
139	8	0	-11.260430	-2.710247	0.421497
140	6	0	-11.014135	-3.905232	-0.344462
141	6	0	-9.724089	-4.614720	0.047921
142	6	0	-8.461349	-3.859721	-0.349143
143	8	0	-8.254941	-2.658998	0.418326
144	1	0	-11.015193	-3.652570	-1.413827
145	1	0	-11.879737	-4.537423	-0.135418
146	1	0	-9.708434	-5.591487	-0.455053
147	1	0	-9.718678	-4.801559	1.127906
148	1	0	-7.573568	-4.462234	-0.144928
149	1	0	-8.473960	-3.606537	-1.418445
150	6	0	-12.452660	-0.065664	-0.007916
151	6	0	-13.043497	1.200560	-0.178127
152	6	0	-14.447777	1.175085	-0.173299
153	6	0	-14.989378	-0.112968	-0.000349
154	16	0	-13.699244	-1.306635	0.161215
155	8	0	-12.261981	2.288453	-0.409740
156	6	0	-12.513031	3.484733	0.352683
157	6	0	-13.803211	4.191517	-0.044052

158	6	0	-15.065320	3.437613	0.356480
159	8	0	-15.270361	2.232855	-0.405240
160	1	0	-12.514422	3.234347	1.422631
161	1	0	-11.647809	4.117804	0.144467
162	1	0	-13.820046	5.170558	0.454393
163	1	0	-13.808274	4.373410	-1.124878
164	1	0	-15.953899	4.037608	0.149210
165	1	0	-15.052567	3.189066	1.426823
166	6	0	-16.361294	-0.456604	0.030096
167	6	0	-16.901027	-1.743378	0.196005
168	6	0	-18.308958	-1.769239	0.207788
169	6	0	-18.894108	-0.505300	0.046540
170	16	0	-17.658821	0.736421	-0.119274
171	8	0	-19.088174	-2.857272	0.453351
172	6	0	-18.863055	-4.045662	-0.328688
173	6	0	-17.569250	-4.759500	0.043211
174	6	0	-16.309310	-4.006290	-0.365149
175	8	0	-16.081030	-2.806101	0.402893
176	1	0	-18.878412	-3.784335	-1.395746
177	1	0	-19.727756	-4.676402	-0.112958
178	1	0	-17.558896	-5.732989	-0.466105
179	1	0	-17.551654	-4.953805	1.121754
180	1	0	-15.420628	-4.612113	-0.175539
181	1	0	-16.334824	-3.746272	-1.432285
182	6	0	-20.288826	-0.216684	0.031176
183	6	0	-20.892155	1.034109	-0.123598
184	6	0	-22.316930	0.990758	-0.156704
185	6	0	-22.807513	-0.298178	-0.012012
186	16	0	-21.525280	-1.466223	0.172305
187	8	0	-20.123592	2.134930	-0.335642
188	6	0	-20.422509	3.331101	0.410323
189	6	0	-21.707098	4.015894	-0.038434
190	6	0	-22.974562	3.248797	0.320691
191	8	0	-23.141771	2.037904	-0.434673
192	1	0	-20.459182	3.085625	1.480814
193	1	0	-19.559514	3.976359	0.231381

194	1	0	-21.754076	4.999261	0.449662
195	1	0	-21.674721	4.188050	-1.120413
196	1	0	-23.858746	3.842118	0.076615
197	1	0	-22.998326	3.015459	1.395212
198	16	0	-24.457090	-0.884584	-0.127676
199	6	0	-25.360906	0.225085	1.020352
200	1	0	-25.335465	1.253571	0.660705
201	1	0	-24.948096	0.152846	2.028917
202	1	0	-26.392252	-0.136911	1.024261

HF= -10703.4208000 hartree

Table S16. Cartesian coordinate of optimized geometry of **12P$_{Hex}^{2+}$** (T) at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.693689	0.178018	-0.010915
2	6	0	1.228887	1.452347	-0.184804
3	6	0	2.646373	1.477739	-0.183141
4	6	0	3.228164	0.223375	-0.007423
5	16	0	1.980956	-1.012190	0.160393
6	8	0	3.417419	2.576494	-0.416663
7	6	0	3.172516	3.749021	0.381962
8	6	0	1.881906	4.469365	0.009102
9	6	0	0.616505	3.702426	0.375941
10	8	0	0.419834	2.523439	-0.425246
11	1	0	3.174446	3.469162	1.444681
12	1	0	4.036763	4.389120	0.190161
13	1	0	1.863927	5.430735	0.541223
14	1	0	1.880346	4.688359	-1.064880
15	1	0	-0.269274	4.311301	0.180536
16	1	0	0.619904	3.422594	1.438764
17	6	0	4.624795	-0.079107	0.018015
18	6	0	5.207614	-1.336298	0.195013
19	6	0	6.620734	-1.310431	0.193796

20	6	0	7.160024	-0.031371	0.017488
21	16	0	5.865974	1.158643	-0.152873
22	8	0	4.433889	-2.431490	0.440185
23	6	0	4.671066	-3.610323	-0.349181
24	6	0	5.961818	-4.328286	0.027737
25	6	0	7.225885	-3.568929	-0.356966
26	8	0	7.434764	-2.376140	0.423955
27	1	0	4.666654	-3.340981	-1.414728
28	1	0	3.806384	-4.246983	-0.148457
29	1	0	5.978130	-5.296629	-0.491491
30	1	0	5.967817	-4.532942	1.104507
31	1	0	8.112519	-4.175178	-0.158418
32	1	0	7.215992	-3.302939	-1.423084
33	6	0	8.538195	0.315759	-0.009421
34	6	0	9.078402	1.598981	-0.186039
35	6	0	10.485674	1.623650	-0.189604
36	6	0	11.074768	0.359315	-0.015882
37	16	0	9.824949	-0.878370	0.157466
38	8	0	11.265250	2.712206	-0.422316
39	6	0	11.016462	3.906759	0.344333
40	6	0	9.726287	4.616007	-0.048004
41	6	0	8.463395	3.859456	0.345980
42	8	0	8.260280	2.660832	-0.424859
43	1	0	11.016981	3.652803	1.413350
44	1	0	11.881835	4.539716	0.136640
45	1	0	9.710135	5.591852	0.456767
46	1	0	9.721808	4.804853	-1.127643
47	1	0	7.575648	4.462007	0.141616
48	1	0	8.474480	3.604351	1.414886
49	6	0	12.458648	0.067384	0.005642
50	6	0	13.049122	-1.199069	0.176755
51	6	0	14.453281	-1.173507	0.171338
52	6	0	14.995235	0.114710	-0.002691
53	16	0	13.704001	1.308403	-0.164699
54	8	0	12.267449	-2.286368	0.411542
55	6	0	12.516341	-3.483547	-0.349738

56	6	0	13.806662	-4.190103	0.046993
57	6	0	15.068561	-3.437662	-0.356665
58	8	0	15.276216	-2.230683	0.401615
59	1	0	12.516713	-3.234833	-1.420099
60	1	0	11.651090	-4.115917	-0.139605
61	1	0	13.823028	-5.170133	-0.449499
62	1	0	13.812773	-4.369861	1.128167
63	1	0	15.957215	-4.037421	-0.149157
64	1	0	15.054566	-3.191313	-1.427459
65	6	0	16.366400	0.457756	-0.033876
66	6	0	16.906519	1.745361	-0.200988
67	6	0	18.313674	1.771015	-0.212593
68	6	0	18.899229	0.506319	-0.050241
69	16	0	17.663516	-0.735598	0.116493
70	8	0	19.094056	2.857683	-0.457966
71	6	0	18.867214	4.049452	0.318958
72	6	0	17.573705	4.761486	-0.057048
73	6	0	16.313726	4.009920	0.354035
74	8	0	16.085782	2.806856	-0.409621
75	1	0	18.881470	3.792093	1.386968
76	1	0	19.732136	4.679274	0.101621
77	1	0	17.563164	5.737110	0.448113
78	1	0	17.556686	4.951262	-1.136399
79	1	0	15.424993	4.614806	0.161928
80	1	0	16.339075	3.753797	1.422112
81	6	0	20.292921	0.218472	-0.034457
82	6	0	20.896810	-1.032874	0.121434
83	6	0	22.321052	-0.989535	0.153669
84	6	0	22.811592	0.299812	0.006949
85	16	0	21.529443	1.468074	-0.178196
86	8	0	20.127811	-2.132539	0.334826
87	6	0	20.427229	-3.331893	-0.406285
88	6	0	21.711566	-4.014941	0.045568
89	6	0	22.978991	-3.249430	-0.316708
90	8	0	23.146214	-2.035535	0.434214
91	1	0	20.464235	-3.090359	-1.477626

92	1	0	19.564017	-3.976141	-0.225057
93	1	0	21.758434	-5.000226	-0.438600
94	1	0	21.679091	-4.182837	1.128204
95	1	0	23.863244	-3.841665	-0.070402
96	1	0	23.002708	-3.019933	-1.392020
97	16	0	24.459686	0.888670	0.121884
98	6	0	25.373409	-0.239431	-0.999898
99	1	0	24.966717	-0.186348	-2.012120
100	1	0	25.348589	-1.261217	-0.621923
101	1	0	26.403477	0.126107	-1.003787
102	6	0	-0.693689	-0.178018	0.010915
103	6	0	-1.228887	-1.452347	0.184804
104	6	0	-2.646373	-1.477739	0.183141
105	6	0	-3.228164	-0.223375	0.007423
106	16	0	-1.980956	1.012190	-0.160393
107	8	0	-3.417419	-2.576494	0.416663
108	6	0	-3.172516	-3.749021	-0.381962
109	6	0	-1.881906	-4.469365	-0.009102
110	6	0	-0.616505	-3.702426	-0.375941
111	8	0	-0.419834	-2.523439	0.425246
112	1	0	-3.174446	-3.469162	-1.444681
113	1	0	-4.036763	-4.389120	-0.190161
114	1	0	-1.863927	-5.430735	-0.541223
115	1	0	-1.880346	-4.688359	1.064880
116	1	0	0.269274	-4.311301	-0.180536
117	1	0	-0.619904	-3.422594	-1.438764
118	6	0	-4.624795	0.079107	-0.018015
119	6	0	-5.207614	1.336298	-0.195013
120	6	0	-6.620734	1.310431	-0.193796
121	6	0	-7.160024	0.031371	-0.017488
122	16	0	-5.865974	-1.158643	0.152873
123	8	0	-4.433889	2.431490	-0.440185
124	6	0	-4.671066	3.610323	0.349181
125	6	0	-5.961818	4.328286	-0.027737
126	6	0	-7.225885	3.568929	0.356966
127	8	0	-7.434764	2.376140	-0.423955

128	1	0	-4.666654	3.340981	1.414728
129	1	0	-3.806384	4.246983	0.148457
130	1	0	-5.978130	5.296629	0.491491
131	1	0	-5.967817	4.532942	-1.104507
132	1	0	-8.112519	4.175178	0.158418
133	1	0	-7.215992	3.302939	1.423084
134	6	0	-8.538195	-0.315759	0.009421
135	6	0	-9.078402	-1.598981	0.186039
136	6	0	-10.485674	-1.623650	0.189604
137	6	0	-11.074768	-0.359315	0.015882
138	16	0	-9.824949	0.878370	-0.157466
139	8	0	-11.265250	-2.712206	0.422316
140	6	0	-11.016462	-3.906759	-0.344333
141	6	0	-9.726287	-4.616007	0.048004
142	6	0	-8.463395	-3.859456	-0.345980
143	8	0	-8.260280	-2.660832	0.424859
144	1	0	-11.016981	-3.652803	-1.413350
145	1	0	-11.881835	-4.539716	-0.136640
146	1	0	-9.710135	-5.591852	-0.456767
147	1	0	-9.721808	-4.804853	1.127643
148	1	0	-7.575648	-4.462007	-0.141616
149	1	0	-8.474480	-3.604351	-1.414886
150	6	0	-12.458648	-0.067384	-0.005642
151	6	0	-13.049122	1.199069	-0.176755
152	6	0	-14.453281	1.173507	-0.171338
153	6	0	-14.995235	-0.114710	0.002691
154	16	0	-13.704001	-1.308403	0.164699
155	8	0	-12.267449	2.286368	-0.411542
156	6	0	-12.516341	3.483547	0.349738
157	6	0	-13.806662	4.190103	-0.046993
158	6	0	-15.068561	3.437662	0.356665
159	8	0	-15.276216	2.230683	-0.401615
160	1	0	-12.516713	3.234833	1.420099
161	1	0	-11.651090	4.115917	0.139605
162	1	0	-13.823028	5.170133	0.449499
163	1	0	-13.812773	4.369861	-1.128167

164	1	0	-15.957215	4.037421	0.149157
165	1	0	-15.054566	3.191313	1.427459
166	6	0	-16.366400	-0.457756	0.033876
167	6	0	-16.906519	-1.745361	0.200988
168	6	0	-18.313674	-1.771015	0.212593
169	6	0	-18.899229	-0.506319	0.050241
170	16	0	-17.663516	0.735598	-0.116493
171	8	0	-19.094056	-2.857683	0.457966
172	6	0	-18.867214	-4.049452	-0.318958
173	6	0	-17.573705	-4.761486	0.057048
174	6	0	-16.313726	-4.009920	-0.354035
175	8	0	-16.085782	-2.806856	0.409621
176	1	0	-18.881470	-3.792093	-1.386968
177	1	0	-19.732136	-4.679274	-0.101621
178	1	0	-17.563164	-5.737110	-0.448113
179	1	0	-17.556686	-4.951262	1.136399
180	1	0	-15.424993	-4.614806	-0.161928
181	1	0	-16.339075	-3.753797	-1.422112
182	6	0	-20.292921	-0.218472	0.034457
183	6	0	-20.896810	1.032874	-0.121434
184	6	0	-22.321052	0.989535	-0.153669
185	6	0	-22.811592	-0.299812	-0.006949
186	16	0	-21.529443	-1.468074	0.178196
187	8	0	-20.127811	2.132539	-0.334826
188	6	0	-20.427229	3.331893	0.406285
189	6	0	-21.711566	4.014941	-0.045568
190	6	0	-22.978991	3.249430	0.316708
191	8	0	-23.146214	2.035535	-0.434214
192	1	0	-20.464235	3.090359	1.477626
193	1	0	-19.564017	3.976141	0.225057
194	1	0	-21.758434	5.000226	0.438600
195	1	0	-21.679091	4.182837	-1.128204
196	1	0	-23.863244	3.841665	0.070402
197	1	0	-23.002708	3.019933	1.392020
198	16	0	-24.459686	-0.888670	-0.121884
199	6	0	-25.373409	0.239431	0.999898

200	1	0	-25.348589	1.261217	0.621923
201	1	0	-24.966717	0.186348	2.012120
202	1	0	-26.403477	-0.126107	1.003787

HF= -10703.4194463 hartree

Table S17. Cartesian coordinate of optimized geometry of **6P**$_{\mathbf{Hex}}^{3+}$ at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.695973	-0.107553	-0.003232
2	6	0	-1.340622	-1.370995	-0.088020
3	6	0	-2.738818	-1.280414	-0.100213
4	6	0	-3.216564	0.057239	-0.021792
5	16	0	-1.874960	1.202870	0.071102
6	8	0	-3.632300	-2.274254	-0.270783
7	6	0	-3.462971	-3.545586	0.403876
8	6	0	-2.232836	-4.314767	-0.050333
9	6	0	-0.926261	-3.706486	0.433543
10	8	0	-0.580504	-2.473410	-0.242674
11	1	0	-3.442164	-3.364268	1.486421
12	1	0	-4.376011	-4.088186	0.155551
13	1	0	-2.303145	-5.328812	0.365233
14	1	0	-2.225769	-4.412033	-1.141830
15	1	0	-0.083830	-4.362831	0.211300
16	1	0	-0.951133	-3.516233	1.514556
17	6	0	-4.564914	0.450987	-0.033890
18	6	0	-5.042267	1.790791	0.053135
19	6	0	-6.436712	1.881546	0.041323
20	6	0	-7.084534	0.612977	-0.063401
21	16	0	-5.905925	-0.698569	-0.138850
22	8	0	-4.145406	2.780486	0.228426
23	6	0	-4.332818	4.071423	-0.405090
24	6	0	-5.560310	4.821804	0.087046
25	6	0	-6.869373	4.236410	-0.415349

26	8	0	-7.207313	2.970599	0.208944
27	1	0	-4.367411	3.921934	-1.492192
28	1	0	-3.418936	4.610684	-0.152391
29	1	0	-5.492683	5.851404	-0.288690
30	1	0	-5.561367	4.877473	1.181485
31	1	0	-7.713419	4.877648	-0.159498
32	1	0	-6.851769	4.090240	-1.502944
33	6	0	-8.467551	0.416187	-0.101697
34	6	0	-9.151100	-0.832370	-0.219212
35	6	0	-10.552102	-0.712724	-0.284439
36	6	0	-10.969336	0.635885	-0.203460
37	16	0	-9.626697	1.751566	-0.051637
38	8	0	-11.457447	-1.678961	-0.535746
39	6	0	-11.352581	-2.969296	0.109314
40	6	0	-10.122976	-3.753083	-0.321127
41	6	0	-8.826613	-3.203662	0.248933
42	8	0	-8.407642	-1.941194	-0.339366
43	1	0	-11.371568	-2.823714	1.197798
44	1	0	-12.267280	-3.481676	-0.191514
45	1	0	-10.232904	-4.781455	0.047875
46	1	0	-10.069576	-3.806490	-1.414388
47	1	0	-7.988231	-3.866648	0.032558
48	1	0	-8.896865	-3.061961	1.334915
49	16	0	-12.521719	1.368864	-0.284422
50	6	0	0.695973	0.107553	0.003232
51	6	0	1.340622	1.370995	0.088020
52	6	0	2.738818	1.280414	0.100213
53	6	0	3.216564	-0.057239	0.021792
54	16	0	1.874960	-1.202870	-0.071102
55	8	0	3.632300	2.274254	0.270783
56	6	0	3.462971	3.545586	-0.403876
57	6	0	2.232836	4.314767	0.050333
58	6	0	0.926261	3.706486	-0.433543
59	8	0	0.580504	2.473410	0.242674
60	1	0	3.442164	3.364268	-1.486421
61	1	0	4.376011	4.088186	-0.155551

62	1	0	2.303145	5.328812	-0.365233
63	1	0	2.225769	4.412033	1.141830
64	1	0	0.083830	4.362831	-0.211300
65	1	0	0.951133	3.516233	-1.514556
66	6	0	4.564914	-0.450987	0.033890
67	6	0	5.042267	-1.790791	-0.053135
68	6	0	6.436712	-1.881546	-0.041323
69	6	0	7.084534	-0.612977	0.063401
70	16	0	5.905925	0.698569	0.138850
71	8	0	4.145406	-2.780486	-0.228426
72	6	0	4.332818	-4.071423	0.405090
73	6	0	5.560310	-4.821804	-0.087046
74	6	0	6.869373	-4.236410	0.415349
75	8	0	7.207313	-2.970599	-0.208944
76	1	0	4.367411	-3.921934	1.492192
77	1	0	3.418936	-4.610684	0.152391
78	1	0	5.492683	-5.851404	0.288690
79	1	0	5.561367	-4.877473	-1.181485
80	1	0	7.713419	-4.877648	0.159498
81	1	0	6.851769	-4.090240	1.502944
82	6	0	8.467551	-0.416187	0.101697
83	6	0	9.151100	0.832370	0.219212
84	6	0	10.552102	0.712724	0.284439
85	6	0	10.969336	-0.635885	0.203460
86	16	0	9.626697	-1.751566	0.051637
87	8	0	11.457447	1.678961	0.535746
88	6	0	11.352581	2.969296	-0.109314
89	6	0	10.122976	3.753083	0.321127
90	6	0	8.826613	3.203662	-0.248933
91	8	0	8.407642	1.941194	0.339366
92	1	0	11.371568	2.823714	-1.197798
93	1	0	12.267280	3.481676	0.191514
94	1	0	10.232904	4.781455	-0.047875
95	1	0	10.069576	3.806490	1.414388
96	1	0	7.988231	3.866648	-0.032558
97	1	0	8.896865	3.061961	-1.334915

98	16	0	12.521719	-1.368864	0.284422
99	6	0	-13.785364	0.041868	-0.298158
100	1	0	-13.736453	-0.550637	0.615313
101	1	0	-13.686974	-0.583677	-1.183518
102	1	0	-14.727900	0.594295	-0.328693
103	6	0	13.785364	-0.041868	0.298158
104	1	0	13.686974	0.583677	1.183518
105	1	0	13.736453	0.550637	-0.615313
106	1	0	14.727900	-0.594295	0.328693

HF= -5789.2143061 hartree

Table S18. Cartesian coordinate of optimized geometry of **8P**$_{\mathbf{Hex}}^{3+}$ at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.677070	0.166256	0.035058
2	6	0	-1.181535	1.471460	0.245035
3	6	0	-2.567561	1.527821	0.297985
4	6	0	-3.187384	0.276366	0.122561
5	16	0	-1.984128	-0.984627	-0.111292
6	8	0	-3.287292	2.616088	0.577207
7	6	0	-3.078750	3.811090	-0.167609
8	6	0	-1.764465	4.485916	0.180295
9	6	0	-0.541379	3.715247	-0.279699
10	8	0	-0.351679	2.489724	0.433710
11	1	0	-3.141788	3.584624	-1.227051
12	1	0	-3.911254	4.442039	0.100013
13	1	0	-1.744174	5.457663	-0.305612
14	1	0	-1.711794	4.653073	1.250193
15	1	0	0.358970	4.273878	-0.080833
16	1	0	-0.586960	3.493371	-1.340466
17	6	0	-4.578890	0.022154	0.136710
18	6	0	-5.188474	-1.231915	-0.029868
19	6	0	-6.589281	-1.186181	-0.019530

20	6	0	-7.113251	0.103263	0.159782
21	16	0	-5.803463	1.275933	0.334183
22	8	0	-4.460428	-2.338245	-0.243599
23	6	0	-4.686789	-3.471040	0.588438
24	6	0	-5.987280	-4.186087	0.264966
25	6	0	-7.234377	-3.386064	0.600422
26	8	0	-7.387960	-2.243841	-0.231638
27	1	0	-4.654415	-3.159932	1.627894
28	1	0	-3.845723	-4.120026	0.398122
29	1	0	-6.013873	-5.108504	0.839389
30	1	0	-6.001238	-4.452976	-0.785879
31	1	0	-8.118207	-3.977990	0.418548
32	1	0	-7.236840	-3.073869	1.640109
33	6	0	-8.484892	0.457779	0.181001
34	6	0	-9.013764	1.747279	0.372678
35	6	0	-10.407531	1.787913	0.369807
36	6	0	-11.013582	0.523624	0.176720
37	16	0	-9.789715	-0.721106	-0.014529
38	8	0	-11.157982	2.868911	0.593919
39	6	0	-10.926758	4.055697	-0.168405
40	6	0	-9.633420	4.752022	0.213151
41	6	0	-8.381332	3.978397	-0.161986
42	8	0	-8.216323	2.795622	0.611665
43	1	0	-10.945903	3.802116	-1.223073
44	1	0	-11.775779	4.683097	0.051459
45	1	0	-9.607056	5.707419	-0.304062
46	1	0	-9.629759	4.955726	1.278045
47	1	0	-7.500590	4.564244	0.050207
48	1	0	-8.377228	3.717668	-1.215650
49	6	0	-12.388294	0.301455	0.147902
50	6	0	-13.038683	-0.945537	-0.064672
51	6	0	-14.422110	-0.865845	-0.082011
52	6	0	-14.878111	0.442319	0.123798
53	16	0	-13.585064	1.573861	0.341904
54	8	0	-12.313559	-2.023196	-0.278540
55	6	0	-12.623180	-3.275905	0.350948

56	6	0	-13.926183	-3.886728	-0.125735
57	6	0	-15.154823	-3.107698	0.303971
58	8	0	-15.262414	-1.860041	-0.375714
59	1	0	-12.625195	-3.120913	1.423862
60	1	0	-11.785764	-3.902119	0.091230
61	1	0	-13.991974	-4.885214	0.297313
62	1	0	-13.916102	-3.988509	-1.205016
63	1	0	-16.054837	-3.637693	0.036065
64	1	0	-15.160373	-2.931421	1.375009
65	16	0	-16.457139	1.108263	0.152635
66	6	0	0.677070	-0.166256	-0.035058
67	6	0	1.181535	-1.471460	-0.245035
68	6	0	2.567561	-1.527821	-0.297985
69	6	0	3.187384	-0.276366	-0.122561
70	16	0	1.984128	0.984627	0.111292
71	8	0	3.287292	-2.616088	-0.577207
72	6	0	3.078750	-3.811090	0.167609
73	6	0	1.764465	-4.485916	-0.180295
74	6	0	0.541379	-3.715247	0.279699
75	8	0	0.351679	-2.489724	-0.433710
76	1	0	3.141788	-3.584624	1.227051
77	1	0	3.911254	-4.442039	-0.100013
78	1	0	1.744174	-5.457663	0.305612
79	1	0	1.711794	-4.653073	-1.250193
80	1	0	-0.358970	-4.273878	0.080833
81	1	0	0.586960	-3.493371	1.340466
82	6	0	4.578890	-0.022154	-0.136710
83	6	0	5.188474	1.231915	0.029868
84	6	0	6.589281	1.186181	0.019530
85	6	0	7.113251	-0.103263	-0.159782
86	16	0	5.803463	-1.275933	-0.334183
87	8	0	4.460428	2.338245	0.243599
88	6	0	4.686789	3.471040	-0.588438
89	6	0	5.987280	4.186087	-0.264966
90	6	0	7.234377	3.386064	-0.600422
91	8	0	7.387960	2.243841	0.231638

92	1	0	4.654415	3.159932	-1.627894
93	1	0	3.845723	4.120026	-0.398122
94	1	0	6.013873	5.108504	-0.839389
95	1	0	6.001238	4.452976	0.785879
96	1	0	8.118207	3.977990	-0.418548
97	1	0	7.236840	3.073869	-1.640109
98	6	0	8.484892	-0.457779	-0.181001
99	6	0	9.013764	-1.747279	-0.372678
100	6	0	10.407531	-1.787913	-0.369807
101	6	0	11.013582	-0.523624	-0.176720
102	16	0	9.789715	0.721106	0.014529
103	8	0	11.157982	-2.868911	-0.593919
104	6	0	10.926758	-4.055697	0.168405
105	6	0	9.633420	-4.752022	-0.213151
106	6	0	8.381332	-3.978397	0.161986
107	8	0	8.216323	-2.795622	-0.611665
108	1	0	10.945903	-3.802116	1.223073
109	1	0	11.775779	-4.683097	-0.051459
110	1	0	9.607056	-5.707419	0.304062
111	1	0	9.629759	-4.955726	-1.278045
112	1	0	7.500590	-4.564244	-0.050207
113	1	0	8.377228	-3.717668	1.215650
114	6	0	12.388294	-0.301455	-0.147902
115	6	0	13.038683	0.945537	0.064672
116	6	0	14.422110	0.865845	0.082011
117	6	0	14.878111	-0.442319	-0.123798
118	16	0	13.585064	-1.573861	-0.341904
119	8	0	12.313559	2.023196	0.278540
120	6	0	12.623180	3.275905	-0.350948
121	6	0	13.926183	3.886728	0.125735
122	6	0	15.154823	3.107698	-0.303971
123	8	0	15.262414	1.860041	0.375714
124	1	0	12.625195	3.120913	-1.423862
125	1	0	11.785764	3.902119	-0.091230
126	1	0	13.991974	4.885214	-0.297313
127	1	0	13.916102	3.988509	1.205016

128	1	0	16.054837	3.637693	-0.036065
129	1	0	15.160373	2.931421	-1.375009
130	16	0	16.457139	-1.108263	-0.152635
131	6	0	-17.650460	-0.249429	-0.045526
132	1	0	-17.586654	-0.945429	0.774760
133	1	0	-17.521283	-0.747120	-0.991153
134	1	0	-18.608329	0.251599	-0.019394
135	6	0	17.650460	0.249429	0.045526
136	1	0	17.521283	0.747120	0.991153
137	1	0	17.586654	0.945429	-0.774760
138	1	0	18.608329	-0.251599	0.019394

HF= -7399.7772013 hartree

Table S19. Cartesian coordinate of optimized geometry of **10P**$_{\mathbf{Hex}}^{3+}$ at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.692283	0.139171	-0.007437
2	6	0	1.287164	1.411006	-0.157194
3	6	0	2.690425	1.377934	-0.156439
4	6	0	3.223855	0.079334	-0.006075
5	16	0	1.928949	-1.111474	0.140382
6	8	0	3.527116	2.421712	-0.373929
7	6	0	3.316263	3.654334	0.347364
8	6	0	2.058549	4.396656	-0.082535
9	6	0	0.768401	3.713025	0.348404
10	8	0	0.500482	2.492744	-0.374424
11	1	0	3.299009	3.437580	1.424098
12	1	0	4.207706	4.243198	0.123685
13	1	0	2.081917	5.393526	0.378148
14	1	0	2.061233	4.538709	-1.169199
15	1	0	-0.095411	4.342462	0.126729
16	1	0	0.777019	3.493875	1.424761
17	6	0	4.593931	-0.265634	0.010471

18	6	0	5.126447	-1.564411	0.162480
19	6	0	6.529878	-1.598061	0.166272
20	6	0	7.125754	-0.326527	0.014644
21	16	0	5.888713	0.924834	-0.136280
22	8	0	4.288843	-2.607949	0.379098
23	6	0	4.502340	-3.841707	-0.339845
24	6	0	5.758503	-4.583750	0.095066
25	6	0	7.050177	-3.901513	-0.333281
26	8	0	7.315297	-2.679346	0.387793
27	1	0	4.523178	-3.626347	-1.416806
28	1	0	3.610110	-4.430242	-0.118253
29	1	0	5.736150	-5.581381	-0.363997
30	1	0	5.752583	-4.724041	1.181940
31	1	0	7.913220	-4.530271	-0.107082
32	1	0	7.045496	-3.684719	-1.410080
33	6	0	8.509755	-0.049877	-0.000779
34	6	0	9.106741	1.222270	-0.158085
35	6	0	10.507535	1.187521	-0.160480
36	6	0	11.041808	-0.115218	-0.002408
37	16	0	9.743764	-1.303857	0.152448
38	8	0	11.348170	2.224473	-0.385183
39	6	0	11.140835	3.470347	0.315499
40	6	0	9.882350	4.206356	-0.121983
41	6	0	8.593586	3.530969	0.325641
42	8	0	8.318555	2.302024	-0.379704
43	1	0	11.127488	3.270894	1.395527
44	1	0	12.032469	4.053295	0.078310
45	1	0	9.909047	5.210403	0.322565
46	1	0	9.880688	4.331227	-1.210752
47	1	0	7.729507	4.158993	0.101024
48	1	0	8.608446	3.325616	1.404677
49	6	0	12.405384	-0.457077	0.017709
50	6	0	12.941252	-1.760037	0.180803
51	6	0	14.340229	-1.791530	0.187168
52	6	0	14.933417	-0.514204	0.024620
53	16	0	13.703720	0.736656	-0.134779

54	8	0	12.098521	-2.795365	0.395071
55	6	0	12.332123	-4.057251	-0.271780
56	6	0	13.588708	-4.774651	0.200440
57	6	0	14.879116	-4.108853	-0.254666
58	8	0	15.138501	-2.857995	0.420821
59	1	0	12.361413	-3.880979	-1.355457
60	1	0	11.440563	-4.640794	-0.035667
61	1	0	13.569699	-5.790750	-0.216023
62	1	0	13.580215	-4.870106	1.292156
63	1	0	15.745059	-4.723690	-0.004667
64	1	0	14.874248	-3.931357	-1.338442
65	6	0	16.315554	-0.246720	-0.006700
66	6	0	16.932635	1.013989	-0.170729
67	6	0	18.346472	0.962517	-0.192293
68	6	0	18.829247	-0.342788	-0.052055
69	16	0	17.544112	-1.513724	0.085808
70	8	0	19.193981	2.001277	-0.392668
71	6	0	19.006025	3.208319	0.373490
72	6	0	17.760753	3.984382	-0.034387
73	6	0	16.459271	3.320178	0.388859
74	8	0	16.157604	2.106356	-0.342572
75	1	0	18.985291	2.956789	1.442614
76	1	0	19.906367	3.791421	0.171842
77	1	0	17.801531	4.970458	0.447726
78	1	0	17.763374	4.150932	-1.117605
79	1	0	15.605210	3.965208	0.175142
80	1	0	16.464951	3.086064	1.461623
81	16	0	20.461751	-0.936628	0.078200
82	6	0	21.429332	0.079613	-1.106623
83	1	0	21.448826	1.125727	-0.809003
84	1	0	21.023897	-0.029631	-2.113913
85	1	0	22.435571	-0.344740	-1.068857
86	6	0	-0.692283	-0.139171	0.007437
87	6	0	-1.287164	-1.411006	0.157194
88	6	0	-2.690425	-1.377934	0.156439
89	6	0	-3.223855	-0.079334	0.006075

90	16	0	-1.928949	1.111474	-0.140382
91	8	0	-3.527116	-2.421712	0.373929
92	6	0	-3.316263	-3.654334	-0.347364
93	6	0	-2.058549	-4.396656	0.082535
94	6	0	-0.768401	-3.713025	-0.348404
95	8	0	-0.500482	-2.492744	0.374424
96	1	0	-3.299009	-3.437580	-1.424098
97	1	0	-4.207706	-4.243198	-0.123685
98	1	0	-2.081917	-5.393526	-0.378148
99	1	0	-2.061233	-4.538709	1.169199
100	1	0	0.095411	-4.342462	-0.126729
101	1	0	-0.777019	-3.493875	-1.424761
102	6	0	-4.593931	0.265634	-0.010471
103	6	0	-5.126447	1.564411	-0.162480
104	6	0	-6.529878	1.598061	-0.166272
105	6	0	-7.125754	0.326527	-0.014644
106	16	0	-5.888713	-0.924834	0.136280
107	8	0	-4.288843	2.607949	-0.379098
108	6	0	-4.502340	3.841707	0.339845
109	6	0	-5.758503	4.583750	-0.095066
110	6	0	-7.050177	3.901513	0.333281
111	8	0	-7.315297	2.679346	-0.387793
112	1	0	-4.523178	3.626347	1.416806
113	1	0	-3.610110	4.430242	0.118253
114	1	0	-5.736150	5.581381	0.363997
115	1	0	-5.752583	4.724041	-1.181940
116	1	0	-7.913220	4.530271	0.107082
117	1	0	-7.045496	3.684719	1.410080
118	6	0	-8.509755	0.049877	0.000779
119	6	0	-9.106741	-1.222270	0.158085
120	6	0	-10.507535	-1.187521	0.160480
121	6	0	-11.041808	0.115218	0.002408
122	16	0	-9.743764	1.303857	-0.152448
123	8	0	-11.348170	-2.224473	0.385183
124	6	0	-11.140835	-3.470347	-0.315499
125	6	0	-9.882350	-4.206356	0.121983

126	6	0	-8.593586	-3.530969	-0.325641
127	8	0	-8.318555	-2.302024	0.379704
128	1	0	-11.127488	-3.270894	-1.395527
129	1	0	-12.032469	-4.053295	-0.078310
130	1	0	-9.909047	-5.210403	-0.322565
131	1	0	-9.880688	-4.331227	1.210752
132	1	0	-7.729507	-4.158993	-0.101024
133	1	0	-8.608446	-3.325616	-1.404677
134	6	0	-12.405384	0.457077	-0.017709
135	6	0	-12.941252	1.760037	-0.180803
136	6	0	-14.340229	1.791530	-0.187168
137	6	0	-14.933417	0.514204	-0.024620
138	16	0	-13.703720	-0.736656	0.134779
139	8	0	-12.098521	2.795365	-0.395071
140	6	0	-12.332123	4.057251	0.271780
141	6	0	-13.588708	4.774651	-0.200440
142	6	0	-14.879116	4.108853	0.254666
143	8	0	-15.138501	2.857995	-0.420821
144	1	0	-12.361413	3.880979	1.355457
145	1	0	-11.440563	4.640794	0.035667
146	1	0	-13.569699	5.790750	0.216023
147	1	0	-13.580215	4.870106	-1.292156
148	1	0	-15.745059	4.723690	0.004667
149	1	0	-14.874248	3.931357	1.338442
150	6	0	-16.315554	0.246720	0.006700
151	6	0	-16.932635	-1.013989	0.170729
152	6	0	-18.346472	-0.962517	0.192293
153	6	0	-18.829247	0.342788	0.052055
154	16	0	-17.544112	1.513724	-0.085808
155	8	0	-19.193981	-2.001277	0.392668
156	6	0	-19.006025	-3.208319	-0.373490
157	6	0	-17.760753	-3.984382	0.034387
158	6	0	-16.459271	-3.320178	-0.388859
159	8	0	-16.157604	-2.106356	0.342572
160	1	0	-18.985291	-2.956789	-1.442614
161	1	0	-19.906367	-3.791421	-0.171842

162	1	0	-17.801531	-4.970458	-0.447726
163	1	0	-17.763374	-4.150932	1.117605
164	1	0	-15.605210	-3.965208	-0.175142
165	1	0	-16.464951	-3.086064	-1.461623
166	16	0	-20.461751	0.936628	-0.078200
167	6	0	-21.429332	-0.079613	1.106623
168	1	0	-21.023897	0.029631	2.113913
169	1	0	-21.448826	-1.125727	0.809003
170	1	0	-22.435571	0.344740	1.068857

HF= -9065.1847194 hartree

Table S20. Cartesian coordinate of optimized geometry of **12P$_{Hex}^{3+}$** at the UB3LYP/6-31G(d) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.686287	0.169458	-0.010859
2	6	0	1.227547	1.462337	-0.157849
3	6	0	2.632331	1.487232	-0.164796
4	6	0	3.220226	0.215101	-0.022779
5	16	0	1.976330	-1.028317	0.124509
6	8	0	3.419045	2.572038	-0.381843
7	6	0	3.168554	3.772382	0.376530
8	6	0	1.879274	4.477079	-0.024170
9	6	0	0.618618	3.729062	0.388725
10	8	0	0.400733	2.518589	-0.364818
11	1	0	3.167340	3.525520	1.447104
12	1	0	4.034345	4.402975	0.164902
13	1	0	1.864414	5.459913	0.466372
14	1	0	1.871372	4.651010	-1.106208
15	1	0	-0.270101	4.329319	0.184075
16	1	0	0.637985	3.484310	1.459578
17	6	0	4.605654	-0.075342	-0.014247
18	6	0	5.192872	-1.346969	0.125878
19	6	0	6.599233	-1.322333	0.119284

20	6	0	7.139252	-0.031013	-0.025627
21	16	0	5.850608	1.167440	-0.159206
22	8	0	4.406909	-2.433053	0.339333
23	6	0	4.658829	-3.630576	-0.423658
24	6	0	5.948116	-4.336809	-0.025693
25	6	0	7.209130	-3.586395	-0.433485
26	8	0	7.424494	-2.380432	0.327228
27	1	0	4.660278	-3.379192	-1.493156
28	1	0	3.793163	-4.262391	-0.214989
29	1	0	5.963094	-5.317185	-0.521149
30	1	0	5.955364	-4.516135	1.055469
31	1	0	8.097543	-4.187799	-0.230786
32	1	0	7.191206	-3.336445	-1.503186
33	6	0	8.514542	0.309824	-0.046587
34	6	0	9.053443	1.602092	-0.190417
35	6	0	10.459279	1.627684	-0.200409
36	6	0	11.048224	0.355246	-0.063332
37	16	0	9.803294	-0.888725	0.082779
38	8	0	11.244211	2.713413	-0.414480
39	6	0	10.994636	3.912208	0.348011
40	6	0	9.703759	4.617113	-0.046599
41	6	0	8.444689	3.865928	0.365618
42	8	0	8.226700	2.659919	-0.394705
43	1	0	10.997169	3.661797	1.417645
44	1	0	11.859479	4.543653	0.135432
45	1	0	9.689772	5.597690	0.448441
46	1	0	9.693077	4.796022	-1.127793
47	1	0	7.555179	4.466925	0.166382
48	1	0	8.466764	3.615557	1.435143
49	6	0	12.432483	0.068138	-0.057091
50	6	0	13.024265	-1.205304	0.082252
51	6	0	14.426471	-1.177207	0.075892
52	6	0	14.966153	0.121569	-0.069161
53	16	0	13.672312	1.317020	-0.202428
54	8	0	12.236930	-2.289749	0.295872
55	6	0	12.495849	-3.495122	-0.452302

56	6	0	13.785685	-4.192489	-0.041130
57	6	0	15.045004	-3.446187	-0.460181
58	8	0	15.259382	-2.226964	0.281373
59	1	0	12.500984	-3.255730	-1.524555
60	1	0	11.631031	-4.126669	-0.239700
61	1	0	13.804051	-5.180159	-0.521620
62	1	0	13.791917	-4.355634	1.042591
63	1	0	15.935326	-4.041230	-0.248458
64	1	0	15.026334	-3.211294	-1.533144
65	6	0	16.332330	0.460980	-0.091906
66	6	0	16.871715	1.760457	-0.240160
67	6	0	18.272177	1.788421	-0.248923
68	6	0	18.862617	0.512568	-0.100539
69	16	0	17.629049	-0.736022	0.045591
70	8	0	19.065039	2.863257	-0.478179
71	6	0	18.822055	4.085177	0.251441
72	6	0	17.530121	4.775631	-0.163002
73	6	0	16.272772	4.040280	0.280542
74	8	0	16.038117	2.808828	-0.438561
75	1	0	18.827259	3.864488	1.327342
76	1	0	19.687910	4.707092	0.018203
77	1	0	17.516345	5.771750	0.299664
78	1	0	17.515902	4.920055	-1.249296
79	1	0	15.382264	4.635707	0.070573
80	1	0	16.303288	3.819929	1.356194
81	6	0	20.247076	0.239992	-0.078996
82	6	0	20.864172	-1.016494	0.075106
83	6	0	22.281064	-0.964541	0.114604
84	6	0	22.763432	0.337557	-0.029430
85	16	0	21.475783	1.502323	-0.217651
86	8	0	20.092922	-2.109152	0.271917
87	6	0	20.421045	-3.339677	-0.413084
88	6	0	21.700991	-3.993768	0.087029
89	6	0	22.966420	-3.236070	-0.292765
90	8	0	23.114741	-1.993001	0.418631
91	1	0	20.474533	-3.136753	-1.491133

92	1	0	19.557608	-3.979189	-0.220406
93	1	0	21.758567	-4.997274	-0.356074
94	1	0	21.655684	-4.119044	1.174835
95	1	0	23.853437	-3.809194	-0.015770
96	1	0	22.999916	-3.041776	-1.374205
97	16	0	24.381729	0.973304	0.082196
98	6	0	25.454765	-0.355781	-0.583183
99	1	0	25.134008	-0.639972	-1.587295
100	1	0	25.469383	-1.216862	0.082250
101	1	0	26.448568	0.095556	-0.635764
102	6	0	-0.686287	-0.169458	0.010859
103	6	0	-1.227547	-1.462337	0.157849
104	6	0	-2.632331	-1.487232	0.164796
105	6	0	-3.220226	-0.215101	0.022779
106	16	0	-1.976330	1.028317	-0.124509
107	8	0	-3.419045	-2.572038	0.381843
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