

Synthesis of monolayer and persistent bilayer graphene fragments by using a radical-mediated coupling approach

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1. General methods

All chemicals were purchased from commercial suppliers (Sigma-Aldrich, AK Scientific, BLDpharm, etc.) and were used without further purification unless otherwise noted. Anhydrous toluene and THF were distilled from sodium-benzophenone immediately prior to use. Thin layer chromatography (TLC) was performed on silica gel 60 F₂₅₄ (Supelco). Column chromatography was carried out on silica gel (QingdaoHaiyang, 200–300 mesh). Boric acid-impregnated silica gel (B-silica gel) was prepared using a modified literature procedure (*Chem. Lett.* **2012**, 41, 972–973. DOI: 10.1246/cl.2012.972). Silica gel (50 g, QingdaoHaiyang, 200–300 mesh) was immersed in ethanol containing 5% w/v boric acid (200 mL) for 1 h with gentle shaking. After removal of solvent by filtration, the gel was washed with ethanol (200 mL) and hexanes (200 mL), dried by evaporation at 60 °C under reduced pressure over 1 h and used in column chromatography. Triethylamine (TEA) deactivated silica gel (TEA-silica gel) was prepared by the following procedures: Silica gel (100 g, QingdaoHaiyang, 200–300 mesh) was immersed in hexanes (200 mL) containing TEA (10 mL) for 1 h with gentle shaking. After removal of solvent by filtration, the gel was washed with hexanes (200 mL), dried by evaporation at 60 °C under reduced pressure over 1 h and used in column chromatography. Activated Zn dust was prepared by the following procedures: To a 500 mL beaker was added zinc dust (100 g, Sigma-Aldrich, <10 μm) and 0.1 M aq HCl (200 mL). After being stirred for 20 min at room temperature, the precipitate was collected by filtration and washed with distilled water, ethanol, and absolute diethyl ether, finally dried by evaporation at 60 °C under reduced pressure over 1 h.

Nuclear magnetic resonance (NMR). NMR Spectra were recorded at 298 K on Bruker Avance 500 spectrometer, with working frequencies of 500 MHz for ¹H, and 125 MHz for ¹³C nuclei, respectively. ¹⁹F NMR spectrum was recorded at 298 K on Bruker Avance 400 spectrometer with working frequency of 376 MHz. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents (CDCl₃: δ_H = 7.26 ppm, δ_C = 77.16 ppm; (CD₃)₂SO: δ_H = 2.50 ppm, δ_C = 39.52 ppm; C₆D₆: δ_H = 7.16 ppm, δ_C = 128.06 ppm; C₆D₅CD₃: δ_H = 7.09 ppm, δ_C = 20.43 ppm; CD₂Cl₂: δ_H = 5.32 ppm, δ_C = 53.84 ppm; CDCl₂CDCl₂: δ_H = 5.36 ppm, δ_C = 73.38 ppm).

High-resolution mass spectrometry (HRMS). HRMS was measured on an Agilent G6546 Liquid Chromatography Quadrupole-time-of-flight Mass Spectrometry (Q-TOF MS) or a Bruker Autoflex III Smartbeam Matrix-assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry (MALDI-TOF MS) with the parameters.

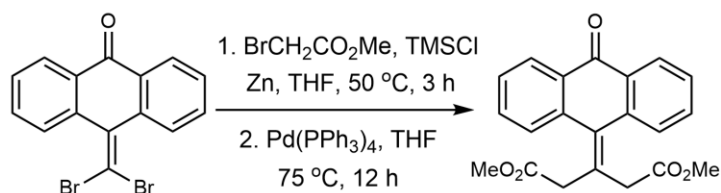
Electron paramagnetic resonance (EPR) spectroscopy. The continuous-wave electron paramagnetic resonance (EPR) spectroscopy was performed at X-band (8-10 GHz) on a JEOL FA200 EPR spectrometer. The VT ESR data was fitted by Bleaney-Bowers equation: $IT = A + C / \{k_B [3 + \exp(-2J/k_B T)]\}$. Where I is the ESR intensity, A and C are constant, k_B is Boltzmann constant, T is the absolute temperature and $-2J$ is correlated to the excitation energy from the ground state to the first excited state.

UV-vis absorption spectroscopy. UV-vis spectra were recorded on a SHIMADZU UV-3600 Plus UV-vis-NIR spectrophotometer.

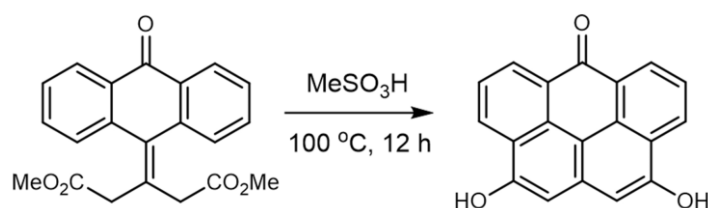
Electrochemical measurements. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were performed in CH₂Cl₂ solutions on an Autolab (Metrohm) potentiostat/galvanostat system equipped with an Ag/AgCl as reference electrode, a gold disk as working electrode, and a Pt wire as counter electrode. Tetrabutylammonium hexafluorophosphate (Bu₄NPF₆, 0.1 M) was used as the supporting electrolyte. The potentials were referenced with the ferrocene/ferrocenium couple used as an internal standard.

2. Synthetic procedures

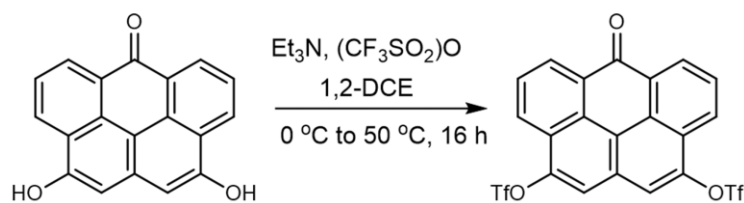
Dibromo **1** was prepared according to literature procedure (*Angew. Chem. Int. Ed.* **2018**, *57*, 16516–16519. DOI: 10.1002/anie.201811314).



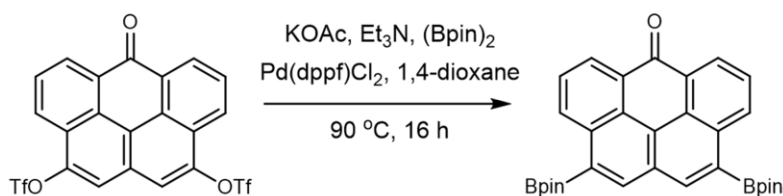
2: Activated Zn dust (2.7 g, 41 mmol) was added to an oven-dried round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N_2 . The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N_2 . Freshly distilled THF (45 mL) and chlorotrimethylsilane (200 μL , 1.58 mmol) were added. The suspension was stirred at room temperature (rt) for 30 min, then methyl bromoacetate (2.0 mL, 21 mmol) was added dropwise at rt. The suspension was further stirred at $50\text{ }^\circ\text{C}$ for 3 h. After cooling to room temperature and zinc powder precipitated, the yellow supernatant solution was transferred to an oven-dried round-bottom flask containing **1** (1.50 g, 4.12 mmol) and $\text{Pd}(\text{PPh}_3)_4$ (0.70 g, 0.61 mmol) by a syringe under N_2 atmosphere. The mixture was further stirred at $75\text{ }^\circ\text{C}$ for 12 h. After cooling to room temperature, the solvent was removed by evaporation under reduced pressure. The residue was poured into water and then extracted with ethyl acetate (2 x 100 mL). The resulting organic extract was washed with brine (3 x 100 mL), dried over anhydrous Na_2SO_4 , and then concentrated to give the crude product. Purification by column chromatography (hexanes/ethyl acetate (6:1); silica gel) yielded the pure **2** (0.66g, 46%) as light brown oil. ^1H NMR (500 MHz, CDCl_3 , 298 K, δ ppm): 8.09 (ddd, $J_1 = 7.6\text{ Hz}$, $J_2 = 1.5\text{ Hz}$, $J_3 = 0.5\text{ Hz}$, 2H), 7.79 (ddd, $J_1 = 7.7\text{ Hz}$, $J_2 = 1.2\text{ Hz}$, $J_3 = 0.5\text{ Hz}$, 2H), 7.55 (dt, $J_1 = 7.6\text{ Hz}$, $J_2 = 1.5\text{ Hz}$, 2H), 7.46 (dt, $J_1 = 7.5\text{ Hz}$, $J_2 = 1.2\text{ Hz}$, 2H), 3.75 (s, 6H), 3.54 (s, 4H). ^{13}C NMR (125 MHz, CDCl_3 , 298 K, δ ppm): 186.2, 171.5, 139.3, 135.7, 133.4, 131.4, 128.1, 127.6, 127.3, 127.0, 52.4, 41.2. HRMS (APCI, m/z): calcd for $\text{C}_{21}\text{H}_{19}\text{O}_5$ $[\text{M}+\text{H}]^+$, 351.1227; found 351.1234.



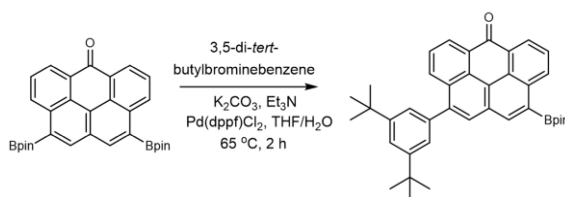
3: **2** (1.32 g, 3.77 mmol) was dissolved in methanesulfonic acid (100 mL). The mixture was stirred at $100\text{ }^\circ\text{C}$ under N_2 atmosphere for 12 h. After cooling to room temperature, 500 mL ice water was added to it and stirred rigorously for 2 h. The orange precipitate was collected by filtration, and washed several times with water, and dried under vacuum. **3** was obtained as orange solid (0.97 g, 90%). ^1H NMR (500 MHz, $(\text{CD}_3)_2\text{SO}$, 298 K, δ ppm): 10.97 (s, 2H), 8.63–8.67 (m, 4H), 7.82 (t, $J = 7.7\text{ Hz}$, 2H), 7.14 (s, 2H). ^{13}C NMR (125 MHz, $(\text{CD}_3)_2\text{SO}$, 298 K, δ ppm): 183.3, 154.8, 136.4, 129.4, 129.1, 128.7, 128.0, 124.8, 123.8, 108.2, 105.7. HRMS (ESI, m/z): calcd for $\text{C}_{19}\text{H}_{11}\text{O}_3$ $[\text{M}+\text{H}]^+$, 287.0703; found 287.0705.



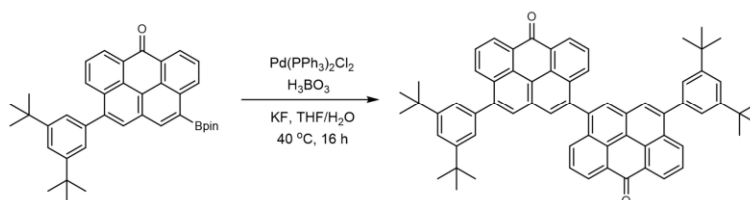
4: 3 (0.50 g, 1.75 mmol) was dispersed in anhydrous 1,2-dichloroethane (100 mL) and stirred for 30 min at 0 °C. Then triethylamine (2.40 mL, 17.2 mmol) was added dropwise to the mixture at 0 °C under N₂ atmosphere. Then trifluoromethanesulfonic anhydride (1.76 mL, 10.5 mmol) was added dropwise to the reaction mixture at 0 °C under N₂ atmosphere. The mixture was slowly heated to 50 °C and stirred overnight. After cooling to room temperature, the reaction was quenched by adding brine (100 mL). The precipitate in the mixture was collected by filtration, and washed with excess amount of water, recovering the **3** (0.15 g, 0.52 mmol, 30%). Organic layer in the mixture was extracted with CH₂Cl₂ and washed with brine (3 x 50 mL), dried by anhydrous Na₂SO₄. After removal of the solvent under vacuum, the crude material was subjected to column chromatography (CH₂Cl₂; silica gel) to afford the **4** (414 mg, 43%) as light-yellow solid. ¹H NMR (500 MHz, CDCl₃, 298 K, δ ppm): 8.98 (dd, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 2H), 8.60 (dd, J_1 = 8.2 Hz, J_2 = 1.2 Hz, 2H), 8.09 (dd, J_1 = 8.2 Hz, J_2 = 7.5 Hz, 2H), 8.03 (s, 2H). ¹³C NMR (125 MHz, CDCl₃, 298 K, δ ppm): 183.1, 146.5, 131.4, 130.2, 129.7, 129.3, 129.2, 128.2, 125.2, 120.8, 120.2, 118.2, 117.6. ¹⁹F NMR (376 MHz, CDCl₃, 298 K, δ ppm): 72.81. HRMS (ESI, m/z): calcd for C₂₁H₉F₆O₇S₂ [M+H]⁺, 550.9688; found 550.9690.



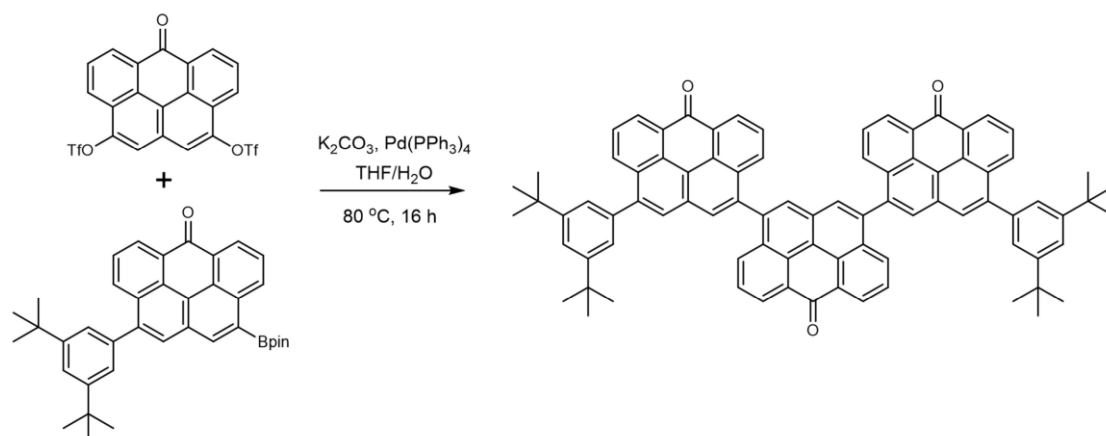
5: 4 (0.75 g, 1.36 mmol), KOAc (1.35 g, 13.8 mmol), triethylamine (1.8 mL, 13 mmol), bis(pinacolato)diboron (2.10 g, 8.27 mmol), and Pd(dppf)Cl₂ (0.15 g, 0.21 mmol) were dispersed in 1,4-dioxane (30 mL). The mixture was bubbling with N₂ for 1 h. Then the mixture was heated to 90 °C and stirred for 16 h under N₂ atmosphere. After cooling to room temperature, the solvent (1,4-dioxane) was removed by evaporation under reduced pressure. The residue was poured into water and then extracted with CH₂Cl₂ (100 mL). The resulting organic extract was washed with brine (3 x 100 mL), dried over anhydrous Na₂SO₄, and then concentrated. Purification by column chromatography (CH₂Cl₂; B-silica gel) yielded the crude product as yellow solid. The crude product was washed by excess hexanes, finally collected by filtration to give the pure **5** as light-yellow solid (0.53g, 77%). ¹H NMR (500 MHz, CDCl₃, 298 K, δ ppm): 9.25 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 8.86 (dd, J_1 = 7.3 Hz, J_2 = 1.3 Hz, 2H), 8.71 (s, 2H), 7.92 (dd, J_1 = 8.1 Hz, J_2 = 7.3 Hz, 2H), 1.49 (s, 24H). ¹³C NMR (125 MHz, CDCl₃, 298 K, δ ppm): 184.9, 138.2, 135.6, 134.7, 130.05, 129.99, 128.9, 128.0, 127.5, 124.9, 84.4, 25.2. HRMS (ESI, m/z): calcd for C₃₁H₃₃B₂O₅ [M+H]⁺, 507.2509; found 507.2518.



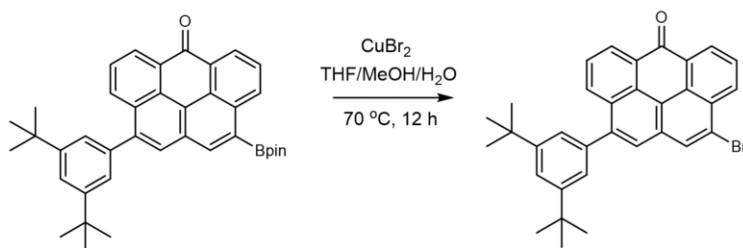
6: **5** (0.52 g, 1.03 mmol), K_2CO_3 (0.71 g, 5.14 mmol), $Pd(dppf)Cl_2$ (45 mg, 0.06 mmol) and 1-bromo-3,5-di-*tert*-butylbenzene (92 mg, 0.34 mmol) were added to a round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N_2 . The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N_2 . THF (15 mL), triethylamine (0.48 mL, 3.4 mmol) and H_2O (1.5 mL) were added. The reaction mixture was further degassed by three freeze-pump-thaw cycles. The reaction mixture was then stirred at 65 °C under an N_2 atmosphere for 2 h. After cooling to room temperature, the reaction mixture was poured into water (50 mL) and then extracted with CH_2Cl_2 (2 x 50 mL). The resulting organic extract was washed with brine (3 x 50 mL), dried over anhydrous Na_2SO_4 , and then concentrated to give the crude product. Purification by column chromatography (from 2% to 10% v/v ethyl acetate in hexanes; B-silica gel) yielded the pure **6** as yellow solid (130 mg, 66%). Together with **6**, **5** was recovered (0.19 g, 0.37 mmol, 36 %). ^1H NMR (500 MHz, $CDCl_3$, 298 K, δ ppm): 9.28 (dd, $J_1 = 8.1$ Hz, $J_2 = 1.2$ Hz, 1H), 8.90 (dd, $J_1 = 7.3$ Hz, $J_2 = 1.2$ Hz, 1H), 8.88 (dd, $J_1 = 7.3$ Hz, $J_2 = 1.2$ Hz, 1H), 8.65 (s, 1H), 8.43 (dd, $J_1 = 8.2$ Hz, $J_2 = 1.2$ Hz, 1H), 8.04 (s, 1H), 7.92 (t, $J = 7.7$ Hz, 1H), 7.85 (t, $J = 7.8$ Hz, 1H), 7.59 (t, $J = 1.8$ Hz, 1H), 7.47 (d, $J = 1.8$ Hz, 2H), 1.51 (s, 12H), 1.44 (s, 18H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K, δ ppm): 184.9, 151.0, 142.4, 139.1, 137.7, 135.8, 134.1, 133.5, 131.1, 130.8, 130.3, 129.7, 129.2, 129.1, 128.5, 128.1, 128.0, 127.2, 127.0, 125.0, 122.3, 121.8, 84.4, 35.2, 31.7, 25.2. HRMS (APCI, m/z): calcd for $C_{39}H_{42}BO_3$ $[M+H]^+$, 569.3222; found 569.3230.



7: **6** (80 mg, 0.14 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (15 mg, 0.02 mmol, 0.15 equiv), and boric acid (44 mg, 0.71 mmol, 5.0 equiv) were dissolved in THF (25 mL). The mixture was then stirred vigorously for 10 min. Potassium fluoride (18 mg, 0.31 mmol, 2.2 equiv) was added to the mixture followed by the addition of water (2.5 mL). The reaction mixture was further stirred at 40 °C under atmosphere for 16 h. The THF was removed by evaporation and the resulting solution was extracted with CH_2Cl_2 (3 x 50 mL). The combined organic layers were washed with brine (3 x 50 mL) then dried over anhydrous Na_2SO_4 and concentrated. Purification by column chromatography (5% v/v ethyl acetate in hexanes; silica gel) yielded **7** as yellow solid (40 mg, 64%). ^1H NMR (500 MHz, $CDCl_3$, 298 K, δ ppm): 8.98 (dd, $J_1 = 7.5$ Hz, $J_2 = 1.3$ Hz, 2H), 8.93 (dd, $J_1 = 7.4$ Hz, $J_2 = 1.2$ Hz, 2H), 8.47 (dd, $J_1 = 8.3$ Hz, $J_2 = 1.2$ Hz, 2H), 8.24 (s, 2H), 8.06 (s, 2H), 7.99 (dd, $J_1 = 8.2$ Hz, $J_2 = 1.3$ Hz, 2H), 7.90 (dd, $J_1 = 8.3$ Hz, $J_2 = 0.9$ Hz, 2H), 7.72 (dd, $J_1 = 8.2$ Hz, $J_2 = 0.8$ Hz, 2H), 7.60 (t, $J = 1.8$ Hz, 2H), 7.49 (d, $J = 1.8$ Hz, 4H), 1.43 (s, 36H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K, δ ppm): 184.7, 151.1, 143.3, 139.0, 138.9, 133.8, 133.7, 131.5, 131.4, 130.9, 130.1, 130.0, 129.7, 129.6, 129.4, 128.7, 128.5, 127.6, 127.11, 127.10, 124.8, 122.0, 120.7, 35.2, 31.7. HRMS (ESI, m/z): calcd for $C_{66}H_{59}O_2$ $[M+H]^+$, 883.451; found 883.4504.

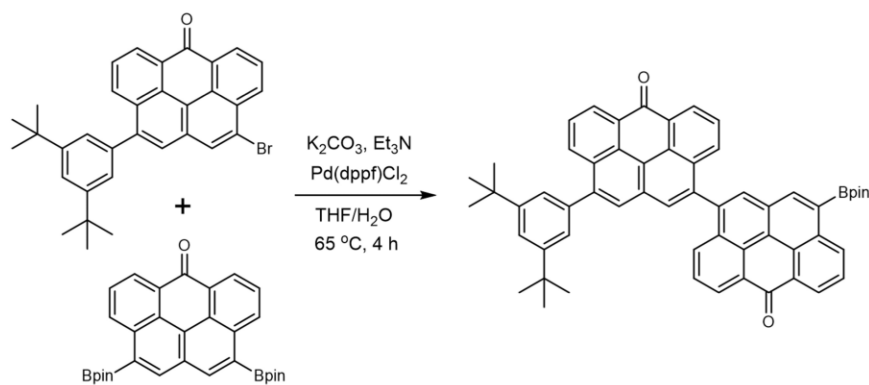


10: 4 (50 mg, 0.09 mmol, 1.0 equiv), K_2CO_3 (300 mg, 2.17 mmol), $Pd(PPh_3)_4$ (25 mg, 0.02 mmol) and **6** (120 mg, 0.21 mmol, 2.3 equiv) were added to a round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N_2 . The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N_2 . THF (25 mL) and H_2O (2.0 mL) were added. The reaction mixture was bubbled with N_2 for 1 h. The reaction mixture was further stirred at 80 °C under an N_2 atmosphere for 16 h. After cooling to room temperature, the reaction mixture was poured into water (100 mL) and then extracted with CH_2Cl_2 (2 x 50 mL). The resulting organic extract was washed with brine (3 x 50 mL), dried over anhydrous Na_2SO_4 , and then concentrated. Purification by column chromatography (20% v/v ethyl acetate in hexanes; silica gel) yielded the crude product with around 90 % purity. The crude product was further dissolved in $CHCl_3$ and purified by preparative GPC to give the pure **10** as yellow solid (83 mg, 81%). Note: It was observed by TLC and column chromatography that **10** has two conformational isomers with different polarities. The two conformational isomers of **10** have very similar NMR spectra. ^1H NMR (500 MHz, $CDCl_3$, 298 K, δ ppm): 8.96–9.00 (m, 4H), 8.94 (dd, $J_1 = 7.4$ Hz, $J_2 = 1.0$ Hz, 2H), 8.45–8.48 (m, 2H), 8.28 (s, 2H), 8.25 (s, 2H), 8.01–8.08 (m, 6H), 7.90 (t, $J = 7.9$ Hz, 2H), 7.72–7.80 (m, 4H), 7.58–7.61 (m, 2H), 7.47–7.50 (m, 4H), 1.41–1.44 (m, 36H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K, δ ppm): 184.7, 184.6, 151.1, 143.3, 139.4, 139.0, 138.7, 133.8, 133.6, 131.8, 131.4, 131.3, 131.1, 130.9, 130.12, 130.07, 129.99, 129.92, 129.71, 129.65, 129.4, 129.2, 128.7, 128.5, 127.58, 127.53, 127.2, 124.8, 122.0, 121.5, 120.7, 35.2, 31.7. HRMS (ESI, m/z): calcd for $C_{85}H_{67}O_3$ $[M+H]^+$, 1135.5085; found 1135.5082.

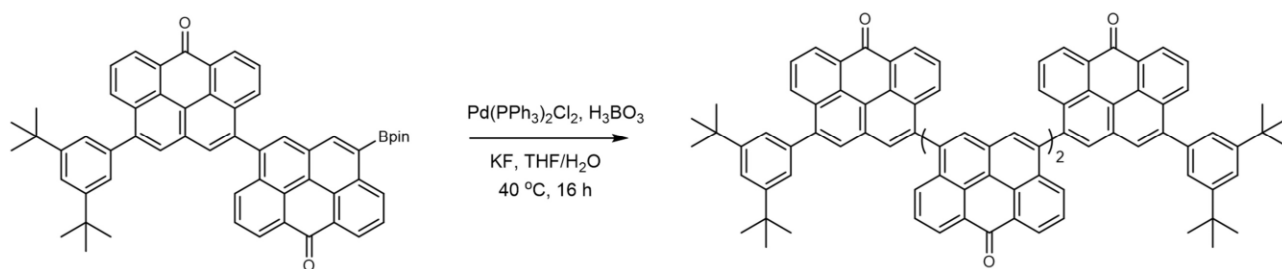


15: 6 (110 mg, 0.19 mmol) was dissolved in a mixture solvent consisting of THF (20 mL) and MeOH (40 mL). Copper (II) bromide (216 mg, 0.97 mmol) in water (10 mL) was added and the mixture was stirred at 70 °C for 12 h. After cooling to room temperature, the solvents (THF and MeOH) were removed by evaporation under reduced pressure. The residue was poured into water and then extracted with CH_2Cl_2 (2 x 50 mL). The resulting organic extract was washed with brine (3 x 50 mL),

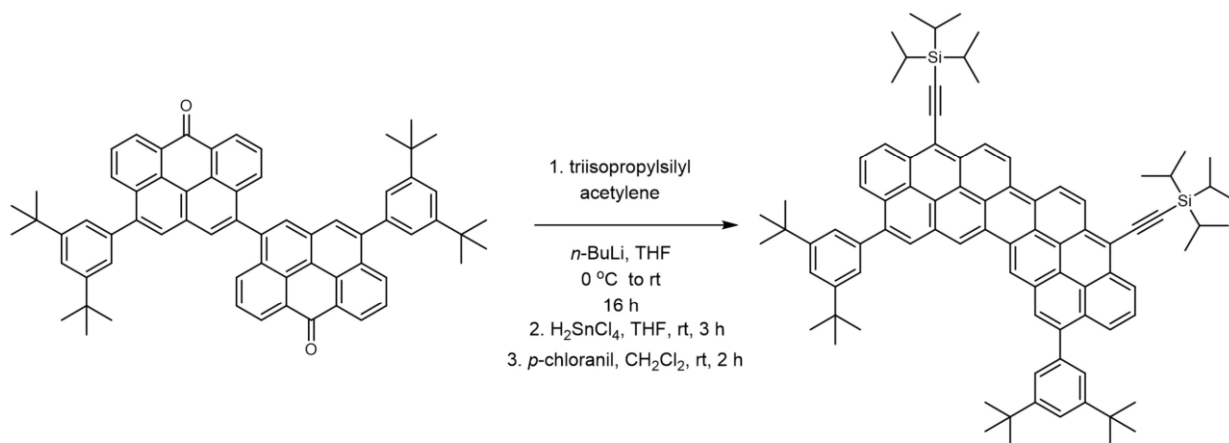
dried over anhydrous Na₂SO₄, and then concentrated. Purification by column chromatography (10% v/v ethyl acetate in hexanes; silica gel) yielded **15** as yellow solid (100 mg, quantitative yield). ¹H NMR (500 MHz, CDCl₃, 298 K, δ ppm): 8.90 (dd, $J_1 = 7.4$ Hz, $J_2 = 1.3$ Hz, 1H), 8.86 (dd, $J_1 = 7.4$ Hz, $J_2 = 1.3$ Hz, 1H), 8.72 (dd, $J_1 = 8.2$ Hz, $J_2 = 1.3$ Hz, 1H), 8.38 (dd, $J_1 = 8.2$ Hz, $J_2 = 1.3$ Hz, 1H), 8.30 (s, 1H), 7.94 (dd, $J_1 = 8.2$ Hz, $J_2 = 7.4$ Hz, 1H), 7.86 (s, 1H), 7.84 (dd, $J_1 = 8.2$ Hz, $J_2 = 7.3$ Hz, 1H), 7.59 (t, $J = 1.8$ Hz, 1H), 7.44 (d, $J = 1.8$ Hz, 2H), 1.43 (s, 18H). ¹³C NMR (125 MHz, CDCl₃, 298 K, δ ppm): 183.6, 151.1, 143.1, 138.8, 133.8, 133.7, 131.8, 130.6, 130.5, 129.9, 129.6, 129.44, 129.40, 129.37, 128.8, 128.2, 127.3, 126.9, 126.5, 124.9, 124.0, 122.0, 119.6, 35.2, 31.8. HRMS (APCI, m/z): calcd for C₃₃H₂₉BrO [M]⁺, 520.1407; found 520.1408.



16: 5 (175 mg, 0.35 mmol), K₂CO₃ (238 mg, 1.72 mmol), Pd(dppf)Cl₂ (20 mg, 0.03 mmol) and **15** (60 mg, 0.12 mmol) were added to a round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N₂. The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N₂. THF (15 mL), triethylamine (0.16 mL, 1.2 mmol) and H₂O (1.5 mL) were added. The reaction mixture was further degassed by three freeze-pump-thaw cycles. The reaction mixture was then stirred at 65 °C under an N₂ atmosphere for 4 h. After cooling to room temperature, the reaction mixture was poured into water (50 mL) and then extracted with CH₂Cl₂ (2 x 50 mL). The resulting organic extract was washed with brine (3 x 50 mL), dried over anhydrous Na₂SO₄, and then concentrated. Purification by column chromatography (from 5% to 10% v/v ethyl acetate in hexanes; B-silica gel) yielded the crude product with around 90 % purity. The crude product was further dissolved in CHCl₃ and purified by preparative GPC to give the pure **16** as yellow solid (60 mg, 64%). ¹H NMR (500 MHz, CDCl₃, 298 K, δ ppm): 9.34 (dd, $J_1 = 8.2$ Hz, $J_2 = 1.3$ Hz, 1H), 8.99 (dd, $J_1 = 7.4$ Hz, $J_2 = 1.3$ Hz, 1H), 8.90–8.96 (m, 3H), 8.72 (s, 1H), 8.48 (dd, $J_1 = 8.3$ Hz, $J_2 = 1.3$ Hz, 1H), 8.25 (s, 1H), 8.20 (s, 1H), 8.05 (s, 1H), 7.96–8.00 (m, 3H), 7.91 (t, $J = 7.9$ Hz, 1H), 7.69–7.75 (m, 2H), 7.59 (t, $J = 1.8$ Hz, 1H), 7.49 (d, $J = 1.8$ Hz, 2H), 1.50 (s, 12H), 1.48 (s, 18H). ¹³C NMR (125 MHz, CDCl₃, 298 K, δ ppm): 184.82, 184.78, 151.1, 143.3, 139.0, 138.9, 138.4, 137.6, 136.0, 134.4, 133.9, 133.6, 133.5, 132.1, 131.5, 131.4, 130.9, 130.5, 130.3, 130.1, 130.0, 129.9, 129.70, 129.65, 129.5, 129.41, 129.39, 128.7, 128.5, 128.4, 128.2, 127.65, 127.61, 127.5, 127.15, 127.12, 124.9, 123.2, 122.0, 120.7, 84.5, 35.2, 31.7, 25.2. HRMS (APCI, m/z): calcd for C₅₈H₅₀BO₄ [M+H]⁺, 821.3797; found 821.3804.

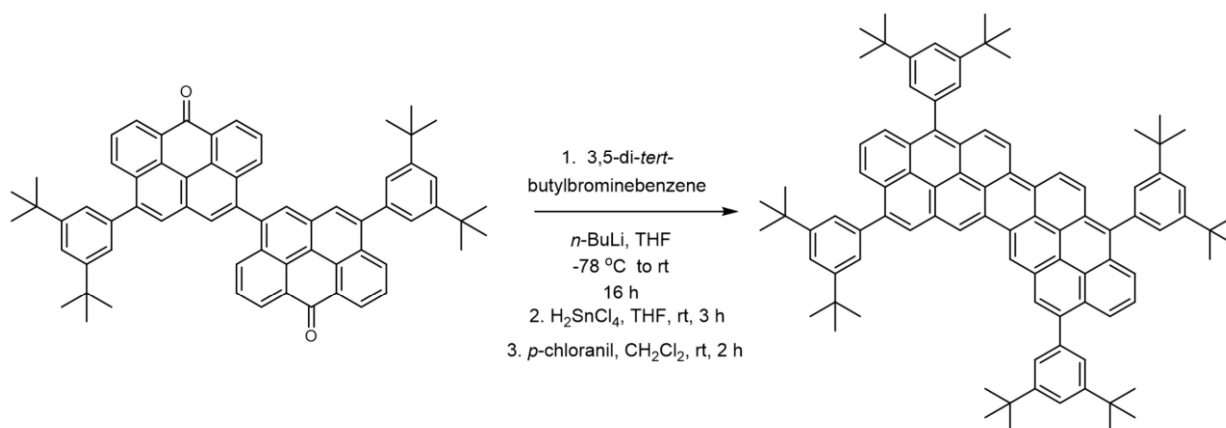


17: **16** (16 mg, 0.020 mmol, 1.0 equiv), Pd(PPh₃)₂Cl₂ (5.5 mg, 0.008 mmol, 0.4 equiv), and boric acid (10 mg, 0.16 mmol, 8.1 equiv) were dissolved in THF (10 mL). The mixture was then stirred vigorously for 10 min. Potassium fluoride (6 mg, 0.10 mmol, 5.2 equiv) was added to the mixture followed by the addition of water (1.0 mL). The reaction mixture was further stirred at 40 °C under atmosphere for 16 h. The THF was removed by evaporation and the resulting solution was extracted with CH₂Cl₂ (2 x 50 mL). The combined organic layers were washed with brine (3 x 50 mL) then dried over anhydrous Na₂SO₄ and concentrated. Purification by column chromatography (5% v/v ethyl acetate in CH₂Cl₂; silica gel) yielded the crude product with around 90 % purity. The crude product was further dissolved in CHCl₃ and purified by preparative GPC to give the pure **17** as yellow solid (10 mg, 74%). It was observed by TLC and column chromatography that **17** has three conformational isomers with different polarities. ¹H NMR (500 MHz, CDCl₂CDCl₂, 298 K, δ ppm): 8.24–8.39 (m, 8H), 7.86–7.93 (m, 2H), 7.43–7.64 (m, 6H), 7.40–7.55 (m, 8H), 7.27–7.33 (m, 2H), 7.09–7.24 (m, 6H), 6.90–6.96 (m, 2H), 6.81–6.88 (m, 4H), 0.75–0.82 (m, 36H). ¹³C NMR (125 MHz, CDCl₂CDCl₂, 298 K, δ ppm): 184.0, 183.9, 150.3, 142.8, 138.65, 138.61, 138.45, 138.42, 138.38, 138.02, 138.00, 137.98, 137.89, 133.5, 133.3, 133.09, 133.05, 131.04, 131.00, 130.8, 130.7, 130.56, 130.52, 130.2, 129.36, 129.33, 129.25, 129.1, 128.94, 128.86, 128.76, 128.66, 127.9, 127.76, 127.71, 127.0, 126.6, 124.1, 121.4, 120.8, 119.8, 34.4, 31.1. HRMS (APCI, m/z): calcd for C₁₀₄H₇₅O₄ [M+H]⁺, 1387.566; found 1387.5654.



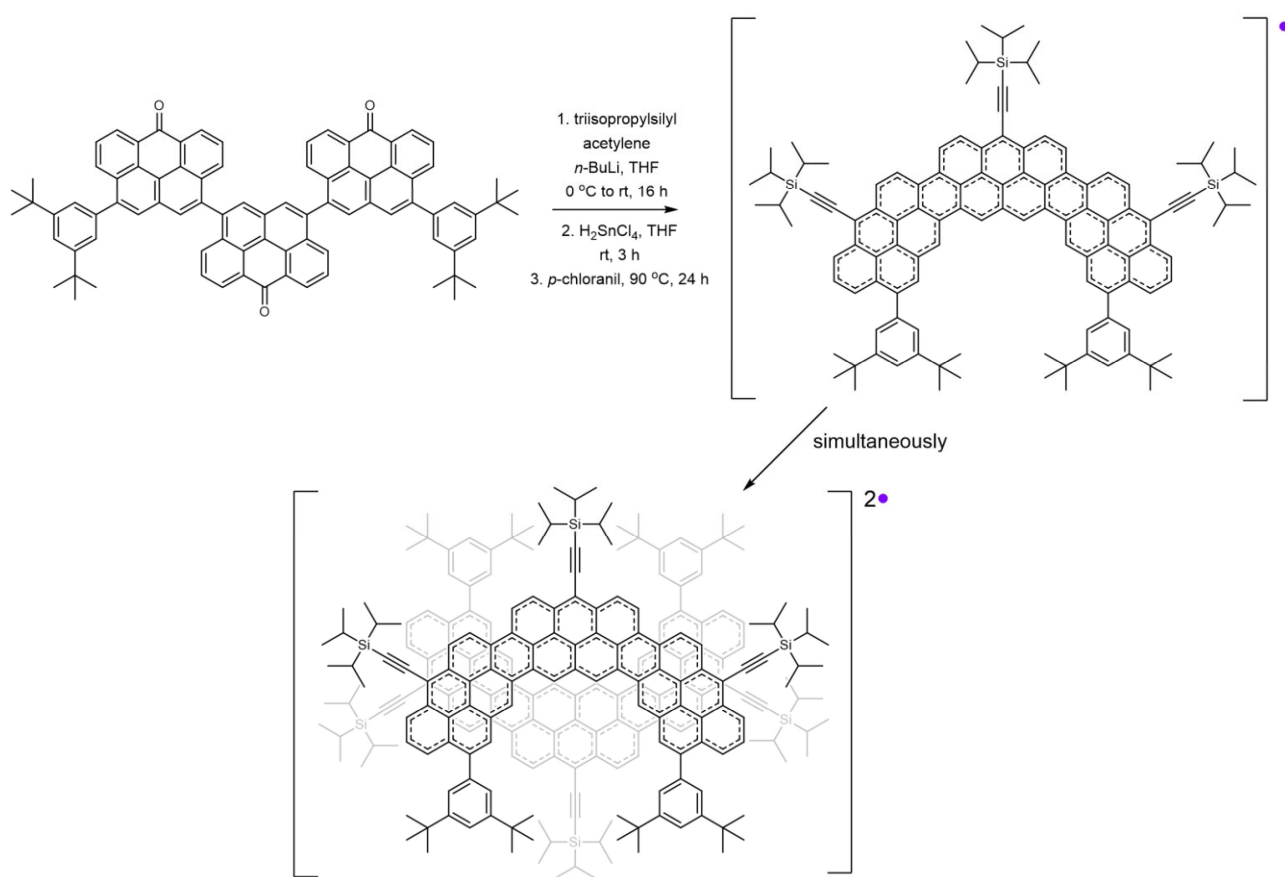
tips-OR-2: Triisopropylsilylacetylene (152 μ L, 0.68 mmol, 30.0 equiv) was dissolved in 5 mL of anhydrous THF, then the solution was cooled to 0 °C by ice bath and kept under N₂ atmosphere. *n*-BuLi in cyclohexane (2.0 M, 226 μ L, 0.45 mmol, 20.0 equiv) was added dropwise at 0 °C. The reaction mixture was stirred for 2 hours at 0 °C and a solution of **7** (20.0 mg, 0.023 mmol) in anhydrous THF (5 mL) was added dropwise. The reaction mixture was warmed to room temperature slowly and stirred for 16 hours. A solution of H₂SnCl₄ in THF was prepared by dissolving anhydrous SnCl₂ (86.0 mg, 0.45 mmol, 20.0 equiv) in anhydrous THF (2 mL) then adding concentrated aqueous HCl (75 μ L, 0.90 mmol, 40.0 equiv) and stirring for 30 min at rt and under N₂ atmosphere. Subsequently, the

H₂SnCl₄ solution was added into the above-mentioned reaction mixture. After addition, the color of the reaction mixture became orange instantaneously and then became green in several minutes. This dark green solution was stirred for additional 3 h. Water (50 mL) was then added to the reaction mixture and the crude organic solids was extracted with CH₂Cl₂ (2 x 50 mL). The resulting organic extract was washed with water (3 x 50 mL), dried over anhydrous Na₂SO₄, and then concentrated. The concentrated crude product was washed with CH₃CN (5 mL) to remove excess triisopropylsilylacetylene and the light-green supernatant was discarded. The blue solid residue was dissolved in CH₂Cl₂ (3 mL), then *p*-chloranil (27.8 mg, 0.11 mmol) was added. The solution was stirred vigorously at rt. The color of the reaction mixture became dark blue immediately. The dark blue solution was stirred for additional 2 h and then concentrated. Purification by column chromatography (10% v/v CH₂Cl₂ in hexanes; silica gel) yielded **tips-OR-2** as dark blue solid (21 mg, 77%). ¹H NMR (500 MHz, C₆D₆, 298 K, δ ppm): 10.00 (s, 2H), 9.59 (d, *J* = 7.9 Hz, 2H), 9.38 (d, *J* = 9.5 Hz, 2H), 8.91 (d, *J* = 9.9 Hz, 2H), 8.64 (d, *J* = 7.5 Hz, 2H), 8.53 (s, 2H), 8.07 (t, *J* = 7.8 Hz, 2H), 7.94 (d, *J* = 1.8 Hz, 4H), 7.84 (t, *J* = 1.8 Hz, 2H), 1.50–1.54 (m, 42H), 1.49 (s, 36H). ¹³C NMR (125 MHz, C₆D₆, 298 K, δ ppm) (one signal could not be detected because of the signal overlap): 151.5, 142.4, 141.0, 134.5, 132.24, 132.20, 130.6, 129.2, 127.4, 127.2, 127.1, 126.2, 125.5, 125.2, 124.9, 124.1, 123.5, 122.9, 122.4, 122.3, 122.0, 116.9, 105.9, 104.2, 35.3, 31.8, 19.4, 12.2. HRMS (APCI, *m/z*): calcd for C₈₈H₉₉Si₂ [M+H]⁺, 1211.728; found 1211.7282.



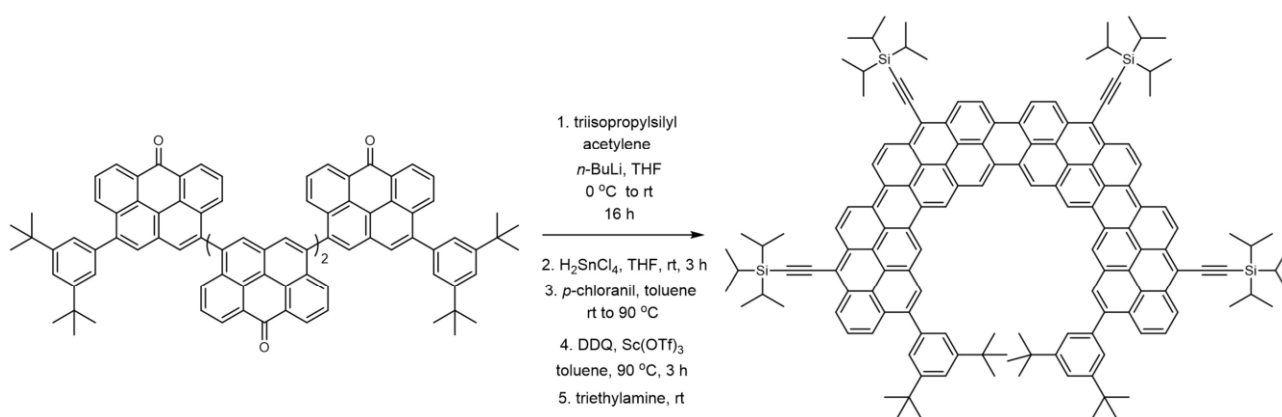
dtbp-OR-2: 3,5-di-*tert*-butylbenzene (43 mg, 0.16 mmol, 15 equiv) was dissolved in 5 mL of anhydrous THF, then the solution was cooled to -78 °C by dry ice/acetone bath and kept under N₂ atmosphere. *n*-BuLi in cyclohexane (2.0 M, 55 μ L, 0.11 mmol, 10 equiv) was added dropwise at -78 °C. The reaction mixture was stirred for 16 hours at -78 °C and a solution of **7** (9.5 mg, 0.011 mmol) in anhydrous THF (5 mL) was added dropwise. The reaction mixture was warmed to room temperature slowly and stirred for 3 hours. A solution of H₂SnCl₄ in THF was prepared by dissolving anhydrous SnCl₂ (46.0 mg, 0.24 mmol, 22 equiv) in anhydrous THF (2 mL) then adding concentrated aqueous HCl (40 μ L, 0.48 mmol, 44 equiv) and stirring for 30 min at rt and under N₂ atmosphere. Subsequently, the H₂SnCl₄ solution was added into the above-mentioned reaction mixture. After addition, the color of the reaction mixture became orange instantaneously and then became green in several minutes. This green solution was stirred for additional 3 h. Water (50 mL) was then added to the reaction mixture and the crude organic solids was extracted with CH₂Cl₂ (2 x 50 mL). The resulting organic extract was washed with water (3 x 50 mL), dried over anhydrous Na₂SO₄, and then concentrated. The concentrated crude product was washed with CH₃CN (5 mL) to remove excess

3,5-di-*tert*-butylbenzene and the light-green supernatant was discarded. The blue solid residue was dissolved in CH₂Cl₂ (5 mL), then *p*-chloranil (13.9 mg, 0.056 mmol) was added. The solution was stirred vigorously at rt. The color of the reaction mixture became pink immediately. The pink solution was stirred for additional 2 h and then concentrated. Purification by column chromatography (10% v/v CH₂Cl₂ in hexanes; silica gel) yielded **dtbp-OR-2** as blue solid (2 mg, 15%). ¹H NMR (500 MHz, C₆D₅CD₃, 298 K, δ ppm): 10.21 (s, 2H), 8.63 (d, *J* = 9.0 Hz, 2H), 8.62 (s, 2H), 8.58 (d, *J* = 7.5 Hz, 2H), 8.52 (d, *J* = 7.5 Hz, 2H), 8.28 (d, *J* = 10.0 Hz, 2H), 7.95 (d, *J* = 2.0 Hz, 4H), 7.87 (t, *J* = 1.8 Hz, 2H), 7.83 (t, *J* = 7.8 Hz, 2H), 7.80 (t, *J* = 2.0 Hz, 2H), 7.78 (d, *J* = 2.0 Hz, 4H), 1.50 (s, 36H), 1.48 (s, 36H). ¹³C NMR (125 MHz, C₆D₅CD₃, 298 K, δ ppm) (three signals could not be detected because of the signal overlap): 151.5, 151.4, 142.2, 141.4, 139.5, 132.2, 131.9, 130.7, 129.9, 129.5, 127.6, 126.8, 126.32, 126.27, 125.9, 124.7, 124.6, 124.4, 124.3, 124.2, 122.9, 122.8, 121.8, 121.6, 121.5, 35.3, 31.8, 1.4. HRMS (MALDI-TOF, *m/z*): calcd for C₉₄H₉₈ [M]⁺, 1227.77; found 1227.83.



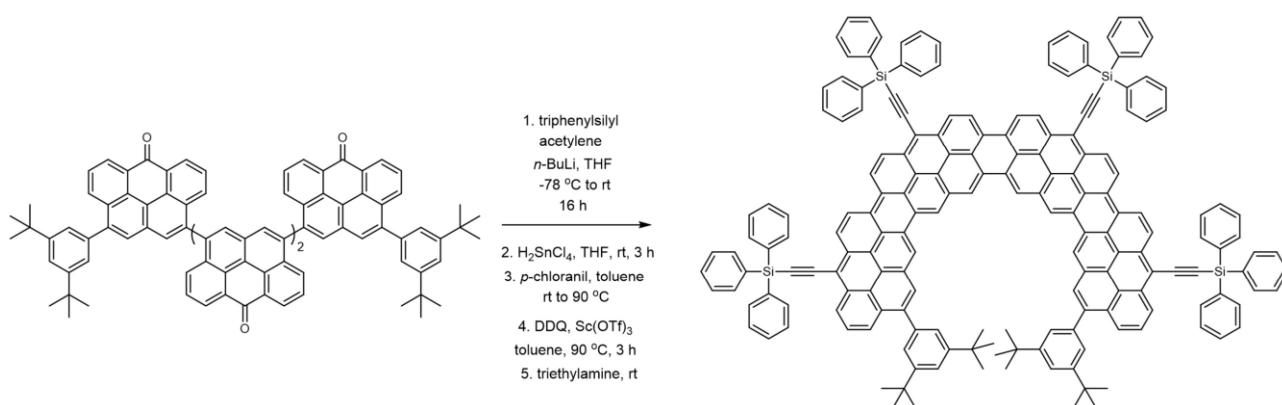
tips-OR-3: Triisopropylsilylacetylene (190 μ L, 0.85 mmol, 45.0 equiv) was dissolved in 5 mL of anhydrous THF, then the solution was cooled to 0 °C by ice bath and kept under N₂ atmosphere. n -BuLi in cyclohexane (2.0 M, 280 μ L, 0.56 mmol, 30.0 equiv) was added dropwise at 0 °C. The reaction mixture was stirred for 2 hours at 0 °C and a solution of **10** (21.0 mg, 0.018 mmol) in anhydrous THF (5 mL) was added dropwise. The reaction mixture was warmed to room temperature slowly and stirred for 16 hours. A solution of H₂SnCl₄ in THF was prepared by dissolving anhydrous SnCl₂ (105.0 mg, 0.55 mmol, 30.0 equiv) in anhydrous THF (4 mL) then adding concentrated aqueous HCl (93 μ L, 1.10 mmol, 60.0 equiv) and stirring for 30 min at rt and under N₂ atmosphere. Subsequently, the H₂SnCl₄ solution was added into the above-mentioned reaction mixture. After addition, the color of

the reaction mixture became orange instantaneously and then became green in several minutes. This dark green solution was stirred for additional 3 h. Water (50 mL) was then added to the reaction mixture and the crude organic solids were extracted with CH₂Cl₂ (2 x 50 mL). The resulting organic extract was washed with water (3 x 50 mL), dried over anhydrous Na₂SO₄, and then concentrated. The concentrated dark green solid and *p*-chloranil (46 mg, 0.18 mmol, 10.0 equiv) were added to a round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N₂. The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N₂. Dry toluene (10 mL) was added. The reaction mixture was stirred for 24 hours at 90 °C. After cooling to room temperature, the solvent (toluene) was removed by evaporation under reduced pressure. The concentrated crude product was washed with CH₃CN (5 mL) to remove excess triisopropylsilylacetylene and the blue supernatant was discarded. The residue was further dissolved in a small amount of mixture of solvents (hexanes : CH₂Cl₂ 7:3, 3 mL) and purified by column chromatography (initially, 100% hexanes as eluent to remove byproducts; then 30% v/v CH₂Cl₂ in hexanes as eluent to remove decomposition; finally, 100:30:4 v/v/v hexanes : CH₂Cl₂ : ethyl acetate; TEA-silica gel) to give the pure **tips-OR-3** as black solid (8 mg, 27%). Further experiments disclosed that **tips-OR-3** simultaneously assembled as its persistent π -dimer – [**tips-OR-3**]₂ in solution and solid-state. Thus, the isolated **tips-OR-3** actually is [**tips-OR-3**]₂. Owing to the paramagnetic property of **tips-OR-3**, only a set of broad peaks corresponding to the [**tips-OR-3**]₂ was observed below 253K. ¹H NMR (500 MHz, C₆D₅CD₃, 223K, δ ppm): 10.06 (br, 2H), 9.85 (br, 2H), 9.76 (br, 2H), 9.11 (br, 2H), 8.69 (br, 2H), 8.64 (br, 2H), 8.18 (br, 2H), 8.01 (br, 2H), 7.90 (br, 2H), 7.48 (br, 2H), 6.30 (br, 2H), 4.74 (br, 2H), 3.83 (br, 2H), 2.04 (br, 36H), 1.75 (br, 9H), 1.66 (br, 36H), 1.38 (br, 18H). HRMS (MALDI-TOF, *m/z*): calcd for C₁₁₈H₁₂₅Si₃ [M]⁺, 1626.91; found 1626.95.



tips-OR-4: Triisopropylsilylacetylene (310 μ L, 1.38 mmol, 60 equiv) was dissolved in 6 mL of anhydrous THF, then the solution was cooled to 0 °C by ice bath and kept under N₂ atmosphere. *n*-BuLi in cyclohexane (2.0 M, 460 μ L, 0.92 mmol, 40 equiv) was added dropwise at 0 °C. The reaction mixture was stirred for 2 hours at 0 °C and a suspension of **17** (32 mg, 0.023 mmol) in anhydrous THF (10 mL) was added dropwise. The reaction mixture was warmed to room temperature slowly and stirred overnight. A solution of H₂SnCl₄ in THF was prepared by dissolving anhydrous SnCl₂ (174 mg, 0.92 mmol, 40 equiv) in anhydrous THF (5 mL) then adding concentrated aqueous HCl (154 μ L, 1.82 mmol, 80 equiv) and stirring for 30 min at rt and under N₂ atmosphere. Subsequently, the H₂SnCl₄ solution was added into the above-mentioned reaction mixture. After addition, the color of

the reaction mixture became orange instantaneously and then became green in several minutes. This dark green solution was stirred for additional 3 h. Water (100 mL) was then added to the reaction mixture and the crude organic solids was extracted with CH₂Cl₂ (2 x 50 mL). The resulting organic extract was washed with water (3 x 50 mL), dried over anhydrous Na₂SO₄, and then concentrated. The concentrated dark green solid and *p*-chloranil (80 mg, 0.33 mmol, 14 equiv) were added to a round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N₂. The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N₂. Dry toluene (15 mL) was added. The reaction mixture was stirred for 12 hours at rt and further 3 hours at 90 °C. A suspension/solution of Sc(OTf)₃ and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) in toluene was prepared by dissolving DDQ (27 mg, 0.12 mmol, 5 equiv) and dispersing Sc(OTf)₃ (58 mg, 0.12 mmol, 5 equiv) in dry toluene (10 mL). Subsequently, the DDQ-Sc(OTf)₃ solution with red color was added into the reaction mixture. The reaction mixture was further stirred for 5 hours at 90 °C. The reaction solution was cooled down to rt and was added triethylamine (0.5 mL) and stirred for 1 h. The crude mixture was further concentrated by rotary evaporation under reduced pressure. The concentrated crude product was washed with CH₃CN (5 mL) to remove excess triisopropylsilylacetylene and the blue supernatant was discarded. The residue was further dissolved in a small amount of mixture of solvents (hexanes : CH₂Cl₂ 7:3, 3 mL) and purified by column chromatography (initially, 100:20:3 v/v/v hexanes : CH₂Cl₂ : ethyl acetate as eluent to remove byproducts with blue color; then 20% v/v ethyl acetate in CH₂Cl₂ as eluent; TEA-silica gel) to collect the crude product with green color. The crude product was further purified by a flash column chromatography (CH₂Cl₂; TEA-silica gel) to give the pure **tips-OR-4** as dark green solid (15 mg, 32%). Its ¹H NMR spectrum is extremely broad as a result of severe aggregation in solution. HRMS (MALDI-TOF, m/z): calcd for C₁₄₈H₁₅₂Si₄ [M]⁺, 2042.10; found 2041.99.



tips-OR-4: (Triphenylsilyl)acetylene (178 mg, 0.63 mmol, 60 equiv) was dissolved in 6 mL of anhydrous THF, then the solution was cooled to -78 °C by dry ice/acetone bath and kept under N₂ atmosphere. *n*-BuLi in cyclohexane (2.0 M, 210 μL, 0.42 mmol, 40 equiv) was added dropwise at -78 °C. The reaction mixture was stirred for 3 hours at -78 °C and a suspension of **17** (14.5 mg, 0.01 mmol) in anhydrous THF (10 mL) was added dropwise. The reaction mixture was warmed to room temperature slowly and stirred overnight. A solution of H₂SnCl₄ in THF was prepared by dissolving anhydrous SnCl₂ (80 mg, 0.42 mmol, 40 equiv) in anhydrous THF (2 mL) then adding concentrated aqueous HCl (70 μL, 0.84 mmol, 80 equiv) and stirring for 30 min at rt and under N₂ atmosphere.

Subsequently, the H_2SnCl_4 solution was added into the above-mentioned reaction mixture. After addition, the color of the reaction mixture became orange instantaneously and then became dark green in several minutes. This dark green solution was stirred for additional 3 h. Water (100 mL) was then added to the reaction mixture and the crude organic solids was extracted with CH_2Cl_2 (2 x 50 mL). The resulting organic extract was washed with water (3 x 50 mL), dried over anhydrous Na_2SO_4 , and then concentrated. The concentrated dark green solid and *p*-chloranil (38 mg, 0.15 mmol, 15 equiv) were added to a round-bottom flask containing a magnetic stirring bar. The flask was sealed with a rubber septum, evacuated with an oil-pump, and refilled with N_2 . The evacuation-filling process was repeated twice more, and then the system was placed under a static pressure of N_2 . Dry toluene (15 mL) was added. The reaction mixture was stirred for 12 hours at rt and further 5 hours at 90 °C. A suspension/solution of $\text{Sc}(\text{OTf})_3$ and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) in toluene was prepared by dissolving DDQ (12 mg, 0.05 mmol, 5 equiv) and dispersing $\text{Sc}(\text{OTf})_3$ (27 mg, 0.05 mmol, 5 equiv) in dry toluene (5 mL). Subsequently, the DDQ- $\text{Sc}(\text{OTf})_3$ solution with red color was added into the reaction mixture. The reaction mixture was further stirred for 3 hours at 90 °C. The reaction solution was cooled down to rt and was added triethylamine (0.5 mL) and stirred for 1 h. The crude mixture was further concentrated by rotary evaporation under reduced pressure. The concentrated crude product was washed with CH_3CN (5 mL) to remove excess (triphenylsilyl)acetylene and the blue supernatant was discarded. The residue was further dissolved in a small amount of mixture of solvents (hexanes : CH_2Cl_2 7:3, 3 mL) and purified by column chromatography (initially, 100:20:3 v/v/v hexanes : CH_2Cl_2 : ethyl acetate as eluent to remove byproducts with blue color; then 20% v/v ethyl acetate in CH_2Cl_2 as eluent; TEA-silica gel) to collect the crude product with green color. The crude product was further purified by a flash column chromatography (CH_2Cl_2 ; TEA-silica gel) to give the pure **tps-OR-4** as dark green solid (8 mg, 30%). HRMS (MALDI-TOF, m/z): calcd for $\text{C}_{184}\text{H}_{128}\text{Si}_4$ $[\text{M}]^+$, 2450.91; found 2451.45.

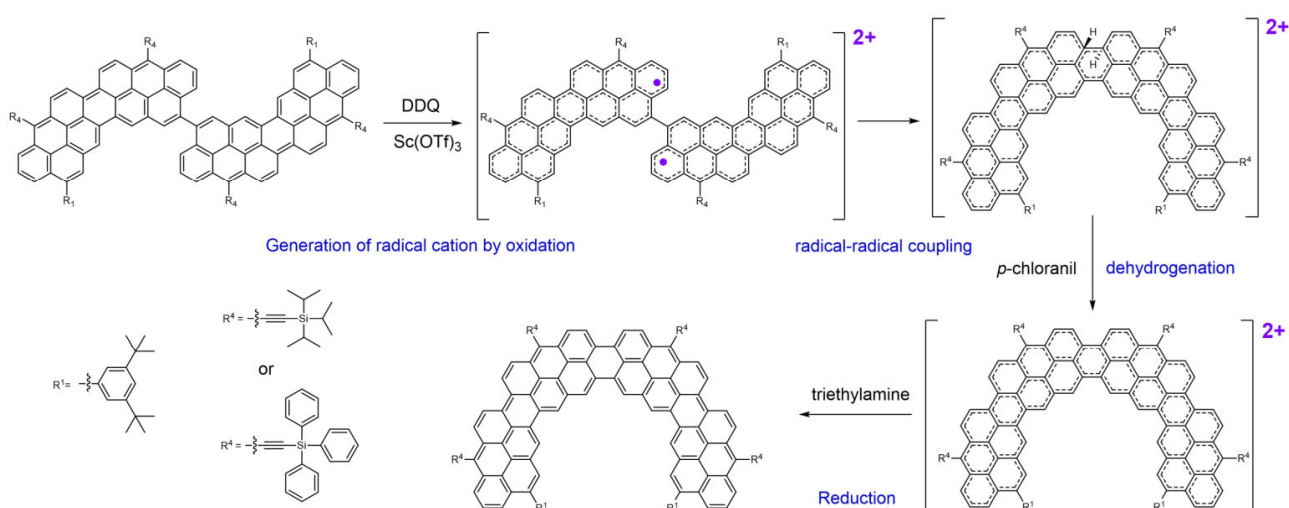


Figure S1. Proposed reaction mechanism of the Scholl reaction step for synthesis of **OR-4**.

3. Additional spectra

The investigation of photoinduced ring-opening reaction of **9** to **8**:

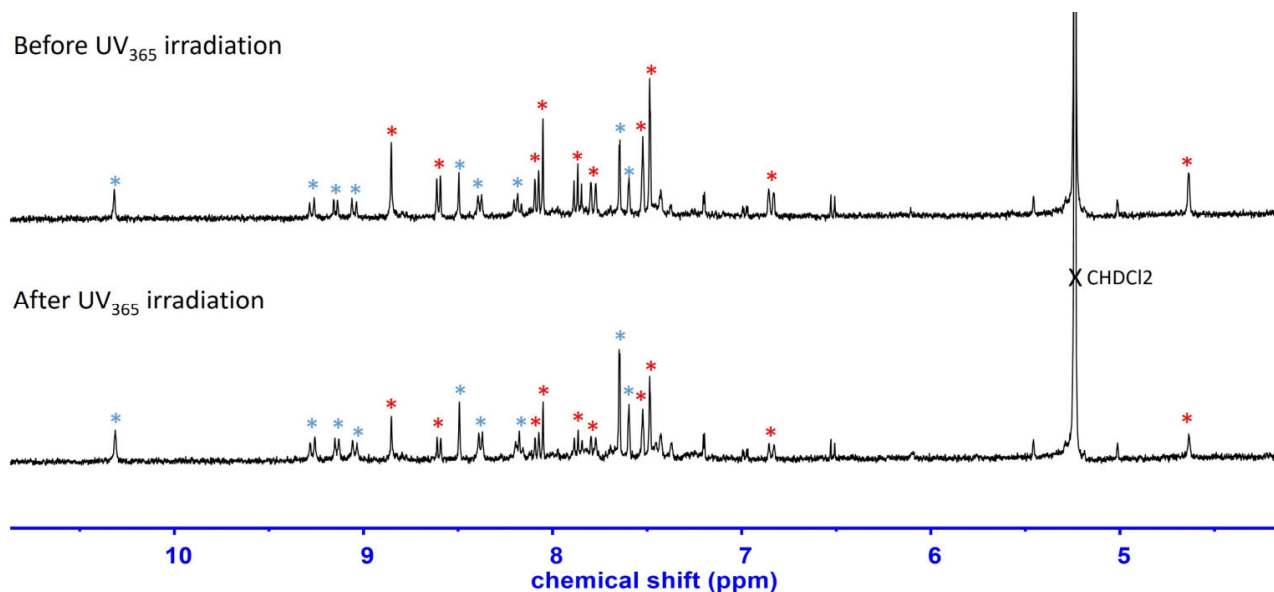


Figure S2. ^1H NMR spectra of the freshly prepared mixture of intermediate **9** and **tips-OR-2** recorded in degassed CD_2Cl_2 at 298 K before irradiation and after irradiation of UV light at 365 nm for 2 mins. Red stars label resonance peaks for **9**. Blue stars label resonance peaks for **tips-OR-2**.

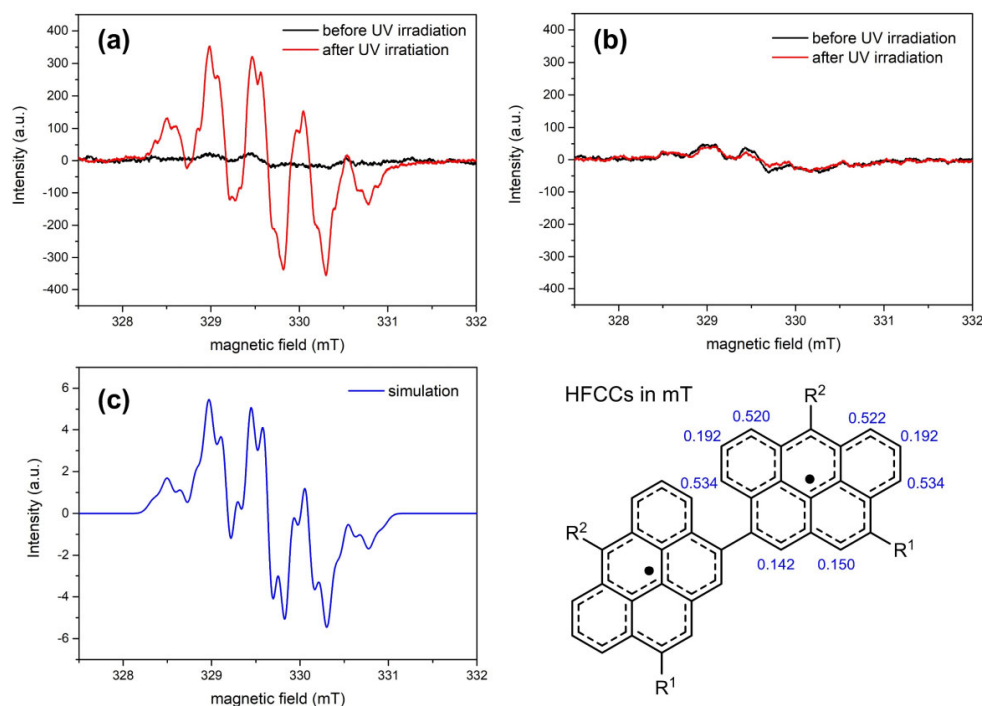


Figure S3. (a) ESR spectra of the freshly prepared mixture of intermediate **9** and **tips-OR-2** recorded in degassed CH_2Cl_2 at 298 K before irradiation and after irradiation of UV light at 365 nm for 2 mins. (b) ESR spectra of the freshly prepared **tips-OR-2** recorded in degassed CH_2Cl_2 at 298 K before irradiation and after irradiation of UV light at 365 nm for 2 mins. (c) Simulated ESR spectrum for intermediate **8** with calculated hyperfine coupling constants (HFCCs).

Irradiation of UV light (365 nm) to the mixture of **9** and **tips-OR-2** in degassed CD₂Cl₂ resulted in the decrease of the intensity of the resonance peaks of **9**, compared with **tips-OR-2** (Figure S2). Note: partial compound **9** has unavoidably transformed to the final compound **tips-OR-2** during the necessary liquid/liquid extraction step because of exposure with air. However, no new set of resonance peaks appears after the irradiation. Due to the “pure” diradical nature, **8** should be NMR silent. We thus used ESR to monitor the signal change after the UV irradiation. Before UV irradiation, the mixture of **9** and **tips-OR-2** in degassed CH₂Cl₂ doesn’t show any ESR signal as expected. In contrast, a well resolved multiline ESR signal was observed after UV irradiation (Figure S3). To rule out the possibility that this ESR signal corresponds to unknown product of **tips-OR-2** or other impurities after irradiation, we did a control experiment for the sample in which **9** has been fully converted to **tips-OR-2**. UV irradiation didn’t generate any observable ESR signal in the control experiment. Thus, we reasoned this ESR signal corresponds to the ring-opening reaction product – **8**, which was further supported by the consistent calculated ESR spectrum of **8**. Here, the observable well resolved ESR signal of **8** also demonstrates the almost “pure” diradical nature of compound **8**. Both the ¹H NMR results and ESR measurements demonstrate the photoinduced ring-opening electrocyclization mechanism of **9** to **8**.

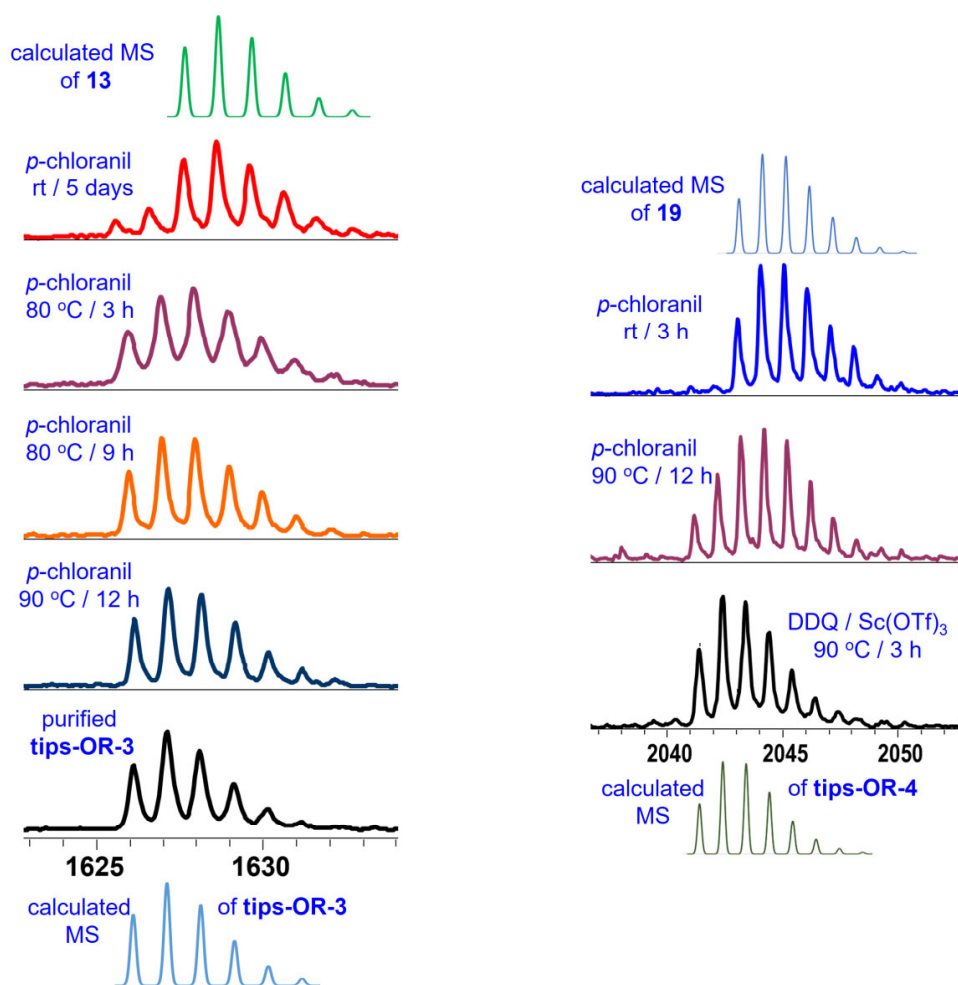


Figure S4. MALDI-TOF MS analyses of the conversion process from **13** to **tips-OR-3** (left), and **19** to **tips-OR-4** (right).

Isolation and characterization of intermediate **13**:

After adding *p*-chloranil (10 equiv.) to the crude mixture of **11/12** in dry toluene and stirring for about 2 hours at rt, the solvent was removed by evaporation under reduced pressure. The residue was further dissolved in a small amount of mixture of solvents (hexane : CH₂Cl₂ 10:1) and purified by column chromatography (10% v/v CH₂Cl₂ in hexanes, TEA-silica gel) to give the **13** as green solid. The freshly prepared **13** was used in the following characterizations.

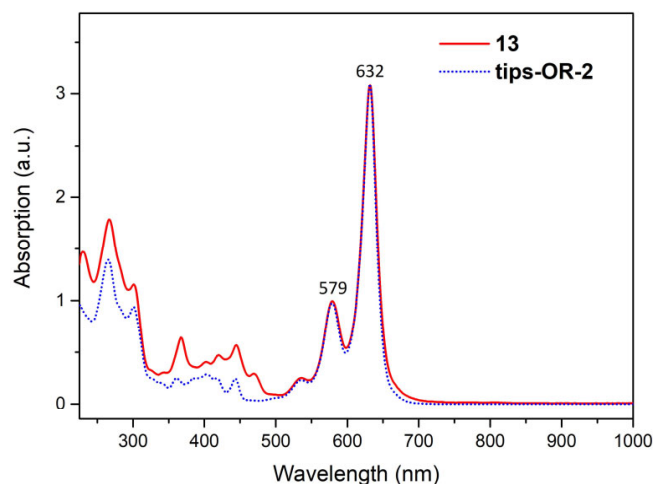


Figure S5. UV-vis-NIR absorption spectra of intermediate **13** (red line) and **tips-OR-2** (blue dash line) in CH₂Cl₂. Intermediate **13** exhibits the absorption features of both **tips-OR-2** (the intense absorption bands at 632 and 579 nm) and olympicenyl monoradical (the absorption bands in the region between 300 – 500 nm).

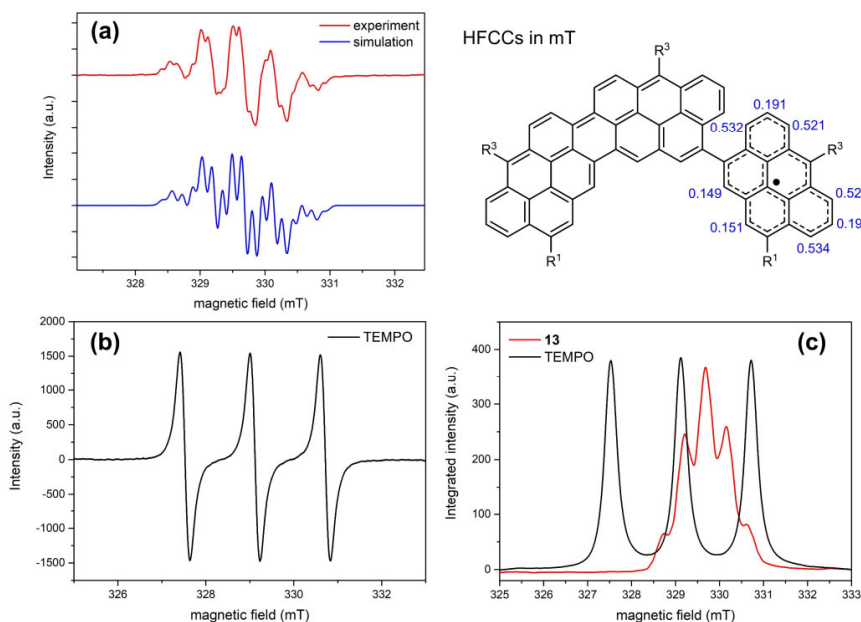


Figure S6. (a) Observed and simulated ESR spectra for intermediate **13** recorded in degassed CH₂Cl₂ (3.2 x 10⁻⁴ M) at 298 K with the calculated hyperfine coupling constants (HFCCs). (b) Observed ESR spectrum for TEMPO recorded in CH₂Cl₂ (2.9 x 10⁻⁴ M) at 298 K. (c) The integrated ESR spectra for intermediate **13** and TEMPO which were recorded at same experimental condition. The integration intensity ratio for **13**/TEMPO = 57.3/70.7 = 81%. Considering the experimental errors and decomposition of samples, we think these results support the monoradical character of **13**.

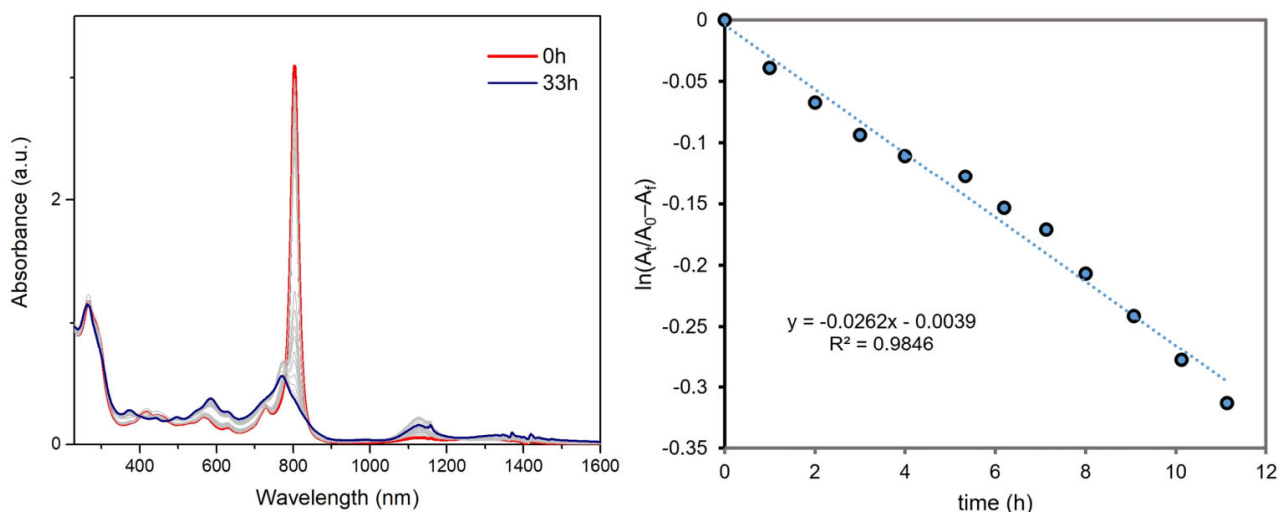
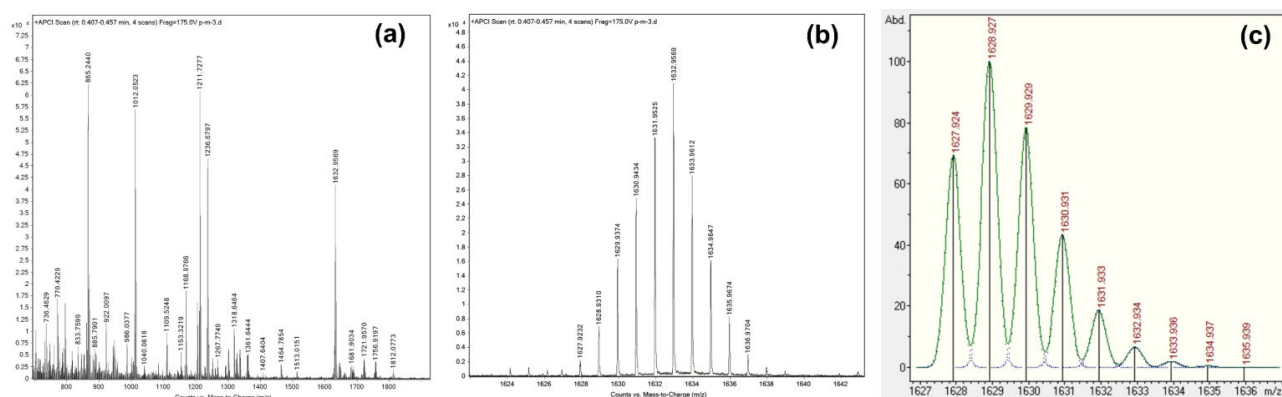


Figure S8. The stability of [tips-OR-3]₂ in CH₂Cl₂ solution under ambient condition. Left: change of absorption spectra of [tips-OR-3]₂. Right: plot of optical density decay at 803.5 nm. The decay half-life is around 26 h.

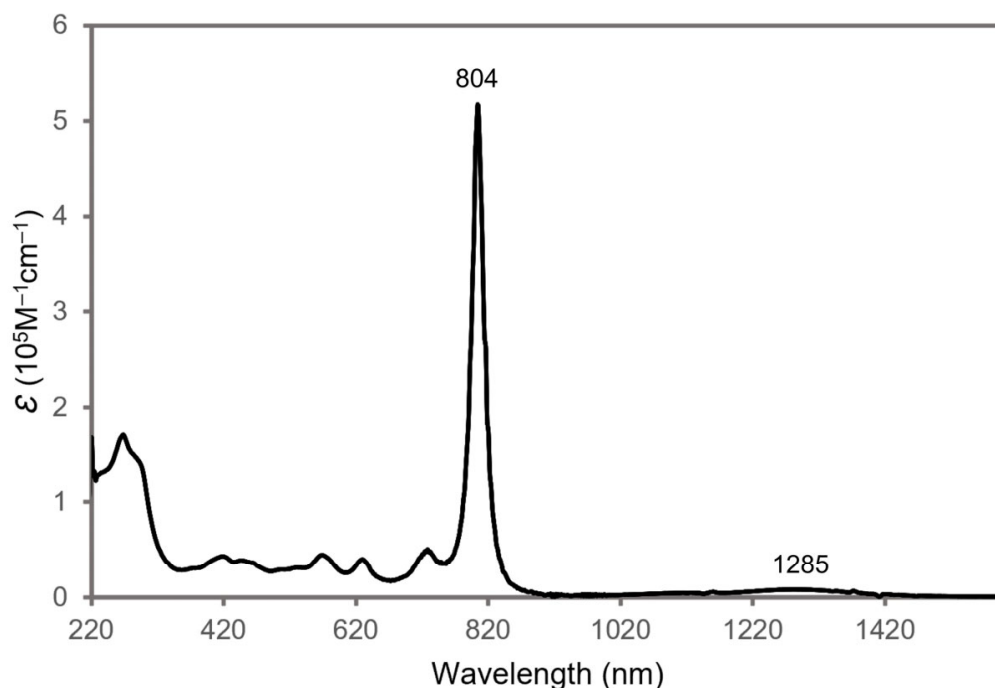


Figure S9. UV-vis-NIR absorption spectrum of **tips-OR-3** in dry CH_2Cl_2 (7.9×10^{-6} M) at rt. It is noteworthy that, **tips-OR-3** exists as π -dimer complex – $[\text{tips-OR-3}]_2$ in solution.

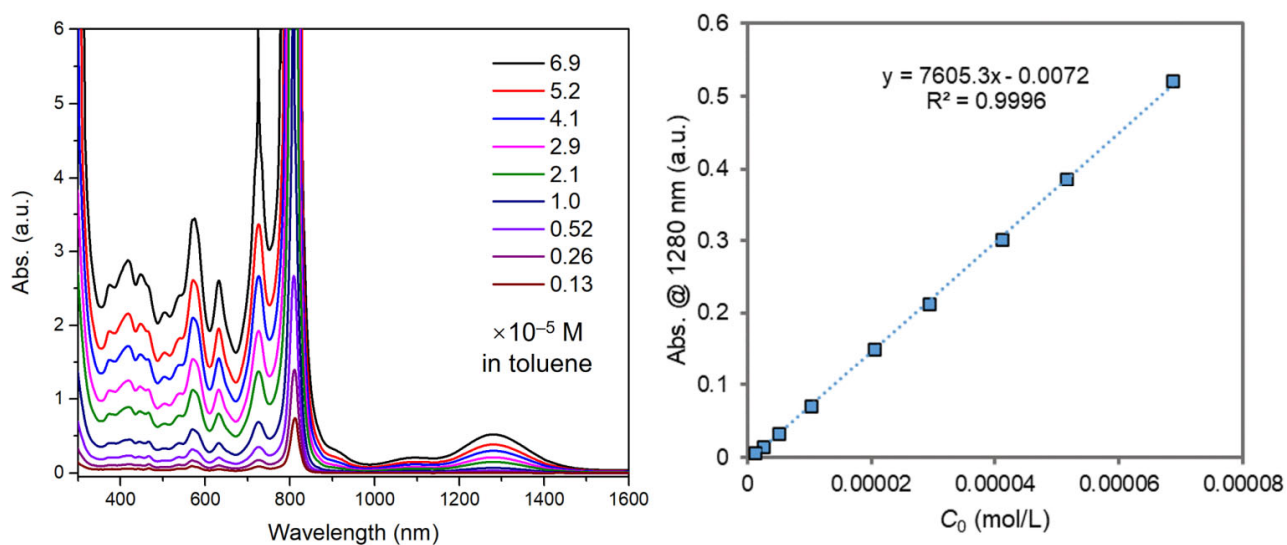


Figure S10. Left: UV-vis-NIR spectra of **tips-OR-3** with different concentrations in toluene. Right: The concentration dependence of the absorption at 1280 nm. The dash line is the fitted curve. The absorption intensity of the band corresponding to the **tips-OR-3** dimer at 1280 nm and the concentration are linearly correlated, suggesting that **tips-OR-3** exists as a homogenous specie in solution which is further demonstrated to be $[\text{tips-OR-3}]_2$.

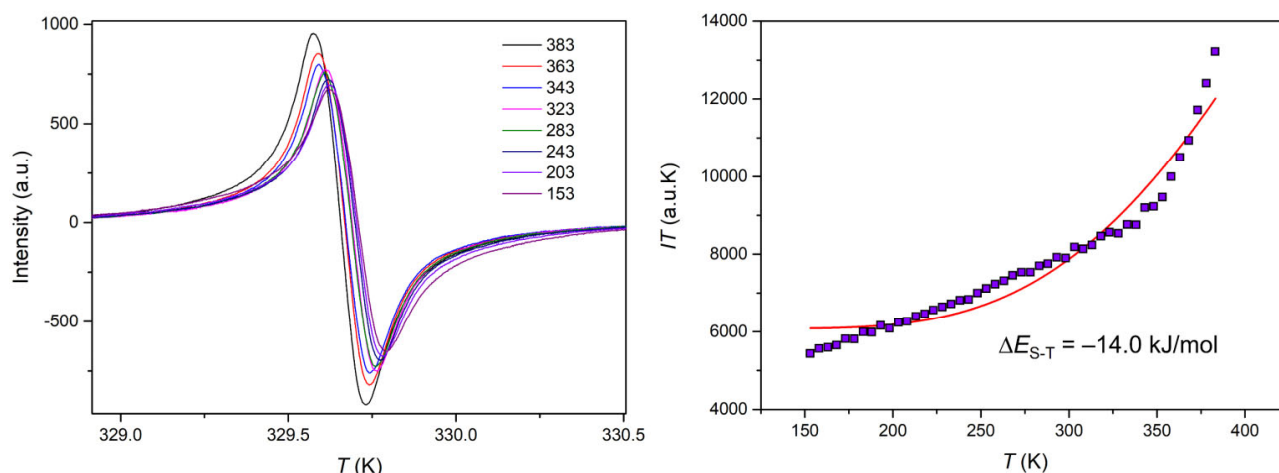


Figure S11. Left: VT-ESR spectra of **[tips-OR-3]₂** in the solid-state. Right: IT - T plot for **[tips-OR-3]₂** in the solid-state, and the fitted curve based on the Bleaney-Bowers equation. As the temperature increases from room temperature to 383 K, the ESR signal become larger, which is consistent with the increase of triplet state specie of **[tips-OR-3]₂**. On cooling the temperature from room temperature to 153 K, the ESR signal become much broader, probably because of the increase of the intermolecular spin interaction extent or the limitation of molecular motion at low temperature. The IT - T plot for **[tips-OR-3]₂** in the solid-state can be roughly fitted by the Bleaney-Bowers equation, to afford the ΔE_{S-T} of -14.0 kJ/mol, which is qualitatively consistent with the result in the solution-phase (-15.4 kJ/mol). We think that the close-stacking of **[tips-OR-3]₂** in the solid-state may cause complex intermolecular spin interaction which is not negligible at low temperature.

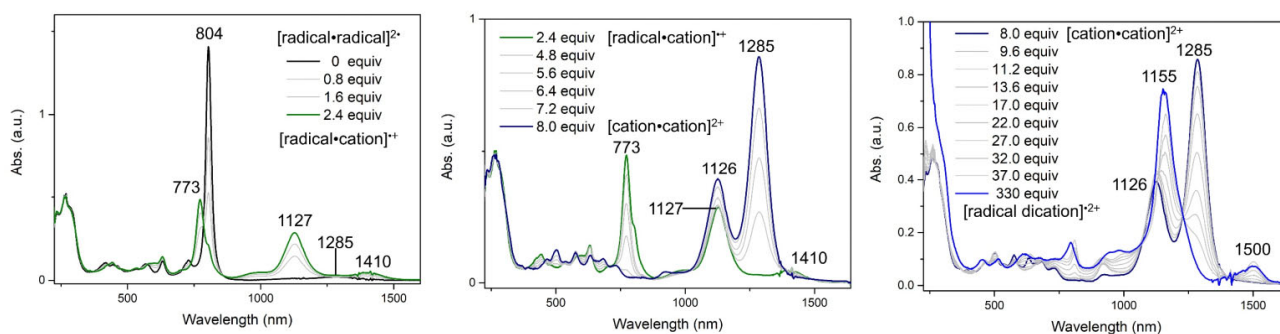


Figure S12. Change of the UV-vis-NIR spectra of **[tips-OR-3]₂** in dry CH_2Cl_2 (2.7×10^{-6} M) during chemical oxidative titration with NOSbF_6 .

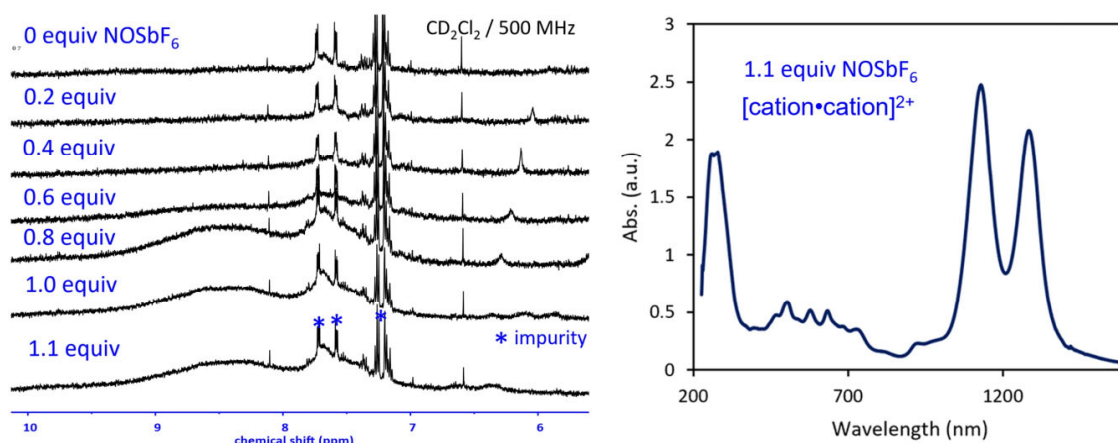


Figure S13. ^1H NMR spectra (500 MHz, CD_2Cl_2 , 298 K) of $[\text{tips-OR-3}]_2$ (0.85 mM) after the addition of different equivalents of NOSbF_6 . After addition of 0.8 – 1.0 equiv NOSbF_6 (relative to the molar concentration of **tips-OR-3**), broad resonance was observed, indicating the formation of $[\text{cation}\cdot\text{cation}]^{2+}$ state of $[\text{tips-OR-3}]_2$ in CD_2Cl_2 . The UV-vis-NIR absorption spectrum of this solution (after the addition of 1.1 equiv NOSbF_6) confirmed the characteristic absorption bands of $[\text{cation}\cdot\text{cation}]^{2+}$ state.

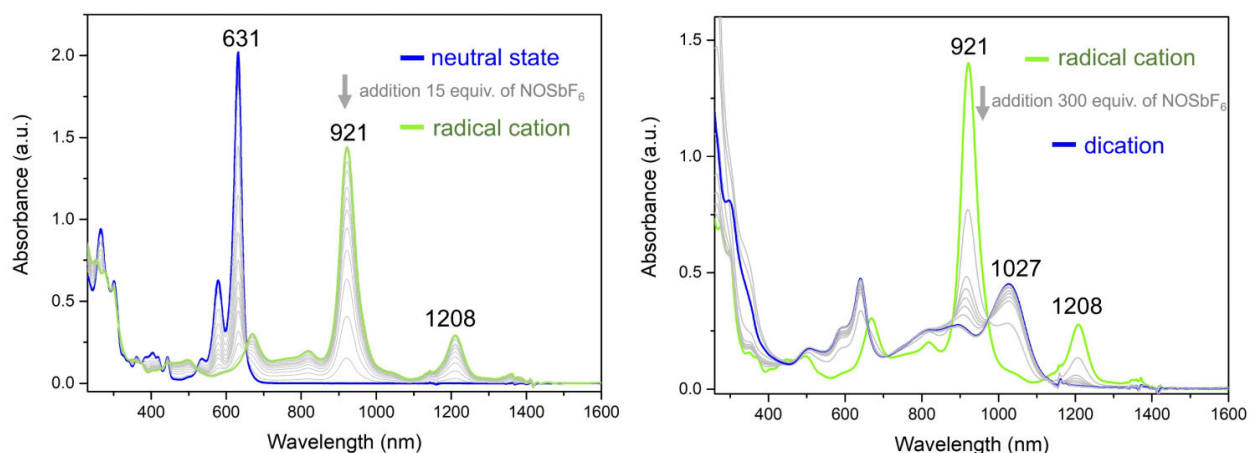


Figure S14. Change of the UV-vis-NIR spectra of **tips-OR-2** in dry CH_2Cl_2 (7.4×10^{-6} M) during chemical oxidative titration with NOSbF_6 .

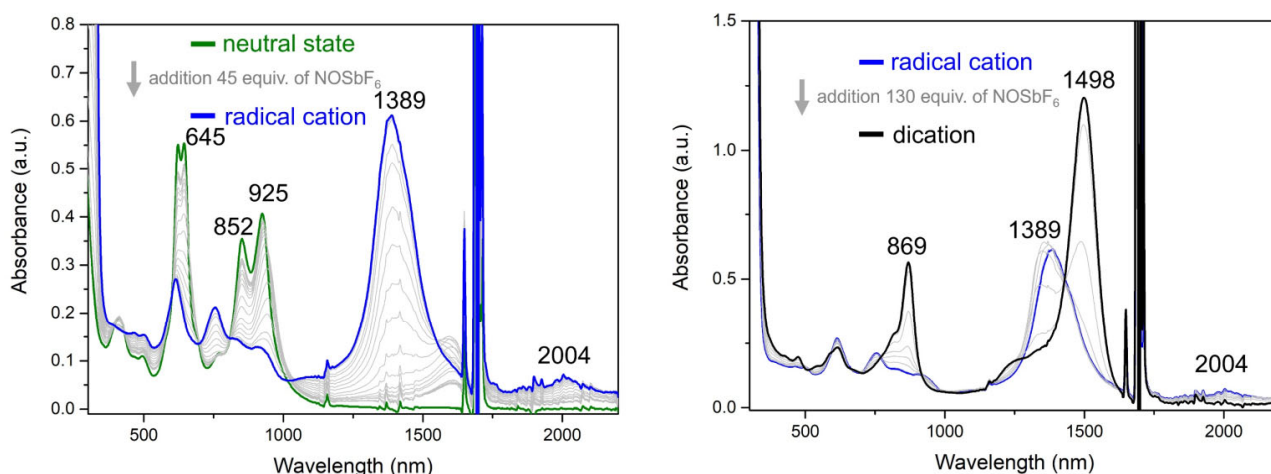


Figure S15. Change of the UV-vis-NIR spectra of **tps-OR-4** in dry CH_2Cl_2 (2.7×10^{-6} M) during oxidative chemical titration with NOSbF_6 .

4. X-ray crystallography

1) dtbp-OR-2

1.1) Methods

Slow vapor diffusion of acetonitrile into the toluene solution of **dtbp-OR-2** at room temperature yielded green block crystals of **dtbp-OR-2**. The crystals were mounted on a MiTeGen holder in Paratone oil on a Bruker APEX-II CCD diffractometer. The crystals were kept at 109 K during data collection. The structure was solved using Olex2 software¹ with the ShelXT² structure solution program by Intrinsic Phasing and refined with the ShelXL³ refinement package using Least Squares minimization.

1.2) Crystal data and structure refinements of **dtbp-OR-2**

Formula: C₉₄H₉₈. Formula weight: 1227.72 g/mol. Crystal size max/min/mim / mm: 0.2/0.15/0.2. Temperature: 109 K. Radiation type: Cu-K α . Wavelength / Å: 1.54178. Bond precision: 0.0085 Å. Crystal color: green. Crystal description: block. Crystal system: monoclinic. Space group: P2₁/c. Unit cell dimensions: $a = 23.302(9)$ Å, $b = 19.284(9)$ Å, $c = 17.653(6)$ Å, $\alpha = 90^\circ$, $\beta = 92.54(2)^\circ$, $\gamma = 90^\circ$. Volume(Å³): 7925(5). Z: 4. ρ (g.cm⁻³): 1.029. F (000): 2648. μ (mm⁻¹): 0.430. θ for data collection (°): 2.976 to 52.628. Limiting indices: $-24 \leq h \leq 24$, $-19 \leq k \leq 19$, $-18 \leq l \leq 18$. Reflection collected: 76561 [R(int) = 0.1660]. Data / restraints / parameters: 8990/276/911. Goodness-of fit on F²: 1.029. R₁(reflections) [$I > 2\sigma(I)$]: 0.1041(5725). wR₂(reflections)(all data): 0.3151(8990). Data completeness: 0.989. CCDC number: 2220240. CheckCif report gives 1 A level alerts : *"THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550 Calculated sin(theta_max)/wavelength = 0.5155"*. Response: Due to the limited crystal quality, despite of long exposure time, the crystal did not exhibit decent diffraction intensity and failed to bring the resolution higher than 0.97 Å. This explanation has been embedded in the cif. The solvent masking⁴ procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. Total solvent accessible volume/cell = 1326.3 Å³ [16.7%] Total electron count/cell = 241.6. The structure with probability ellipsoids is shown in Fig. 4a.

1.3) Solid-State (Super-) structures of **dtbp-OR-2**

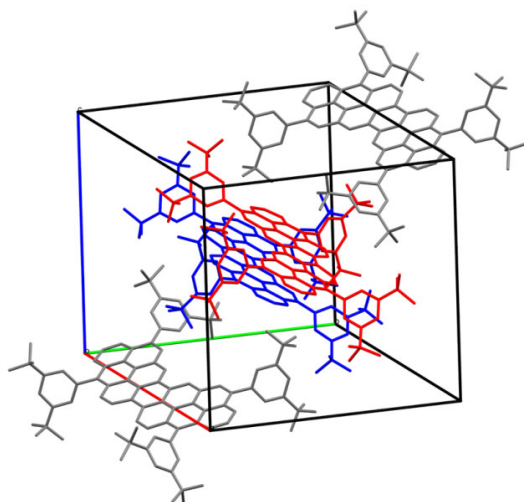


Figure S16. Super-structure of **dtbp-OR-2**.

2) tips-OR-3

2.1) Methods

Slow vapor diffusion of *n*-hexane into the chlorobenzene solution of **tips-OR-3** at room temperature in the glovebox yielded black plate crystals of **tips-OR-3**. The crystals were mounted on a MiTeGen holder in Paratone oil on a Bruker APEX-II CCD diffractometer. The crystals were kept at 110 K during data collection. The structure was solved using Olex2 software¹ with the ShelXT² structure solution program by Intrinsic Phasing and refined with the ShelXL³ refinement package using Least Squares minimization.

2.2) Crystal data and structure refinements of **tips-OR-3**

Formula: $2(\text{C}_{118}\text{H}_{125}\text{Si}_3) \cdot \text{C}_6\text{H}_5\text{Cl}$, Formula weight: 3367.43 g/mol. Crystal size max/min/min / mm: 0.18/0.08/0.14. Temperature: 110 K. Radiation type: Cu-K α . Wavelength / Å: 1.54178. Bond precision: 0.0034 Å. Crystal color: black. Crystal description: plate. Crystal system: triclinic. Space group: $P\bar{1}$. Unit cell dimensions: $a = 15.3514(6)$ Å, $b = 25.8344(10)$ Å, $c = 27.5106(11)$ Å, $\alpha = 83.956(2)^\circ$, $\beta = 79.178(2)^\circ$, $\gamma = 89.681(2)^\circ$. Volume(Å³): 10655.8(7). Z: 2. ρ (g.cm⁻³): 1.050. F (000): 3616. μ (mm⁻¹): 0.863. θ for data collection ($^\circ$): 2.250 to 72.685. Limiting indices: $-18 \leq h \leq 18$, $-31 \leq k \leq 31$, $-33 \leq l \leq 33$. Reflection collected: 268381 [R(int) = 0.0804]. Data / restraints / parameters: 41975/5105/2714. Goodness-of fit on F²: 1.048. R_1 (reflections) [$I > 2\sigma(I)$]: 0.0685(30987). wR_2 (reflections)(all data): 0.2121(41975). Data completeness: 0.992. CCDC number: 2220242. No A or B level alerts were found in CheckCif report. SQUEEZE function⁵ of PLATON⁶ was employed to remove the contribution of the electron density associated with these highly disordered solvent molecules (hexanes), which gave a potential solvent accessible void of 1598 Å³ per unit cell (a total of approximately 324 electrons). The structure with probability ellipsoids is shown in Fig. 4b.

2.3) Solid-State (Super-) structures of **tips-OR-3**

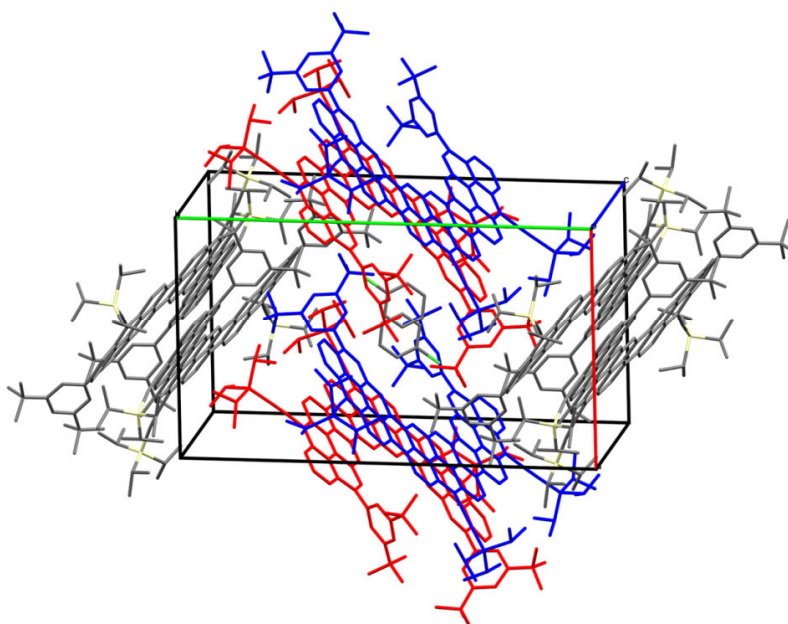


Figure S17. Super-structure of **tips-OR-3**.

5. DFT calculations

All calculations were performed with Gaussian 09.⁷ Geometry optimization of all the minima involved was carried out at the (u)m06-2x level of theory⁸ with the 6-31g(d) or 6-31g(d,p) basis set.⁹ The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. The single-point energy was computed at the (u)m06-2x level of theory with the 6-311g(d,p) basis set, based on the gas-phase optimized structures. Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD model.¹⁰ The transition states (TS) were identified by one imaginary frequency at the saddle point, and ZPVE and thermal corrections were applied to the relative energies. The 3D diagrams of molecules were generated using CYLView.¹¹ NOON (natural orbital occupation number) calculations were done by spin unrestricted ucam-b3lyp/6-31g(d,p) method based on the optimized structure and the diradical character (y_0) was calculated according to Yamaguchi's scheme: $y_0 = 1 - (2T/(1+T^2))$, and $T = (n_{\text{HONO}} - n_{\text{LUNO}})/2$ (n_{HONO} is the occupation number of the HONO, n_{LUNO} is the occupation number of the LUNO). For **tips-OR-2**, $y_0 = 0.004$, $n_{\text{HONO}} = 1.91612$, $n_{\text{LUNO}} = 0.08388$. For **tips-OR-4**, $y_0 = 0.07$, $n_{\text{HONO}} = 1.68404$, $n_{\text{LUNO}} = 0.31596$. Time-dependent DFT (TD-DFT) calculations were performed at the (u)m06-2x/6-31g(d,p) level of theory. NICS values were calculated using the standard GIAO (GIAO=NMR) at the level of m06-2x/6-31g(d,p). The ICSS calculations were carried out to analyze 2D-NICS along the XY planes. The 2D ICSS_{zz,1} maps were visualized by Multiwfn software.¹² NMR values were calculated using the standard GIAO (GIAO=NMR) at the level of m06-2x/6-311g(d,p). For the gauge-including magnetically induced current (GIMIC) calculation, the nuclear shielding calculation were performed at the level of GIAO-um06-2x/6-311g(d,p) functional. Magnetically induced current densities were calculated using the Gimic 2.0 program.¹³ The external magnetic field was applied along the x, y, z-axis, respectively. The origin and length of grid were calculated by Multiwfn software. The visualization of the three-dimensional current density has been done with the streamline plugin of ParaView 5.6.1¹⁴ using an inspection sphere of radius 0.5 Bohr. The inspection sphere has been placed in the geometric center of the dimer.

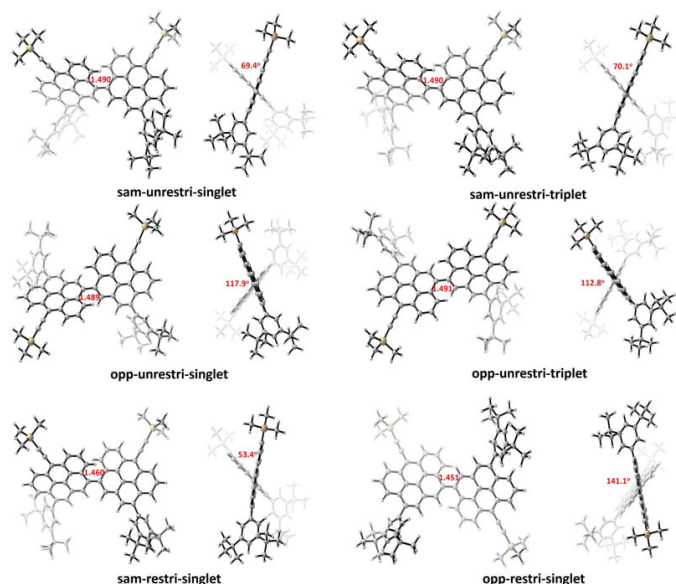


Figure S18. Optimized structures of the covalent linked olympicenyl radical dimer by DFT at the (u)m06-2x/6-31g(d) level of theory. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K.

Table S1. Detailed computed energies, and diradical character of calculated structures of the covalent linked olympicenyl radical dimer. All structures were optimized at (u)m06-2x/6-31g(d) level of theory.

structure	sam-unrestris-singlet	sam-unrestris-triplet	opp-unrestris-singlet	opp-unrestris-triplet	sam-restris-singlet	opp-restris-singlet
Initial guess spin-multiplicity	singlet	triplet	singlet	triplet	singlet	singlet
Spin-restricted/broken-symmetry unrestricted	unrestricted	unrestricted	unrestricted	unrestricted	restricted	restricted
Electronic Energy (EE, in Hartress)	— 3519.651043	— 3519.650975	— 3519.649927	— 3519.649751	— 3519.618004	— 3519.623931
Thermal correction to free energy (in Hartress)	1.179575	1.178449	1.179631	1.178802	1.182505	1.183339
EE+Thermal free energy correction (in Hartress)	— 3518.471468	— 3518.472526	— 3518.470295	— 3518.470949	— 3518.435499	— 3518.440592
Free energy difference (ΔG , in kJ/mol)	+2.8	0	+5.9	+4.1	+97.2	+83.8
Imaginary frequency (cm^{-1})	—	—	—	—	—	—
Diradical character (y_0), occupation number of HONO (n_{HONO}), and LUNO (n_{LUNO})	$Y_0 = 0.992$ $n_{\text{HONO}} = 1.00387$ $n_{\text{LUNO}} = 0.99613$	$Y_0 = 1$ $n_{\text{HONO}} = 1.00000$ $n_{\text{LUNO}} = 1.00000$	$Y_0 = 0.906$ $n_{\text{HONO}} = 1.04691$ $n_{\text{LUNO}} = 0.95309$	$Y_0 = 1$ $n_{\text{HONO}} = 1.00000$ $n_{\text{LUNO}} = 1.00000$	$Y_0 = 0$ $n_{\text{HONO}} = 2.00000$ $n_{\text{LUNO}} = 0$	$Y_0 = 0$ $n_{\text{HONO}} = 2.00000$ $n_{\text{LUNO}} = 0$

The optimized structure **sam-unrestris-triplet** for compound **8**, has lowest computed free energy (EE + thermal free energy correction) in comparison with other optimized structures. These calculated results suggest the electronic structure of ground state of **8** is almost “pure” diradical because the diradical character of corresponding optimized structure with minimum free energy is 1.

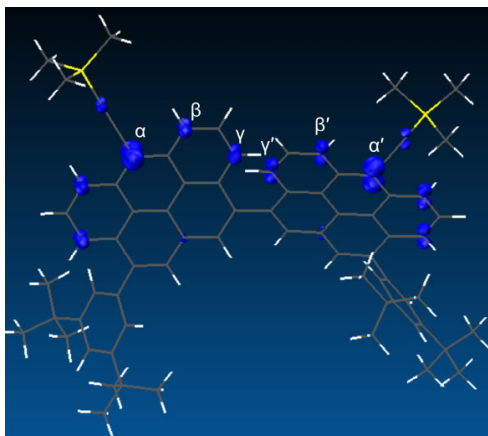


Figure S19. Calculated spin density distribution of the open-shell triplet state of **8** at um06-2x/6-311g(d,p) level of theory. The triisopropyl groups are replaced with trimethyl groups during the DFT calculations. Iso-surface value: 0.015.

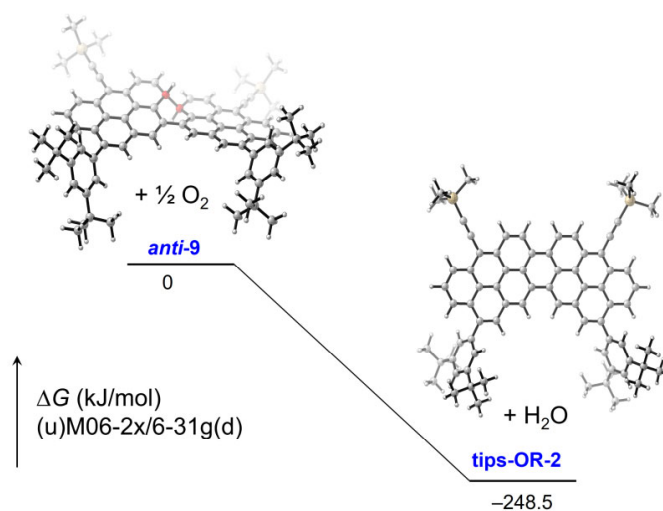


Figure S20. Calculated energy diagram of dehydrogenation by O₂. Zero-point vibrational energy (ZPVE) and thermal corrections were applied to the relative energies. The triisopropyl groups were replaced with trimethyl groups during DFT-calculation.

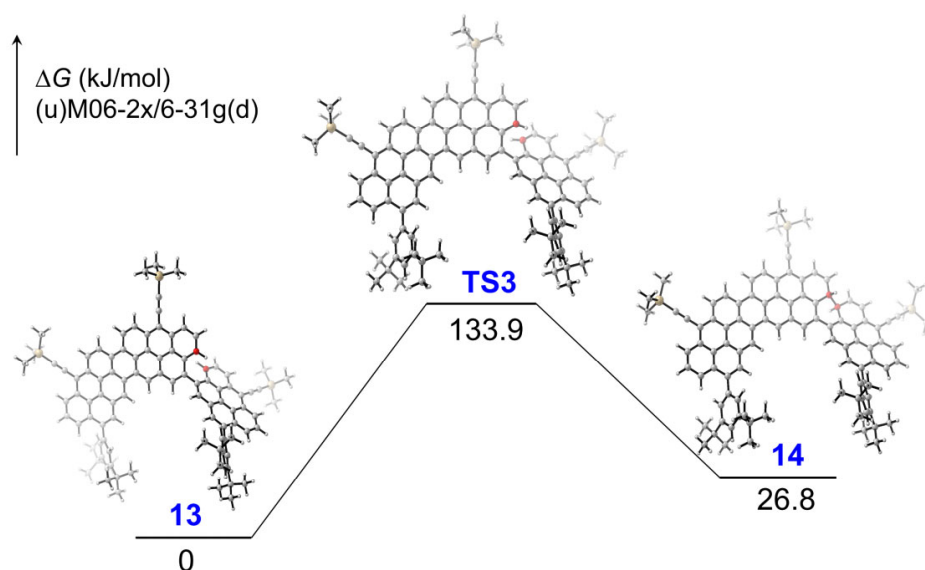


Figure S21. Calculated energy diagram of radical-mediated ring-closure from **13** to **14**. Transition states (TS) were identified by one imaginary frequency at the saddle point. Zero-point vibrational energy (ZPVE) and thermal corrections were applied to the relative energies. The triisopropyl groups were replaced with trimethyl groups during DFT-calculation.

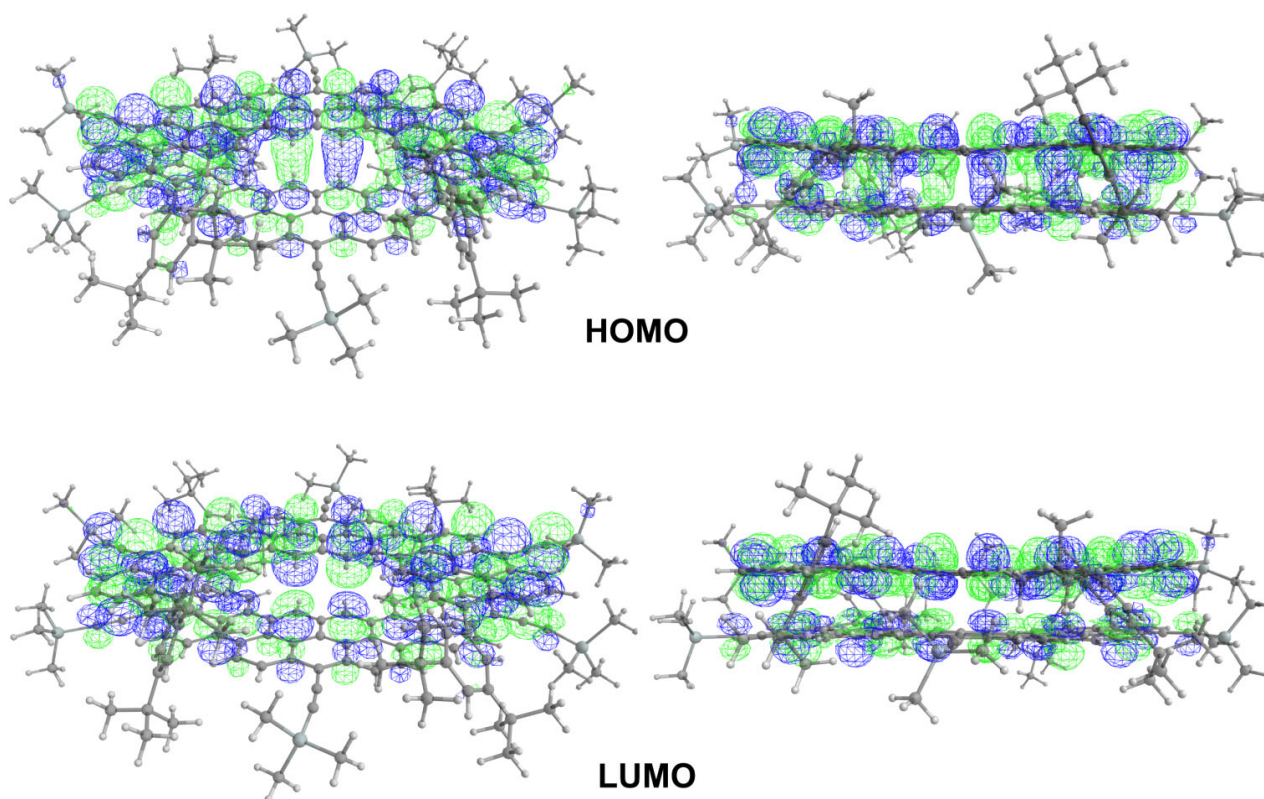


Figure S22. Calculated HOMO and LUMO of $[\text{tips-OR-3}]_2$ at the level of um06-2x/6-311g(d,p) theory. The triisopropyl groups were replaced with trimethyl groups during DFT-calculation.

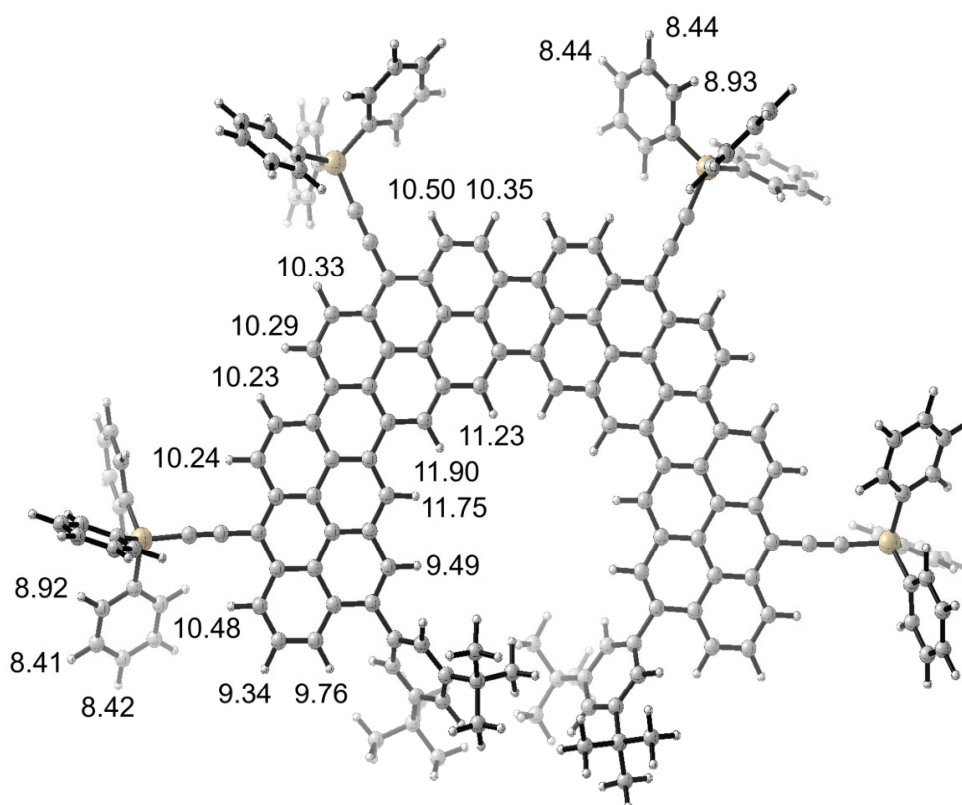


Figure S23. Calculated ^1H NMR of **tips-OR-4** by using DFT (keyword `nmr=giao`) at the level of m06-2x/6-311g(d,p) theory. The resonance values were calibrated by subtracting the value (32.0620) of shielding tensor of tetramethylsilane.

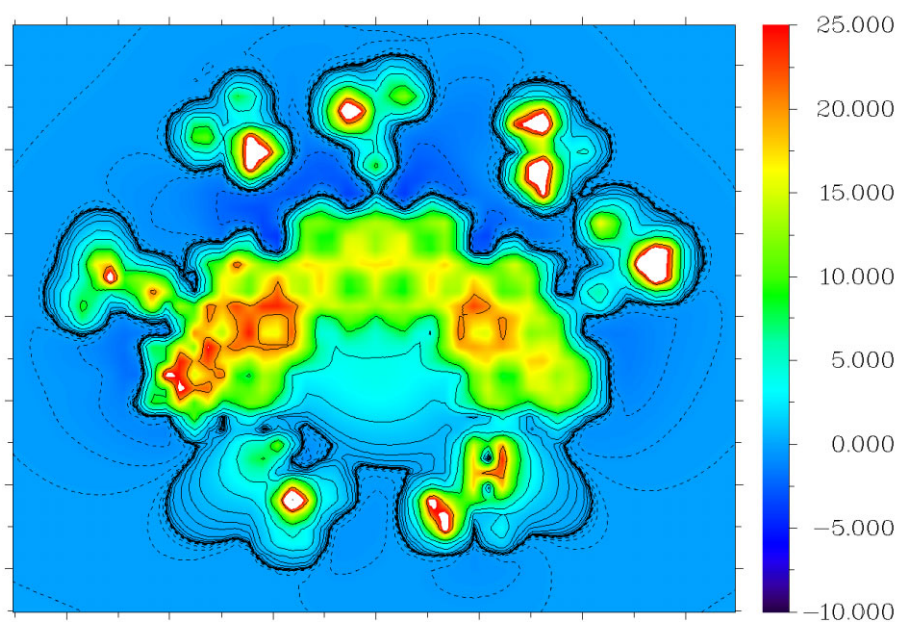


Figure S24. Calculated 2D $\text{ICSS}_{zz,1}$ map of **[tips-OR-3]₂** by using DFT at the level of m06-2x/6-31g(d,p) theory. The triisopropyl groups were replaced with trimethyl groups during DFT-calculation.

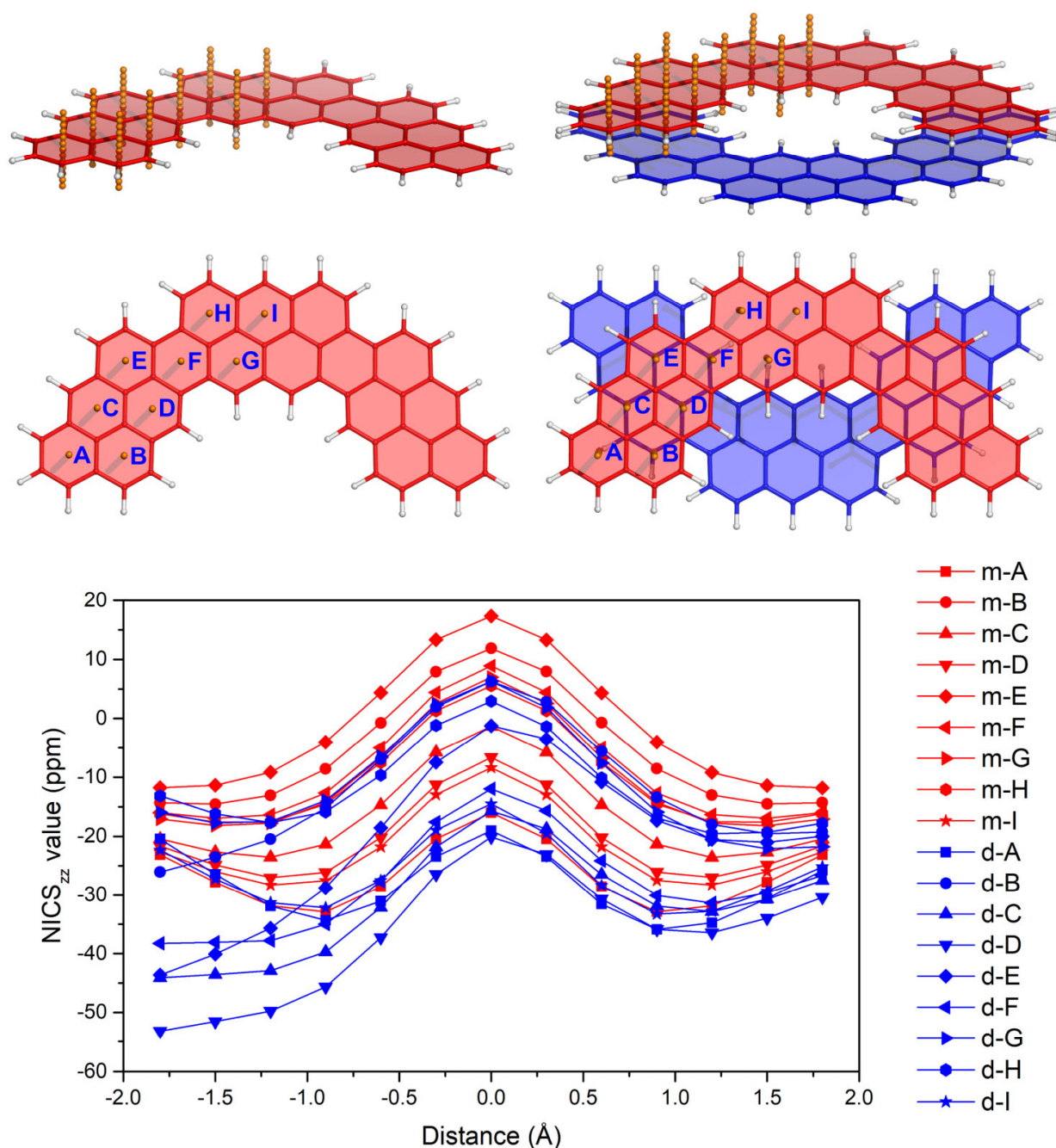
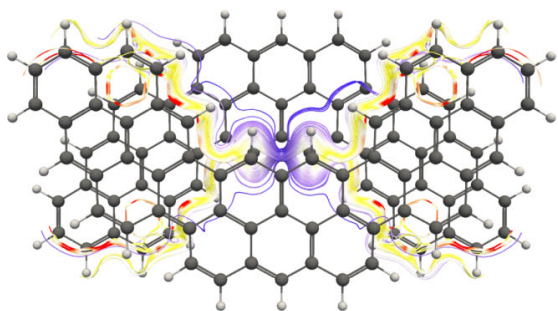


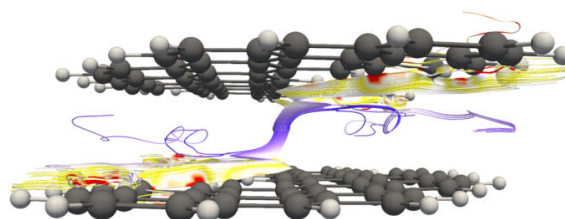
Figure S25. NICS_{zz} scan analysis on rings A to I for the monomer and dimer of **tips-OR-3**, and the molecular models with ghost atoms (shown as orange balls) are shown. The positive and negative values of distance denote up and down directions from the molecular plane. Compared with the monomer, all rings of the dimer, especially rings B, C, D, E, F which have large intermolecular overlap, exhibited enhanced aromaticity with more negative NICS_{zz} values. In addition, the NICS scan curve of the dimer showed an asymmetric pattern, with the negative distance region more magnetically shielded, suggesting an enhanced aromaticity of the interior of the dimer compared to the exterior space.

Magnetic field direction: 0,0,1

Top view

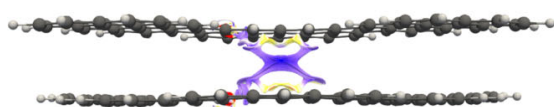


Side view

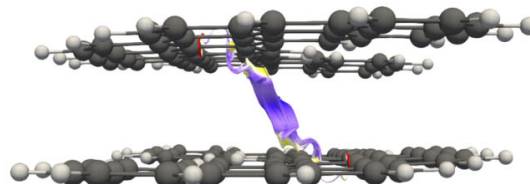


Magnetic field direction: 0,1,0

Top view

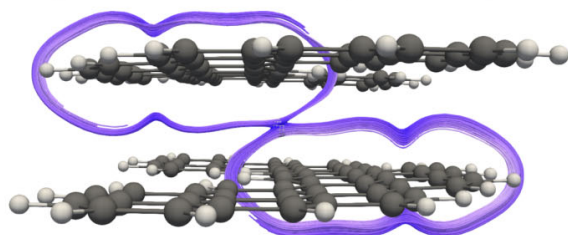


Side view



Magnetic field direction: 1,0,0

Top view



Side view

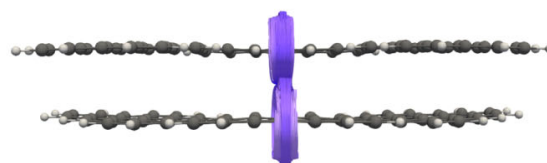


Figure S26. Calculated magnetically induced current in **[tips-OR-3]₂** with the GIMIC method. The external magnetic field was applied along the x, y, z-axis, respectively. The ring currents started from each monomer, indeed form consecutive circuits through the interior space between the two monomers, especially on the position of the carbons which have the shortest C•••C distance – 2.99 Å. This calculation further supports the enhanced 3D aromaticity in **[tips-OR-3]₂**.

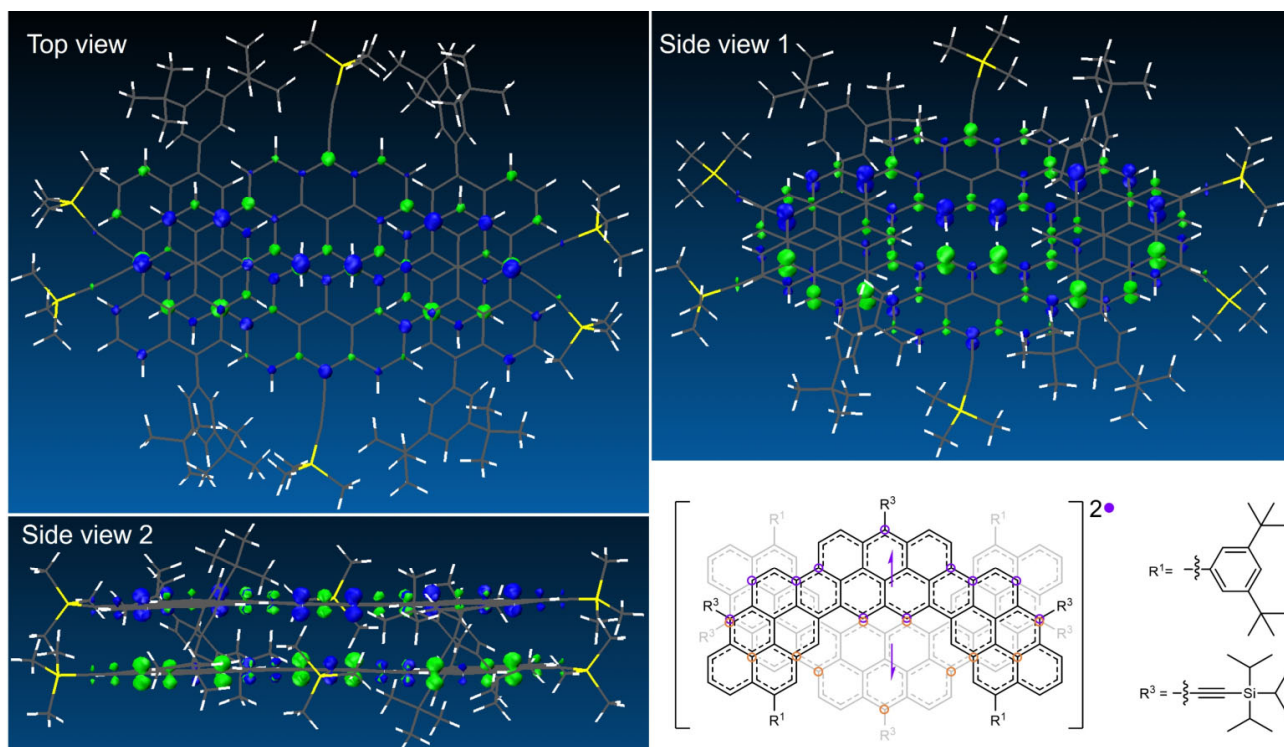


Fig. S27. Calculated spin density distribution of the open-shell singlet state of **[tips-OR-3]₂** at um06-2x/6-311g(d,p) level of theory. The triisopropyl groups are replaced with trimethyl groups during the DFT calculations. Iso-surface value: 0.005.

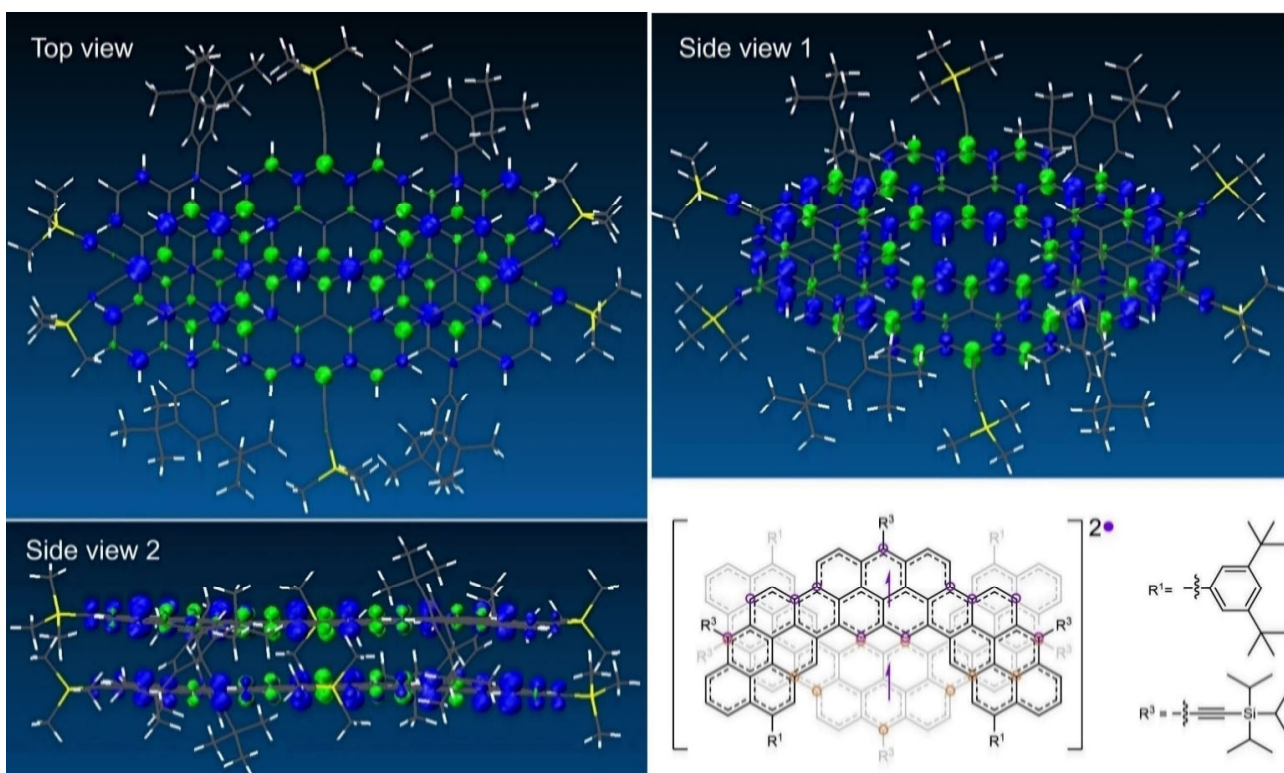


Fig. S28. Calculated spin density distribution of the open-shell triplet state of **[tips-OR-3]₂** at um06-2x/6-311g(d,p) level of theory. The triisopropyl groups are replaced with trimethyl groups during the DFT calculations. Iso-surface value: 0.005.

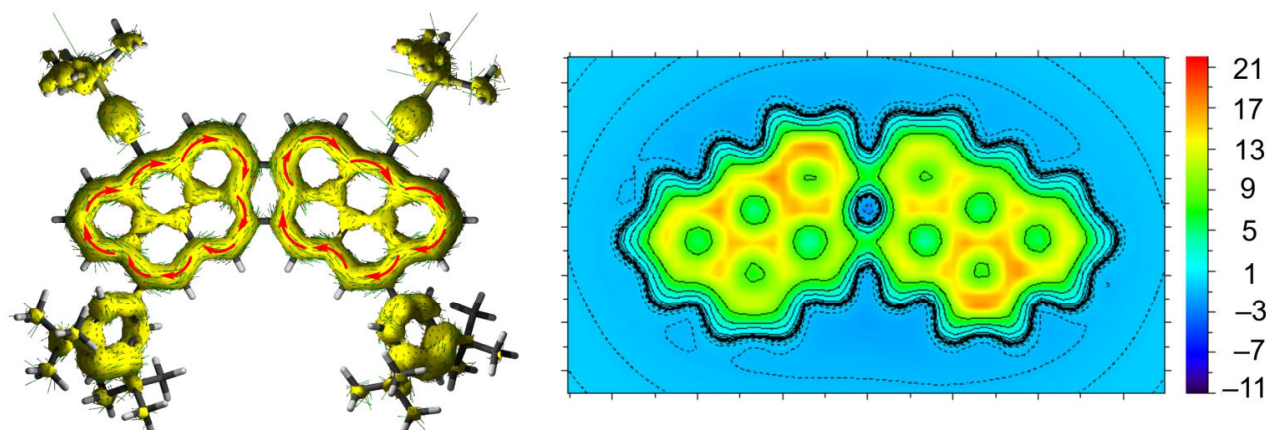


Figure S29. Calculated AICD plot and 2D ICSS_{zz,1} map of dication state of **tips-OR-2** by using DFT at the level of m06-2x/6-31g(d,p) theory. The triisopropyl groups were replaced with trimethyl groups during DFT-calculation.

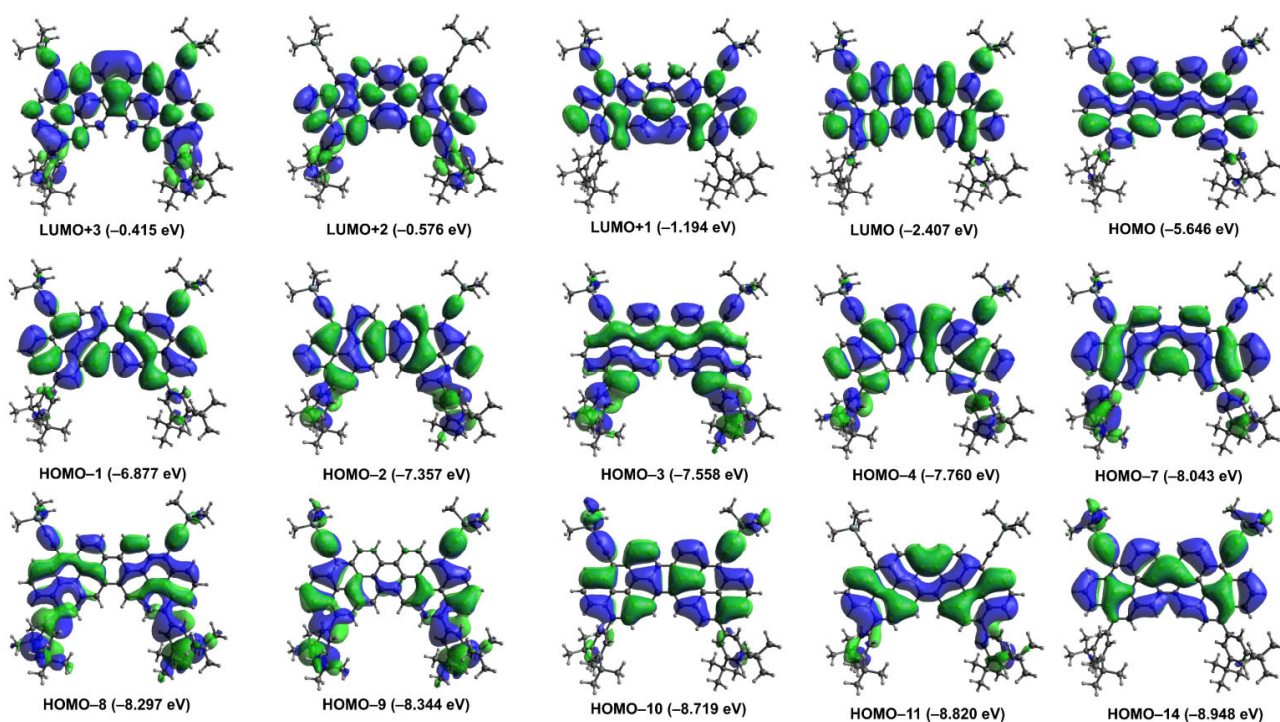


Figure S30. The frontier molecular orbitals of **tips-OR-2** calculated by DFT (m06-2x/6-311g(d,p)). The triisopropyl groups were replaced with trimethyl groups during calculation.

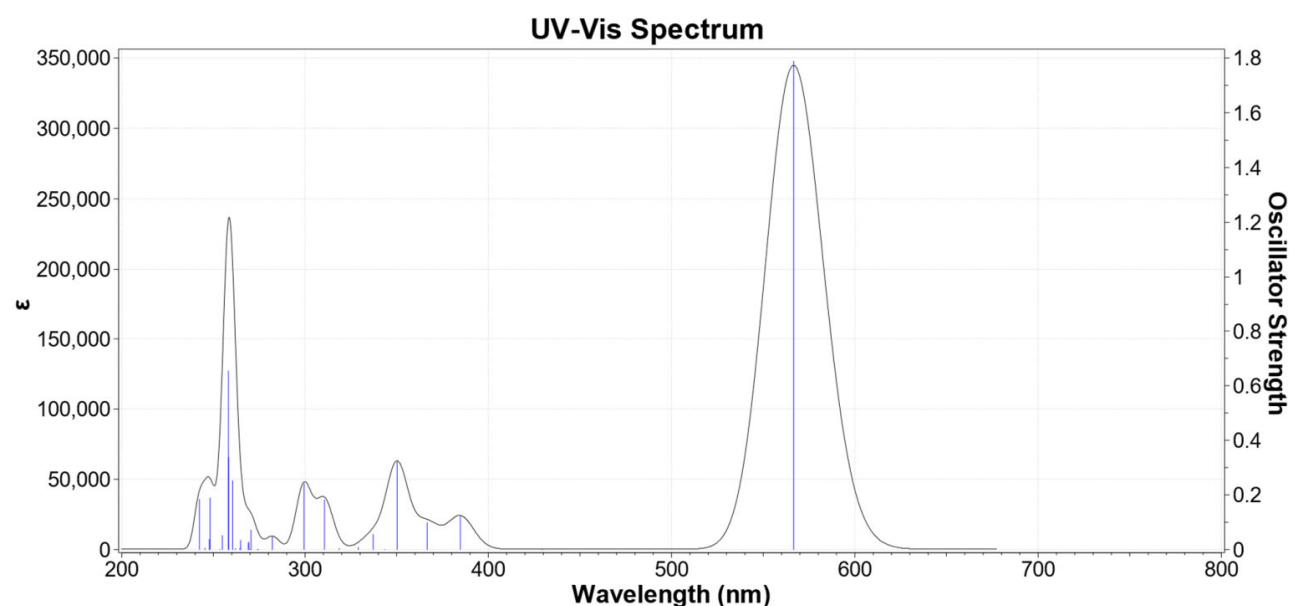


Figure S31. Calculated UV-vis absorption spectrum of **tips-OR-2** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S2. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of **tips-OR-2**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
2.1882	566.60	1.7881	HOMO->LUMO (99%)
3.2224	384.75	0.1220	H-1->LUMO (66%) HOMO->L+1 (27%)
3.5398	350.26	0.3199	HOMO->L+2 (38%) HOMO->L+3 (32%) H-2->LUMO (11%) H-4->LUMO (9%)
3.9918	310.60	0.1816	H-4->LUMO (43%) HOMO->L+2 (27%) HOMO->L+3 (14%) H-2->LUMO (10%)
4.1405	299.44	0.2407	H-1-> L+1 (57%) HOMO->L+5 (12%) H-7->LUMO (12%) H-5->LUMO (7%)

4.7594	260.51	0.2516	H-9->LUMO (32%) H-14->LUMO (15%) H-4-> L+1 (8%)
4.8000	258.30	0.3369	H-3-> L+1 (29%) H-1-> L+4 (12%) H-1-> L+2 (11%) H-2-> L+1 (8%)
4.8023	258.18	0.6536	H-1-> L+2 (22%) H-3-> L+1 (17%) H-2-> L+1 (14%)
4.9957	248.18	0.1884	H-1-> L+3 (22%) H-11-> LUMO (14%)
5.1149	242.40	0.1834	HOMO->L+13 (20%) HOMO->L+14 (11%)

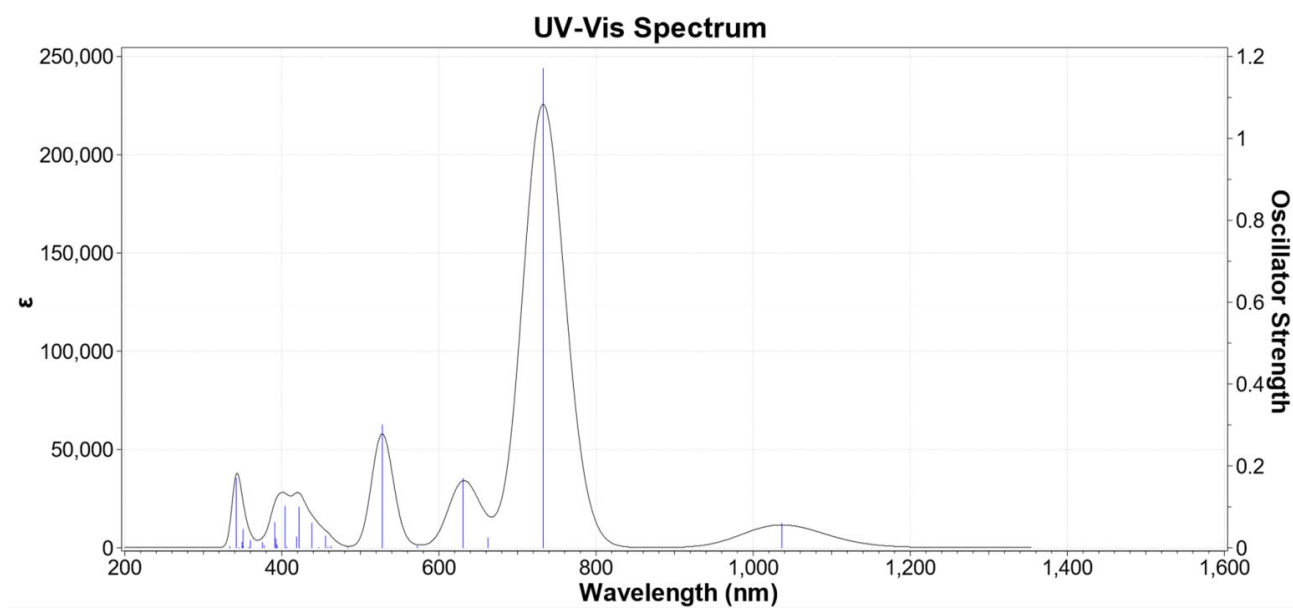


Figure S32. Calculated UV-vis-NIR absorption spectrum of radical cation state of **tips-OR-2** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S3. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of radical cation state of **tips-OR-2**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.1961	1036.59	0.0598	HOMO α (SOMO)->LUMO α (59%) HOMO β ->LUMO β (34%)
1.6922	732.70	1.1705	HOMO β ->LUMO β (60%) HOMO α (SOMO)->LUMO α (32%)
1.9658	630.70	0.1693	H-2 β ->LUMO β (62%) H-6 β ->LUMO β (10%) H-1 β ->LUMO β (7%)
2.3493	527.75	0.3000	H-7 β ->LUMO β (62%) H-5 β ->LUMO β (22%)
2.9391	421.84	0.0988	H-2 α ->LUMO α (25%) H-6 β ->LUMO β (14%) H-1 α ->LUMO α (11%)
3.0678	404.14	0.1014	HOMO α (SOMO)->L+1 α (24%) H-13 β ->LUMO β (17%) H-6 α ->LUMO α (15%)
3.6274	341.80	0.1700	HOMO α (SOMO)->L+2 α (24%) H-13 β ->LUMO β (20%) H-8 α ->LUMO α (11%)

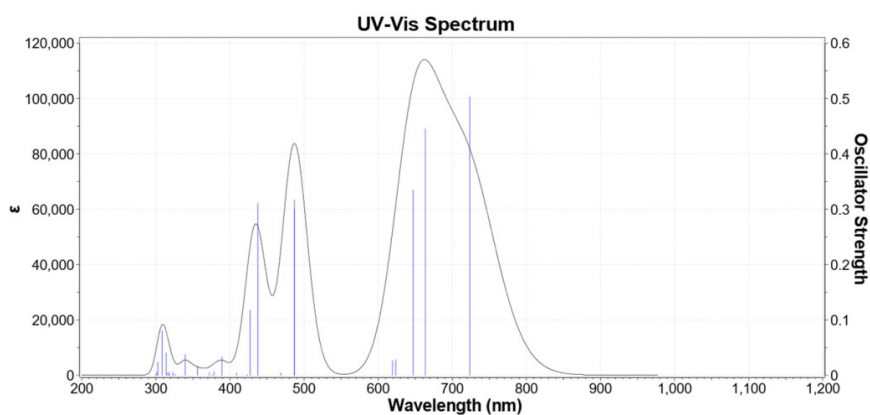


Figure S33. Calculated UV-vis-NIR absorption spectrum of dication state of **tips-OR-2** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S4. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of dication state of **tips-OR-2**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.7132	723.70	0.5032	HOMO->LUMO (88%)
1.8688	663.43	0.4455	H-1->LUMO (90%)
1.9156	647.24	0.3349	H-4->LUMO (64%) H-2->LUMO (20%)
2.5447	487.23	0.3170	H-7->LUMO (44%) H-8->LUMO (18%)
2.5457	487.04	0.3006	H-7->LUMO (40%) H-8->LUMO (20%)
2.8344	437.43	0.3110	H-6->LUMO (54%) H-8->LUMO (26%)

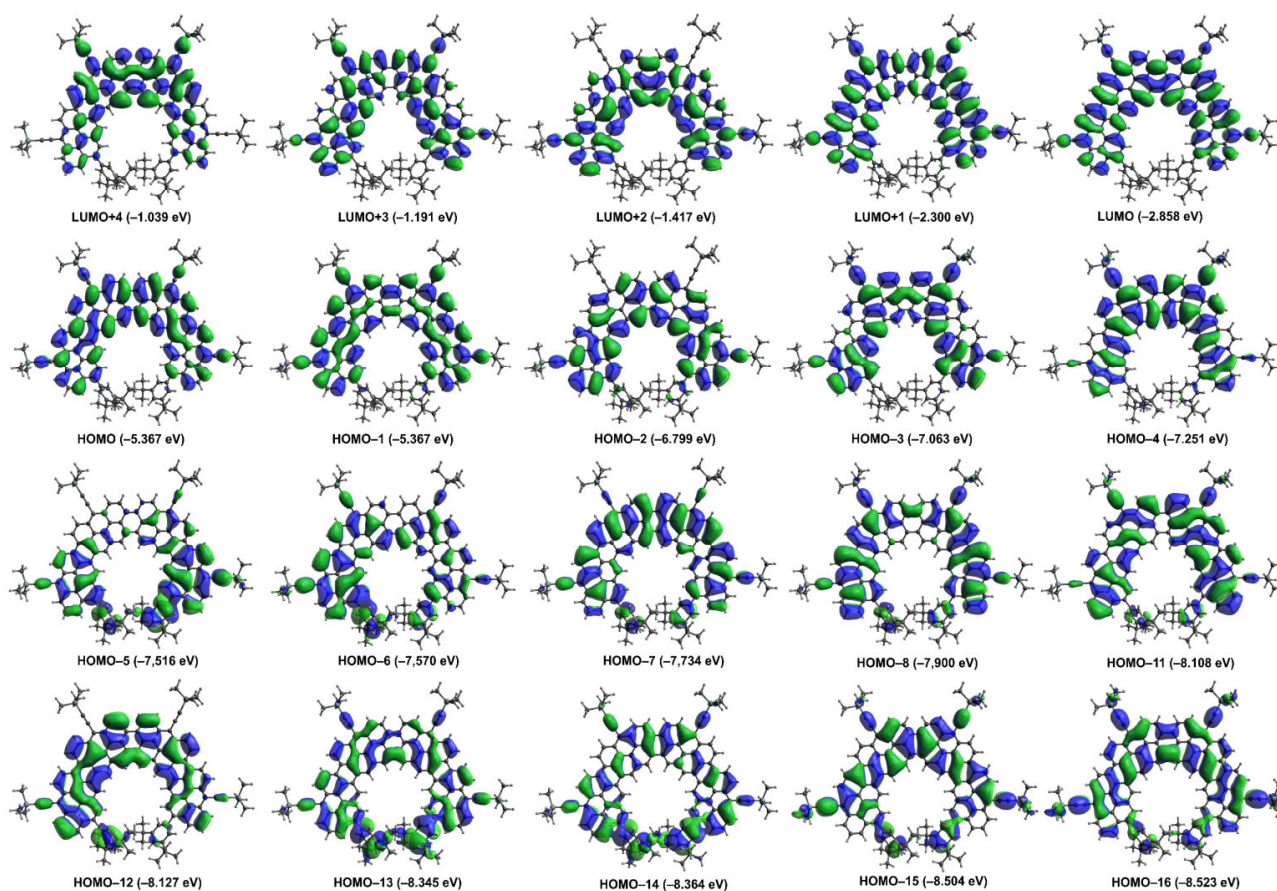


Figure S34. The frontier molecular orbitals of **tips-OR-4** calculated by DFT (m06-2x/6-311g(d,p)). The triisopropyl groups were replaced with trimethyl groups during calculation.

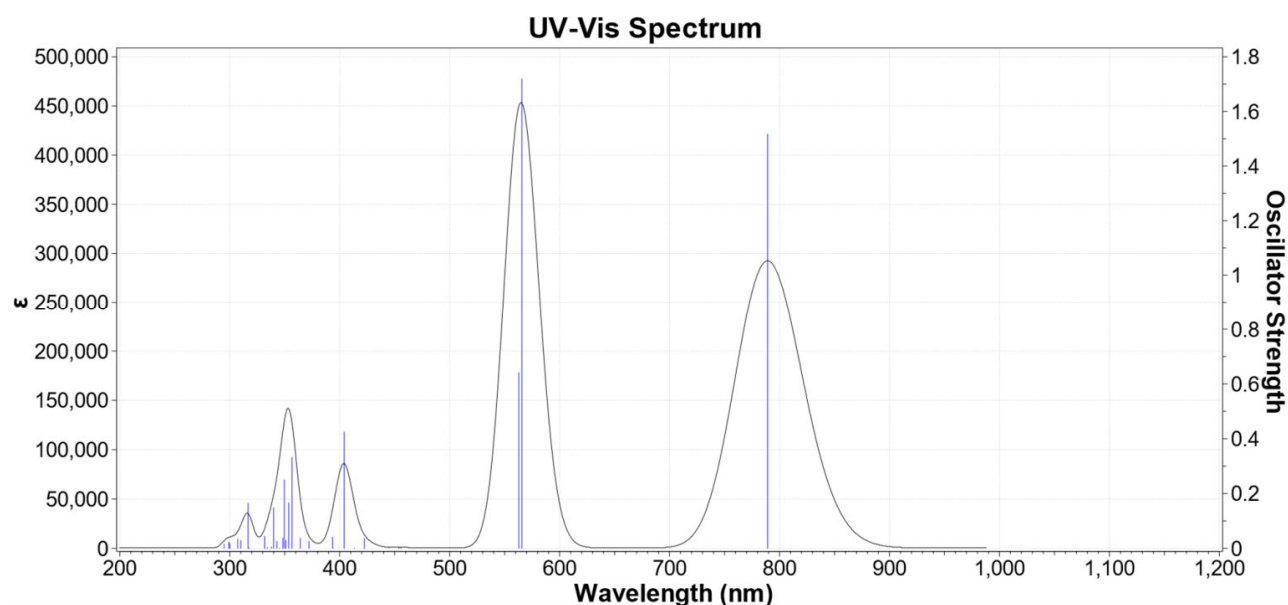


Figure S35. Calculated UV-vis-NIR absorption spectrum of **tips-OR-4** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S5. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of **tips-OR-4**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.5712	789.11	1.5165	HOMO->LUMO (95%)
2.1919	565.66	1.7191	HOMO->L+1 (91%)
2.2027	562.86	0.6409	H-1->LUMO (90%)
3.0688	404.02	0.4244	H-4->LUMO (47%) HOMO->L+5 (12%) HOMO->L+4 (11%) HOMO->L+2 (10%)
3.4775	356.53	0.3319	H-6->LUMO (32%) H-5->L+1 (13%) H-7->LUMO (8%)
3.5061	353.62	0.1660	HOMO->L+6 (27%) H-1->L+4 (15%) H-1->L+2 (10%)
3.5466	349.58	0.2494	H-7->LUMO (32%) HOMO->L+7 (13%)

			HOMO->L+5 (11%)
3.6473	339.93	0.1480	HOMO->L+7 (36%) H-7->LUMO (16%) H-1->L+6 (12%)
3.9153	316.66	0.1643	H-8->LUMO (32%) HOMO->L+8 (15%) H-1->L+4 (14%)

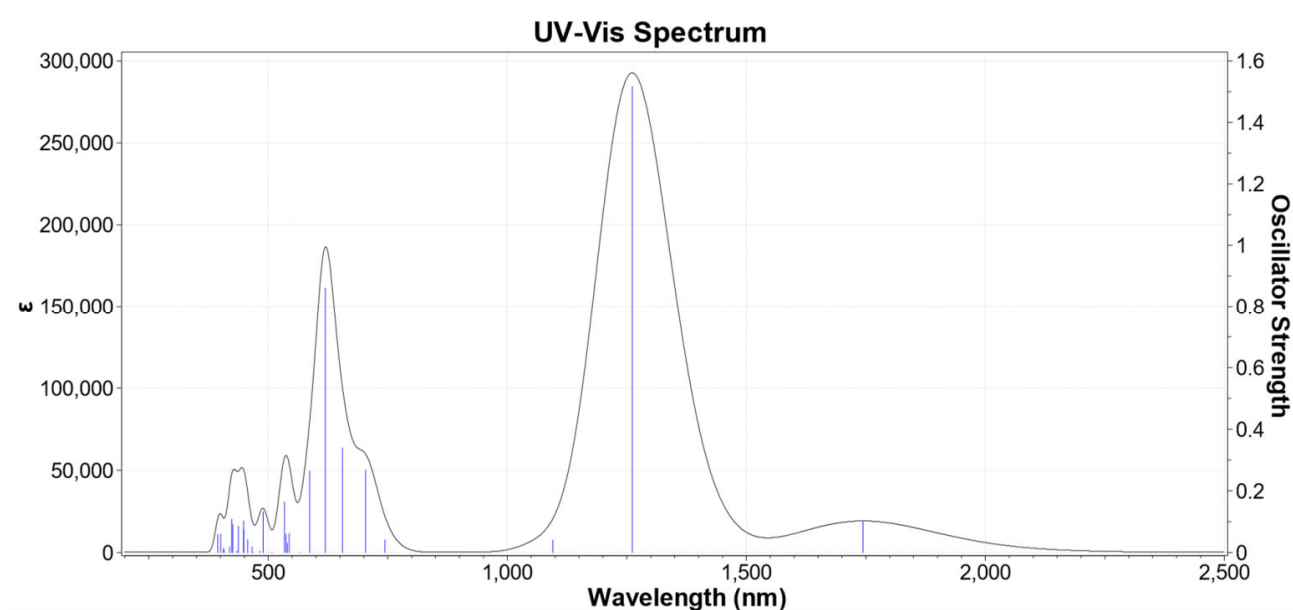


Figure S36. Calculated UV-vis-NIR absorption spectrum of radical cation state of **tips-OR-4** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S6. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of radical cation state of **tips-OR-4**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
0.7109	1743.99	0.0985	HOMO β ->LUMO β (65%) HOMO α ->LUMO α (31%)
0.9828	1261.54	1.5170	HOMO α ->LUMO α (56%) HOMO β ->LUMO β (29%)
1.7623	703.53	0.2669	H-1 β ->LUMO β (73%) H-1 α ->LUMO α (8%)

1.8917	655.40	0.3383	H-1 α ->LUMO α (51%) HOMO β ->L+1 β (31%)
2.0016	619.43	0.8605	HOMO α ->L+1 (55%) HOMO β ->L+1 β (30%)
2.1131	586.73	0.2643	H-3 β ->LUMO β (72%)
2.3211	534.16	0.1637	H-5 β ->LUMO β (15%) H-2 α ->LUMO α (14%) HOMO β ->L+2 β (9%)
2.5328	489.51	0.1318	H-8 β ->LUMO β (66%)

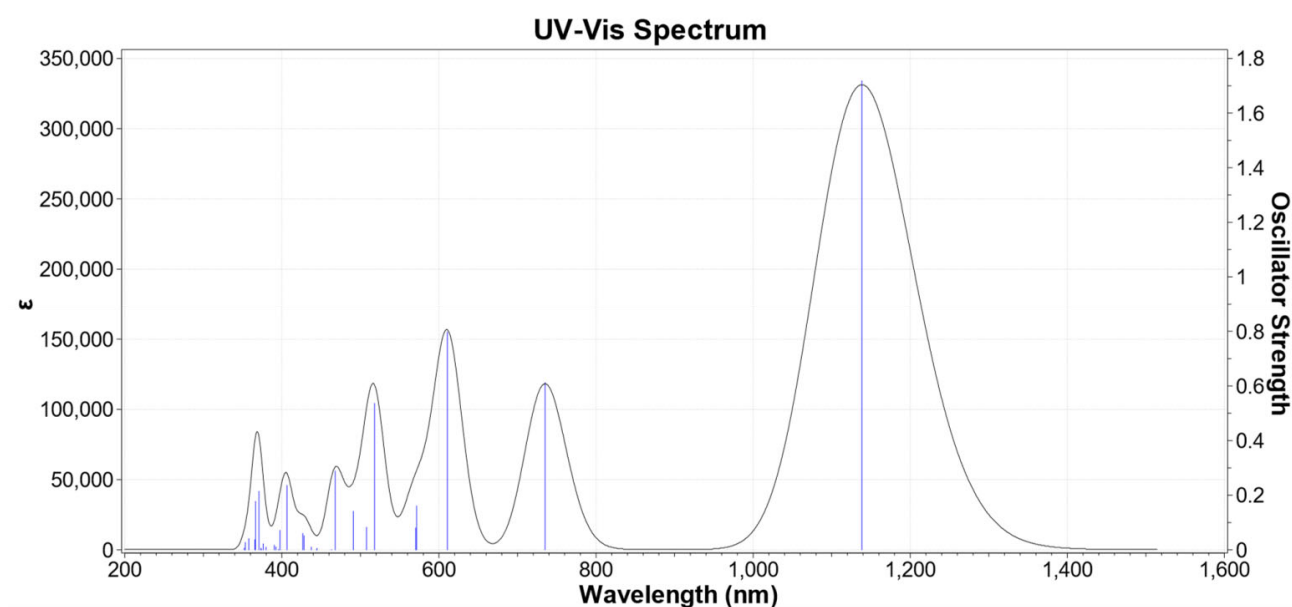


Figure S37. Calculated UV-vis-NIR absorption spectrum of dication state of **tips-OR-4** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S7. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of dication state of **tips-OR-4**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.0890	1138.49	1.7182	HOMO->LUMO (97%)
1.6866	735.09	0.6121	HOMO->L+1 (94%)
2.0302	610.69	0.7973	H-1->LUMO (90%)
2.1692	571.57	0.1607	H-3->LUMO (58%) H-2->LUMO (20%)
2.3938	517.94	0.5363	H-4->LUMO (66%)

2.5250	491.02	0.1411	HOMO->L+2 (94%)
2.6500	467.86	0.2886	H-8->LUMO (72%)
3.0493	406.60	0.2358	HOMO->L+3 (57%)
3.3434	370.83	0.2142	HOMO->L+4 (51%)
3.3830	366.50	0.1772	HOMO->L+5 (57%)

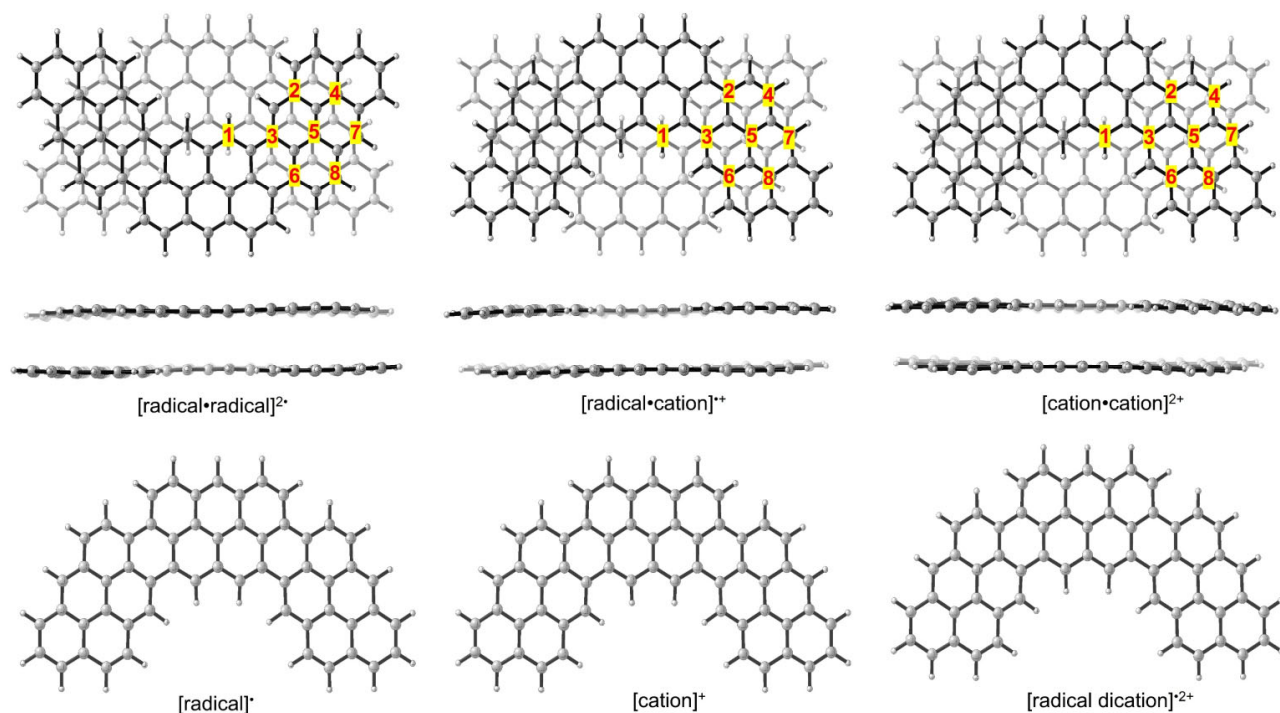


Figure S38. Calculated structures of truncated $[\text{radical}\bullet\text{radical}]^{2+}$, $[\text{radical}\bullet\text{cation}]^{+}$, $[\text{cation}\bullet\text{cation}]^{2+}$ state of $[\text{tips-OR-3}]_2$, $[\text{radical}]^\bullet$, $[\text{cation}]^+$, $[\text{radical dication}]^{2+}$ state of **tips-OR-3** by DFT at the (u)m06-2x/6-31g(d,p) level of theory.

Table S8. Selected C•••C distances (in Å) from the crystallographic structure of $[\text{radical}\bullet\text{radical}]^{2+}$ state of $[\text{tips-OR-3}]_2$ and the calculated structures of $[\text{radical}\bullet\text{radical}]^{2+}$, $[\text{radical}\bullet\text{cation}]^{+}$, $[\text{cation}\bullet\text{cation}]^{2+}$ states of truncated $[\text{tips-OR-3}]_2$. The number assignment of selected C•••C distances is shown in **Figure S38** and **Figure 4e**.

	1	2	3	4	5	6	7	8
$[\text{radical}\bullet\text{radical}]^{2+}$ (crystallographic)	2.99	3.24	3.17	3.31	3.25	3.24	3.35	3.31
$[\text{radical}\bullet\text{radical}]^{2+}$ (calculated)	2.991	3.189	3.170	3.185	3.237	3.189	3.146	3.185
$[\text{radical}\bullet\text{cation}]^{+}$	3.087	3.200	3.192	3.206	3.249	3.200	3.187	3.206

(calculated)								
[cation•cation] ²⁺	3.218	3.228	3.230	3.267	3.289	3.228	3.281	3.267
(calculated)								

Table S9. Detailed computed energies (in Hartrees) of calculated structures of truncated [radical•radical]^{2•}, [radical•cation]^{•+}, [cation•cation]²⁺ state of **[tips-OR-3]₂**, [radical][•], [cation]⁺ state of **tips-OR-3** at (u)m06-2x/6-311g(d,p)-SMD(DCM)//(u)m06-2x/6-311g(d,p)-SMD(DCM) level of theory.

Structure	[radical] [•] state	[cation] ⁺ state	[radical•radical] ^{2•} state	[radical•cation] ^{•+} state	[cation•cation] ²⁺ state
Electronic Energy (EE)	-2187.043732	-2186.881546	-4374.149901	-4373.991637	-4373.816341
Zero-point Energy Correction	0.632892	0.635992	1.266294	1.269236	1.269927
Thermal Correction to Energy	0.667229	0.670210	1.336661	1.338898	1.340410
Thermal Correction to Enthalpy	0.668173	0.671154	1.337605	1.339842	1.341354
Thermal Correction to Free Energy	0.570280	0.573883	1.170723	1.175224	1.172297
Imaginary Frequency (cm ⁻¹)	—	—	—	—	—

DFT calculations were performed to evaluate the free energy change (ΔG), which is defined as the free energy difference between the dimer complex and the corresponding unbound monomers, for the formation of truncated [radical•radical]^{2•}, [radical•cation]^{•+}, [cation•cation]²⁺ state of **[tips-OR-3]₂**. The ΔG values for the formation of truncated [radical•radical]^{2•}, [radical•cation]^{•+}, [cation•cation]²⁺ state of **[tips-OR-3]₂** were calculated to be -84.9 , -92.5 , and -75.3 kJ mol⁻¹, respectively. The ΔG values indicate that the formation of [radical•radical]^{2•}, [radical•cation]^{•+}, and [cation•cation]²⁺ states of **[tips-OR-3]₂** is thermodynamic favored in dichloromethane solution. The

driving forces contain not only the radical delocalization, but also the π - π interactions between the two π -surfaces. (It is noteworthy that, the ΔG values calculated here, are for the formation of truncated dimer complex without side chains. Thus, the ΔG values do not contain the contribution of interactions from side chains). The two partially overlapped redox waves on 0.46 V and 0.56 V (Fig. 5c) suggest the existence of a metastable redox state between $[\text{cation}\bullet\text{cation}]^{2+}$ state of **[tips-OR-3]₂** and $[\text{radical dication}]^{2+}$ state of **[tips-OR-3]**. During the oxidation titration measured by UV-vis-NIR spectroscopy, we indeed observed a metastable state (blue trace in Fig. 5d). This metastable state is very unstable, shaking the UV cuvette led to the transformation of the state to radical dication state of **[tips-OR-3]**. Thus, both the electrochemical and titration experimental results indicate the existence of metastable state – $[\text{cation}\bullet\text{radical dication}]^{\bullet 3+}$ states of **[tips-OR-3]₂** which immediately dissociated to two separate **tips-OR-3** in $[\text{cation}]^+$ and $[\text{radical dication}]^{\bullet 2+}$ state.

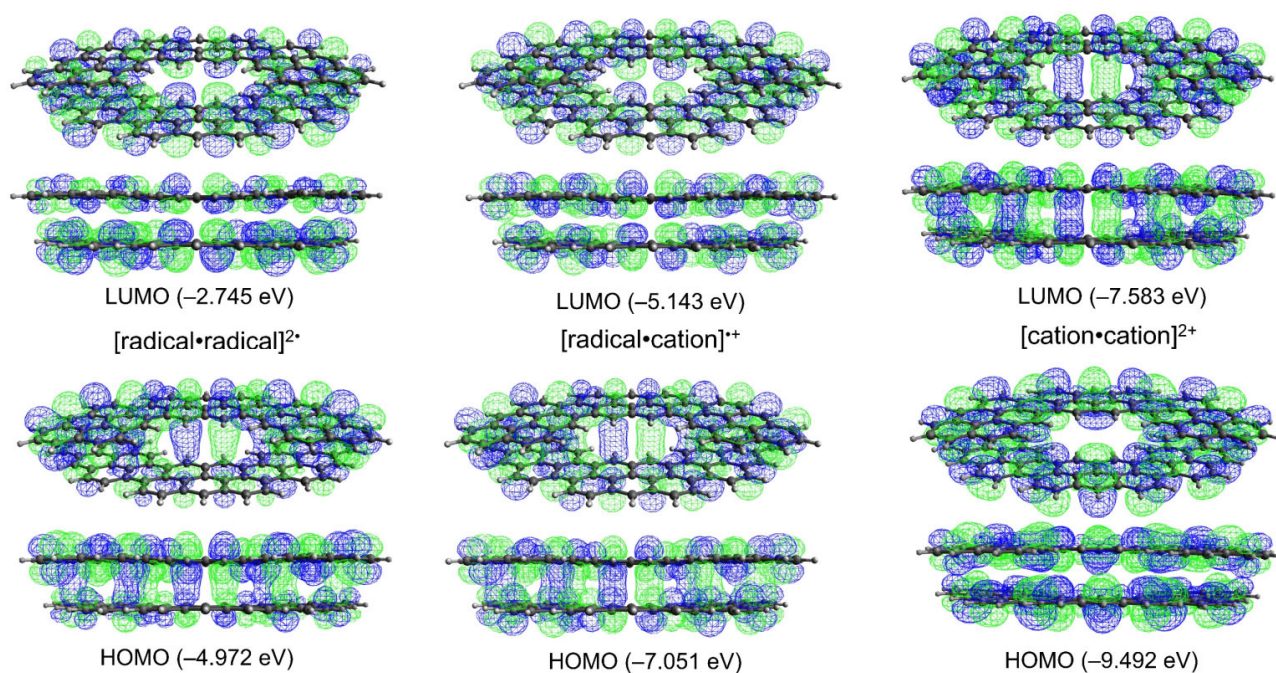


Figure S39. The frontier molecular orbitals of truncated $[\text{radical}\bullet\text{radical}]^{2\bullet}$, $[\text{radical}\bullet\text{cation}]^{\bullet+}$, $[\text{cation}\bullet\text{cation}]^{2+}$ state of **[tips-OR-3]₂** calculated by DFT (um06-2x/6-311g(d,p)).

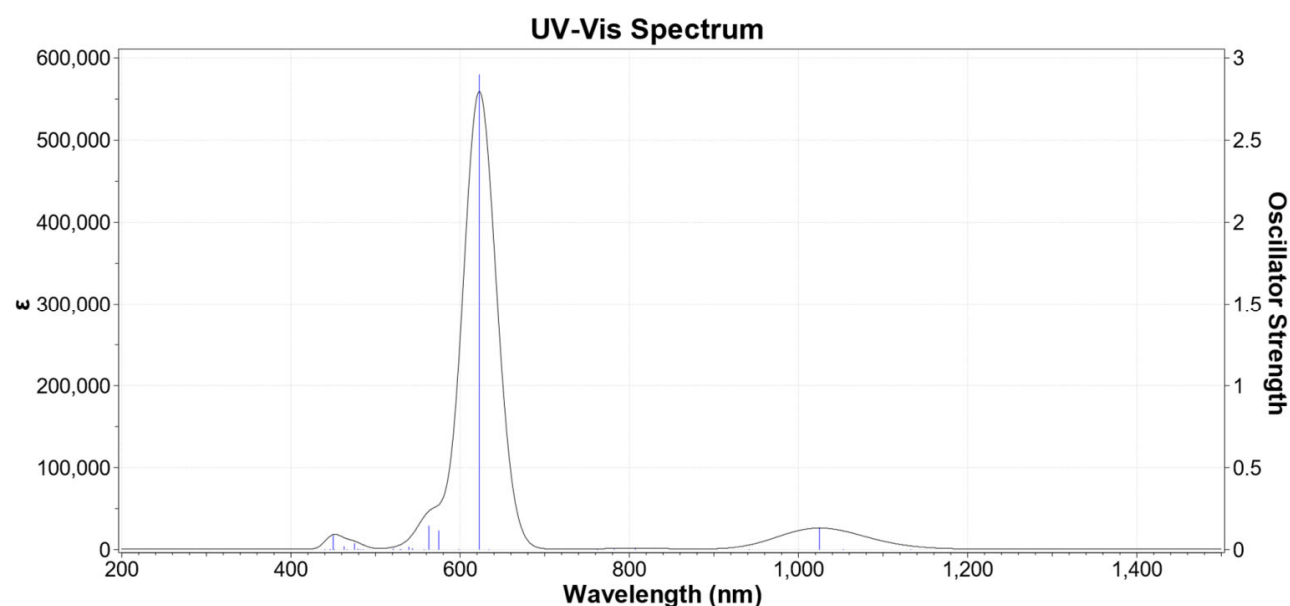


Figure S40. Calculated UV-vis-NIR absorption spectrum of truncated [radical•radical]^{2•} state of [tips-OR-3]₂ by TD-DFT at the um06-2x/6-31g(d,p) level of theory.

Table S10. Selected TD-DFT (um06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of truncated [radical•radical]^{2•} state of [tips-OR-3]₂.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.2098	1024.82	0.1333	HOMO α ->LUMO α (49%) HOMO β ->LUMO β (49%)
1.9908	622.7	2.8981	HOMO α ->L+1 α (24%) HOMO β ->L+1 β (24%) H-1 α ->LUMO α (19%) H-1 β ->LUMO β (19%)

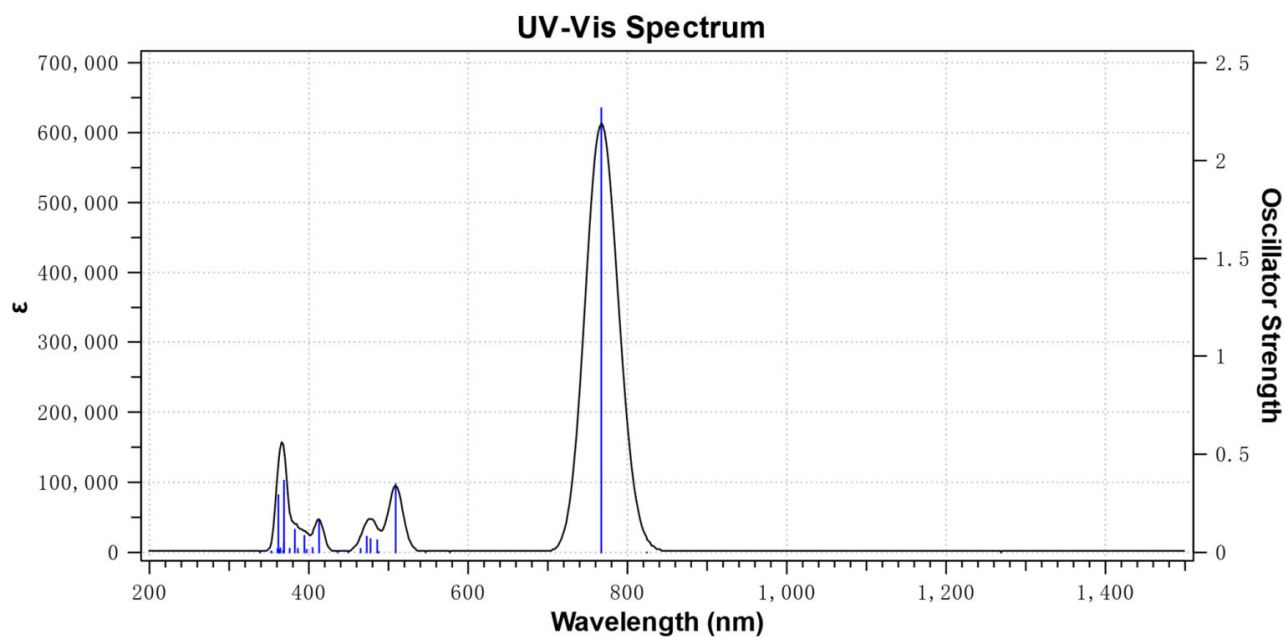


Figure S41. Calculated UV-vis-NIR absorption spectrum of [radical][•] state of **tips-OR-3** by TD-DFT at the m06-2x/6-31g(d,p) level of theory.

Table S11. Selected TD-DFT (m06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of [radical][•] state of **tips-OR-3**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
0.9769	1269.15	0	HOMO α ->LUMO α (48%) HOMO β ->LUMO β (47%)
1.6161	767.18	2.2675	HOMO α ->LUMO α (48%) HOMO β ->LUMO β (47%)

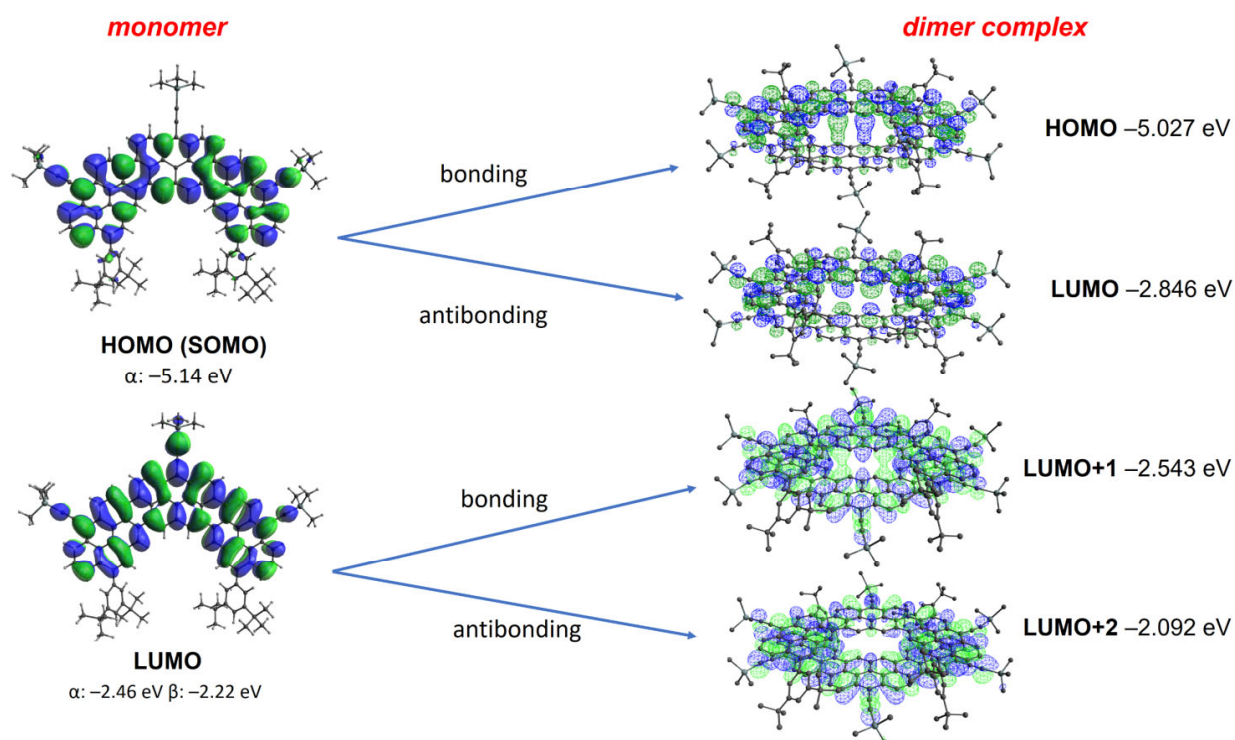


Figure S42. Calculated molecular orbitals of **tips-OR-3** and **[tips-OR-3]₂** by DFT at the (u)m06-2x/6-311g(d,p) level of theory. The triisopropyl groups are replaced with trimethyl groups during the DFT calculations.

As shown in **Fig. S40**, calculated UV-vis-NIR absorption spectrum of **[tips-OR-3]₂** is well consistent with the experimental absorption spectrum. Based on TD-DFT calculation, the broad absorption band of **[tips-OR-3]₂** at 1285 nm can be attributed to the transition from HOMO to LUMO of **[tips-OR-3]₂** formed by the linear combination of two SOMOs of each **tips-OR-3**. The sharp absorption band of **[tips-OR-3]₂** at 804 nm can be mainly attributed to the transition from HOMO to LUMO+1 of **[tips-OR-3]₂**.

In addition, we also calculated the UV-vis-NIR absorption spectrum of the hypothetical **tips-OR-3** monomer (**Fig. S41**). For the hypothetical **tips-OR-3** monomer, the oscillator strength (f) of the transition (from SOMO α -spin to LUMO α -spin, and HOMO β -spin to LUMO β -spin) corresponding to calculated absorption band at 1269 nm is zero, in other words, the calculated absorption band at 1269 nm is forbidden in the case of **tips-OR-3** monomer. For **[tips-OR-3]₂**, the 32-center-2-electron pancake bond makes the two SOMOs of each **tips-OR-3** combine into new HOMO and LUMO of **[tips-OR-3]₂**. Particularly, the transition from HOMO to LUMO of **[tips-OR-3]₂** is unforbidden ($f = 0.133$). Thus, the 32-center-2-electron pancake bond leads to the generation of the experimental broad absorption band at 1285 nm corresponding to the HOMO to LUMO transition of **[tips-OR-3]₂**.

Furthermore, both the calculated UV-vis-NIR spectra of **[tips-OR-3]₂** and hypothetical **tips-OR-3** monomer show a sharp absorption band at 623 and 767 nm, respectively, which is consistent with the experimental sharp absorption band at 804 nm. Based on orbital analysis, the corresponding transition from HOMO to LUMO+1 of **[tips-OR-3]₂** is homologous to the transition from SOMO to LUMO of **tips-OR-3** monomer, because the LUMO+1 of **[tips-OR-3]₂** is formed by the linear

combination of LUMO of **tips-OR-3** monomer (Fig. S34). Thus, **[tips-OR-3]₂** maintains the sharp absorption band at 804 nm from the **tips-OR-3** monomer.

In conclusion, the origin of the sharp and broad absorption bands of **[tips-OR-3]₂** at 804 and 1285 nm can be attributed to the transitions from HOMO to LUMO+1, and HOMO to LUMO of **[tips-OR-3]₂**, respectively. The 32-center-2-electron pancake bond makes the forbidden absorption band for **tips-OR-3** monomer become the observable broad charge-transfer band at 1285 nm for **[tips-OR-3]₂**.

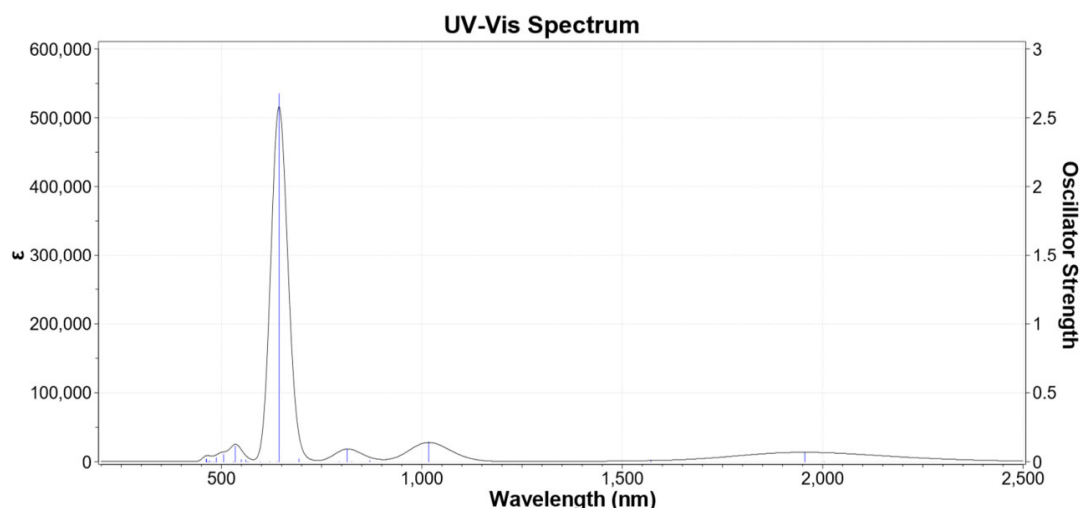


Figure S43. Calculated UV-vis-NIR absorption spectrum of truncated [radical•cation]^{•+} state of **[tips-OR-3]₂** by TD-DFT at the um06-2x/6-31g(d,p) level of theory.

Table S12. Selected TD-DFT (um06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of truncated [radical•cation]^{•+} state of **[tips-OR-3]₂**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
0.6340	1955.47	0.0687	HOMO α ->LUMO α (93%)
1.2187	1017.33	0.1437	HOMO α ->L+1 α (44%) H-1 α ->LUMO α (33%)
1.9261	643.70	2.6749	HOMO α ->L+1 α (38%) HOMO β ->L+1 β (19%) H-1 α ->LUMO α (16%)

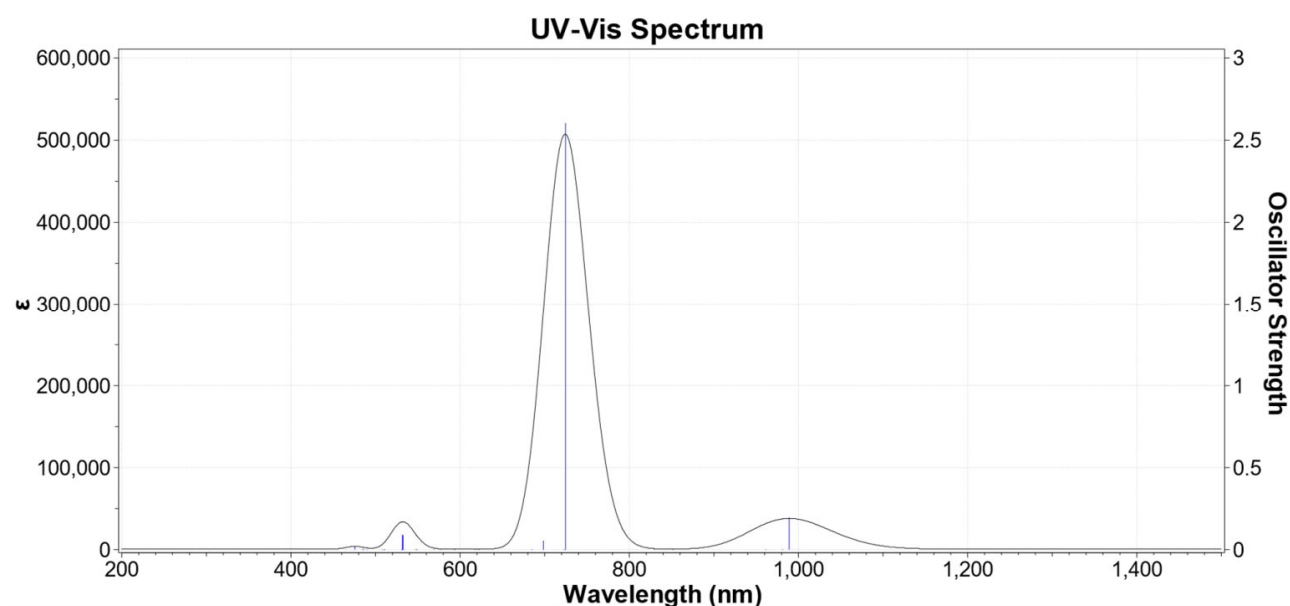


Figure S44. Calculated UV-vis-NIR absorption spectrum of truncated $[\text{cation}\bullet\text{cation}]^{2+}$ state of **[tips-OR-3]₂** by TD-DFT at the um06-2x/6-31g(d,p) level of theory. The calculated spectrum is not consistent well with the experimental result (see Fig. 5 in main text), may because the TD-DFT calculation in this case is not suitable to describe experimental result or the two $[\text{cation}]^+$ state of **tips-OR-3** within $[\text{cation}\bullet\text{cation}]^{2+}$ state of **[tips-OR-3]₂** is weak coupled.

Table S13. Selected TD-DFT (um06-2x/6-31g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of truncated $[\text{cation}\bullet\text{cation}]^{2+}$ state of **[tips-OR-3]₂**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.2537	988.97	0.1948	H-1 α ->LUMO α (36%) H-1 β ->LUMO β (36%)
1.7112	724.54	2.6023	HOMO α ->L+1 α (35%) HOMO β ->L+1 β (35%) H-1 α ->LUMO α (14%) H-1 β ->LUMO β (14%)
2.3279	532.59	0.0855	HOMO α ->L+2 α (45%) HOMO β ->L+2 β (45%)

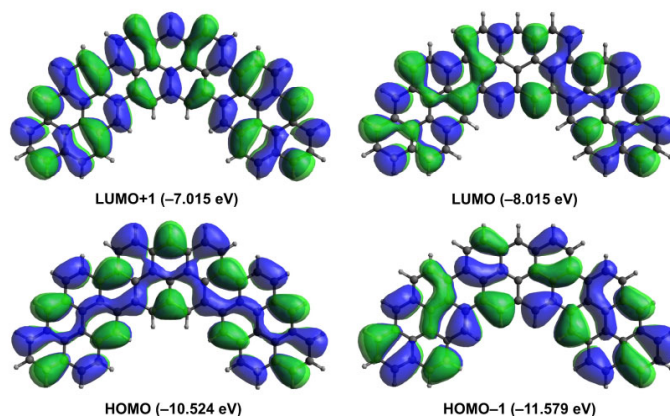


Figure S45. The frontier molecular orbitals of truncated [radical dication] $\bullet^{2+}$ state of **tips-OR-3** calculated by DFT (m06-2x/6-311g(d,p)).

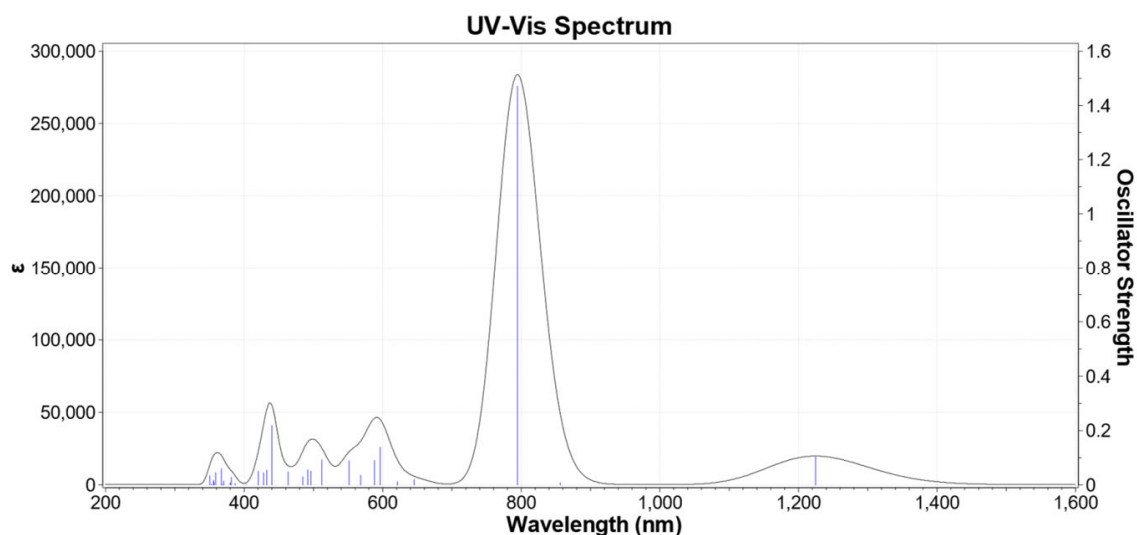


Figure S46. Calculated UV-vis-NIR absorption spectrum of truncated [radical dication] $\bullet^{2+}$ state of **tips-OR-3** by TD-DFT at the m06-2x/6-311g(d,p) level of theory.

Table S14. Selected TD-DFT (m06-2x/6-311g(d,p)) calculated excitation energies, wavelengths, oscillator strengths and compositions of major electronic transitions of truncated [radical dication] $\bullet^{2+}$ state of **tips-OR-3**.

Energy (eV)	Wavelength (nm)	Oscillator strength	Major contributions
1.0123	1224.76	0.1024	HOMO α ->LUMO α (65%) HOMO β ->LUMO β (30%)
1.5605	794.50	1.4705	HOMO β ->LUMO β (60%) HOMO α ->LUMO α (30%)

6. Resonance forms analysis of OR-2

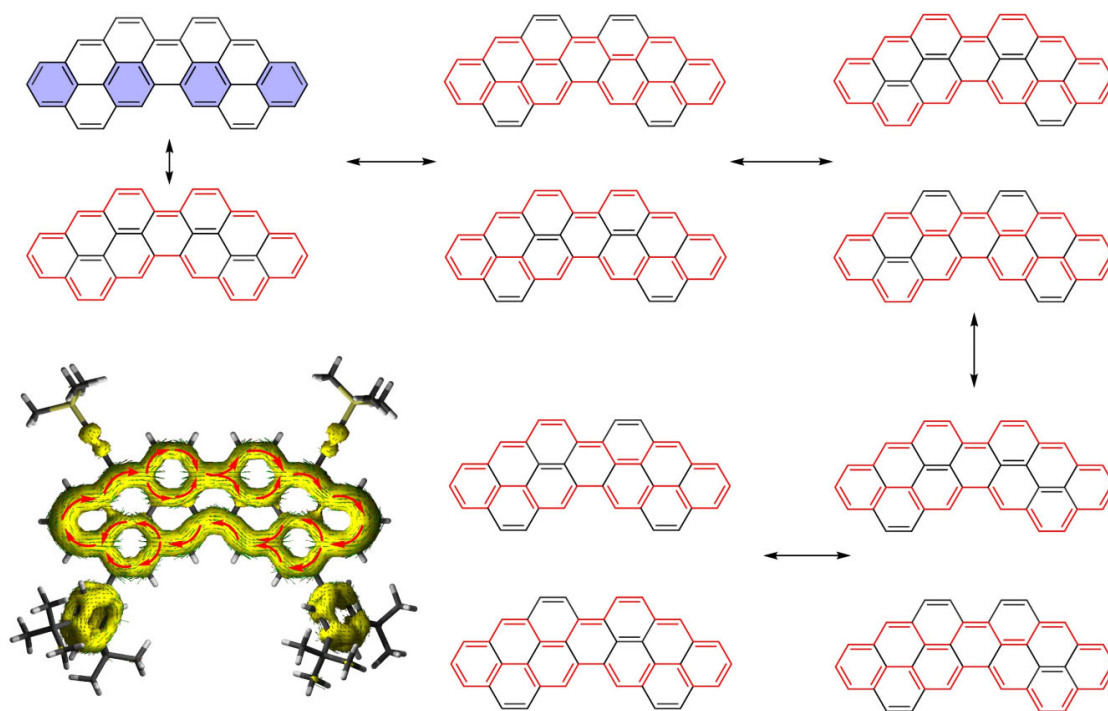


Figure S47. Representative resonance forms of **OR-2** containing inner formal $[30]\pi$ annulene. The formal $[30]\pi$ annulene obeys Hückel aromaticity rule and calculated ACID plot. Therefore, we believe that the global aromaticity (inner $[30]\pi$ annulene) at least partially contribute to the aromatic character of **OR-2**.

7. NMR and HRMS spectra

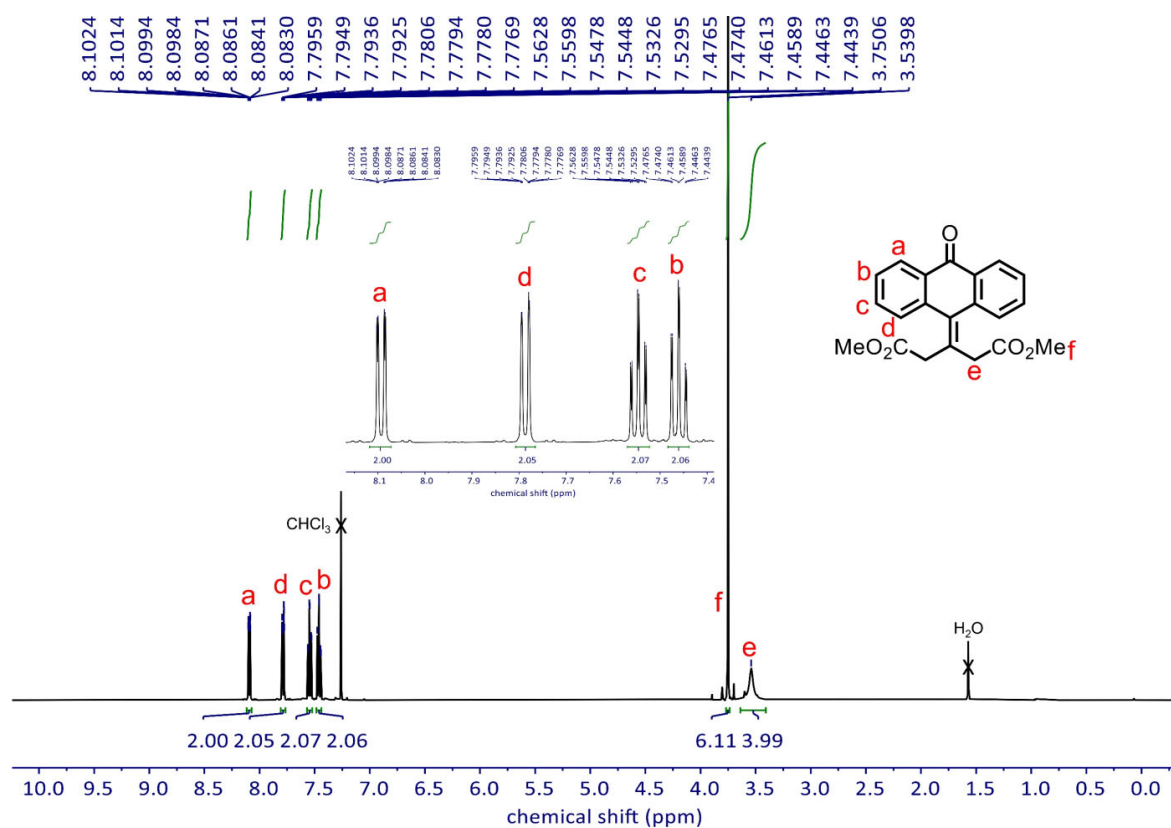


Figure S48. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of 2.

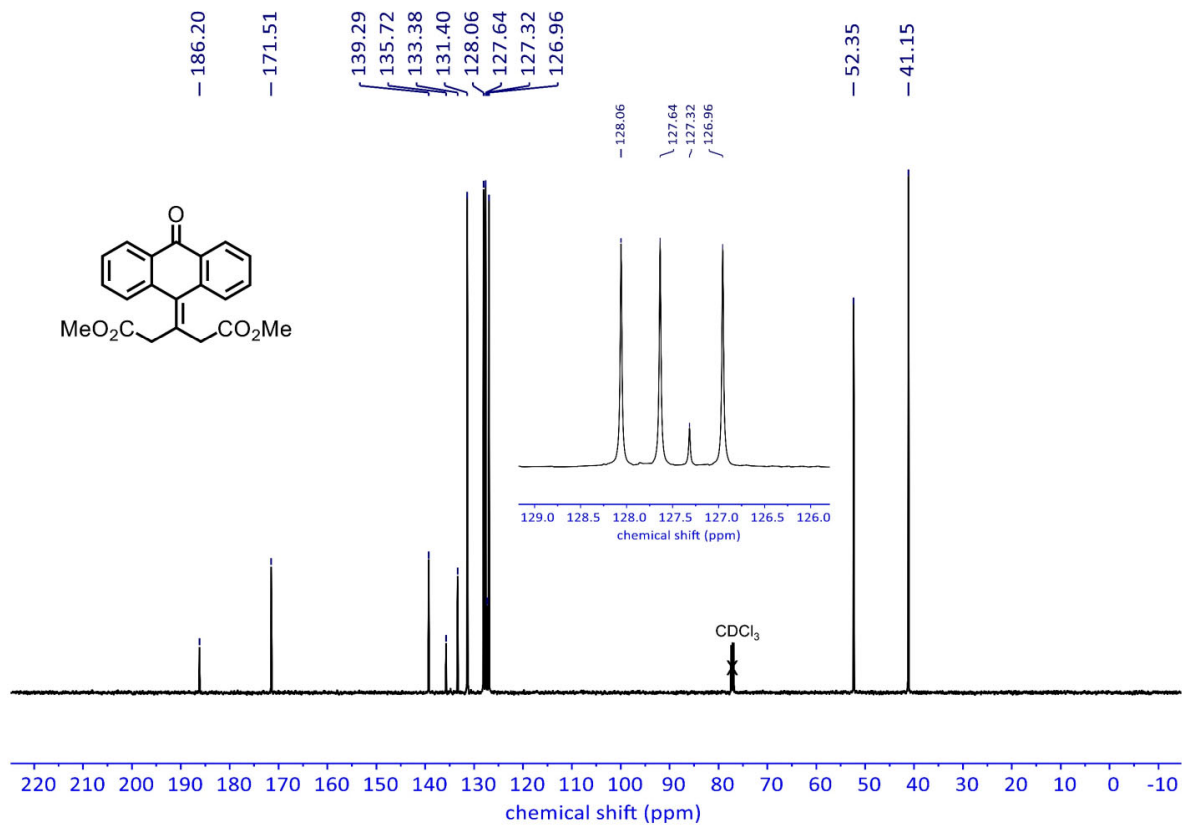


Figure S49. ¹³C NMR Spectrum (125 MHz, CDCl₃, 298K) of 2.

Mass Spectrum SmartFormula Report

Sample Name	CH2CO2Me	Data File	D:\MassHunter\Data\Chemistry\2021\202109\20210909\CH2CO2Me.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union_APCI-1.m	Acquired Time	9/9/2021 10:52:38 AM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
351.1234	1	C21 H19 O5	351.1227	1.99

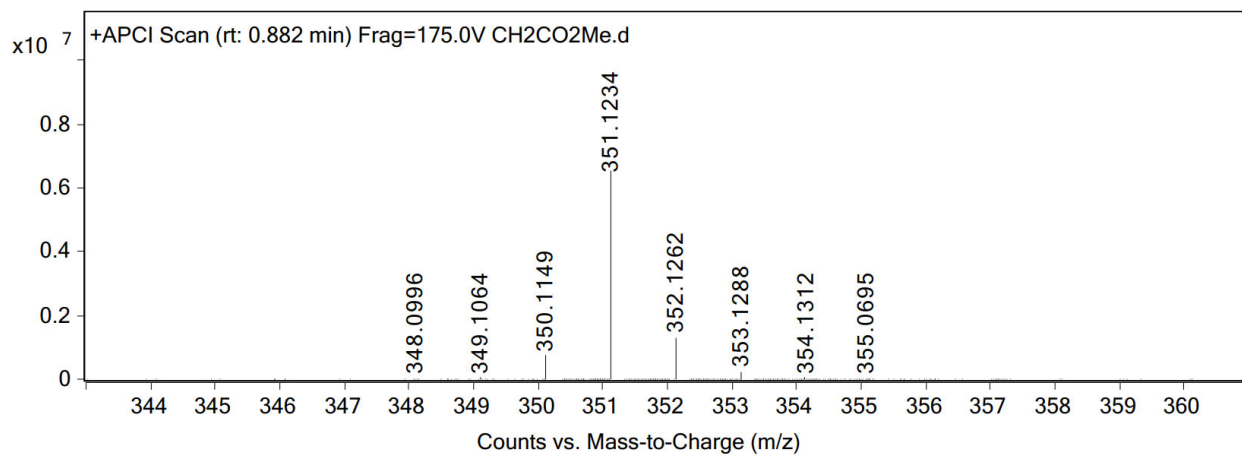


Figure S50. HR-APCI-MS of **2**.

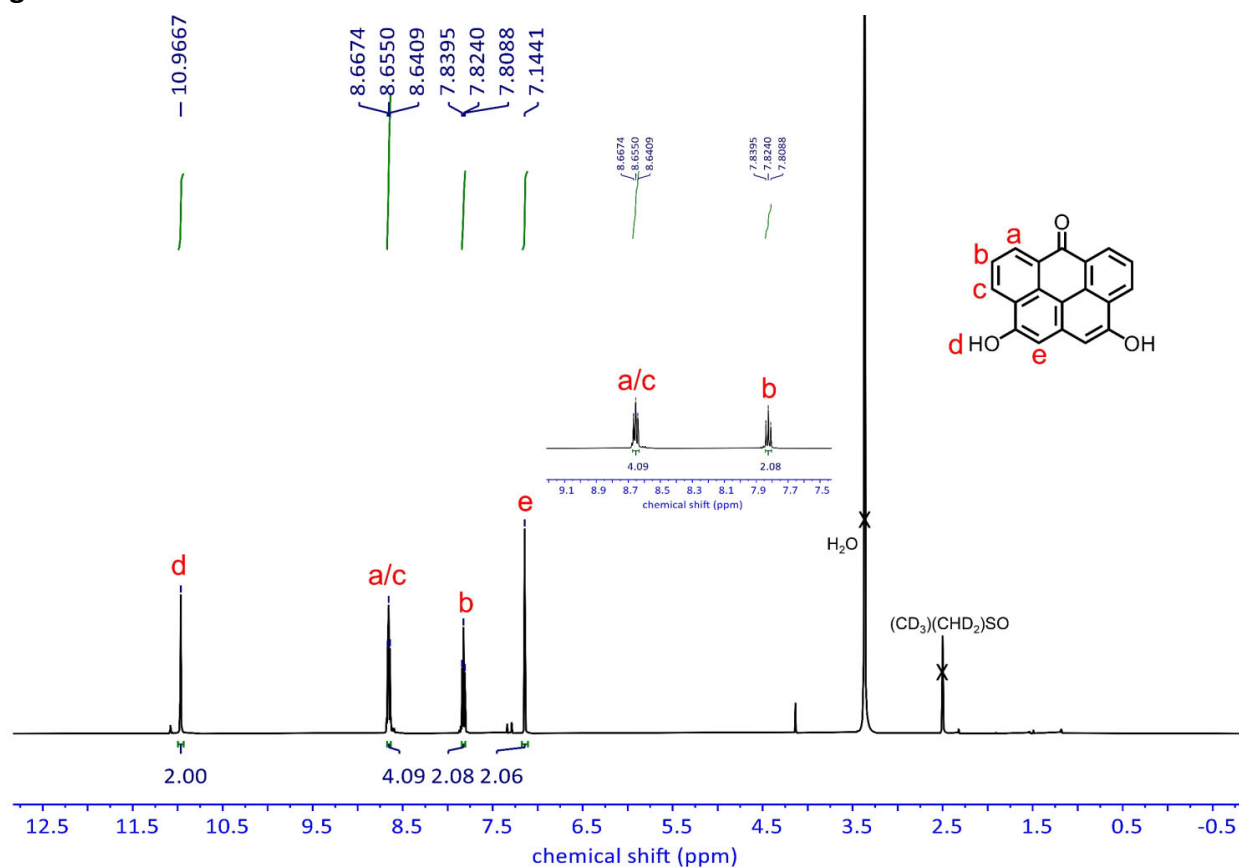


Figure S51. ^1H NMR Spectrum (500 MHz, $(\text{CD}_3)_2\text{SO}$, 298K) of **3**.

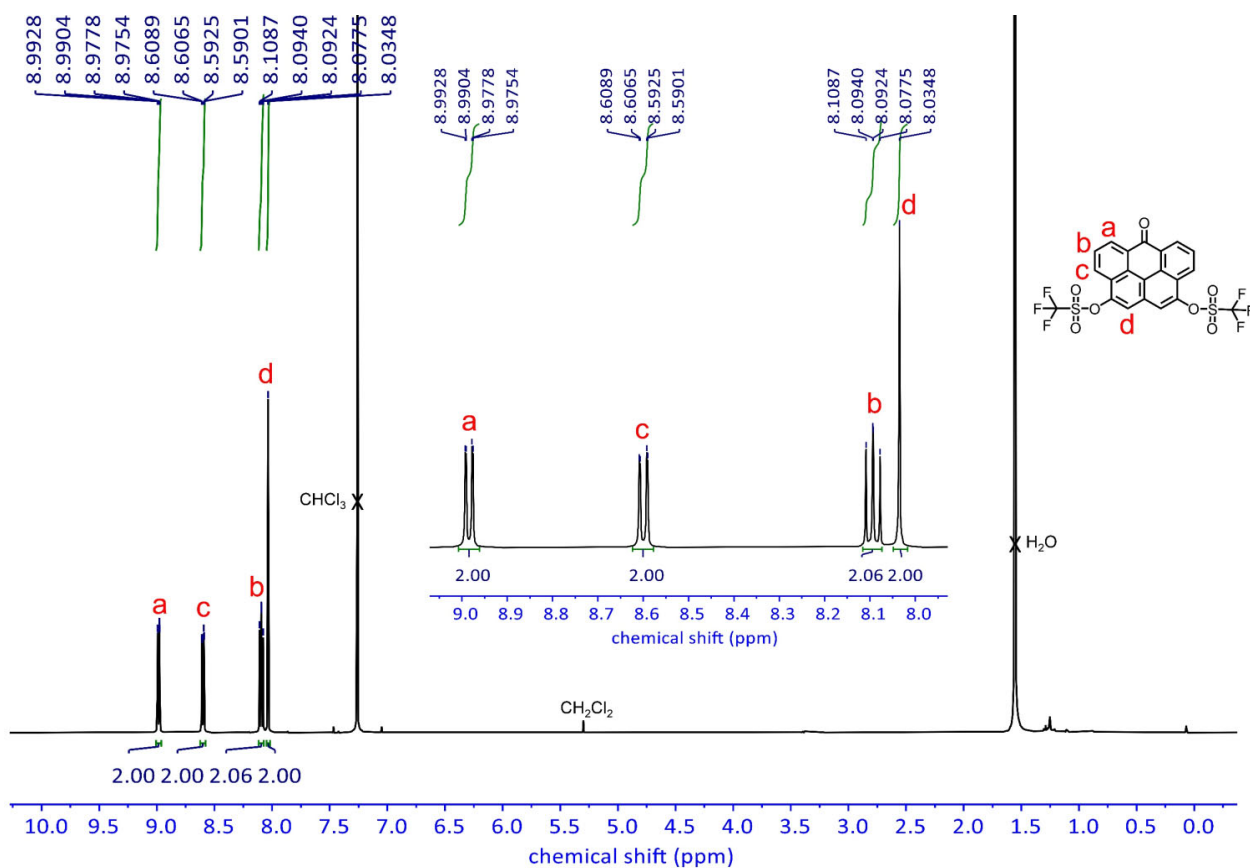


Figure S54. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of **4**.

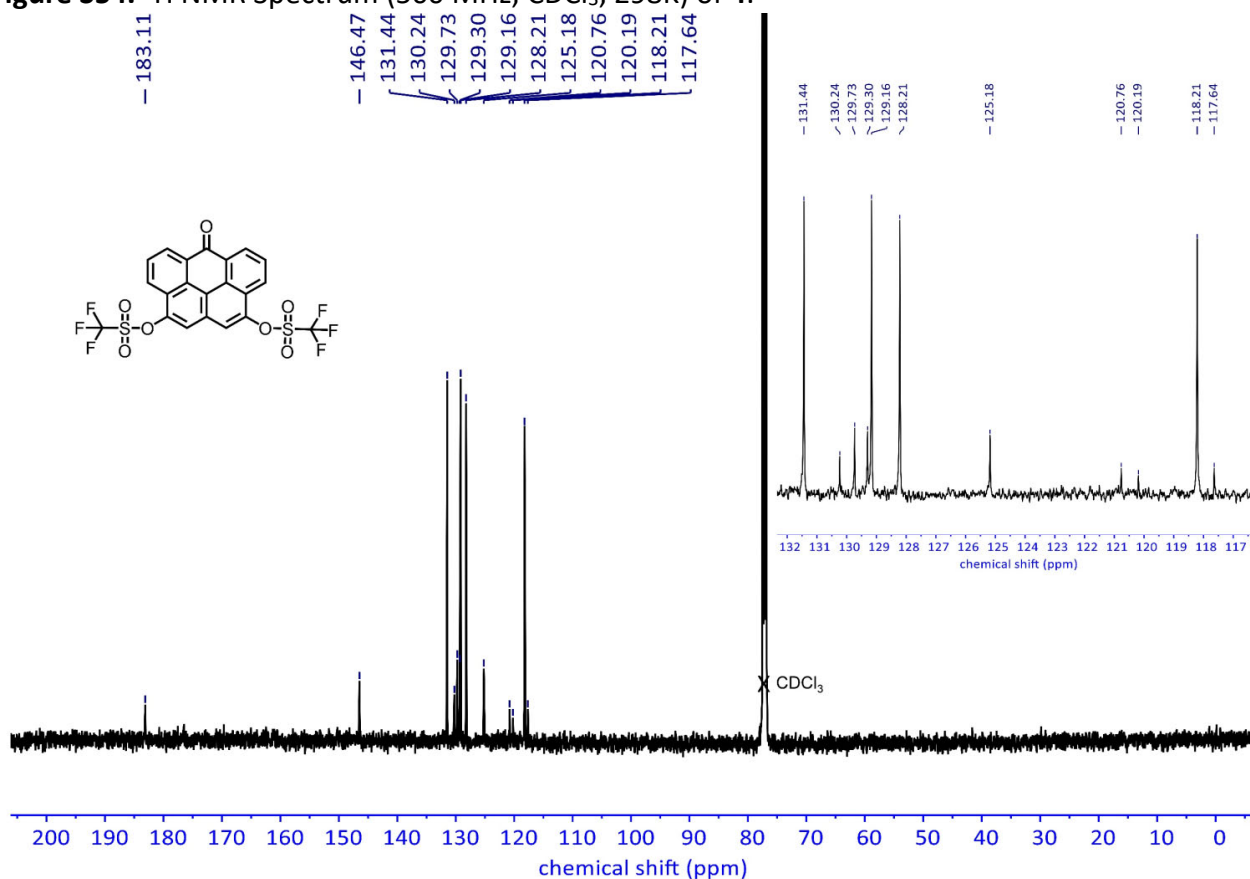


Figure S55. ¹³C NMR Spectrum (125 MHz, CDCl₃, 298K) of **4**.

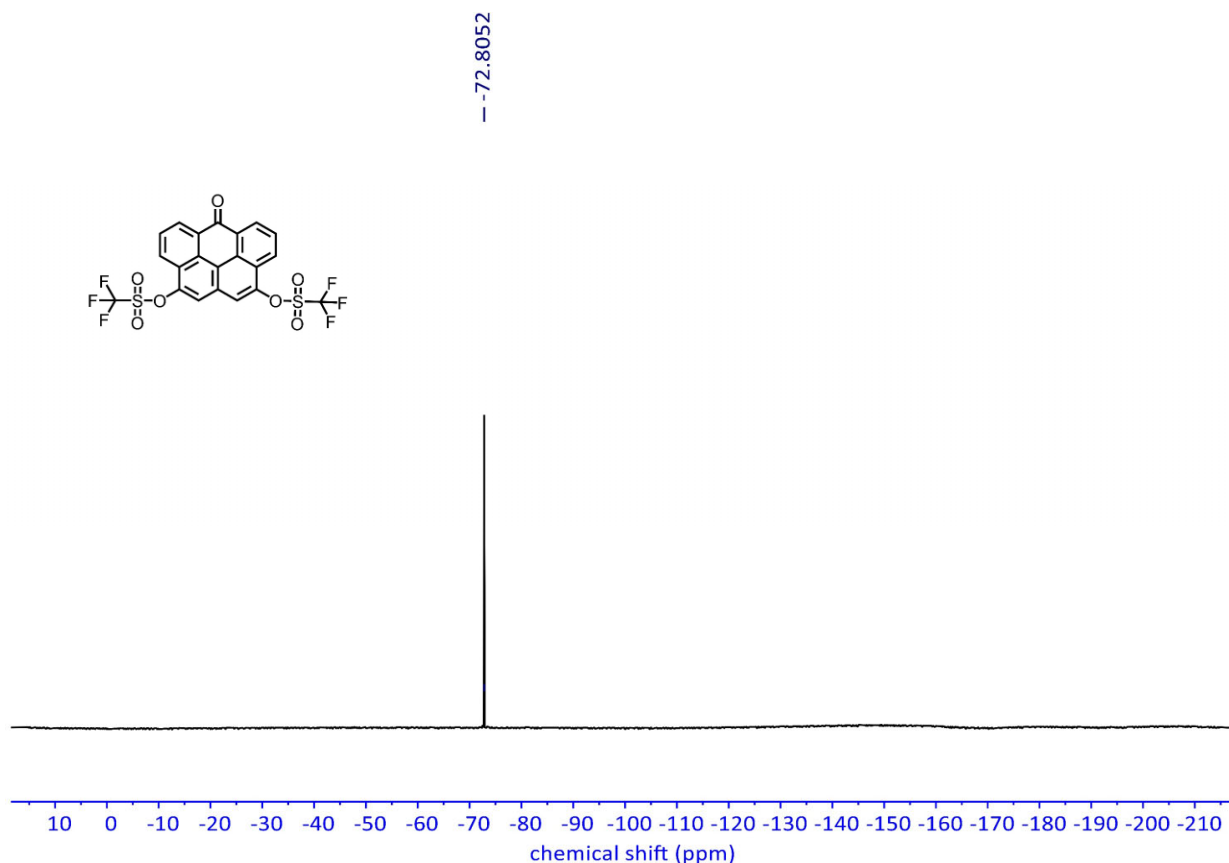


Figure S56. ^{19}F NMR Spectrum (376 MHz, CDCl_3 , 298K) of **4**.

Mass Spectrum SmartFormula Report

Sample Name	oly-OTf	Data File	D:\MassHunter\Data\Chemistry\2021\202108\20210816\oly-OTf.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union-1.m	Acquired Time	16/8/2021 3:26:04 PM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
550.969	1	$\text{C}_{21}\text{H}_9\text{F}_6\text{O}_7\text{S}_2$	550.9688	0.36

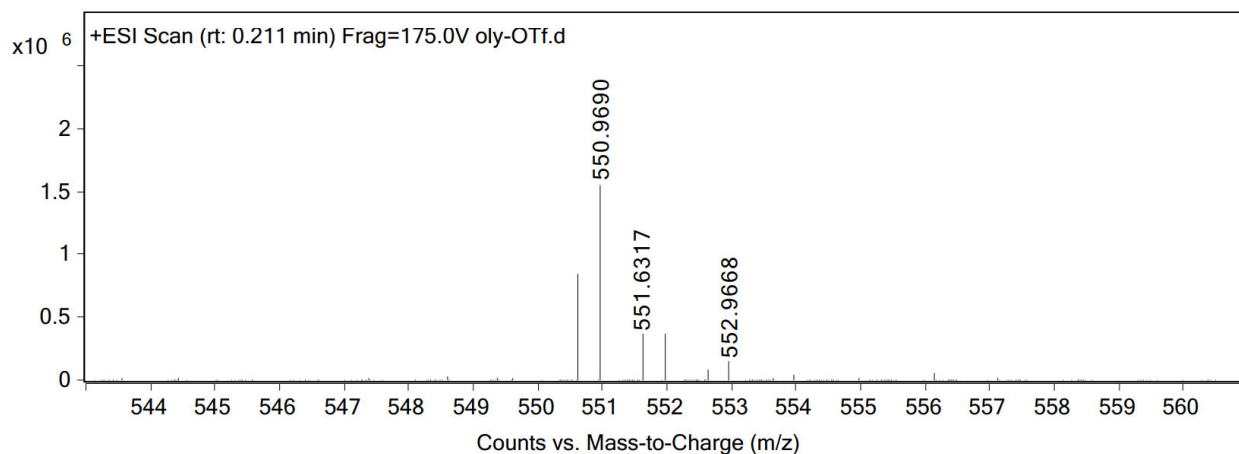


Figure S57. HR-ESI-MS of **4**.

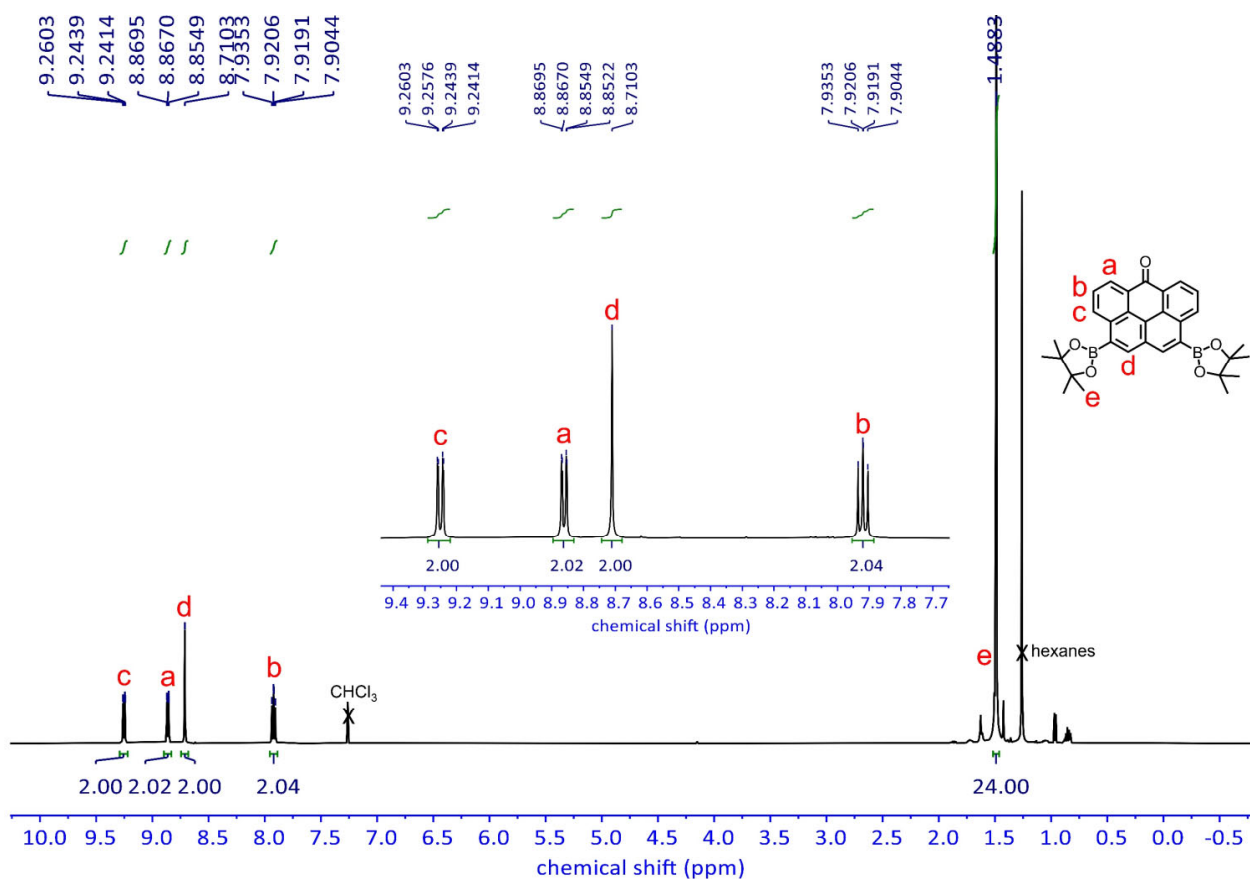


Figure S58. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of 5.

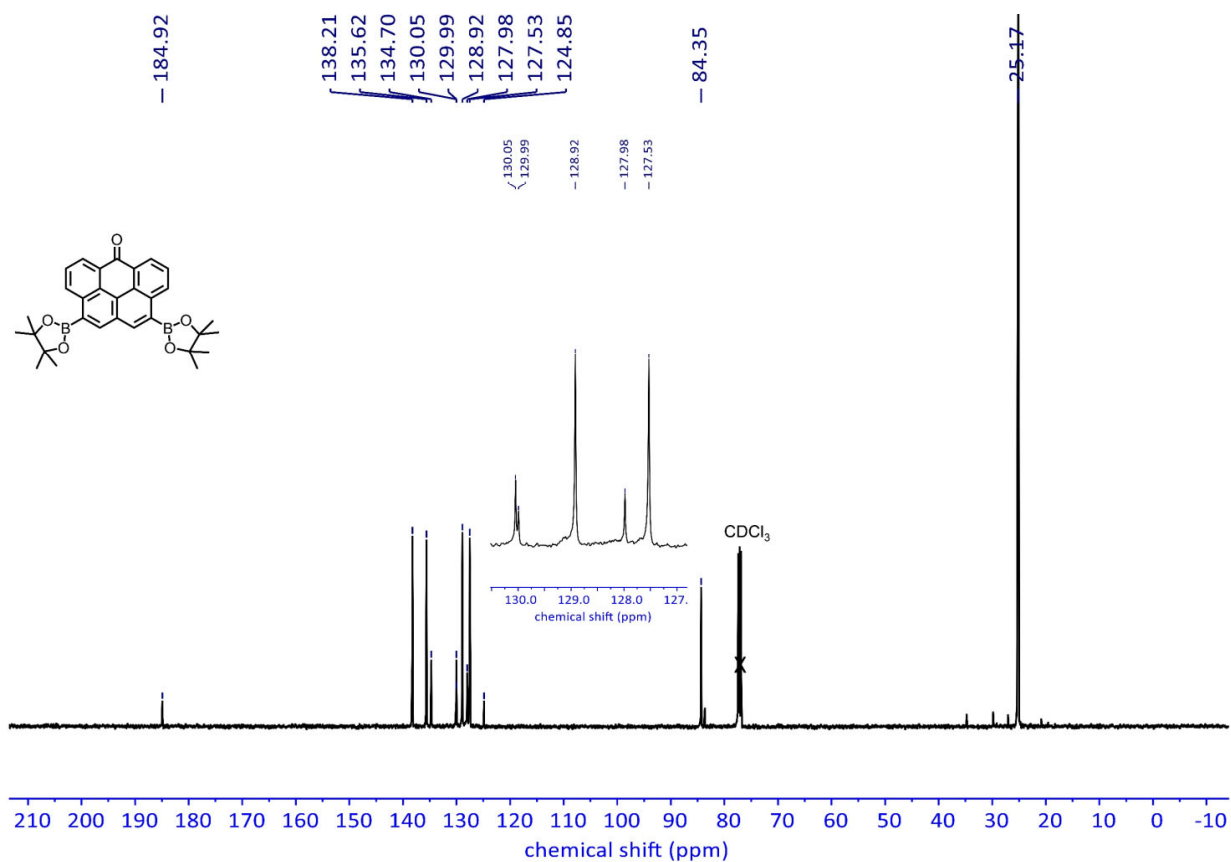


Figure S59. ¹³C NMR Spectrum (125 MHz, CDCl₃, 298K) of 5.

Mass Spectrum SmartFormula Report

Sample Name	olym-2bpin	Data File	D:\MassHunter\Data\Chemistry\2021\202108\20210811\olym-2bpin.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union-1.m	Acquired Time	11/8/2021 11:54:30 AM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
507.2518	1	C ₃₁ H ₃₃ [11B] ₂ O ₅	507.2509	1.77

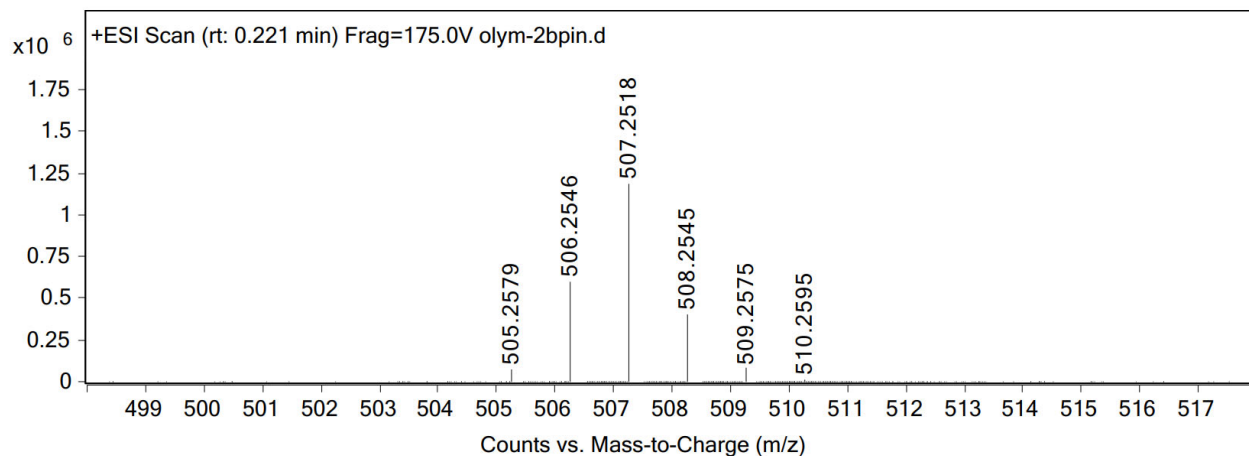


Figure S60. HR-ESI-MS of 5.

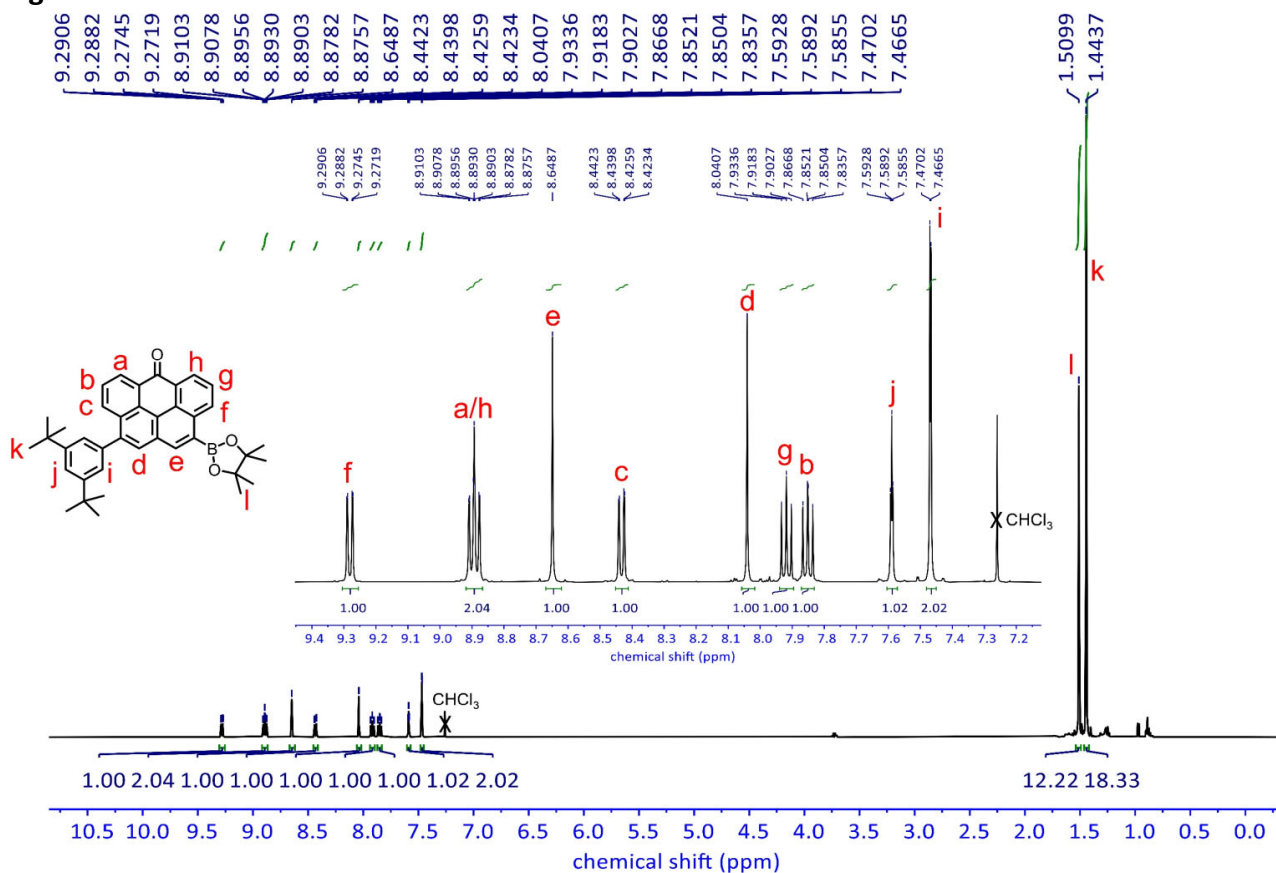


Figure S61. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of 6.

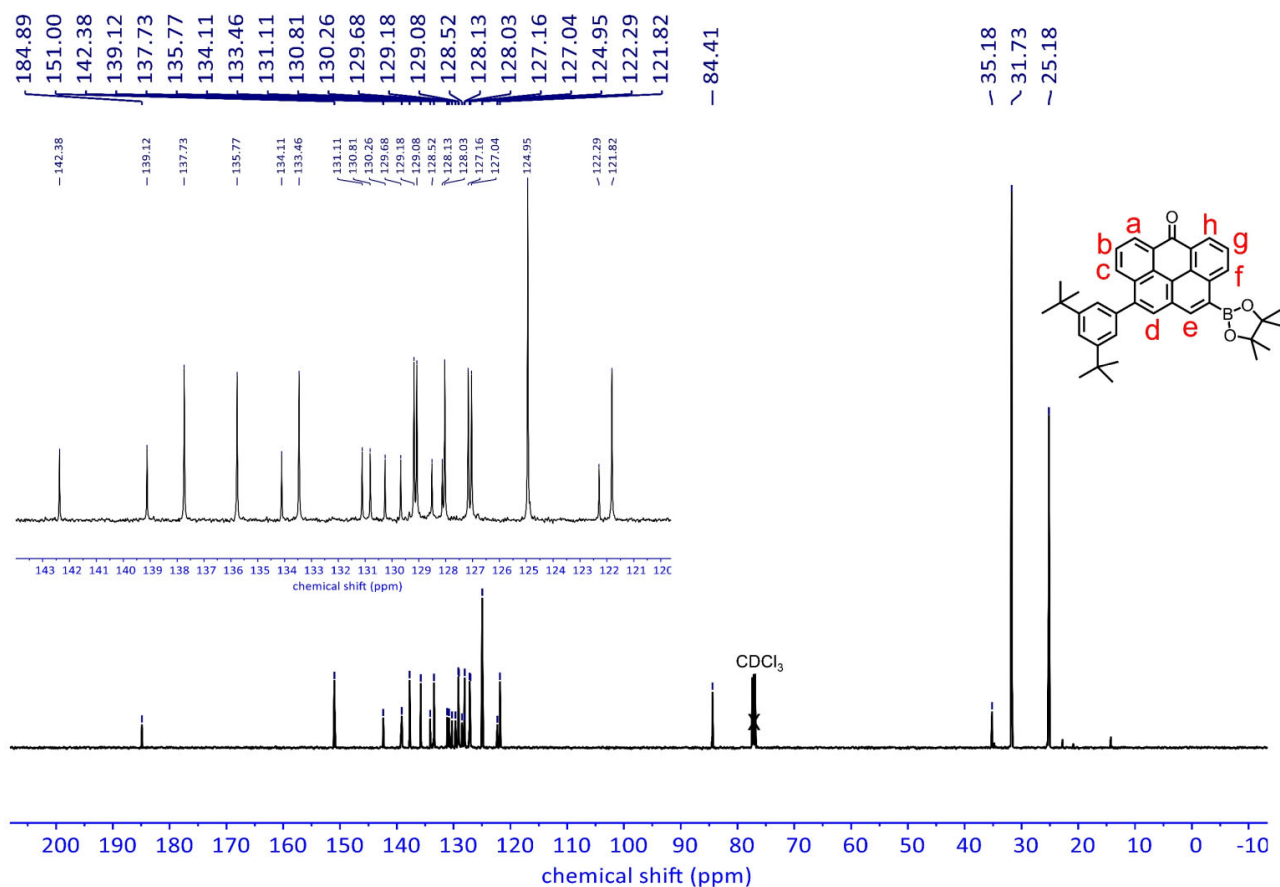


Figure S62. ^{13}C NMR Spectrum (125 MHz, CDCl_3 , 298K) of **6**.

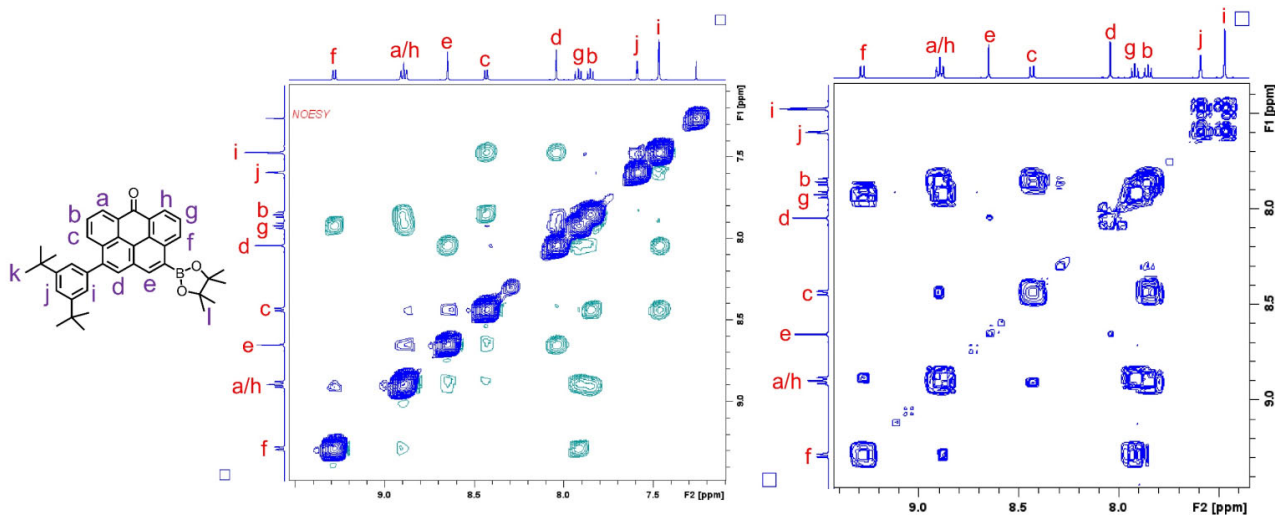


Figure S63. ^1H - ^1H NOESY and COSY spectra (500 MHz, CDCl_3 , 298K) of **6**. Left: NOESY spectrum. Right: COSY spectrum.

Mass Spectrum SmartFormula Report

Sample Name	boly-bpin	Data File	D:\MassHunter\Data\Chemistry\2021\202108\20210813-APCI\boly-bpin.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union_APCI.m	Acquired Time	13/8/2021 5:52:52 PM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
569.323	1	C ₃₉ H ₄₂ [11B] O ₃	569.3222	1.41

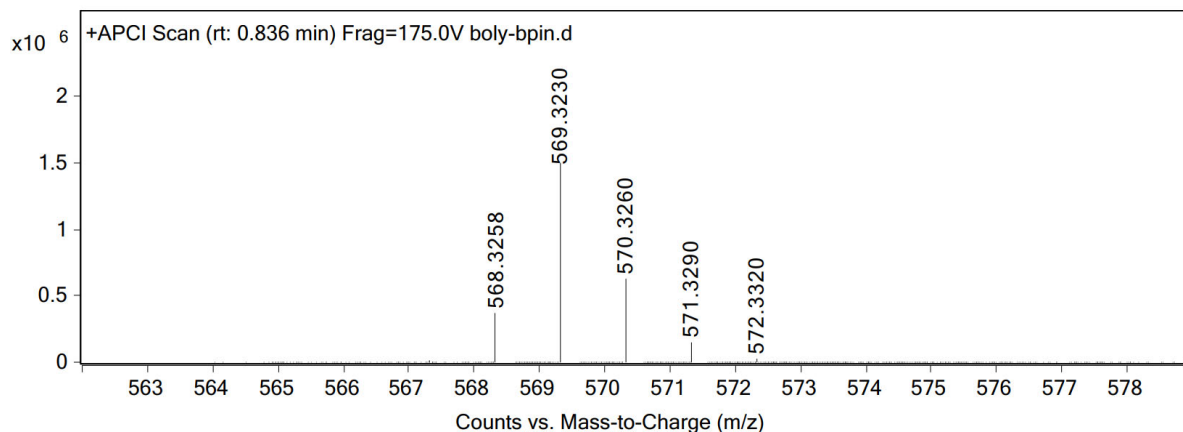


Figure S64. HR-APCI-MS of **6**.

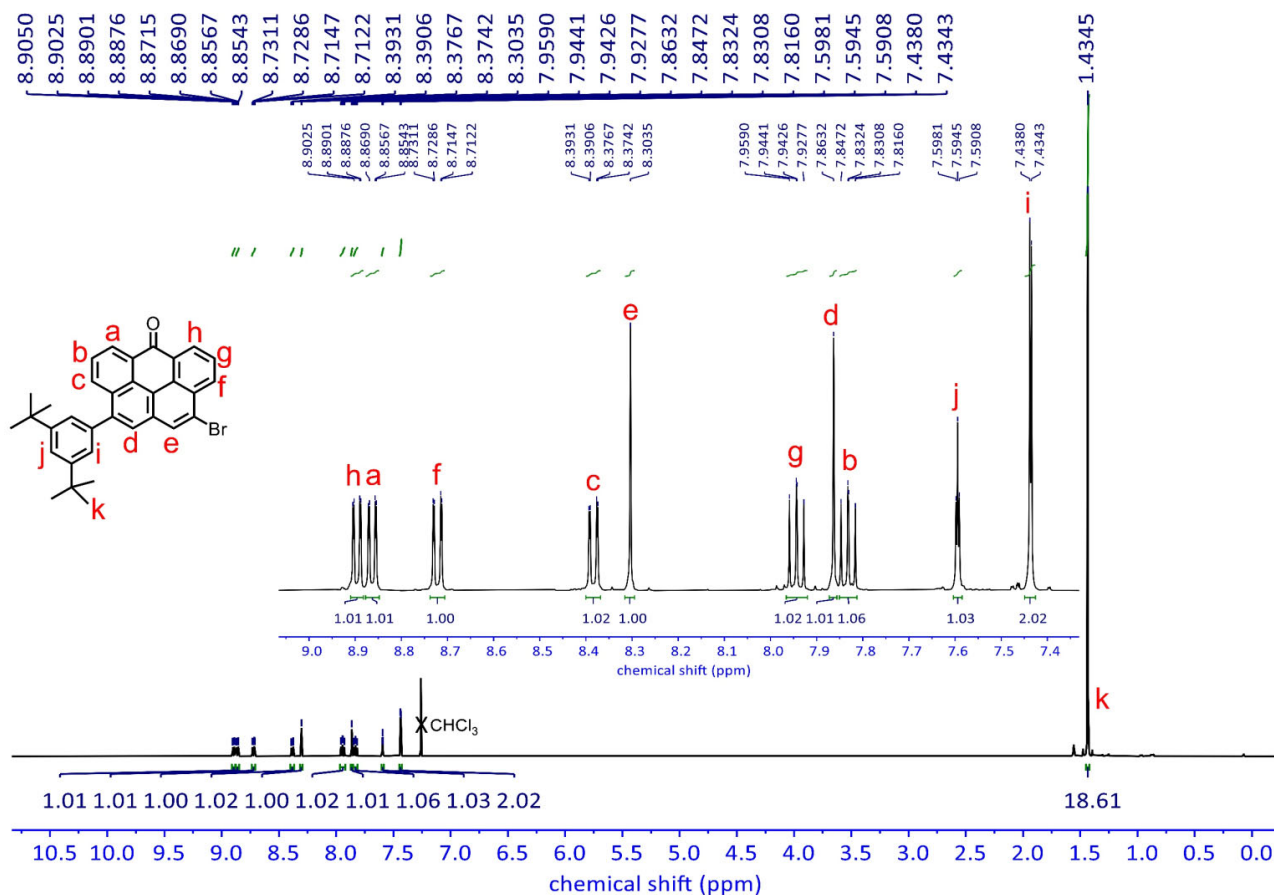


Figure S65. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of **15**.

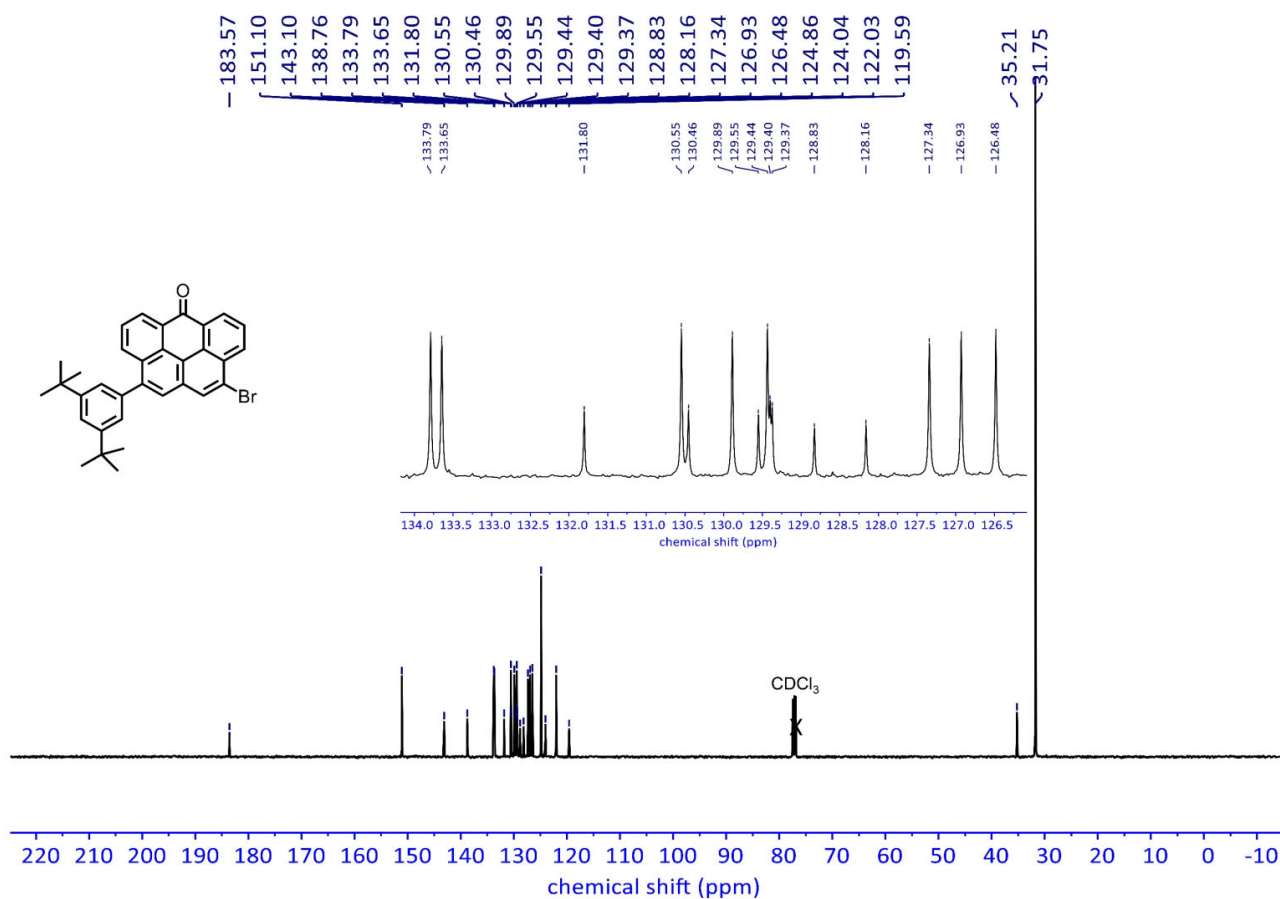


Figure S66. ^{13}C NMR Spectrum (125 MHz, CDCl_3 , 298K) of **15**.

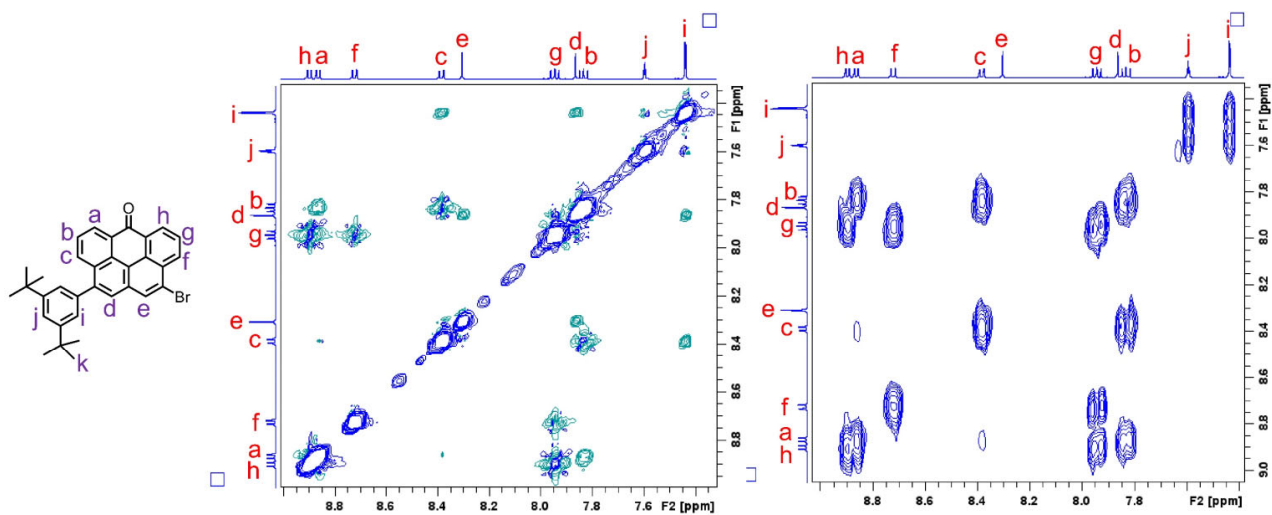


Figure S67. ^1H - ^1H NOESY and COSY spectra (500 MHz, CDCl_3 , 298K) of **15**. Left: NOESY spectrum. Right: COSY spectrum.

Mass Spectrum SmartFormula Report

Sample Name	ben-olm-Br	Data File	D:\MassHunter\Data\Chemistry\2021\202109\20210908\ben-olm-Br-1.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union_APCI_negative-1.m	Acquired Time	8/9/2021 5:00:33 PM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
520.1408	1	C33 H29 Br O	520.1407	0.19

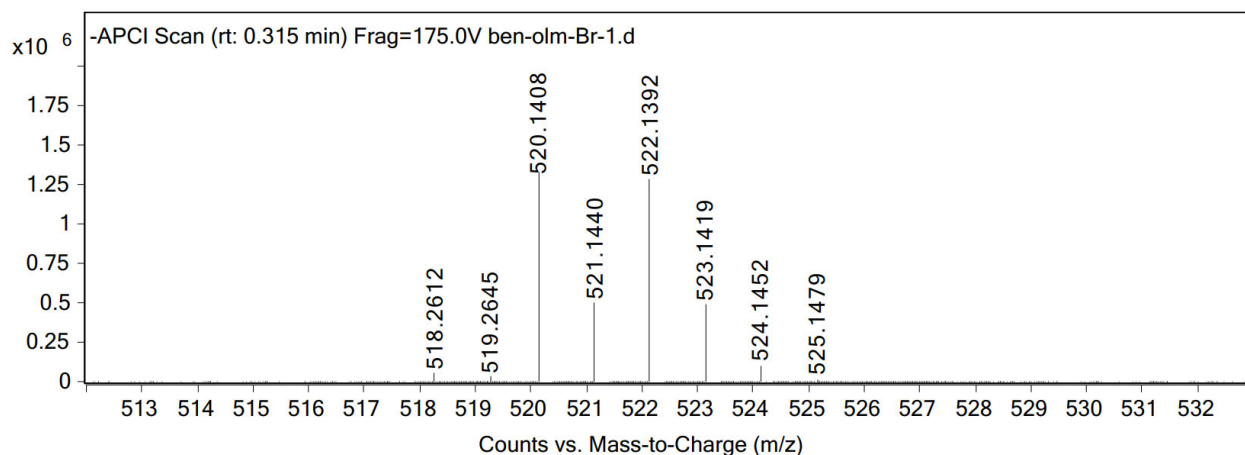


Figure S68. HR-APCI-MS of **15**.

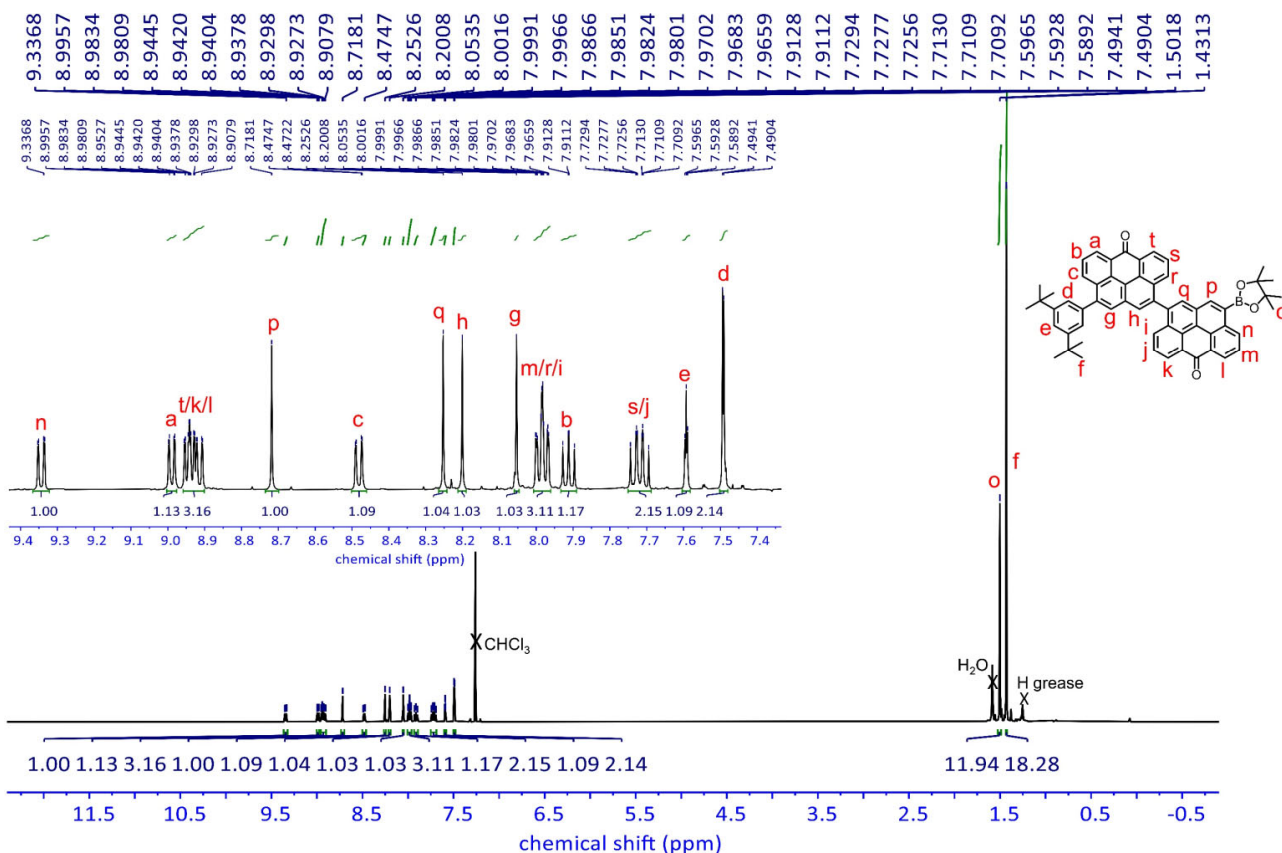


Figure S69. ^1H NMR Spectrum (500 MHz, CDCl_3 , 298K) of **16**.

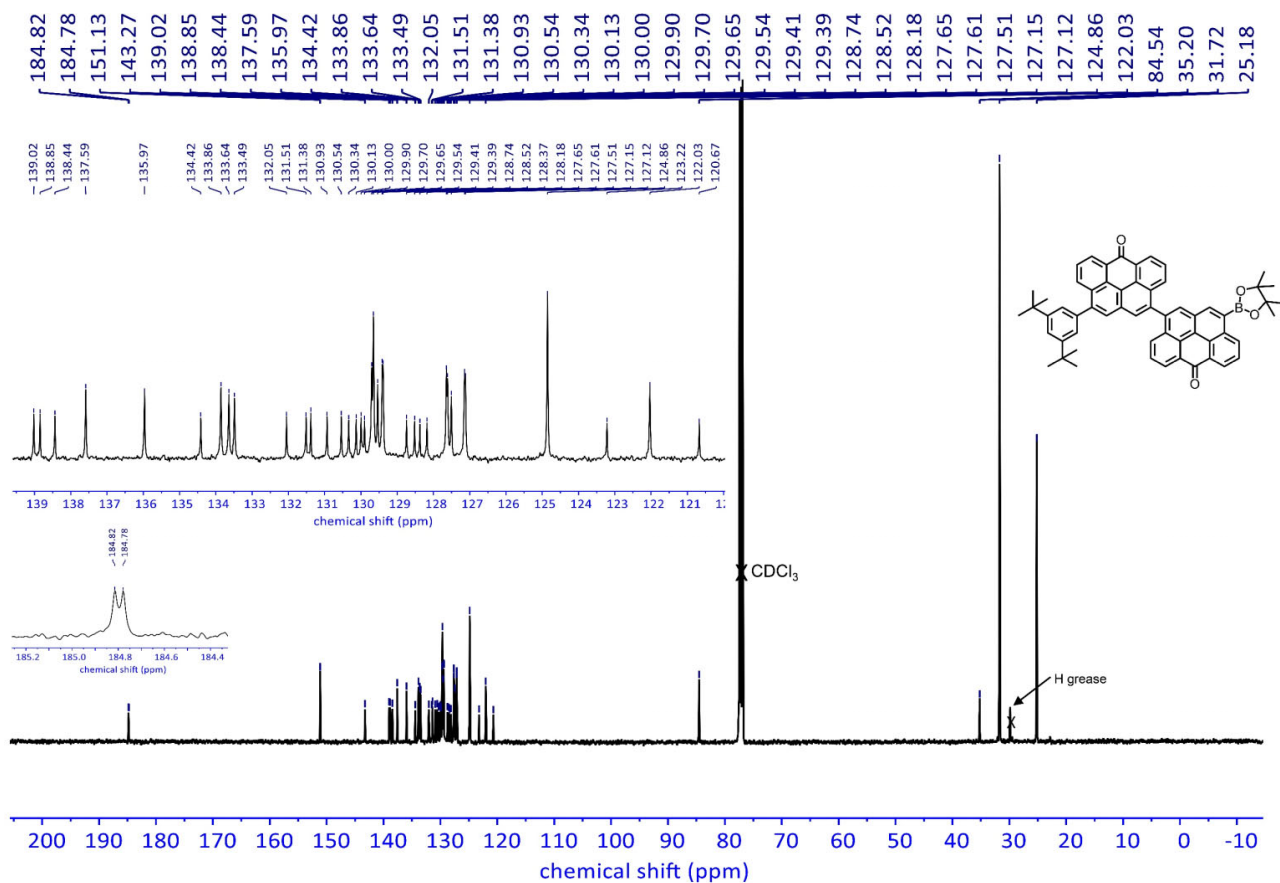


Figure S70. ¹³C NMR Spectrum (125 MHz, CDCl₃, 298K) of **16**.

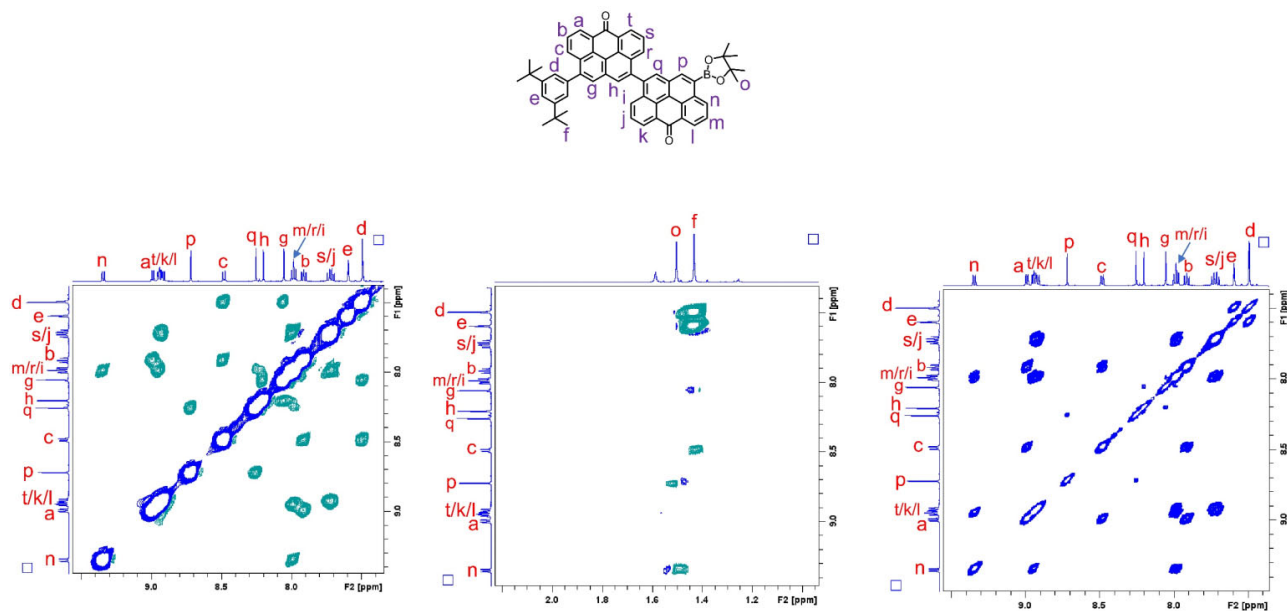


Figure S71. ¹H-¹H NOESY and COSY spectra (500 MHz, CDCl₃, 298K) of **16**. Left and middle: NOESY spectrum. Right: COSY spectrum.

Mass Spectrum SmartFormula Report

Sample Name	ben-olm2-bpin	Data File	D:\MassHunter\Data\Chemistry\2021\202109\20210908\ben-olm2-bpin.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union_APCI-1.m	Acquired Time	8/9/2021 4:33:29 PM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
821.3804	1	C ₅₈ H ₅₀ [11B]O ₄	821.3797	0.85

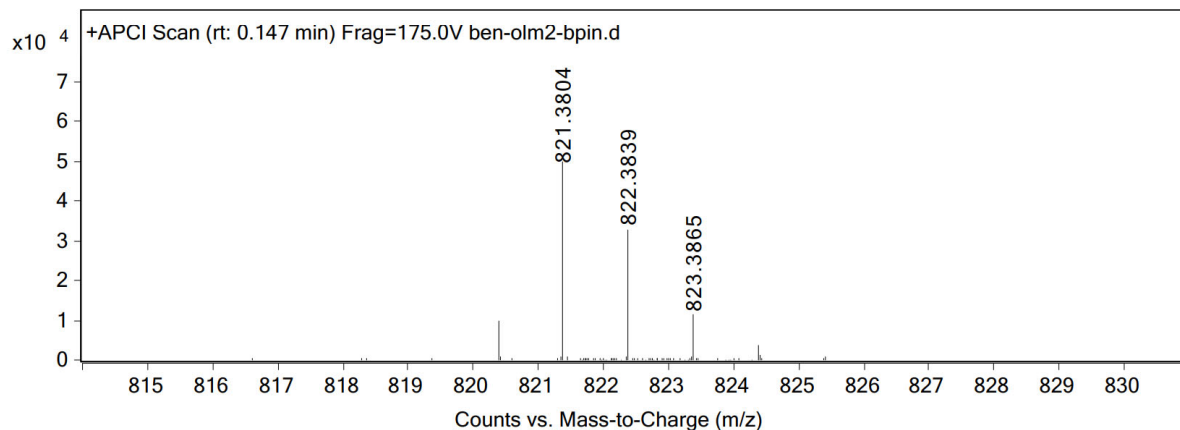


Figure S72. HR-APCI-MS of **16**.

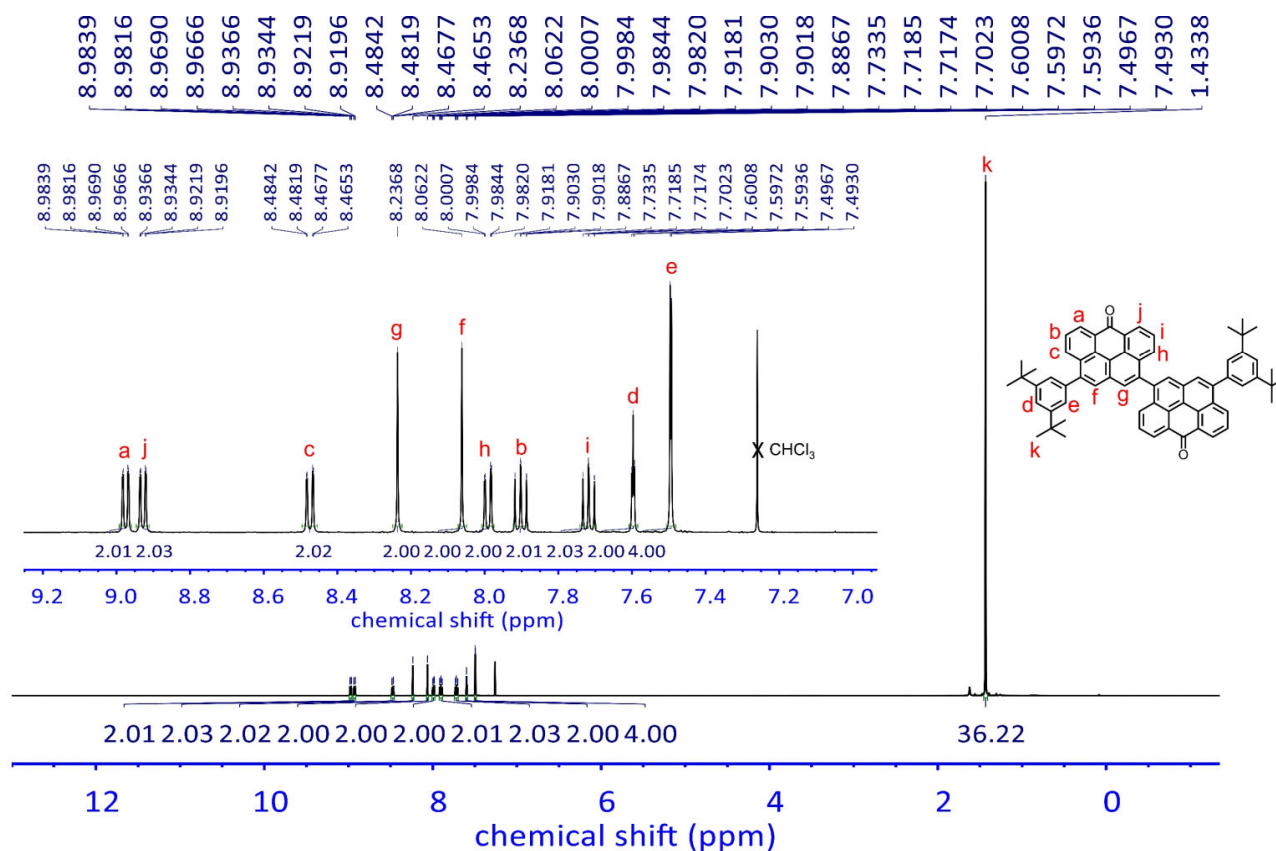


Figure S73. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of **7**.

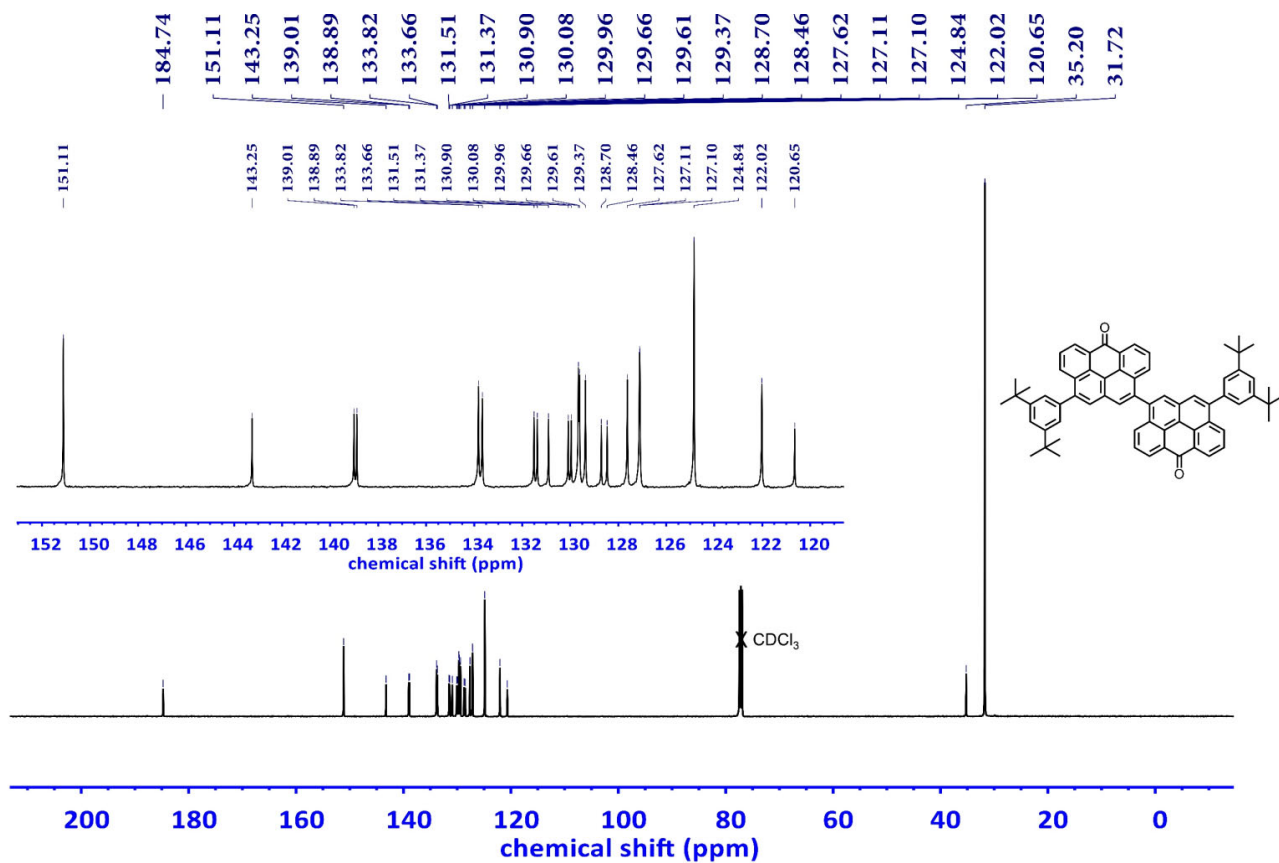


Figure S74. ^{13}C NMR Spectrum (125 MHz, CDCl_3 , 298K) of **7**.

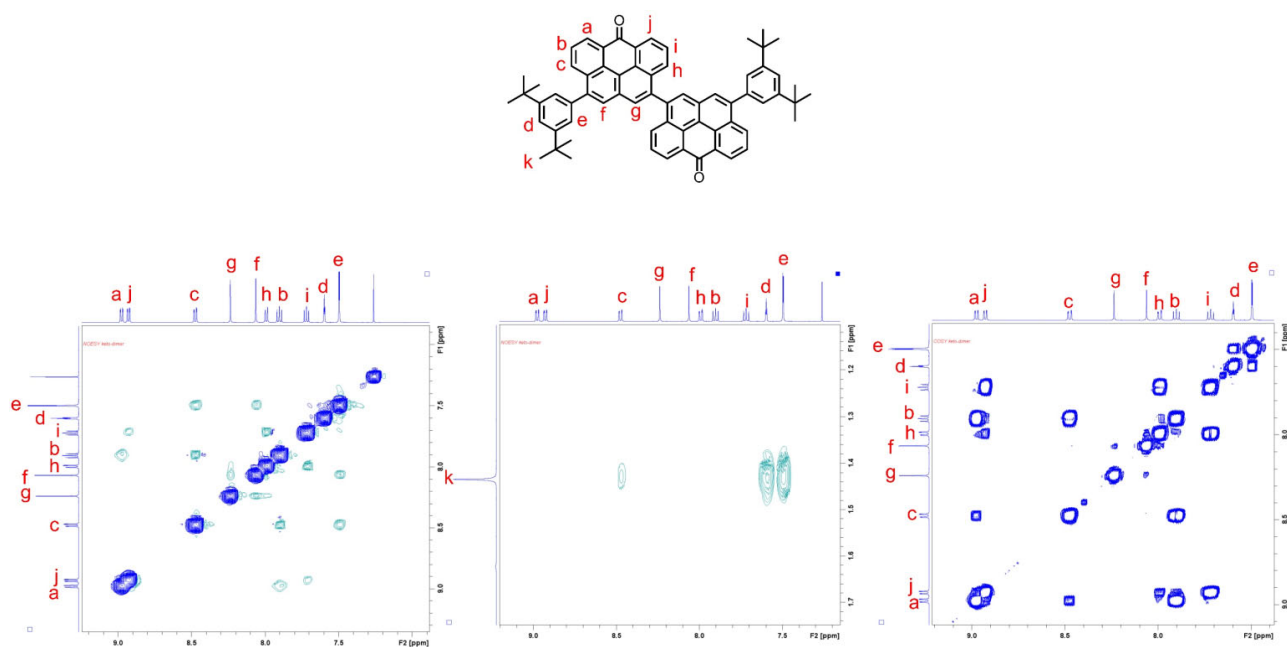


Figure S75. ^1H - ^1H NOESY and COSY spectra (500 MHz, CDCl_3 , 298K) of **7**. Left and middle: NOESY spectrum. Right: COSY spectrum.

Mass Spectrum SmartFormula Report

Sample Name	olym-di	Data File	D:\MassHunter\Data\Chemistry\2021\202108\20210811\olym-di.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union-1.m	Acquired Time	11/8/2021 11:59:25 AM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
883.4504	1	C ₆₆ H ₅₉ O ₂	883.451	0.68

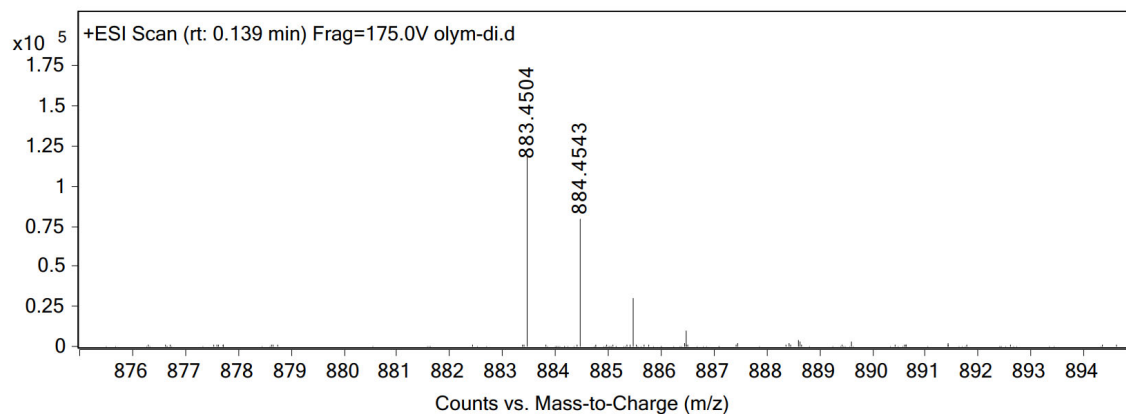


Figure S76. HR-ESI-MS of **7**.

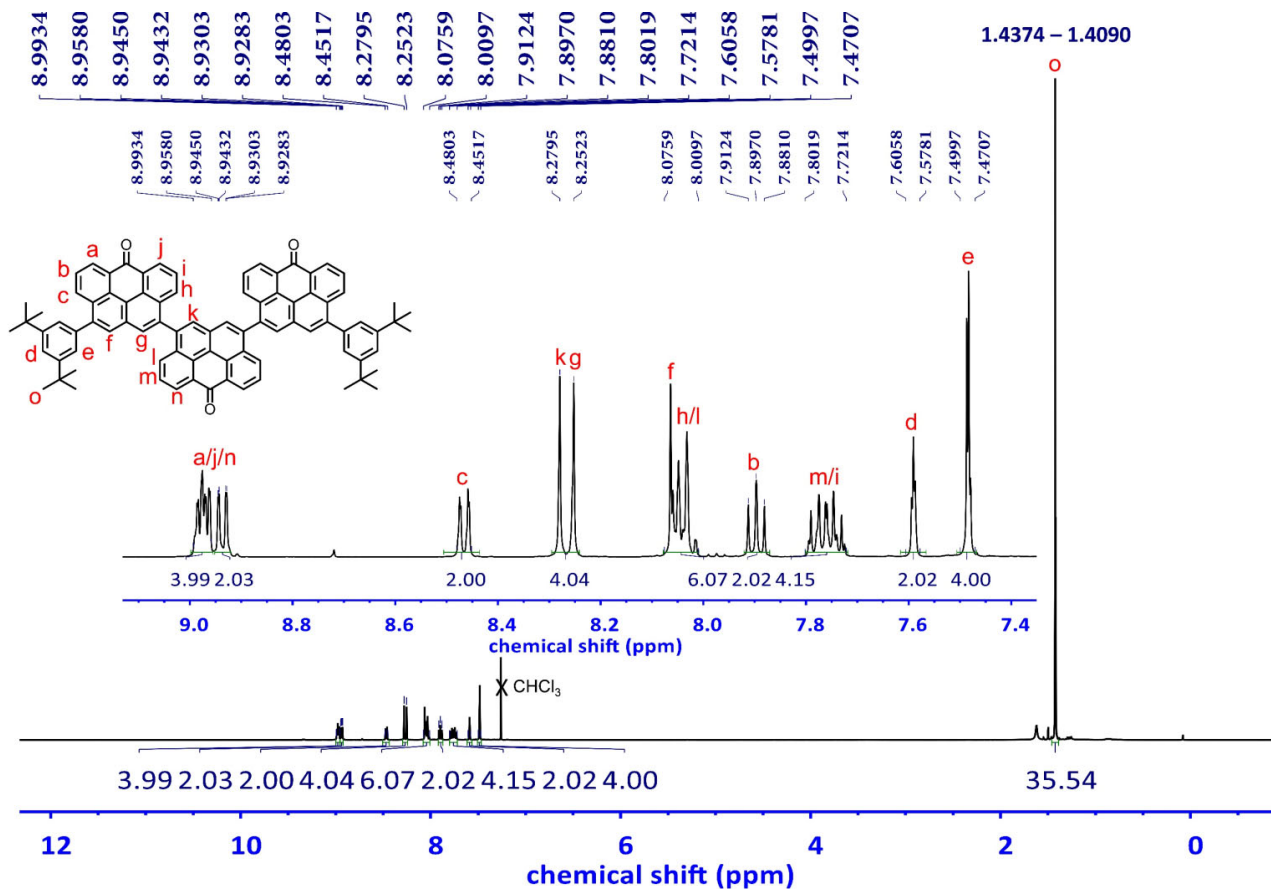


Figure S77. ¹H NMR Spectrum (500 MHz, CDCl₃, 298K) of **10**.

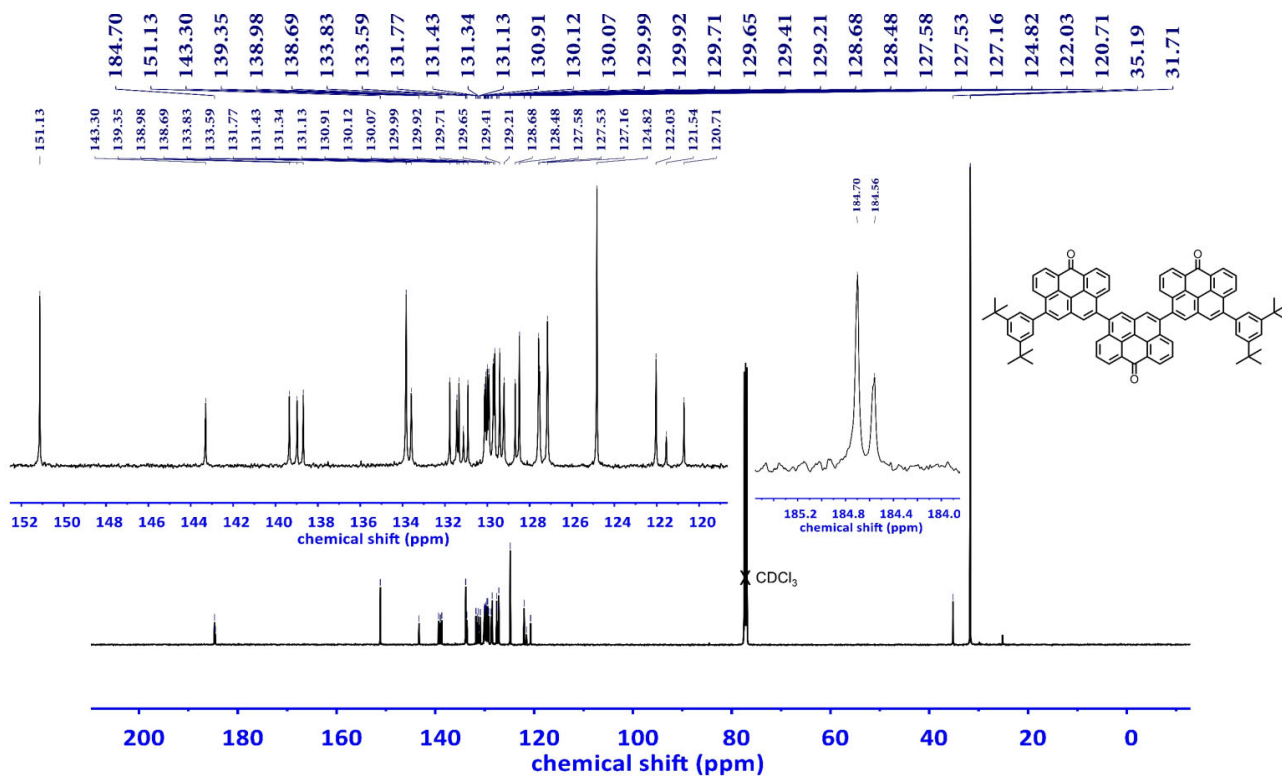


Figure S78. ¹³C NMR Spectrum (125 MHz, CDCl₃, 298K) of **10**.

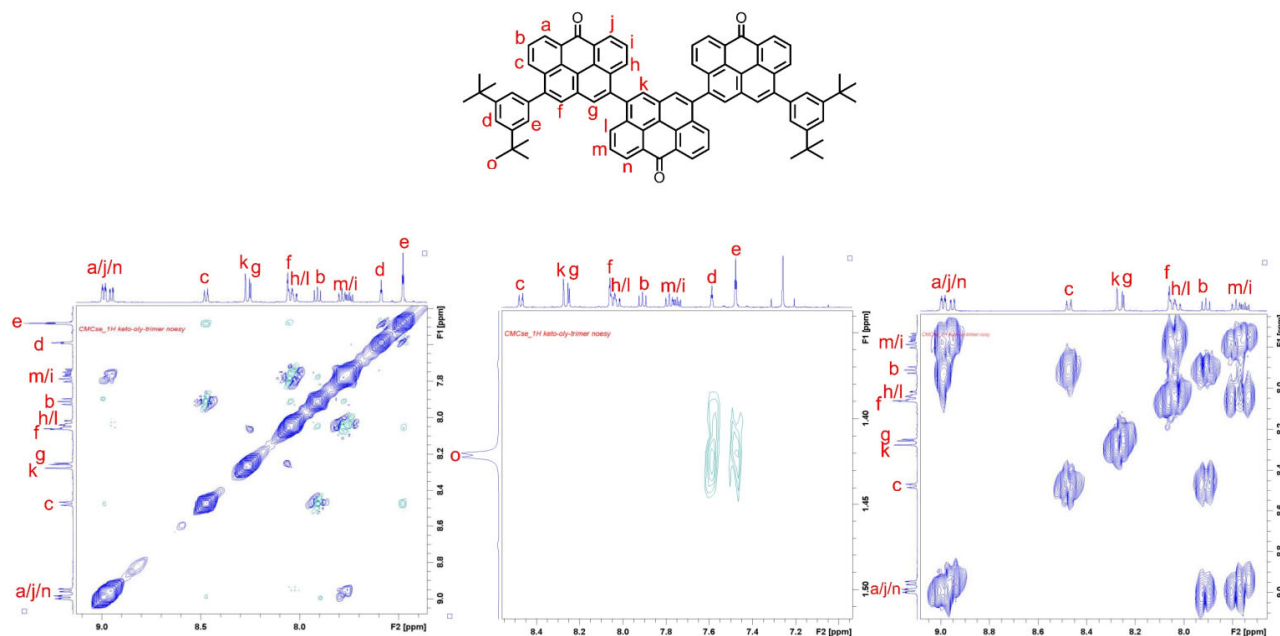


Figure S79. ¹H-¹H NOESY and COSY spectra (500 MHz, CDCl₃, 298K) of **10**. Left and middle: NOESY spectrum. Right: COSY spectrum.

Mass Spectrum SmartFormula Report

Sample Name	olym-tri	Data File	D:\MassHunter\Data\Chemistry\2021\202108\20210811\olym-tri-1.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union-1.m	Acquired Time	11/8/2021 12:09:07 PM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
1135.5082	1	C ₈₅ H ₆₇ O ₃	1135.5085	0.26

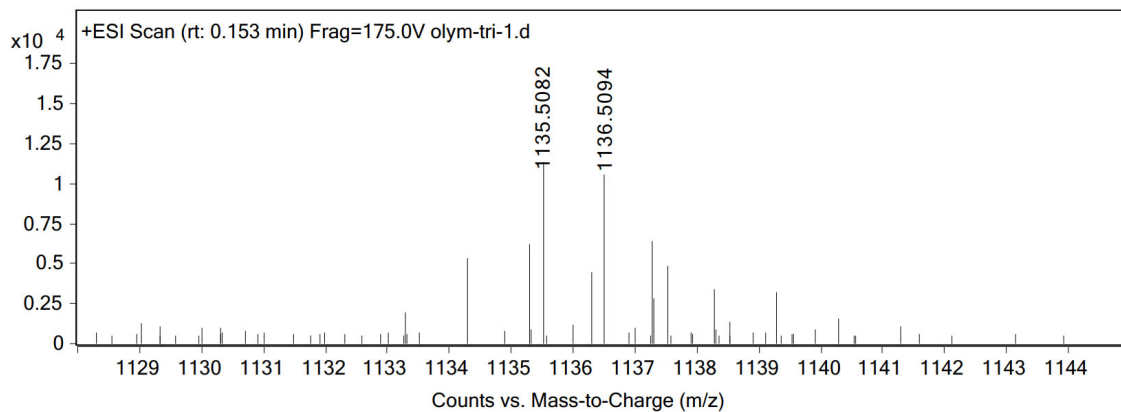


Figure S80. HR-ESI-MS of 10.

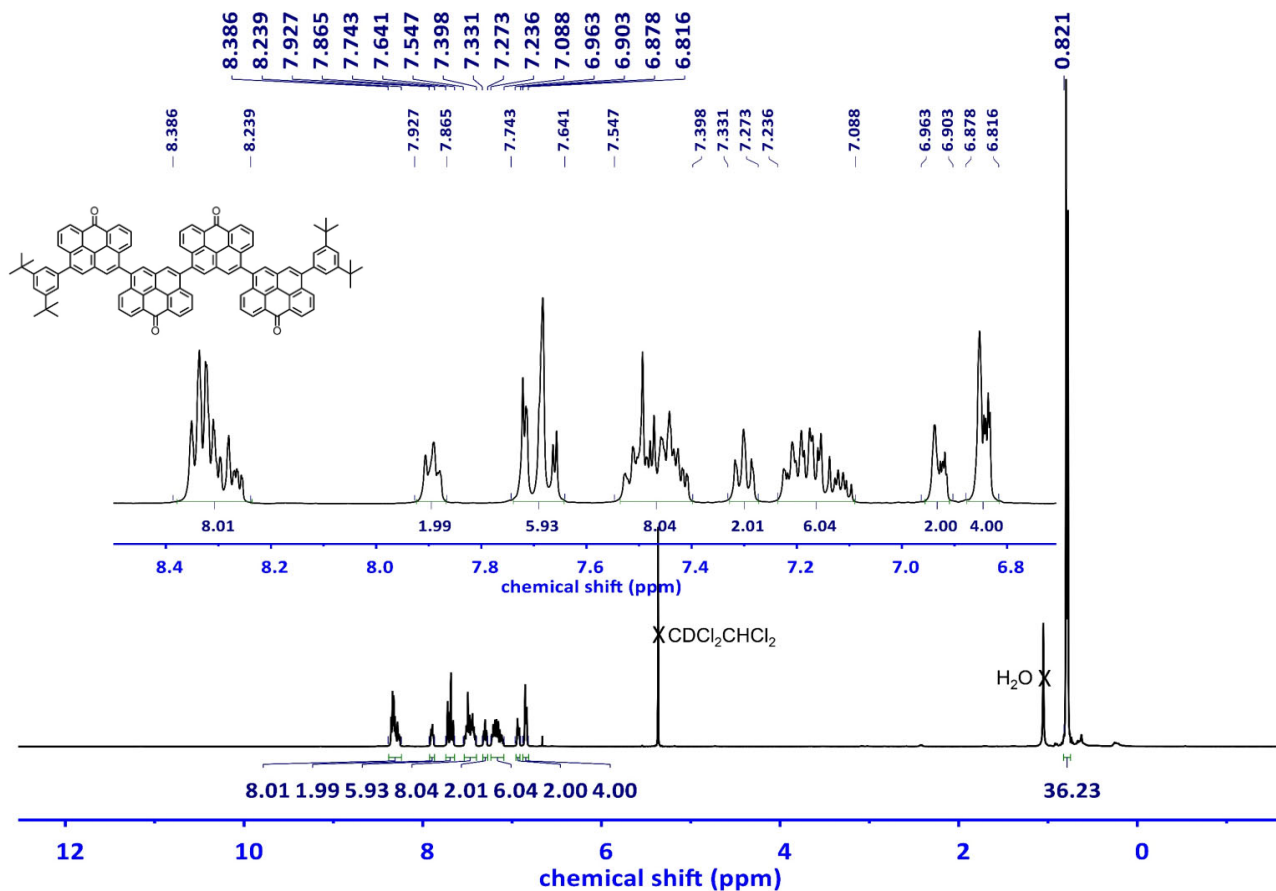


Figure S81. ¹H NMR Spectrum (500 MHz, CDCl₂CDCl₂, 298K) of 17.

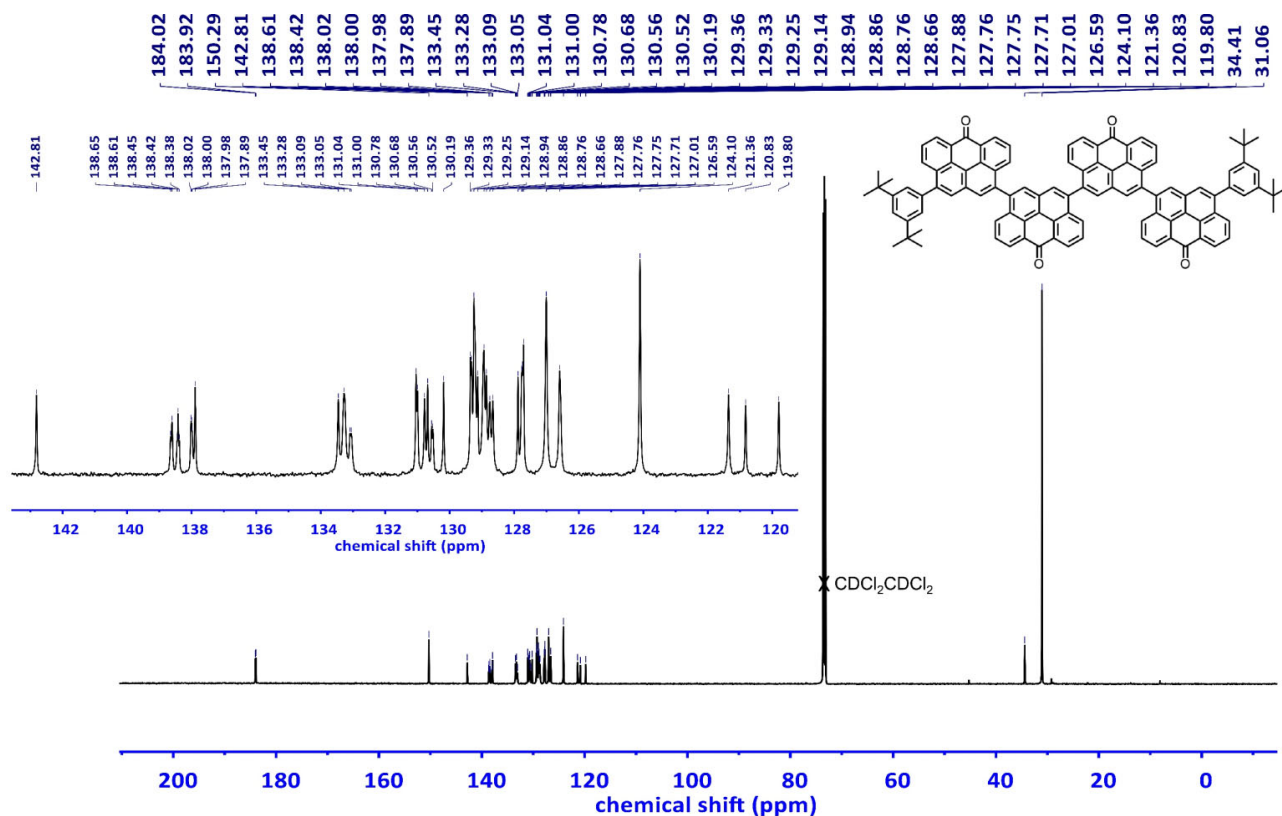


Figure S82. ^{13}C NMR Spectrum (125 MHz, $\text{CDCl}_2\text{CDCl}_2$, 298K) of **17**.

Mass Spectrum SmartFormula Report

Sample Name	olm-tetramer	Data File	D:\MassHunter\Data\Chemistry\2021\202109\20210909\olm-tetramer-1.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union_APCI-1.m	Acquired Time	9/9/2021 10:46:22 AM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
1387.5654	1	$\text{C}_{104}\text{H}_{75}\text{O}_4$	1387.566	0.43

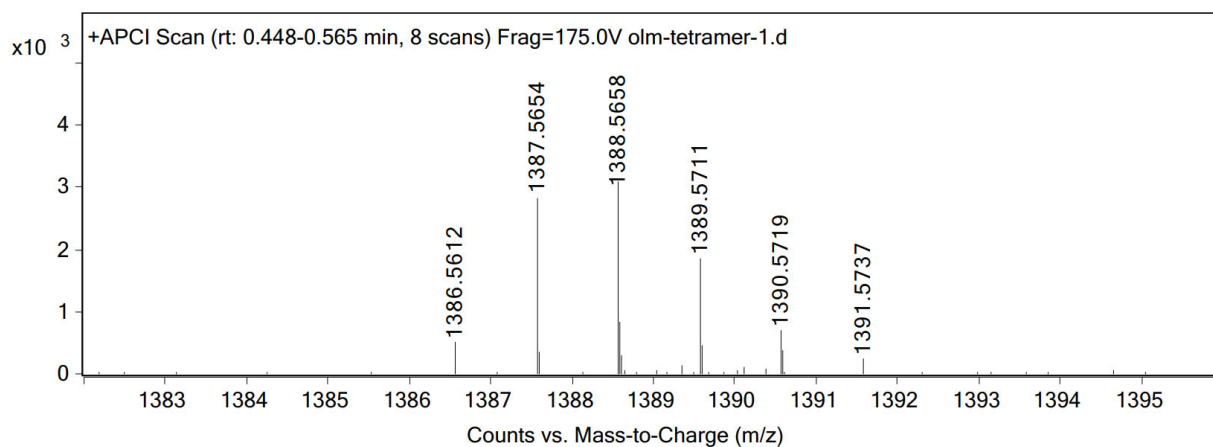


Figure S83. HR-APCI-MS of **17**.

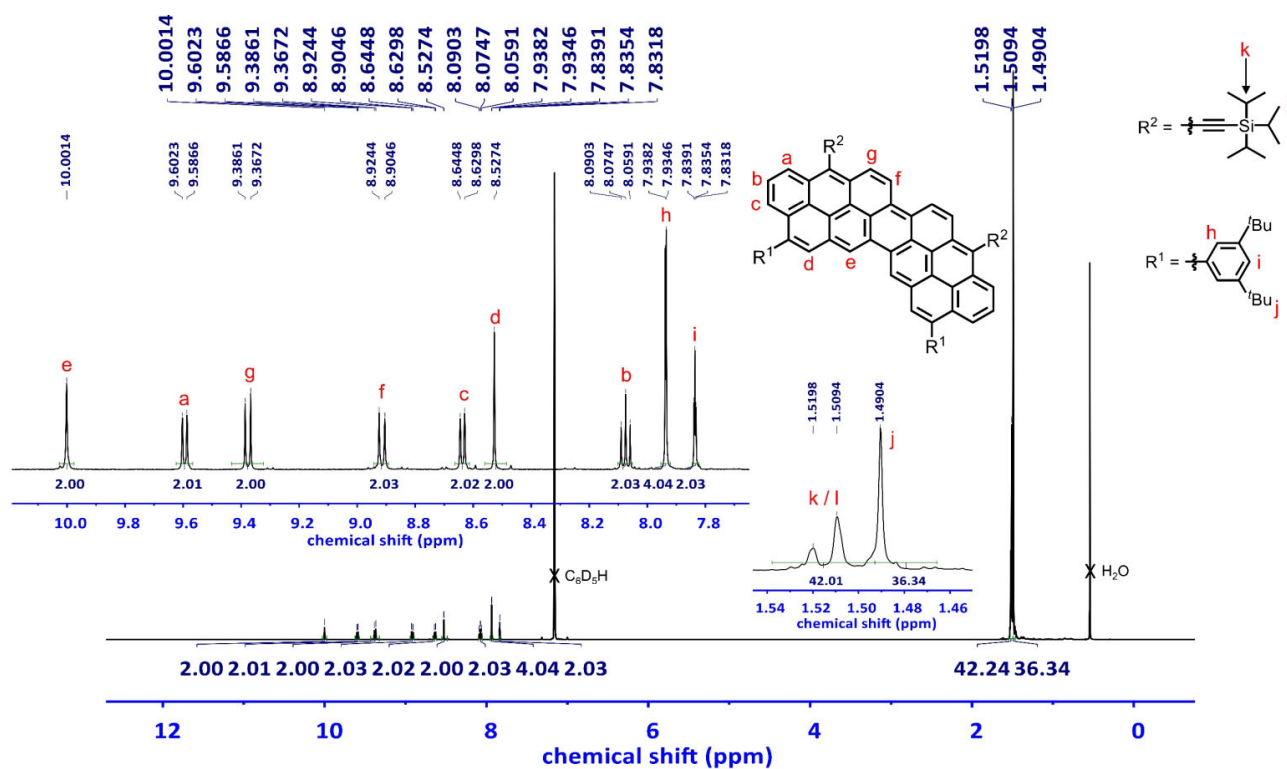


Figure S84. ¹H NMR Spectrum (500 MHz, C₆D₆, 298K) of tips-OR-2.

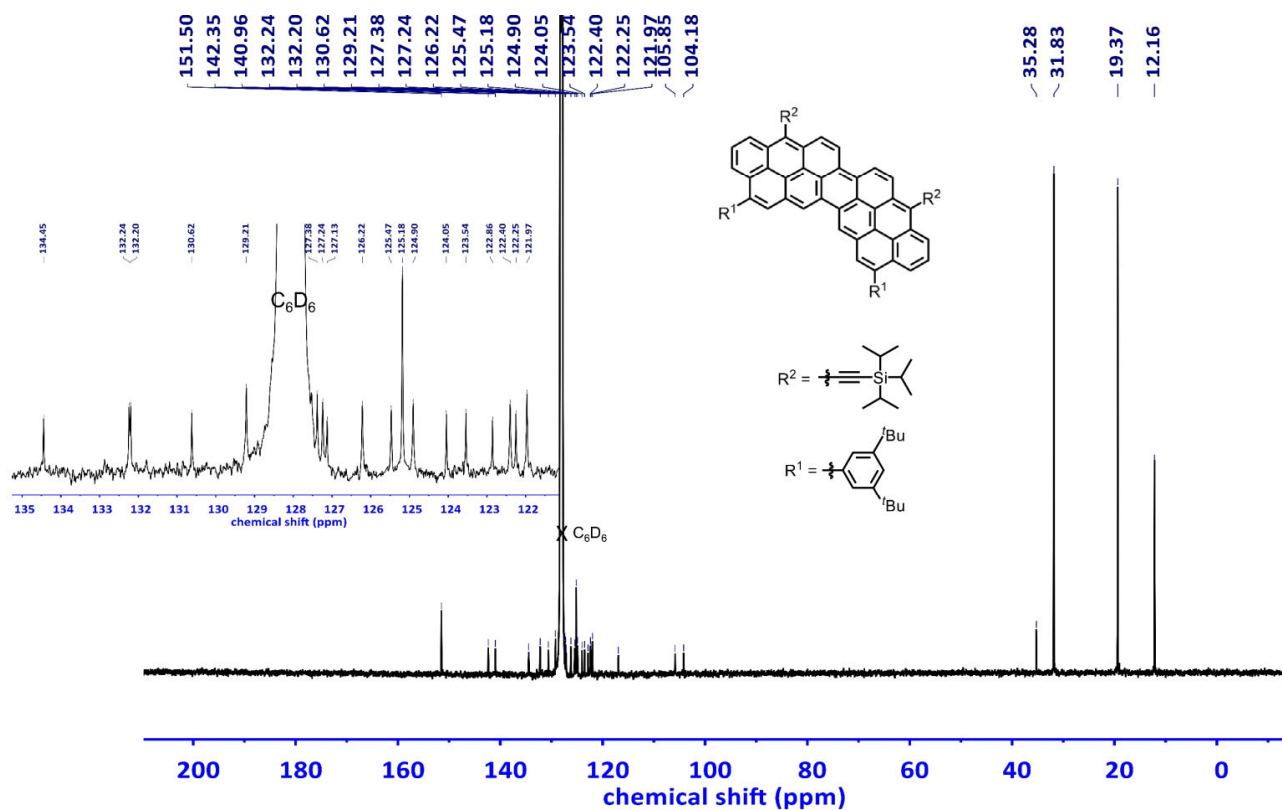


Figure S85. ¹³C NMR Spectrum (125 MHz, C₆D₆, 298K) of tips-OR-2.

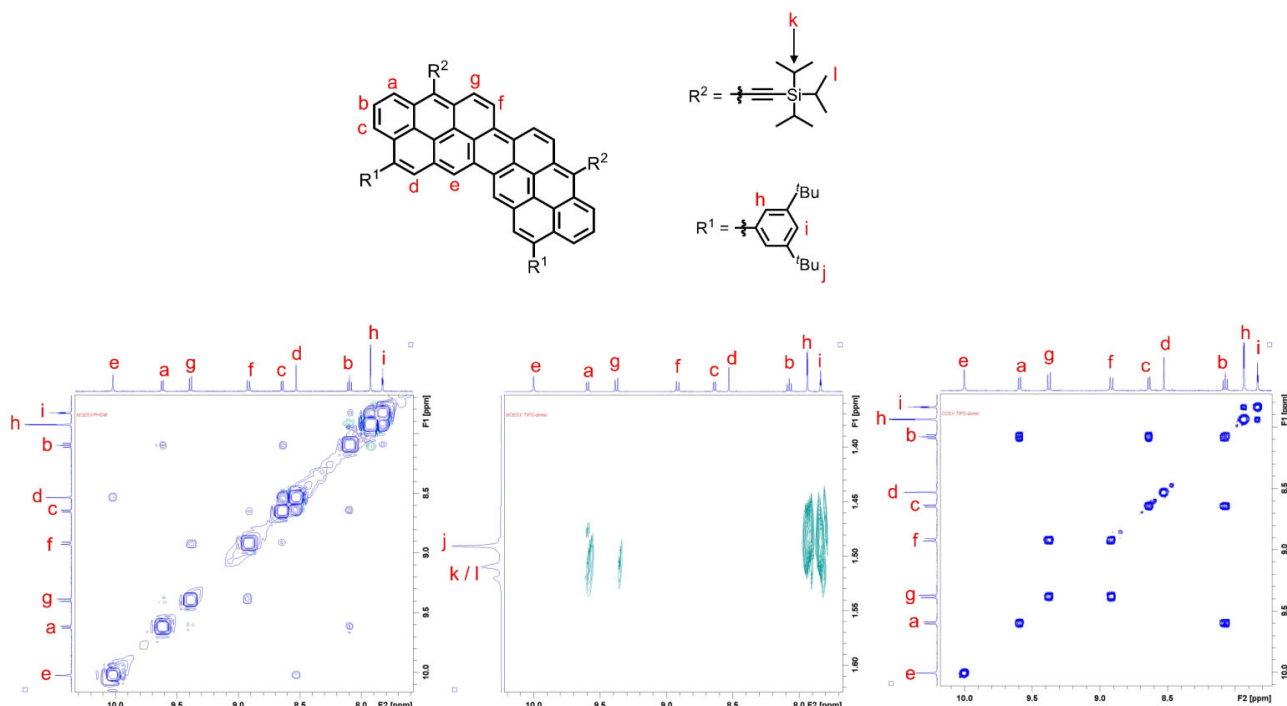


Figure S86. ^1H - ^1H NOESY and COSY spectra (500 MHz, C_6D_6 , 298K) of **tips-OR-2**. Left and middle: NOESY spectrum. Right: COSY spectrum.

Mass Spectrum SmartFormula Report

Sample Name	TIPS-dimer	Data File	D:\MassHunter\Data\Chemistry\2022\202201\20220119\TIPS-dimer.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union_APCI-1.m	Acquired Time	19/1/2022 5:49:21 PM (UTC+08:00)
Comment	Prof Wu Jishan	Operator	WLK

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
1211.7282	1	$\text{C}_{88}\text{H}_{99}\text{Si}_2$	1211.728	0.17

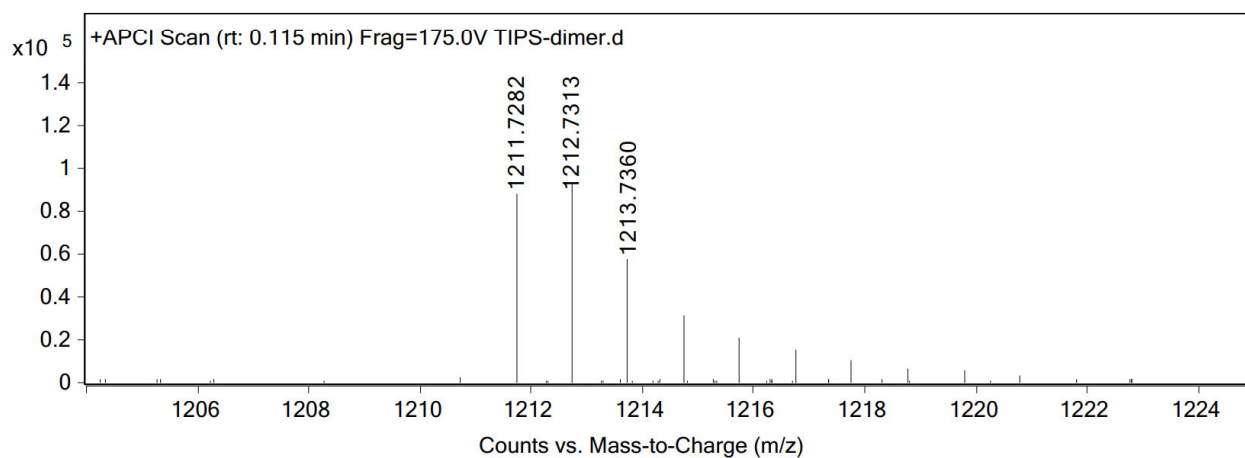


Figure S87. HR-APCI-MS of **tips-OR-2**.

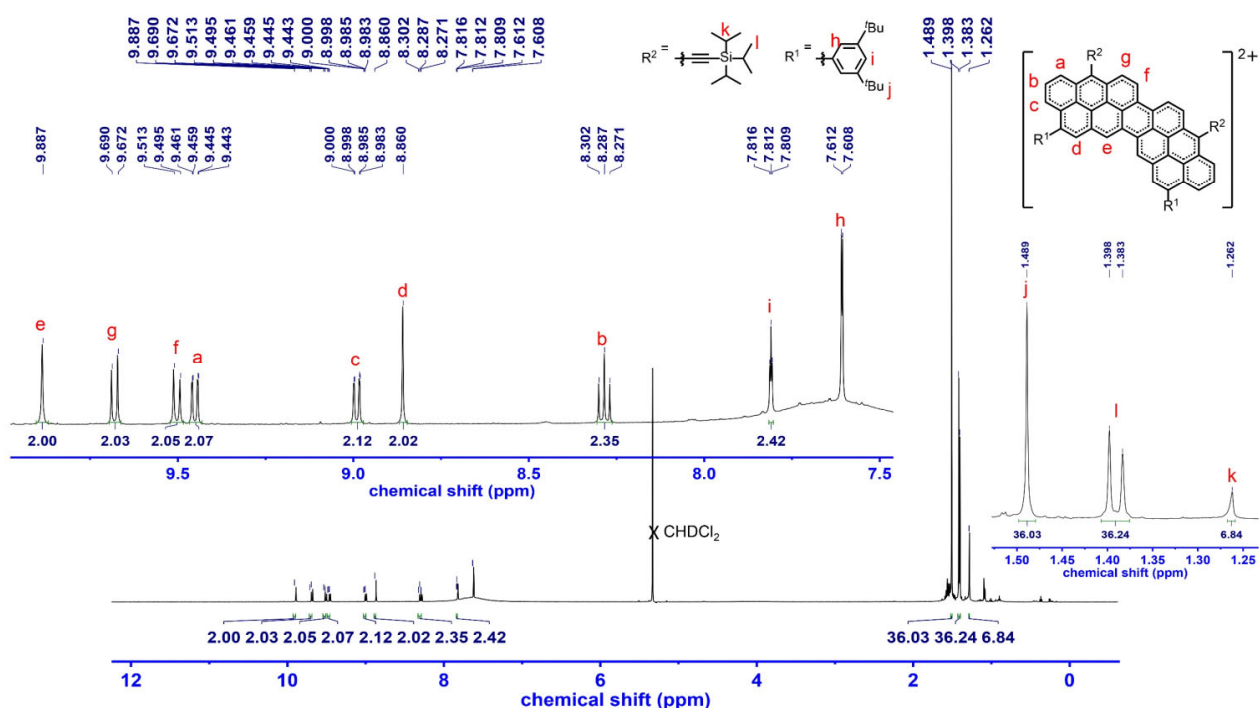


Figure S88. ^1H NMR Spectrum (500 MHz, CD_2Cl_2 , 298K) of dication state of **tips-OR-2**. The dication state of **tips-OR-2** was obtained by dissolving excess NOSbF_6 in the CD_2Cl_2 solution of **tips-OR-2** under N_2 gas.

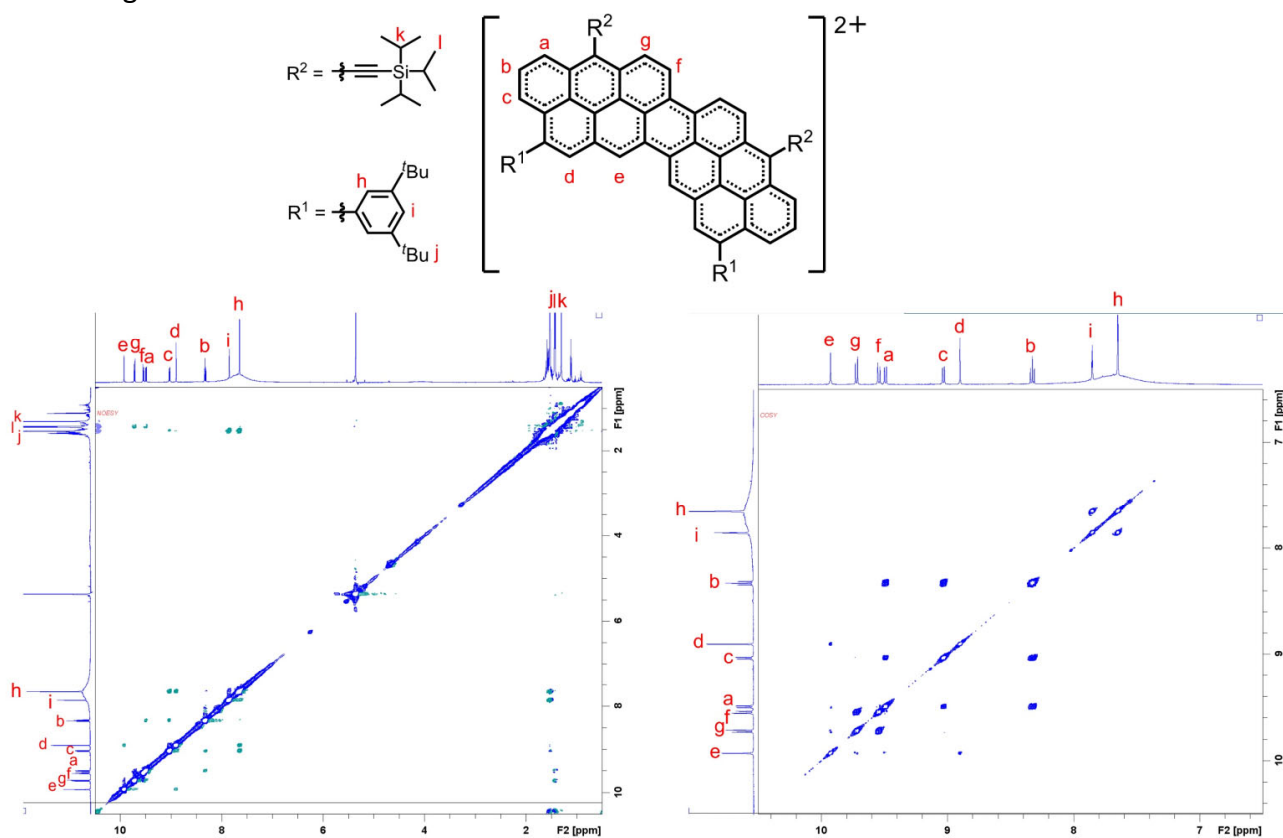


Figure S89. ^1H - ^1H NOESY and COSY spectra (500 MHz, CD_2Cl_2 , 298K) of dication state of **tips-OR-2**. Left: NOESY spectrum. Right: COSY spectrum.

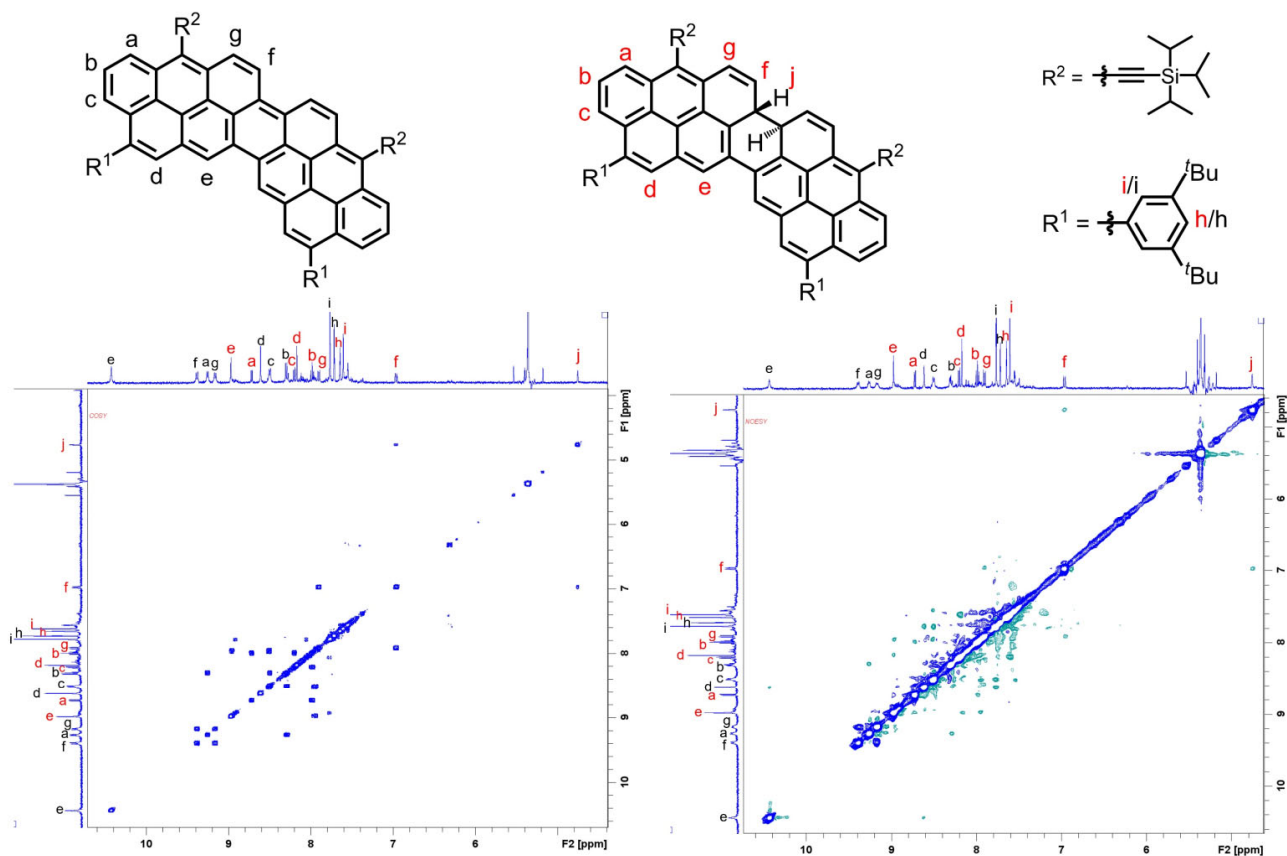


Figure S90. ^1H - ^1H COSY and NOESY spectra (500 MHz, CD_2Cl_2 , 298K) of the freshly prepared intermediate **9**. Left: COSY spectrum. Right: NOESY spectrum.

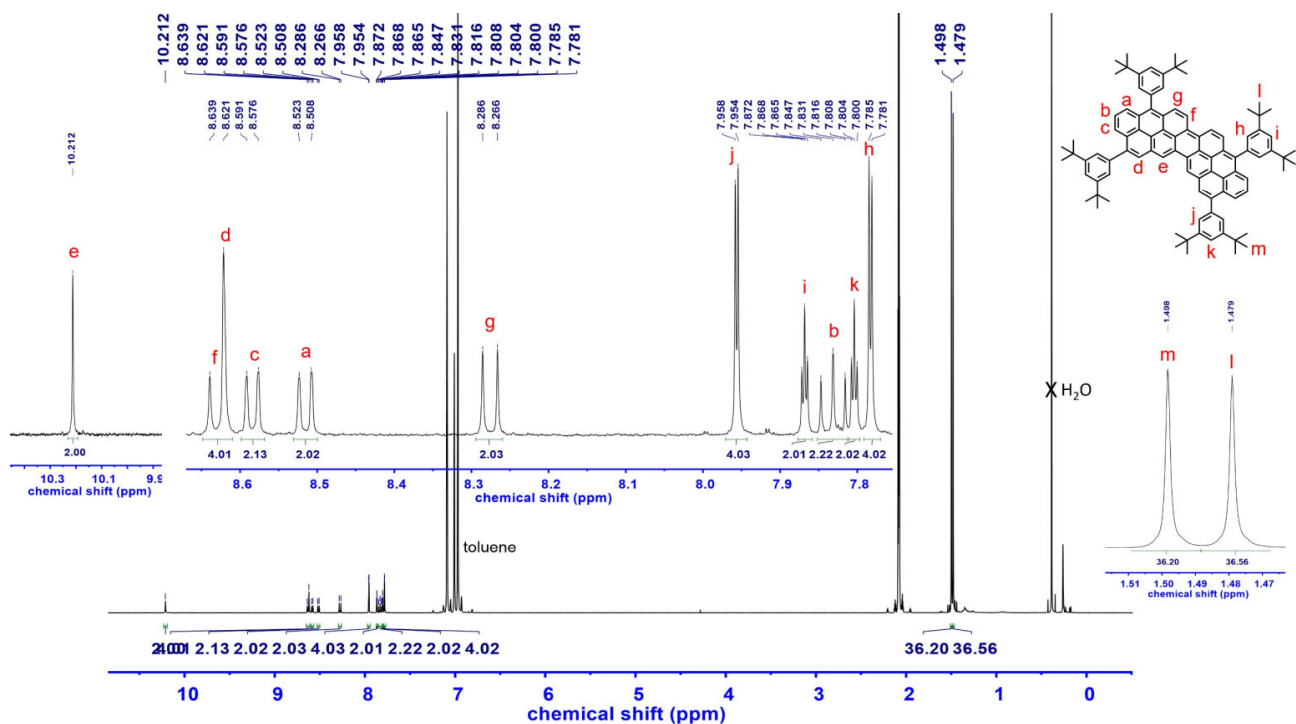


Figure S91. ^1H NMR Spectrum (500 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 298K) of **dtbp-OR-2**.

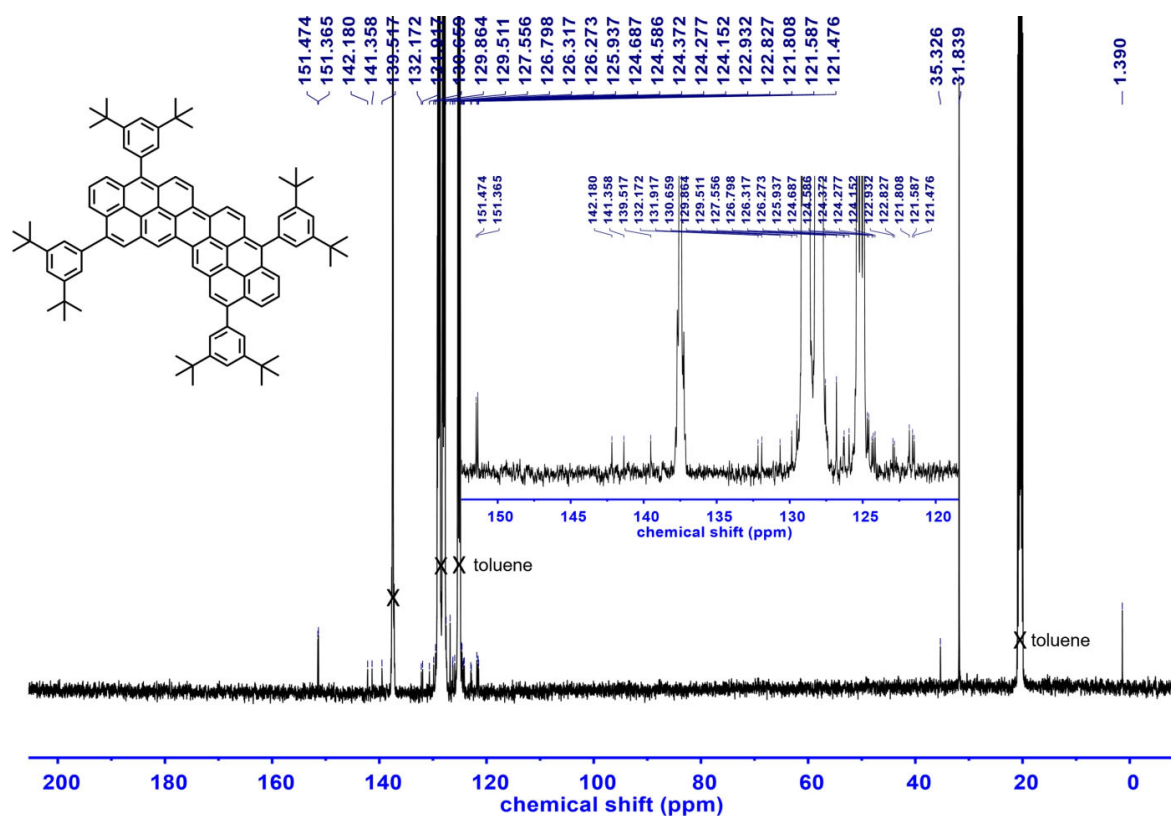


Figure S92. ^{13}C NMR Spectrum (125 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 298K) of **dtbp-OR-2**.

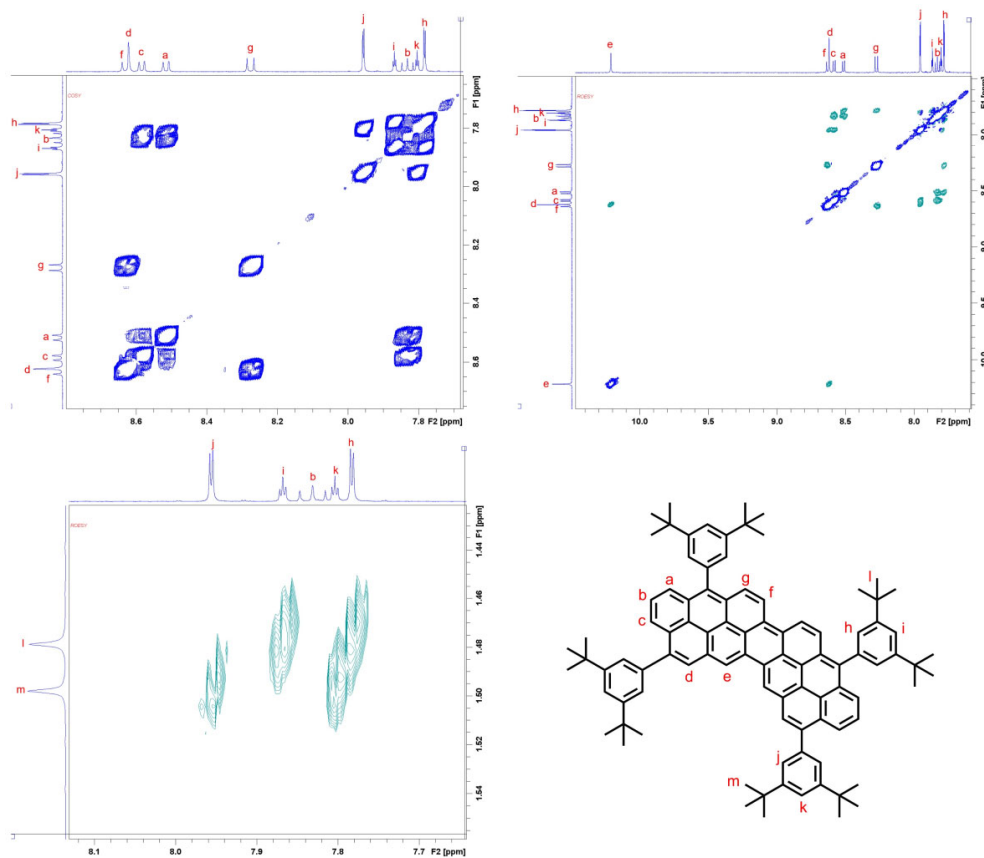


Figure S93. ^1H - ^1H COSY and ROESY spectra (500 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 298K) of **dtbp-OR-2**. Left: COSY spectrum. Middle and right: ROESY spectrum.

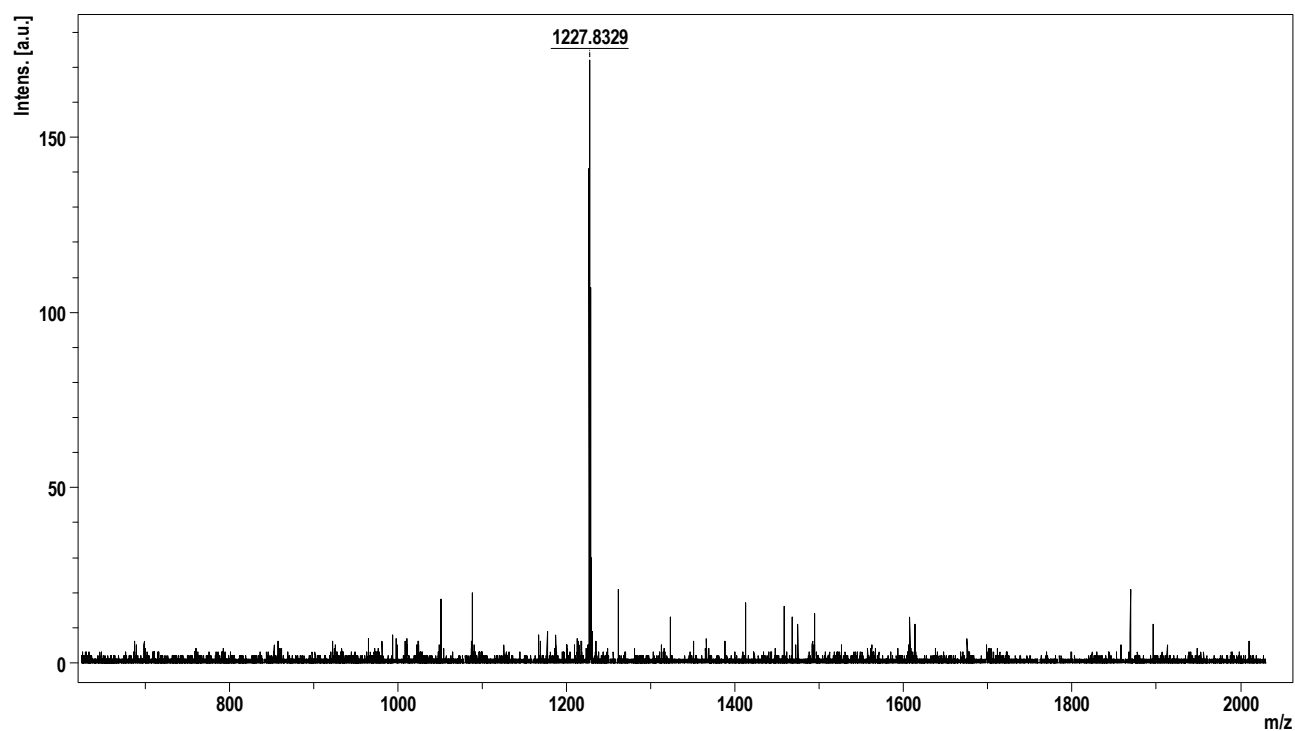


Figure S94. MALDI-TOF spectrum of **dtbp-OR-2**, showing the observed peak for $[M]^+$.

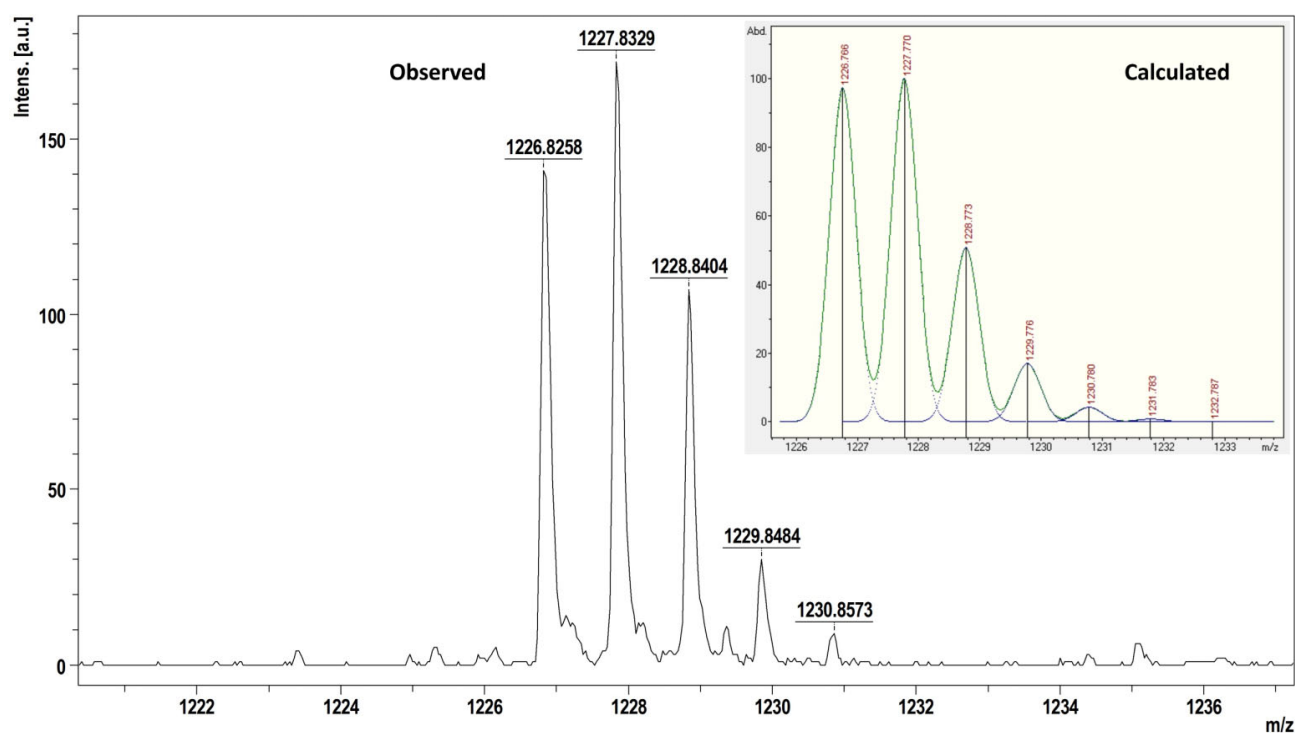


Figure S95. Calculated and observed isotopic distribution for the $[M]^+$ peak in the MALDI-TOF spectrum of **dtbp-OR-2**.

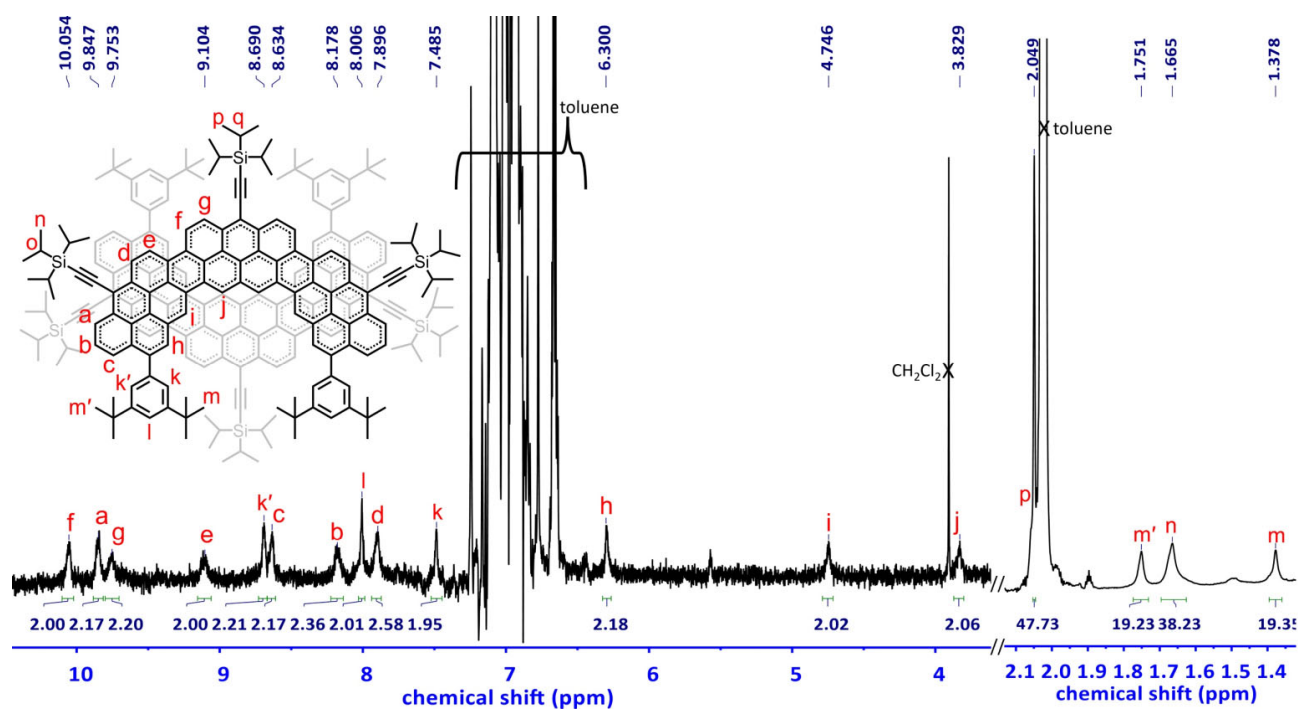


Figure S96. ¹H NMR Spectrum (500 MHz, C₆D₅CD₃, 223 K) of **[tips-OR-3]₂**.

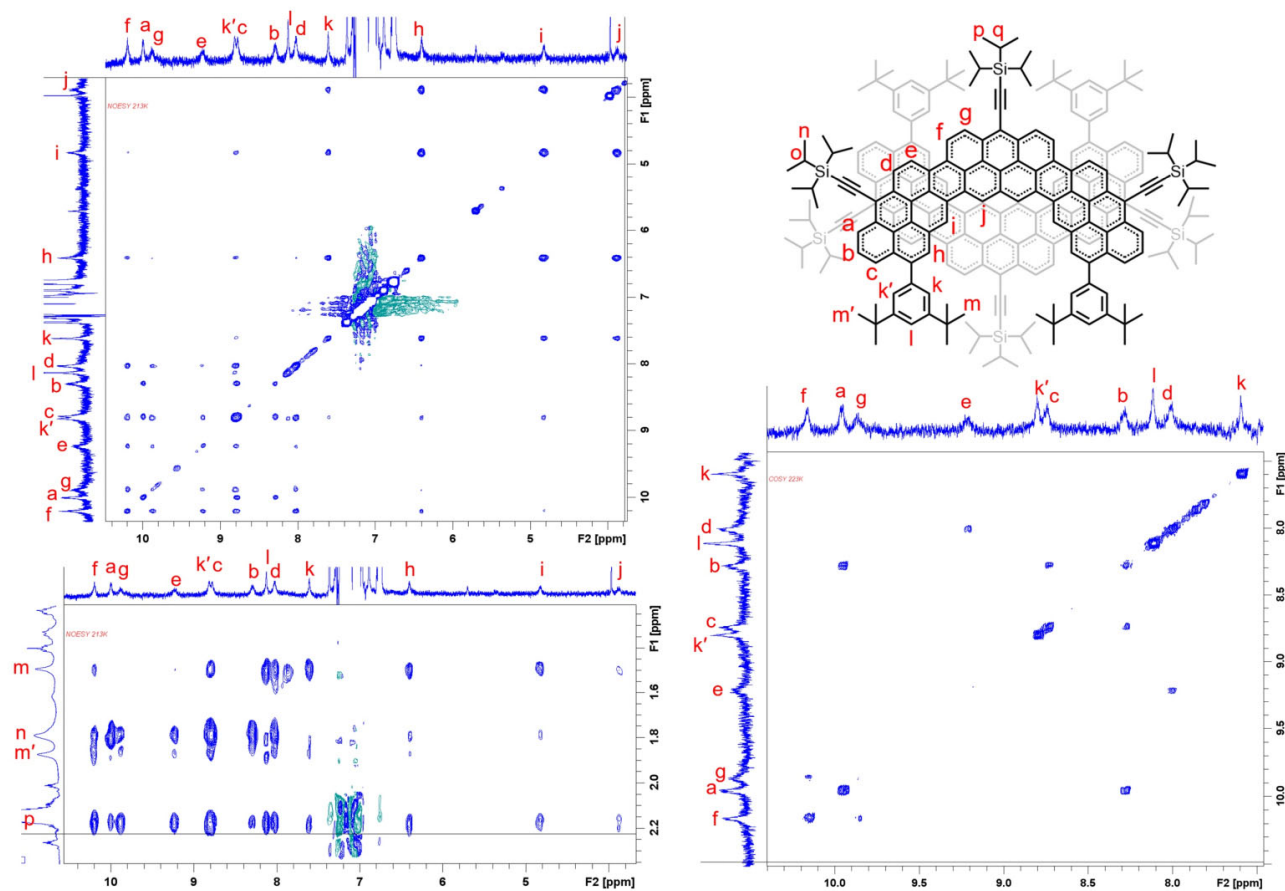


Figure S97. ¹H-¹H NOESY and COSY spectra (500 MHz, C₆D₅CD₃, 213 K / 223 K) of **[tips-OR-3]₂**. Left: NOESY spectrum. Right: COSY spectrum.

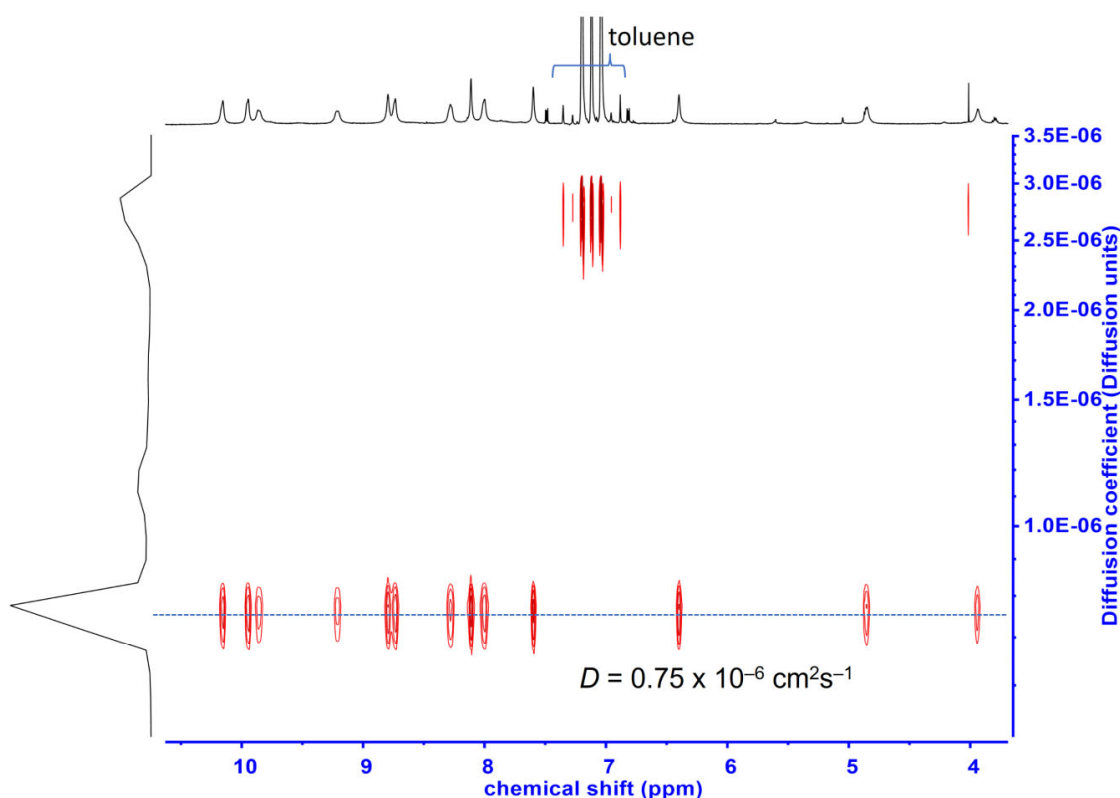


Figure S98. ^1H DOSY spectrum of **[tips-OR-3]₂** (500 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 223 K). The D value is $0.75 \times 10^{-10} \text{ m}^2\text{s}^{-1}$. By applying this value in the Stokes-Einstein relationship ($D = kT/6\pi\eta R_h$),¹⁵ we determined the apparent hydrodynamic radius (R_h) of 10.9 Å for **[tips-OR-3]₂**.

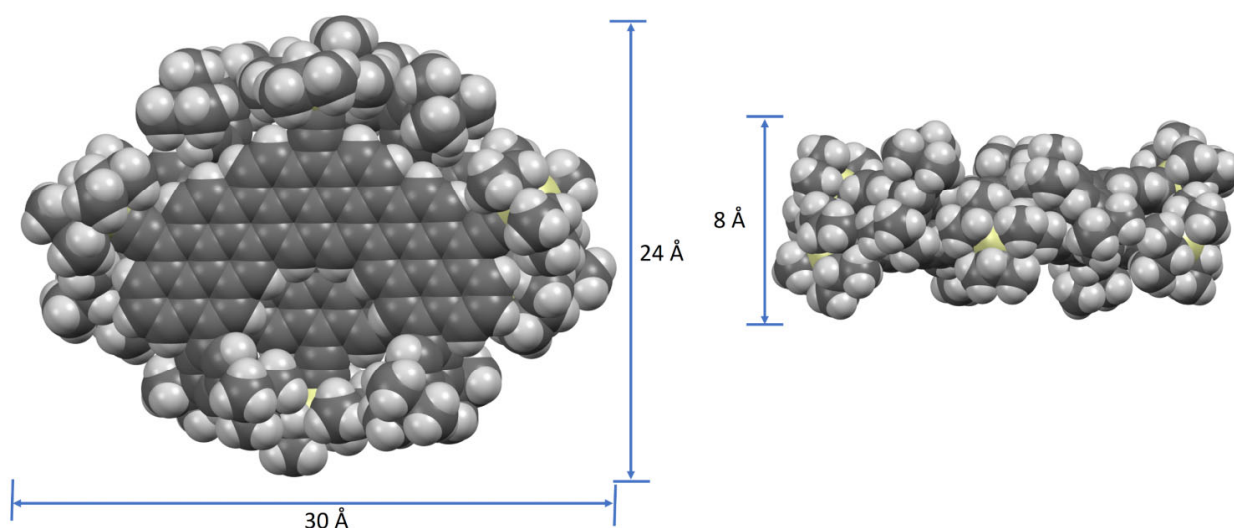


Figure S99. Size of **[tips-OR-3]₂** measured from crystal structure. The thickness (t) was determined to be 8 Å. The average radius (r) was determined to be $((24+30)/2)/2 = 13.5$ Å. By applying these

values in the Equation $R_h = \frac{3}{2}r\left\{1 + \left(\frac{t}{2r}\right)^2\right\}^{\frac{1}{2}} + \frac{2r}{t} \ln \left[\frac{t}{2r} + \left[1 + \left(\frac{t}{2r}\right)^2\right]^{\frac{1}{2}} \right] - \frac{t}{2r} \right\}^{-1}$,¹⁶ the expected hydrodynamic radius value for **[tips-OR-3]₂** was determined to be 11.7 Å, which is consistent with the R_h value (10.9 Å) measured from DOSY.

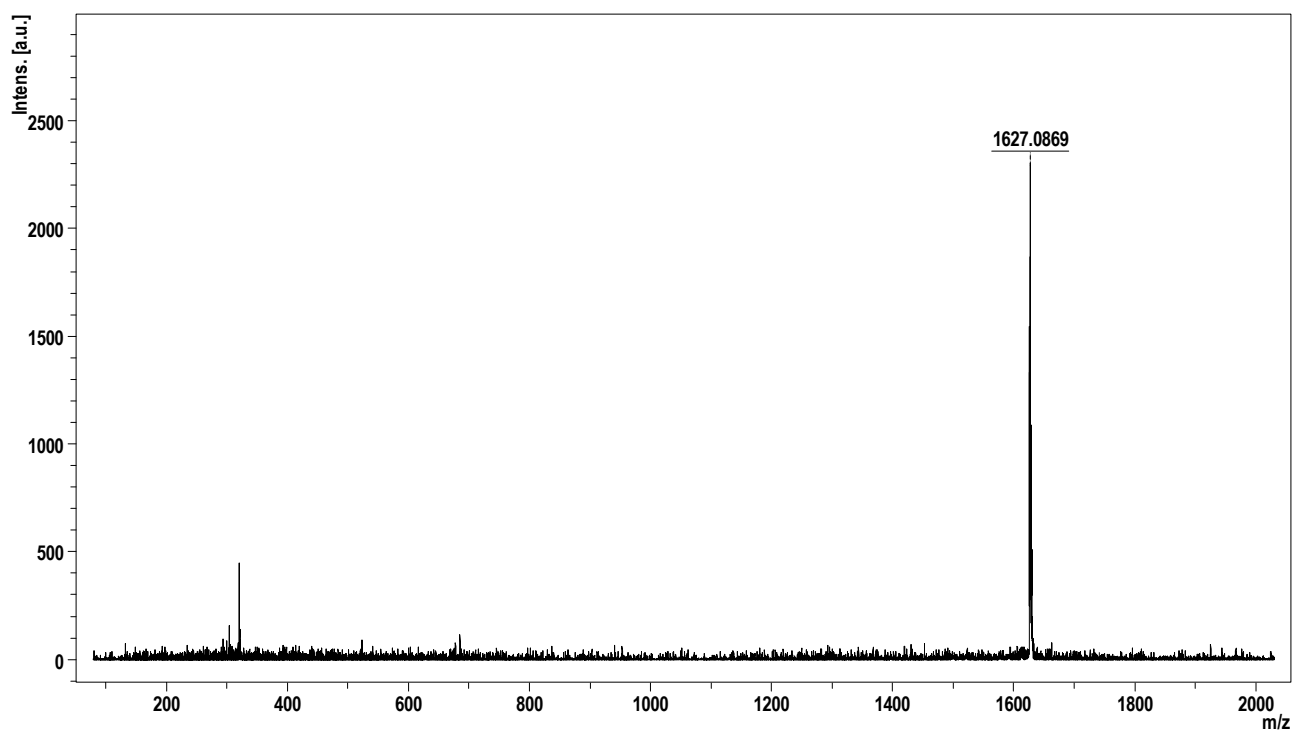


Figure S100. MALDI-TOF spectrum of **tips-OR-3**, showing the observed peak for $[M]^+$.

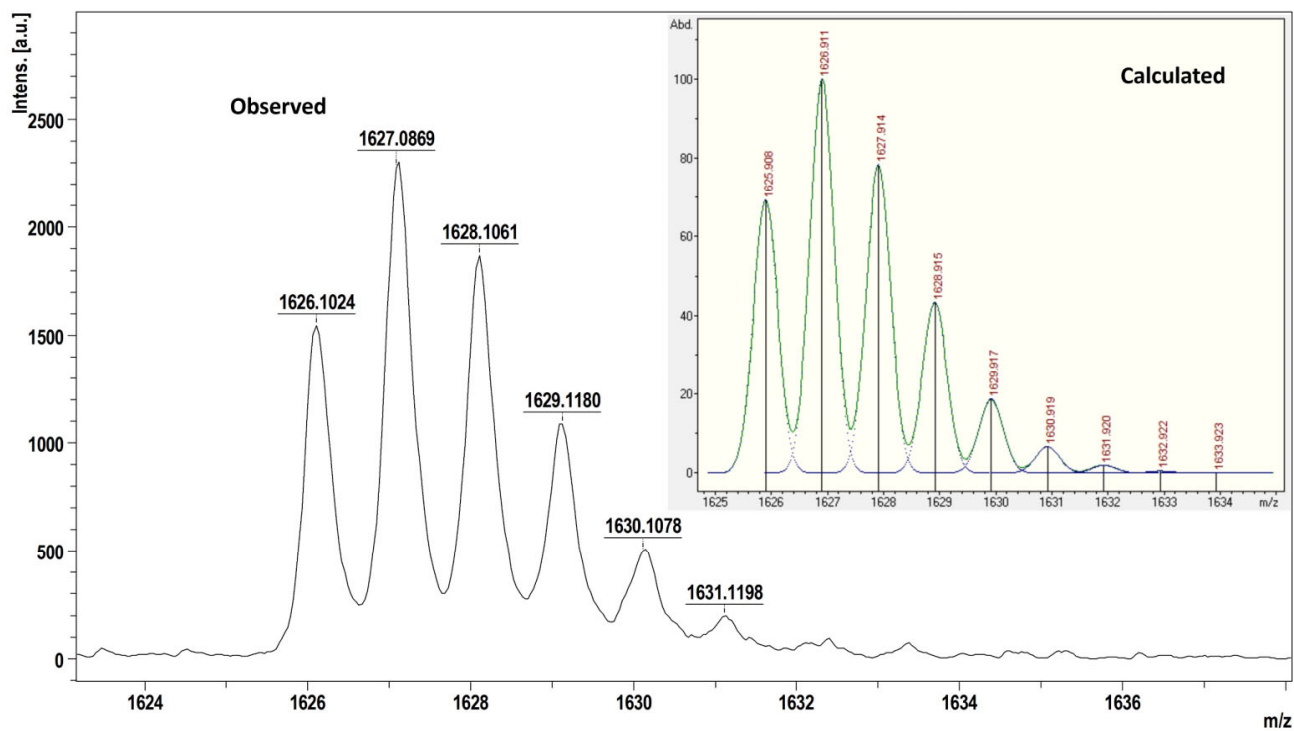


Figure S101. Calculated and observed isotopic distribution for the $[M]^+$ peak in the MALDI-TOF spectrum of **tips-OR-3**.

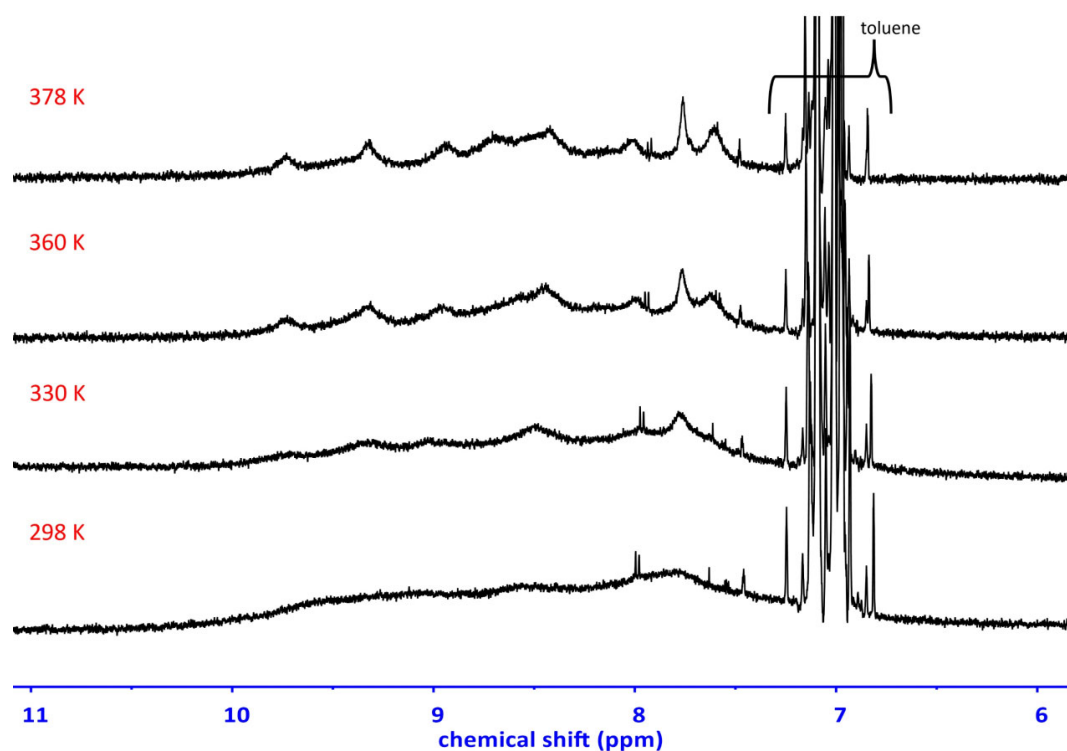


Figure S102. VT ^1H NMR spectra of **tips-OR-4** (500 MHz, $\text{C}_6\text{D}_5\text{CD}_3$). As the temperature increases from 298 K to 378 K, the resonance peaks of **tips-OR-4** in the aromatic region become much sharper, indicating that its aggregation behavior are inhibited to some extent.

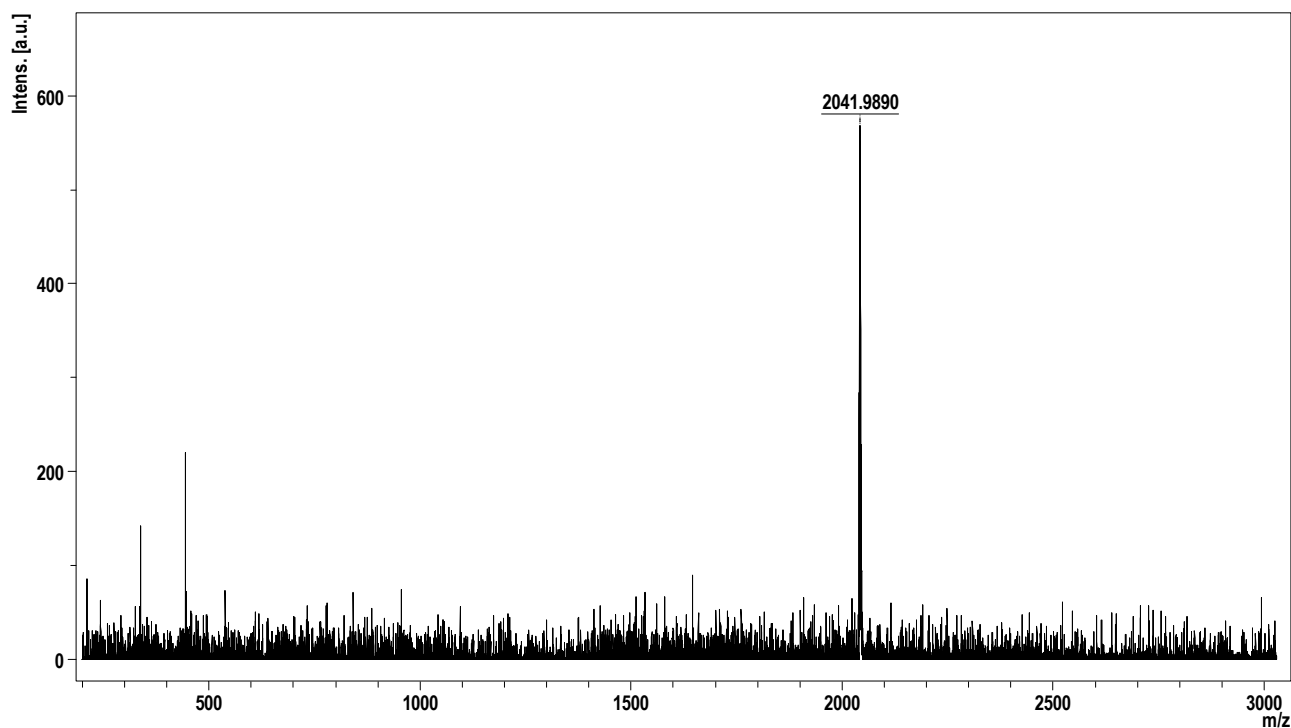


Figure S103. MALDI-TOF spectrum of **tips-OR-4**, showing the observed peak for $[M]^+$.

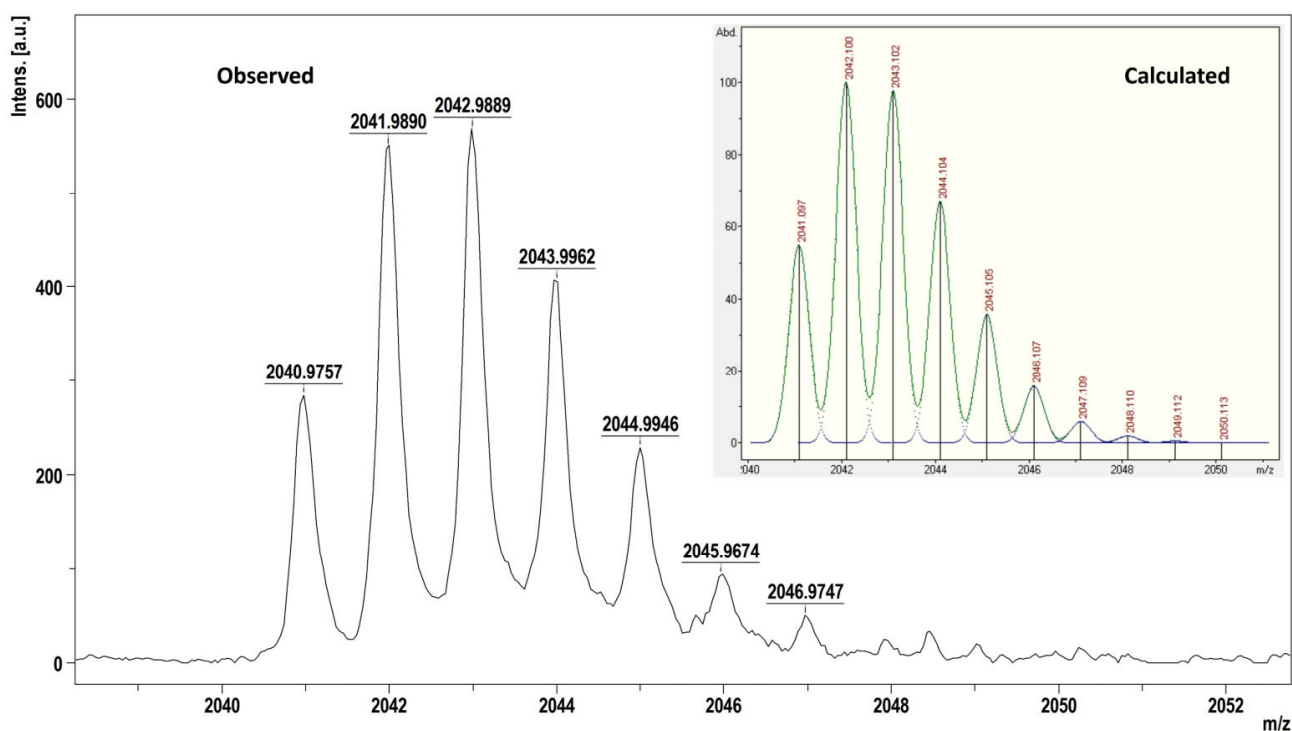


Figure S104. Calculated and observed isotopic distribution for the $[M]^+$ peak in the MALDI-TOF spectrum of **tps-OR-4**.

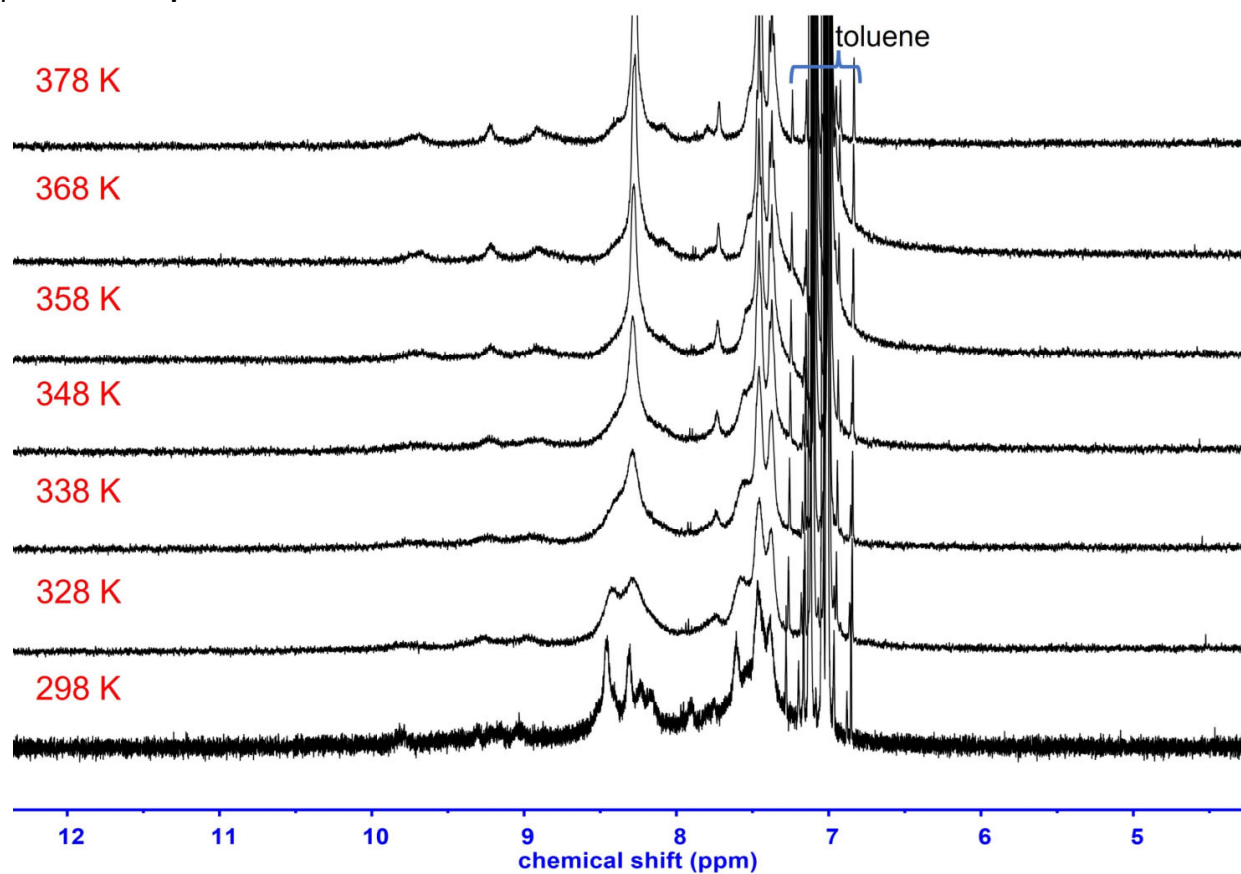


Figure S105. VT ^1H NMR spectra of **tps-OR-4** (500 MHz, $\text{C}_6\text{D}_5\text{CD}_3$). As the temperature increases from 298 K to 378 K, the resonance peaks of **tps-OR-4** in the aromatic region become much sharper, indicating that its aggregation behavior is inhibited to some extent.

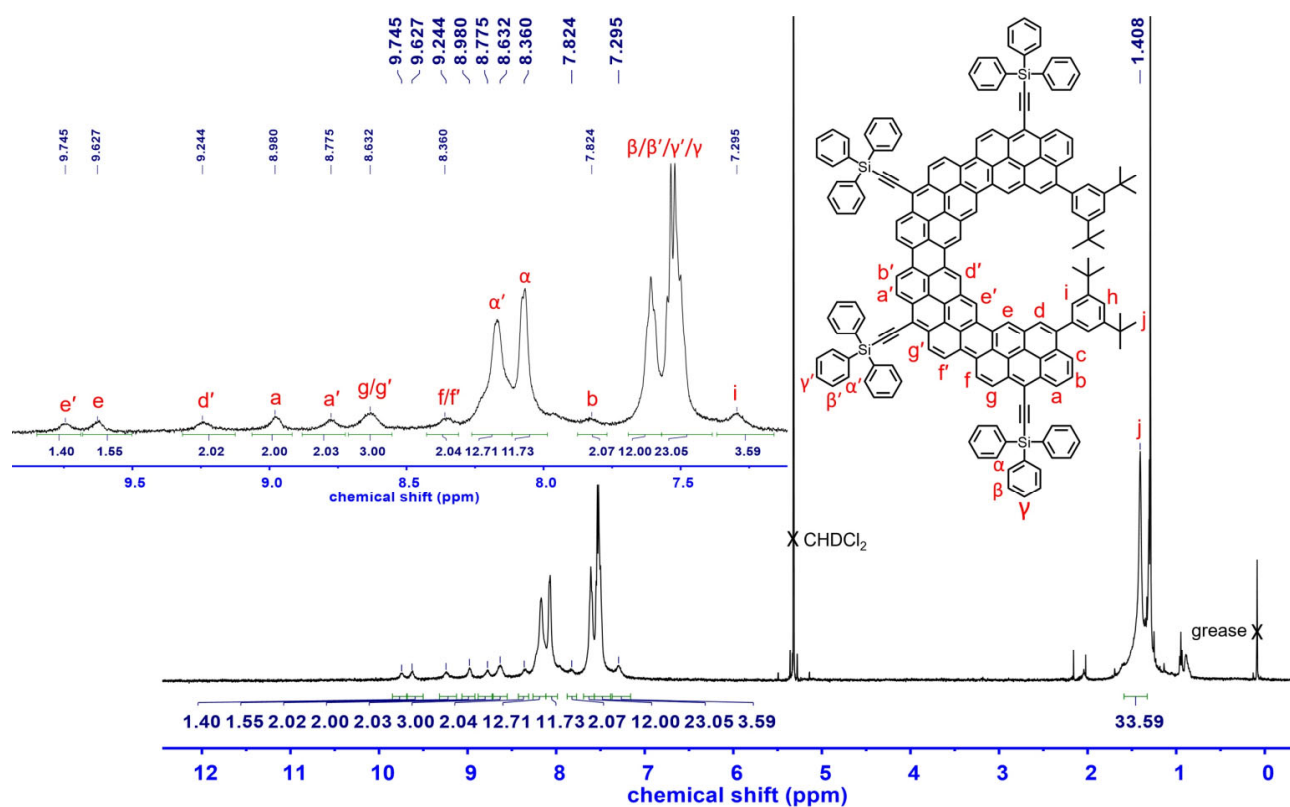


Figure S106. ¹H NMR Spectrum (500 MHz, 1:3 v/v CD₂Cl₂:CS₂, 298 K) of tps-OR-4.

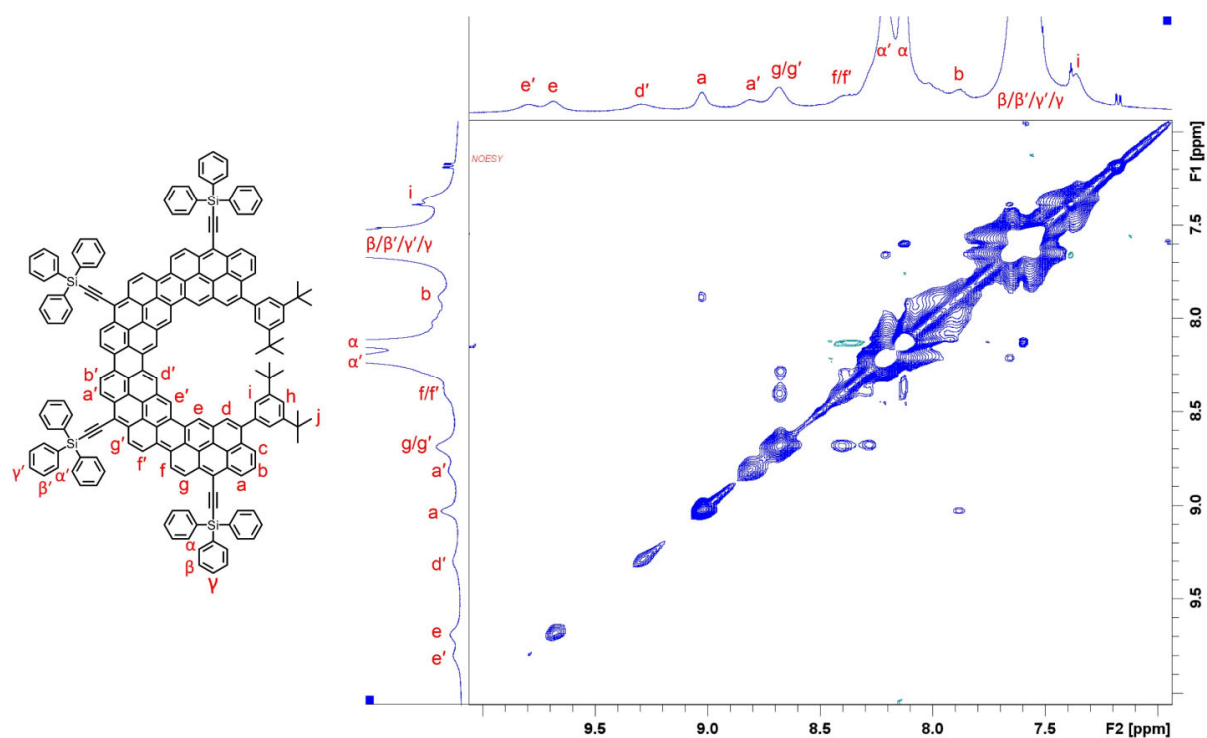


Figure S107. ¹H-¹H NOESY Spectrum (500 MHz, 1:3 v/v CD₂Cl₂:CS₂, 298 K) of tps-OR-4.

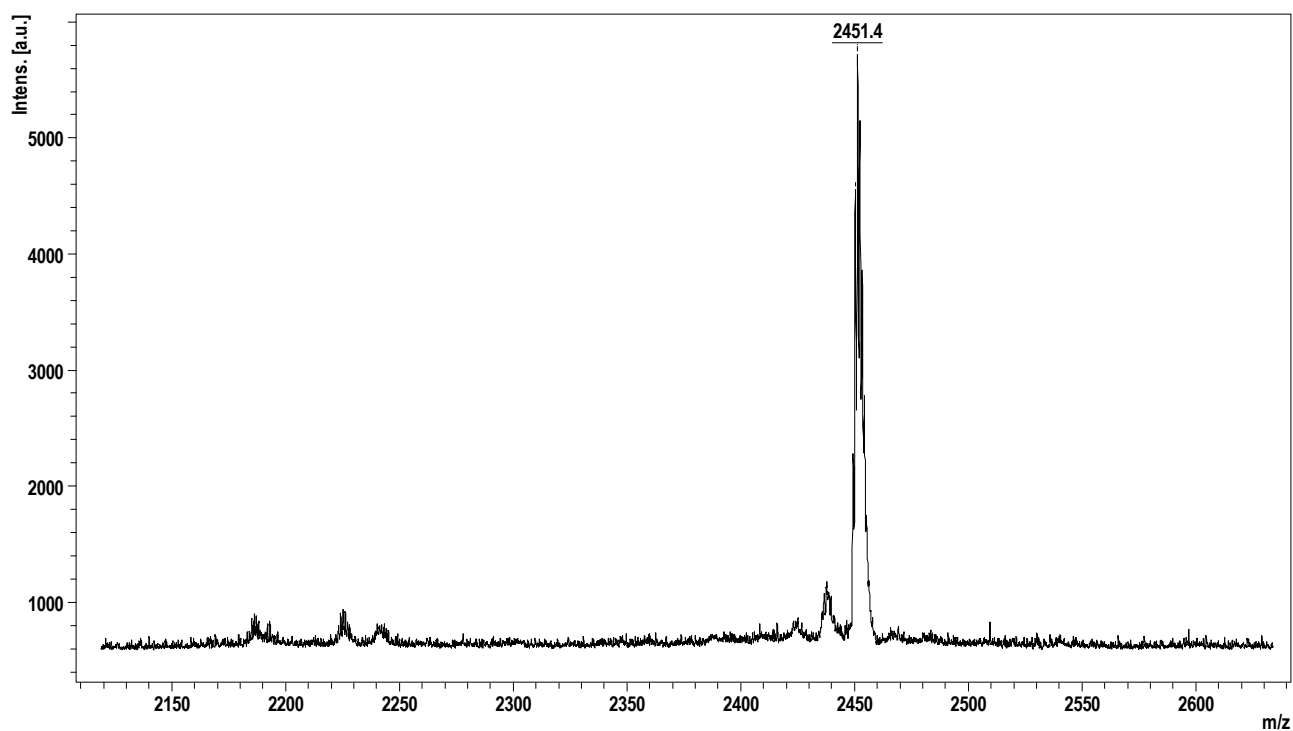


Figure S108. MALDI-TOF spectrum of **tps-OR-4**, showing the observed peak for $[M]^+$.

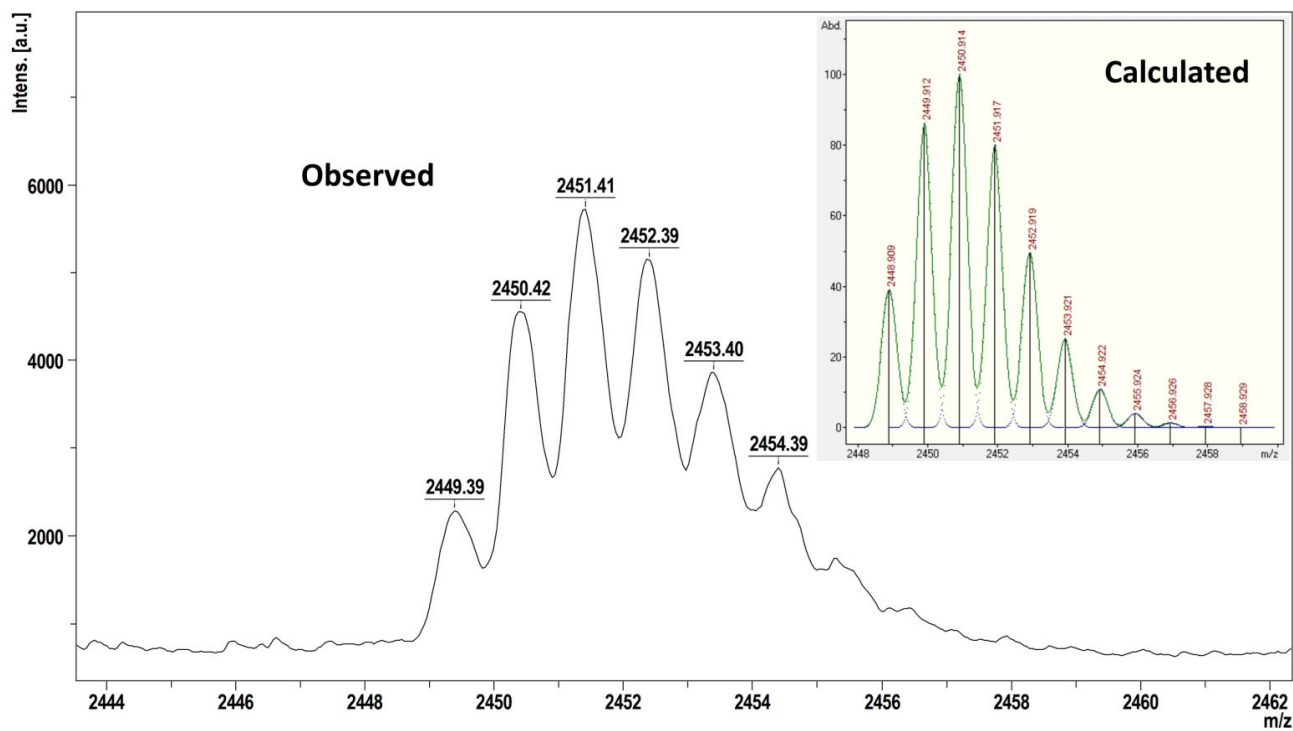


Figure S109. Calculated and observed isotopic distribution for the $[M]^+$ peak in the MALDI-TOF spectrum of **tps-OR-4**.

8. References

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9. Cartesian coordinates for the optimized structure

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C 3.01848900 1.52666300 -0.78880000	C -4.14533100 2.54381800 -1.49637400
C 2.12238500 2.61005300 -0.92797300	C -3.87073800 3.78735200 -2.16347200
C 2.37345100 3.83056100 -0.20921800	C -2.74276100 3.94329900 -2.90501500
C 3.47026800 3.91185800 0.65282600	C -1.74980300 2.91666800 -2.95747900
C 0.99347100 2.50458000 -1.80059400	C -5.62827100 1.03214400 -0.23405200
C 0.37336100 3.72432100 -2.19759000	C -5.35121700 2.30811700 -0.83030700
C 0.56199800 4.89959500 -1.40459100	C -6.13132800 -1.48992700 0.90609400
C 1.48380500 4.94013100 -0.40858500	C -7.06964100 -0.45694700 1.01495800
C 4.88363200 -0.63172400 -0.71769100	C -6.83548100 0.77893300 0.44893800
C 3.74713200 -0.73255000 -1.45440500	C -6.33461100 3.33927100 -0.74799900
C 2.76227500 0.31372700 -1.49823500	C -4.18352300 -3.72536900 0.58443800
C 1.53859300 0.15192500 -2.12174600	C -5.30858300 -4.43650900 0.17474800
C 0.55862400 1.16992600 -2.15504000	C -5.54347400 -5.74495100 0.61325800
C -0.84921400 0.78699300 -2.09624400	C -4.60782900 -6.32263500 1.46898400
C 5.87175300 -1.74260300 -0.74827100	C -3.45767200 -5.64146900 1.89533800
C 5.46352900 -3.05268800 -0.49582400	C -3.26234200 -4.33932200 1.44353700
C 6.36215200 -4.12057700 -0.56107000	C -6.80551100 -6.47471100 0.14400400
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C -2.73824800 -2.07028700 -0.51209200	C -1.28064500 -5.45789200 3.19614900
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C -4.93344500 -1.29854600 0.22072400	C 3.89472300 6.10841600 2.06722800

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anti-9

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C 7.10672100 -0.43575500 -0.25823300	C 8.10960100 7.46597100 0.16800200
C 7.76757300 0.75509300 -0.52987700	C 8.22016200 6.87201200 -2.85682400
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syn-9

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C -2.88901700 1.79620300 -0.86576900	C -9.35002300 -4.40770700 -0.76159800
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C -3.43176700 -1.81906000 -0.01938300	C -3.74941300 -5.47509800 3.72167300
C -4.77341300 -1.88347200 0.19585600	C -4.43031200 -7.46233600 2.38908700
C -5.57404500 -0.67060900 0.11445400	C 5.28027500 5.72331900 1.65665500
C -4.93667800 0.55270700 -0.24294700	C -6.46052000 5.20401100 -0.85755300
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C -2.98048400 4.24723300 -1.32000500	Si -7.43900600 6.76280200 -0.96084100
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C -0.83411300 3.03038400 -1.68129400	C 6.92727300 6.94232600 3.88318200
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C -7.67381000 0.52796600 0.32368400	C -8.54091300 6.88337200 0.55596600
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H 4.76137800 -3.73486700 0.66316200	H -9.07261000 -6.78161000 0.58784400
H 8.18452600 -5.70437900 -1.00443700	H -7.93193600 -7.55835300 -0.53154600
H 7.42194200 -1.58082200 -1.88439300	H -9.54282400 -7.08697300 -1.09029500
H -0.80737200 -1.44705800 -0.40678800	H -6.91021100 -6.21652800 -2.44538200
H -2.83767900 -2.72825800 0.03874500	H -7.39738200 -4.53644800 -2.71879500
H -3.56702200 5.16050800 -1.33177900	H -8.56430800 -5.84345600 -2.97371600
H -1.20473400 5.19981600 -1.92068400	H -9.69186200 -4.32670200 0.27567200
H -0.69148600 2.79412500 -2.75001800	H -9.05152200 -3.40982500 -1.09831200
H -7.43622600 -1.56484800 0.72500300	H -10.19576900 -4.73157000 -1.37854100
H -8.73353300 0.52006300 0.55920900	H -6.41549100 -5.44096000 4.39668000
H -7.63833700 2.63534200 -0.12287700	H -6.89978300 -6.88911500 3.50012500
H -6.82054500 -3.07460600 -1.08562200	H -5.69517600 -7.01557400 4.79156700
H -6.93118100 -6.65969400 1.26279000	H -2.89796300 -5.28557200 3.05952400
H -4.07847900 -3.58240500 2.14158700	H -3.41105900 -6.14543400 4.51833900
H 6.98867500 -7.57992300 -0.72257300	H -4.04452800 -4.52763900 4.18445200
H 6.58284000 -8.22945300 0.87228800	H -3.61944100 -7.30247900 1.67097600
H 7.95356200 -7.12528100 0.69840500	H -4.05721400 -8.10787000 3.19215800
H 3.84701400 -5.78844600 0.34594700	H -5.23535700 -7.99651700 1.87531800
H 4.58233500 -6.75049200 -0.94640200	H 4.59350100 9.23454700 3.37777800
H 4.25740900 -7.48578500 0.63743900	H 3.65790000 8.47832500 2.07804500
H 5.25095100 -5.12169900 2.39500000	H 3.73362500 7.71459400 3.67354800
H 6.94332800 -5.62995600 2.50104700	H 7.27103100 7.87103900 4.35122300
H 5.64218500 -6.82843600 2.65942500	H 7.80977700 6.36565400 3.58996500
H 8.15582300 -3.91504500 -4.27552400	H 6.38243300 6.36518500 4.63617700
H 9.71781300 -3.09358100 -4.47487100	H 7.13897400 9.24033800 1.52063300

H 6.17852200 8.49437800 0.23224900
H 7.67943600 7.72858100 0.77244900
H -6.77650500 9.15671300 -1.07671800
H -5.61331700 8.23098400 -0.11369700
H -5.57465200 8.13516900 -1.88135400
H -9.07204000 7.64316300 -2.61312800
H -9.17160800 5.87724300 -2.51804400
H -7.85085300 6.64043300 -3.41444900
H -9.13537700 7.80290400 0.52729000
H -7.94622100 6.89262400 1.47420800
H -9.23184400 6.03660600 0.61050800

tips-OR-2 (neutral state)

C 7.77464900 0.86424100 -0.39015900
C 7.08099800 -0.34823300 -0.33911700
C 5.69242400 -0.37435000 -0.21733300
C 4.98186900 0.86558900 -0.18683300
C 5.69765500 2.09356800 -0.23364900
C 7.10197900 2.06831600 -0.32775800
C 3.55971700 0.88082800 -0.12820100
C 2.84651400 2.09912100 -0.10032500
C 3.57450900 3.33652200 -0.12891100
C 4.96492100 3.32948300 -0.19426300
C 1.42229100 2.09847200 -0.04722500
C 0.70375200 3.34033300 -0.01933300
C 1.47383300 4.55962500 -0.04281900
C 2.82392300 4.56247100 -0.09414000
C 4.93792000 -1.62191900 -0.15723400
C 3.58125200 -1.58425600 -0.12160200
C 2.84269800 -0.35091400 -0.10758000
C 1.45958500 -0.33495800 -0.05503800
C 0.72075700 0.86015100 -0.02328000
C -0.72692600 0.86323900 0.03285500

C 5.62809600 -2.93927700 -0.12575900
C 5.29315100 -3.92205300 -1.05113100
C 5.88695500 -5.19143600 -1.01513500
C 6.82840800 -5.43934200 -0.02046900
C 7.19011500 -4.47297100 0.93262600
C 6.57816300 -3.22621500 0.86611200
C 5.48657100 -6.23737800 -2.05979300
C 8.23044500 -4.82603400 1.99997100
C 5.68727200 4.56131000 -0.22758400
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C -3.59767500 -1.56873100 0.12980200
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C -1.46413200 4.56584800 0.05306600
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C -5.69830300 2.11777400 0.24569100
C -4.96066100 3.35043100 0.20747900
C -7.09293800 -0.31726600 0.34999800
C -7.78083700 0.89845300 0.40190400
C -7.10250300 2.09924300 0.33971200
C -5.67272700 4.58821600 0.24340800
C -5.65027600 -2.91539200 0.13073000
C -6.60993800 -3.19130900 -0.83985900
C -7.24435200 -4.43757900 -0.90311700
C -6.87883900 -5.40234100 0.03346100

C -5.90996600 -5.16418900 1.01987900	H 0.95242200 -1.29286600 -0.03818000
C -5.30530800 -3.91078500 1.05457800	H 4.56325600 -3.68016700 -1.81981200
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C -5.56581800 -6.27640900 2.01547700	H 6.81314300 -2.45348400 1.59061200
C 3.97554700 -6.50553700 -1.95682400	H -0.96780600 -1.28873600 0.04680600
C 6.22407000 -7.56579400 -1.86420700	H -3.04192200 -2.50197800 0.07434800
C 5.81554600 -5.70475700 -3.46460600	H -3.35878900 5.51303400 0.12241700
C 7.72330200 -6.01399100 2.83468700	H -0.94890100 5.51734600 0.02758100
C 8.50561900 -3.65424800 2.94769900	H -7.64656500 -1.24727400 0.41706500
C 9.55231100 -5.21106400 1.31423900	H -8.86235700 0.89472000 0.49556600
C -7.66410100 -4.51475200 -3.37141800	H -7.63758800 3.04239700 0.37559400
C -8.90398200 -6.08984200 -1.89685600	H -6.85520400 -2.41753800 -1.56335500
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C -5.04318900 -7.50290200 1.24850200	H 3.71611200 -6.88423000 -0.96278800
C -6.82867700 -6.66622700 2.80208900	H 3.39154000 -5.59771700 -2.13611200
C 6.31848900 5.60358500 -0.25507100	H 3.67288300 -7.25182100 -2.69990100
C -6.28021200 5.64446200 0.27279600	H 6.00946300 -8.00601200 -0.88455700
Si 7.31059300 7.15690200 -0.30231400	H 7.30823300 -7.44289700 -1.95871700
Si -7.15913500 7.26486400 0.30870400	H 5.90117400 -8.27909600 -2.62930200
C 9.10831600 6.68691700 -0.58204600	H 5.27868400 -4.77616700 -3.68037000
C 7.11640100 8.05214700 1.33773500	H 6.88762500 -5.50519600 -3.56176100
C 6.68743700 8.23084800 -1.71200600	H 5.53193200 -6.44217000 -4.22395200
C -7.96723100 7.48100500 1.99076600	H 7.55208000 -6.89941500 2.21479700
C -5.89064000 8.61937500 0.01343900	H 6.78122700 -5.76281000 3.33267000
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O₂

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H₂O

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13

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 Si 12.81516400 2.13449500 -0.75292800
 Si 1.04550400 10.55494100 -1.51072800
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C -7.75938700 -3.71168800 -7.39481900	H 3.41134300 -8.54876500 -2.41453300
C -5.97669300 -2.10982200 -6.72905800	H 5.07586200 -8.44877300 -1.80326200
C -8.38945200 -1.42275000 -6.65101400	H 8.43534000 -6.25961300 3.76751800
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Si -10.25058300 1.70763500 6.31794400	H 8.09100100 -7.15270200 5.25583100
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H 4.28671300 -5.32703500 -0.62849200	H 12.01983300 4.47646900 -0.45532000
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H 6.91564500 -4.97200800 2.71227900	H 13.89958100 0.97147500 1.16616600
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H 3.26407100 6.93175200 -0.98296000	H 2.18805300 11.91374600 -3.24820800

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 H 1.87751800 12.47060000 -0.16608000
 H 2.81488800 11.00937600 0.18497400
 H 1.20312700 11.21452400 0.88573000
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 H -5.01218600 -1.07367300 -2.46069800
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 H -4.34291800 3.58038400 4.32038000
 H -2.91535300 3.15064500 2.35436000
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 H -11.78376200 5.65959300 0.42521800
 H -12.68526600 4.45861400 -0.51093900
 H -14.57709700 2.82002400 2.07894400
 H -13.41829800 1.58240400 2.59118200
 H -13.72166500 1.85191000 0.86760700
 H -12.97660700 4.96618900 3.75534600
 H -11.24065600 5.17487400 3.47380100
 H -11.83862100 3.70220700 4.25146900

tips-OR-2 (radical cation state)

C -7.78533400 0.86489600 0.42437900
 C -7.08975500 -0.34344900 0.36322500
 C -5.69515200 -0.37498700 0.22548900
 C -4.98689100 0.86041300 0.20076400
 C -5.70287900 2.09041600 0.25781800
 C -7.10862900 2.06872800 0.36052300
 C -3.56849600 0.87049900 0.13807700
 C -2.85116600 2.09003600 0.11278000

C -3.56835600 3.32433200 0.14863600	C 1.45822100 4.53768200 -0.06609900
C -4.97778200 3.32222400 0.22134300	C 0.71608800 3.32349700 -0.03482100
C -1.42937100 2.08689000 0.05434100	C 5.70218700 2.11064200 -0.27013900
C -0.72080400 3.32098100 0.02559900	C 4.97319300 3.33971000 -0.23400700
C -1.46726000 4.53247900 0.05767000	C 7.09838600 -0.31750000 -0.37703600
C -2.83057700 4.53868400 0.11715600	C 7.78923000 0.89359900 -0.43787500
C -4.95482800 -1.62191300 0.15259000	C 7.10783200 2.09460200 -0.37291900
C -3.58948700 -1.58541700 0.11818500	C 5.67454000 4.57646700 -0.27745800
C -2.86024400 -0.35859600 0.11087200	C 5.66624100 -2.91338600 -0.11329700
C -1.45982100 -0.34213200 0.05359500	C 6.64239900 -3.16262800 0.84856200
C -0.72759300 0.83772300 0.02475100	C 7.28482300 -4.40449300 0.92380100
C 0.73157100 0.84033000 -0.03503100	C 6.90959400 -5.38450800 0.00733200
C -5.64878400 -2.93388100 0.10668500	C 5.92322800 -5.17243300 -0.96875000
C -5.29985700 -3.93244100 1.01043100	C 5.30730600 -3.92531500 -1.01413800
C -5.90552000 -5.19547600 0.96500300	C 8.35880100 -4.62864300 1.99212400
C -6.86458000 -5.41809700 -0.01971000	C 5.57430300 -6.30388600 -1.93995200
C -7.23612000 -4.43690400 -0.95355100	C -3.99209100 -6.53790600 1.85965300
C -6.61617800 -3.19438000 -0.87598300	C -6.25026200 -7.58032500 1.77821900
C -5.49984000 -6.26122200 1.98715800	C -5.80757800 -5.74784500 3.40405700
C -8.29295400 -4.76839000 -2.01101200	C -7.80075300 -5.94449600 -2.87141500
C -5.68812700 4.55384100 0.26302900	C -8.57665900 -3.57987600 -2.93506300
C 1.46789300 -0.33682900 -0.06411900	C -9.60557100 -5.16007100 -1.31110400
C 2.86844700 -0.34834300 -0.12165700	C 7.73519200 -4.44819000 3.38642200
C 3.57247000 0.88322500 -0.14923900	C 8.97015800 -6.03099300 1.91376500
C 2.85082800 2.10031100 -0.12352100	C 9.48469800 -3.59834100 1.79749900
C 1.42900300 2.09204300 -0.06443100	C 4.47775400 -5.89745300 -2.92950800
C 3.60176700 -1.57238200 -0.12846100	C 5.07879500 -7.52255600 -1.14272000
C 4.96735400 -1.60452400 -0.16196900	C 6.82898200 -6.69177600 -2.74082800
C 5.70379600 -0.35501800 -0.23727800	C -6.31023700 5.60203700 0.29774800
C 4.99082200 0.87788300 -0.21258000	C 6.27281100 5.63843300 -0.31283900
C 3.56357900 3.33717700 -0.15962400	Si -7.30424100 7.17776700 0.35621400
C 2.82143700 4.54903400 -0.12650200	Si 7.16491600 7.27434000 -0.36097400

C -9.09002200 6.69051700 0.65290200	H -5.25894700 -4.82827600 3.63026000
C -7.09505400 8.04089700 -1.29469800	H -6.87649200 -5.54146800 3.51874400
C -6.63473500 8.21840300 1.76444600	H -5.52160400 -6.50034800 4.14681300
C 7.96050100 7.43561200 -2.05046500	H -7.62577200 -6.84122500 -2.26931000
C 5.88046000 8.61160900 -0.07955700	H -6.86512100 -5.68957400 -3.37952000
C 8.44773400 7.25940700 1.00557300	H -8.54869700 -6.19247500 -3.63215500
H -8.86492400 0.85633500 0.52838100	H -7.68246000 -3.27532300 -3.48918900
H -7.63507400 -1.27819000 0.43361100	H -9.34128300 -3.85983200 -3.66604900
H -7.64641200 3.01026400 0.40401000	H -8.95119400 -2.71452800 -2.37700200
H -0.95696300 5.48595100 0.03612000	H -9.97621800 -4.33787100 -0.69009800
H -3.37411900 5.47720000 0.14313000	H -9.47820000 -6.03718300 -0.66963400
H -3.03502600 -2.51816200 0.05602700	H -10.37139200 -5.39932400 -2.05662700
H -0.95915400 -1.30316700 0.03044500	H 6.92757000 -5.16953900 3.54677100
H -4.55743100 -3.70973300 1.77291900	H 7.32319000 -3.44307000 3.51970400
H -7.34788300 -6.38760300 -0.07508200	H 8.49414100 -4.60444500 4.16051200
H -6.85405900 -2.41271700 -1.59020400	H 8.21729600 -6.80937300 2.07656800
H 0.97066900 -1.29964700 -0.04105300	H 9.73381700 -6.13985300 2.68992000
H 3.05012700 -2.50676000 -0.06593800	H 9.45080000 -6.20925100 0.94600500
H 3.36109600 5.48998800 -0.15144800	H 9.11576800 -2.57170000 1.89346100
H 0.94452000 5.48929400 -0.04313500	H 10.26396600 -3.74391100 2.55318500
H 7.64836600 -1.24940700 -0.44964100	H 9.94227100 -3.70545700 0.80837100
H 8.86876200 0.88887300 -0.54275200	H 3.54834800 -5.63065200 -2.41467800
H 7.64117300 3.03847700 -0.41571300	H 4.78709300 -5.05010400 -3.55054900
H 6.88999300 -2.37933100 1.56113300	H 4.25922700 -6.73654600 -3.59705700
H 7.39640400 -6.35321500 0.04340800	H 4.18548900 -7.27062700 -0.56190800
H 4.55318600 -3.70555900 -1.76262600	H 5.84038900 -7.89074500 -0.44884500
H -3.74709100 -6.90114700 0.85629800	H 4.82561800 -8.34020000 -1.82610300
H -3.39790300 -5.63863000 2.05054000	H 7.20256300 -5.83840200 -3.31591300
H -3.68729600 -7.29982700 2.58505700	H 6.59286100 -7.50079800 -3.44038900
H -6.05128500 -8.00679500 0.78931400	H 7.63521300 -7.03902200 -2.08767000
H -7.33200300 -7.45214300 1.89028500	H -9.46558000 6.05094600 -0.15164000
H -5.92297200 -8.30827200 2.52686200	H -7.45042600 7.41492200 -2.11835900

H -6.72052600 7.69510300 2.72120100
 H 7.21218000 7.40450600 -2.84770500
 H 5.11327700 8.59529300 -0.85968400
 H 7.98319800 7.12175500 1.98629200
 H -5.58207100 8.47217200 1.60826500
 H -7.19746800 9.15468900 1.84162600
 H -9.72565500 7.58109800 0.69637800
 H 6.35127200 9.60012300 -0.09429400
 H 8.99269300 8.20914600 1.02145300
 H 9.17691700 6.45716200 0.85890700
 H 8.68197700 6.63322000 -2.23008500
 H -9.20279500 6.15233000 1.59885000
 H -7.67086700 8.97234000 -1.30747500
 H -6.04738700 8.29137800 -1.48535000
 H 8.49337600 8.38937700 -2.12588500
 H 5.38705000 8.49045100 0.88949000

tips-OR-2 (dication state)

C 7.79044900 0.85831700 -0.58198500
 C 7.09489800 -0.34638000 -0.45676000
 C 5.70246900 -0.38073100 -0.26038100
 C 4.99079800 0.84950300 -0.27099800
 C 5.70207200 2.07958400 -0.39357400
 C 7.10915900 2.05917700 -0.53576500
 C 3.57869800 0.85341600 -0.18120800
 C 2.85557800 2.07147200 -0.18231000
 C 3.55924500 3.30402000 -0.27428300
 C 4.98399200 3.30672000 -0.38524600
 C 1.43550600 2.06500000 -0.09192900
 C 0.73488600 3.29053300 -0.06313600
 C 1.45728300 4.49829600 -0.16032000
 C 2.82831400 4.50905100 -0.26650200

C 4.98204900 -1.62635200 -0.11152500
 C 3.60441200 -1.59208100 -0.06592900
 C 2.88249800 -0.37672900 -0.09772400
 C 1.46384600 -0.36094700 -0.01824300
 C 0.73605500 0.80409800 -0.02461500
 C -0.73563300 0.80573100 0.03546900
 C 5.68191800 -2.92159100 0.01088900
 C 5.27600600 -4.00204900 -0.77027300
 C 5.90004600 -5.24998200 -0.65460700
 C 6.92659300 -5.37426000 0.28065600
 C 7.35134800 -4.31314700 1.09726900
 C 6.71727500 -3.08467700 0.94742900
 C 5.44449200 -6.40674900 -1.54868600
 C 8.47537800 -4.54617300 2.11015400
 C 5.67863200 4.53506400 -0.49071100
 C -1.46571800 -0.35770000 0.03166600
 C -2.88456900 -0.37046100 0.11137100
 C -3.57829700 0.86138200 0.19290300
 C -2.85268600 2.07805400 0.19113800
 C -1.43255300 2.06836400 0.09997000
 C -3.60860900 -1.58409500 0.08108700
 C -4.98663900 -1.61536600 0.12486800
 C -5.70473900 -0.36832900 0.27536200
 C -4.99024700 0.86045000 0.28346400
 C -3.55370400 3.31228400 0.28094900
 C -2.82022200 4.51593600 0.26871500
 C -1.44938700 4.50178400 0.16130000
 C -0.72947800 3.29219800 0.06751500
 C -5.69874000 2.09236800 0.40439100
 C -4.97861100 3.31779400 0.39405700
 C -7.09683200 -0.33022200 0.47575900
 C -7.78971700 0.87647400 0.59744800

C -7.10575300 2.07551100 0.54687700	H 8.86482300 0.84640800 -0.72579700
C -5.66647900 4.54997800 0.49963100	H 7.63788100 -1.28328200 -0.52564400
C -5.69066500 -2.90719000 -0.00101000	H 7.64060800 3.00119600 -0.62886200
C -6.73015000 -3.05960400 -0.91971300	H 0.94337600 5.44967600 -0.16141700
C -7.38716200 -4.28662000 -1.06929700	H 3.36290000 5.45003800 -0.34499600
C -6.96278600 -5.34611100 -0.26987600	H 3.05872900 -2.52432800 0.04962000
C -5.91273400 -5.23315100 0.65779800	H 0.97179300 -1.32420800 0.05317700
C -5.27832900 -4.00149100 0.77537900	H 4.48497700 -3.85517700 -1.50159700
C -8.52533700 -4.40982600 -2.08624800	H 7.42144200 -6.33295500 0.39096600
C -5.52047600 -6.45121400 1.49779500	H 6.98682700 -2.24616500 1.58160200
C 3.95034800 -6.67790500 -1.30247400	H -0.97566100 -1.32212900 -0.03764100
C 6.22186500 -7.69644500 -1.26697000	H -3.06453700 -2.51739900 -0.03319900
C 5.65953100 -6.02065000 -3.02221500	H -3.35235800 5.45871600 0.34424100
C 8.04535900 -5.64045700 3.10215600	H -0.93352200 5.45211000 0.15877800
C 8.80824500 -3.27776300 2.90210800	H -7.64252100 -1.26515400 0.55117600
C 9.74228500 -4.99852300 1.36357700	H -8.86389900 0.86692300 0.74297100
C -7.98065100 -4.11718300 -3.49466200	H -7.63435500 3.01917000 0.63732700
C -9.14964500 -5.80865200 -2.08736800	H -7.00588600 -2.21859500 -1.55157600
C -9.62260800 -3.38898300 -1.73769500	H -7.46087100 -6.30493200 -0.36370400
C -4.35905500 -6.14504100 2.44857100	H -4.47927700 -3.85772600 1.49523800
C -5.09280800 -7.59446400 0.56120300	H 3.76983000 -6.94912100 -0.25731500
C -6.72975600 -6.89944100 2.33670500	H 3.33441200 -5.80440000 -1.54075500
C 6.29200800 5.58727300 -0.58198400	H 3.61192400 -7.50525100 -1.93459300
C -6.25743900 5.61503400 0.58975600	H 6.08923100 -8.03281200 -0.23327400
Si 7.28225700 7.18423800 -0.72712300	H 7.29277000 -7.57466800 -1.45985200
Si -7.16319000 7.26174400 0.72886900	H 5.85674200 -8.49140900 -1.92369400
C 9.04832000 6.67554300 -1.07689000	H 5.08537400 -5.13014900 -3.29768000
C 7.10522100 8.06277000 0.91591600	H 6.71654000 -5.81895600 -3.22233700
C 6.52545200 8.15093600 -2.13965800	H 5.33858600 -6.83974900 -3.67393200
C -7.88433000 7.31839200 2.45467500	H 7.84147400 -6.58909600 2.59661700
C -5.87932200 8.59534500 0.45104600	H 7.14209600 -5.34321800 3.64458200
C -8.48093100 7.25459100 -0.59938200	H 8.84182200 -5.81638100 3.83236700

H 7.95053000 -2.92625000 3.48574200
 H 9.62074200 -3.48851300 3.60331900
 H 9.14149200 -2.46597000 2.24527100
 H 10.06881600 -4.23628500 0.64841800
 H 9.58151700 -5.93102800 0.81459400
 H 10.55483400 -5.16871300 2.07716200
 H -7.19450400 -4.82942100 -3.76420900
 H -7.56474300 -3.10717600 -3.56911800
 H -8.78585400 -4.20122500 -4.23164500
 H -8.42026400 -6.57708800 -2.36384600
 H -9.96071400 -5.84425800 -2.82041600
 H -9.57357400 -6.06462800 -1.11064000
 H -9.24786200 -2.36009700 -1.77673000
 H -10.44808800 -3.46656400 -2.45245200
 H -10.02151100 -3.57211500 -0.73444300
 H -3.45896200 -5.84146500 1.90226100
 H -4.61730100 -5.35712700 3.16434400
 H -4.11108700 -7.04327400 3.02140500
 H -4.23392100 -7.29878900 -0.05011000
 H -5.90114100 -7.89393200 -0.11233400
 H -4.80896600 -8.47233600 1.15058400
 H -7.05534400 -6.10099600 3.01116100
 H -6.46146200 -7.77127400 2.94207900
 H -7.57955500 -7.18014000 1.70737400
 H 9.45755300 6.06490600 -0.26643000
 H 7.49423300 7.45785400 1.73987800
 H 6.57729400 7.59600400 -3.08071600
 H -7.10536500 7.25744100 3.21995900
 H -5.08757600 8.55266000 1.20504400
 H -8.04702800 7.15360000 -1.59823700
 H 5.47848500 8.39946600 -1.94316600
 H 7.07079800 9.09067700 -2.27643900

H 9.68107800 7.56393700 -1.17377000
 H -6.34729000 9.58303600 0.51771700
 H -9.03761600 8.19722000 -0.57095400
 H -9.19713200 6.44121900 -0.45135100
 H -8.59501200 6.50404600 2.62187700
 H 9.12615300 6.11016900 -2.01028800
 H 7.67159700 8.99981400 0.89366900
 H 6.06178200 8.30895000 1.13246100
 H -8.42003200 8.26282500 2.59762400
 H -5.42156000 8.51187000 -0.53911100

tips-OR-4 (neutral state)

C 8.93719100 -5.74055700 -0.38227600
 C 7.53992500 -5.68642600 -0.41366500
 C 6.87026700 -4.46544800 -0.35937100
 C 7.64406900 -3.26122600 -0.30555400
 C 9.06446100 -3.32656000 -0.26903700
 C 9.69190300 -4.58680600 -0.30223100
 C 7.00473500 -1.99064300 -0.30046400
 C 7.75167400 -0.79301200 -0.23591800
 C 9.18324500 -0.86346400 -0.18540200
 C 9.81997100 -2.10366000 -0.20622200
 C 7.08893400 0.46892100 -0.21748800
 C 7.84374500 1.68714900 -0.13745100
 C 9.27966200 1.57082900 -0.09373700
 C 9.91313000 0.37457400 -0.11700800
 C 5.41362700 -4.36971600 -0.38935200
 C 4.82967500 -3.14442300 -0.40785300
 C 5.58440100 -1.92618600 -0.36386400
 C 4.95570800 -0.69592500 -0.35119900
 C 5.66932500 0.50856500 -0.27322200
 C 4.99150800 1.78398800 -0.23224800

C 4.52001800 -5.56022100 -0.37039100	C 2.82279900 -9.74712500 1.71911000
C 3.47118400 -5.64225000 -1.29790100	C 5.25045400 -9.22289100 1.79584500
C 2.52066200 -6.65628000 -1.22846000	C 3.62712100 -7.90580800 3.18984800
C 2.65328000 -7.61201900 -0.20916600	C 12.46293200 -2.22844700 -0.13119400
C 3.69618600 -7.57771400 0.71497200	C 6.46980100 8.96041600 0.24146500
C 4.62336500 -6.53136700 0.62224200	Si 14.30547500 -2.28186200 -0.07195500
C 1.32942900 -6.73426500 -2.18995100	Si 7.35210400 10.57691300 0.34421000
C 3.84107700 -8.60852800 1.83852800	C 14.82922300 -3.53959700 1.22126500
C 11.24589400 -2.17057400 -0.16549900	C 14.95250900 -2.77557400 -1.76501600
C 3.59650500 1.86559300 -0.27234700	C 14.92321100 -0.56888100 0.39099900
C 2.92649600 3.07441100 -0.19243400	C 6.05874600 11.93993100 0.35735100
C 3.66198700 4.28652100 -0.08400400	C 8.36275600 10.61649000 1.92710200
C 5.07302900 4.23829200 -0.06611700	C 8.47296200 10.75049200 -1.15327000
C 5.75025900 2.98464600 -0.13296500	C -1.36849700 3.14278100 0.12670800
C 1.50591500 3.12129900 -0.19183200	C -2.79018500 3.12149000 0.13019600
C 0.81205000 4.28711700 -0.05991200	C -3.50116400 4.35089000 0.05202700
C 1.53267300 5.54150700 -0.00442300	C -2.77677700 5.57294500 0.00019700
C 2.96105400 5.52025000 -0.00475300	C -1.34860300 5.56787400 -0.00065300
C 5.81022200 5.46369500 0.02533900	C -3.48484200 1.92409000 0.18742800
C 7.24526100 5.37881400 0.04634600	C -4.88203000 1.87073400 0.15554300
C 7.88576200 4.18650000 -0.00895600	C -5.61490500 3.09018500 0.08073500
C 7.18165700 2.93108900 -0.09599300	C -4.91277000 4.33120900 0.03668000
C 3.69652100 6.73194900 0.07339100	C -3.48818100 6.80044200 -0.04882600
C 5.12973000 6.68272900 0.08852100	C -2.74480100 7.99924000 -0.08267100
C 0.83889200 6.76404200 0.03435200	C -1.36985000 7.98245000 -0.05781000
C 1.60024800 7.95285100 0.11126500	C -0.63153300 6.77793100 -0.00992800
C 2.97544300 7.94353300 0.13612500	C -5.62519000 5.57341200 -0.02695500
C 5.86069500 7.90712200 0.17145000	C -4.92134000 6.77998300 -0.06441000
C -0.65277000 4.29890900 0.02338500	C -7.04688200 3.06949900 0.04600900
C 1.42231100 -5.69275600 -3.31035100	C -7.72562900 4.34030200 -0.01447200
C 1.25800200 -8.12700300 -2.83747300	C -7.06143500 5.51987000 -0.04657500
C 0.03690200 -6.47655600 -1.39696900	C -5.63241400 8.01770700 -0.11981700

C -5.58915200 0.60907800 0.18484900
C -4.90641200 -0.61531300 0.25457400
C -5.56583300 -1.83092700 0.26358700
C -6.98848600 -1.85699000 0.20134900
C -7.70439100 -0.64011600 0.14230200
C -7.00996800 0.60463900 0.13196100
C -6.23634900 9.07526200 -0.16633400
Si -7.17664800 10.66105500 -0.22326200
C -7.11359500 11.34174700 -1.97286300
C -8.95217400 10.30450600 0.27708100
C -6.38637300 11.86909200 0.97867700
C -4.84532700 -3.07255200 0.31109000
C -5.46669200 -4.27948600 0.29692500
C -6.92558500 -4.33332400 0.26538900
C -7.66443500 -3.10889800 0.20741500
C -9.13784300 -0.67292500 0.09258300
C -9.83730200 0.58233900 0.03042400
C -9.17430900 1.76192800 0.01865200
C -7.73634000 1.84098300 0.06687700
C -9.08613200 -3.13645600 0.17209300
C -9.80834700 -1.89462300 0.10964900
C -7.62881900 -5.53522600 0.32609800
C -9.02668900 -5.55200800 0.29407000
C -9.74879500 -4.37824500 0.20896800
C -4.63139600 -5.51244100 0.30834700
C -11.23558900 -1.92241400 0.06835300
C -4.76193600 -6.48342400 -0.69642100
C -3.93316900 -7.60061300 -0.72564000
C -2.96255000 -7.73227700 0.28155500
C -2.80730100 -6.79301200 1.29773000
C -3.65736500 -5.67786000 1.28900200
C -4.04897700 -8.68793200 -1.79921900

C -1.78098000 -6.94794300 2.42585400
C -0.96554700 -8.23929300 2.30129500
C -0.80336700 -5.76109700 2.40888200
C -2.52066100 -6.97917300 3.77487500
C -5.18210800 -8.40300500 -2.79025100
C -2.73121200 -8.77931400 -2.58684600
C -4.33255800 -10.04013900 -1.12231300
C -12.45375400 -1.94585300 0.03338800
Si -14.29707300 -1.94285200 -0.02712200
C -14.95990000 -2.43816900 1.65936300
C -14.86155000 -0.20587100 -0.46817900
C -14.85805200 -3.16737500 -1.33652100
H 9.43317100 -6.70524300 -0.42472600
H 6.96865000 -6.60545600 -0.49231400
H 10.77554300 -4.63376500 -0.27401100
H 9.88411400 2.46774600 -0.03845200
H 10.99664300 0.32671200 -0.08124400
H 3.74504600 -3.06907200 -0.41292100
H 3.87331700 -0.69408500 -0.39450500
H 3.41914400 -4.88567600 -2.07348700
H 1.91392200 -8.40394800 -0.14322800
H 5.42228700 -6.44501000 1.35460000
H 2.99208900 0.97033600 -0.35255700
H 0.98965300 2.17333900 -0.29494100
H 7.81029500 6.30289800 0.11150400
H 8.96854400 4.18776400 0.01415300
H 1.09903800 8.91211200 0.16322400
H 3.52535800 8.87692200 0.20245600
H 0.56865800 -5.80677300 -3.98610000
H 1.39837900 -4.67136000 -2.91669900
H 2.33784000 -5.81500400 -3.89871800
H 0.40463900 -8.17665100 -3.52361800

H 1.12986800 -8.91842400 -2.09253100	H -9.75589300 2.67389900 -0.03176500
H 2.16953800 -8.34070300 -3.40512800	H -7.08357200 -6.46902900 0.41024100
H 0.06498900 -5.49317400 -0.91522600	H -9.54885500 -6.50256500 0.34092600
H -0.83731700 -6.50785700 -2.05679500	H -10.83331700 -4.39448500 0.18109500
H -0.11205800 -7.23026700 -0.61585900	H -5.51623000 -6.33255200 -1.46170500
H 2.99249800 -10.47399100 2.52000500	H -2.31706400 -8.60488700 0.26348700
H 1.79444100 -9.38332100 1.81548900	H -3.57780100 -4.92436300 2.06879200
H 2.91677300 -10.27191400 0.76223800	H -0.25734900 -8.30448500 3.13455800
H 5.36280000 -9.96287600 2.59594700	H -1.60419500 -9.12849800 2.33392900
H 6.03002500 -8.46692300 1.93008700	H -0.38495700 -8.26281800 1.37157500
H 5.42528600 -9.72364500 0.83779100	H -0.10213200 -5.83966400 3.24757600
H 2.62656500 -7.46182100 3.23712000	H -1.32793400 -4.80482100 2.49898500
H 3.72649600 -8.62355200 4.01204000	H -0.22300300 -5.74762800 1.48052300
H 4.35831400 -7.10675600 3.34673300	H -3.23069800 -7.81187400 3.80852800
H 14.45542300 -4.53826400 0.97581300	H -1.80415200 -7.10296000 4.59453600
H 14.58183200 -3.76250400 -2.05757900	H -3.07701100 -6.05407800 3.95223000
H 16.01734600 -0.55267000 0.43787100	H -5.23188100 -9.20766000 -3.53085800
H 5.38951800 11.83799400 1.21716400	H -6.15349000 -8.35034200 -2.28681800
H 7.72177400 10.50101300 2.80612500	H -5.02147400 -7.46310100 -3.32842900
H 9.21768100 9.94952200 -1.18478100	H -2.78724100 -9.58619200 -3.32642500
H -0.86929700 2.18343900 0.20596500	H -1.87751700 -8.98054900 -1.93080800
H -2.89866400 1.01470600 0.24422500	H -2.53384900 -7.84196800 -3.11838100
H -3.27773500 8.94353800 -0.12590600	H -5.26220300 -9.99635600 -0.54555600
H -0.85047900 8.93296500 -0.08644500	H -4.43321500 -10.82641100 -1.87874800
H -8.80803200 4.36452100 -0.03325300	H -3.52656300 -10.33083000 -0.44180300
H -7.60748000 6.45665600 -0.08999000	H -14.62755900 -1.73998900 2.43330800
H -3.82406000 -0.63947400 0.29962300	H -14.52242500 0.51925600 0.27803100
H -7.55759600 10.63955700 -2.68471000	H -15.95133500 -3.18719900 -1.40041600
H -9.41621500 9.58458400 -0.40410600	H -9.55047000 11.22168300 0.25681400
H -6.40493100 11.47674500 1.99976600	H -8.99997200 9.89192200 1.28932700
H -3.75864900 -3.03123200 0.32366800	H -7.66661500 12.28508100 -2.03739200
H -10.92150300 0.56117600 -0.00838300	H -6.92326800 12.82377500 0.97235000

H -5.34368400 12.06712000 0.71232100	C 7.08406800 0.46070400 -0.17499700
H -6.08276300 11.53208500 -2.28616500	C 7.83567500 1.67506800 -0.12092300
H 6.53477400 12.92463200 0.41472000	C 9.26068400 1.57172100 -0.08376400
H 9.00624000 11.70682000 -1.12449100	C 9.90131000 0.36962300 -0.09764400
H 5.44956600 11.91190400 -0.55126500	C 5.42525100 -4.38211400 -0.32428400
H 7.89680500 10.71155400 -2.08246100	C 4.83595700 -3.15495300 -0.34329400
H 8.89534100 11.56928100 2.01847100	C 5.58734500 -1.94063200 -0.30150600
H 9.10446800 9.81229500 1.94304800	C 4.95187200 -0.70369800 -0.28594000
H 14.60648500 0.17588600 -0.34565000	C 5.65824200 0.49412200 -0.21301800
H 14.64054400 -2.05835000 -2.52998600	C 4.97742700 1.77601600 -0.16712500
H 16.04725700 -2.81269200 -1.76126800	C 4.53590400 -5.57454700 -0.30573200
H 15.92141200 -3.59395600 1.28376700	C 3.48942300 -5.65687900 -1.23607300
H 14.53845500 -0.26298400 1.36855200	C 2.54330300 -6.67481400 -1.16920100
H 14.44632200 -3.26995000 2.20998100	C 2.67648200 -7.62798400 -0.14722700
H -14.46596900 -2.89718900 -2.32148300	C 3.71550900 -7.59130400 0.78105900
H -14.51544400 -4.18009100 -1.10345100	C 4.64156300 -6.54343000 0.68876000
H -14.46696700 0.10054300 -1.44165200	C 1.35708000 -6.76055800 -2.13599000
H -15.95463000 -0.15527900 -0.51505000	C 3.85873400 -8.62095200 1.90571900
H -16.05526300 -2.44294700 1.65466100	C 11.24728400 -2.16623300 -0.13785500
H -14.61876900 -3.43915500 1.93986700	C 3.59629700 1.85466000 -0.16159400

tips-OR-4 (radical cation state)

C 8.95131400 -5.74369900 -0.32929400	C 3.65294900 4.29176800 -0.06505600
C 7.55501200 -5.69031500 -0.35537400	C 5.06632200 4.24318600 -0.07146700
C 6.87863100 -4.46915200 -0.29824300	C 5.74322400 2.98702400 -0.11482000
C 7.64826900 -3.26546800 -0.25058900	C 1.51414100 3.11623500 -0.08743600
C 9.07001900 -3.32753000 -0.22208100	C 0.81039300 4.30012900 -0.02092900
C 9.70249100 -4.58603200 -0.25495900	C 1.52947400 5.54341800 -0.00168400
C 7.00448000 -1.99918300 -0.24499400	C 2.95624200 5.52305000 -0.01773800
C 7.74932600 -0.79794700 -0.19118300	C 5.80319600 5.46331700 -0.03006800
C 9.17718000 -0.86102200 -0.15174300	C 7.22739100 5.38495700 -0.03027100
C 9.82382300 -2.10705500 -0.16970300	C 7.86939600 4.18351500 -0.06149600
	C 7.16304100 2.93984800 -0.10122000

C 3.69667400 6.73892500 0.01429900	C -3.47834900 6.81053900 0.03333800
C 5.11419400 6.69724500 0.00879300	C -2.72730700 8.01843600 0.02004900
C 0.83093400 6.77696000 0.02793400	C -1.36125500 8.00466000 0.01900100
C 1.60359000 7.97471200 0.05726300	C -0.61352100 6.79112300 0.02500500
C 2.96980500 7.96134500 0.05366300	C -5.61003500 5.57896700 0.04764000
C 5.85117000 7.91921300 0.04392000	C -4.89578900 6.79873500 0.03355800
C -0.64446500 4.31345300 0.02560800	C -7.02312800 3.08667200 0.06514200
C 1.44955500 -5.71974400 -3.25703500	C -7.70272500 4.34567400 0.04801500
C 1.29671900 -8.15469200 -2.78171700	C -7.03540100 5.53298800 0.04295500
C 0.05977400 -6.50883900 -1.34856100	C -5.61102000 8.03403400 0.01745400
C 2.83425100 -9.75431300 1.79007600	C -5.57672300 0.60275400 0.15138400
C 5.26547400 -9.24120900 1.85887400	C -4.90278500 -0.61543100 0.22236600
C 3.65218300 -7.91543900 3.25688200	C -5.57017300 -1.83714600 0.22277600
C 12.46496300 -2.21573400 -0.11104700	C -6.98867000 -1.85597300 0.14946900
C 6.47128700 8.96766300 0.07286800	C -7.70088000 -0.63484800 0.09680000
Si 14.32079400 -2.26844600 -0.06492500	C -7.00301400 0.60589700 0.10025600
Si 7.37828400 10.58547800 0.11464700	C -6.22498400 9.08640100 0.00374800
C 14.83074000 -3.53328300 1.22275000	Si -7.18489600 10.67387500 -0.00742000
C 14.92911300 -2.75652800 -1.77081400	C -7.13639100 11.37556900 -1.74670900
C 14.92214900 -0.55269600 0.39961100	C -8.94517800 10.27396200 0.50590600
C 6.08970000 11.95012200 0.13366900	C -6.37968000 11.84829100 1.21424800
C 8.42605300 10.62978400 1.67022400	C -4.85445800 -3.07578900 0.27167800
C 8.44967800 10.69513300 -1.42152800	C -5.48202900 -4.28364800 0.24275400
C -1.37212100 3.14225700 0.06896000	C -6.93700300 -4.32744300 0.19643000
C -2.77613900 3.13047200 0.08740400	C -7.67008200 -3.10288800 0.14192000
C -3.48558900 4.36101600 0.06654500	C -9.12989800 -0.65913400 0.04087700
C -2.76380500 5.57891900 0.04369500	C -9.82218400 0.58932200 -0.01066400
C -1.33722400 5.57136900 0.02995500	C -9.15098100 1.77387600 -0.00212800
C -3.48192100 1.92025400 0.11919700	C -7.72470400 1.83887400 0.05539500
C -4.86501700 1.87023600 0.12300500	C -9.09262000 -3.12590600 0.09671100
C -5.60298300 3.10011500 0.08745100	C -9.81159100 -1.88571600 0.04177100
C -4.89951900 4.34232900 0.06865900	C -7.64853800 -5.52915100 0.24421200

C -9.04496200 -5.54399000 0.20025300	H 2.98848300 0.95829300 -0.18853500
C -9.76157200 -4.36539700 0.11852200	H 1.00031100 2.16330100 -0.13054400
C -4.65371600 -5.52023100 0.25715400	H 7.79498500 6.30907700 -0.00237300
C -11.23572200 -1.90443600 -0.00797600	H 8.95208300 4.18628600 -0.05845600
C -4.77433100 -6.48074400 -0.75866900	H 1.10553400 8.93556600 0.08906300
C -3.95240700 -7.60345200 -0.78171500	H 3.52532000 8.89320100 0.08062200
C -3.00375400 -7.74952100 0.24430900	H 0.59972900 -5.83908500 -3.93640100
C -2.86094600 -6.82117200 1.27258700	H 1.41842100 -4.69767900 -2.86489400
C -3.69980900 -5.69778100 1.25536100	H 2.36756100 -5.83835600 -3.84217900
C -4.05371900 -8.68056100 -1.86674400	H 0.44777900 -8.20934600 -3.47262700
C -1.86212700 -6.99737600 2.42200600	H 1.16817900 -8.94590100 -2.03677000
C -1.05674000 -8.29558600 2.30289400	H 2.21197500 -8.36484100 -3.34435100
C -0.87399100 -5.81919200 2.43921400	H 0.07995600 -5.52429700 -0.86836700
C -2.63315100 -7.03474300 3.75333200	H -0.81072900 -6.54688200 -2.01276300
C -5.16465000 -8.37920600 -2.87782500	H -0.08837800 -7.26208200 -0.56688400
C -2.72034000 -8.77266400 -2.62786500	H 3.00020800 -10.47902100 2.59326100
C -4.35898400 -10.03662500 -1.20702700	H 1.80777300 -9.38465500 1.88589700
C -12.45388200 -1.91791300 -0.05019100	H 2.92515500 -10.28398000 0.83570600
Si -14.30970700 -1.91140100 -0.11982400	H 5.37647900 -9.98158700 2.65830000
C -14.95467600 -2.40367800 1.57139100	H 6.04868700 -8.48866600 1.99308700
C -14.85008700 -0.17080200 -0.56668800	H 5.43634200 -9.74299700 0.90076000
C -14.84314200 -3.14106900 -1.43180200	H 2.65364600 -7.46750000 3.30832200
H 9.44904000 -6.70674100 -0.37312400	H 3.75131500 -8.63334100 4.07847500
H 6.98456900 -6.61014700 -0.43189100	H 4.38783800 -7.12010100 3.41246300
H 10.78638800 -4.62915900 -0.23227700	H 14.45488300 -4.52972300 0.97194300
H 9.86367900 2.46952300 -0.03920900	H 14.55346500 -3.74241000 -2.06004700
H 10.98529300 0.32800600 -0.06631900	H 16.01617100 -0.53010800 0.44214600
H 3.75139900 -3.08490300 -0.34701500	H 5.44504900 11.87246800 1.01448000
H 3.86952100 -0.70813800 -0.33020400	H 7.80717300 10.53711900 2.56749900
H 3.43734000 -4.90220700 -2.01360200	H 9.18440600 9.88508200 -1.45257300
H 1.93939900 -8.42190200 -0.08238800	H -0.87679800 2.17890100 0.09422300
H 5.43684000 -6.45458800 1.42491800	H -2.89394000 1.01007600 0.12950100

H -3.26453000 8.96108200 0.01137900
 H -0.84365800 8.95556700 0.00751100
 H -8.78491000 4.37211300 0.04395600
 H -7.58266600 6.46977600 0.03345400
 H -3.82123700 -0.64660100 0.28087600
 H -7.58035800 10.68151600 -2.46638800
 H -9.40846600 9.56562300 -0.18778600
 H -6.38080400 11.42998000 2.22508200
 H -3.76819200 -3.04072300 0.29668500
 H -10.90626400 0.57537600 -0.05731200
 H -9.72976100 2.68729600 -0.04609000
 H -7.10576000 -6.46458500 0.32724300
 H -9.57003200 -6.49271000 0.23661300
 H -10.84588700 -4.37680400 0.08258500
 H -5.51100200 -6.31831300 -1.53879100
 H -2.36580400 -8.62756600 0.23240700
 H -3.62997700 -4.95230800 2.04377800
 H -0.36812100 -8.37524700 3.15088100
 H -1.70446200 -9.17848800 2.31454600
 H -0.45619300 -8.31813600 1.38590500
 H -0.19168600 -5.91455100 3.29142300
 H -1.39178400 -4.85917900 2.53113600
 H -0.27440300 -5.79957600 1.52316100
 H -3.35204000 -7.86021700 3.76254100
 H -1.93704800 -7.17508500 4.58744200
 H -3.18343400 -6.10553200 3.92886100
 H -5.20410200 -9.17637600 -3.62659400
 H -6.14620700 -8.32703000 -2.39428700
 H -4.98774100 -7.43568800 -3.40473400
 H -2.76705300 -9.57195300 -3.37578000
 H -1.88174200 -8.98721200 -1.95666700
 H -2.50592400 -7.83195600 -3.14700900

H -5.29950500 -9.99303900 -0.64828000
 H -4.44988000 -10.81478400 -1.97250700
 H -3.56829400 -10.33977100 -0.51419600
 H -14.62020400 -1.70371700 2.34265700
 H -14.51347500 0.55267900 0.18219000
 H -15.93527800 -3.16331900 -1.50976000
 H -9.55665900 11.18237200 0.51540200
 H -8.97521300 9.83783600 1.50888100
 H -7.69804000 12.31466300 -1.79291500
 H -6.92232900 12.79913100 1.24206100
 H -5.34309500 12.06189200 0.93659300
 H -6.10991200 11.58140900 -2.06417800
 H 6.57230100 12.93284900 0.15636500
 H 8.99511500 11.64469400 -1.43717900
 H 5.45643000 11.90779300 -0.75772700
 H 7.84475000 10.63864600 -2.33123400
 H 8.97238000 11.57686600 1.73333900
 H 9.15922500 9.81779200 1.67924000
 H 14.60015600 0.19196200 -0.33479100
 H 14.60713300 -2.03577500 -2.52812600
 H 16.02352200 -2.79543300 -1.78563200
 H 15.92248900 -3.59218600 1.28554900
 H 14.54158500 -0.25175300 1.38027200
 H 14.45012700 -3.26654400 2.21303600
 H -14.44063500 -2.87336200 -2.41313200
 H -14.50328900 -4.15258800 -1.19018000
 H -14.44789400 0.13147700 -1.53827400
 H -15.94219400 -0.11224300 -0.62196900
 H -16.04986100 -2.40882200 1.57233200
 H -14.61333500 -3.40460900 1.85131200

tips-OR-4 (dication state)

C 8.99766500 -5.72972700 -0.32570600
C 7.60074900 -5.67976400 -0.35005400
C 6.91337100 -4.46257700 -0.28518400
C 7.67440600 -3.25641000 -0.23994500
C 9.09713000 -3.31140100 -0.21438800
C 9.73987500 -4.56673100 -0.24941000
C 7.02236900 -1.99738000 -0.23587000
C 7.76028100 -0.79171300 -0.18528600
C 9.18495600 -0.84404200 -0.14896100
C 9.84542500 -2.09189900 -0.16563800
C 7.08833200 0.46195300 -0.17075900
C 7.83287800 1.67435800 -0.12938800
C 9.25190300 1.58650400 -0.09232100
C 9.90148100 0.38294900 -0.10032800
C 5.46202900 -4.38969300 -0.30869900
C 4.86355800 -3.16158900 -0.33513900
C 5.60705600 -1.94882600 -0.29480800
C 4.96047500 -0.70698800 -0.27973700
C 5.65604300 0.48683500 -0.20254200
C 4.96951100 1.77393900 -0.14811600
C 4.58349600 -5.58680600 -0.27986200
C 3.52451200 -5.67266800 -1.19657000
C 2.59123400 -6.70105500 -1.12083000
C 2.74742100 -7.65412000 -0.10135900
C 3.79553800 -7.61066600 0.81610100
C 4.71276600 -6.55578100 0.71239800
C 1.39607000 -6.80159000 -2.07477100
C 3.96124800 -8.64116000 1.93670900
C 11.26560200 -2.13988500 -0.13672100
C 3.59996800 1.84774100 -0.11006700
C 2.90830000 3.08043500 -0.06586200
C 3.64281200 4.29454600 -0.06008800

C 5.05845800 4.24783200 -0.08612700
C 5.73801200 2.99312100 -0.12141600
C 1.51779400 3.10996900 -0.02976000
C 0.80636300 4.30601900 0.00955900
C 1.52344400 5.53980500 0.00780200
C 2.94817700 5.52295200 -0.02367800
C 5.79300000 5.46436700 -0.07299200
C 7.20817700 5.39470100 -0.09110800
C 7.85506400 4.18782200 -0.11149700
C 7.14934400 2.95365300 -0.12312500
C 3.69087700 6.74383000 -0.01844700
C 5.09490700 6.71057700 -0.04219300
C 0.81828400 6.78382800 0.03620700
C 1.59913800 7.98948600 0.03854800
C 2.95712200 7.97421000 0.01392500
C 5.83660800 7.92863700 -0.03455000
C -0.64129600 4.31931100 0.04804900
C 1.45573500 -5.74952100 -3.18737500
C 1.35675100 -8.19171700 -2.73088500
C 0.10312400 -6.58164900 -1.27007700
C 2.92397600 -9.76528700 1.84869700
C 5.36188400 -9.27102200 1.84863700
C 3.79875900 -7.93531400 3.29385500
C 12.48433500 -2.17962900 -0.11248000
C 6.46536800 8.97243100 -0.02856700
Si 14.35578800 -2.22652000 -0.07324500
Si 7.38583400 10.59323200 -0.02027600
C 14.84813200 -3.49854800 1.21007800
C 14.92728400 -2.70793700 -1.79079300
C 14.93304500 -0.50658100 0.39505100
C 6.09633700 11.95479000 -0.00884200
C 8.44344400 10.64087500 1.52655500

C 8.43644900 10.66010500 -1.57116200	C -5.51726700 -4.29102100 0.24469300
C -1.37658400 3.13652400 0.06799800	C -6.96834900 -4.32164100 0.16851100
C -2.76802200 3.13283000 0.09591900	C -7.69278900 -3.09534100 0.10901200
C -3.47676300 4.36267500 0.10283900	C -9.13427900 -0.64504500 -0.00049300
C -2.75740900 5.57764100 0.09022200	C -9.81905300 0.59926200 -0.05422900
C -1.33275800 5.56718200 0.06591400	C -9.14029800 1.78546900 -0.02327000
C -3.48628900 1.91330500 0.11665900	C -7.72171400 1.83590800 0.05948100
C -4.85797400 1.86717900 0.14066200	C -9.11496300 -3.11230500 0.03706500
C -5.59881600 3.10455500 0.12029000	C -9.82858500 -1.87354700 -0.02093000
C -4.89307100 4.34527700 0.11426200	C -7.69045800 -5.52026400 0.19904000
C -3.47458400 6.81364200 0.09892200	C -9.08614700 -5.53271000 0.12744900
C -2.71676000 8.02939100 0.09240800	C -9.79309500 -4.34906200 0.03822700
C -1.35879400 8.01833900 0.07452200	C -4.69972600 -5.53210300 0.25877500
C -0.60263100 6.79740300 0.05866100	C -11.24798200 -1.88209400 -0.09541500
C -5.60187100 5.57749300 0.11319200	C -4.81687300 -6.48096300 -0.76875900
C -4.87860800 6.80932300 0.10962700	C -4.00536100 -7.61144000 -0.78997300
C -7.01024400 3.09773500 0.09713500	C -3.07700400 -7.77630100 0.25175800
C -7.69005300 4.34648000 0.10281300	C -2.94072100 -6.86060200 1.29280800
C -7.01827000 5.53906900 0.11549000	C -3.76311600 -5.72551900 1.27084800
C -5.59910600 8.04012500 0.11334700	C -4.09781100 -8.67582400 -1.88797400
C -5.57535800 0.59436300 0.17078200	C -1.96647000 -7.06282800 2.45874000
C -4.91273600 -0.61898700 0.25961100	C -1.18206900 -8.37417800 2.34333100
C -5.59031300 -1.84582800 0.24378800	C -0.96016100 -5.90067900 2.50158400
C -7.00472000 -1.85548100 0.13855400	C -2.76185100 -7.09687500 3.77583000
C -7.70998400 -0.63052300 0.07955400	C -5.18494500 -8.35050300 -2.91727800
C -7.00680300 0.60537600 0.10090200	C -2.75005400 -8.77406400 -2.62297500
C -6.22327800 9.08666600 0.11614500	C -4.43064800 -10.03500300 -1.24807100
Si -7.19874600 10.67486300 0.12869900	C -12.46593300 -1.88638400 -0.15859300
C -7.14464900 11.39082200 -1.60276400	Si -14.33575100 -1.87494700 -0.25713200
C -8.95199000 10.24115600 0.63351700	C -14.97571000 -2.37523200 1.43067200
C -6.39506500 11.82475600 1.37175900	C -14.84498100 -0.12799700 -0.70420100
C -4.88250000 -3.08252400 0.30163900	C -14.82540400 -3.10297000 -1.58359100

H 9.49954600 -6.68975600 -0.37435500	H 3.91472600 -8.65622100 4.11006900
H 7.03471800 -6.60226300 -0.43166800	H 4.54607400 -7.14768800 3.43269200
H 10.82423600 -4.60204800 -0.22864800	H 14.47415400 -4.49358000 0.95152100
H 9.84943500 2.48734800 -0.05176700	H 14.55001500 -3.69388500 -2.07711900
H 10.98603100 0.34947800 -0.06928500	H 16.02678300 -0.47473100 0.43655600
H 3.77896300 -3.10028000 -0.33853500	H 5.46030000 11.89160400 0.87931500
H 3.87850200 -0.71964500 -0.32992100	H 7.83175500 10.56161700 2.42995400
H 3.45535600 -4.91863100 -1.97347200	H 9.16648000 9.84563200 -1.59495800
H 2.01912500 -8.45513300 -0.02894500	H -0.88097500 2.17321700 0.06496700
H 5.51404400 -6.46098500 1.44138500	H -2.89916700 1.00198000 0.10283600
H 2.99309500 0.94972100 -0.10590100	H -3.25769500 8.96978900 0.10173700
H 1.00399700 2.15632200 -0.03806100	H -0.84159000 8.96889700 0.06936500
H 7.77462600 6.31974900 -0.08561100	H -8.77203300 4.37652000 0.10418600
H 8.93751500 4.19510200 -0.12330600	H -7.56482400 6.47612300 0.12389500
H 1.10125300 8.95003000 0.06279500	H -3.83329300 -0.65731700 0.34557500
H 3.51602200 8.90430200 0.01836500	H -7.58089300 10.70246300 -2.33247100
H 0.59918500 -5.87742300 -3.85635700	H -9.40783000 9.54140400 -0.07369300
H 1.41271900 -4.73123300 -2.78582500	H -6.39330200 11.38829900 2.37483100
H 2.36659500 -5.84814100 -3.78711700	H -3.79728400 -3.05560600 0.35053800
H 0.50052300 -8.25839800 -3.41131200	H -10.90245800 0.59285200 -0.12061700
H 1.25460200 -8.99142700 -1.99114800	H -9.71330400 2.70157900 -0.07113700
H 2.26820700 -8.37824100 -3.30748900	H -7.15281000 -6.45826700 0.29041700
H 0.10880200 -5.59993200 -0.78345900	H -9.61504600 -6.47908800 0.14999900
H -0.77269300 -6.63302000 -1.92610900	H -10.87671900 -4.35346300 -0.01841600
H -0.02110700 -7.34322300 -0.49227400	H -5.53603900 -6.30287600 -1.56185800
H 3.10076300 -10.48735200 2.65148500	H -2.45014300 -8.66208600 0.24319000
H 1.90330300 -9.38511900 1.96535300	H -3.69803400 -4.98937300 2.06838900
H 2.98919800 -10.30187400 0.89621200	H -0.51060400 -8.47233100 3.20257900
H 5.49090500 -10.01226900 2.64406600	H -1.84551700 -9.24517000 2.33824300
H 6.15341800 -8.52326900 1.96225400	H -0.56647000 -8.40238800 1.43672300
H 5.50248000 -9.77386400 0.88628500	H -0.29054200 -6.01718900 3.36090100
H 2.80617300 -7.47911300 3.37583600	H -1.46374100 -4.93347300 2.59951500

H -0.34931500 -5.87968100 1.59291700
 H -3.49472800 -7.90974300 3.76661500
 H -2.08307900 -7.25651900 4.62031300
 H -3.29817600 -6.15932400 3.95094200
 H -5.21815400 -9.13845600 -3.67554400
 H -6.17588100 -8.29491300 -2.45338400
 H -4.98760900 -7.40346600 -3.43076800
 H -2.79281500 -9.56142600 -3.38315300
 H -1.92886300 -9.01176300 -1.93822300
 H -2.51238400 -7.82908100 -3.12419700
 H -5.38179100 -9.98830000 -0.70797500
 H -4.51442000 -10.80353600 -2.02351500
 H -3.65724000 -10.35490800 -0.54345700
 H -14.64606600 -1.67841000 2.20665900
 H -14.51890800 0.58914600 0.05524800
 H -15.91528000 -3.12685700 -1.68724400
 H -9.57361700 11.14224600 0.65851800
 H -8.97847600 9.78861400 1.62927100
 H -7.71318900 12.32601000 -1.64113400
 H -6.94272300 12.77188100 1.41852900
 H -5.36052700 12.05066000 1.09646300
 H -6.11866800 11.60942900 -1.91300700
 H 6.58029400 12.93700400 -0.00408300
 H 8.98795500 11.60530100 -1.61195500
 H 5.45588100 11.90229600 -0.89449800
 H 7.82070900 10.59150200 -2.47267800
 H 8.99547600 11.58534300 1.57625000
 H 9.17323500 9.82592500 1.53726800
 H 14.60629200 0.23716100 -0.33805900
 H 14.59550100 -1.98432500 -2.54091900
 H 16.02130400 -2.74586300 -1.82193300
 H 15.93944900 -3.55910800 1.27712500

H 14.55333500 -0.21172700 1.37780200
 H 14.46587900 -3.23635300 2.20082800
 H -14.40254800 -2.83225500 -2.55537500
 H -14.49164100 -4.11475300 -1.33523300
 H -14.42534000 0.17587500 -1.66779500
 H -15.93532800 -0.06075300 -0.77896300
 H -16.07080700 -2.38020100 1.42734800
 H -14.63742800 -3.37820700 1.70638800

[tips-OR-3]₂ (neutral radical • radical state, open-shell singlet)

Si -0.48150100 -9.49748100 1.53326100
 Si -12.59994900 -2.11211100 1.90602800
 Si 12.07594200 -2.75440600 1.29110200
 C 3.73775600 1.37200600 1.59944900
 H 2.81291800 1.93742700 1.62727400
 C 3.71982100 -0.02450700 1.57059700
 C 2.51168700 -2.20436700 1.51398400
 C -1.18835100 -2.95354500 1.45270500
 C 1.24556400 -0.12710600 1.49098900
 H 1.18712000 0.95576300 1.47155100
 C -2.41914300 -0.80843400 1.54615100
 C 3.75272200 -2.89550200 1.52927800
 C -3.60232600 -4.37939100 1.41284400
 H -4.52145000 -4.95028100 1.34703200
 C 2.47640700 -0.77058600 1.53638800
 C -1.19882300 -0.14538700 1.50046800
 H -1.15673400 0.93849200 1.50199400
 C 4.92166000 2.09805300 1.57575400
 C 3.72185700 -4.32622000 1.46561000
 H 4.64985900 -4.88804900 1.44108200
 C 1.29080100 -4.36060600 1.41639300

C 5.93031300 5.74713200 1.41791000	C -7.38074800 2.01665400 1.73843600
C 4.97800400 -2.15884500 1.55382400	C -8.58832000 -0.12590700 1.82027100
C 4.96061600 -0.73281700 1.55619800	C -4.95686500 3.43860900 1.49425700
C -2.42860500 -2.24241700 1.51093200	H -4.01417900 3.94772600 1.30590900
C 0.04167100 -2.25032600 1.47017800	C -1.17278800 -4.37728000 1.39452100
C 6.16691100 1.41513000 1.51361800	C 8.63407200 0.04862900 1.36034900
C 6.18352100 0.00010100 1.51781500	C -7.33271600 -2.25838100 1.75635600
C -4.89284000 -2.24730300 1.63050000	H -8.27175000 -2.80404700 1.77746700
C 0.04353600 -6.49217200 1.37920800	C -8.60997700 1.30718700 1.83380900
C -7.37675400 -0.83123400 1.77025500	C 8.62239800 1.48183100 1.36011200
C 1.28272500 -2.93522500 1.46228200	C 5.50068400 8.48296800 1.23301900
C -4.90061200 -0.82194900 1.66027600	H 5.32292000 9.55156700 1.16603100
C 6.04971100 4.26488700 1.48064200	C 6.50500200 8.53690600 -1.13297300
C -3.72541300 1.31048300 1.59737000	C -9.82616700 -0.82783700 1.85558100
H -2.81401500 1.89450200 1.52965600	C 8.54118000 4.29451300 1.36053200
C 0.06559200 -5.06359000 1.38253200	H 8.52608000 5.37960700 1.37611300
C -3.67625900 -0.08664900 1.60600200	C 4.49868200 8.61184100 3.55897100
C -6.13743300 -0.11603300 1.72116300	C 9.76217600 3.61786300 1.28684000
C 7.41952600 -2.11570000 1.47764600	H 10.68323100 4.18997800 1.24328800
H 8.36601000 -2.64716800 1.43032100	C -5.09345800 6.42738700 1.51763400
C -6.15369300 1.29813800 1.69958700	H -4.41903800 6.05925000 2.28605200
C 7.43874200 -0.68578500 1.45283200	C 4.12637900 7.71728900 4.74574000
C -13.02474400 -2.60156900 3.66928300	H 3.38742800 6.96014800 4.46319200
H -14.04535100 -2.99563000 3.72346600	H 3.69067200 8.32943100 5.54189500
C 6.33163500 6.44860200 0.28433900	H 5.00334600 7.20756400 5.15798100
H 6.81338800 5.90018500 -0.52313500	C 5.51233700 9.66186000 4.04491500
C -6.14769600 -2.92520800 1.69590200	H 6.43001100 9.18014000 4.39768100
H -6.16848600 -4.00856300 1.69649500	H 5.08773900 10.24201500 4.87191800
C -2.42448100 -5.05981400 1.34782000	H 5.78242000 10.36060900 3.24709200
H -2.42546900 -6.14080700 1.25447900	C -9.81613200 2.03129500 1.92941600
C 4.90994400 3.53182500 1.57182100	H -10.74977600 1.48239900 2.00286300
H 3.94650900 4.03681300 1.59098000	C 1.06902700 -10.54432600 1.36689900

H 1.47761000 -10.48529100 0.35375500
 C -10.90327200 -1.39959800 1.87188100
 C -8.59828000 4.11681700 1.81197300
 H -8.61074400 5.20181300 1.82146100
 C 3.22469800 9.32045900 3.07194200
 H 3.43452600 10.01977500 2.25652600
 H 2.77151100 9.88761800 3.89299500
 H 2.49180200 8.59190900 2.70916200
 C -4.96587300 7.73247700 1.03722300
 C 10.85451900 -1.37654400 1.22226100
 C -6.84995900 7.32416500 -0.47004500
 C 6.15314800 10.02781000 -1.11023400
 H 5.07565400 10.18619500 -0.98898600
 H 6.45458800 10.48916900 -2.05609400
 H 6.67304600 10.55282100 -0.30192900
 C -3.84834800 8.63115900 1.57822800
 C -2.50008200 8.09154900 1.07077200
 H -2.34524500 7.04759100 1.36469200
 H -1.66907000 8.68388300 1.47528800
 H -2.44744900 8.14042800 -0.02226700
 C 8.02243000 8.39864900 -1.34119100
 H 8.56990100 8.86271600 -0.51427800
 H 8.32358500 8.89038000 -2.27294400
 H 8.32721500 7.34905700 -1.40135800
 C -13.76153300 -0.77724500 1.27519900
 H -13.45076600 -0.46008000 0.27341600
 C -7.82999700 7.76699100 -1.56080800
 C -3.99816500 10.08377100 1.11233200
 H -3.91383200 10.17499200 0.02448400
 H -3.20323400 10.69330400 1.55571100
 H -4.95965300 10.50748500 1.42237500
 C -9.25700100 7.74923500 -0.98706400

H -9.53243000 6.75074900 -0.63200900
 H -9.97993500 8.04306700 -1.75691900
 H -9.34519300 8.44590500 -0.14673300
 C -3.86016000 8.62515800 3.11585700
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 H -3.07820400 9.29134300 3.49652500
 H -3.67199400 7.62903000 3.52553800
 C 13.17700100 -2.79315100 -0.23144000
 H 12.59664900 -2.74652200 -1.15741000
 C -7.52919900 9.17866400 -2.07386200
 H -7.61900300 9.92539700 -1.27793000
 H -8.24424300 9.44259400 -2.85961800
 H -6.52223900 9.24593100 -2.49947900
 C -3.65565200 -2.95533600 1.52961900
 C 0.02889700 -0.82623100 1.49677500
 C -12.69399200 -3.61119900 0.77698100
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 C 2.55328100 -5.02566600 1.40917500
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 C -7.74856600 6.79338500 -2.74942100
 H -6.73302600 6.76212800 -3.15897500
 H -8.43059800 7.11214000 -3.54556900
 H -8.03024900 5.77522600 -2.46093500
 C 7.33864100 3.59201900 1.42124200
 C 5.32480300 6.43975600 2.47356200
 H 5.02983700 5.87272600 3.34986500
 C 7.37461100 2.16262700 1.43825500
 C -4.92548400 2.01126500 1.63001000
 C 6.24957200 -2.80834400 1.54201600
 H 6.29541700 -3.89101800 1.55954900
 C 6.10342500 7.82521600 0.16186000
 C 5.11614000 7.81450000 2.40590400

C -6.12178400 4.13973200 1.44939100	C 1.18861500 2.95330900 -1.45331000
C -0.06743900 -7.70615100 1.40421800	C -1.24554700 0.12707700 -1.49196300
C -7.38487800 3.44405700 1.66700200	H -1.18720200 -0.95580600 -1.47288700
C -1.28389500 -9.78347700 3.20841100	C 2.41923800 0.80811800 -1.54710000
H -1.57448800 -10.83356000 3.32228900	C -3.75245900 2.89570700 -1.52941700
C -6.08136200 5.56588600 1.03576600	C 3.60269400 4.37895900 -1.41366000
C 9.86282300 -0.66792700 1.28506700	H 4.52189000 4.94971000 -1.34786000
C -1.69224500 -9.90403500 0.15335800	C -2.47633900 0.77067200 -1.53707200
H -2.05808400 -10.93332700 0.24349800	C 1.19885700 0.14516100 -1.50152900
C 9.81032200 2.23633300 1.27484700	H 1.15668400 -0.93871400 -1.50328000
H 10.75890300 1.71077800 1.21252500	C -4.92186300 -2.09775100 -1.57670700
C 5.76531400 7.88642300 -2.31511100	C -3.72146600 4.32641200 -1.46541100
H 6.03374000 6.83112400 -2.43073500	H -4.64941200 4.88832200 -1.44079100
H 6.01830400 8.39833300 -3.25025000	C -1.29042200 4.36057000 -1.41624900
H 4.68015700 7.94510200 -2.17306200	C -5.93083900 -5.74668900 -1.41841200
C -6.95218800 6.03145600 0.04486000	C -4.97781800 2.15916100 -1.55420600
H -7.71164700 5.35495700 -0.34069200	C -4.96055600 0.73313200 -1.55688300
C -9.79865600 3.41197900 1.95156400	C 2.42880200 2.24209200 -1.51182000
H -10.72809400 3.96354600 2.06529600	C -0.04146300 2.25019400 -1.47074000
C -5.85251300 8.15949700 0.04219000	C -6.16706300 -1.41471600 -1.51473500
H -5.76520100 9.16771400 -0.34187700	C -6.18353500 0.00031500 -1.51875200
C 11.05302000 -4.33121700 1.40652100	C 4.89303800 2.24685000 -1.63180700
H 11.68754400 -5.22424200 1.38486600	C -0.04289200 6.49201100 -1.37803700
C 13.14635700 -2.55192300 2.82248800	C 7.37684900 0.83059600 -1.77165400
H 13.85541300 -3.38244400 2.90900400	C -1.28246400 2.93520600 -1.46254500
Si 0.48317300 9.49732700 -1.52818800	C 4.90072200 0.82148700 -1.66135900
Si 12.60009400 2.11121100 -1.90804300	C -6.05016000 -4.26447900 -1.48173700
Si -12.07599700 2.75506700 -1.29206200	C 3.72540600 -1.31086700 -1.59784000
C -3.73788600 -1.37180500 -1.60023800	H 2.81397800 -1.89480700 -1.52983600
H -2.81308900 -1.93730500 -1.62793800	C -0.06515400 5.06343900 -1.38226900
C -3.71982200 0.02470600 -1.57132600	C 3.67632600 0.08626900 -1.60684400
C -2.51149200 2.20445700 -1.51432000	C 6.13748800 0.11548000 -1.72222700

C -7.41935100 2.11623100 -1.47830700
 H -8.36579300 2.64776800 -1.43100200
 C 6.15367000 -1.29868400 -1.70029000
 C -7.43869800 0.68631400 -1.45382700
 C 13.02451900 2.60097400 -3.67130400
 H 14.04501700 2.99528800 -3.72565900
 C -6.33446000 -6.44793300 -0.28550800
 H -6.81823800 -5.89951000 0.52075500
 C 6.14792400 2.92465500 -1.69761500
 H 6.16890400 4.00800100 -1.69851900
 C 2.42493500 5.05946600 -1.34821700
 H 2.42604300 6.14043300 -1.25462600
 C -4.91029000 -3.53152600 -1.57265100
 H -3.94688800 -4.03659600 -1.59134400
 C 7.38068300 -2.01726900 -1.73908900
 C 8.58836900 0.12520500 -1.82162000
 C 4.95675600 -3.43904100 -1.49424700
 H 4.01406500 -3.94804000 -1.30562200
 C 1.17316900 4.37704000 -1.39478600
 C -8.63412000 -0.04800000 -1.36175100
 C 7.33289300 2.25773900 -1.75813400
 H 8.27194800 2.80335500 -1.77955500
 C 8.60993900 -1.30789100 -1.83479400
 C -8.62260300 -1.48119100 -1.36189300
 C -5.50146600 -8.48248700 -1.23205200
 H -5.32381300 -9.55106800 -1.16446800
 C -6.51083500 -8.53596600 1.13179500
 C 9.82625800 0.82704900 -1.85722300
 C -8.54172200 -4.29386400 -1.36300700
 H -8.52676300 -5.37895100 -1.37895300
 C -4.49473200 -8.61179000 -3.55595200
 C -9.76267300 -3.61709800 -1.28969300

H -10.68384100 -4.18907100 -1.24671000
 C 5.09302800 -6.42778300 -1.51647600
 H 4.41835600 -6.05979500 -2.28474100
 C -4.12000900 -7.71744700 -4.74211700
 H -3.38155200 -6.96032600 -4.45821900
 H -3.68278100 -8.32974000 -5.53731800
 H -4.99612000 -7.20771500 -5.15616100
 C -5.50734700 -9.66192500 -4.04379900
 H -6.42428300 -9.18029400 -4.39860400
 H -5.08100800 -10.24224800 -4.86978900
 H -5.77910600 -10.36050400 -3.24639900
 C 9.81603300 -2.03209000 -1.93038100
 H 10.74970500 -1.48328700 -2.00410000
 C -1.06727300 10.54442600 -1.36238200
 H -1.47686300 10.48457300 -0.34968600
 C 10.90340900 1.39871900 -1.87370400
 C 8.59809500 -4.11751900 -1.81225200
 H 8.61049900 -5.20251800 -1.82146800
 C -3.22174700 -9.32029500 -3.06615000
 H -3.43332400 -10.01960900 -2.25118600
 H -2.76673800 -9.88745900 -3.88619300
 H -2.48968000 -8.59169600 -2.70179100
 C 4.96547800 -7.73270900 -1.03563200
 C -10.85449300 1.37727400 -1.22352400
 C 6.85024300 -7.32419800 0.47072400
 C -6.15950900 -10.02700600 1.10984800
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C 3.99813500 -10.08414900 -1.11062800
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H 3.20290300 -10.69368100 -1.55346400
H 4.95942300 -10.50749500 -1.42181700
C 9.25745900 -7.74929000 0.98695100
H 9.53283400 -6.75090500 0.63157100
H 9.98065700 -8.04300900 1.75660000
H 9.34528600 -8.44615200 0.14674000
C 3.85770000 -8.62485200 -3.11345300
H 4.82218900 -8.97210300 -3.49811500
H 3.07570100 -9.29133900 -3.49349100
H 3.66851300 -7.62869900 -3.52260400
C 7.52997300 -9.17832400 2.07477300
H 7.61939700 -9.92527300 1.27900000
H 8.24531700 -9.44210100 2.86030800
H 6.52318200 -9.24540300 2.50082000
C 3.65589900 2.95492500 -1.53066000
C -0.02880800 0.82609900 -1.49766800
C 12.69427100 3.61013100 -0.77879200
H 13.65602500 4.11924900 -0.90498200
C -2.55282900 5.02574700 -1.40881700
H -2.56867700 6.11013700 -1.35827800
C 7.74972800 -6.79288000 2.74960900

H 6.73435700 -6.76151800 3.15957200
H 8.43209200 -7.11142000 3.54555900
H 8.03128000 -5.77479700 2.46072900
C -7.33906300 -3.59149400 -1.42293000
C -5.32311200 -6.43953300 -2.47265000
H -5.02640300 -5.87268500 -3.34848200
C -7.37486500 -2.16209900 -1.43976100
C 4.92543100 -2.01173000 -1.63039500
C -6.24932300 2.80877800 -1.54236600
H -6.29507100 3.89145700 -1.55969900
C -6.10648400 -7.82452900 -0.16231300
C -5.11455500 -7.81425000 -2.40429100
C 6.12164600 -4.14021400 -1.44933500
C 0.06828400 7.70599400 -1.40190600
C 7.38474800 -3.44465700 -1.66729300
C 1.28774800 9.78544600 -3.20191600
H 1.57939600 10.83550200 -3.31339600
C 6.08123300 -5.56624300 -1.03525700
C -9.86282100 0.66864200 -1.28650000
C 1.69249800 9.90166600 -0.14637400
H 2.05872400 10.93097500 -0.23472300
C -9.81065200 -2.23557100 -1.27727600
H -10.75920200 -1.70992900 -1.21520400
C -5.77320200 -7.88566000 2.31530300
H -6.04118100 -6.83014700 2.43007300
H -6.02848300 -8.39715000 3.25004900
H -4.68778100 -7.94506600 2.17555900
C 6.95238400 -6.03162400 -0.04455700
H 7.71204500 -5.35509500 0.34054500
C 9.79849300 -3.41277700 -1.95216700
H 10.72790100 -3.96440400 -2.06586500
C 5.85251700 -8.15956900 -0.04088000

H 5.76531000 -9.16770300 0.34342700
 C -11.05321200 4.33202500 -1.40677700
 H -11.68779100 5.22498900 -1.38427400
 C -13.14613600 2.55306200 -2.82370700
 H -13.85510100 3.38367100 -2.91012500
 H 14.79449000 1.13689200 -1.22115800
 H 12.60930800 3.30952200 0.27039900
 H 13.74101300 -0.10305100 -1.92913600
 H 12.95585100 1.74231700 -4.34566100
 H 11.89709900 4.32777500 -0.99465400
 H 13.88082600 -1.95583300 -0.23231900
 H 13.75953400 -3.72122900 -0.24335000
 H -14.79411400 -1.13778600 1.21819600
 H -13.74100300 0.10203200 1.92694000
 H -12.95601300 -1.74284700 4.34354800
 H -11.89631200 -4.32840600 0.99241100
 H -12.60977000 -3.31062400 -0.27228200
 H 12.53565800 -2.53034800 3.72985100
 H -10.35076300 4.38721800 -0.56696800
 H -0.84052600 11.59517400 -1.57320600
 H -13.72075500 1.62254100 -2.78183100
 H -12.53523200 2.53173400 -3.73094100
 H 13.72089500 -1.62137000 2.78018100
 H 10.35085700 -4.38693600 0.56651000
 H 0.84264300 -11.59491700 1.57890400
 H -2.55749400 -9.23078500 0.17124600
 H 2.55759800 9.22821300 -0.16427600
 H 12.34299800 3.37354800 -4.03983600
 H 10.47343600 -4.34919000 2.33600300
 H -0.59823300 -9.53031100 4.02246100
 H -2.18201700 -9.16857300 3.32313500
 H -12.34349700 -3.37427000 4.03805000

H -10.47395000 4.35069600 -2.33644600
 H 0.60278500 9.53450500 -4.01724200
 H 2.18546700 9.16999800 -3.31682800
 H 1.84665400 -10.21930100 2.06560200
 H -1.21322900 -9.80044700 -0.82558000
 H 1.21244400 9.79684900 0.83193300
 H -1.84428600 10.22014300 -2.06210800
 C -13.17735400 2.79329600 0.23025900
 H -13.76101300 3.72068200 0.24139200
 H -13.88017500 1.95514100 0.23151300
 H -12.59718200 2.74804700 1.15641300

[tips-OR-3]₂ (neutral radical • radical state, open-shell triplet)

Si -0.57900500 -9.50558800 1.38275500
 Si -12.64401300 -2.18014600 2.09834700
 Si 12.07176300 -2.74623700 1.37306000
 C 3.67085800 1.34279400 1.66199200
 H 2.74901800 1.91343500 1.67598700
 C 3.64594300 -0.05547400 1.64494100
 C 2.42721700 -2.22349800 1.54498100
 C -1.27302700 -2.95818500 1.44923900
 C 1.16649000 -0.14403800 1.61831300
 H 1.11248000 0.93862300 1.64846100
 C -2.49588200 -0.80856300 1.58545800
 C 3.66938700 -2.92289600 1.55712400
 C -3.68884800 -4.37265800 1.38693500
 H -4.60982200 -4.93879200 1.31415800
 C 2.39765600 -0.79342700 1.61065100
 C -1.28059200 -0.15159000 1.60754400
 H -1.23559900 0.93112500 1.65774300
 C 4.85795500 2.06098700 1.63481100

C 3.63255100 -4.35441500 1.45494500	H -2.51745000 -6.13562000 1.18404200
H 4.55908300 -4.91831700 1.41937800	C 4.85685800 3.49400000 1.62153200
C 1.20068800 -4.37347100 1.38871400	H 3.89804000 4.00660000 1.65855000
C 5.88966900 5.70258000 1.45522900	C -7.46206000 2.02184600 1.73986800
C 4.89077600 -2.19916800 1.62344500	C -8.67114500 -0.11881000 1.89953900
C 4.88059300 -0.76893100 1.62800500	C -5.03763100 3.43089700 1.45617400
C -2.51062100 -2.24556600 1.51849000	H -4.09375100 3.93718300 1.26630400
C -0.03989800 -2.25825400 1.49266300	C -1.26213600 -4.37926100 1.35921800
C 6.09878600 1.36910200 1.56607900	C 8.55434900 -0.01643700 1.41852000
C 6.10697800 -0.04500200 1.58378100	C -7.41536500 -2.25274000 1.83451600
C -4.97883300 -2.24657600 1.66182900	H -8.35237200 -2.79953300 1.88145900
C -0.04773000 -6.49858500 1.29965100	C -8.69033400 1.31551800 1.87140300
C -7.45975900 -0.82823600 1.82999800	C 8.55039400 1.41814000 1.37051000
C 1.19753600 -2.94725700 1.46951000	C 5.47142300 8.44351500 1.31408500
C -4.98493900 -0.81976300 1.68570300	H 5.29712300 9.51369500 1.26372700
C 6.00029900 4.21882000 1.50348300	C 6.40990000 8.51871900 -1.07839000
C -3.80699900 1.30586600 1.58587500	C -9.90763800 -0.81932700 1.97025800
H -2.89617800 1.88706100 1.48721700	C 8.48719100 4.22883100 1.29859600
C -0.02145400 -5.07060400 1.33443600	H 8.48006900 5.31404600 1.29007700
C -3.76001800 -0.08558200 1.62508300	C 4.54524000 8.55154300 3.67292900
C -6.22024700 -0.11445100 1.75067700	C 9.70001300 3.54205900 1.20055300
C 7.33439800 -2.17246100 1.57657100	H 10.62270500 4.10568900 1.10718800
H 8.27998700 -2.70677100 1.54945500	C -5.17143200 6.41867500 1.45529500
C -6.23532800 1.30071700 1.70763700	H -4.51456100 6.05876200 2.24273400
C 7.35988800 -0.73950600 1.52540000	C 4.19648900 7.64404400 4.85703900
C -13.00664000 -2.69155600 3.86918500	H 3.44018100 6.90015800 4.58533700
H -14.00040000 -3.14643900 3.94238400	H 3.79183500 8.24968500 5.67428100
C 6.26603500 6.41584300 0.32060100	H 5.07853100 7.11771400 5.23619800
H 6.72450600 5.87517300 -0.50529900	C 5.58840700 9.57973400 4.14300900
C -6.22773800 -2.92129300 1.75306500	H 6.50919200 9.07990300 4.46075600
H -6.24892600 -4.00489700 1.76636500	H 5.19747500 10.15372600 4.99067000
C -2.51167800 -5.05678200 1.30077600	H 5.84435500 10.28598900 3.34710600

C -9.89241500 2.04311800 1.96344700	H -3.27942100 10.68455100 1.48505500
H -10.82538700 1.49803900 2.06823400	H -5.02941500 10.50007200 1.28633800
C 0.97731700 -10.54784100 1.24568500	C -9.27177200 7.73278700 -1.15950100
H 1.42824000 -10.45543500 0.25322900	H -9.56517500 6.74559100 -0.78804500
C -10.98198700 -1.39496300 2.02445100	H -9.97544900 8.01665200 -1.95063400
C -8.68061500 4.12417100 1.74985600	H -9.36985600 8.44909500 -0.33696000
H -8.69228500 5.20892300 1.72125200	C -4.00703200 8.65038900 3.06103000
C 3.26757300 9.28568900 3.23663500	H -4.98600800 9.00806400 3.39629200
H 3.46258000 9.99603900 2.42715900	H -3.23973700 9.32243100 3.46077700
H 2.84766000 9.84485300 4.08050700	H -3.83991700 7.66202900 3.49785300
H 2.51367200 8.57374000 2.88417100	C 13.19137700 -2.68158400 -0.13455200
C -5.03027000 7.71734900 0.96120300	H 12.61962500 -2.71276400 -1.06634300
C 10.78861000 -1.42632000 1.31631400	C -7.50545600 9.12053600 -2.23829000
C -6.88139600 7.29212500 -0.58263800	H -7.60662400 9.88507300 -1.46085000
C 6.04431500 10.00598200 -1.03866300	H -8.19903000 9.37455700 -3.04623600
H 4.96809500 10.15264100 -0.89236200	H -6.48804400 9.16883300 -2.64102900
H 6.32002500 10.47571800 -1.98825300	C -3.73703100 -2.95488200 1.53010100
H 6.57705300 10.53183300 -0.23935600	C -0.04789600 -0.83663000 1.57672300
C -3.93095200 8.62476000 1.52518000	C -12.67619500 -3.67909500 0.96485100
C -2.56274000 8.07455400 1.08711000	H -13.61521800 -4.23048700 1.08359400
H -2.42589100 7.03322800 1.39841100	C 2.46305100 -5.04463800 1.37190500
H -1.75001100 8.66806500 1.52531700	H 2.47288900 -6.12721700 1.29348600
H -2.45717600 8.11396600 -0.00261200	C -7.73680200 6.72480700 -2.86986700
C 7.92419700 8.39508400 -1.31635300	H -6.71288800 6.67403500 -3.25609800
H 8.48339700 8.85986400 -0.49774800	H -8.39727700 7.03510400 -3.68722700
H 8.20344100 8.89358500 -2.25134500	H -8.03611000 5.71561400 -2.56794600
H 8.23623600 7.34816300 -1.38709600	C 7.28167600 3.53634100 1.41521900
C -13.89466100 -0.91468600 1.49388500	C 5.31779700 6.38693600 2.53502500
H -13.66996400 -0.63557400 0.45891000	H 5.04339400 5.81140400 3.41242700
C -7.83300300 7.72306700 -1.70301300	C 7.30925600 2.10837000 1.45940300
C -4.05792400 10.06749400 1.02341100	C -5.00948100 2.01018100 1.61841700
H -3.93020900 10.13519900 -0.06203600	C 6.16284900 -2.85715600 1.63352800

H 6.20166400 -3.93973500 1.66786000	H -2.74902900 -1.91342400 -1.67599200
C 6.04027900 7.79463400 0.21916600	C -3.64597800 0.05547300 -1.64492000
C 5.11753600 7.76378600 2.49028600	C -2.42727100 2.22350700 -1.54499100
C -6.20309500 4.13367200 1.39629200	C 1.27297000 2.95821500 -1.44929000
C -0.16050900 -7.71264600 1.29864400	C -1.16653100 0.14405100 -1.61825300
C -7.46465100 3.44466500 1.62393900	H -1.11251700 -0.93861200 -1.64835700
C -1.43248200 -9.82430700 3.02653700	C 2.49584200 0.80859700 -1.58547100
H -1.72243000 -10.87737400 3.11127400	C -3.66944700 2.92289800 -1.55714000
C -6.15231900 5.55388200 0.96473600	C 3.68878100 4.37270900 -1.38700400
C 9.78451700 -0.73506100 1.35609400	H 4.60975200 4.93884800 -1.31422600
C -1.74905500 -9.88274100 -0.03949600	C -2.39769900 0.79343400 -1.61062000
H -2.12393200 -10.91097600 0.02195000	C 1.28055300 0.15161600 -1.60751400
C 9.73917700 2.15988000 1.22955100	H 1.23556400 -0.93110000 -1.65768400
H 10.68197900 1.62711900 1.14727400	C -4.85796500 -2.06100100 -1.63482700
C 5.65370100 7.87016200 -2.25102700	C -3.63261700 4.35442500 -1.45506800
H 5.93555300 6.82075800 -2.38662000	H -4.55914900 4.91833100 -1.41955600
H 5.87689500 8.39696300 -3.18548500	C -1.20075400 4.37349000 -1.38884500
H 4.57126100 7.90924500 -2.08356000	C -5.88964400 -5.70261200 -1.45536800
C -7.00162500 6.00795000 -0.04988200	C -4.89083300 2.19915600 -1.62342300
H -7.75515300 5.32738300 -0.44062400	C -4.88063300 0.76891800 -1.62798700
C -9.87660700 3.42530800 1.93002700	C 2.51056900 2.24560300 -1.51852500
H -10.80542700 3.97974300 2.03434100	C 0.03984700 2.25827600 -1.49268800
C -5.89231600 8.13163500 -0.06030800	C -6.09880400 -1.36913100 -1.56609500
H -5.79232200 9.13351800 -0.45768500	C -6.10701000 0.04497300 -1.58377600
C 11.12868800 -4.37451400 1.43109700	C 4.97877500 2.24663800 -1.66187400
H 11.80542100 -5.23495400 1.38490200	C 0.04764900 6.49861400 -1.29986000
C 13.10716800 -2.53220300 2.92678300	C 7.45971800 0.82833400 -1.83000800
H 13.85407900 -3.32978400 3.00420800	C -1.19759200 2.94727300 -1.46956000
Si 0.57896400 9.50560700 -1.38311100	C 4.98489800 0.81982400 -1.68573400
Si 12.64418200 2.17990000 -2.09765000	C -6.00028500 -4.21885100 -1.50356500
Si -12.07177500 2.74619800 -1.37272900	C 3.80698600 -1.30582300 -1.58593400
C -3.67087700 -1.34279400 -1.66199000	H 2.89617300 -1.88703300 -1.48730000

C 0.02138800 5.07063200 -1.33458000	H -8.48004800 -5.31410400 -1.29026800
C 3.75998500 0.08562800 -1.62511600	C -4.54524600 -8.55146600 -3.67323000
C 6.22021600 0.11453000 -1.75070200	C -9.70002100 -3.54213900 -1.20071800
C -7.33445600 2.17241300 -1.57651300	H -10.62268400 -4.10584400 -1.10747600
H -8.28005000 2.70671100 -1.54936500	C 5.17144300 -6.41859300 -1.45532300
C 6.23531600 -1.30063900 -1.70766600	H 4.51458300 -6.05867700 -2.24276900
C -7.35992800 0.73945800 -1.52538000	C -4.19654700 -7.64390900 -4.85731100
C 13.00799200 2.69005100 -3.86860500	H -3.44024800 -6.90001700 -4.58559800
H 14.00210800 3.14420500 -3.94154000	H -3.79190200 -8.24950500 -5.67459100
C -6.26596900 -6.41592800 -0.32075900	H -5.07861200 -7.11758100 -5.23642300
H -6.72442700 -5.87531200 0.50518500	C -5.58841700 -9.57964700 -4.14332000
C 6.22767000 2.92137500 -1.75313300	H -6.50921900 -9.07981200 -4.46101200
H 6.24883600 4.00498000 -1.76648900	H -5.19750900 -10.15359500 -4.99102200
C 2.51160700 5.05682800 -1.30087100	H -5.84432900 -10.28594200 -3.34744100
H 2.51736900 6.13566700 -1.18415700	C 9.89241700 -2.04297300 -1.96334500
C -4.85685000 -3.49401500 -1.62157700	H 10.82538600 -1.49788600 -2.06807800
H -3.89802400 -4.00660000 -1.65859400	C -0.97736700 10.54785300 -1.24610800
C 7.46205800 -2.02175100 -1.73986900	H -1.42832800 10.45541000 -0.25367200
C 8.67111200 0.11892500 -1.89950400	C 10.98198000 1.39504900 -2.02417400
C 5.03765000 -3.43083900 -1.45625300	C 8.68066300 -4.12405200 -1.74979900
H 4.09377300 -3.93714000 -1.26641700	H 8.69235400 -5.20880400 -1.72119300
C 1.26207000 4.37929500 -1.35931400	C -3.26755500 -9.28561700 -3.23701600
C -8.55438000 0.01637300 -1.41850200	H -3.46252800 -9.99601500 -2.42757400
C 7.41530500 2.25283800 -1.83455800	H -2.84766000 -9.84472600 -4.08093300
H 8.35230600 2.79964100 -1.88151900	H -2.51365400 -8.57367600 -2.88453500
C 8.69032000 -1.31540000 -1.87136300	C 5.03025600 -7.71725800 -0.96121500
C -8.55041500 -1.41820500 -1.37053800	C -10.78860500 1.42629300 -1.31611600
C -5.47135000 -8.44354700 -1.31434900	C 6.88136000 -7.29203500 0.58265200
H -5.29702900 -9.51372600 -1.26403800	C -6.04410200 -10.00611300 1.03835700
C -6.40973500 -8.51886500 1.07815600	H -4.96788400 -10.15272900 0.89199200
C 9.90760600 0.81944800 -1.97012100	H -6.31974300 -10.47589100 1.98794700
C -8.48717800 -4.22888800 -1.29874100	H -6.57686600 -10.53195500 0.23906200

C 3.93094900 -8.62467700 -1.52520200
 C 2.56272100 -8.07448600 -1.08717400
 H 2.42590100 -7.03313900 -1.39842100
 H 1.75001700 -8.66796100 -1.52547400
 H 2.45707100 -8.11396000 0.00253800
 C -7.92402400 -8.39528700 1.31618800
 H -8.48324700 -8.86005700 0.49759300
 H -8.20321200 -8.89383000 2.25117500
 H -8.23609600 -7.34837900 1.38698200
 C 13.89408200 0.91449200 -1.49153200
 H 13.66770700 0.63512100 -0.45698700
 C 7.83293100 -7.72296800 1.70306100
 C 4.05792600 -10.06740700 -1.02342200
 H 3.93016000 -10.13511300 0.06201800
 H 3.27945500 -10.68447700 -1.48510200
 H 5.02943800 -10.49996700 -1.28630200
 C 9.27171500 -7.73272800 1.15959000
 H 9.56514800 -6.74554700 0.78812000
 H 9.97536300 -8.01658900 1.95074900
 H 9.36980800 -8.44905600 0.33706800
 C 4.00706400 -8.65032000 -3.06105300
 H 4.98606800 -9.00794100 -3.39628800
 H 3.23981700 -9.32241300 -3.46080700
 H 3.83989900 -7.66197400 -3.49789000
 C 7.50534600 -9.12041800 2.23836500
 H 7.60651300 -9.88497500 1.46094400
 H 8.19889900 -9.37443500 3.04633000
 H 6.48792600 -9.16868400 2.64108600
 C 3.73697100 2.95493000 -1.53015100
 C 0.04785400 0.83665000 -1.57669600
 C 12.67608100 3.67963400 -0.96516000
 H 13.61476200 4.23143100 -1.08472500

C -2.46311700 5.04465600 -1.37210500
 H -2.47292200 6.12724700 -1.29385900
 C 7.73671400 -6.72467800 2.86988900
 H 6.71278800 -6.67387600 3.25608500
 H 8.39715600 -7.03496700 3.68727700
 H 8.03605000 -5.71549800 2.56795100
 C -7.28166900 -3.53638600 -1.41530300
 C -5.31779600 -6.38691700 -2.53521000
 H -5.04342800 -5.81134400 -3.41259600
 C -7.30926800 -2.10841400 -1.45944500
 C 5.00947800 -2.01012000 -1.61847700
 C -6.16291700 2.85712400 -1.63347600
 H -6.20175300 3.93970200 -1.66776700
 C -6.04018400 -7.79471900 -0.21938800
 C -5.11751000 -7.76376600 -2.49053400
 C 6.20312400 -4.13359800 -1.39633600
 C 0.16044200 7.71267500 -1.29891100
 C 7.46467700 -3.44457100 -1.62393900
 C 1.43249500 9.82424600 -3.02688100
 H 1.72238100 10.87732500 -3.11167400
 C 6.15234000 -5.55380600 -0.96476700
 C -9.78454400 0.73499500 -1.35600900
 C 1.74900100 9.88280800 0.03913900
 H 2.12392200 10.91102300 -0.02236400
 C -9.73920000 -2.15996000 -1.22963600
 H -10.68200200 -1.62719900 -1.14736800
 C -5.65350400 -7.87033000 2.25078600
 H -5.93540800 -6.82095000 2.38645500
 H -5.87661200 -8.39719800 3.18522700
 H -4.57107200 -7.90934200 2.08324900
 C 7.00162400 -6.00787200 0.04986900
 H 7.75515600 -5.32731200 0.44061700

C 9.87664900 -3.42516200 -1.92990600
 H 10.80550400 -3.97955800 -2.03414600
 C 5.89227800 -8.13153700 0.06032100
 H 5.79225800 -9.13341000 0.45771600
 C -11.12874200 4.37449900 -1.43080900
 H -11.80547200 5.23491700 -1.38413200
 C -13.10733800 2.53210900 -2.92633700
 H -13.85422000 3.32971600 -3.00376300
 H 14.91237200 1.31651100 -1.52175400
 H 12.59998400 3.36990700 0.08222500
 H 13.86727900 0.00496500 -2.09994500
 H 12.97888500 1.82705800 -4.54034100
 H 11.84867700 4.36273100 -1.18004100
 H 13.79588200 -1.76991600 -0.14059500
 H 13.87543800 -3.53756700 -0.12788500
 H -14.91294200 -1.31659800 1.52585500
 H -13.86679400 -0.00503200 2.10205900
 H -12.97778200 -1.82891000 4.54138000
 H -11.84924000 -4.36276000 1.17966400
 H -12.59941400 -3.36868100 -0.08227600
 H 12.48150900 -2.56471100 3.82361200
 H -10.43397200 4.43561200 -0.58534600
 H -0.74415100 11.60486300 -1.41413200
 H -13.63636600 1.57420800 -2.91886900
 H -12.48174600 2.56452300 -3.82321600
 H 13.63615700 -1.57427900 2.91942300
 H 10.43422800 -4.43582800 0.58539500
 H 0.74407300 -11.60484200 1.41373800
 H -2.61030900 -9.20373500 -0.03494500
 H 2.61022500 9.20376500 0.03463300
 H 12.27516300 3.41947600 -4.22636800
 H 10.54566400 -4.45147100 2.35554300

H -0.77387800 -9.58448200 3.86656500
 H -2.33652400 -9.21519800 3.12473200
 H -12.27311700 -3.42066200 4.22617900
 H -10.54607000 4.45170400 -2.35545500
 H 0.77395500 9.58432100 -3.86692900
 H 2.33658300 9.21518900 -3.12497700
 H 1.72458300 -10.24553300 1.98649500
 H -1.24136200 -9.76511900 -1.00226000
 H 1.24129400 9.76526200 1.00190500
 H -1.72459600 10.24553000 -1.98695000
 C -13.19109600 2.68152700 0.13508900
 H -13.87595300 3.53686800 0.12800700
 H -13.79473400 1.76929500 0.14193600
 H -12.61911700 2.71391300 1.06670100

tips-OR-3 (neutral radical state)

C 9.84126700 -2.24441000 -0.21549700
 C 8.63497400 -2.94533500 -0.16484100
 C 7.41517000 -2.26907300 -0.07652200
 C 7.42016000 -0.84103800 -0.08201100
 C 8.65629500 -0.13575800 -0.12636400
 C 9.86047500 -0.86302300 -0.18528900
 C 6.19501400 -0.11631000 -0.06000500
 C 6.18565300 1.29852900 -0.06149500
 C 7.43199100 2.00607300 -0.08412400
 C 8.64087600 1.29886300 -0.11880900
 C 4.95130300 2.01049900 -0.04197500
 C 4.95156400 3.43887900 -0.03077800
 C 6.21301900 4.10783700 -0.05049500
 C 7.39406500 3.43388300 -0.07739700
 C 6.13992100 -2.96927600 -0.01578000
 C 4.98174100 -2.25560800 -0.01774700

C 4.96131800 -0.82250700 -0.04267600
C 3.76495700 -0.11160400 -0.02845500
C 3.72067200 1.28428400 -0.03131100
C 2.45960800 2.01366400 -0.02179600
C 6.07680800 -4.45327600 0.06106600
C 5.30336500 -5.16618400 -0.84882700
C 5.18305400 -6.56062000 -0.76949200
C 5.86571500 -7.21384600 0.25263900
C 6.65302100 -6.52755200 1.19178700
C 6.74675000 -5.14472700 1.08188000
C 4.32178600 -7.29958000 -1.79808300
C 7.36812700 -7.31890800 2.29106200
C 9.87917900 2.00468100 -0.15055200
C 1.23306700 1.36328900 -0.03492200
C 0.00797500 2.05387400 -0.01902100
C 0.01220500 3.47799400 0.01364700
C 1.24852000 4.17003000 0.02274000
C 2.48173800 3.44875200 0.00097300
C -1.22131000 1.37065700 -0.03462000
C -2.44389600 2.02822800 -0.01775200
C -2.45752800 3.46304400 0.02251400
C -1.21997200 4.17707700 0.03542100
C 1.24697600 5.59524100 0.05334300
C 2.49981400 6.27290000 0.05745900
C 3.67151500 5.58259300 0.03080400
C 3.71581400 4.15390200 0.00021100
C -1.20995500 5.60212800 0.07045800
C 0.02054000 6.29505900 0.07945900
C -3.68739900 4.17489500 0.05039800
C -3.63454200 5.60318200 0.08516800
C -2.45862400 6.28679300 0.09403100
C 0.02616000 7.72347200 0.11568100

C -3.70933300 1.30661500 -0.03907500
C 4.30114300 -8.81259000 -1.55897300
C 4.87854600 -7.04113400 -3.20820800
C 2.87670600 -6.77899500 -1.71699400
C 8.18085400 -6.41124200 3.21998600
C 8.32941200 -8.33121200 1.64528800
C 6.32852800 -8.07105900 3.13877900
C 10.94597200 2.59487100 -0.17692100
C 0.03505200 8.94172500 0.14782000
Si 12.58189000 3.44454900 -0.21508100
Si 0.06781500 10.78550900 0.18513600
C 13.91846800 2.12366900 -0.21780400
C 12.73682700 4.53020700 1.31026200
C 12.68854100 4.48779400 -1.77365700
C -0.14053500 11.36039700 1.96125300
C 1.72267900 11.35624200 -0.49718800
C -1.33886000 11.42876700 -0.88078300
C -3.76178900 -0.08779000 -0.09275500
C -4.96238200 -0.79155000 -0.11021900
C -6.19208500 -0.07951600 -0.07042400
C -6.17441600 1.33445700 -0.02066200
C -4.93580700 2.03916900 -0.00496100
C -4.99031900 -2.22400800 -0.14607500
C -6.15186600 -2.93219900 -0.14506500
C -7.42482000 -2.22447800 -0.14428700
C -7.42152600 -0.79712100 -0.09206100
C -7.41672200 2.04858800 0.01070400
C -7.37037400 3.47507800 0.06592600
C -6.18516000 4.14210400 0.08047700
C -4.92760000 3.46676200 0.04253400
C -8.65419600 -0.08429900 -0.07876900
C -8.63017800 1.34898000 -0.01896500

C -8.65106000 -2.89009400 -0.22893400	H 7.32928200 -4.56968800 1.79400500
C -9.85383300 -2.18150800 -0.22045600	H 1.18354300 0.28059100 -0.06116500
C -9.86394000 -0.80236100 -0.13528900	H -1.17820000 0.28764000 -0.05862200
C -9.86450500 2.06208700 0.00396300	H 2.50122000 7.35764000 0.08138800
C -6.09443100 -4.41826200 -0.13545300	H 4.59431400 6.14832900 0.03636900
C -6.74895100 -5.15218700 0.85053700	H -4.55392700 6.17420600 0.10258800
C -6.67144500 -6.54934900 0.89069400	H -2.45324300 7.37144700 0.11845200
C -5.90836300 -7.18718300 -0.08511700	H 3.88886000 -9.06001300 -0.57493200
C -5.22745700 -6.48109000 -1.08840800	H 5.30406400 -9.24621900 -1.63333500
C -5.33316200 -5.09313600 -1.09901400	H 3.67260600 -9.29355300 -2.31531200
C -7.42251100 -7.30799500 1.98874500	H 4.87416500 -5.97529700 -3.45517600
C -4.41094300 -7.25623700 -2.12711200	H 4.27018000 -7.56258600 -3.95570600
C -7.24187000 -8.82488800 1.87459100	H 5.90881800 -7.40232500 -3.28997300
C -8.92408600 -6.99090400 1.88245400	H 2.82241000 -5.70637300 -1.92675800
C -6.90232000 -6.86145400 3.36535600	H 2.45845700 -6.95072600 -0.71978400
C -3.73712600 -6.32800200 -3.14267600	H 2.24688700 -7.29692300 -2.44899500
C -5.33747300 -8.21607100 -2.89255100	H 8.95442800 -5.86229900 2.67217600
C -3.31518600 -8.06556400 -1.41296600	H 7.54257200 -5.68573900 3.73493500
C -10.92735200 2.65965200 0.02255500	H 8.67848700 -7.01918000 3.98234100
Si -12.55652000 3.52265300 0.04766800	H 9.07953000 -7.81778600 1.03482300
C -12.67006200 4.55900300 1.61040200	H 7.79911300 -9.04039600 1.00244800
C -13.90417600 2.21322300 0.03009600	H 8.85016000 -8.90447100 2.42047500
C -12.68696100 4.61733800 -1.47347200	H 5.74575600 -8.77295500 2.53444700
H 10.77498200 -2.79406200 -0.28257700	H 6.82802300 -8.64210100 3.92945300
H 8.64262400 -4.02883400 -0.20533800	H 5.63139900 -7.36964500 3.60847700
H 10.79950600 -0.32026300 -0.21942800	H 13.85256800 1.49665800 0.67661000
H 6.24691400 5.18980000 -0.04818700	H 12.66064300 3.93576400 2.22552500
H 8.33484000 3.97376000 -0.09523200	H 12.58580900 3.86838000 -2.66955700
H 4.03123200 -2.78130400 0.03749000	H 0.66432400 10.97812700 2.59609000
H 2.84782100 -0.68968400 -0.00930300	H 2.55113300 10.96902900 0.10400300
H 4.79855700 -4.61686000 -1.63980200	H -1.23587100 11.08831300 -1.91539100
H 5.79135200 -8.29322000 0.33399600	H -2.84801400 -0.67065100 -0.12336000

H -4.04145600 -2.75544500 -0.13803700
 H -8.30810500 4.01974600 0.09470700
 H -6.21273300 5.22339300 0.12327700
 H -8.66761600 -3.97095000 -0.31403100
 H -10.79212300 -2.72355500 -0.28562600
 H -10.80014900 -0.25380800 -0.12438100
 H -7.32016800 -4.61608700 1.60461300
 H -5.83503000 -8.26973000 -0.07594600
 H -4.84005200 -4.50293600 -1.86421300
 H -7.61907700 -9.20540500 0.91933200
 H -7.79933800 -9.32092700 2.67557400
 H -6.18989500 -9.11385100 1.97136400
 H -9.12033200 -5.92057000 2.00154600
 H -9.31666500 -7.30097200 0.90825200
 H -9.47975600 -7.52309200 2.66266000
 H -5.83311200 -7.07546500 3.46332600
 H -7.04772300 -5.78868500 3.52365600
 H -7.43492100 -7.39439300 4.16100100
 H -4.47281900 -5.74441500 -3.70582900
 H -3.16382700 -6.92451400 -3.85958400
 H -3.04442800 -5.63334600 -2.65585100
 H -6.12788800 -7.66168400 -3.40879200
 H -4.76545200 -8.77713700 -3.64009300
 H -5.81373200 -8.93835200 -2.22252000
 H -2.64222400 -7.40242300 -0.85968700
 H -3.73927200 -8.78344800 -0.70431800
 H -2.72236400 -8.62571600 -2.14482300
 H -12.58095800 3.93441600 2.50416400
 H -13.82714500 1.55867600 0.90364800
 H -12.60636100 4.02703600 -2.39103400
 H -0.12369400 12.45437300 2.01440400
 H -1.09123900 11.01601400 2.37902700

H 1.86305400 11.01367100 -1.52674200
 H -2.30761900 11.08364700 -0.50676000
 H -1.34928200 12.52402100 -0.88367200
 H -14.89580800 2.67807500 0.04245100
 H -13.83465100 1.59028200 -0.86692000
 H -13.65004400 5.13893400 -1.48907800
 H -11.87629800 5.31129800 1.64458200
 H -11.89426000 5.37137200 -1.48731100
 H 11.95058400 5.29068400 1.33601000
 H 13.70424700 5.04386500 1.31880700
 H 13.82718400 1.47437600 -1.09394100
 H 11.90044800 5.24643000 -1.79646100
 H -13.63215800 5.08068600 1.65559000
 H 1.78521500 12.44971800 -0.49251600
 H 13.65430500 5.00202400 -1.82563400
 H 14.91384400 2.58017900 -0.23788700

truncated OR-3 (neutral state)

C -3.77250700 -1.57357300 -0.00260800
 H -2.85791100 -2.15551000 -0.00452600
 C -3.71820500 -0.17386700 -0.00097200
 C -2.47057100 1.98098500 -0.00113100
 C 1.23344700 2.69359700 -0.00172200
 C -1.22844500 -0.11146800 -0.00019800
 H -1.18590300 -1.19447400 0.00080900
 C 2.45420000 0.54649100 -0.00079300
 C -3.70022800 2.69835600 -0.00064900
 C 3.64548700 4.13178700 -0.00187700
 H 4.56501600 4.70225000 -0.00251400
 C -2.45420100 0.54649100 -0.00078700
 C 1.22844500 -0.11146800 -0.00020100
 H 1.18590400 -1.19447400 0.00081200

C -4.97108900 -2.27505300 -0.00220600
 C -3.64548800 4.13178700 -0.00190600
 H -4.56501700 4.70225000 -0.00254600
 C -1.21889500 4.12087700 -0.00243800
 C -4.93686900 1.99332400 0.00107300
 C -4.94160000 0.56250600 0.00051300
 C 2.47057000 1.98098500 -0.00112200
 C 0.00000000 1.99865800 -0.00147900
 C -6.20087400 -1.55371700 -0.00004700
 C -6.17884000 -0.14113100 0.00124000
 C 4.93686900 1.99332400 0.00112300
 C 7.42756600 0.57101400 0.00336300
 C -1.23344700 2.69359700 -0.00172800
 C 4.94160100 0.56250600 0.00053100
 C -6.18774400 -4.38344600 -0.00321500
 C 3.77250700 -1.57357300 -0.00267900
 H 2.85791100 -2.15551000 -0.00464200
 C 0.00000000 4.79942700 -0.00287200
 C 3.71820500 -0.17386700 -0.00099100
 C 6.17884000 -0.14113000 0.00126000
 C -7.38158300 2.00391400 0.00459000
 H -8.32010100 2.55049000 0.00657900
 C 6.20087500 -1.55371700 -0.00007200
 C -7.42756600 0.57101400 0.00329600
 C 6.20003800 2.67154000 0.00356200
 H 6.22533900 3.75345000 0.00492500
 C 2.46908800 4.81030500 -0.00277300
 H 2.46276600 5.89646000 -0.00378700
 C -5.01109000 -3.71406900 -0.00386700
 H -4.06788900 -4.25310800 -0.00561700
 C 7.43607500 -2.25841400 0.00060600
 C 8.62343700 -0.12241100 0.00419300

C 5.01109000 -3.71406900 -0.00399500
 H 4.06788900 -4.25310800 -0.00578500
 C 1.21889500 4.12087700 -0.00242900
 C 7.38158300 2.00391400 0.00470200
 H 8.32010000 2.55049000 0.00673300
 C 8.66474900 -1.53847900 0.00285600
 C -8.66474900 -1.53847900 0.00283200
 C -8.67053500 -4.35240900 -0.00004900
 H -8.67855800 -5.43855700 -0.00120500
 C -9.87541300 -3.64226500 0.00221700
 H -10.81598100 -4.18338900 0.00287800
 C 9.87787100 -2.25981600 0.00364500
 H 10.81501400 -1.71084200 0.00540700
 C 8.67053500 -4.35240900 -0.00012200
 H 8.67855800 -5.43855700 -0.00131600
 C 3.70022800 2.69835600 -0.00062000
 C 0.00000000 0.57258400 -0.00059800
 C -2.46908900 4.81030500 -0.00279100
 H -2.46276600 5.89646000 -0.00380200
 C -7.44759200 -3.68180200 -0.00087400
 C -7.43607500 -2.25841400 0.00063200
 C 4.97108900 -2.27505300 -0.00228100
 C -6.20003900 2.67154000 0.00346000
 H -6.22533900 3.75345000 0.00478400
 C 6.18774400 -4.38344500 -0.00334200
 C 7.44759300 -3.68180200 -0.00094900
 C -9.87787100 -2.25981600 0.00362000
 H -10.81501400 -1.71084200 0.00534300
 C 9.87541400 -3.64226400 0.00219500
 H 10.81598100 -4.18338900 0.00285700
 H 0.00000000 5.88685700 -0.00345600
 H 9.55956000 0.43070500 0.00589600

H 6.20613900 -5.46956700 -0.00463400
H -6.20613900 -5.46956700 -0.00446800
C -8.62343700 -0.12241100 0.00412300
H -9.55956000 0.43070500 0.00578700

truncated OR-3 (cation state)

C -3.76445600 -1.58298900 -0.00053500
H -2.85331300 -2.16952500 -0.00079400
C -3.71015000 -0.18560300 -0.00034700
C -2.46462000 1.97857000 -0.00024700
C 1.23169100 2.69232700 -0.00024600
C -1.22569200 -0.11183500 -0.00061400
H -1.18216900 -1.19528700 -0.00082500
C 2.44961800 0.54271600 -0.00041900
C -3.69213500 2.69616900 -0.00009100
C 3.64313900 4.12960000 -0.00007100
H 4.56231800 4.69970200 -0.00010800
C -2.44961900 0.54271600 -0.00041200
C 1.22569200 -0.11183500 -0.00061700
H 1.18216900 -1.19528700 -0.00082700
C -4.96813400 -2.28137400 -0.00039000
C -3.64313900 4.12960000 -0.00006100
H -4.56231800 4.69970200 -0.00009300
C -1.21859100 4.12134200 -0.00011500
C -4.92533100 1.98558900 0.00005900
C -4.93252800 0.55388100 -0.00005600
C 2.46461900 1.97857000 -0.00025200
C 0.00000000 1.99936500 -0.00034900
C -6.19478900 -1.55589500 -0.00002700
C -6.16924400 -0.14511200 0.00012100
C 4.92533100 1.98558900 0.00005500
C 7.41282200 0.56990100 0.00045300

C -1.23169100 2.69232700 -0.00024200
C 4.93252900 0.55388100 -0.00005900
C -6.19203200 -4.38349000 -0.00037800
C 3.76445600 -1.58298900 -0.00055000
H 2.85331300 -2.16952500 -0.00081700
C 0.00000000 4.80114300 -0.00006500
C 3.71015000 -0.18560300 -0.00035600
C 6.16924400 -0.14511200 0.00012000
C -7.36768800 2.00125200 0.00056600
H -8.30532100 2.54936200 0.00080200
C 6.19479000 -1.55589500 -0.00003100
C -7.41282200 0.56990100 0.00044800
C 6.18766300 2.67047600 0.00038600
H 6.21185300 3.75116300 0.00052500
C 2.46886400 4.81135900 -0.00008000
H 2.46456400 5.89669900 -0.00006900
C -5.01103300 -3.71994800 -0.00057300
H -4.07134900 -4.26366000 -0.00087700
C 7.43087100 -2.25451700 0.00017400
C 8.61184400 -0.11810500 0.00067000
C 5.01103300 -3.71994800 -0.00059000
H 4.07134900 -4.26366000 -0.00090200
C 1.21859000 4.12134300 -0.00011900
C 7.36768800 2.00125200 0.00057200
H 8.30532100 2.54936200 0.00081000
C 8.65687300 -1.53280600 0.00054500
C -8.65687300 -1.53280600 0.00053600
C -8.67402800 -4.33844400 0.00022100
H -8.68768600 -5.42454400 0.00009600
C -9.87950600 -3.62744200 0.00059000
H -10.82024000 -4.16651800 0.00075700
C 9.87532900 -2.24527100 0.00075700

H 10.80979600 -1.69217500 0.00105400
 C 8.67402800 -4.33844400 0.00022300
 H 8.68768600 -5.42454400 0.00009500
 C 3.69213500 2.69616900 -0.00009800
 C 0.00000000 0.57641200 -0.00054600
 C -2.46886400 4.81135900 -0.00007100
 H -2.46456400 5.89669900 -0.00005800
 C -7.44695500 -3.67524500 0.00000900
 C -7.43087100 -2.25451700 0.00017400
 C 4.96813400 -2.28137400 -0.00040300
 C -6.18766300 2.67047500 0.00038500
 H -6.21185300 3.75116200 0.00052500
 C 6.19203200 -4.38349000 -0.00039100
 C 7.44695500 -3.67524500 0.00000600
 C -9.87532900 -2.24527100 0.00074300
 H -10.80979600 -1.69217500 0.00103400
 C 9.87950600 -3.62744200 0.00060100
 H 10.82024000 -4.16651800 0.00077200
 H 0.00000000 5.88768200 0.00003300
 H 9.54591700 0.43874200 0.00093700
 H 6.21454800 -5.46920200 -0.00052600
 H -6.21454800 -5.46920200 -0.00051000
 C -8.61184400 -0.11810500 0.00066000
 H -9.54591700 0.43874200 0.00092200

truncated OR-3 (radical dication state)

C -3.78030700 -1.57851600 -0.00255800
 H -2.87295100 -2.17088100 -0.00422000
 C -3.72155200 -0.19334600 -0.00114900
 C -2.46410600 1.97102500 -0.00109700
 C 1.23315300 2.68168300 -0.00153200
 C -1.23129700 -0.12157600 -0.00082200

H -1.18719900 -1.20463100 -0.00035900
 C 2.44979100 0.53350200 -0.00107200
 C -3.68725200 2.69446100 -0.00055100
 C 3.64534000 4.11416900 -0.00126800
 H 4.56196900 4.68750700 -0.00141900
 C -2.44979100 0.53350200 -0.00106100
 C 1.23129700 -0.12157600 -0.00082900
 H 1.18719900 -1.20463100 -0.00036300
 C -4.99782800 -2.28335700 -0.00206100
 C -3.64534000 4.11416900 -0.00131600
 H -4.56196900 4.68750700 -0.00147300
 C -1.22241800 4.10850500 -0.00198300
 C -4.94458500 1.97687400 0.00083300
 C -4.94750200 0.55441600 0.00029300
 C 2.46410600 1.97102500 -0.00108300
 C 0.00000000 1.98657500 -0.00145900
 C -6.21617400 -1.55435800 -0.00007000
 C -6.18520900 -0.14055700 0.00102700
 C 4.94458500 1.97687400 0.00091600
 C 7.41986400 0.57789000 0.00298700
 C -1.23315300 2.68168300 -0.00154100
 C 4.94750200 0.55441600 0.00032200
 C -6.22888000 -4.37622400 -0.00267200
 C 3.78030700 -1.57851600 -0.00268100
 H 2.87295200 -2.17088100 -0.00441600
 C 0.00000000 4.79172300 -0.00230600
 C 3.72155200 -0.19334600 -0.00118500
 C 6.18520900 -0.14055700 0.00106100
 C -7.38078700 1.99742000 0.00385300
 H -8.31492800 2.55097300 0.00544900
 C 6.21617400 -1.55435800 -0.00011400
 C -7.41986400 0.57789000 0.00287400

C 6.18828400 2.66668700 0.00297100
 H 6.21257000 3.74724000 0.00392600
 C 2.46165500 4.80015400 -0.00204600
 H 2.46034900 5.88553600 -0.00267400
 C -5.03931000 -3.71283200 -0.00341000
 H -4.10346100 -4.26225500 -0.00500900
 C 7.45240500 -2.24647400 0.00063400
 C 8.63347100 -0.11580500 0.00386500
 C 5.03931000 -3.71283200 -0.00362600
 H 4.10346100 -4.26225400 -0.00529300
 C 1.22241800 4.10850500 -0.00197000
 C 7.38078700 1.99742000 0.00404100
 H 8.31492800 2.55097300 0.00570700
 C 8.67886700 -1.52058900 0.00272700
 C -8.67886700 -1.52058900 0.00268400
 C -8.71058000 -4.32257500 0.00028500
 H -8.72743400 -5.40885900 -0.00066300
 C -9.91503600 -3.61307500 0.00232400
 H -10.85633500 -4.15010000 0.00296500
 C 9.90449900 -2.22958200 0.00355000
 H 10.83707300 -1.67313900 0.00518400
 C 8.71058000 -4.32257500 0.00016400
 H 8.72743400 -5.40885900 -0.00084800
 C 3.68725200 2.69446100 -0.00050300
 C 0.00000000 0.56917300 -0.00101700
 C -2.46165500 4.80015400 -0.00207400
 H -2.46034900 5.88553600 -0.00269900
 C -7.47219800 -3.66255400 -0.00057000
 C -7.45240500 -2.24647400 0.00067600
 C 4.99782800 -2.28335700 -0.00219000
 C -6.18828400 2.66668700 0.00280000
 H -6.21257100 3.74724000 0.00369300

C 6.22888000 -4.37622400 -0.00288600
 C 7.47219900 -3.66255300 -0.00069600
 C -9.90449900 -2.22958200 0.00350400
 H -10.83707400 -1.67313900 0.00507200
 C 9.91503600 -3.61307500 0.00228900
 H 10.85633500 -4.15010000 0.00293200
 H 0.00000000 5.87849300 -0.00273800
 H 9.56451000 0.44643300 0.00545000
 H 6.25290300 -5.46168800 -0.00395200
 H -6.25290200 -5.46168800 -0.00367200
 C -8.63347100 -0.11580500 0.00374500
 H -9.56451000 0.44643300 0.00526400

truncated [tips-OR-3]₂ (neutral radical•radical state)

C 3.75553600 -1.32606700 -1.64375600
 H 2.83938500 -1.90633100 -1.64526100
 C 3.70918000 0.07419400 -1.58337000
 C 2.47196000 2.22809500 -1.44535900
 C -1.23438600 2.94034600 -1.37477200
 C 1.22598900 0.13729300 -1.48907900
 H 1.18185700 -0.94642100 -1.50385600
 C -2.45348500 0.79659100 -1.51627300
 C 3.70227800 2.94198800 -1.43307000
 C -3.64957300 4.37099000 -1.31757200
 H -4.57223600 4.93626400 -1.28157500
 C 2.45352500 0.79662800 -1.51613100
 C -1.22594800 0.13724400 -1.48951400
 H -1.18180200 -0.94647400 -1.50455400
 C 4.95156300 -2.02855600 -1.68014800
 C 3.64962400 4.37101700 -1.31782800
 H 4.57229100 4.93630000 -1.28196500

C 1.22038900 4.36432800 -1.27816400	H -8.32230900 2.77568900 -1.43935000
C 4.93666000 2.23433900 -1.50180400	C -8.64724500 -1.30974000 -1.62295600
C 4.93577500 0.80758000 -1.57497600	C 8.64723900 -1.30979800 -1.62301700
C -2.47192300 2.22805000 -1.44529500	C 8.63851900 -4.12447400 -1.68032700
C 0.00001100 2.24676900 -1.40904200	H 8.64234300 -5.21063800 -1.70156000
C 6.18513700 -1.31331800 -1.66485500	C 9.84810200 -3.41994400 -1.61783200
C 6.16997300 0.09845200 -1.61568200	H 10.78534300 -3.96666000 -1.59328500
C -4.93662000 2.23433700 -1.50169700	C -9.85692600 -2.03875900 -1.58944400
C -7.41957700 0.80496100 -1.57283100	H -10.79602600 -1.49433000 -1.54195100
C 1.23441200 2.94036600 -1.37482700	C -8.63856800 -4.12441300 -1.68027800
C -4.93574100 0.80757600 -1.57492500	H -8.64240700 -5.21057700 -1.70153500
C 6.15648900 -4.14391200 -1.72963700	C -3.70223500 2.94196100 -1.43289900
C -3.75552800 -1.32608600 -1.64390200	C 0.00000200 0.82224200 -1.47535300
H -2.83940100 -1.90641100 -1.64567000	C 2.47389200 5.04924300 -1.24131100
C -3.70915100 0.07417600 -1.58346200	H 2.47077100 6.13228100 -1.15676100
C -6.16995500 0.09847500 -1.61562700	C 7.42187500 -3.44820500 -1.70648900
C 7.38071200 2.23561300 -1.50056500	C 7.41662900 -2.02312400 -1.67676100
H 8.32235100 2.77563100 -1.43919400	C -4.95157800 -2.02854200 -1.68022900
C -6.18514300 -1.31329200 -1.66481400	C 6.20207100 2.90833900 -1.47626600
C 7.41960200 0.80492200 -1.57286900	H 6.23236300 3.98814000 -1.40827700
C -6.20202700 2.90835700 -1.47623700	C -6.15654000 -4.14388100 -1.72968300
H -6.23231500 3.98816200 -1.40834700	C -7.42191400 -3.44816000 -1.70643500
C -2.47385200 5.04922600 -1.24109100	C 9.85691000 -2.03883600 -1.58949300
H -2.47073500 6.13225700 -1.15646400	H 10.79601800 -1.49442200 -1.54198500
C 4.98341900 -3.46933400 -1.71561000	C -9.84814000 -3.41986700 -1.61778300
H 4.03590100 -4.00175900 -1.71203700	H -10.78538900 -3.96657100 -1.59324700
C -7.41664600 -2.02308100 -1.67668900	C -3.75554500 1.32608600 1.64393300
C -8.61258000 0.10491800 -1.56944300	H -2.83941800 1.90641300 1.64573100
C -4.98346200 -3.46931800 -1.71574800	C -3.70916600 -0.07417400 1.58346700
H -4.03595300 -4.00175700 -1.71232100	C -2.47193500 -2.22804600 1.44526800
C -1.22035100 4.36431500 -1.27806600	C 1.23440000 -2.94035500 1.37472200
C -7.38067400 2.23565300 -1.50058600	C -1.22596500 -0.13723800 1.48947900

H -1.18182400 0.94648000 1.50452100	C 6.20205700 -2.90834200 1.47622900
C 2.45351500 -0.79661800 1.51604500	H 6.23234400 -3.98814400 1.40823600
C -3.70224600 -2.94195900 1.43288100	C 2.47388000 -5.04923000 1.24116700
C 3.64961200 -4.37100500 1.31768700	H 2.47075900 -6.13226600 1.15659500
H 4.57228000 -4.93628600 1.28179700	C -4.98348100 3.46931500 1.71582500
C -2.45349900 -0.79658700 1.51625900	H -4.03597300 4.00175500 1.71240900
C 1.22597700 -0.13728400 1.48901200	C 7.41662900 2.02311500 1.67682600
H 1.18184300 0.94643000 1.50381800	C 8.61258900 -0.10486900 1.56950100
C -4.95159600 2.02854100 1.68027500	C 4.98342300 3.46933400 1.71567700
C -3.64958300 -4.37098700 1.31755300	H 4.03590700 4.00176200 1.71210800
H -4.57224500 -4.93626500 1.28158400	C 1.22037700 -4.36431600 1.27804700
C -1.22036300 -4.36430700 1.27799500	C 7.38070000 -2.23562100 1.50055900
C -4.93663200 -2.23433600 1.50167900	H 8.32233800 -2.77564200 1.43920900
C -4.93575500 -0.80757600 1.57492100	C 8.64723700 1.30978600 1.62308900
C 2.47194900 -2.22808500 1.44525100	C -8.64726200 1.30973400 1.62299400
C -0.00000100 -2.24676000 1.40896400	C -8.63858800 4.12440700 1.68037700
C -6.18516000 1.31328900 1.66484600	H -8.64242800 5.21057000 1.70165700
C -6.16997100 -0.09847700 1.61563200	C -9.84816000 3.41986100 1.61787000
C 4.93664900 -2.23433600 1.50173200	H -10.78540900 3.96656400 1.59334900
C 7.41959400 -0.80492900 1.57286900	C 9.85691100 2.03882100 1.58961700
C -1.23439700 -2.94033900 1.37471300	H 10.79601900 1.49440500 1.54211700
C 4.93576600 -0.80757700 1.57492100	C 8.63852600 4.12446100 1.68050100
C -6.15656000 4.14387700 1.72977500	H 8.64235400 5.21062400 1.70177600
C 3.75553400 1.32607300 1.64372100	C 3.70226700 -2.94198000 1.43295900
H 2.83938600 1.90634100 1.64522000	C -0.00001100 -0.82223300 1.47528800
C 0.00000100 -5.04040200 1.22506800	C -2.47386200 -5.04922000 1.24104700
C 3.70917300 -0.07418700 1.58330500	H -2.47074400 -6.13225200 1.15642300
C 6.16996700 -0.09845500 1.61566300	C -7.42193400 3.44815500 1.70651600
C -7.38068700 -2.23565400 1.50055300	C -7.41666400 2.02307600 1.67673900
H -8.32232100 -2.77569100 1.43930700	C 4.95156300 2.02855700 1.68015900
C 6.18513500 1.31331500 1.66486800	C -6.20203800 -2.90835700 1.47620200
C -7.41959100 -0.80496400 1.57282400	H -6.23232500 -3.98816000 1.40829200

C 6.15649500 4.14390600 1.72976000
 C 7.42187900 3.44819600 1.70660800
 C -9.85694400 2.03875300 1.58950000
 H -10.79604400 1.49432400 1.54199800
 C 9.84810800 3.41992800 1.61800500
 H 10.78535100 3.96664200 1.59350200
 H -0.00000600 -6.12547000 1.15144000
 H 6.16965600 -5.23045900 -1.75101700
 H -6.16972100 -5.23042800 -1.75111900
 H 9.54958800 -0.65462800 1.50993300
 H -9.54957200 0.65469000 -1.50992400
 H 6.16966500 5.23045300 1.75118400
 H -6.16974200 5.23042300 1.75123200
 C -8.61259500 -0.10492200 1.56945000
 H -9.54958700 -0.65469400 1.50992200
 C 0.00001200 5.04041200 -1.22516900
 H 0.00000500 6.12548100 -1.15154900
 C 8.61259500 0.10485800 -1.56946200
 H 9.54959400 0.65461500 -1.50987800

truncated [tips-OR-3]₂ (neutral radical•cation state)

C -3.75749300 -1.33797600 1.64809000
 H -2.84411000 -1.92238300 1.64840400
 C -3.70857500 0.06098900 1.59494900
 C -2.46893100 2.21804100 1.45114100
 C 1.23327300 2.92961100 1.37584300
 C -1.22558300 0.12898900 1.53810400
 H -1.18101800 -0.95447400 1.57589100
 C 2.45169400 0.78613400 1.53623100
 C -3.69730500 2.93378400 1.43503000
 C 3.64695500 4.36168500 1.31059900

H 4.56884700 4.92747500 1.27320600
 C -2.45176500 0.78608200 1.53626500
 C 1.22551700 0.12902300 1.53783100
 H 1.18099900 -0.95445400 1.57534300
 C -4.95777600 -2.03723400 1.68184300
 C -3.64710100 4.36167200 1.31162900
 H -4.56899400 4.92749400 1.27475800
 C -1.21990700 4.35366100 1.26864900
 C -4.93101700 2.22602700 1.51252900
 C -4.93314400 0.79743400 1.58280100
 C 2.46883500 2.21806300 1.45082800
 C -0.00005300 2.23695800 1.41809100
 C -6.18807200 -1.31749000 1.66627500
 C -6.16815500 0.09365200 1.62201200
 C 4.93090300 2.22611600 1.51196900
 C 7.41441600 0.80478500 1.58632700
 C -1.23339000 2.92960500 1.37608600
 C 4.93305800 0.79753700 1.58255100
 C -6.17194100 -4.14672700 1.71721100
 C 3.75743600 -1.33788100 1.64893200
 H 2.84404300 -1.92229800 1.65066800
 C 3.70850200 0.06106400 1.59503500
 C 6.16808600 0.09380500 1.62195300
 C -7.37346700 2.23507200 1.52342000
 H -8.31388400 2.77855500 1.47862400
 C 6.18803300 -1.31732200 1.66658200
 C -7.41450200 0.80460200 1.58648100
 C 6.19378600 2.90623400 1.49585400
 H 6.22105900 3.98622900 1.44189000
 C 2.47207400 5.04017300 1.22771000
 H 2.46890200 6.12220200 1.13750700
 C -4.99464800 -3.47734600 1.70992300

H -4.05026200 -4.01462300 1.71208200
 C 7.42189400 -2.02156200 1.67596800
 C 8.61023800 0.11067200 1.58981100
 C 4.99467100 -3.47719100 1.71120000
 H 4.05030400 -4.01449800 1.71371100
 C 1.21975400 4.35365500 1.26829300
 C 7.37334600 2.23524400 1.52302600
 H 8.31375200 2.77874600 1.47825500
 C 8.64992600 -1.30444600 1.63212800
 C -8.64996200 -1.30467400 1.63182100
 C -8.65383900 -4.11515200 1.66839300
 H -8.66315900 -5.20125400 1.68454700
 C -9.86157900 -3.40752700 1.61773600
 H -10.80028200 -3.95059900 1.59634300
 C 9.86374300 -2.02520100 1.60117800
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 C 8.65387700 -4.11491300 1.66944100
 H 8.66322600 -5.20100900 1.68590000
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 H -2.46909800 6.12223100 1.13860100
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 C -7.42191300 -2.02176900 1.67549500
 C 4.95774900 -2.03709000 1.68260800
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 C 6.17198400 -4.14653800 1.71845900
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 C -9.86376100 -2.02545300 1.60066900
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 C 9.86159800 -3.40726900 1.61859400

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 C 3.75748600 1.33787500 -1.64896200
 H 2.84408900 1.92228700 -1.65071800
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 C 2.46889700 -2.21807400 -1.45089600
 C -1.23332700 -2.92962300 -1.37620600
 C 1.22557400 -0.12904200 -1.53802400
 H 1.18105000 0.95443200 -1.57559900
 C -2.45169700 -0.78610600 -1.53647500
 C 3.69725200 -2.93383700 -1.43442000
 C -3.64704000 -4.36168100 -1.31165500
 H -4.56893400 -4.92749800 -1.27474000
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 C -1.22551900 -0.12901300 -1.53836100
 H -1.18095400 0.95444800 -1.57619800
 C 4.95779800 2.03709000 -1.68258400
 C 3.64701900 -4.36168800 -1.31058600
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 C 1.21981600 -4.35366600 -1.26833200
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 C 4.93311700 -0.79753800 -1.58255600
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 C 0.00000900 -2.23697600 -1.41823300
 C 6.18808400 1.31732800 -1.66652600
 C 6.16814300 -0.09380000 -1.62191200
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 C -7.41442900 -0.80459200 -1.58644200
 C 1.23333500 -2.92962500 -1.37593100
 C -4.93307300 -0.79744500 -1.58291300
 C 6.17202400 4.14654500 -1.71836000
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 H 8.31381800 -2.77873100 -1.47816200
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 C -7.42182100 2.02178000 -1.67543500
 C -8.61022900 -0.11043300 -1.58965500
 C -4.99454500 3.47733600 -1.71007400
 H -4.05015400 4.01460400 -1.71231000
 C -1.21984500 -4.35367400 -1.26870500
 C -7.37340200 -2.23506300 -1.52338400
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 C -8.64987300 1.30469600 -1.63166100
 C 8.64997600 1.30446300 -1.63199200
 C 8.65391500 4.11493100 -1.66926900
 H 8.66325900 5.20102700 -1.68571400
 C 9.86163700 3.40729300 -1.61839700
 H 10.80035200 3.95035000 -1.59713100
 C -9.86366300 2.02548600 -1.60040000
 H -10.80075200 1.47707400 -1.56613700
 C -8.65372700 4.11517400 -1.66820700
 H -8.66303800 5.20127600 -1.68435600
 C -3.69724300 -2.93379800 -1.43511200
 C 0.00001400 -0.81535800 -1.50860000

C 2.47213800 -5.04017800 -1.22770200
 H 2.46896700 -6.12220400 -1.13746300
 C 7.43252600 3.44475100 -1.69668600
 C 7.42194200 2.02157400 -1.67586100
 C -4.95768500 2.03722300 -1.68199800
 C 6.19385200 -2.90622900 -1.49582200
 H 6.22112900 -3.98622400 -1.44186200
 C -6.17183300 4.14672700 -1.71725500
 C -7.43235800 3.44496400 -1.69585100
 C 9.86378900 2.02522400 -1.60099900
 H 10.80086300 1.47679100 -1.56666400
 C -9.86146900 3.40756000 -1.61745400
 H -10.80016600 3.95064000 -1.59597800
 H -0.00003200 -6.11425100 -1.13009300
 H -6.18963900 -5.23298100 1.73738200
 H 6.18971500 -5.23278600 1.73893600
 H -9.54564700 -0.66424200 -1.54471400
 H 9.54564300 0.66450100 1.54485000
 H -6.18952300 5.23298100 -1.73742100
 H 6.18975000 5.23279300 -1.73881900
 C 8.61029400 -0.11065500 -1.58969400
 H 9.54570000 -0.66448000 -1.54470700
 C -0.00008400 5.03022200 1.21014400
 H -0.00009500 6.11424500 1.13011600
 C -8.61030800 0.11045400 1.58979200
 H -9.54572400 0.66427100 1.54492500

truncated [tips-OR-3]₂ (cation•cation state)

C -3.76657200 1.34023200 -1.65660400
 H -2.85723500 1.93095600 -1.64981100
 C -3.71128100 -0.05663200 -1.61366800
 C -2.46550100 -2.21316900 -1.44748400

C 1.23209100 -2.92188900 -1.35958000	C -7.41184300 -0.82355700 -1.62126000
C -1.22652900 -0.12675400 -1.60390800	C 6.18323300 -2.91950700 -1.53540100
H -1.18359300 0.95467700 -1.68566300	H 6.20427900 -3.99991400 -1.50205700
C 2.45069800 -0.78133300 -1.56019600	C 2.46891900 -5.03490900 -1.18208800
C -3.69146400 -2.93276800 -1.42811000	H 2.46451800 -6.11505400 -1.07566900
C 3.64297100 -4.35845100 -1.28259100	C -5.01994100 3.47196400 -1.70734700
H 4.56385800 -4.92498000 -1.24033300	H -4.08048100 4.01722200 -1.71409000
C -2.45049900 -0.78126700 -1.55982400	C 7.43738000 2.00106700 -1.68234500
C 1.22672900 -0.12678900 -1.60409900	C 8.61277400 -0.13876000 -1.63416900
H 1.18380600 0.95465000 -1.68575400	C 5.02026500 3.47181900 -1.70883700
C -4.97382400 2.03368200 -1.68980800	H 4.08081700 4.01708500 -1.71640000
C -3.64284200 -4.35838200 -1.28257800	C 1.21877100 -4.34557400 -1.22944000
H -4.56374300 -4.92488800 -1.24032500	C 7.36554100 -2.25394000 -1.57375100
C -1.21864100 -4.34555200 -1.22940600	H 8.30313700 -2.80355000 -1.55641200
C -4.92467600 -2.22956200 -1.53115500	C 8.66114800 1.27625400 -1.65509700
C -4.93257800 -0.79926800 -1.60011600	C -8.66088100 1.27643700 -1.65560700
C 2.46566900 -2.21321700 -1.44767300	C -8.68592100 4.08303300 -1.66056600
C 0.00008600 -2.22958700 -1.41523000	H -8.70367100 5.16917900 -1.66807500
C -6.19881600 1.30615700 -1.67644900	C -9.88960900 3.36906700 -1.62793100
C -6.17033900 -0.10459000 -1.64132000	H -10.83160800 3.90571300 -1.61061200
C 4.92485100 -2.22965900 -1.53101500	C 9.88128300 1.98562400 -1.62757800
C 7.41206800 -0.82371300 -1.62066700	H 10.81493600 1.43070200 -1.61221100
C -1.23193300 -2.92186700 -1.35949200	C 8.68623400 4.08284900 -1.66077000
C 4.93278900 -0.79937300 -1.60018400	H 8.70400600 5.16899100 -1.66857300
C -6.20395800 4.13319200 -1.70648500	C 3.69162500 -2.93284000 -1.42817200
C 3.76683200 1.34012300 -1.65775900	C 0.00009800 -0.81233500 -1.54814900
H 2.85751500 1.93088800 -1.65192000	C -2.46879900 -5.03486100 -1.18205100
C 3.71149800 -0.05672600 -1.61420900	H -2.46442000 -6.11500700 -1.07563200
C 6.17057400 -0.10473200 -1.64123800	C -7.45693300 3.42206700 -1.68857800
C -7.36535200 -2.25379000 -1.57458800	C -7.43709100 2.00123900 -1.68227400
H -8.30296100 -2.80339000 -1.55763600	C 4.97411400 2.03353800 -1.69077400
C 6.19908900 1.30600500 -1.67671200	C -6.18306100 -2.91938800 -1.53599400

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C 6.20428900 4.13303100 -1.70769000	C 1.23185200 2.92186700 1.35912400
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C -9.88101600 1.98582100 -1.62832600	C 6.20412400 -4.13302300 1.70734500
H -10.81468200 1.43090800 -1.61340800	C -3.76680400 -1.34024100 1.65696000
C 9.88989800 3.36887100 -1.62752300	H -2.85746700 -1.93096700 1.65036400
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C 2.46544100 2.21317900 1.44694000	H 8.30288000 2.80359500 1.55688800
C -1.23217400 2.92187000 1.35957100	C -6.19904900 -1.30616900 1.67654500
C 1.22651600 0.12674300 1.60340500	C 7.41182500 0.82375000 1.62101500
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C -3.64307800 4.35846200 1.28361600	H -2.46467100 6.11511800 1.07690100
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C 2.45047500 0.78128500 1.55935000	H 4.08064400 -4.01713000 1.71476700
C -1.22674700 0.12672600 1.60359900	C -7.43732700 -2.00125800 1.68226200
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C 1.21852500 4.34556300 1.22915600	C -7.36559400 2.25376700 1.57444700
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C 6.17034200 0.10474200 1.64113700	C 9.88975400 -3.36877400 1.62902300
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H 6.20401100 3.99991700 1.50168900
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H 10.81475500 -1.43058500 1.61413200
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H -6.22898100 5.21925000 -1.72296600
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H 9.54504700 -0.69936200 -1.61198300
H -6.22922200 -5.21926100 1.72344200
H 6.22919900 -5.21907500 1.72412500
C 8.61254500 0.13882400 1.63505100
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H 0.00005400 -6.10437600 -1.06383000
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