Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

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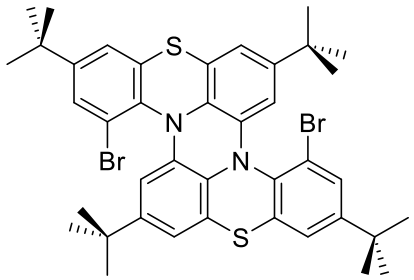
1. General remarks

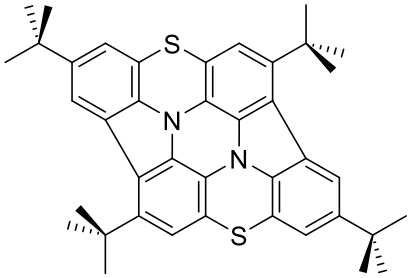
All reagents and solvents were commercially available and were used without further purification unless otherwise noted. For thin layer chromatography Silica gel 60 F254 plates from Merck were used and examined under UV-light irradiation (254 nm and 365 nm). Flash column chromatography was performed on silica gel (particle size: 200-300 mesh). Melting points were measured with a MPA100 OptiMelt. IR-Spectra were recorded as KBr-pellets on a Bruker VERTEX 80V spectrometer. NMR spectra were taken on Bruker AVANCE NEO (400 MHz). Chemical shifts (δ) are reported in parts per million (ppm) relative to traces of C_6H_6 in the deuterated solvent. HRMS experiments were carried out on a ThermoFisher LTQ Orbitrap XL. Absorption spectra were recorded on a Shimadzu UV2600. Emission spectra, absolute quantum yields, as well as fluorescence lifetimes were measured on FluoroMax-4 spectrometer equipped with an integral sphere and a time-correlated single photon counting system with a NanoLED laser. Crystal structure analysis was accomplished with SuperNova Dual AtlasS2 diffractometer with a Cu source. Electrochemical data were obtained in dichloromethane solution of tetrabutylammonium hexafluorophosphate (0.1 M) with ferrocene as an internal standard. Cyclic voltammograms (CV) was obtained using a glassy carbon working electrode, a platinum counter electrode, and a silver wire reference electrode tested on CHI660E station. EPR spectrum was measured on a Bruker EMX 10/12 apparatus. 1,9-dibromo-3,7-di-*tert*-butylphenothiazine **4** was synthesized according to the reported method.[S1]

2. Experimental section

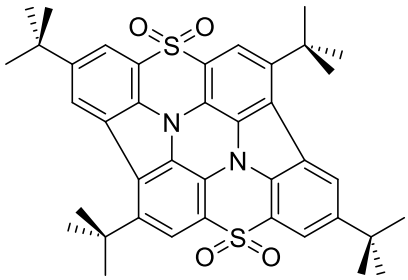


A 38 mL screw capped glass vial was charged with 1,9-dibromo-3,7-di-*tert*-butylphenothiazine **4** (1.88 g, 4 mmol), CuI (152 mg, 0.8 mmol), 18-crown-6 (211 mg, 0.8 mmol) and anhydrous K_2CO_3 (830 mg, 6 mmol). Under the protection of argon, dry *o*-dichlorobenzene (6 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 180 ºC for 2 days. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 1:50) to give the product **5** as pale yellow solid (1.18 g, 76%). m.p. 338-339 ºC; ^{1}H NMR (400 MHz, benzene-d_6) δ (ppm) = 7.52 (d, J = 2.1 Hz, 2H), 7.26 (d, J = 2.1 Hz, 2H), 7.00 (d, J = 1.8 Hz, 2H), 6.93 (d, J = 1.7 Hz, 2H), 1.06 (s, 18H), 0.99 (s, 18H); ^{13}C NMR (100 MHz,

benzene-d_6) δ (ppm) = 149.4, 148.4, 137.9, 135.4, 134.7, 132.4, 130.8, 125.2, 124.5, 118.3, 115.2, 114.6, 34.5, 34.3, 31.2, 31.0; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3070, 2960, 2910, 2869, 1620, 1575, 1475, 1448, 1408, 1329, 1261, 1221, 1122, 1020, 866, 739, 694, 624, 603, 472; HRMS(ESI) (*m/z*) : $[M]^+$ calcd. for $C_{40}H_{44}Br_2N_2S_2$, 776.1292; found, 776.1312.



A 38 mL screw capped glass vial was charged with compound **5** (466 mg, 0.60 mmol), $Pd(OAc)_2$ (27 mg, 0.12 mmol) and anhydrous K_2CO_3 (498 g, 3.6 mmol). Under the protection of argon, dry *N,N*-dimethylacetamide (2.4 mL) and PCy_3HBF_4 (88 mg, 0.24 mmol) were added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 170 °C for 48 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 1:50) to give the product **6** as yellow solid (181 mg, 49%). m.p. > 400 °C (dec.); ^{1}H NMR (400 MHz, benzene-d_6) δ (ppm) = 7.85 (d, J = 1.1 Hz, 2H), 7.07 (d, J = 1.1 Hz, 2H), 6.73 (s, 2H), 1.45 (s, 18H), 1.28 (s, 18H); ^{13}C NMR (100 MHz, benzene-d_6) δ (ppm) = 147.2, 145.6, 134.4, 132.0, 124.6, 121.2, 120.6, 120.5, 119.8, 117.1, 116.1, 110.6, 35.6, 35.4, 32.0, 29.8; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 2956, 2914, 2867, 1620, 1548, 1510, 1475, 1365, 1309, 1271, 1183, 11143, 1109, 1055, 926, 858, 729, 627, 606, 519, 472; HRMS(ESI) (*m/z*) : $[M]^+$ calcd. for $C_{40}H_{42}N_2S_2$, 614.2789; found, 614.2811.



A 100 mL single neck flask was charged with compound **6** (87 mg, 0.14 mmol), chloroform (8 mL), acetic acid (8 mL) and hydrogen peroxide aqueous solution (30%, 0.30 mL, 2.94 mmol). The reaction mixture was stirred at 60 °C for 12 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL) and washed with water (2 x 200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 2:1) to give the product **7** as yellow solid (67 mg, 70%). m.p. > 400 °C (dec.); ^{1}H NMR (400 MHz, benzene-d_6) δ (ppm) = 8.58 (d, J = 1.2 Hz, 2H), 8.25 (d, J = 1.2 Hz, 2H), 7.75 (s, 2H), 1.67 (s, 18H), 1.51 (s, 18H); ^{13}C NMR (100 MHz, benzene-d_6) δ (ppm) = 148.4, 147.4,

134.5, 130.6, 128.7, 126.1, 124.7, 124.3, 121.8, 121.0, 119.4, 113.9, 36.2, 36.1, 31.9, 29.4; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3072, 2960, 2875, 1624, 1493, 1396, 1367, 1315, 1138, 887, 822, 777, 748, 706, 658, 615, 571, 544, 492; HRMS(ESI) (*m/z*) : $[M]^+$ calcd. for $C_{40}H_{42}N_2S_2$, 678.2586; found, 678.2610.

Chemical oxidation of 6 with $AgSbF_6$

Compound **6** (31 mg, 0.05 mmol) was dissolved in dry dichloromethane (10 mL) and $AgSbF_6$ (18 mg, 0.05 mmol) was quickly added in solution. The reaction was stirred at room temperature for 20 minutes. The solution was then passed through a PTFE filter to the remove the Ag powder. After removal of the solvent by rotatory evaporation, the obtained powder was washed with hexane to give the monocation $\mathbf{6}^{\bullet+}SbF_6^-$ (33 mg, 77%).

Compound **6** (31 mg, 0.05 mmol) was dissolved in dry dichloromethane (10 mL) and $AgSbF_6$ (36 mg, 0.1 mmol) was quickly added in solution. The reaction was stirred at room temperature for 20 minutes. The solution was then passed through a PTFE filter to the remove the Ag powder. After removal of the solvent by rotatory evaporation, the obtained powder was washed with hexane to the dication $\mathbf{6}^{2+}[SbF_6]^{2-}$ (52 mg, 96%).

3. NMR Spectra

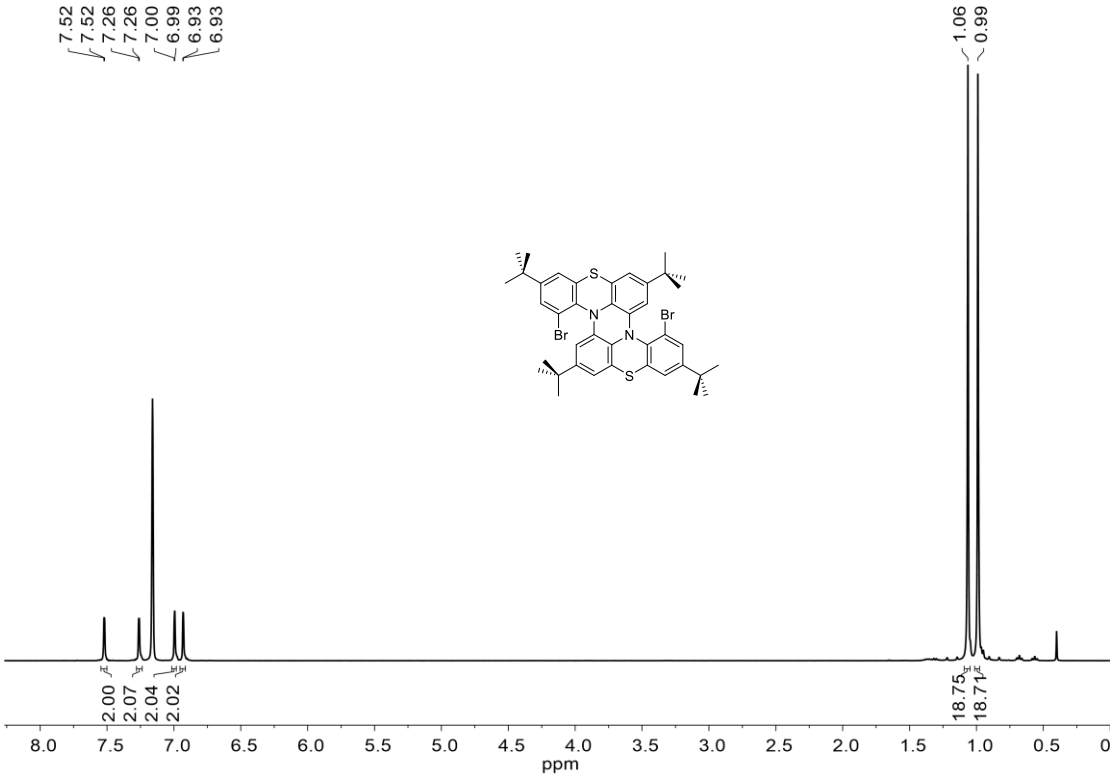


Figure S1. ^{1}H NMR spectrum (400 MHz, C_6D_6) of compound **5**.

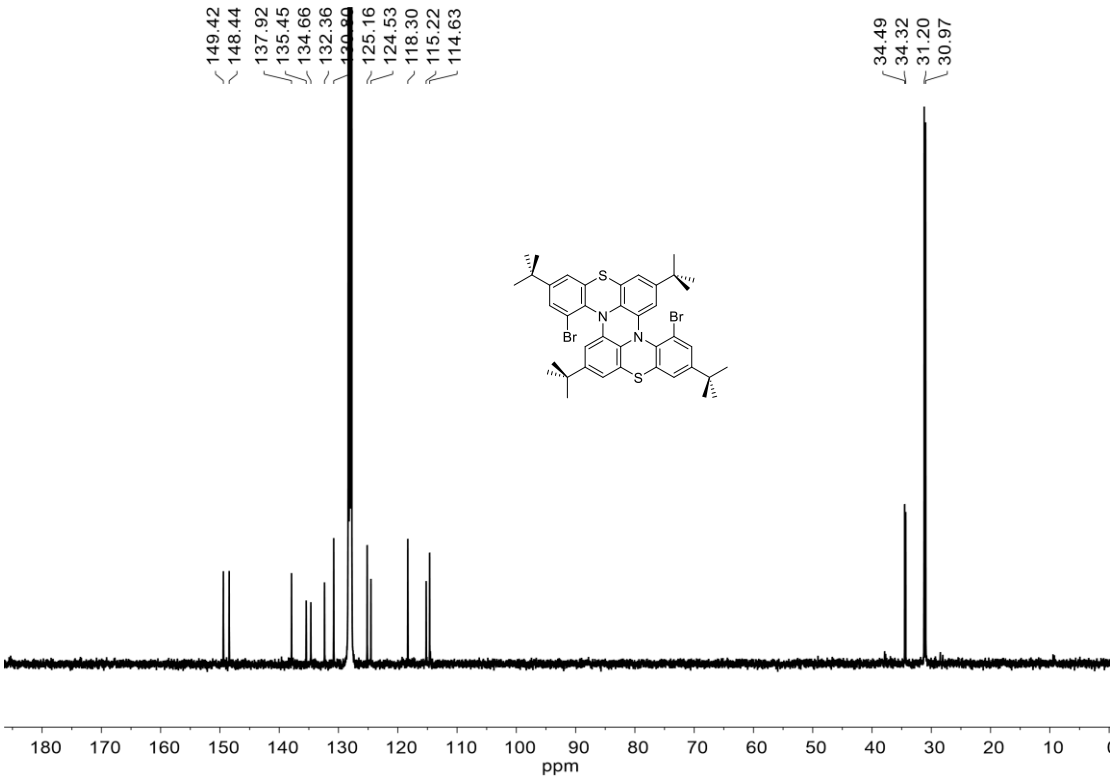


Figure S2. ^{13}C NMR spectrum (100 MHz, C_6D_6) of compound **5**.

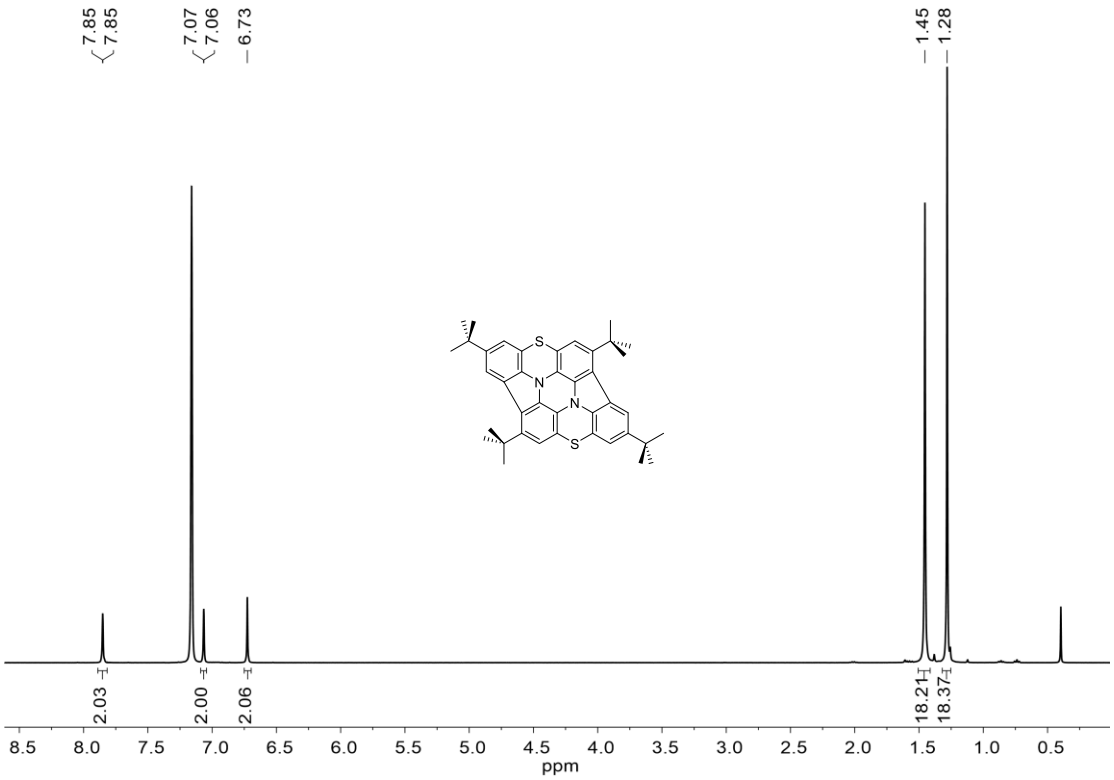


Figure S3. ^{1}H NMR spectrum (400 MHz, C_6D_6) of compound **6**.

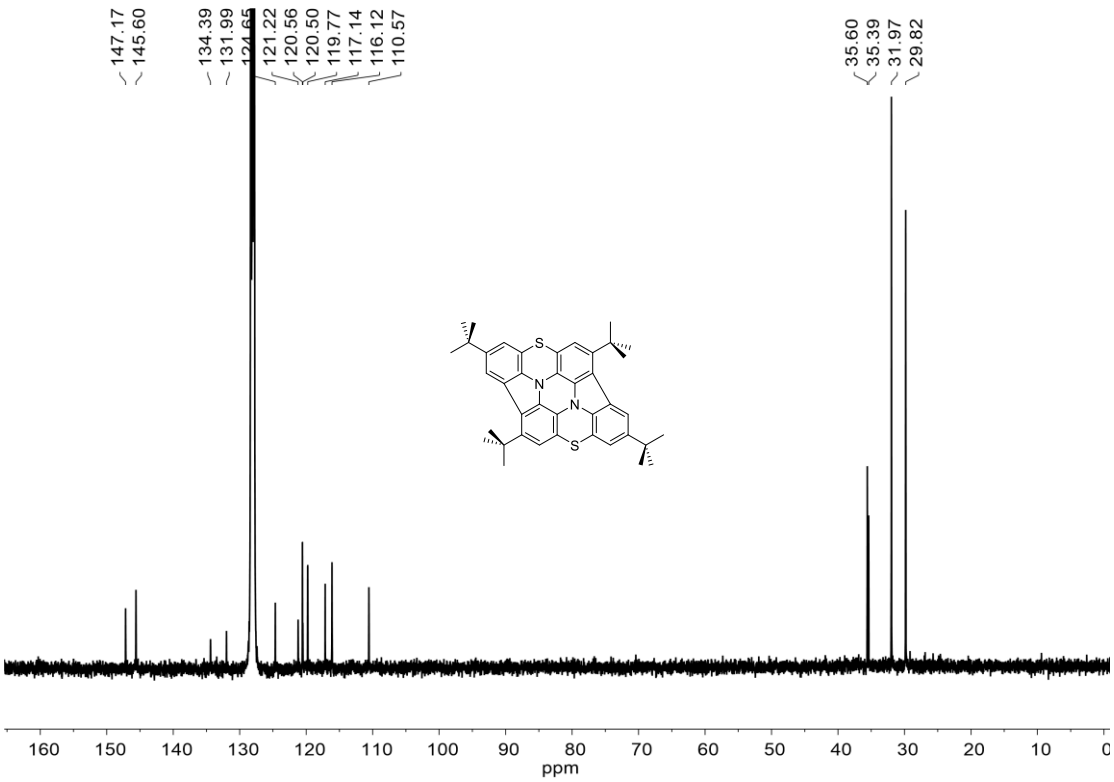


Figure S4. ^{13}C NMR spectrum (100 MHz, C_6D_6) of compound **6**.

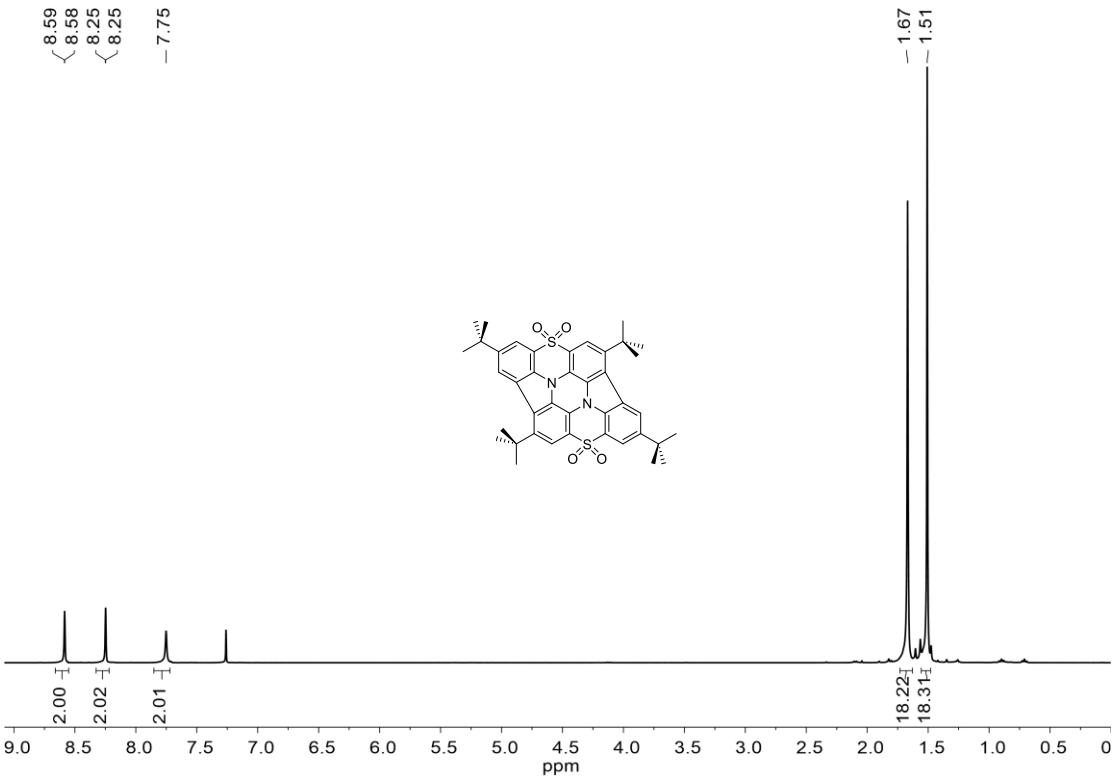


Figure S5. ^{1}H NMR spectrum (400 MHz, C_6D_6) of compound **7**.

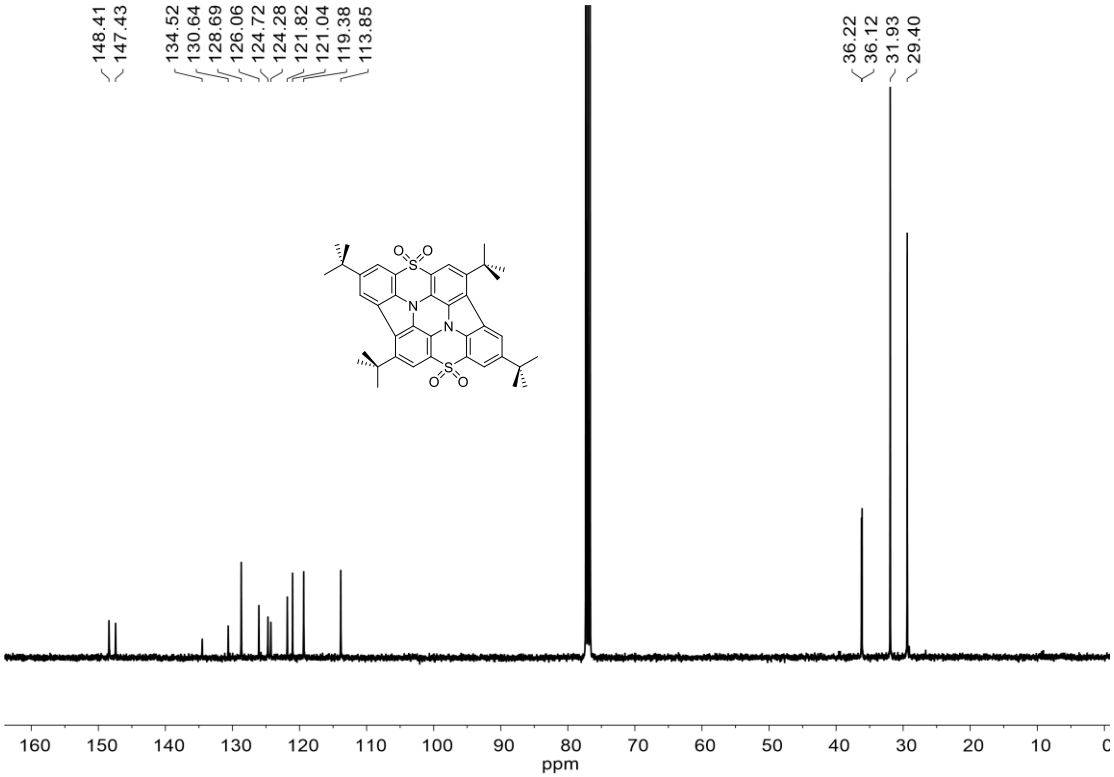


Figure S6. ^{13}C NMR spectrum (100 MHz, C_6D_6) of compound **7**.

4. Mass Spectra

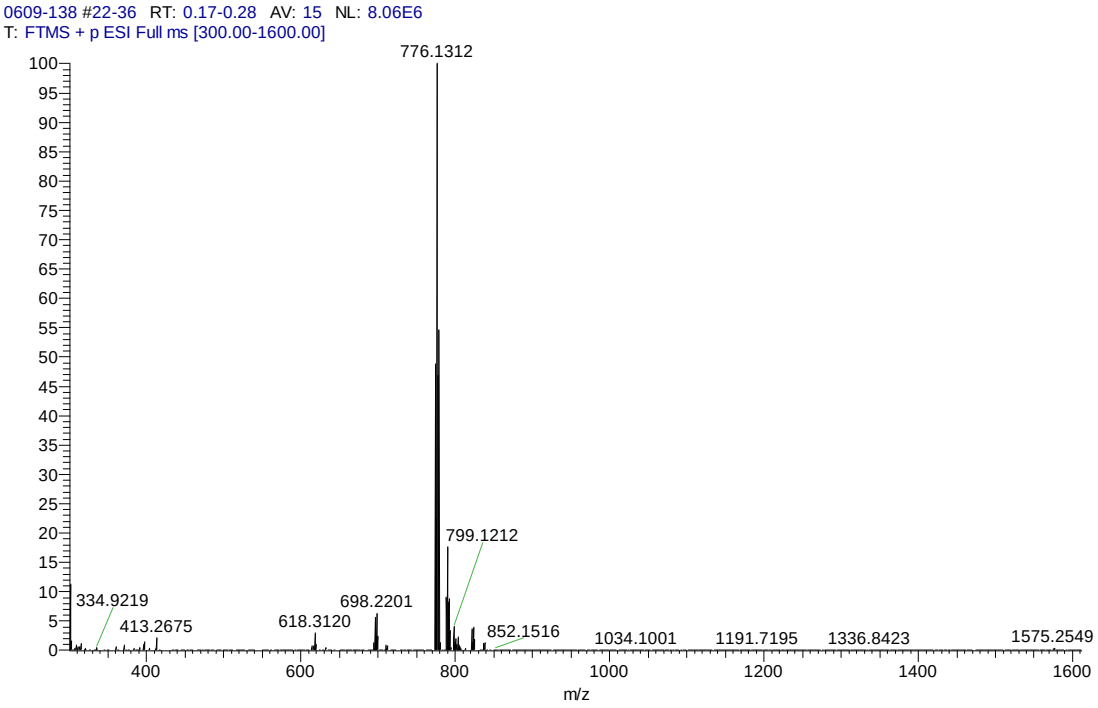


Figure S7. Mass spectrum (ESI) of compound **5**.

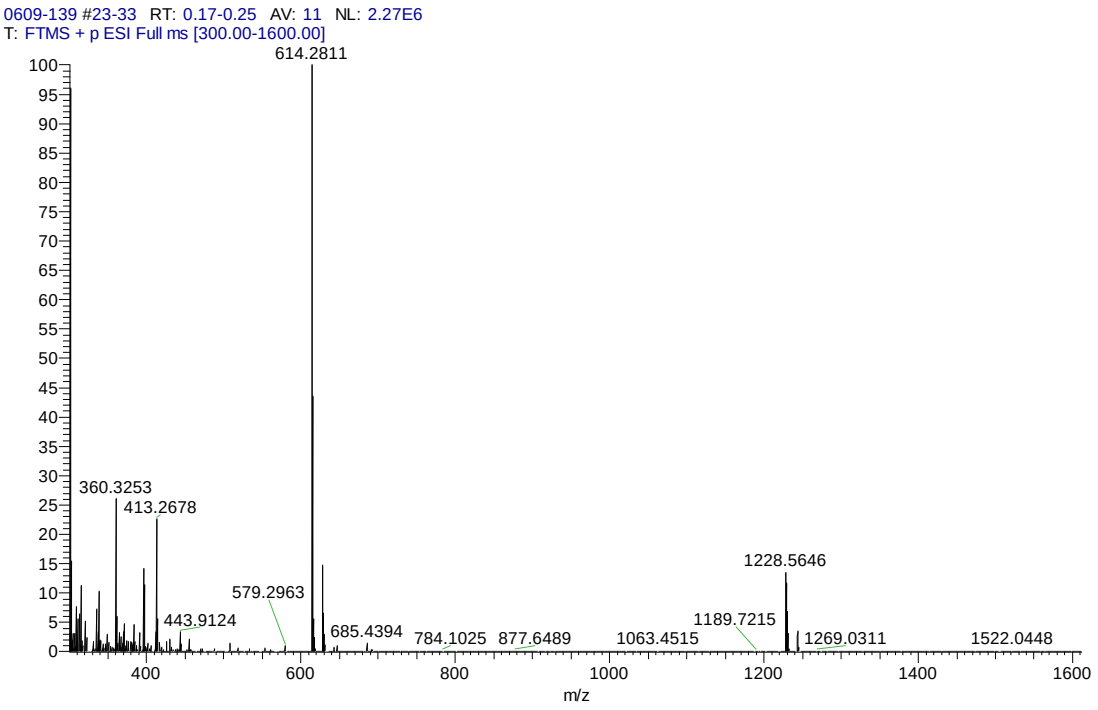


Figure S8. Mass spectrum (ESI) of compound **6**.

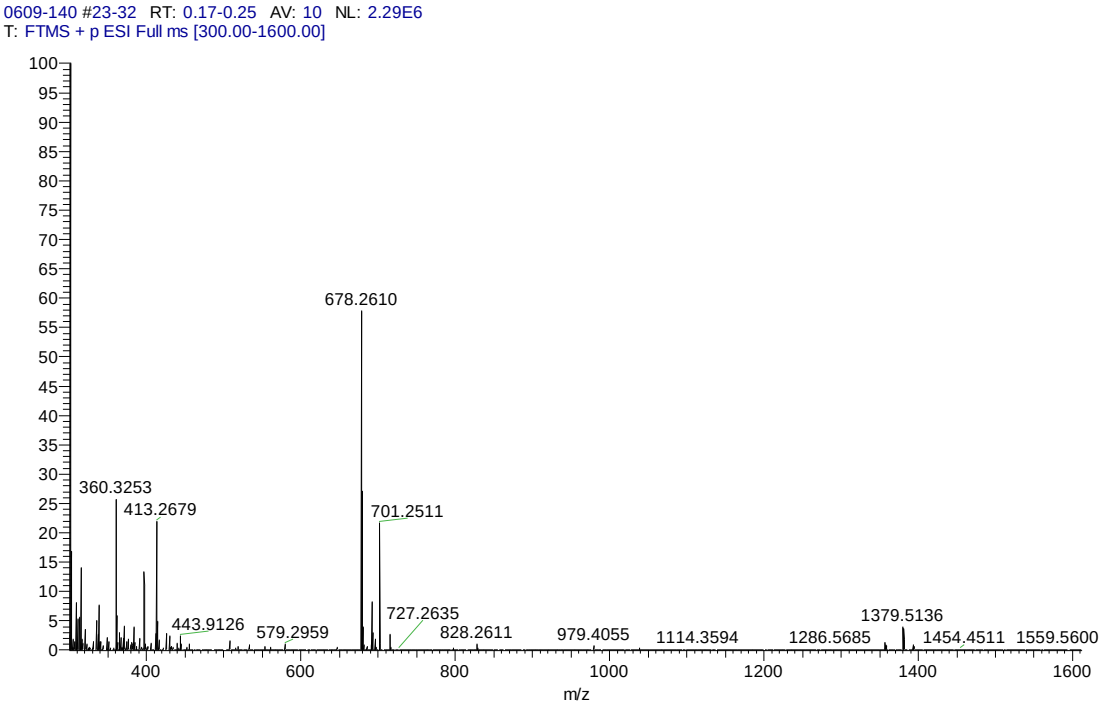


Figure S9. Mass spectrum (ESI) of compound **7**.

5. X-ray crystallographic structures

Table S1 Crystal data and structure refinement for **6** (CCDC 2024841).

Empirical formula	$C_{40}H_{42}N_2S_2$
Formula weight	614.87
Temperature/K	293(2)
Crystal system	tetragonal
Space group	$P4_32_12$
a/Å	17.7483(2)
b/Å	17.7483(2)
c/Å	12.1031(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3812.50(11)
Z	4
ρ_{calc}g/cm^3	1.071
μ/mm^{-1}	1.459
F(000)	1312.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.044 to 147.034
Index ranges	$-19 \leq h \leq 21$, $-21 \leq k \leq 14$, $-14 \leq l \leq 10$
Reflections collected	7563
Independent reflections	3735 [R_{int} = 0.0216, R_{sigma} = 0.0290]
Data/restraints/parameters	3735/0/206
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0379, wR_2 = 0.1035
Final R indexes [all data]	R_1 = 0.0400, wR_2 = 0.1053
Largest diff. peak/hole / e Å^{-3}	0.23/-0.21
Flack parameter	0.017(9)

Table S2 Crystal data and structure refinement for **6**-C_{60} (CCDC 2024844)**.**

Empirical formula	$C_{77}H_{50}N_2S_2$
Formula weight	1067.31
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	13.2343(7)
b/Å	13.6338(5)
c/Å	16.3052(6)
α/°	75.744(3)
β/°	69.165(4)
γ/°	89.458(3)
Volume/Å^3	2655.0(2)
Z	2
ρ_{calc}g/cm^3	1.335
μ/mm^{-1}	1.299
F(000)	1116.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.006 to 147.296
Index ranges	$-15 \leq h \leq 16$, $-14 \leq k \leq 16$, $-20 \leq l \leq 18$
Reflections collected	19135
Independent reflections	10392 [R_{int} = 0.0469, R_{sigma} = 0.0605]
Data/restraints/parameters	10392/7/765
Goodness-of-fit on F^2	1.081
Final R indexes [I>=2σ (I)]	R_1 = 0.0552, wR_2 = 0.1440
Final R indexes [all data]	R_1 = 0.0635, wR_2 = 0.1529
Largest diff. peak/hole / e Å^{-3}	0.84/-0.85

Table S3 Crystal data and structure refinement for $\mathbf{6}^{\cdot+}$ SbF_6^- (CCDC 2024842).

Empirical formula	$C_{41}H_{44}Cl_2F_6N_2S_2Sb$
Formula weight	935.55
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.2189(5)
b/Å	12.4989(4)
c/Å	15.4497(6)
α/°	103.886(3)
β/°	92.811(4)
γ/°	102.498(3)
Volume/Å^3	2041.57(15)
Z	2
ρ_{calc}g/cm^3	1.522
μ/mm^{-1}	8.030
F(000)	950.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.926 to 147.476
Index ranges	$-11 \leq h \leq 13$, $-15 \leq k \leq 14$, $-19 \leq l \leq 18$
Reflections collected	14048
Independent reflections	7985 [R_{int} = 0.0625, R_{sigma} = 0.0741]
Data/restraints/parameters	7985/0/499
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0759, wR_2 = 0.2103
Final R indexes [all data]	R_1 = 0.0899, wR_2 = 0.2221
Largest diff. peak/hole / e Å^{-3}	1.87/-1.75

Table S4 Crystal data and structure refinement for $\mathbf{6}^{2+}$ $[SbF_6^-]_2$ (CCDC 2024843).

Empirical formula	$C_{42}H_{46}Cl_4F_{12}N_2S_2Sb_2$
Formula weight	1256.23
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.3204(5)
b/Å	10.4195(5)
c/Å	14.2747(6)
α/°	100.389(4)
β/°	104.598(4)
γ/°	111.290(5)
Volume/Å^3	1191.81(11)
Z	1
ρ_{calc}g/cm^3	1.750
μ/mm^{-1}	12.588
F(000)	622.0
Crystal size/mm^3	0.11 × 0.09 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.71 to 147.416
Index ranges	$-10 \leq h \leq 11$, $-12 \leq k \leq 12$, $-17 \leq l \leq 10$
Reflections collected	7952
Independent reflections	4644 [R_{int} = 0.0344, R_{sigma} = 0.0476]
Data/restraints/parameters	4644/0/295
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0343, wR_2 = 0.0850
Final R indexes [all data]	R_1 = 0.0367, wR_2 = 0.0868
Largest diff. peak/hole / e Å^{-3}	0.80/-1.28

Table S5 Crystal data and structure refinement for **7** (CCDC 2036398).

Empirical formula	$C_{47}H_{50}N_2O_4S_2$
Formula weight	771.01
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.0384(6)
b/Å	14.0757(7)
c/Å	14.1533(8)
α/°	100.408(4)
β/°	103.832(5)
γ/°	105.597(4)
Volume/Å^3	1984.86(19)
Z	2
ρ_{calc}g/cm^3	1.290
μ/mm^{-1}	0.182
F(000)	820.0
Crystal size/mm^3	0.14 × 0.13 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.02 to 49.998
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -15 ≤ l ≤ 16
Reflections collected	14009
Independent reflections	6992 [R_{int} = 0.0322, R_{sigma} = 0.0540]
Data/restraints/parameters	6992/0/509
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0459, wR_2 = 0.1068
Final R indexes [all data]	R_1 = 0.0576, wR_2 = 0.1172
Largest diff. peak/hole / e Å^{-3}	0.32/-0.37

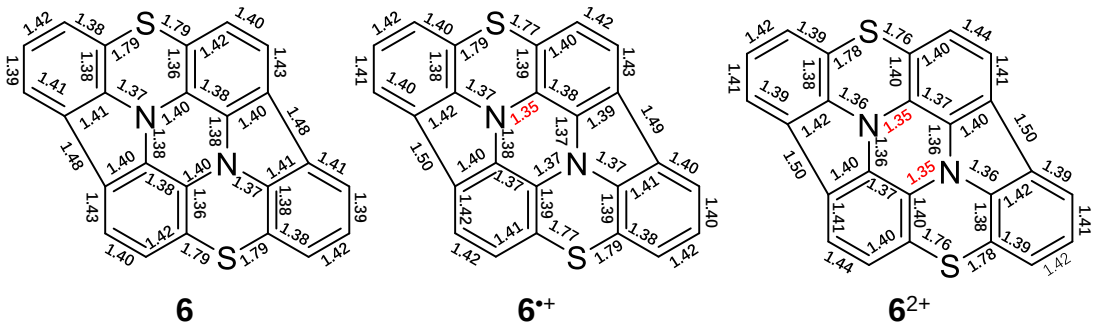


Figure S10. Bond lengths of crystal structures of buckybowl **6** in different oxidative state.

6. Fluorescence decay curves

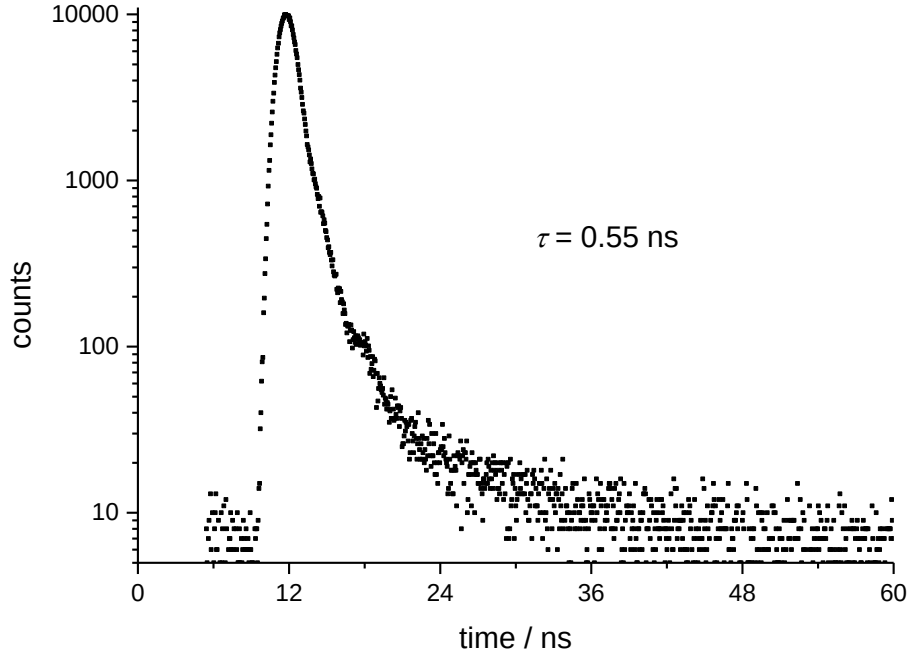


Figure S11. Fluorescence decay curve of **6** in dichloromethane at room temperature.

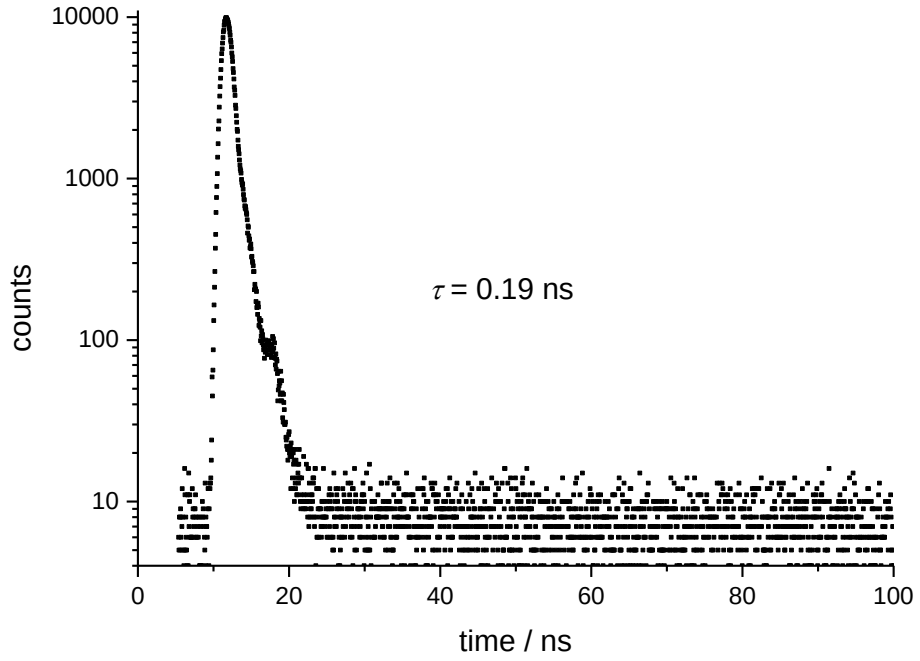


Figure S12. Fluorescence decay curve of **6** in solid state at room temperature.

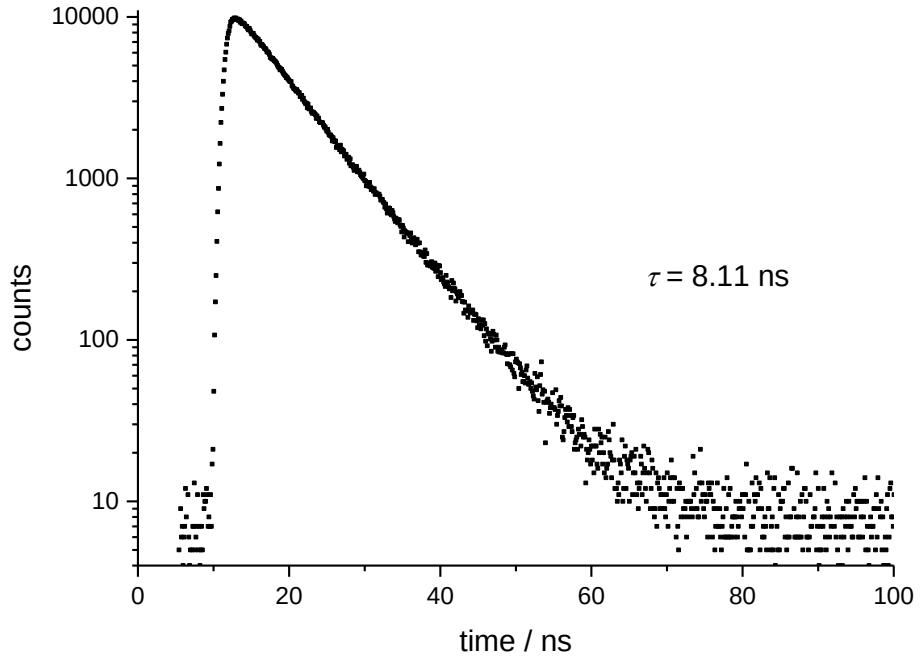


Figure S13. Fluorescence decay curve of **7** in dichloromethane at room temperature.

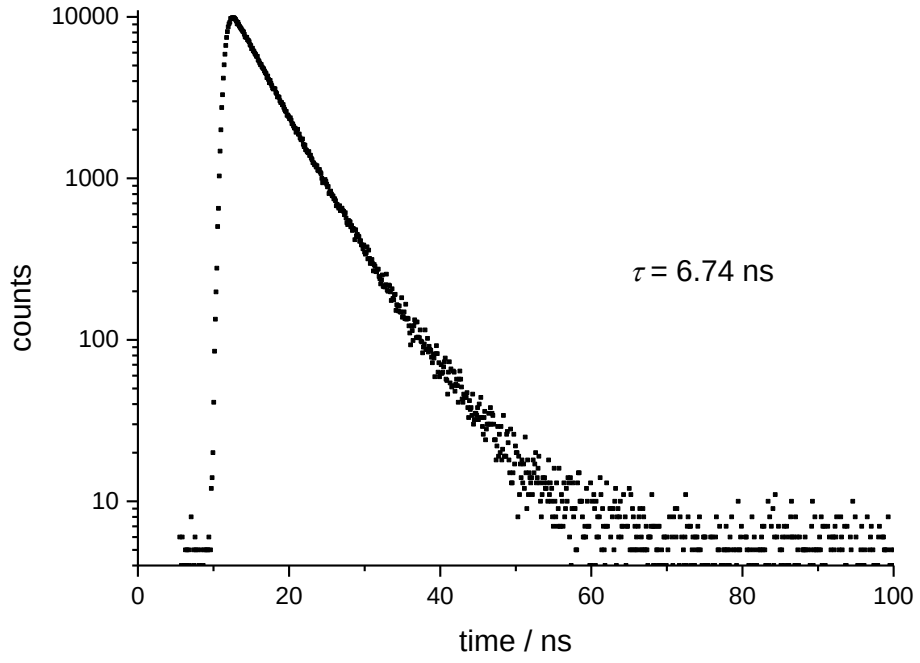


Figure S14. Fluorescence decay curve of **7** in solid state at room temperature.

7. Association behavior of 6 and 7 with C_{60}

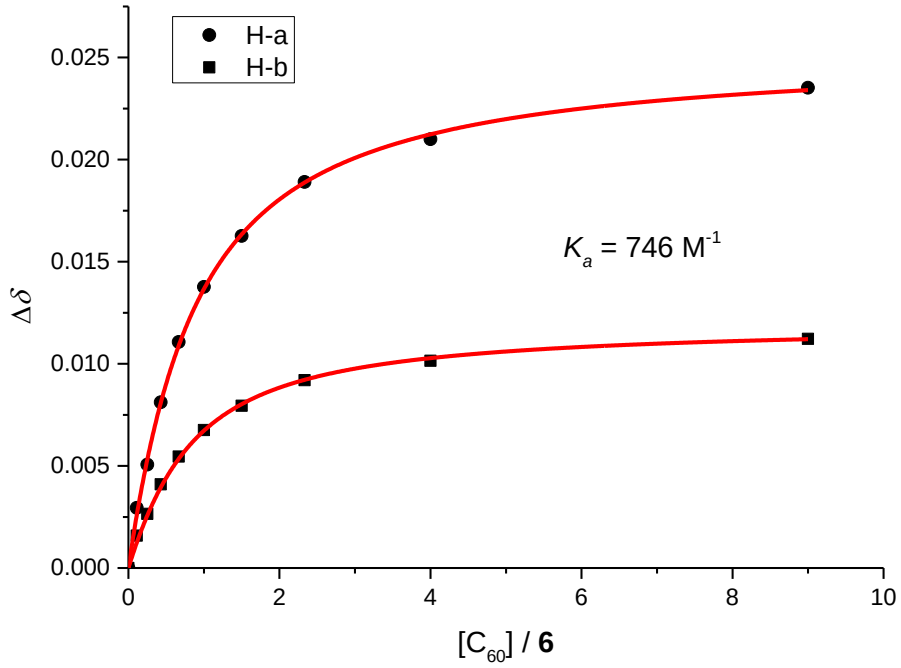


Figure S15. The binding isotherms and average binding constant of **6** and C_{60}.

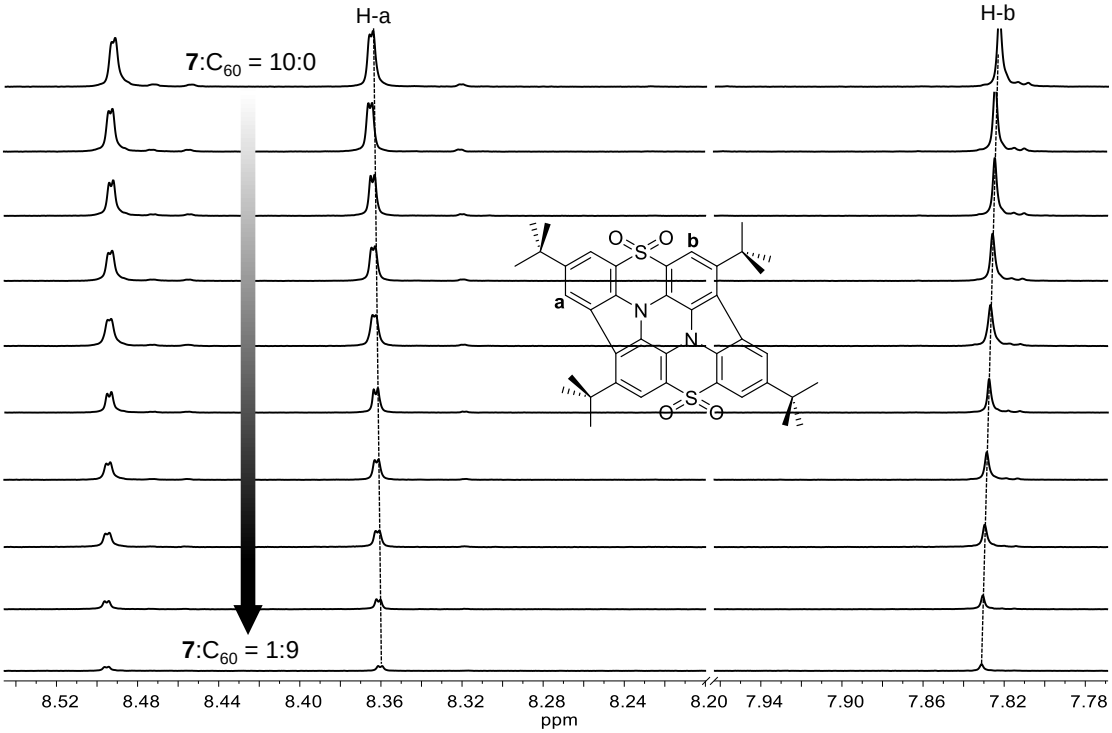


Figure S16. ^{1}H NMR spectra (400 MHz) of **7** when titrated with C_{60} ([**7**] + [C_{60}] = 1.8 × 10^{-3} M, toluene-d_8, 298 K).

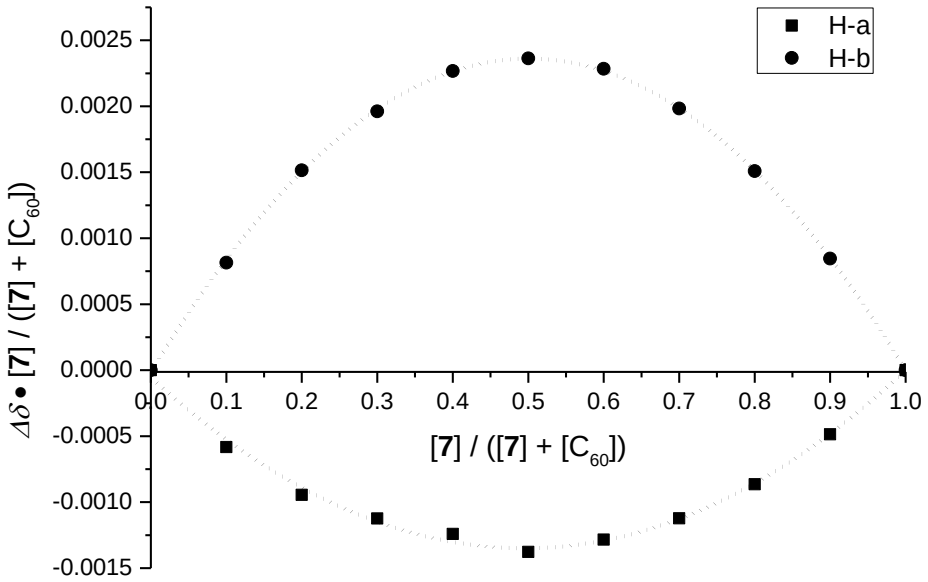


Figure S17. Job plot based on ^{1}H NMR titration of **7** with C_{60} in toluene-d_8.

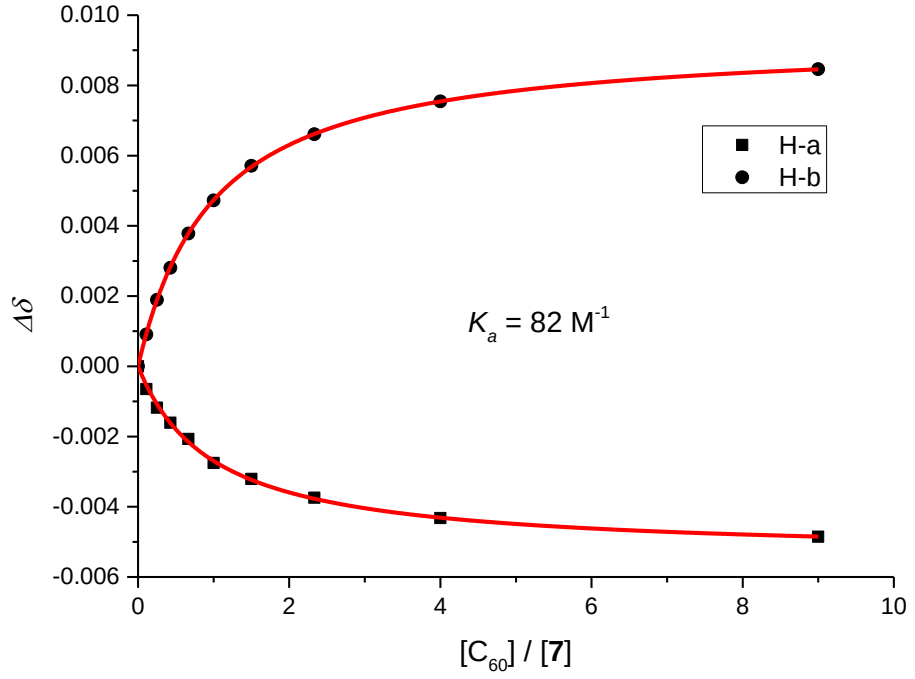


Figure S18. The binding isotherms and average binding constant of **7** and C_{60}..

8. Theoretical calculation

All the theoretical calculations were carried out using a *Gaussian 16* software. [S2] All the calculations were based on the optimized geometries at B3LYP/6-31G(d,p) level of theory. The bowl-to-bowl inversion energy was calculated at B3LYP/6-311+G(2d,p) level of theory for the single-point energy, the planar transition state was checked by frequency calculations at B3LYP/6-31G(d,p) level of theory. [S3] The frontier molecular orbitals are calculated at the B3LYP/6-311+G(d,p) level of theory. The nucleus-independent chemical shift (NICS) calculation was done at GIAO-B3LYP/6-311+G(d,p) level of theory. Bq atoms were inserted at the calculated positions and the Bq positions that are at the 1 Å away above and below the bowls were fixed with the assistant of Multiwfn software, as well as the calculated NICS values at the *zz* tensor.[S4] The calculations of excited state properties were performed using time-depended DFT methods at (U)B3LYP/6-311+G(d,p) level of theory in the solvent dichloromethane.

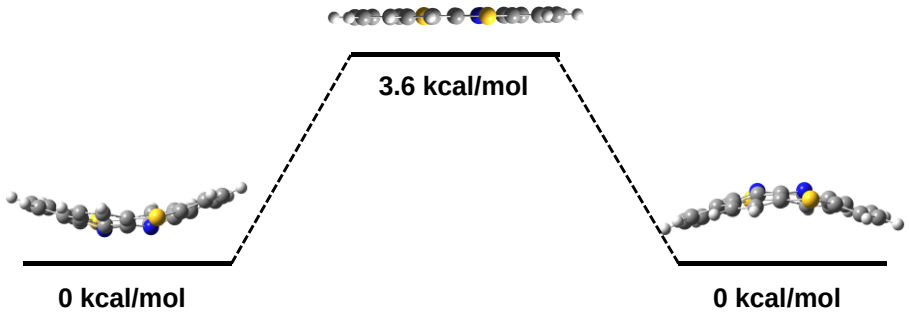


Figure S19. Energy diagram of the inversion process of the non-substituted **6**.

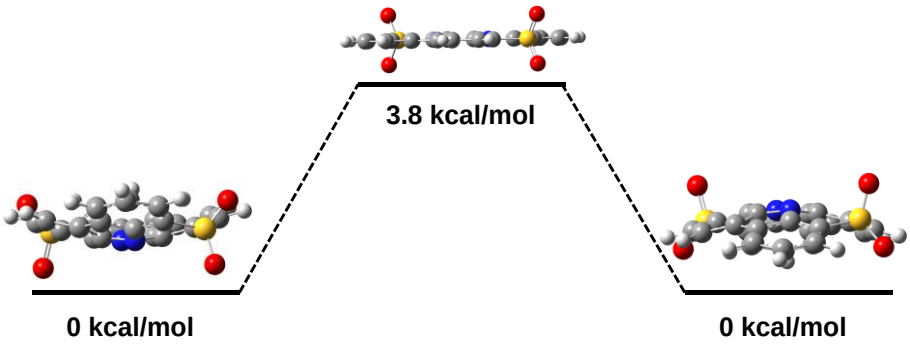


Figure S20. Energy diagram of the inversion process of the non-substituted **7**.

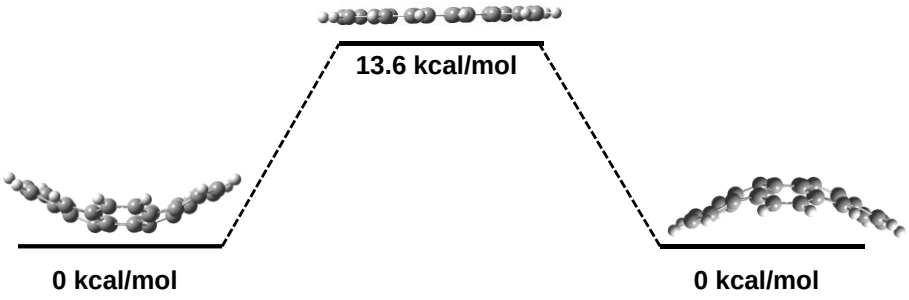


Figure S21. Energy diagram of the inversion process of buckybowl **1**.

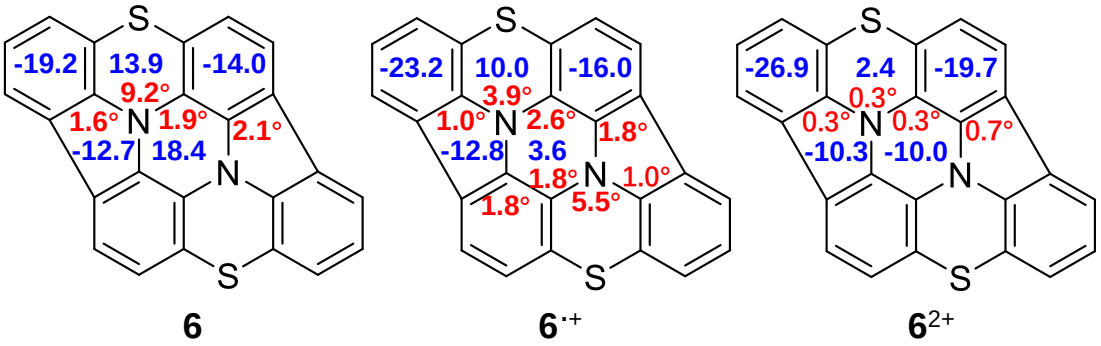


Figure S22. Average NICS(1)$_{zz}$ values and POAV angles of the non-substituted **6** in different oxidative state. The POAV angles are calculated based on the crystal structures.

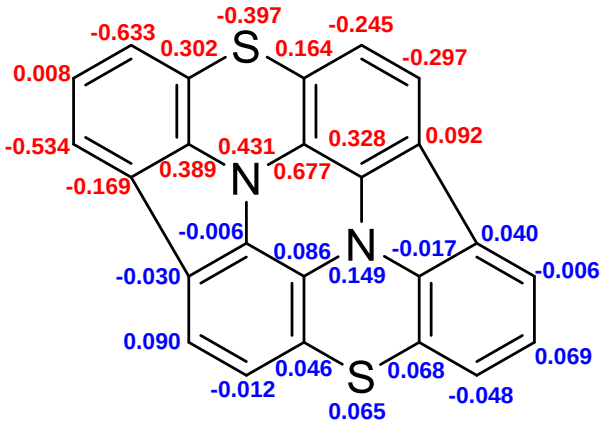


Figure S23. Calculated Muliken atom charge (red) and spin density (blue) of **6**$^{\bullet+}$ at UB3LYP/6-311+G(d,p) level of theory. *tert*-Butyl groups are omitted for clarity.

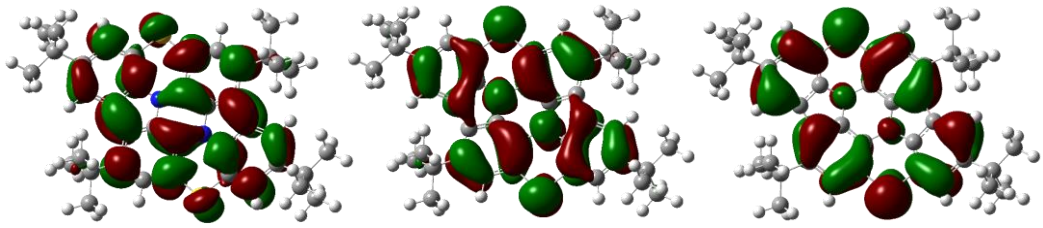


Figure S24. Calculated frontier molecular orbitals and energy levels of **6** at B3LYP/6-311+G(d,p) level of theory.

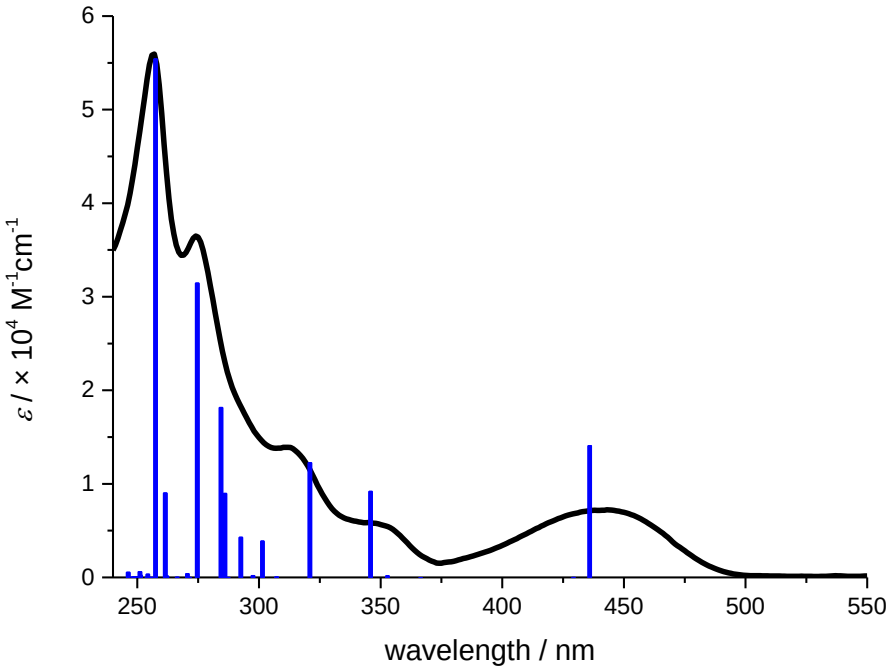


Figure S25. UV/Vis absorption spectrum of **6** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

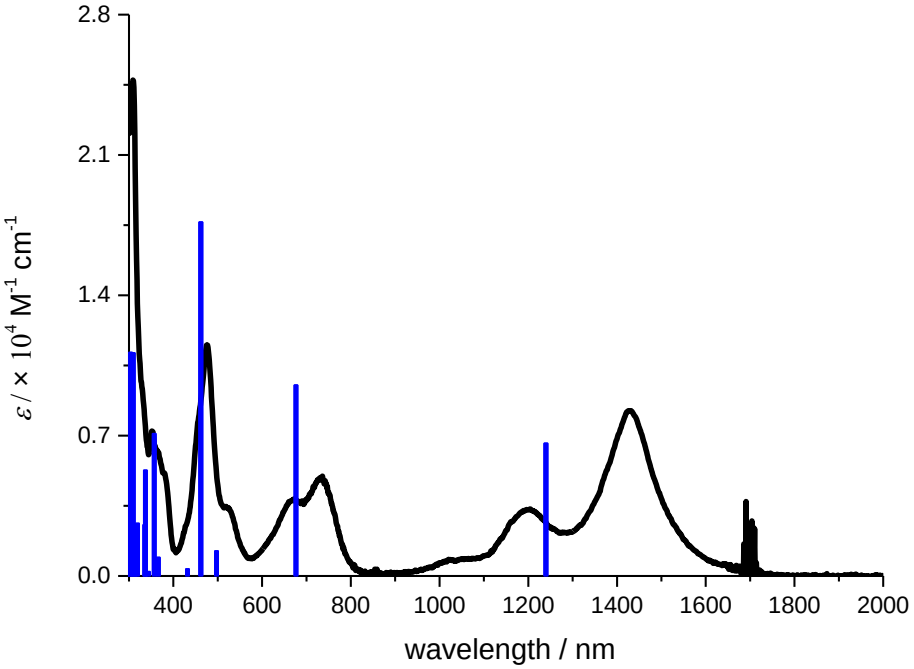


Figure S26. UV/Vis absorption spectrum of $\mathbf{6}^{\bullet+}$ and TD-DFT calculated oscillator strength (blue column) in dichloromethane at UB3LYP/6-311+G(d,p) level.

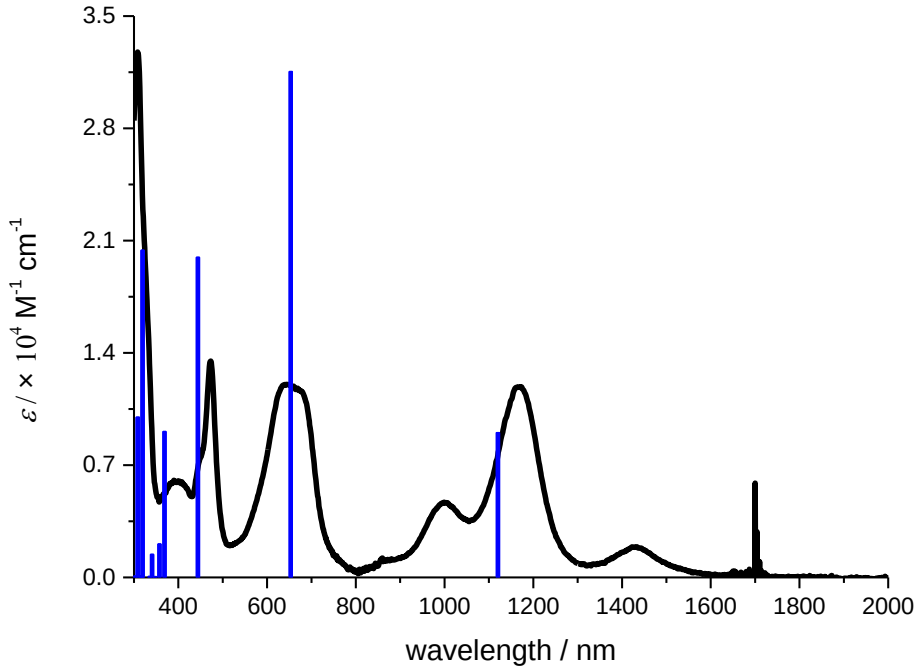


Figure S27. UV/Vis absorption spectrum of $\mathbf{6}^{2+}$ and TD-DFT calculated oscillator strength (blue column) in dichloromethane at UB3LYP/6-311+G(d,p) level.

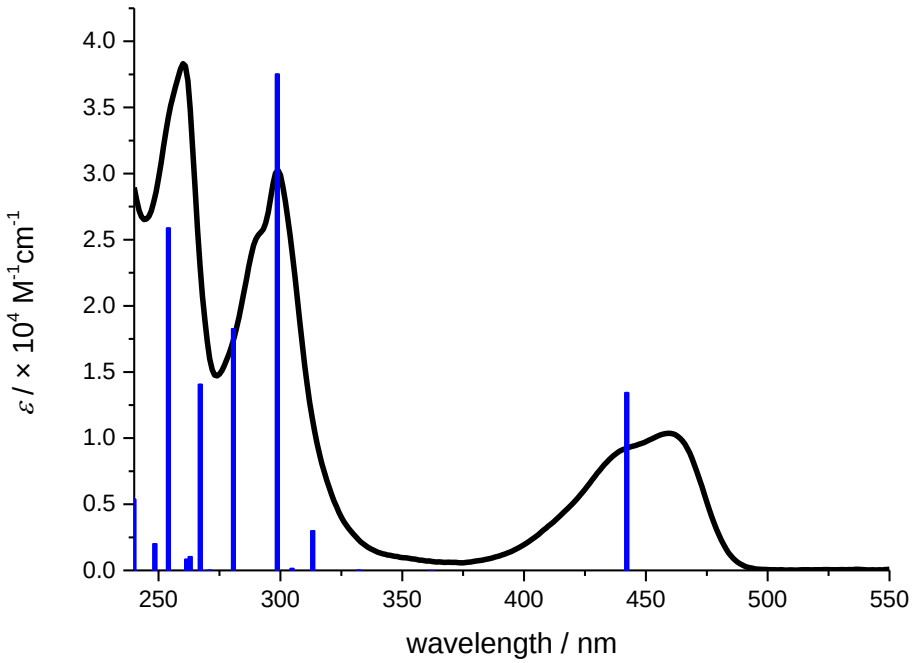


Figure S28. UV/Vis absorption spectrum of **7** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

Table S6. TD-DFT calculated first-ten electron transitions of **6** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State 1: Singlet-A	2.8422 eV	436.22 nm	f=0.2117	<S**2>=0.000
164 -> 165	0.69545			
Excited State 2: Singlet-A	2.8862 eV	429.58 nm	f=0.0006	<S**2>=0.000
164 -> 166	0.70164			
Excited State 3: Singlet-A	3.3808 eV	366.73 nm	f=0.0002	<S**2>=0.000
163 -> 165	0.22708			
164 -> 167	0.66435			
Excited State 4: Singlet-A	3.5114 eV	353.09 nm	f=0.0034	<S**2>=0.000
163 -> 165	0.65594			
164 -> 167	-0.22978			
Excited State 5: Singlet-A	3.5817 eV	346.16 nm	f=0.1384	<S**2>=0.000
163 -> 166	0.62673			
164 -> 168	0.30010			
Excited State 6: Singlet-A	3.8597 eV	321.23 nm	f=0.1845	<S**2>=0.000
162 -> 165	0.10926			
163 -> 166	-0.30020			
164 -> 168	0.61966			
Excited State 7: Singlet-A	4.0310 eV	307.58 nm	f=0.0015	<S**2>=0.000
161 -> 165	-0.18699			
162 -> 166	0.20549			
163 -> 168	-0.11197			
164 -> 169	0.62484			
Excited State 8: Singlet-A	4.1093 eV	301.72 nm	f=0.0589	<S**2>=0.000
161 -> 166	-0.11399			
162 -> 165	0.40224			
163 -> 167	0.37945			
164 -> 171	0.27866			
164 -> 172	0.27264			
Excited State 9: Singlet-A	4.1627 eV	297.84 nm	f=0.0036	<S**2>=0.000
161 -> 165	0.10587			
162 -> 166	-0.21311			
164 -> 170	0.62640			
164 -> 175	-0.17949			
Excited State 10: Singlet-A	4.2156 eV	294.11 nm	f=0.0000	<S**2>=0.000
161 -> 165	-0.15882			
162 -> 166	0.56480			
163 -> 168	0.17367			
164 -> 169	-0.20432			
164 -> 170	0.23837			

164: HOMO, 165: LUMO

Table S7. TD-DFT calculated first-ten electron transitions of $\mathbf{6}^{\bullet+}$ in dichloromethane at UB3LYP / 6-311+G(d,p) level

Excited State 1: 2.017-A	0.9991 eV	1240.92 nm	f=0.0945	<S**2>=0.767
163B -> 164B	0.98957			
Excited State 2: 2.038-A	1.8167 eV	682.48 nm	f=0.0000	<S**2>=0.788
160B -> 164B	0.24886			
161B -> 164B	0.95865			
Excited State 3: 2.032-A	1.8293 eV	677.77 nm	f=0.1360	<S**2>=0.783
162B -> 164B	0.98061			
Excited State 4: 2.057-A	2.2083 eV	561.46 nm	f=0.0000	<S**2>=0.808
164A -> 166A	-0.19484			
160B -> 164B	0.93383			
161B -> 164B	-0.25606			
Excited State 5: 2.086-A	2.4867 eV	498.59 nm	f=0.0179	<S**2>=0.837
163A -> 166A	0.10409			
164A -> 165A	0.85819			
159B -> 164B	0.45299			
Excited State 6: 2.109-A	2.5713 eV	482.19 nm	f=0.0000	<S**2>=0.862
164A -> 166A	0.93850			
164A -> 167A	-0.11832			
160B -> 164B	0.21095			
Excited State 7: 2.064-A	2.6763 eV	463.27 nm	f=0.2521	<S**2>=0.815
164A -> 165A	-0.41324			
159B -> 164B	0.87158			
Excited State 8: 2.337-A	2.7673 eV	448.04 nm	f=0.0000	<S**2>=1.116
163A -> 165A	-0.31376			
158B -> 164B	0.89028			
163B -> 165B	0.24115			
Excited State 9: 3.329-A	2.8616 eV	433.27 nm	f=0.0050	<S**2>=2.520
160A -> 165A	-0.14159			
163A -> 166A	-0.58094			
163A -> 167A	-0.10521			
164A -> 165A	0.20288			
164A -> 168A	0.23558			
160B -> 165B	0.12672			
160B -> 168B	0.10674			
163B -> 166B	0.63406			
163B -> 167B	-0.12034			
Excited State 10: 2.928-A	2.8988 eV	427.71 nm	f=0.0000	<S**2>=1.893
160A -> 166A	-0.11870			
163A -> 165A	-0.44472			
164A -> 166A	0.13492			
164A -> 167A	0.50814			
158B -> 164B	-0.36833			

160B -> 166B	0.14932			
162B -> 165B	-0.10769			
163B -> 165B	0.48431			
163B -> 168B	0.11282			

164: HOMO, 165: LUMO

Table S8. TD-DFT calculated first-ten electron transitions of $\mathbf{6}^{2+}$ in dichloromethane at UB3LYP / 6-311+G(d,p) level

Excited State 1: 3.000-A	0.3750 eV	3306.21 nm	f=0.0000	<S**2>=2.000
163A -> 164A	-0.75591			
163B -> 164B	0.75591			
163A <- 164A	-0.27449			
163B <- 164B	0.27449			
Excited State 2: 1.000-A	1.1043 eV	1122.74 nm	f=0.1160	<S**2>=0.000
162A -> 164A	-0.15659			
163A -> 164A	0.69493			
162B -> 164B	-0.15659			
163B -> 164B	0.69493			
163A <- 164A	-0.11298			
163B <- 164B	-0.11298			
Excited State 3: 3.000-A	1.4024 eV	884.10 nm	f=0.0000	<S**2>=2.000
162A -> 164A	-0.70285			
162B -> 164B	0.70285			
Excited State 4: 3.000-A	1.4715 eV	842.59 nm	f=0.0000	<S**2>=2.000
160A -> 164A	-0.10508			
161A -> 164A	0.69590			
160B -> 164B	0.10508			
161B -> 164B	-0.69590			
Excited State 5: 3.000-A	1.8830 eV	658.46 nm	f=0.0000	<S**2>=2.000
160A -> 164A	-0.68649			
161A -> 164A	-0.11007			
160B -> 164B	0.68649			
161B -> 164B	0.11007			
Excited State 6: 1.000-A	1.8904 eV	655.88 nm	f=0.4053	<S**2>=0.000
162A -> 164A	0.68402			
163A -> 164A	0.16186			
162B -> 164B	0.68402			
163B -> 164B	0.16186			
Excited State 7: 1.000-A	1.9325 eV	641.56 nm	f=0.0000	<S**2>=0.000
160A -> 164A	-0.35662			
161A -> 164A	0.60731			
160B -> 164B	-0.35662			

161B -> 164B	0.60731			
Excited State 8: 1.000-A	2.1765 eV	569.66 nm	f=0.0000	<S**2>=0.000
160A -> 164A	0.60864			
161A -> 164A	0.35711			
160B -> 164B	0.60864			
161B -> 164B	0.35711			
Excited State 9: 3.000-A	2.1927 eV	565.44 nm	f=0.0000	<S**2>=2.000
158A -> 164A	0.69872			
158B -> 164B	-0.69872			
Excited State 10: 3.000-A	2.3137 eV	535.88 nm	f=0.0000	<S**2>=2.000
159A -> 164A	0.68191			
163A -> 165A	0.12505			
159B -> 164B	-0.68191			
163B -> 165B	-0.12505			

164: HOMO, 165: LUMO

Table S9. TD-DFT calculated first-ten electron transitions of **7** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State 1: Singlet-A	2.8040 eV	442.17 nm	f=0.2536	<S**2>=0.000
180 -> 181	0.70063			
Excited State 2: Singlet-A	3.4258 eV	361.92 nm	f=0.0004	<S**2>=0.000
180 -> 182	0.69947			
Excited State 3: Singlet-A	3.7318 eV	332.24 nm	f=0.0008	<S**2>=0.000
177 -> 181	0.10278			
179 -> 181	0.68248			
180 -> 183	0.10005			
Excited State 4: Singlet-A	3.8291 eV	323.79 nm	f=0.0000	<S**2>=0.000
177 -> 181	0.15408			
179 -> 181	-0.12828			
180 -> 183	0.67024			
Excited State 5: Singlet-A	3.9572 eV	313.31 nm	f=0.0571	<S**2>=0.000
178 -> 181	0.54848			
180 -> 184	-0.43886			
Excited State 6: Singlet-A	4.0675 eV	304.82 nm	f=0.0033	<S**2>=0.000
177 -> 181	0.66459			
178 -> 182	-0.11342			
180 -> 183	-0.16642			
Excited State 7: Singlet-A	4.1495 eV	298.79 nm	f=0.7066	<S**2>=0.000
178 -> 181	0.41633			
179 -> 182	0.17062			
180 -> 184	0.53210			
Excited State 8: Singlet-A	4.3904 eV	282.40 nm	f=0.0000	<S**2>=0.000

178 -> 182	0.21269				
180 -> 185	0.65281				
Excited State 9: Singlet-A	4.4155 eV	280.80 nm	f=0.3444	<S**2>=0.000	
176 -> 181	-0.33714				
178 -> 184	0.11590				
179 -> 182	0.55594				
180 -> 187	-0.14993				
Excited State 10: Singlet-A	4.5752 eV	270.99 nm	f=0.0009	<S**2>=0.000	
175 -> 181	0.50193				
178 -> 182	0.23166				
180 -> 185	-0.12793				
180 -> 186	0.40185				

180: HOMO, 181: LUMO

Cartesian coordinates for theoretically optimized structures of 6, $6^{\bullet+}$, 6^{2+}, 7 and 1.

6

C	2.29296562	1.47181634	-0.39889590
C	1.08911317	0.82988030	-0.73192603
C	-0.16783310	1.41053833	-0.75106486
C	-0.27772280	2.76291682	-0.50845088
C	0.92096700	3.47873057	-0.26981217
C	2.19831753	2.89333908	-0.20381351
C	-3.00507039	2.12838736	-0.28509454
C	-2.53888138	0.83631955	-0.50527371
C	-3.26450419	-0.35322449	-0.25192562
C	-4.61487864	-0.17720400	0.11999599
C	-5.14940762	1.10405057	0.30127621
C	-4.32461995	2.24756208	0.13034204
H	0.83059892	4.54454953	-0.10697450
H	-5.24549676	-1.03708956	0.28698350
H	-4.72819164	3.23445661	0.33058099
C	-1.08911907	-0.82989446	-0.73191568
C	0.16782839	-1.41055327	-0.75104413
C	-2.29296884	-1.47182800	-0.39887353
C	0.27772449	-2.76292622	-0.50841253
C	-2.19831990	-2.89335304	-0.20378599
C	2.53887893	-0.83632946	-0.50526785
C	-0.92096377	-3.47873920	-0.26977015
C	3.26450441	0.35321952	-0.25194864
C	3.00507944	-2.12839054	-0.28509093
H	-0.83058982	-4.54455782	-0.10694681

C	4.61488792	0.17721302	0.11993119
C	4.32463835	-2.24755567	0.13032391
C	5.14942325	-1.10403954	0.30123511
H	5.24551531	1.03710763	0.28684823
H	4.72822134	-3.23445080	0.33053739
N	-1.25109174	0.53501076	-0.88084095
N	1.25108436	-0.53502608	-0.88081649
S	-1.90526332	3.54730134	-0.52957168
S	1.90526922	-3.54730931	-0.52954212
C	6.62051973	-1.32406227	0.71399700
C	7.33583408	-2.17392538	-0.36344441
H	8.38173185	-2.34296998	-0.08358657
H	6.86465227	-3.15269918	-0.49199058
H	7.32110998	-1.66744607	-1.33394556
C	7.39501541	-0.00105157	0.86502973
H	7.41915991	0.56712370	-0.07051928
H	6.96686497	0.63753797	1.64453799
H	8.43084759	-0.21365524	1.14779662
C	6.67514072	-2.06507576	2.07152152
H	7.71549716	-2.22910126	2.37400566
H	6.18107221	-1.48165067	2.85514984
H	6.18663265	-3.04271271	2.02630271
C	-3.43117695	-3.76533058	0.10049518
C	-3.99258284	-3.38773553	1.49363549
H	-4.20919269	-2.32264796	1.58719527
H	-4.91632848	-3.94199437	1.69547459
H	-3.26864472	-3.64287603	2.27431706
C	-4.49344342	-3.56023465	-1.00630320
H	-5.40559545	-4.11745839	-0.76519325
H	-4.76404769	-2.51285797	-1.14578225
H	-4.11736621	-3.92968251	-1.96601734
C	-3.10836122	-5.27332066	0.13576528
H	-2.68850943	-5.62467827	-0.81217814
H	-2.41163527	-5.52974313	0.93997228
H	-4.03129357	-5.83364153	0.31610800
C	-6.62050751	1.32410303	0.71400726
C	-7.33588784	2.17347928	-0.36378417
H	-6.86474811	3.15222037	-0.49272506
H	-7.32111893	1.66660046	-1.33407588
H	-8.38180149	2.34257415	-0.08401263
C	-6.67519925	2.06565195	2.07123038
H	-7.71557670	2.22969561	2.37363092
H	-6.18108613	1.48258388	2.85509642
H	-6.18679606	3.04332554	2.02564492

C	-7.39488481	0.00108786	0.86559872
H	-7.41903423	-0.56747001	-0.06971900
H	-6.96663558	-0.63714735	1.64534131
H	-8.43072419	0.21371655	1.14831973
C	3.43117143	3.76529944	0.10051143
C	4.49347175	3.56020203	-1.00626072
H	4.11742760	3.92965933	-1.96598305
H	5.40562593	4.11741218	-0.76512384
H	4.76406604	2.51282051	-1.14574013
C	3.99252196	3.38770046	1.49367410
H	4.91627451	3.94193424	1.69555346
H	3.26856299	3.64285661	2.27433084
H	4.20909842	2.32260637	1.58724331
C	3.10833869	5.27328325	0.13576668
H	2.68853570	5.62462974	-0.81220175
H	2.41156420	5.52970741	0.93993166
H	4.03125813	5.83360808	0.31616735

unsubstituted **6**

C	-1.41138428	-2.28932263	-0.09819582
C	-0.61741820	-1.20474903	-0.49218549
C	0.76722906	-1.20388236	-0.50263456
C	1.45166505	-2.37192796	-0.20433896
C	0.68089498	-3.52276782	0.09727038
C	-0.71789496	-3.49354202	0.15961748
C	3.62184925	-0.61740391	0.06071750
C	2.64965864	0.34046400	-0.20678097
C	2.75885044	1.72466169	0.08369864
C	4.00439637	2.17845267	0.54562082
C	5.01915654	1.24479987	0.75926475
C	4.83330053	-0.13945659	0.55896362
H	1.19536736	-4.45144733	0.32270416
H	4.17393605	3.22822130	0.76282209
H	5.63425638	-0.82942848	0.80498878
C	0.61742091	1.20475491	-0.49216688
C	-0.76722627	1.20388837	-0.50262418
C	1.41138479	2.28932383	-0.09815976
C	-1.45166397	2.37193036	-0.20431855
C	0.71789392	3.49354008	0.15966413
C	-2.64965757	-0.34046155	-0.20680068
C	-0.68089566	3.52276657	0.09730931
C	-2.75885091	-1.72466259	0.08366196
C	-3.62184955	0.61740320	0.06070417
H	-1.19536942	4.45144332	0.32275128

C	-4.00439924	-2.17845912	0.54557226
C	-4.83330343	0.13944996	0.55893826
C	-5.01916054	-1.24480890	0.75922194
H	-4.17394003	-3.22823041	0.76275985
H	-5.63426056	0.82941892	0.80496748
N	1.37377392	0.05113004	-0.65330194
N	-1.37377036	-0.05112216	-0.65331153
S	3.26004126	-2.36929795	-0.21604597
S	-3.26004008	2.36930046	-0.21603648
H	-1.24935367	-4.39504256	0.44645539
H	-5.98175887	-1.58635761	1.12674036
H	1.24935092	4.39503724	0.44651579
H	5.98175289	1.58634427	1.12679231

6$^{\bullet+}$

C	-2.32202500	-1.48911200	-0.00011800
C	-1.08522900	-0.83269300	-0.00015800
C	0.17369600	-1.40480800	-0.00018500
C	0.28680200	-2.79222400	-0.00017400
C	-0.92779200	-3.50605700	-0.00015200
C	-2.22576400	-2.91833200	-0.00012800
C	3.04374000	-2.13534900	-0.00012200
C	2.55827800	-0.83207100	-0.00014300
C	3.31653600	0.36645000	-0.00006300
C	4.70911000	0.18339900	0.00001000
C	5.26556100	-1.11117500	0.00001300
C	4.42892000	-2.25838100	-0.00004400
H	-0.86651900	-4.58589700	-0.00014600
H	5.37102500	1.03587400	0.00007000
H	4.87895500	-3.24457900	-0.00002000
C	1.08523400	0.83269100	-0.00011500
C	-0.17369200	1.40480600	-0.00010300
C	2.32203000	1.48911000	-0.00004500
C	-0.28679900	2.79222100	-0.00001000
C	2.22576600	2.91833000	0.00002600
C	-2.55827500	0.83206900	-0.00008200
C	0.92779500	3.50605500	0.00004500
C	-3.31653200	-0.36645300	-0.00006800
C	-3.04373700	2.13534600	0.00001800
H	0.86652300	4.58589600	0.00011500
C	-4.70910600	-0.18340400	0.00002200
C	-4.42891800	2.25837700	0.00011100
C	-5.26555800	1.11117000	0.00010400
H	-5.37102000	-1.03588000	0.00003500

H	-4.87895300	3.24457400	0.00019600
N	1.22737600	-0.53133800	-0.00018700
N	-1.22737100	0.53133600	-0.00015100
S	1.91442900	-3.55026500	-0.00019100
S	-1.91442700	3.55026300	0.00002600
C	-6.79282500	1.33249800	0.00020900
C	-7.19388500	2.13045700	-1.26468700
H	-8.27628200	2.29220000	-1.27535100
H	-6.71526800	3.11324500	-1.30428500
H	-6.92390600	1.58774600	-2.17608700
C	-7.57999300	0.00832800	0.00021500
H	-7.37102900	-0.59530300	-0.88909300
H	-7.37090300	-0.59536800	0.88945000
H	-8.65168400	0.22524100	0.00029900
C	-7.19372500	2.13037400	1.26520600
H	-8.27612000	2.29212200	1.27601500
H	-6.92363500	1.58760200	2.17653600
H	-6.71510000	3.11315800	1.30481100
C	3.47165100	3.82065400	0.00009900
C	4.29906500	3.53347500	1.27791600
H	4.56873700	2.48124400	1.38327800
H	5.22380300	4.11863000	1.26049400
H	3.73737900	3.82024600	2.17235600
C	4.29916900	3.53354200	-1.27766500
H	5.22391000	4.11868800	-1.26013300
H	4.56884000	2.48131500	-1.38306600
H	3.73755900	3.82036900	-2.17213500
C	3.13347700	5.32489300	0.00012400
H	2.57070500	5.62398600	-0.88979900
H	2.57060100	5.62393300	0.88999900
H	4.06490400	5.89770000	0.00019500
C	6.79282800	-1.33250400	0.00009600
C	7.19387500	-2.13041800	-1.26483200
H	6.71525500	-3.11320300	-1.30446200
H	6.92389000	-1.58767400	-2.17621000
H	8.27627100	-2.29216500	-1.27551000
C	7.19374000	-2.13042600	1.26506100
H	8.27613500	-2.29217200	1.27585500
H	6.92365600	-1.58768700	2.17641300
H	6.71511700	-3.11321200	1.30463500
C	7.57999700	-0.00833500	0.00014300
H	7.37103300	0.59532400	-0.88914700
H	7.37090600	0.59533500	0.88939500
H	8.65168700	-0.22524800	0.00022000

C	-3.47165700	-3.82064500	-0.00010100
C	-4.29916900	-3.53345800	-1.27785200
H	-3.73756100	-3.82024400	-2.17233600
H	-5.22391700	-4.11859400	-1.26035100
H	-4.56882800	-2.48122200	-1.38319600
C	-4.29907300	-3.53351300	1.27772500
H	-5.22381600	-4.11865900	1.26027500
H	-3.73739200	-3.82032400	2.17215500
H	-4.56873700	-2.48128400	1.38312800
C	-3.13350900	-5.32489200	-0.00014700
H	-2.57074800	-5.62395500	-0.89008700
H	-2.57063500	-5.62398300	0.88971100
H	-4.06494600	-5.89768100	-0.00009900

unsubstituted **6**$^{\bullet+}$

C	-0.34129100	4.67718400	0.16605700
C	-0.02644000	3.32304500	0.01187800
C	-1.13838500	2.44019600	-0.07183200
C	-2.48773400	2.76196700	0.02696900
C	-2.75931300	4.12361500	0.18664100
C	-1.69368000	5.04394100	0.24224200
C	-2.81607500	-0.05142300	-0.06379300
C	-1.42417100	0.00281100	-0.17927700
C	-0.68633900	-1.16709000	-0.18512700
C	-1.18497300	-2.46603800	-0.05485200
C	-2.59071500	-2.52622900	0.03940300
C	-3.37302100	-1.34590900	0.03019500
H	0.42953500	5.43674000	0.23510100
H	-3.77958500	4.48134600	0.27495900
H	-1.93856600	6.09386800	0.36361500
H	-3.10654300	-3.47502700	0.14124700
H	-4.44920100	-1.45050600	0.11909200
C	0.68633900	1.16709000	-0.18512700
C	1.42417100	-0.00281100	-0.17927700
C	1.18497300	2.46603800	-0.05485200
C	2.81607500	0.05142300	-0.06379300
C	2.59071500	2.52622900	0.03940300
C	1.13838500	-2.44019600	-0.07183200
C	3.37302100	1.34590900	0.03019500
H	3.10654300	3.47502700	0.14124700
C	0.02644000	-3.32304500	0.01187800
C	2.48773400	-2.76196700	0.02696900
H	4.44920100	1.45050600	0.11909200
C	0.34129100	-4.67718400	0.16605700

C	2.75931300	-4.12361500	0.18664100
C	1.69368000	-5.04394100	0.24224200
H	-0.42953500	-5.43674000	0.23510100
H	3.77958500	-4.48134600	0.27495900
H	1.93856600	-6.09386800	0.36361500
N	-0.68633900	1.15581300	-0.21044000
N	0.68633900	-1.15581300	-0.21044000
S	-3.75937500	1.47703300	-0.03449800
S	3.75937500	-1.47703300	-0.03449800

6^{2+}

C	-2.31325100	-1.49475100	-0.00374100
C	-1.08046900	-0.83299900	-0.00636200
C	0.18658200	-1.39426100	-0.00606100
C	0.30777100	-2.79808800	-0.00348500
C	-0.89943600	-3.50509500	-0.00179000
C	-2.21312500	-2.91894300	-0.00177900
C	3.04533400	-2.13748300	-0.00181100
C	2.55772800	-0.82896800	-0.00385300
C	3.31450100	0.37482200	-0.00249700
C	4.69912500	0.19551600	0.00025100
C	5.26271800	-1.10817300	0.00187400
C	4.43120600	-2.25809000	0.00105600
H	-0.84423400	-4.58543200	0.00005900
H	5.36463000	1.04496300	0.00138700
H	4.88636300	-3.24148900	0.00289700
C	1.08043500	0.83301500	-0.00646400
C	-0.18662200	1.39428500	-0.00605200
C	2.31327200	1.49471100	-0.00388800
C	-0.30781700	2.79809800	-0.00345300
C	2.21300600	2.91894200	-0.00187400
C	-2.55776600	0.82896800	-0.00370700
C	0.89938100	3.50514700	-0.00181200
C	-3.31455800	-0.37484700	-0.00240300
C	-3.04529700	2.13752000	-0.00166100
H	0.84418500	4.58548100	0.00009100
C	-4.69917700	-0.19540200	0.00019700
C	-4.43116100	2.25820500	0.00121200
C	-5.26269900	1.10833100	0.00194700
H	-5.36483200	-1.04471500	0.00110300
H	-4.88627800	3.24162200	0.00310500
N	1.22964900	-0.53301500	-0.00644100
N	-1.22967700	0.53300600	-0.00633300
S	1.92739500	-3.54145900	-0.00250500

S	-1.92737700	3.54149400	-0.00235200
C	-6.78694100	1.31875300	0.00532700
C	-7.18753900	2.12113500	-1.26015000
H	-8.27060200	2.27211300	-1.26491400
H	-6.72080000	3.10964800	-1.29464200
H	-6.91802000	1.58428100	-2.17474800
C	-7.56732600	-0.00939200	0.00498500
H	-7.36297700	-0.61039700	-0.88728400
H	-7.35980300	-0.61269600	0.89496900
H	-8.63846900	0.20590700	0.00720500
C	-7.18215600	2.11731400	1.27492400
H	-8.26514200	2.26861800	1.28460000
H	-6.90903700	1.57749900	2.18670800
H	-6.71489900	3.10554500	1.31056400
C	3.44384700	3.83534100	0.00055000
C	4.27025700	3.55028600	1.28242400
H	4.55566600	2.50206800	1.38746500
H	5.18618100	4.14738400	1.26187900
H	3.70781500	3.83197500	2.17740600
C	4.27357000	3.55251200	-1.27966700
H	5.18955800	4.14938800	-1.25564800
H	4.55906000	2.50443600	-1.38595000
H	3.71352300	3.83596800	-2.17559500
C	3.08962200	5.33619000	0.00133300
H	2.52957500	5.63420700	-0.89063300
H	2.52788600	5.63293700	0.89266100
H	4.01645800	5.91491900	0.00264700
C	6.78696900	-1.31852400	0.00516200
C	7.18751000	-2.12100500	-1.26027100
H	6.72086600	-3.10956600	-1.29461400
H	6.91785000	-1.58427500	-2.17490100
H	8.27058600	-2.27188000	-1.26512900
C	7.18232800	-2.11694000	1.27480100
H	8.26532100	-2.26820300	1.28439800
H	6.90926500	-1.57704600	2.18655300
H	6.71510800	-3.10518400	1.31057300
C	7.56728200	0.00966400	0.00461600
H	7.36278300	0.61059000	-0.88767300
H	7.35985000	0.61302300	0.89458400
H	8.63843800	-0.20557500	0.00671200
C	-3.44389300	-3.83548400	0.00042800
C	-4.27334800	-3.55296700	-1.28002200
H	-3.71299000	-3.83639300	-2.17577000
H	-5.18920300	-4.15005200	-1.25620200

H	-4.55904300	-2.50497400	-1.38653200
C	-4.27072000	-3.55089100	1.28210300
H	-5.18632400	-4.14846200	1.26129800
H	-3.70835000	-3.83233500	2.17720800
H	-4.55672700	-2.50285700	1.38716000
C	-3.08925700	-5.33630100	0.00124000
H	-2.52843900	-5.63410000	-0.89029300
H	-2.52822600	-5.63315600	0.89295400
H	-4.01599700	-5.91519500	0.00169900

unsubstituted $\mathbf{6}^{2+}$

C	2.14423400	4.18005300	-0.00016100
C	1.71176800	2.85683700	0.00005500
C	0.29701800	2.67783000	0.00015600
C	-0.69698900	3.65867300	0.00000200
C	-0.21840500	4.97579900	-0.00015000
C	1.16874500	5.20282900	-0.00022800
C	-2.43498700	1.44088800	0.00004400
C	-1.20198400	0.74994000	0.00012000
C	-1.18897800	-0.63704300	0.00000600
C	-2.29685000	-1.48664200	0.00001900
C	-3.52431600	-0.80172400	0.00001000
C	-3.57864000	0.62358300	0.00000600
H	3.19621300	4.44258900	-0.00024100
H	-0.89925300	5.82028600	-0.00021700
H	1.50974600	6.23303900	-0.00040600
H	-4.46829700	-1.33690200	0.00007100
H	-4.56041600	1.08589800	-0.00001400
C	1.18897800	0.63704300	0.00000600
C	1.20198400	-0.74994000	0.00012000
C	2.29685000	1.48664200	0.00001900
C	2.43498700	-1.44088800	0.00004400
C	3.52431600	0.80172400	0.00001000
C	-0.29701800	-2.67783000	0.00015600
C	3.57864000	-0.62358300	0.00000600
H	4.46829700	1.33690200	0.00007100
C	-1.71176800	-2.85683700	0.00005500
C	0.69698900	-3.65867300	0.00000200
H	4.56041600	-1.08589800	-0.00001400
C	-2.14423400	-4.18005300	-0.00016100
C	0.21840500	-4.97579900	-0.00015000
C	-1.16874500	-5.20282900	-0.00022800
H	-3.19621300	-4.44258900	-0.00024100
H	0.89925300	-5.82028600	-0.00021700

H	-1.50974600	-6.23303900	-0.00040600
N	0.01238400	1.34351200	0.00011400
N	-0.01238400	-1.34351200	0.00011400
S	-2.43498700	3.22387600	0.00004500
S	2.43498700	-3.22387600	0.00004500

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C	-2.12741800	-1.68496700	-0.39241700
C	-1.00299500	-0.93386600	-0.76328300
C	0.30695900	-1.38680500	-0.78901400
C	0.53574600	-2.72205500	-0.51404500
C	-0.57643600	-3.55121300	-0.24158500
C	-1.89998800	-3.09002200	-0.16637700
C	3.18006700	-1.82811100	-0.26296400
C	2.59716800	-0.59188000	-0.51560000
C	3.19857200	0.66102700	-0.22831900
C	4.53161300	0.60303400	0.21563800
C	5.18011400	-0.62504100	0.43754500
C	4.48043400	-1.83562100	0.22605500
H	-0.36737600	-4.59529000	-0.05266800
H	5.06906800	1.51641000	0.42099900
H	4.94692000	-2.78759100	0.45327600
C	1.00302100	0.93388500	-0.76337100
C	-0.30693500	1.38682100	-0.78898300
C	2.12744900	1.68497900	-0.39249100
C	-0.53572000	2.72206800	-0.51400100
C	1.90003200	3.09003900	-0.16645800
C	-2.59713800	0.59189300	-0.51546900
C	0.57647300	3.55122900	-0.24161100
C	-3.19854700	-0.66103100	-0.22823400
C	-3.18005400	1.82812300	-0.26288100
H	0.36743500	4.59531100	-0.05269100
C	-4.53161800	-0.60303900	0.21562200
C	-4.48047000	1.83562300	0.22602300
C	-5.18014500	0.62503300	0.43748000
H	-5.06910000	-1.51640700	0.42094900
H	-4.94699700	2.78758300	0.45318100
N	1.29619600	-0.41479200	-0.90376800
N	-1.29617100	0.41480700	-0.90362700
C	-6.63877300	0.69977900	0.93661800
C	-7.49061200	1.48350800	-0.09057100
H	-8.52927300	1.54940100	0.25107500
H	-7.12391900	2.50392200	-0.23379300
H	-7.48454000	0.98691200	-1.06615400

C	-7.27145300	-0.69292600	1.11728700
H	-7.29507200	-1.25737300	0.17925500
H	-6.74326400	-1.29076000	1.86746900
H	-8.30517600	-0.58164500	1.45831100
C	-6.68046100	1.42714200	2.30187900
H	-7.71211800	1.49112800	2.66443600
H	-6.08988800	0.88993400	3.05100700
H	-6.28995700	2.44675000	2.23729200
C	3.03832500	4.06822500	0.17854700
C	3.58681200	3.73635100	1.58856800
H	3.89571100	2.69486200	1.69050600
H	4.45026100	4.37041900	1.81832700
H	2.81979900	3.92381900	2.34663000
C	4.14761700	3.97033700	-0.89615000
H	4.99376300	4.61038200	-0.62407100
H	4.52345300	2.95533200	-1.03237200
H	3.76827100	4.30909500	-1.86556400
C	2.57091900	5.53821500	0.20677500
H	2.14335000	5.85033800	-0.75114600
H	1.83359100	5.72549700	0.99329900
H	3.43148800	6.18286800	0.41058500
C	6.63868900	-0.69984500	0.93678600
C	7.49062300	-1.48324900	-0.09059300
H	7.12389800	-2.50359800	-0.23419400
H	7.48465300	-0.98631200	-1.06599900
H	8.52924700	-1.54927900	0.25113900
C	6.68029300	-1.42762600	2.30181700
H	7.71191800	-1.49171500	2.66444600
H	6.08965300	-0.89066600	3.05107100
H	6.28979800	-2.44722100	2.23690600
C	7.27129700	0.69283100	1.11792800
H	7.29522300	1.25745500	0.18000900
H	6.74285500	1.29051900	1.86804500
H	8.30491100	0.58148800	1.45926200
C	-3.03827600	-4.06820500	0.17865900
C	-4.14753600	-3.97039800	-0.89607400
H	-3.76814800	-4.30915500	-1.86547100
H	-4.99366500	-4.61047400	-0.62401200
H	-4.52341300	-2.95541300	-1.03231700
C	-3.58682600	-3.73624800	1.58863700
H	-4.45027200	-4.37032100	1.81839300
H	-2.81984300	-3.92365800	2.34674500
H	-3.89575000	-2.69475700	1.69049000
C	-2.57084900	-5.53818000	0.20700700

H	-2.14321500	-5.85036500	-0.75086700
H	-1.83356100	-5.72539300	0.99358500
H	-3.43141500	-6.18284200	0.41080500
S	2.23395100	-3.33412000	-0.60931300
O	2.49612400	-3.72924200	-2.00171300
O	2.46446500	-4.30336400	0.47139500
S	-2.23393000	3.33416000	-0.60910400
O	-2.46437000	4.30326300	0.47174900
O	-2.49617800	3.72949000	-2.00143000

unsubstituted **7**

C	-0.64786700	2.60042500	0.04990800
C	-0.22395300	1.33704600	0.47318700
C	1.09676100	0.91490100	0.48659800
C	2.09105900	1.82902100	0.16078400
C	1.71278900	3.15226200	-0.17075600
C	0.37221000	3.53979500	-0.23769900
C	3.62778700	-0.49402000	-0.13028200
C	2.41917000	-1.11325900	0.16726300
C	2.10177600	-2.46303500	-0.14703900
C	3.13585700	-3.24391900	-0.67426000
C	4.38037400	-2.65179600	-0.92597000
C	4.62738300	-1.28804500	-0.69277400
H	2.49152200	3.86489000	-0.41975300
H	2.97453600	-4.28739900	-0.92593600
H	5.58094100	-0.84719500	-0.96270700
C	0.22394500	-1.33705200	0.47317100
C	-1.09677000	-0.91490700	0.48656900
C	0.64786500	-2.60042600	0.04988500
C	-2.09106200	-1.82902300	0.16072800
C	-0.37220700	-3.53979200	-0.23775000
C	-2.41917400	1.11325700	0.16724000
C	-1.71278700	-3.15226000	-0.17082300
C	-2.10177500	2.46303700	-0.14704100
C	-3.62778500	0.49402100	-0.13033400
H	-2.49151600	-3.86488500	-0.41984200
C	-3.13584500	3.24392600	-0.67427300
C	-4.62737000	1.28805200	-0.69283700
C	-4.38035700	2.65180500	-0.92601300
H	-2.97451900	4.28740900	-0.92593300
H	-5.58092300	0.84720400	-0.96279200
N	1.29540700	-0.45901900	0.61584600
N	-1.29541800	0.45901200	0.61583600

S	3.81224800	1.27130600	0.22949400
O	4.27465700	1.41007000	1.61764800
O	4.56844900	1.90500100	-0.85842600
S	-3.81225100	-1.27130800	0.22942200
O	-4.56843900	-1.90499200	-0.85851300
O	-4.27467700	-1.41008400	1.61756900
H	5.17465700	-3.25801500	-1.34864700
H	0.12869300	4.54937600	-0.55059300
H	-5.17463300	3.25803000	-1.34869800
H	-0.12868600	-4.54937000	-0.55065200

1

C	0.22586100	4.38914300	-0.62505600
C	-0.05136500	3.21677100	0.04157000
C	1.09209100	2.39902200	0.36571600
C	2.41207000	2.55855200	-0.11435000
C	2.64464100	3.82492000	-0.75181200
C	1.59032800	4.69337300	-0.96332400
C	3.26407500	1.41215400	-0.11700800
C	2.78321400	0.12641200	0.25702100
C	1.46261300	0.04886400	0.80463400
C	0.77220900	-1.17572700	0.84836100
C	1.26691400	-2.37089700	0.33315000
C	2.64464100	-2.34451400	-0.05919400
C	3.37086200	-1.15598600	-0.06891500
H	-0.55545000	5.07246800	-0.94747100
H	3.63577100	4.08365000	-1.11518300
H	1.78539700	5.63353800	-1.47122300
H	4.25821500	1.50066900	-0.54962700
H	3.13167900	-3.24467100	-0.42531000
H	4.39538400	-1.18238600	-0.43114400
C	-0.77220900	1.17572700	0.84836100
C	-1.46261300	-0.04886400	0.80463400
C	-1.26691400	2.37089700	0.33315000
C	-2.78321400	-0.12641200	0.25702100
C	-2.64464100	2.34451400	-0.05919400
C	-1.09209100	-2.39902200	0.36571600
C	-3.26407500	-1.41215400	-0.11700800
C	-3.37086200	1.15598600	-0.06891500
H	-3.13167900	3.24467100	-0.42531000
C	0.05136500	-3.21677100	0.04157000
C	-2.41207000	-2.55855200	-0.11435000
H	-4.25821500	-1.50066900	-0.54962700
H	-4.39538400	1.18238600	-0.43114400

C	-0.22586100	-4.38914300	-0.62505600
C	-2.64464100	-3.82492000	-0.75181200
C	-1.59032800	-4.69337300	-0.96332400
H	0.55545000	-5.07246800	-0.94747100
H	-3.63577100	-4.08365000	-1.11518300
H	-1.78539700	-5.63353800	-1.47122300
C	-0.66597800	-1.18635700	0.87253500
C	0.66597800	1.18635700	0.87253500

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