Supplementary Information

Pyrrole-Fused Azacoronene Family: The Influence of Replacement with Dialkoxybenzenes on the Optical and Electronic Properties in Neutral and Oxidized States

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S1. Materials and methods

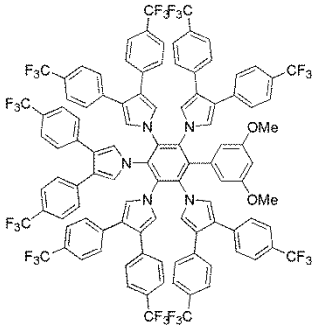
^{1}H-, ^{13}C- and ^{19}F-NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer operating at 500.13 MHz for ^{1}H, 125.76 MHz for ^{13}C, and 470.59 MHz for ^{19}F with use of tetramethylsilane (0 ppm) or residual solvent for ^{1}H (5.31 ppm for CD_2Cl_2) and ^{13}C (77.01 ppm for $CDCl_3$, 53.85 ppm for CD_2Cl_2) signals, and hexafluorobenzene for ^{19}F signal (-164.9 ppm) as an internal standard, and if not otherwise noted, all spectra measured at 298K. Electron impact (EI) mass spectra and atmospheric pressure chemical ionization (APCI) mass spectra were obtained on SHIMADZU GC–MS QP2020 and Bruker MicrOTOF II, respectively. Melting points were determined with Yanako MP–500D and not corrected. Thermogravimetric analysis (TGA) was carried out with Rigaku DSC8230L under nitrogen atmosphere. Elemental analysis was performed with Exeter Analytical, Inc. CE–440F in the microanalysis laboratory of Tokyo Metropolitan University. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were performed on BAS-ALS620B electrochemical analyzer using a standard three-electrode cell consisting of a Pt working electrodes, a Pt wire counter electrode, and a $Ag/AgNO_3$ reference electrode under argon atmosphere. The potentials were calibrated with ferrocene as an external standard. ESR spectra were recorded on JEOL JES–RE3X instruments. Magnetic measurement was carried out on a Quantum Design SQUID MPMS-XL magnetometer on powder samples. Electronic spectra were recorded on SHIMADZU UV–Vis–NIR scanning spectrophotometer (Model UV–3101–PC). Fluorescence and phosphorescence spectra were measured with JASCO FP–6500 spectrofluorometer. Fluorescence quantum yield was determined by comparison with quinine sulfate in 0.5 M H_2SO_4 solution ($\Phi_F = 0.51$). The calculation of the fluorescence quantum yield of a sample solution (Φ_s), relative to the reference sample of known quantum yield (Φ_r), is given by $\Phi_s = \Phi_r(A_r/A_s)(I_s/I_r)(n_s/n_r)^2$ where A_s and A_r are the absorbances of the sample and the reference solutions, I_s and I_r are the corresponding relative integrated fluorescence intensities, and n_s and n_r are the measured refractive indexes of solvents (Parker-Ress method). Fluorescence and phosphorescence lifetimes were measured by time-correlated single-photon counting (TCSPC) and multi-channel scaling (MCS) techniques, respectively. These measurements were carried out with HORIBA Jobin Yvon photon counting system (FluoroCube). The excitation wavelength was 375 nm (fluorescence, TCSPC) and 370 nm (phosphorescence, MCS). The total instrument response function has an FWHM of ca. 200 ps for the fluorescence measurements.

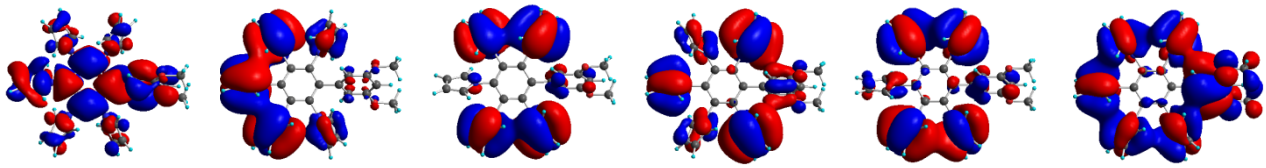
All reactions were carried out under nitrogen atmosphere. THF was freshly distilled from sodium benzophenone ketyl before use, and other solvents were purified with standard methods. Column chromatography was carried out using Daiso silica gel 1001W. *N*-Benzenesulfonyl-3,4-dibromopyrrole[1] 3,5-didodecyloxy-bromobenzene[2] and 3,5-dibuthoxy-bromobenzene[3] were synthesized according to the literature procedures.

S2. Molecular orbitals for 9 and 10

The GAUSSIAN 09[4] series of programs was used for all calculations. All molecules were fully optimized using the hybrid density functional at B3LYP level of theory with the 6-31G(d) basis set. Frequency calculations were conducted to ensure that these structures were indeed local minima.

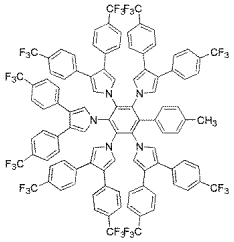
1. Molecular orbitals for **9c**

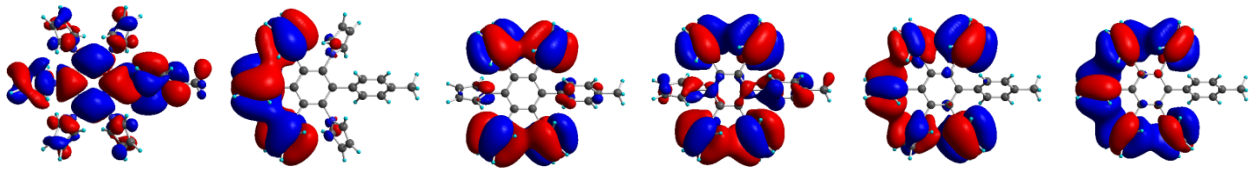




LUMO	HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4
-1.27 eV	-5.56 eV	-5.60 eV	-5.65 eV	-5.67 eV	-5.79 eV

2. Molecular orbitals for **10**

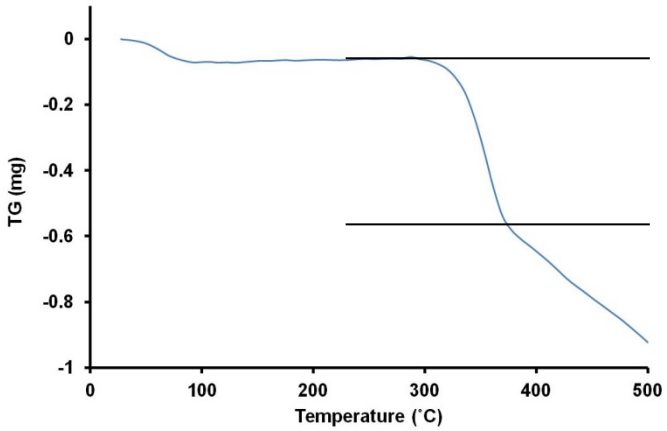




LUMO	HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4
-1.16 eV	-5.51 eV	-5.52 eV	-5.57 eV	-5.58 eV	-5.71 eV

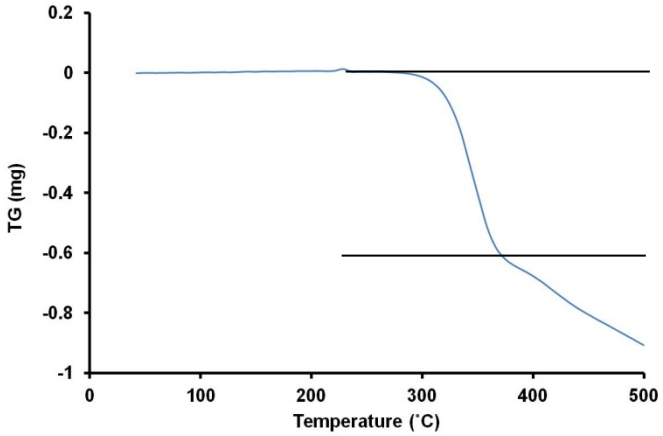
S3. TGA analyses of 2a, 3a and 4a

1. TGA analysis of **2a**



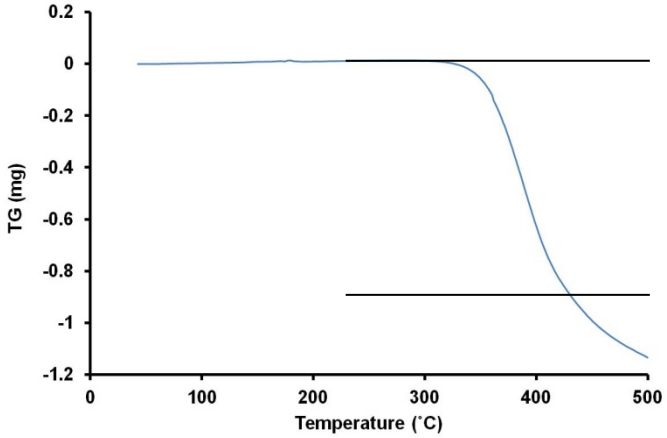
Sample weight: 3.162 mg
Weight loss: 0.474 mg
Losing weight%: 15.0%
Percentages of alkyl chains weight of whole molecule: 14.9%

2. TGA analysis of **3a**



Sample weight: 2.143 mg
Weight loss: 0.585 mg
Losing weight%: 27.3%
Percentages of alkyl chains weight of whole molecule: 28.6%

3. TGA analysis of **4a**

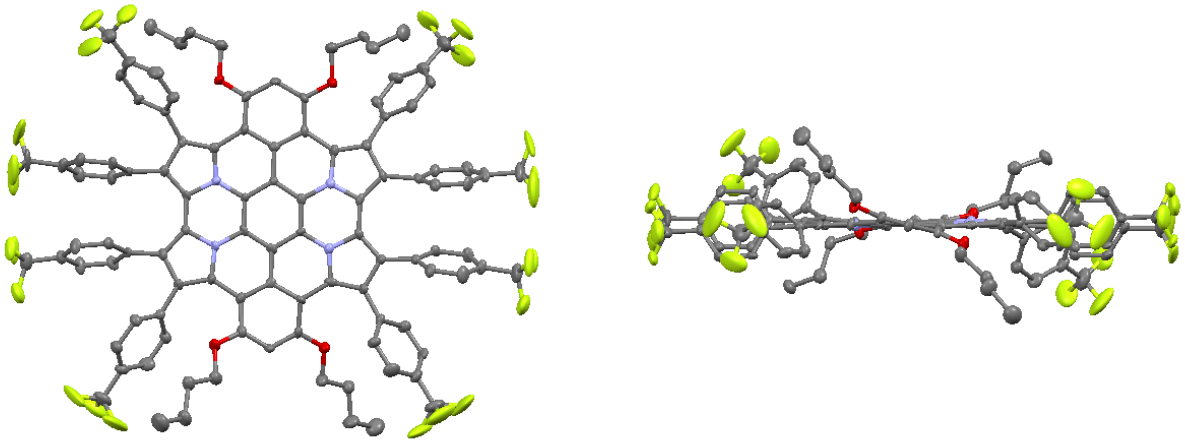


Sample weight: 2.497 mg
Weight loss: 0.887 mg
Losing weight%: 35.5 %
Percentage of alkyl chains weight of whole molecule: 41.3%

S4. X-ray crystal structures of 3b, 4a, and 12b

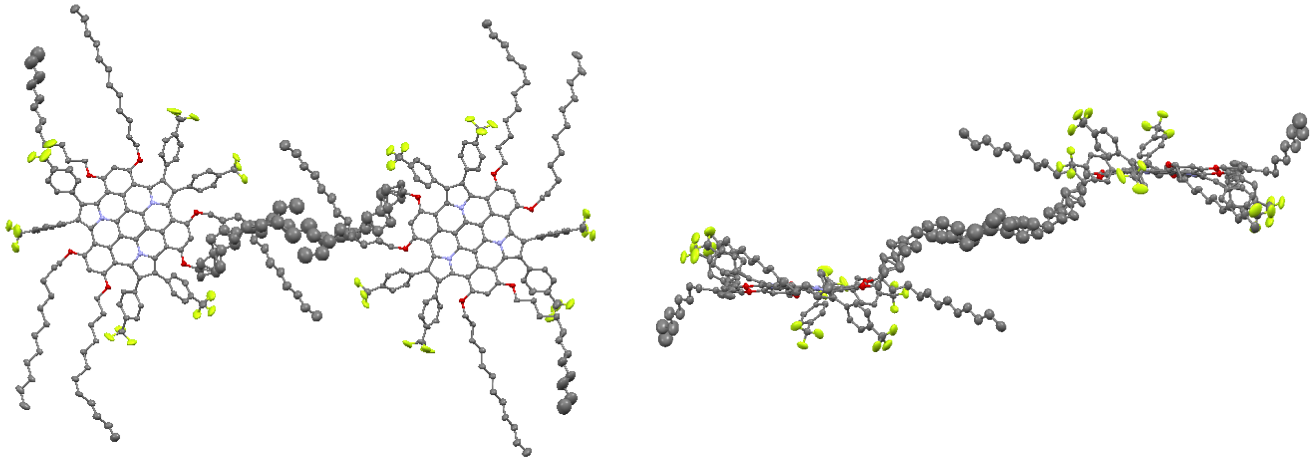
X-ray data were taken on Bruker SMART APEX and SMART APEXII ULTRA diffractometer equipped with a CCD area detector with monochromated Mo-K$_\alpha$ irradiation (λ = 0.71073 Å). The structures were solved by direct methods (SHELXS) and refined by the full-matrix least-squares method on F^2 (SHELXL-97). Non-hydrogen atoms were refined anisotropically, and hydrogen atoms were placed using AFIX instructions.

Table S4a. Crystal data and structure refinement for **3b**.



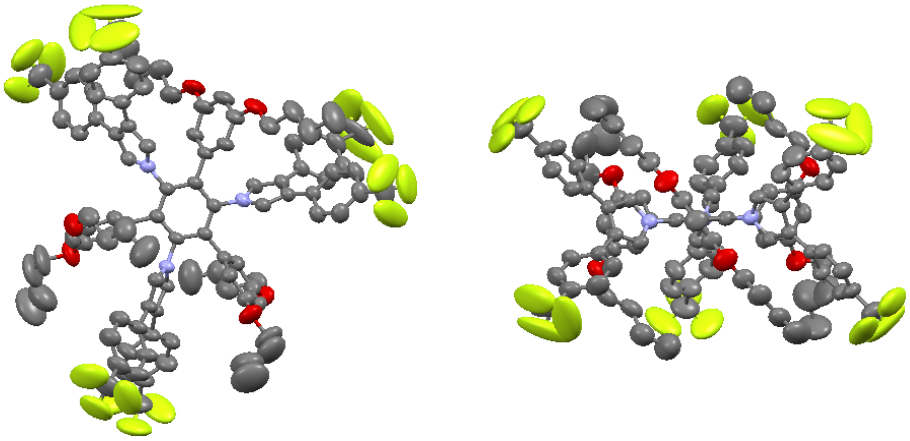
Identification code	**3b**	
Empirical formula	$C_{106}\,H_{70}\,F_{24}\,N_4\,O_4$	
Formula weight	1919.66	
Temperature	123 K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.648(4) Å	α = 90.00°.
	b = 38.150(8) Å	β = 125.87(3)°.
	c = 15.294(3) Å	γ = 90.00°.
Volume	8817(3) Å^3	
Z	4	
Density (calculated)	1.446 Mg/m^3	
Absorption coefficient	0.123 mm^{-1}	
F(000)	3928	
Crystal size	0.30 x 0.20 x 0.02 mm^3	
Theta range for data collection	1.96 to 23.31°.	
Index ranges	-20<=h<=20, -42<=k<=37, -15<=l<=17	
Reflections collected	19072	
Independent reflections	6371 [R(int) = 0.1466]	
Completeness to theta = 23.31°	99.7 %	
Absorption correction	Empirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6371 / 72 / 683	
Goodness-of-fit on F^2	0.905	
Final R indices [I>2sigma(I)]	R1 = 0.0665, wR2 = 0.1457	
R indices (all data)	R1 = 0.1743, wR2 = 0.1915	
Largest diff. peak and hole	0.515 and -0.304 e.Å^{-3}	

Table S4b. Crystal data and structure refinement for **4a**.



Identification code	**4a**	
Empirical formula	$C_{150}\ H_{177}\ F_{18}\ N_3\ O_6$	
Formula weight	2459.95	
Temperature	93 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.1224(17) Å	α= 102.3660(10)°.
	b = 18.0032(17) Å	β= 93.7450(10)°.
	c = 23.929(2) Å	γ = 113.2540(10)°.
Volume	6526.8(11) $Å^3$	
Z	2	
Density (calculated)	1.252 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	2616	
Crystal size	0.42 x 0.10 x 0.05 mm^3	
Theta range for data collection	2.14 to 25.03°.	
Index ranges	-20<=h<=16, -20<=k<=21, -26<=l<=28	
Reflections collected	31195	
Independent reflections	22605 [R(int) = 0.0309]	
Completeness to theta = 25.03°	98.1 %	
Absorption correction	Multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	22605 / 3416 / 1850	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0843, wR2 = 0.2319	
R indices (all data)	R1 = 0.1507, wR2 = 0.2790	
Largest diff. peak and hole	0.995 and -0.611 $e.Å^{-3}$	

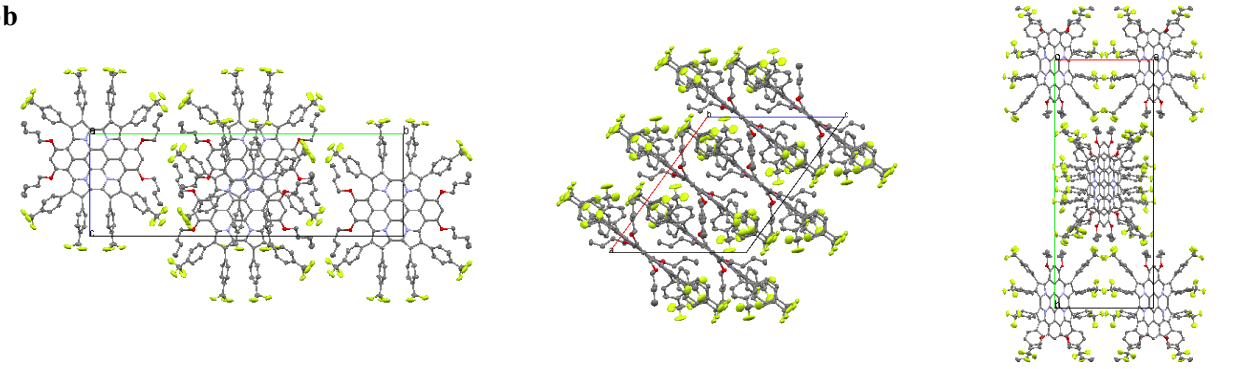
Table S4c. Crystal data and structure refinement for **12b**.



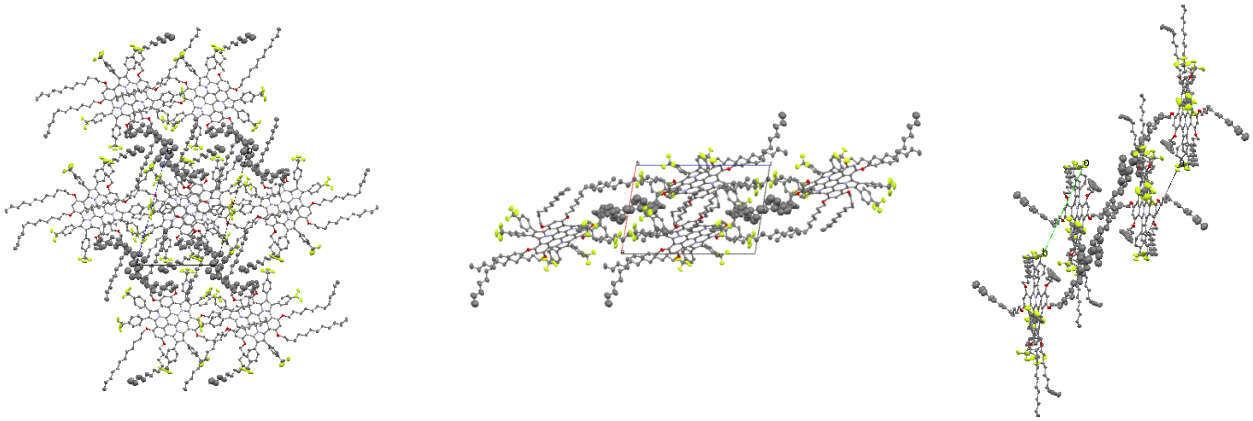
Identification code	**12b**	
Empirical formula	$C_{102}\ H_{93}\ F_{18}\ N_3\ O_6$	
Formula weight	1798.79	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.880(3) Å	α= 99.12(3)°.
	b = 16.898(3) Å	β= 104.64(3)°.
	c = 20.940(4) Å	γ = 118.83(3)°.
Volume	4778(3) $Å^3$	
Z	2	
Density (calculated)	1.250 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	1872	
Crystal size	0.20 x 0.10 x 0.08 mm^3	
Theta range for data collection	1.06 to 23.43°.	
Index ranges	-18<=h<=18, -16<=k<=18, -23<=l<=12	
Reflections collected	20809	
Independent reflections	13719 [R(int) = 0.0222]	
Completeness to theta = 23.43°	97.9 %	
Absorption correction	Empirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13719 / 0 / 1168	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0784, wR2 = 0.2253	
R indices (all data)	R1 = 0.1333, wR2 = 0.2708	
Largest diff. peak and hole	0.436 and -0.370 $e.Å^{-3}$	

S5. Packing structures of 3b and 4a

3b



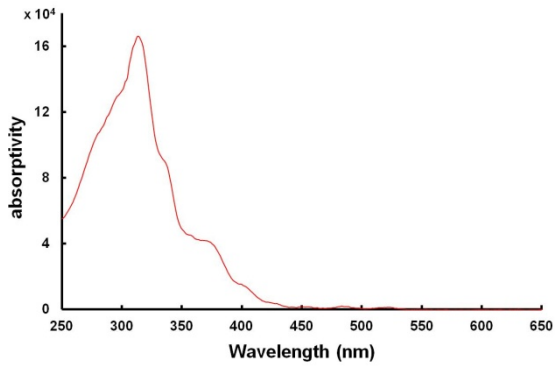
4a



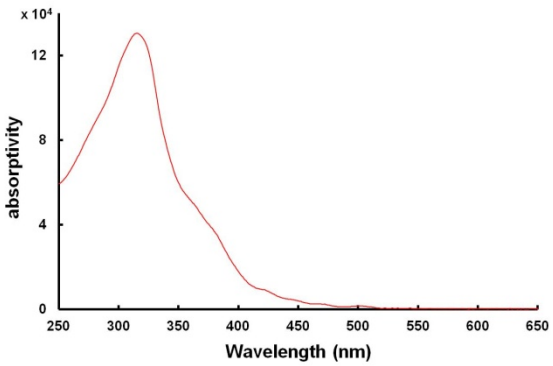
S6. Absorption spectra of 1a–4a with absorptivity

Absorption spectra were all measured in CH_2Cl_2 at room temperature.

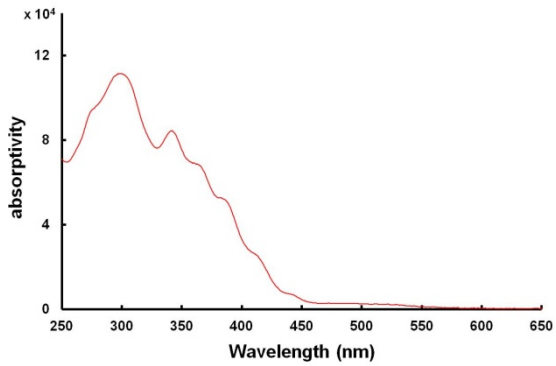
1a



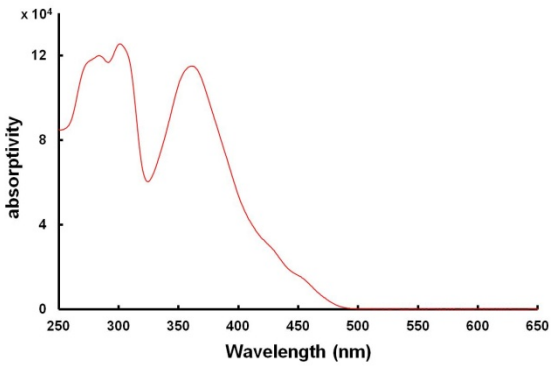
2a



3a

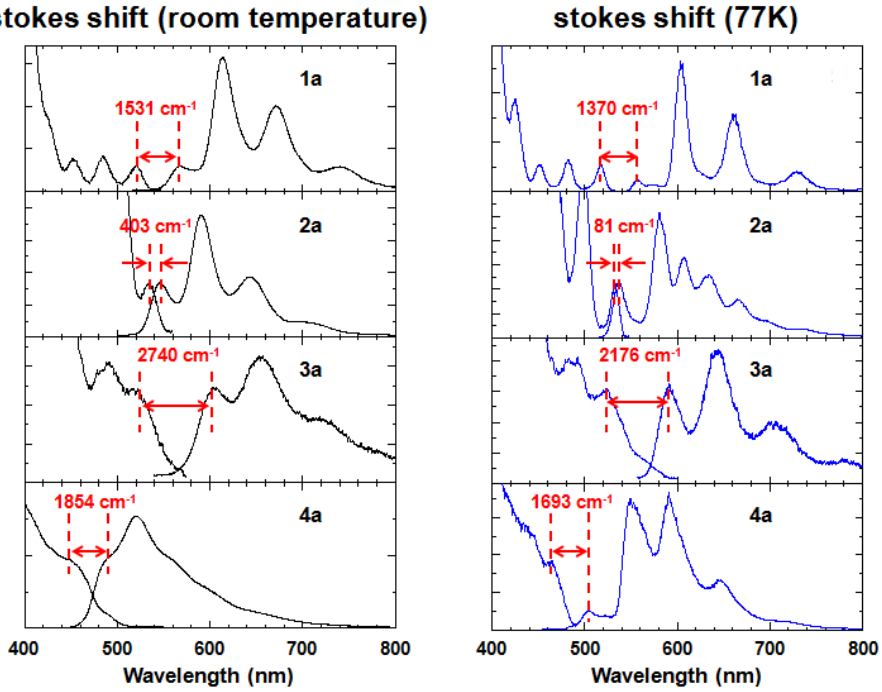


4a



S7. Stokes shifts of 1a–4a

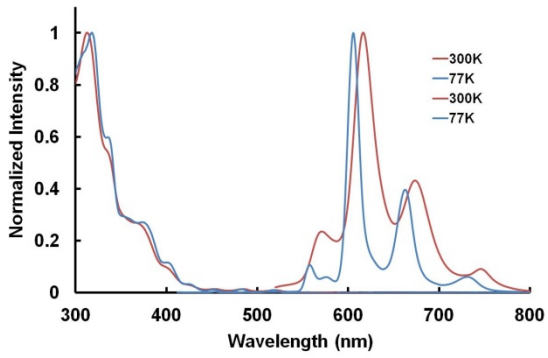
Stokes shifts of **1a**–**4a** at 300K (left) and 77K (right) in MTHF. All excitation wavelengths are 375 nm.



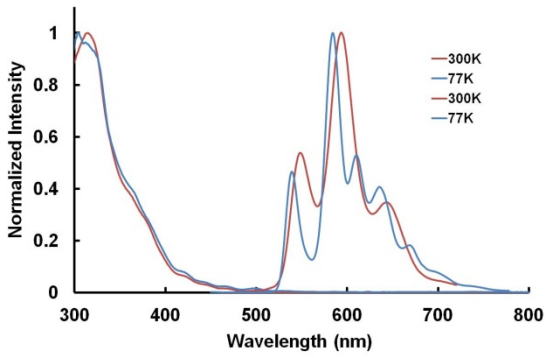
S8. Low temperature measurements of UV and PL spectra of 1a–4a

Following spectra were all measured in MTHF excited at 375 nm.

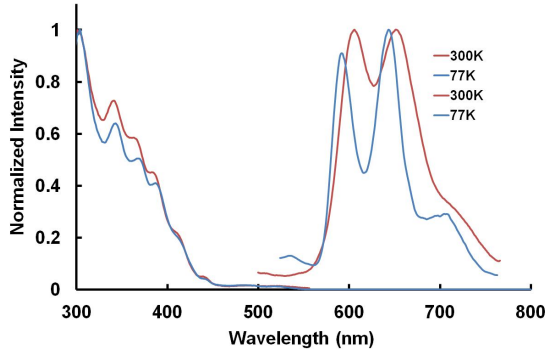
1a



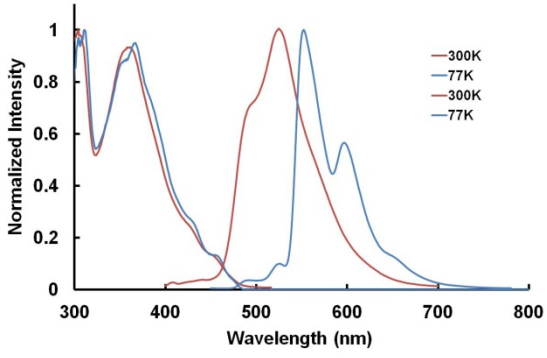
2a



3a

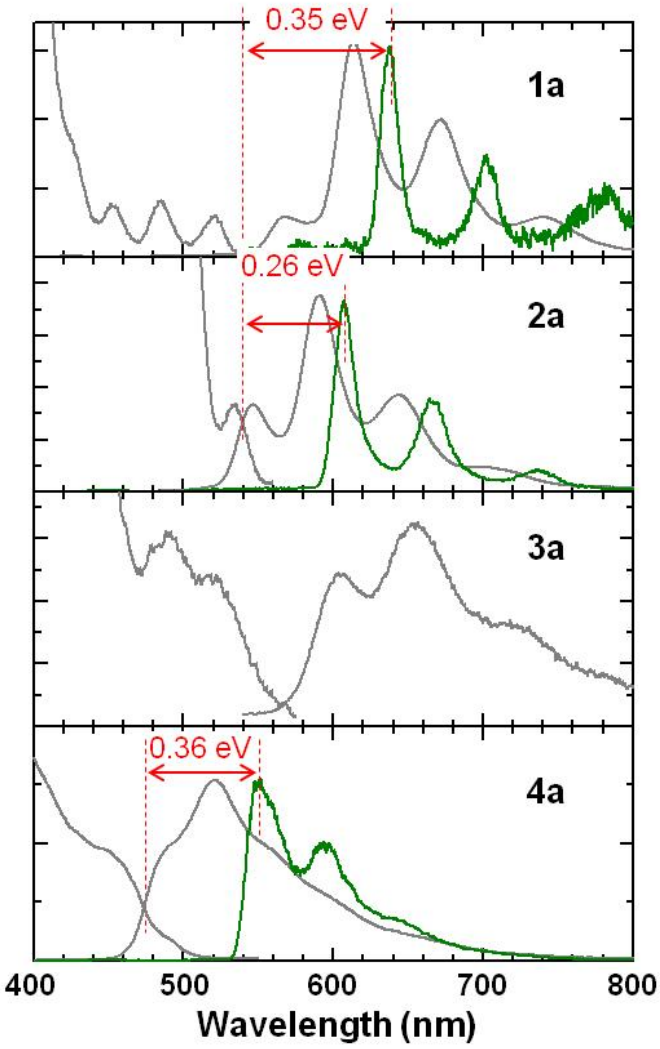


4a



S9. S–T gaps of 1a, 2a, and 4a

Following spectra were all measured in MTHF excited at 375 nm. The S–T gaps were estimated from the 0–0 transition energy and phosphorescence spectra.



S10. Calculated S–T gaps of 1c–4c

1. S–T gap of **1c**

	S	Energy	Transfer orbitals	T	Energy	Transfer orbitals
1c	S2	3.07 eV	117->119			
				T5	2.75 eV	117->120
				T4	2.75 eV	117->119
				T3	2.65 eV	113->118 115->120 116->118 116->119 117->122
				T2	2.65 eV	114->118 115->118 115->119 116->120 117->121
	S1	2.43 eV	117->118			
				T1	2.00 eV	117->118

2. S–T gap of **2c**

	S	Energy	Transfer orbitals	T	Energy	Transfer orbitals
2c	S2	2.86 eV	135->137 136->138			
				T6	2.76 eV	134->137 135->138 136->141
				T5	2.75 eV	135->139 136->138 136->140 136->142
				T4	2.62 eV	135->137 135->139 136->138
				T3	2.53 eV	135->138 136->137 136->139
	S1	2.46 eV	136->137			
				T2	2.34 eV	133->138 134->138 135->137 135->139 136->138 136->140
				T1	2.14 eV	136->137 136->139

3. S–T gap of **3c**

	S	Energy	Transfer orbitals	T	Energy	Transfer orbitals
3c	S2	2.32 eV	154->156			
	S1	2.28 eV	155->156			
				T2	2.12 eV	155->156
				T1	2.00 eV	154->156 155->157

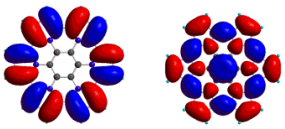
4. S–T gap of **4c**

	S	Energy	Transfer orbitals	T	Energy	Transfer orbitals
4c	S2	2.90 eV	172->176 173->175 173->177 174->176 174->179			
	S1	2.90 eV	172->175 173->176 174->177			
				T9	2.75 eV	172->176 172->179 173->175 173->177 173->178 174->176 174->179
				T8	2.75 eV	172->175 172->177 172->178 173->176 173->179 174->175 174->178
				T7	2.72 eV	172->175 172->178 173->176 173->179 174->177
				T6	2.63 eV	172->176 173->175 173->177 174->176 174->179
				T5	2.63 eV	172->175 172->177 173->176 174->175 174->178
				T4	2.61 eV	172->175 173->176 174->181
				T3	2.44 eV	172->176 173->175 174->180
				T2	2.37 eV	172->179 173->177 173->178 174->176 174->179
				T1	2.37 eV	172->177 172->178 173->179 174->175 174->178

S11. Molecular orbitals of 1c–4c

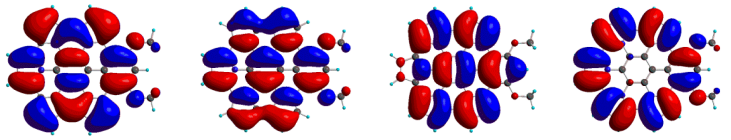
The GAUSSIAN 09[4] series of programs was used for all calculations. All molecules were fully optimized using the hybrid density functional at B3LYP level of theory with the 6-31G(d) basis set. Frequency calculations were conducted to ensure that these structures were indeed local minima.

1c

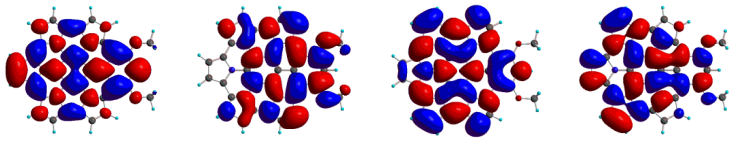


117 (HOMO) 118 (LUMO)

2c

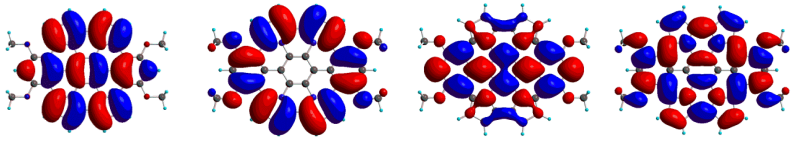


133 134 135 136 (HOMO)



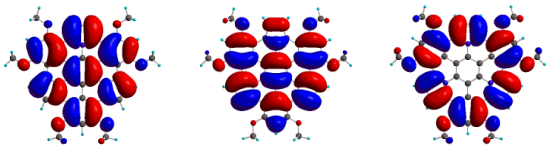
137 (LUMO) 138 139 140

3c

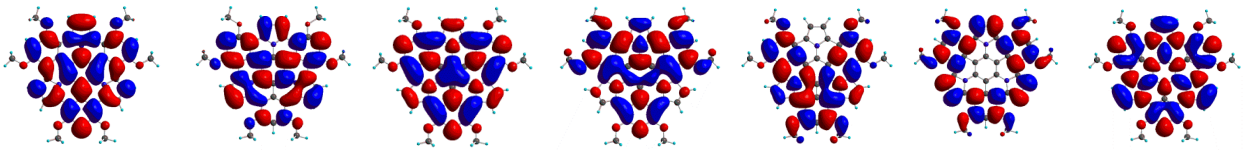


154 156 (HOMO) 157 (LUMO) 158

4c



172 173 174 (HOMO)

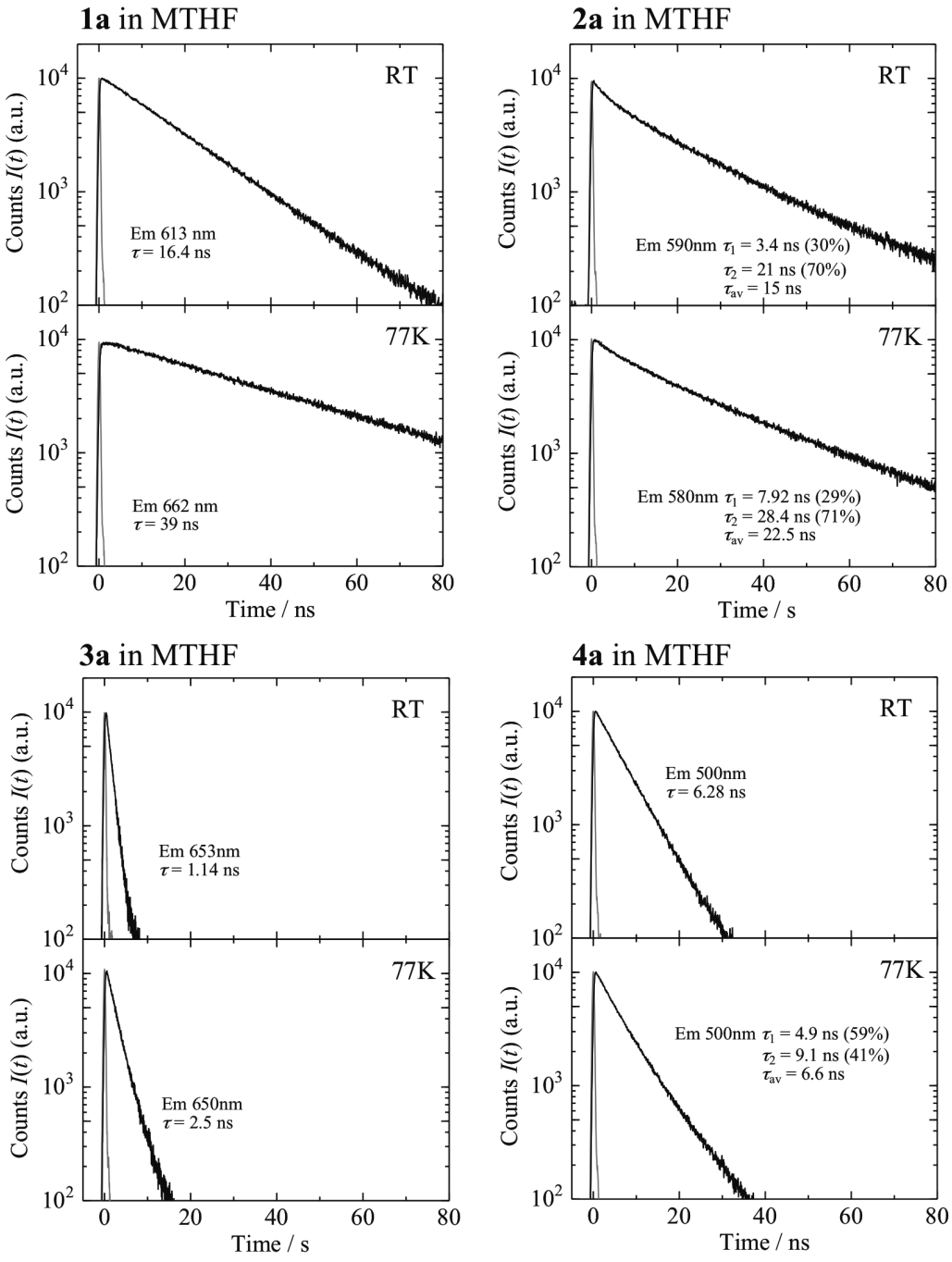


175 (LUMO1) 176 (LUMO2) 177 178 179 180 181

S12. Fluorescence and phosphorescence lifetimes

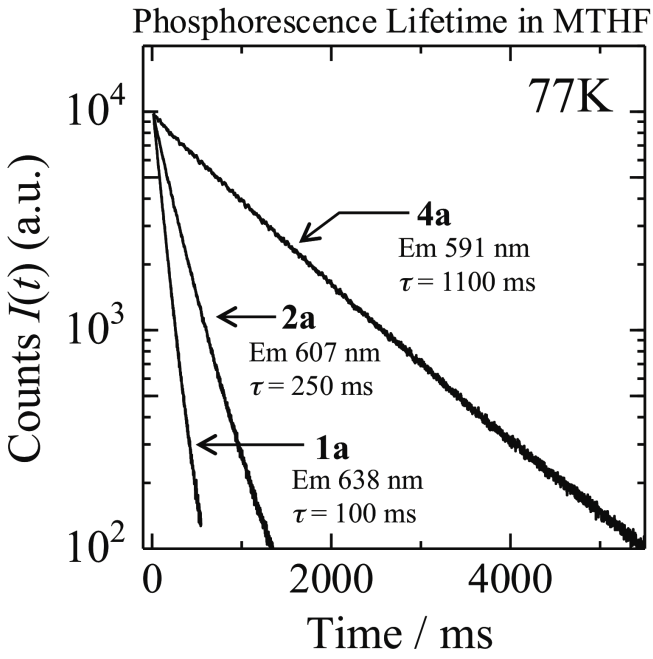
1. Fluorescence lifetimes

The fluorescence decay curve $I(t)$ was fitted with a single or double exponential function, $I(t) = I_0 \sum_i G_i \, exp(-t/\tau_i)$. Excitation wavelength was 375 nm for all samples. Monitor wavelength at RT was 613, 590, 653, and 500 nm for **1a**, **2a**, **3a**, and **4a**, respectively. Monitor wavelength at 77K was 662, 580, 650, and 500 nm for **1a**, **2a**, **3a**, and **4a**, respectively. The gray lines show an excitation laser pulse.



2. Phosphorescence lifetimes

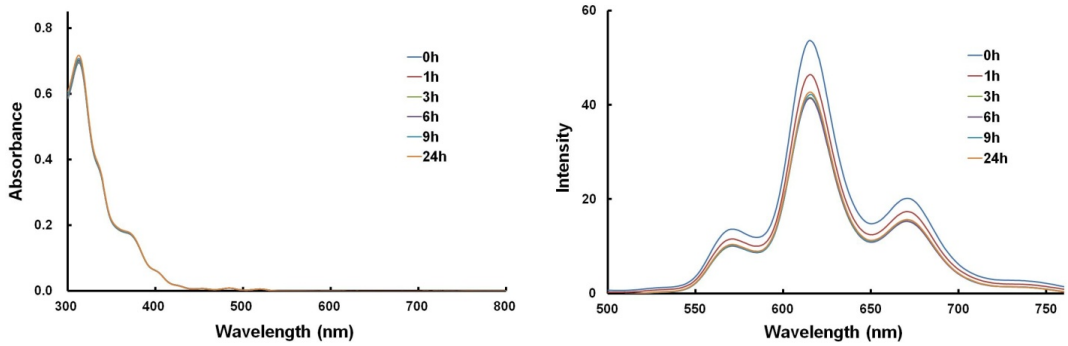
The phosphorescence decay curve $I(t)$ was fitted with a single exponential function, $I(t) = I_0 \, exp(-t/\tau)$. Excitation wavelength was 370 nm for all samples. Monitor wavelength was 638, 607, and 591 nm for **1a**, **2a**, and **4a**, respectively.



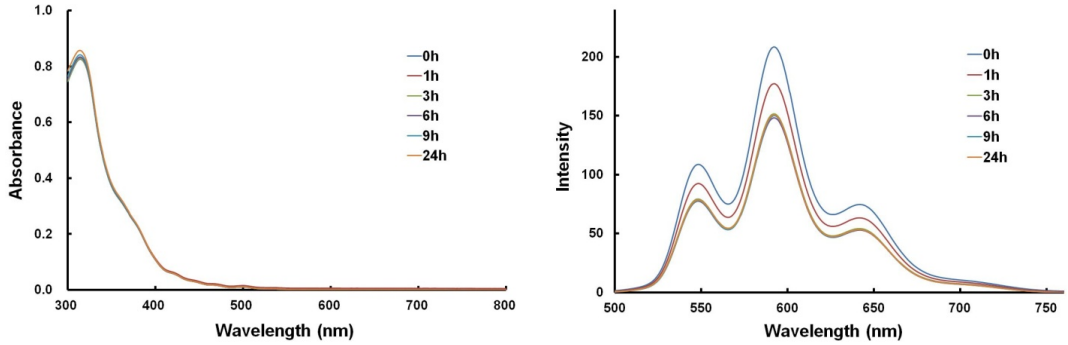
S13. Time dependent UV and PL spectra of 1a–4a

Time dependent changes of the UV-PL spectra of **1a–4a** were measured in MTHF. The solutions were capped under nitrogen atmosphere and stored in ambient laboratory conditions.

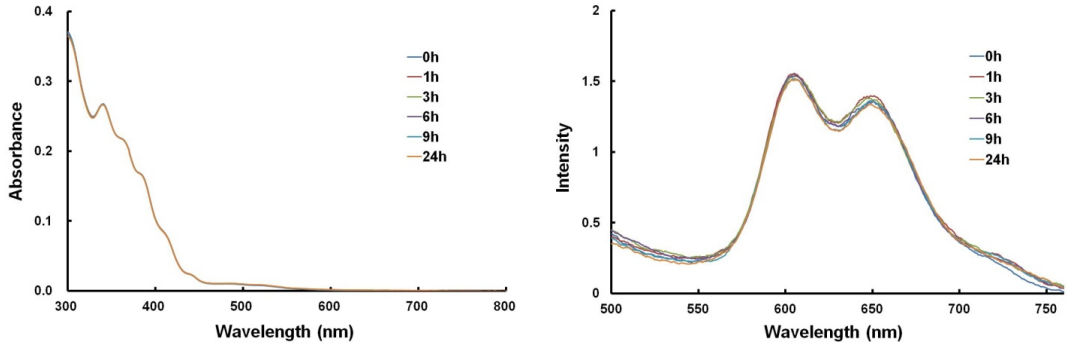
1a



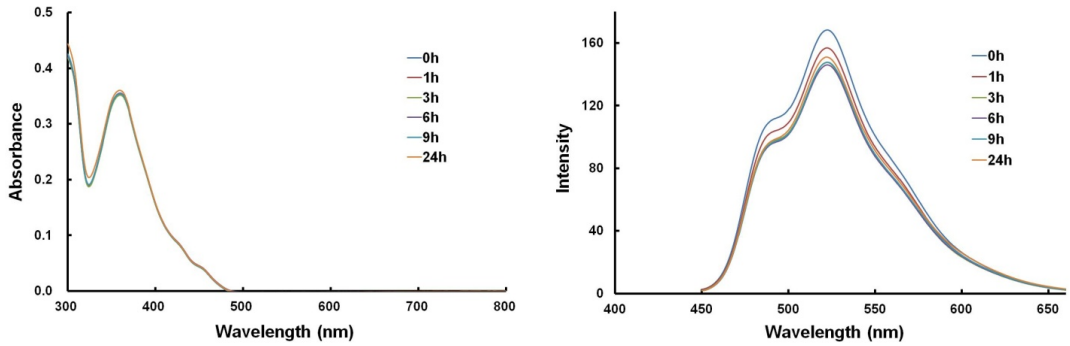
2a



3a



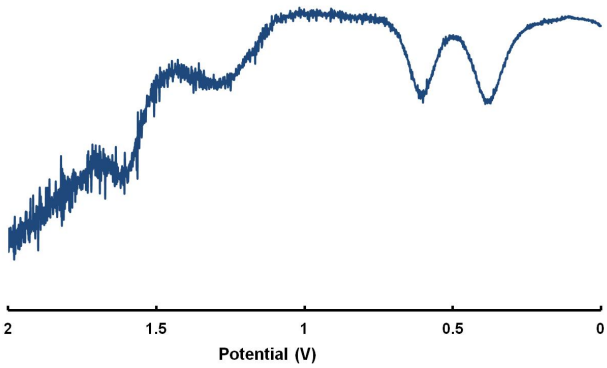
4a



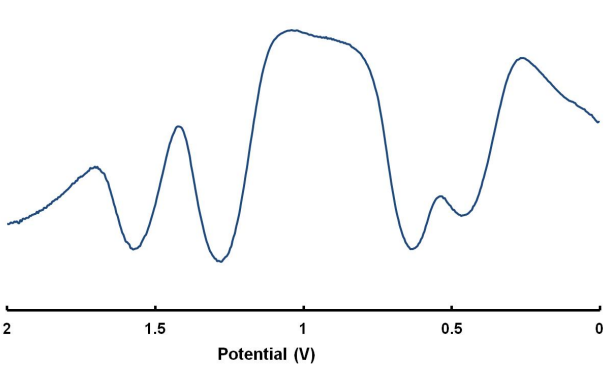
S14. Differential pulse voltammograms of 1a–4a

Differential pulse voltammograms (DPV) of **1a**–**4a** were measured under following conditions: 0.1 M *n*-Bu_4NClO_4 in CH_2Cl_2, $Ag/AgNO_3$ reference electrode, Pt working electrode and Pt counter electrode, scan rate: 100 mV s^{-1}; V vs. Fc/Fc^+.

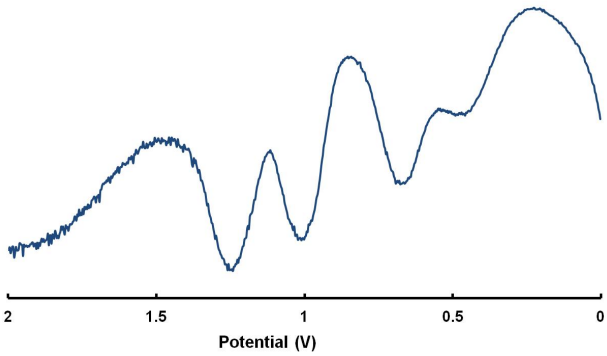
1a



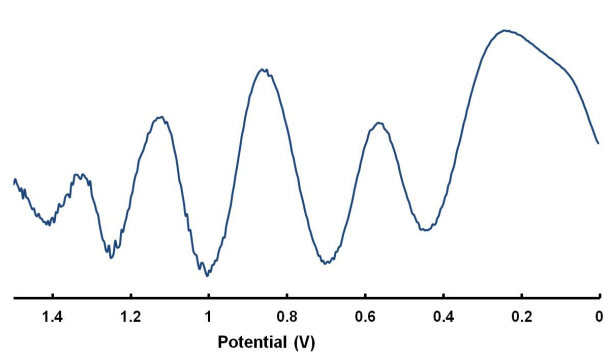
2a



3a



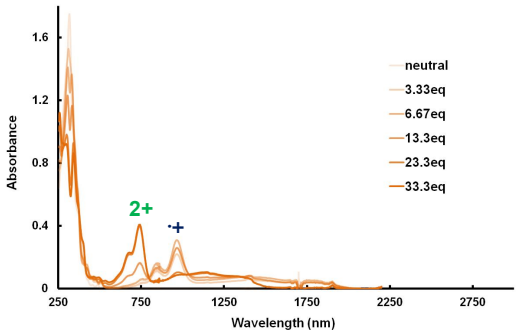
4a



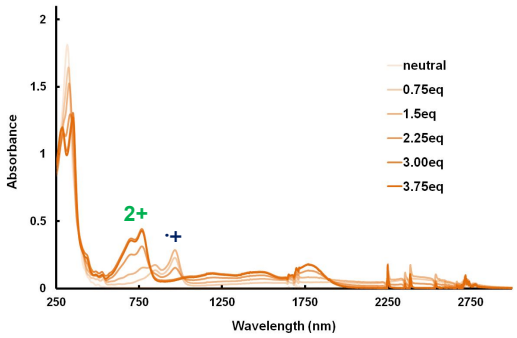
S15. Stepwise chemical oxidations of 1a and 2b–4b

UV-Vis-NIR spectra of **1a** and **2b–4b** in CH_2Cl_2 (1.05 x 10^{-5} M) oxidized by $SbCl_5$.

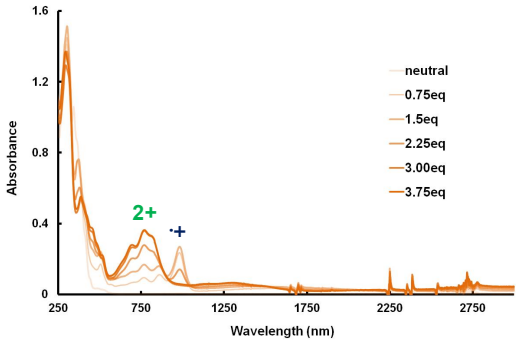
1a



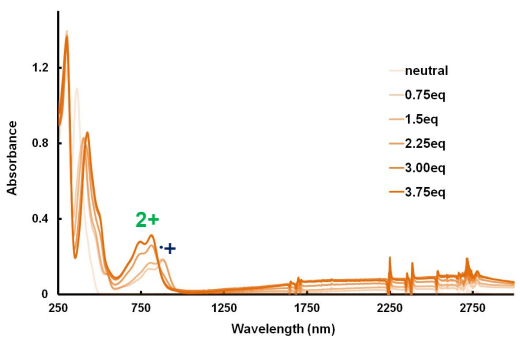
2b



3b

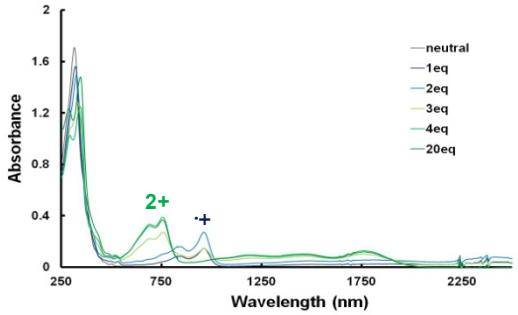


4b

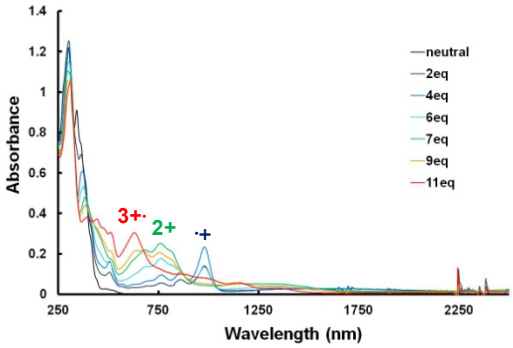


UV–Vis–NIR spectra of **2b–4b** in CH_2Cl_2 and MeCN (4:1, *v*/*v*, 1.05 x 10^{-5} M) oxidized by $Fe(ClO_4)_3$.

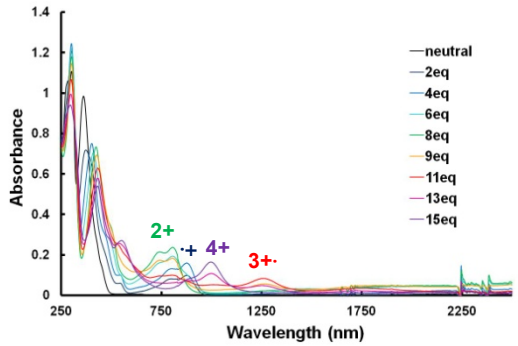
2b



3b

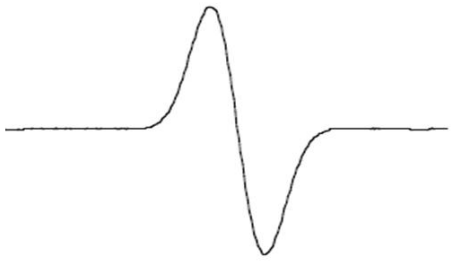


4b



S16. ESR spectra of $1a^{\cdot+}$ and $2b^{\cdot+}$–$4b^{\cdot+}$ in CH_2Cl_2

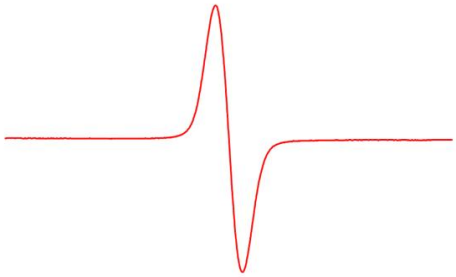
1. ESR spectrum of $\mathbf{1a}^{\cdot+}$ [4]



g factor: 2.0023

ΔH: 0.30 mT

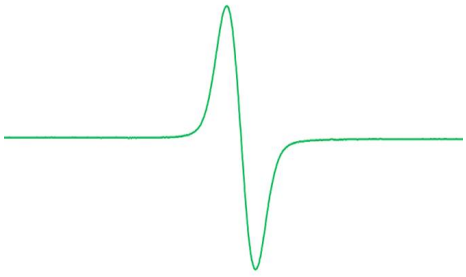
2. ESR spectrum of $\mathbf{2b}^{\cdot+}$



g factor: 2.0033

ΔH: 0.30 mT

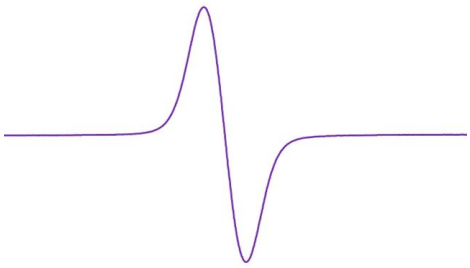
3. ESR spectrum of $\mathbf{3b}^{\cdot+}$



g factor: 2.0034

ΔH: 0.25 mT

4. ESR spectrum of $\mathbf{4b}^{\cdot+}$



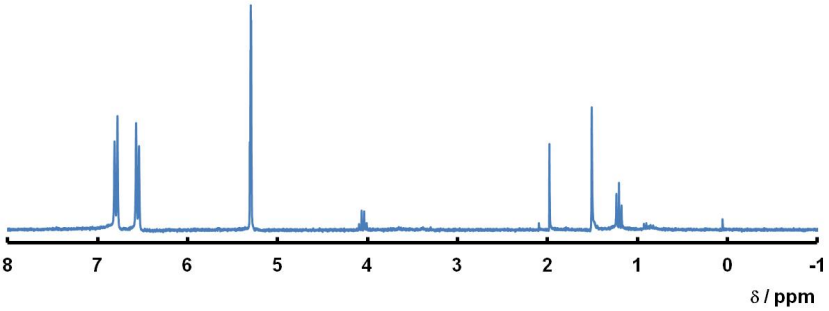
g factor: 2.0034

ΔH: 0.24 mT

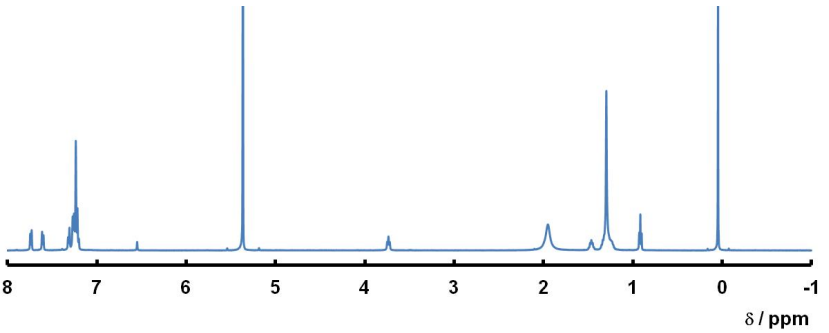
S17. NMR spectra of $1a^{2+}$–$4a^{2+}$ in CD_2Cl_2

The 1.0 mM solutions of $1a^{2+}$–$4a^{2+}$ were prepared by the CD_3CN solutions of $NOSbF_6$ (1 M) and measured at 298 K (for $1a^{2+}$ and $2a^{2+}$) or 233 K (for $3a^{2+}$ and $4a^{2+}$) with or without $Fc(OAc)_2 \cdot AgBF_4$ as a radical scavenger. The circles indicate the peaks of radical scavenger.

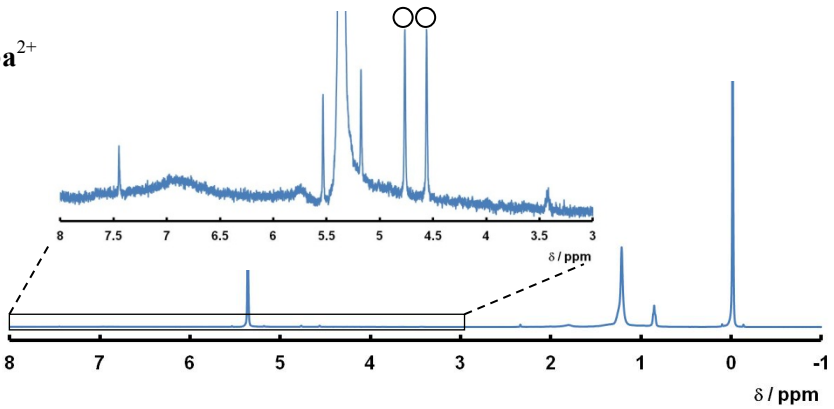
$1a^{2+}$ [4]



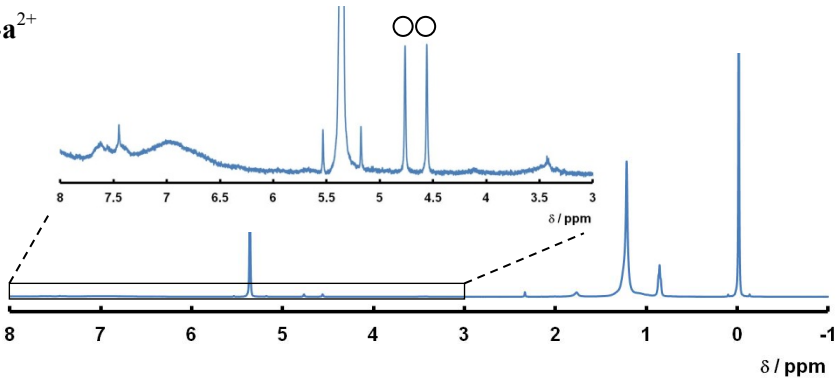
$2a^{2+}$



$3a^{2+}$



$4a^{2+}$



S18. Thermal dependence of $\chi_M T$ and X-ray crystal structure for $4b^{2+}(SbCl_6^-)_2$

Magnetic measurements were carried out for a powder sample in a gelatinous capsule under an applied field of 500 Oe. The χ_p values were obtained from the dc susceptibility, subtracting the diamagnetic susceptibility including a sample holder, –0.0000523 emu K mol^{-1}, evaluated by assuming that χ_p follows the Curie-Weiss law within the temperature range of 100 K – 300 K.

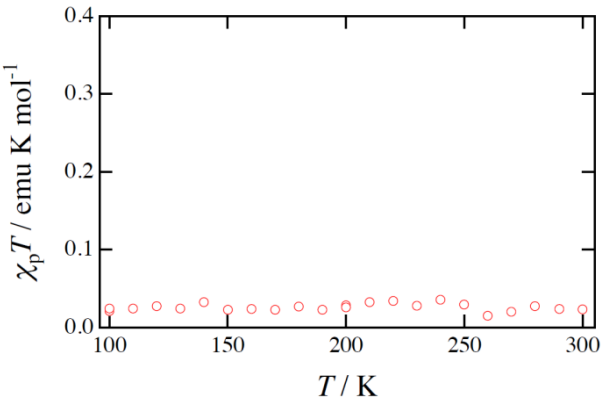
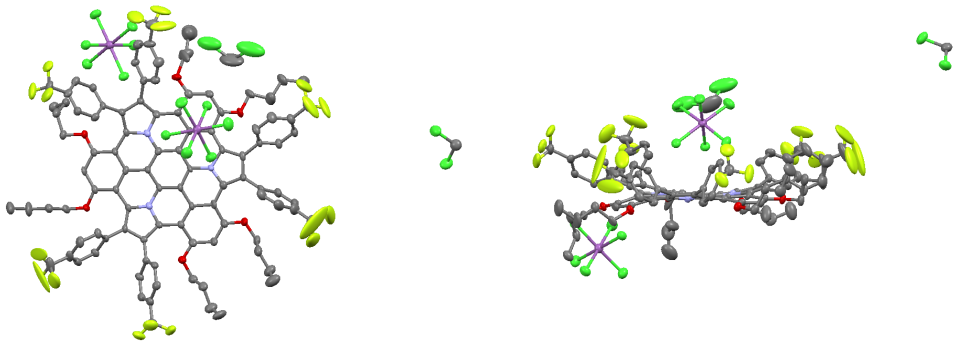


Table S18. Crystal data and structure refinement for **4b**$^{2+}$$(SbCl_6^-)_2$.

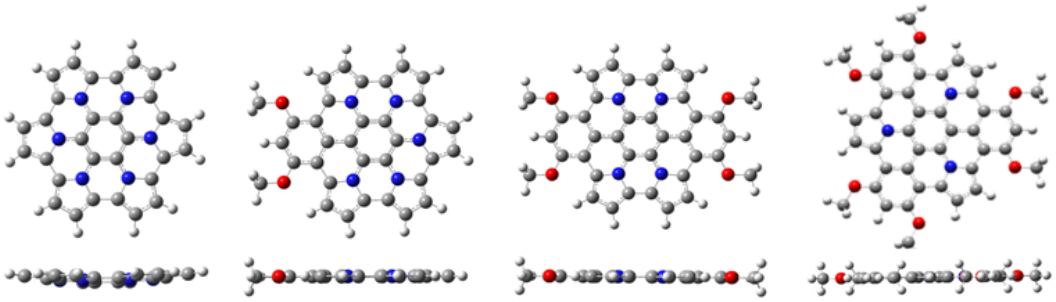


Identification code	**4b**$^{2+}$$(SbCl_6^-)_2$	
Empirical formula	$C_{103.5}H_{84}Cl_{15}F_{18}N_3O_6Sb_2$	
Formula weight	2582.99	
Temperature	100 K	
Wavelength	0.71070 Å	
Crystal system	Orthorhombic	
Space group	Fdd2	
Unit cell dimensions	a = 44.931(3) Å	α= 90.00°.
	b = 47.822(4) Å	β= 90.00°.
	c = 20.0654(15) Å	γ = 90.00°.
Volume	43114(6) Å^3	
Z	16	
Density (calculated)	1.592 Mg/m^3	
Absorption coefficient	0.959 mm^{-1}	
F(000)	20688	
Crystal size	0.10 x 0.05 x 0.02 mm^3	
Theta range for data collection	3.11 to 25.04°.	
Index ranges	-53<=h<=53, -56<=k<=52, -23<=l<=23	
Reflections collected	19030	
Independent reflections	16554 [R(int) = 0.0589]	
Completeness to theta = 25.04°	99.7 %	
Absorption correction	Multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19030 / 1 / 1335	
Goodness-of-fit on F^2	1.095	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1349	
R indices (all data)	R1 = 0.0659, wR2 = 0.1465	
Largest diff. peak and hole	1.431 and -1.048 e.Å^{-3}	

S19. Optimized structures and their atomic coordinations of 1c–4c and $1c^{2+}$–$4c^{2+}$

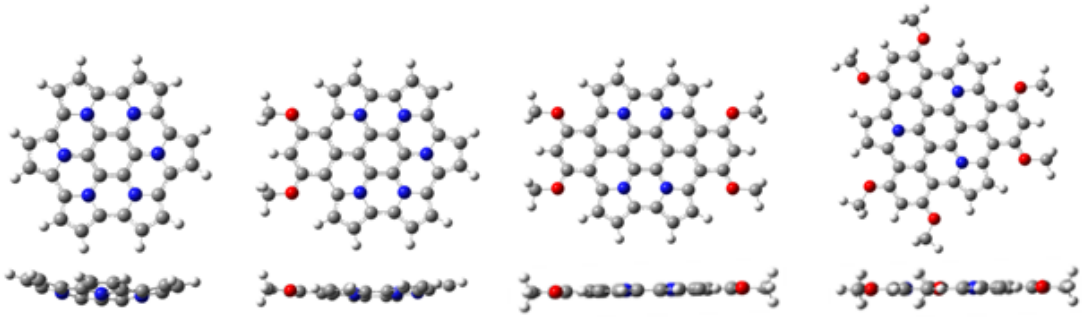
DFT calculations were performed with GAUSSIAN 09[4] series. All geometry optimizations were carried out at the B3LYP/6–31G(d) basis set. Frequency calculations were conducted to ensure that these structures were indeed local minima. For singlet biradical states, symmetry-broken UB3LYP/6–31G(d) method was employed with a keyword "guess=mix", and the biradical index was determined on the basis of the LUMO occupation number in natural orbital analysis.

Optimized structures of **1c**–**4c**.



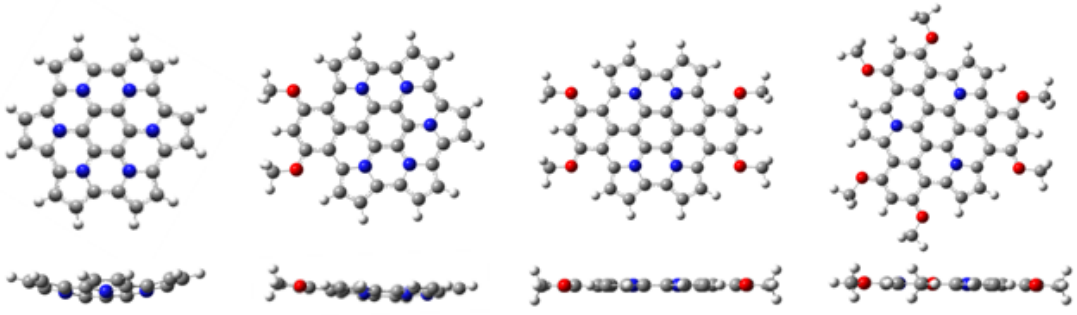
1c (C_{6v}) **2c** (C_{2v}) **3c** (D_{2h}) **4c** (D_{3h})

Optimized structures of $\mathbf{1c}^{2+}$–$\mathbf{4c}^{2+}$ (closed shell singlet).



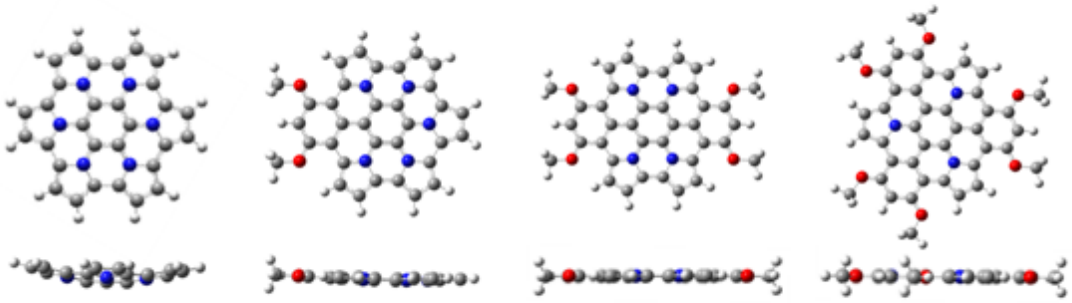
1c (C_{6v}) **2c** (C_s) **3c** (D_{2h}) **4c** (D_{3h})

Optimized structures of $\mathbf{1c}^{2+}$–$\mathbf{4c}^{2+}$ (open shell singlet).



1c (C_{2v}) **2c** (C_s) **3c** (D_{2h}) **4c** (C_{2v})

Optimized structures of **1c**$^{2+}$–**4c**$^{2+}$ (triplet).



1c (C_{2v}) **2c** (C_s) **3c** (D_{2h}) **4c** (C_s)

Atomic coordination of **1c** (C_{6v} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.378165	0.000000	-0.263505
2	6	0	0.689083	1.193526	-0.263505
3	6	0	-0.689083	1.193526	-0.263505
4	6	0	-1.378165	0.000000	-0.263505
5	6	0	-0.689083	-1.193526	-0.263505
6	6	0	0.689083	-1.193526	-0.263505
7	7	0	-1.369138	-2.371417	-0.136434
8	6	0	-0.736953	-3.610209	-0.013385
9	6	0	-2.758056	-2.443324	-0.013385
10	6	0	-1.781858	-4.515225	0.158808
11	6	0	-3.019370	-3.800747	0.158808
12	1	0	-1.675046	-5.583524	0.286756
13	1	0	-3.997950	-4.242394	0.286756
14	7	0	2.738276	0.000000	-0.136434
15	6	0	3.495009	1.166885	-0.013385
16	6	0	3.495009	-1.166885	-0.013385
17	6	0	4.801229	0.714478	0.158808
18	6	0	4.801229	-0.714478	0.158808
19	1	0	5.672996	1.341129	0.286756
20	1	0	5.672996	-1.341129	0.286756
21	7	0	1.369138	2.371417	-0.136434
22	6	0	0.736953	3.610209	-0.013385
23	6	0	2.758056	2.443324	-0.013385
24	6	0	1.781858	4.515225	0.158808
25	6	0	3.019370	3.800747	0.158808
26	1	0	1.675046	5.583524	0.286756
27	1	0	3.997950	4.242394	0.286756
28	7	0	-1.369138	2.371417	-0.136434
29	6	0	-2.758056	2.443324	-0.013385
30	6	0	-0.736953	3.610209	-0.013385
31	6	0	-3.019370	3.800747	0.158808
32	6	0	-1.781858	4.515225	0.158808
33	1	0	-3.997950	4.242394	0.286756
34	7	0	-2.738276	0.000000	-0.136434
35	6	0	-3.495009	-1.166885	-0.013385
36	6	0	-3.495009	1.166885	-0.013385
37	6	0	-4.801229	-0.714478	0.158808
38	6	0	-4.801229	0.714478	0.158808
39	1	0	-5.672996	-1.341129	0.286756
40	1	0	-5.672996	1.341129	0.286756
41	7	0	1.369138	-2.371417	-0.136434
42	6	0	2.758056	-2.443324	-0.013385
43	6	0	0.736953	-3.610209	-0.013385
44	6	0	3.019370	-3.800747	0.158808
45	6	0	1.781858	-4.515225	0.158808
46	1	0	3.997950	-4.242394	0.286756
47	1	0	1.675046	-5.583524	0.286756
48	1	0	-1.675046	5.583524	0.286756

HF = -1478.94481600 hartree

Atomic coordination of **1c**$^{2+}$ (Closed shell, C_{6v} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.380243	0.000000	0.577874
2	6	0	0.690121	-1.195325	0.577874
3	6	0	-0.690121	-1.195325	0.577874
4	6	0	-1.380243	0.000000	0.577874
5	6	0	-0.690121	1.195325	0.577874
6	6	0	0.690121	1.195325	0.577874
7	7	0	-1.361179	2.357631	0.300317
8	6	0	-0.716361	3.560730	0.017265
9	6	0	-2.725502	2.400752	0.017265
10	6	0	-1.760183	4.443965	-0.373478
11	6	0	-2.968495	3.746345	-0.373478
12	1	0	-1.630725	5.482023	-0.647454
13	1	0	-3.932209	4.153260	-0.647454
14	7	0	2.722357	0.000000	0.300317

15	6	0	3.441863	-1.159978	0.017265
16	6	0	3.441863	1.159978	0.017265
17	6	0	4.728678	-0.697620	-0.373478
18	6	0	4.728678	0.697620	-0.373478
19	1	0	5.562933	-1.328762	-0.647454
20	1	0	5.562933	1.328762	-0.647454
21	7	0	1.361179	-2.357631	0.300317
22	6	0	0.716361	-3.560730	0.017265
23	6	0	2.725502	-2.400752	0.017265
24	6	0	1.760183	-4.443965	-0.373478
25	6	0	2.968495	-3.746345	-0.373478
26	1	0	1.630725	-5.482023	-0.647454
27	1	0	3.932209	-4.153260	-0.647454
28	7	0	-1.361179	-2.357631	0.300317
29	6	0	-2.725502	-2.400752	0.017265
30	6	0	-0.716361	-3.560730	0.017265
31	6	0	-2.968495	-3.746345	-0.373478
32	6	0	-1.760183	-4.443965	-0.373478
33	1	0	-3.932209	-4.153260	-0.647454
34	7	0	-2.722357	0.000000	0.300317
35	6	0	-3.441863	1.159978	0.017265
36	6	0	-3.441863	-1.159978	0.017265
37	6	0	-4.728678	0.697620	-0.373478
38	6	0	-4.728678	-0.697620	-0.373478
39	1	0	-5.562933	1.328762	-0.647454
40	1	0	-5.562933	-1.328762	-0.647454
41	7	0	1.361179	2.357631	0.300317
42	6	0	2.725502	2.400752	0.017265
43	6	0	0.716361	3.560730	0.017265
44	6	0	2.968495	3.746345	-0.373478
45	6	0	1.760183	4.443965	-0.373478
46	1	0	3.932209	4.153260	-0.647454
47	1	0	1.630725	5.482023	-0.647454
48	1	0	-1.630725	-5.482023	-0.647454

HF = -1478.42427922 hartree

Atomic coordination of **1c**$^{2+}$ (C_{2v} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.380198	0.576902
2	6	0	1.195261	0.690079	0.576226
3	6	0	1.195261	-0.690079	0.576226
4	6	0	0.000000	-1.380198	0.576902
5	6	0	-1.195261	-0.690079	0.576226
6	6	0	-1.195261	0.690079	0.576226
7	7	0	-2.357854	-1.361429	0.300750
8	6	0	-3.560291	-0.716295	0.015253
9	6	0	-2.400604	-2.725900	0.017742
10	6	0	-4.443375	-1.760385	-0.375592
11	6	0	-3.746069	-2.968761	-0.374020
12	1	0	-5.481291	-1.631335	-0.650317
13	1	0	-4.153481	-3.932472	-0.647277
14	7	0	0.000000	2.723090	0.302901
15	6	0	1.160039	3.442326	0.018936
16	6	0	-1.160039	3.442326	0.018936
17	6	0	0.697572	4.729496	-0.370927
18	6	0	-0.697572	4.729496	-0.370927
19	1	0	1.328469	5.564174	-0.644221
20	1	0	-1.328469	5.564174	-0.644221
21	7	0	2.357854	1.361429	0.300750
22	6	0	3.560291	0.716295	0.015253
23	6	0	2.400604	2.725900	0.017742
24	6	0	4.443375	1.760385	-0.375592
25	6	0	3.746069	2.968761	-0.374020
26	1	0	5.481291	1.631335	-0.650317
27	1	0	4.153481	3.932472	-0.647277
28	7	0	2.357854	-1.361429	0.300750
29	6	0	2.400604	-2.725900	0.017742
30	6	0	3.560291	-0.716295	0.015253
31	6	0	3.746069	-2.968761	-0.374020
32	6	0	4.443375	-1.760385	-0.375592
33	1	0	4.153481	-3.932472	-0.647277
34	7	0	0.000000	-2.723090	0.302901
35	6	0	-1.160039	-3.442326	0.018936
36	6	0	1.160039	-3.442326	0.018936
37	6	0	-0.697572	-4.729496	-0.370927
38	6	0	0.697572	-4.729496	-0.370927
39	1	0	-1.328469	-5.564174	-0.644221
40	1	0	1.328469	-5.564174	-0.644221
41	7	0	-2.357854	1.361429	0.300750
42	6	0	-2.400604	2.725900	0.017742
43	6	0	-3.560291	0.716295	0.015253
44	6	0	-3.746069	2.968761	-0.374020
45	6	0	-4.443375	1.760385	-0.375592
46	1	0	-4.153481	3.932472	-0.647277
47	1	0	-5.481291	1.631335	-0.650317
48	1	0	5.481291	-1.631335	-0.650317

HF = -1478.42434503 hartree

Atomic coordination of **1c**$^{2+}$ (triplet, C_{2v} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.379501	0.475085
2	6	0	1.200865	0.687518	0.483999
3	6	0	1.200865	-0.687518	0.483999
4	6	0	0.000000	-1.379501	0.475085
5	6	0	-1.200865	-0.687518	0.483999
6	6	0	-1.200865	0.687518	0.483999

7	7	0	-2.360583	-1.365333	0.246224
8	6	0	-3.589277	-0.715694	0.007155
9	6	0	-2.421534	-2.727351	0.012482
10	6	0	-4.482645	-1.767142	-0.315395
11	6	0	-3.780692	-2.978378	-0.312924
12	1	0	-5.532548	-1.648232	-0.544992
13	1	0	-4.198696	-3.948773	-0.542713
14	7	0	0.000000	2.710771	0.230715
15	6	0	1.165679	3.461937	0.015383
16	6	0	-1.165679	3.461937	0.015383
17	6	0	0.706606	4.752692	-0.284933
18	6	0	-0.706606	4.752692	-0.284933
19	1	0	1.331166	5.607856	-0.503228
20	1	0	-1.331166	5.607856	-0.503228
21	7	0	2.360583	1.365333	0.246224
22	6	0	3.589277	0.715694	0.007155
23	6	0	2.421534	2.727351	0.012482
24	6	0	4.482645	1.767142	-0.315395
25	6	0	3.780692	2.978378	-0.312924
26	1	0	5.532548	1.648232	-0.544992
27	1	0	4.198696	3.948773	-0.542713
28	7	0	2.360583	-1.365333	0.246224
29	6	0	2.421534	-2.727351	0.012482
30	6	0	3.589277	-0.715694	0.007155
31	6	0	3.780692	-2.978378	-0.312924
32	6	0	4.482645	-1.767142	-0.315395
33	1	0	4.198696	-3.948773	-0.542713
34	7	0	0.000000	-2.710771	0.230715
35	6	0	-1.165679	-3.461937	0.015383
36	6	0	1.165679	-3.461937	0.015383
37	6	0	-0.706606	-4.752692	-0.284933
38	6	0	0.706606	-4.752692	-0.284933
39	1	0	-1.331166	-5.607856	-0.503228
40	1	0	1.331166	-5.607856	-0.503228
41	7	0	-2.360583	1.365333	0.246224
42	6	0	-2.421534	2.727351	0.012482
43	6	0	-3.589277	0.715694	0.007155
44	6	0	-3.780692	2.978378	-0.312924
45	6	0	-4.482645	1.767142	-0.315395
46	1	0	-4.198696	3.948773	-0.542713
47	1	0	-5.532548	1.648232	-0.544992
48	1	0	5.532548	-1.648232	-0.544992

HF = -1478.39815415 hartree

Atomic coordination of **2c** (C_{2v} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.257863
2	6	0	0.000000	1.191081	1.567652
3	6	0	0.000000	1.189246	0.185099
4	6	0	0.000000	0.000000	-0.540256
5	6	0	0.000000	-1.189246	0.185099
6	6	0	0.000000	-1.191081	1.567652
7	6	0	0.000000	0.000000	-1.973606
8	6	0	0.000000	-1.266397	-2.632624
9	6	0	0.000000	1.266397	-2.632624
10	6	0	0.000000	-1.225439	-4.041788
11	6	0	0.000000	1.225439	-4.041788
12	6	0	0.000000	0.000000	-4.723264
13	7	0	0.000000	2.392957	-0.458537
14	6	0	0.000000	3.629549	0.192573
15	6	0	0.000000	2.511152	-1.846624
16	6	0	0.000000	4.569654	-0.834811
17	6	0	0.000000	3.887419	-2.083480
18	1	0	0.000000	5.643073	-0.702761
19	1	0	0.000000	4.349622	-3.057716
20	7	0	0.000000	2.367744	2.267450
21	6	0	0.000000	2.439012	3.661744
22	6	0	0.000000	3.618630	1.656876
23	6	0	0.000000	3.803478	3.942032
24	6	0	0.000000	4.528215	2.712738
25	1	0	0.000000	4.242260	4.930332
26	1	0	0.000000	5.605136	2.617177
27	7	0	0.000000	0.000000	3.624675
28	6	0	0.000000	-1.165314	4.393056
29	6	0	0.000000	1.165314	4.393056
30	6	0	0.000000	-0.714824	5.709731
31	6	0	0.000000	0.714824	5.709731
32	1	0	0.000000	-1.342284	6.590317
33	1	0	0.000000	1.342284	6.590317
34	7	0	0.000000	-2.367744	2.267450
35	6	0	0.000000	-3.618630	1.656876
36	6	0	0.000000	-2.439012	3.661744
37	6	0	0.000000	-4.528215	2.712738
38	6	0	0.000000	-3.803478	3.942032
39	1	0	0.000000	-5.605136	2.617177
40	1	0	0.000000	-4.242260	4.930332
41	7	0	0.000000	-2.392957	-0.458537
42	6	0	0.000000	-3.629549	0.192573
43	6	0	0.000000	-2.511152	-1.846624
44	6	0	0.000000	-4.569654	-0.834811
45	6	0	0.000000	-3.887419	-2.083480
46	1	0	0.000000	-5.643073	-0.702761
47	1	0	0.000000	-4.349622	-3.057716
48	8	0	0.000000	2.432325	-4.677317
49	8	0	0.000000	-2.432325	-4.677317
50	6	0	0.000000	2.466634	-6.095534
51	1	0	-0.896198	1.986522	-6.510344
52	1	0	0.000000	3.523651	-6.367117
53	1	0	0.896198	1.986522	-6.510344
54	6	0	0.000000	-2.466634	-6.095534
55	1	0	0.896198	-1.986522	-6.510344
56	1	0	0.000000	-3.523651	-6.367117
57	1	0	-0.896198	-1.986522	-6.510344
58	1	0	0.000000	0.000000	-5.803653

HF = -1730.09968202 hartree

Atomic coordination of **2c**$^{2+}$ (closed shell, C_s symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330230	-2.253107	0.000000
2	6	0	-0.332145	-1.564664	1.187707
3	6	0	-0.325143	-0.184711	1.185433
4	6	0	-0.321037	0.539447	0.000000
5	6	0	-0.325143	-0.184711	-1.185433
6	6	0	-0.332145	-1.564664	-1.187707
7	6	0	-0.186129	1.962651	0.000000
8	6	0	-0.099128	2.610295	-1.266766
9	6	0	-0.099128	2.610295	1.266766
10	6	0	0.028978	4.039373	-1.228459
11	6	0	0.028978	4.039373	1.228459
12	6	0	0.081155	4.715535	0.000000
13	7	0	-0.196448	0.455136	2.381031
14	6	0	-0.052190	-0.209919	3.608933
15	6	0	-0.086139	1.828901	2.492197
16	6	0	0.115738	0.831718	4.553709
17	6	0	0.092572	2.058925	3.885398
18	1	0	0.248884	0.695103	5.618094
19	1	0	0.204640	3.029462	4.341935
20	7	0	-0.172832	-2.257711	2.356283
21	6	0	0.017765	-3.643456	2.405204
22	6	0	-0.022325	-1.641863	3.586251
23	6	0	0.245726	-3.914747	3.785282
24	6	0	0.220488	-2.715990	4.495294
25	1	0	0.420554	-4.894308	4.208602
26	1	0	0.373895	-2.609791	5.560226
27	7	0	-0.158370	-3.610368	0.000000
28	6	0	0.032613	-4.350719	-1.163614
29	6	0	0.032613	-4.350719	1.163614
30	6	0	0.296875	-5.673557	-0.696467
31	6	0	0.296875	-5.673557	0.696467
32	1	0	0.481148	-6.532812	-1.326555
33	1	0	0.481148	-6.532812	1.326555
34	7	0	-0.172832	-2.257711	-2.356283
35	6	0	-0.022325	-1.641863	-3.586251
36	6	0	0.017765	-3.643456	-2.405204
37	6	0	0.220488	-2.715990	-4.495294
38	6	0	0.245726	-3.914747	-3.785282
39	1	0	0.373895	-2.609791	-5.560226
40	1	0	0.420554	-4.894308	-4.208602
41	7	0	-0.196448	0.455136	-2.381031
42	6	0	-0.052190	-0.209919	-3.608933
43	6	0	-0.086139	1.828901	-2.492197
44	6	0	0.115738	0.831718	-4.553709
45	6	0	0.092572	2.058925	-3.885398
46	1	0	0.248884	0.695103	-5.618094
47	1	0	0.204640	3.029462	-4.341935
48	8	0	0.092120	4.647520	2.408997
49	8	0	0.092120	4.647520	-2.408997
50	6	0	0.218062	6.082606	2.496238
51	1	0	-0.648107	6.568670	2.038040
52	1	0	0.245234	6.301998	3.562269
53	1	0	1.147603	6.413248	2.023715
54	6	0	0.218062	6.082606	-2.496238
55	1	0	1.147603	6.413248	-2.023715
56	1	0	0.245234	6.301998	-3.562269
57	1	0	-0.648107	6.568670	-2.038040
58	1	0	0.173370	5.791713	0.000000

HF = -1729.59523357 hartree

Atomic coordination of **2c**$^{2+}$ (open shell singlet, C_s symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.332221	-2.253221	0.000000
2	6	0	-0.333797	-1.564729	1.187734
3	6	0	-0.326108	-0.184759	1.185442
4	6	0	-0.321844	0.539407	0.000000
5	6	0	-0.326108	-0.184759	-1.185442
6	6	0	-0.333797	-1.564729	-1.187734
7	6	0	-0.186304	1.962582	0.000000
8	6	0	-0.099145	2.610234	-1.266729
9	6	0	-0.099145	2.610234	1.266729
10	6	0	0.029167	4.039297	-1.228444
11	6	0	0.029167	4.039297	1.228444
12	6	0	0.081328	4.715497	0.000000
13	7	0	-0.196711	0.455089	2.380979
14	6	0	-0.052211	-0.209938	3.608868
15	6	0	-0.086001	1.828818	2.492114
16	6	0	0.116309	0.831649	4.553564
17	6	0	0.093173	2.058857	3.885239
18	1	0	0.249727	0.695004	5.617916
19	1	0	0.205699	3.029393	4.341673
20	7	0	-0.174107	-2.257773	2.356328
21	6	0	0.017549	-3.643365	2.405137
22	6	0	-0.022564	-1.641875	3.586164
23	6	0	0.247153	-3.914538	3.784933
24	6	0	0.221520	-2.715821	4.495025
25	1	0	0.423040	-4.894014	4.208026
26	1	0	0.375785	-2.609466	5.559823
27	7	0	-0.159893	-3.610490	0.000000
28	6	0	0.032302	-4.350630	-1.163558
29	6	0	0.032302	-4.350630	1.163558
30	6	0	0.298237	-5.673115	-0.696476
31	6	0	0.298237	-5.673115	0.696476
32	1	0	0.483660	-6.532074	-1.326638
33	1	0	0.483660	-6.532074	1.326638
34	7	0	-0.174107	-2.257773	-2.356328
35	6	0	-0.022564	-1.641875	-3.586164
36	6	0	0.017549	-3.643365	-2.405137
37	6	0	0.221520	-2.715821	-4.495025
38	6	0	0.247153	-3.914538	-3.784933

39	1	0	0.375785	-2.609466	-5.559823
40	1	0	0.423040	-4.894014	-4.208026
41	7	0	-0.196711	0.455089	-2.380979
42	6	0	-0.052211	-0.209938	-3.608868
43	6	0	-0.086001	1.828818	-2.492114
44	6	0	0.116309	0.831649	-4.553564
45	6	0	0.093173	2.058857	-3.885239
46	1	0	0.249727	0.695004	-5.617916
47	1	0	0.205699	3.029393	-4.341673
48	8	0	0.092292	4.647409	2.409002
49	8	0	0.092292	4.647409	-2.409002
50	6	0	0.218396	6.082447	2.496278
51	1	0	-0.647850	6.568743	2.038405
52	1	0	0.245596	6.301825	3.562309
53	1	0	1.147801	6.413002	2.023430
54	6	0	0.218396	6.082447	-2.496278
55	1	0	1.147801	6.413002	-2.023430
56	1	0	0.245596	6.301825	-3.562309
57	1	0	-0.647850	6.568743	-2.038405
58	1	0	0.173617	5.791664	0.000000

HF = -1729.5952335 hartree

Atomic coordination of **2c**$^{2+}$ (triplet, C_s symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.098949	-2.251509	0.000000
2	6	0	-0.104343	-1.560533	1.191715
3	6	0	-0.105703	-0.186045	1.189666
4	6	0	-0.105875	0.541434	0.000000
5	6	0	-0.105703	-0.186045	-1.189666
6	6	0	-0.104343	-1.560533	-1.191715
7	6	0	-0.061266	1.955922	0.000000
8	6	0	-0.033373	2.615959	-1.274878
9	6	0	-0.033373	2.615959	1.274878
10	6	0	0.008364	4.039942	-1.233159
11	6	0	0.008364	4.039942	1.233159
12	6	0	0.024864	4.712203	0.000000
13	7	0	-0.064987	0.458390	2.384256
14	6	0	-0.017572	-0.207403	3.627830
15	6	0	-0.029632	1.831128	2.499716
16	6	0	0.035259	0.841453	4.579337
17	6	0	0.027408	2.065786	3.907638
18	1	0	0.077889	0.709675	5.651628
19	1	0	0.062769	3.041314	4.366411
20	7	0	-0.051920	-2.260219	2.359122
21	6	0	0.007675	-3.642865	2.429470
22	6	0	-0.007141	-1.639321	3.613977
23	6	0	0.077705	-3.923950	3.817720
24	6	0	0.068432	-2.717979	4.532157
25	1	0	0.133405	-4.911943	4.253199
26	1	0	0.115566	-2.623528	5.608078
27	7	0	-0.040483	-3.601631	0.000000
28	6	0	0.013376	-4.373019	-1.168120
29	6	0	0.013376	-4.373019	1.168120
30	6	0	0.090325	-5.696475	-0.707570
31	6	0	0.090325	-5.696475	0.707570
32	1	0	0.145491	-6.578024	-1.331013
33	1	0	0.145491	-6.578024	1.331013
34	7	0	-0.051920	-2.260219	-2.359122
35	6	0	-0.007141	-1.639321	-3.613977
36	6	0	0.007675	-3.642865	-2.429470
37	6	0	0.068432	-2.717979	-4.532157
38	6	0	0.077705	-3.923950	-3.817720
39	1	0	0.115566	-2.623528	-5.608078
40	1	0	0.133405	-4.911943	-4.253199
41	7	0	-0.064987	0.458390	-2.384256
42	6	0	-0.017572	-0.207403	-3.627830
43	6	0	-0.029632	1.831128	-2.499716
44	6	0	0.035259	0.841453	-4.579337
45	6	0	0.027408	2.065786	-3.907638
46	1	0	0.077889	0.709675	-5.651628
47	1	0	0.062769	3.041314	-4.366411
48	8	0	0.030818	4.654928	2.418059
49	8	0	0.030818	4.654928	-2.418059
50	6	0	0.073200	6.093822	2.496774
51	1	0	-0.817339	6.529361	2.033721
52	1	0	0.083941	6.321935	3.561435
53	1	0	0.983772	6.476983	2.026382
54	6	0	0.073200	6.093822	-2.496774
55	1	0	0.983772	6.476983	-2.026382
56	1	0	0.083941	6.321935	-3.561435
57	1	0	-0.817339	6.529361	-2.033721
58	1	0	0.055578	5.792323	0.000000

HF = -1729.58546038 hartree

Atomic coordination of **3c** (D_{2h} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.422538	0.000000	0.000000
2	6	0	0.695189	1.187943	0.000000
3	6	0	-0.695189	1.187943	0.000000
4	6	0	-1.422538	0.000000	0.000000
5	6	0	-0.695189	-1.187943	0.000000
6	6	0	0.695189	-1.187943	0.000000
7	6	0	-2.862183	0.000000	0.000000
8	6	0	-3.527422	-1.260541	0.000000
9	6	0	-3.527422	1.260541	0.000000
10	6	0	-4.936683	-1.222718	0.000000
11	6	0	-4.936683	1.222718	0.000000
12	6	0	-5.620267	0.000000	0.000000

13	1	0	-6.700654	0.000000	0.000000
14	6	0	2.862183	0.000000	0.000000
15	6	0	3.527422	-1.260541	0.000000
16	6	0	3.527422	1.260541	0.000000
17	6	0	4.936683	-1.222718	0.000000
18	6	0	4.936683	1.222718	0.000000
19	6	0	5.620267	0.000000	0.000000
20	1	0	6.700654	0.000000	0.000000
21	7	0	1.357366	2.387350	0.000000
22	6	0	0.726683	3.629220	0.000000
23	6	0	2.746574	2.500942	0.000000
24	6	0	1.756376	4.565684	0.000000
25	6	0	2.997121	3.873953	0.000000
26	1	0	1.628183	5.639449	0.000000
27	1	0	3.976398	4.324872	0.000000
28	7	0	-1.357366	2.387350	0.000000
29	6	0	-0.726683	3.629220	0.000000
30	6	0	-2.746574	2.500942	0.000000
31	6	0	-1.756376	4.565684	0.000000
32	6	0	-2.997121	3.873953	0.000000
33	1	0	-1.628183	5.639449	0.000000
34	1	0	-3.976398	4.324872	0.000000
35	7	0	-1.357366	-2.387350	0.000000
36	6	0	-0.726683	-3.629220	0.000000
37	6	0	-2.746574	-2.500942	0.000000
38	6	0	-1.756376	-4.565684	0.000000
39	6	0	-2.997121	-3.873953	0.000000
40	1	0	-1.628183	-5.639449	0.000000
41	1	0	-3.976398	-4.324872	0.000000
42	7	0	1.357366	-2.387350	0.000000
43	6	0	0.726683	-3.629220	0.000000
44	6	0	2.746574	-2.500942	0.000000
45	6	0	1.756376	-4.565684	0.000000
46	6	0	2.997121	-3.873953	0.000000
47	1	0	1.628183	-5.639449	0.000000
48	1	0	3.976398	-4.324872	0.000000
49	8	0	-5.571501	2.431120	0.000000
50	8	0	-5.571501	-2.431120	0.000000
51	8	0	5.571501	-2.431120	0.000000
52	8	0	5.571501	2.431120	0.000000
53	6	0	6.989000	2.465206	0.000000
54	1	0	7.404724	1.985165	0.895699
55	1	0	7.404724	1.985165	-0.895699
56	1	0	7.261001	3.522205	0.000000
57	6	0	-6.989000	2.465206	0.000000
58	1	0	-7.404724	1.985165	-0.895699
59	1	0	-7.404724	1.985165	0.895699
60	1	0	-7.261001	3.522205	0.000000
61	6	0	-6.989000	-2.465206	0.000000
62	1	0	-7.404724	-1.985165	0.895699
63	1	0	-7.404724	-1.985165	-0.895699
64	1	0	-7.261001	-3.522205	0.000000
65	6	0	6.989000	-2.465206	0.000000
66	1	0	7.404724	-1.985165	-0.895699
67	1	0	7.404724	-1.985165	0.895699
68	1	0	7.261001	-3.522205	0.000000

HF = -1981.24942783 hartree

Atomic coordination of **3c**$^{2+}$ (closed shell, D_{2h} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.418415	0.000000	0.000000
2	6	0	0.692432	1.181636	0.000000
3	6	0	-0.692432	1.181636	0.000000
4	6	0	-1.418415	0.000000	0.000000
5	6	0	-0.692432	-1.181636	0.000000
6	6	0	0.692432	-1.181636	0.000000
7	6	0	-2.851763	0.000000	0.000000
8	6	0	-3.507535	-1.262984	0.000000
9	6	0	-3.507535	1.262984	0.000000
10	6	0	-4.944015	-1.226085	0.000000
11	6	0	-4.944015	1.226085	0.000000
12	6	0	-5.624468	0.000000	0.000000
13	1	0	-6.704513	0.000000	0.000000
14	6	0	2.851763	0.000000	0.000000
15	6	0	3.507535	-1.262984	0.000000
16	6	0	3.507535	1.262984	0.000000
17	6	0	4.944015	-1.226085	0.000000
18	6	0	4.944015	1.226085	0.000000
19	6	0	5.624468	0.000000	0.000000
20	1	0	6.704513	0.000000	0.000000
21	7	0	1.352063	2.378167	0.000000
22	6	0	0.714213	3.616305	0.000000
23	6	0	2.735619	2.486571	0.000000
24	6	0	1.766189	4.566674	0.000000
25	6	0	2.985356	3.886584	0.000000
26	1	0	1.638390	5.640199	0.000000
27	1	0	3.963751	4.339567	0.000000
28	7	0	-1.352063	2.378167	0.000000
29	6	0	-0.714213	3.616305	0.000000
30	6	0	-2.735619	2.486571	0.000000
31	6	0	-1.766189	4.566674	0.000000
32	6	0	-2.985356	3.886584	0.000000
33	1	0	-1.638390	5.640199	0.000000
34	1	0	-3.963751	4.339567	0.000000
35	7	0	-1.352063	-2.378167	0.000000
36	6	0	-0.714213	-3.616305	0.000000
37	6	0	-2.735619	-2.486571	0.000000
38	6	0	-1.766189	-4.566674	0.000000
39	6	0	-2.985356	-3.886584	0.000000
40	1	0	-1.638390	-5.640199	0.000000
41	1	0	-3.963751	-4.339567	0.000000
42	7	0	1.352063	-2.378167	0.000000
43	6	0	0.714213	-3.616305	0.000000
44	6	0	2.735619	-2.486571	0.000000
45	6	0	1.766189	-4.566674	0.000000
46	6	0	2.985356	-3.886584	0.000000

47	1	0	1.638390	-5.640199	0.000000
48	1	0	3.963751	-4.339567	0.000000
49	8	0	-5.554889	2.406688	0.000000
50	8	0	-5.554889	-2.406688	0.000000
51	8	0	5.554889	-2.406688	0.000000
52	8	0	5.554889	2.406688	0.000000
53	6	0	6.994437	2.494588	0.000000
54	1	0	7.405012	2.029383	0.900989
55	1	0	7.405012	2.029383	-0.900989
56	1	0	7.214947	3.560775	0.000000
57	6	0	-6.994437	2.494588	0.000000
58	1	0	-7.405012	2.029383	-0.900989
59	1	0	-7.405012	2.029383	0.900989
60	1	0	-7.214947	3.560775	0.000000
61	6	0	-6.994437	-2.494588	0.000000
62	1	0	-7.405012	-2.029383	0.900989
63	1	0	-7.405012	-2.029383	-0.900989
64	1	0	-7.214947	-3.560775	0.000000
65	6	0	6.994437	-2.494588	0.000000
66	1	0	7.405012	-2.029383	-0.900989
67	1	0	7.405012	-2.029383	0.900989
68	1	0	7.214947	-3.560775	0.000000

HF = -1980.75990959 hartree

Atomic coordination of **3c**$^{2+}$ (open shell singlet, D_{2h} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.419588	0.000000	0.000000
2	6	0	0.691577	1.184989	0.000000
3	6	0	-0.691577	1.184989	0.000000
4	6	0	-1.419588	0.000000	0.000000
5	6	0	-0.691577	-1.184989	0.000000
6	6	0	0.691577	-1.184989	0.000000
7	6	0	-2.846246	0.000000	0.000000
8	6	0	-3.508462	-1.264935	0.000000
9	6	0	-3.508462	1.264935	0.000000
10	6	0	-4.936601	-1.227884	0.000000
11	6	0	-4.936601	1.227884	0.000000
12	6	0	-5.614627	0.000000	0.000000
13	1	0	-6.694865	0.000000	0.000000
14	6	0	2.846246	0.000000	0.000000
15	6	0	3.508462	-1.264935	0.000000
16	6	0	3.508462	1.264935	0.000000
17	6	0	4.936601	-1.227884	0.000000
18	6	0	4.936601	1.227884	0.000000
19	6	0	5.614627	0.000000	0.000000
20	1	0	6.694865	0.000000	0.000000
21	7	0	1.352711	2.378883	0.000000
22	6	0	0.711841	3.623189	0.000000
23	6	0	2.731054	2.489648	0.000000
24	6	0	1.764518	4.572273	0.000000
25	6	0	2.982030	3.890818	0.000000
26	1	0	1.637393	5.645865	0.000000
27	1	0	3.962105	4.340138	0.000000
28	7	0	-1.352711	2.378883	0.000000
29	6	0	-0.711841	3.623189	0.000000
30	6	0	-2.731054	2.489648	0.000000
31	6	0	-1.764518	4.572273	0.000000
32	6	0	-2.982030	3.890818	0.000000
33	1	0	-1.637393	5.645865	0.000000
34	1	0	-3.962105	4.340138	0.000000
35	7	0	-1.352711	-2.378883	0.000000
36	6	0	-0.711841	-3.623189	0.000000
37	6	0	-2.731054	-2.489648	0.000000
38	6	0	-1.764518	-4.572273	0.000000
39	6	0	-2.982030	-3.890818	0.000000
40	1	0	-1.637393	-5.645865	0.000000
41	1	0	-3.962105	-4.340138	0.000000
42	7	0	1.352711	-2.378883	0.000000
43	6	0	0.711841	-3.623189	0.000000
44	6	0	2.731054	-2.489648	0.000000
45	6	0	1.764518	-4.572273	0.000000
46	6	0	2.982030	-3.890818	0.000000
47	1	0	1.637393	-5.645865	0.000000
48	1	0	3.962105	-4.340138	0.000000
49	8	0	-5.549837	2.413039	0.000000
50	8	0	-5.549837	-2.413039	0.000000
51	8	0	5.549837	-2.413039	0.000000
52	8	0	5.549837	2.413039	0.000000
53	6	0	6.988146	2.493832	0.000000
54	1	0	7.398673	2.027327	0.900656
55	1	0	7.398673	2.027327	-0.900656
56	1	0	7.215062	3.558853	0.000000
57	6	0	-6.988146	2.493832	0.000000
58	1	0	-7.398673	2.027327	-0.900656
59	1	0	-7.398673	2.027327	0.900656
60	1	0	-7.215062	3.558853	0.000000
61	6	0	-6.988146	-2.493832	0.000000
62	1	0	-7.398673	-2.027327	0.900656
63	1	0	-7.398673	-2.027327	-0.900656
64	1	0	-7.215062	-3.558853	0.000000
65	6	0	6.988146	-2.493832	0.000000
66	1	0	7.398673	-2.027327	-0.900656
67	1	0	7.398673	-2.027327	0.900656
68	1	0	7.215062	-3.558853	0.000000

HF = -1980.76557642 hartree

Atomic coordination of **3c**$^{2+}$ (triplet, D_{2h} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.420145	0.000000	0.000000
2	6	0	0.691048	1.187071	0.000000
3	6	0	-0.691048	1.187071	0.000000
4	6	0	-1.420145	0.000000	0.000000
5	6	0	-0.691048	-1.187071	0.000000
6	6	0	0.691048	-1.187071	0.000000
7	6	0	-2.843012	0.000000	0.000000
8	6	0	-3.508562	-1.267032	0.000000
9	6	0	-3.508562	1.267032	0.000000
10	6	0	-4.933232	-1.229259	0.000000
11	6	0	-4.933232	1.229259	0.000000
12	6	0	-5.609201	0.000000	0.000000
13	1	0	-6.689638	0.000000	0.000000
14	6	0	2.843012	0.000000	0.000000
15	6	0	3.508562	-1.267032	0.000000
16	6	0	3.508562	1.267032	0.000000
17	6	0	4.933232	-1.229259	0.000000
18	6	0	4.933232	1.229259	0.000000
19	6	0	5.609201	0.000000	0.000000
20	1	0	6.689638	0.000000	0.000000
21	7	0	1.353093	2.379246	0.000000
22	6	0	0.710716	3.626566	0.000000
23	6	0	2.729459	2.490629	0.000000
24	6	0	1.763624	4.575045	0.000000
25	6	0	2.980265	3.892865	0.000000
26	1	0	1.637190	5.648717	0.000000
27	1	0	3.960943	4.341005	0.000000
28	7	0	-1.353093	2.379246	0.000000
29	6	0	-0.710716	3.626566	0.000000
30	6	0	-2.729459	2.490629	0.000000
31	6	0	-1.763624	4.575045	0.000000
32	6	0	-2.980265	3.892865	0.000000
33	1	0	-1.637190	5.648717	0.000000
34	1	0	-3.960943	4.341005	0.000000
35	7	0	-1.353093	-2.379246	0.000000
36	6	0	-0.710716	-3.626566	0.000000
37	6	0	-2.729459	-2.490629	0.000000
38	6	0	-1.763624	-4.575045	0.000000
39	6	0	-2.980265	-3.892865	0.000000
40	1	0	-1.637190	-5.648717	0.000000
41	1	0	-3.960943	-4.341005	0.000000
42	7	0	1.353093	-2.379246	0.000000
43	6	0	0.710716	-3.626566	0.000000
44	6	0	2.729459	-2.490629	0.000000
45	6	0	1.763624	-4.575045	0.000000
46	6	0	2.980265	-3.892865	0.000000
47	1	0	1.637190	-5.648717	0.000000
48	1	0	3.960943	-4.341005	0.000000
49	8	0	-5.547896	2.416739	0.000000
50	8	0	-5.547896	-2.416739	0.000000
51	8	0	5.547896	-2.416739	0.000000
52	8	0	5.547896	2.416739	0.000000
53	6	0	6.985236	2.493953	0.000000
54	1	0	7.396003	2.026760	0.900424
55	1	0	7.396003	2.026760	-0.900424
56	1	0	7.215736	3.558315	0.000000
57	6	0	-6.985236	2.493953	0.000000
58	1	0	-7.396003	2.026760	-0.900424
59	1	0	-7.396003	2.026760	0.900424
60	1	0	-7.215736	3.558315	0.000000
61	6	0	-6.985236	-2.493953	0.000000
62	1	0	-7.396003	-2.026760	0.900424
63	1	0	-7.396003	-2.026760	-0.900424
64	1	0	-7.215736	-3.558315	0.000000
65	6	0	6.985236	-2.493953	0.000000
66	1	0	7.396003	-2.026760	-0.900424
67	1	0	7.396003	-2.026760	0.900424
68	1	0	7.215736	-3.558315	0.000000

HF = -1980.76533037 hartree

Atomic coordination of **4c** (D_{3h} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.381013	0.000000
2	6	0	-1.229891	0.710078	0.000000
3	6	0	-1.195993	-0.690507	0.000000
4	6	0	0.000000	-1.420156	0.000000
5	6	0	1.195993	-0.690507	0.000000
6	6	0	1.229891	0.710078	0.000000
7	6	0	0.000000	-2.863125	0.000000
8	6	0	1.252266	-3.540374	0.000000
9	6	0	-1.252266	-3.540374	0.000000
10	6	0	1.218327	-4.949692	0.000000
11	6	0	-1.218327	-4.949692	0.000000
12	6	0	0.000000	-5.636910	0.000000
13	1	0	0.000000	-6.717227	0.000000
14	6	0	2.479539	1.431562	0.000000
15	6	0	3.692186	0.685693	0.000000
16	6	0	2.439921	2.854681	0.000000
17	6	0	4.895723	1.419744	0.000000
18	6	0	3.677396	3.529949	0.000000
19	6	0	4.881707	2.818455	0.000000
20	1	0	5.817290	3.358614	0.000000
21	6	0	-2.479539	1.431562	0.000000
22	6	0	-3.692186	0.685693	0.000000
23	6	0	-2.439921	2.854681	0.000000
24	6	0	-4.895723	1.419744	0.000000
25	6	0	-3.677396	3.529949	0.000000
26	6	0	-4.881707	2.818455	0.000000
27	1	0	-5.817290	3.358614	0.000000
28	7	0	-2.381757	-1.375108	0.000000

29	6	0	-3.637676	-0.768427	0.000000
30	6	0	-2.484315	-2.766106	0.000000
31	6	0	-4.558287	-1.815048	0.000000
32	6	0	-3.851021	-3.040068	0.000000
33	1	0	-5.629479	-1.695565	0.000000
34	1	0	-4.283142	-4.027490	0.000000
35	7	0	2.381757	-1.375108	0.000000
36	6	0	3.637676	-0.768427	0.000000
37	6	0	2.484315	-2.766106	0.000000
38	6	0	4.558287	-1.815048	0.000000
39	6	0	3.851021	-3.040068	0.000000
40	1	0	5.629479	-1.695565	0.000000
41	1	0	4.283142	-4.027490	0.000000
42	7	0	0.000000	2.750216	0.000000
43	6	0	1.153361	3.534533	0.000000
44	6	0	-1.153361	3.534533	0.000000
45	6	0	0.707266	4.855116	0.000000
46	6	0	-0.707266	4.855116	0.000000
47	1	0	1.346338	5.723054	0.000000
48	1	0	-1.346338	5.723054	0.000000
49	8	0	3.621585	4.895507	0.000000
50	8	0	2.428841	-5.584138	0.000000
51	8	0	-6.050426	0.688631	0.000000
52	8	0	6.050426	0.688631	0.000000
53	8	0	-3.621585	4.895507	0.000000
54	8	0	-2.428841	-5.584138	0.000000
55	6	0	4.831320	5.633205	0.000000
56	1	0	5.432263	5.425781	0.895551
57	1	0	5.432263	5.425781	-0.895551
58	1	0	4.538921	6.684915	0.000000
59	6	0	2.462839	-7.000648	0.000000
60	1	0	1.982732	-7.417369	0.895551
61	1	0	1.982732	-7.417369	-0.895551
62	1	0	3.519846	-7.273279	0.000000
63	6	0	-7.294159	1.367443	0.000000
64	1	0	-7.414996	1.991588	0.895551
65	1	0	-7.414996	1.991588	-0.895551
66	1	0	-8.058767	0.588364	0.000000
67	6	0	7.294159	1.367443	0.000000
68	1	0	7.414996	1.991588	-0.895551
69	1	0	7.414996	1.991588	0.895551
70	1	0	8.058767	0.588364	0.000000
71	6	0	-4.831320	5.633205	0.000000
72	1	0	-5.432263	5.425781	-0.895551
73	1	0	-5.432263	5.425781	0.895551
74	1	0	-4.538921	6.684915	0.000000
75	6	0	-2.462839	-7.000648	0.000000
76	1	0	-1.982732	-7.417369	-0.895551
77	1	0	-1.982732	-7.417369	0.895551
78	1	0	-3.519846	-7.273279	0.000000

HF = -2232.39686436 hartree

Atomic coordination of **4c**$^{2+}$ (closed shell, D_{3h} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.374858	0.000000
2	6	0	-1.225629	0.707617	0.000000
3	6	0	-1.190662	-0.687429	0.000000
4	6	0	0.000000	-1.415235	0.000000
5	6	0	1.190662	-0.687429	0.000000
6	6	0	1.225629	0.707617	0.000000
7	6	0	0.000000	-2.851805	0.000000
8	6	0	1.254036	-3.521893	0.000000
9	6	0	-1.254036	-3.521893	0.000000
10	6	0	1.220665	-4.957437	0.000000
11	6	0	-1.220665	-4.957437	0.000000
12	6	0	0.000000	-5.642121	0.000000
13	1	0	0.000000	-6.722035	0.000000
14	6	0	2.469735	1.425902	0.000000
15	6	0	3.677066	0.674920	0.000000
16	6	0	2.423031	2.846973	0.000000
17	6	0	4.903599	1.421592	0.000000
18	6	0	3.682934	3.535846	0.000000
19	6	0	4.886220	2.821061	0.000000
20	1	0	5.821453	3.361017	0.000000
21	6	0	-2.469735	1.425902	0.000000
22	6	0	-3.677066	0.674920	0.000000
23	6	0	-2.423031	2.846973	0.000000
24	6	0	-4.903599	1.421592	0.000000
25	6	0	-3.682934	3.535846	0.000000
26	6	0	-4.886220	2.821061	0.000000
27	1	0	-5.821453	3.361017	0.000000
28	7	0	-2.374623	-1.370989	0.000000
29	6	0	-3.624839	-0.760753	0.000000
30	6	0	-2.471251	-2.758826	0.000000
31	6	0	-4.557951	-1.827163	0.000000
32	6	0	-3.861345	-3.033720	0.000000
33	1	0	-5.629347	-1.709914	0.000000
34	1	0	-4.295502	-4.020200	0.000000
35	7	0	2.374623	-1.370989	0.000000
36	6	0	3.624839	-0.760753	0.000000
37	6	0	2.471251	-2.758826	0.000000
38	6	0	4.557951	-1.827163	0.000000
39	6	0	3.861345	-3.033720	0.000000
40	1	0	5.629347	-1.709914	0.000000
41	1	0	4.295502	-4.020200	0.000000
42	7	0	0.000000	2.741978	0.000000
43	6	0	1.153588	3.519579	0.000000
44	6	0	-1.153588	3.519579	0.000000
45	6	0	0.696606	4.860882	0.000000
46	6	0	-0.696606	4.860882	0.000000
47	1	0	1.333844	5.730114	0.000000
48	1	0	-1.333844	5.730114	0.000000
49	8	0	3.619588	4.867181	0.000000
50	8	0	2.405308	-5.568245	0.000000
51	8	0	-6.024896	0.701065	0.000000
52	8	0	6.024896	0.701065	0.000000

53	8	0	-3.619588	4.867181	0.000000	67	6	0	7.311473	1.346739	0.000000
54	8	0	-2.405308	-5.568245	0.000000	68	1	0	7.435109	1.956257	-0.900373
55	6	0	4.822047	5.658552	0.000000	69	1	0	7.435109	1.956257	0.900373
56	1	0	5.411723	5.460865	0.900373	70	1	0	8.038769	0.536253	0.000000
57	1	0	5.411723	5.460865	-0.900373	71	6	0	-4.822047	5.658552	0.000000
58	1	0	4.483794	6.693652	0.000000	72	1	0	-5.411723	5.460865	-0.900373
59	6	0	2.489426	-7.005291	0.000000	73	1	0	-5.411723	5.460865	0.900373
60	1	0	2.023386	-7.417122	0.900373	74	1	0	-4.483794	6.693652	0.000000
61	1	0	2.023386	-7.417122	-0.900373	75	6	0	-2.489426	-7.005291	0.000000
62	1	0	3.554976	-7.229905	0.000000	76	1	0	-2.023386	-7.417122	-0.900373
63	6	0	-7.311473	1.346739	0.000000	77	1	0	-2.023386	-7.417122	0.900373
64	1	0	-7.435109	1.956257	0.900373	78	1	0	-3.554976	-7.229905	0.000000
65	1	0	-7.435109	1.956257	-0.900373						
66	1	0	-8.038769	0.536253	0.000000						

HF = -2231.91992422 hartree

Atomic coordination of **4c**$^{2+}$ (open shell singlet, C_{2v} symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.375461
2	6	0	0.000000	1.225782	0.707898
3	6	0	0.000000	1.190752	-0.687072
4	6	0	0.000000	0.000000	-1.415035
5	6	0	0.000000	-1.190752	-0.687072
6	6	0	0.000000	-1.225782	0.707898
7	6	0	0.000000	0.000000	-2.851248
8	6	0	0.000000	-1.254160	-3.521678
9	6	0	0.000000	1.254160	-3.521678
10	6	0	0.000000	-1.220811	-4.956907
11	6	0	0.000000	1.220811	-4.956907
12	6	0	0.000000	0.000000	-5.641594
13	6	0	0.000000	-2.469787	1.426266
14	6	0	0.000000	-3.677500	0.674797
15	6	0	0.000000	-2.423493	2.846944
16	6	0	0.000000	-4.904341	1.421061
17	6	0	0.000000	-3.683483	3.535397
18	6	0	0.000000	-4.886906	2.820443
19	1	0	0.000000	-5.821924	3.360843
20	6	0	0.000000	2.469787	1.426266
21	6	0	0.000000	3.677500	0.674797
22	6	0	0.000000	2.423493	2.846944
23	6	0	0.000000	4.904341	1.421061
24	6	0	0.000000	3.683483	3.535397
25	6	0	0.000000	4.886906	2.820443
26	1	0	0.000000	5.821924	3.360843
27	7	0	0.000000	2.374519	-1.370857
28	6	0	0.000000	3.624968	-0.760322
29	6	0	0.000000	2.471281	-2.758358
30	6	0	0.000000	4.558060	-1.826975
31	6	0	0.000000	3.861641	-3.033329
32	1	0	0.000000	5.629313	-1.709329
33	1	0	0.000000	4.295530	-4.019864
34	7	0	0.000000	-2.374519	-1.370857
35	6	0	0.000000	-3.624968	-0.760322
36	6	0	0.000000	-2.471281	-2.758358
37	6	0	0.000000	-4.558060	-1.826975
38	6	0	0.000000	-3.861641	-3.033329
39	1	0	0.000000	-5.629313	-1.709329
40	1	0	0.000000	-4.295530	-4.019864
41	7	0	0.000000	0.000000	2.742069
42	6	0	0.000000	-1.153780	3.520147
43	6	0	0.000000	1.153780	3.520147
44	6	0	0.000000	-0.696909	4.860650
45	6	0	0.000000	0.696909	4.860650
46	1	0	0.000000	-1.333735	5.730180
47	1	0	0.000000	1.333735	5.730180
48	8	0	0.000000	-3.620535	4.866842
49	8	0	0.000000	-2.405555	-5.567829
50	8	0	0.000000	6.025710	0.700169
51	8	0	0.000000	-6.025710	0.700169
52	8	0	0.000000	3.620535	4.866842
53	8	0	0.000000	2.405555	-5.567829
54	6	0	0.000000	-4.823179	5.657688
55	1	0	-0.900490	-5.412510	5.459525
56	1	0	0.900490	-5.412510	5.459525
57	1	0	0.000000	-4.485450	6.692959
58	6	0	0.000000	-2.489348	-7.004848
59	1	0	-0.900391	-2.023148	-7.416514
60	1	0	0.900391	-2.023148	-7.416514
61	1	0	0.000000	-3.554833	-7.229790
62	6	0	0.000000	7.312008	1.345872
63	1	0	-0.900458	7.435310	1.955330
64	1	0	0.900458	7.435310	1.955330
65	1	0	0.000000	8.039464	0.535530
66	6	0	0.000000	-7.312008	1.345872
67	1	0	0.900458	-7.435310	1.955330
68	1	0	-0.900458	-7.435310	1.955330
69	1	0	0.000000	-8.039464	0.535530
70	6	0	0.000000	4.823179	5.657688
71	1	0	0.900490	5.412510	5.459525
72	1	0	-0.900490	5.412510	5.459525
73	1	0	0.000000	4.485450	6.692959
74	6	0	0.000000	2.489348	-7.004848
75	1	0	0.900391	2.023148	-7.416514
76	1	0	-0.900391	2.023148	-7.416514

77	1	0	0.000000	3.554833	-7.229790
78	1	0	0.000000	0.000000	-6.721428

HF = -2231.91993625 hartree

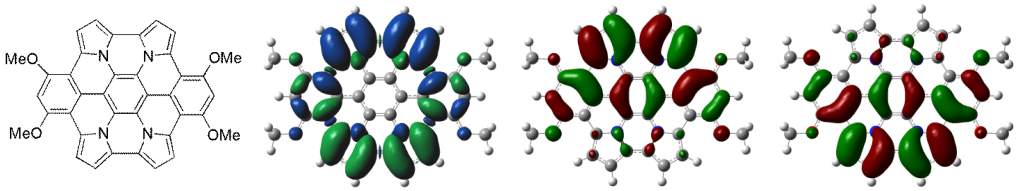
Atomic coordination of **4c**$^{2+}$ (triplet, C_s symmetry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.202379	-0.685657	0.000000
2	6	0	1.227062	0.719100	0.000000
3	6	0	0.000000	1.376311	0.000000
4	6	0	-1.227669	0.699973	0.000000
5	6	0	-1.184149	-0.701566	0.000000
6	6	0	0.006702	-1.422485	0.000000
7	6	0	-2.465634	1.405472	0.000000
8	6	0	-3.679740	0.649220	0.000000
9	6	0	-2.433488	2.836287	0.000000
10	6	0	-4.899887	1.384523	0.000000
11	6	0	-3.687976	3.511585	0.000000
12	6	0	-4.884827	2.784895	0.000000
13	1	0	-5.823325	3.319844	0.000000
14	6	0	0.016890	-2.856662	0.000000
15	6	0	-1.244170	-3.539130	0.000000
16	6	0	1.264874	-3.521696	0.000000
17	6	0	-1.207859	-4.973995	0.000000
18	6	0	1.234010	-4.952656	0.000000
19	6	0	0.014911	-5.647042	0.000000
20	1	0	0.024601	-6.727087	0.000000
21	6	0	2.465983	1.440816	0.000000
22	6	0	2.410703	2.874362	0.000000
23	6	0	3.674145	0.706070	0.000000
24	6	0	3.663458	3.574062	0.000000
25	6	0	4.889206	1.461587	0.000000
26	6	0	4.865352	2.864550	0.000000
27	1	0	5.799642	3.406590	0.000000
28	7	0	-0.013733	2.741126	0.000000
29	6	0	1.144562	3.531117	0.000000
30	6	0	-1.162744	3.509234	0.000000
31	6	0	0.676063	4.871286	0.000000
32	6	0	-0.712825	4.859749	0.000000
33	1	0	1.309386	5.743119	0.000000
34	1	0	-1.361322	5.720662	0.000000
35	7	0	-2.365198	-1.384780	0.000000
36	6	0	-2.454926	-2.784826	0.000000
37	6	0	-3.611512	-0.787772	0.000000
38	6	0	-3.845946	-3.064115	0.000000
39	6	0	-4.543813	-1.862500	0.000000
40	1	0	-4.274055	-4.052974	0.000000
41	1	0	-5.614994	-1.743356	0.000000
42	7	0	2.378290	-1.355671	0.000000
43	6	0	2.488928	-2.752839	0.000000
44	6	0	3.635909	-0.739421	0.000000
45	6	0	3.864496	-3.013160	0.000000
46	6	0	4.561174	-1.790285	0.000000
47	1	0	4.309943	-3.994545	0.000000
48	1	0	5.632505	-1.672917	0.000000
49	8	0	2.423736	-5.556444	0.000000
50	8	0	-6.023335	0.654685	0.000000
51	8	0	3.586914	4.909052	0.000000
52	8	0	-2.395348	-5.588019	0.000000
53	8	0	6.015286	0.745677	0.000000
54	8	0	-3.632573	4.850263	0.000000
55	6	0	2.517297	-6.992371	0.000000
56	1	0	2.054310	-7.407764	0.900365
57	1	0	2.054310	-7.407764	-0.900365
58	1	0	3.584313	-7.210124	0.000000
59	6	0	-7.307466	1.300897	0.000000
60	1	0	-7.433186	1.911021	0.900056
61	1	0	-7.433186	1.911021	-0.900056
62	1	0	-8.036856	0.491998	0.000000
63	6	0	4.786164	5.703075	0.000000
64	1	0	5.377133	5.507313	0.900179
65	1	0	5.377133	5.507313	-0.900179
66	1	0	4.446381	6.737790	0.000000
67	6	0	-2.467853	-7.024572	0.000000
68	1	0	-1.998299	-7.433426	-0.900168
69	1	0	-1.998299	-7.433426	0.900168
70	1	0	-3.531370	-7.259137	0.000000
71	6	0	7.298234	1.397098	0.000000
72	1	0	7.419639	2.007088	-0.900387
73	1	0	7.419639	2.007088	0.900387
74	1	0	8.029470	0.590107	0.000000
75	6	0	-4.843168	5.625543	0.000000
76	1	0	-5.432168	5.422656	-0.900066
77	1	0	-5.432168	5.422656	0.900066
78	1	0	-4.519208	6.665442	0.000000

HF = -2231.923508 hartree

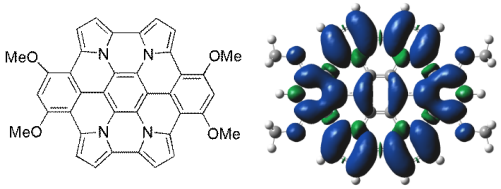
S20. Spin density maps and possible resonance structures of 3^{2+} and 4^{2+}

Spin density map and MOs of **3c**$^{2+}$ in singlet biradical state.

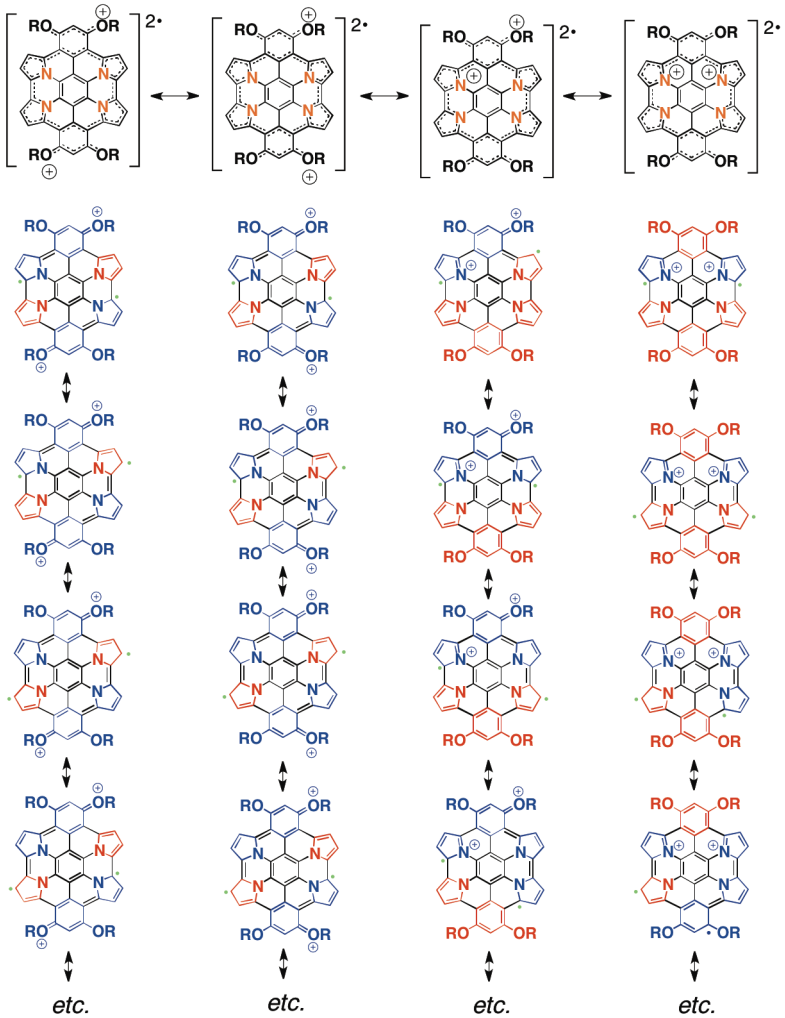


Spin density map MO for α-spin MO for β-spin

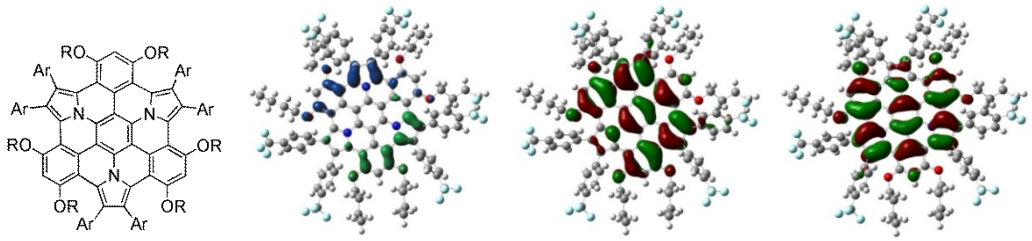
Spin density maps of **3c**$^{2+}$ in triplet state.



Possible resonance structures of **3c**$^{2+}$

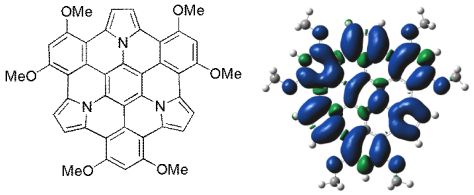


Spin density map and MOs of **4b**$^{2+}$ (R = *n*-C_4H_9) in singlet biradical state. The geometry was taken from the crystal structure.



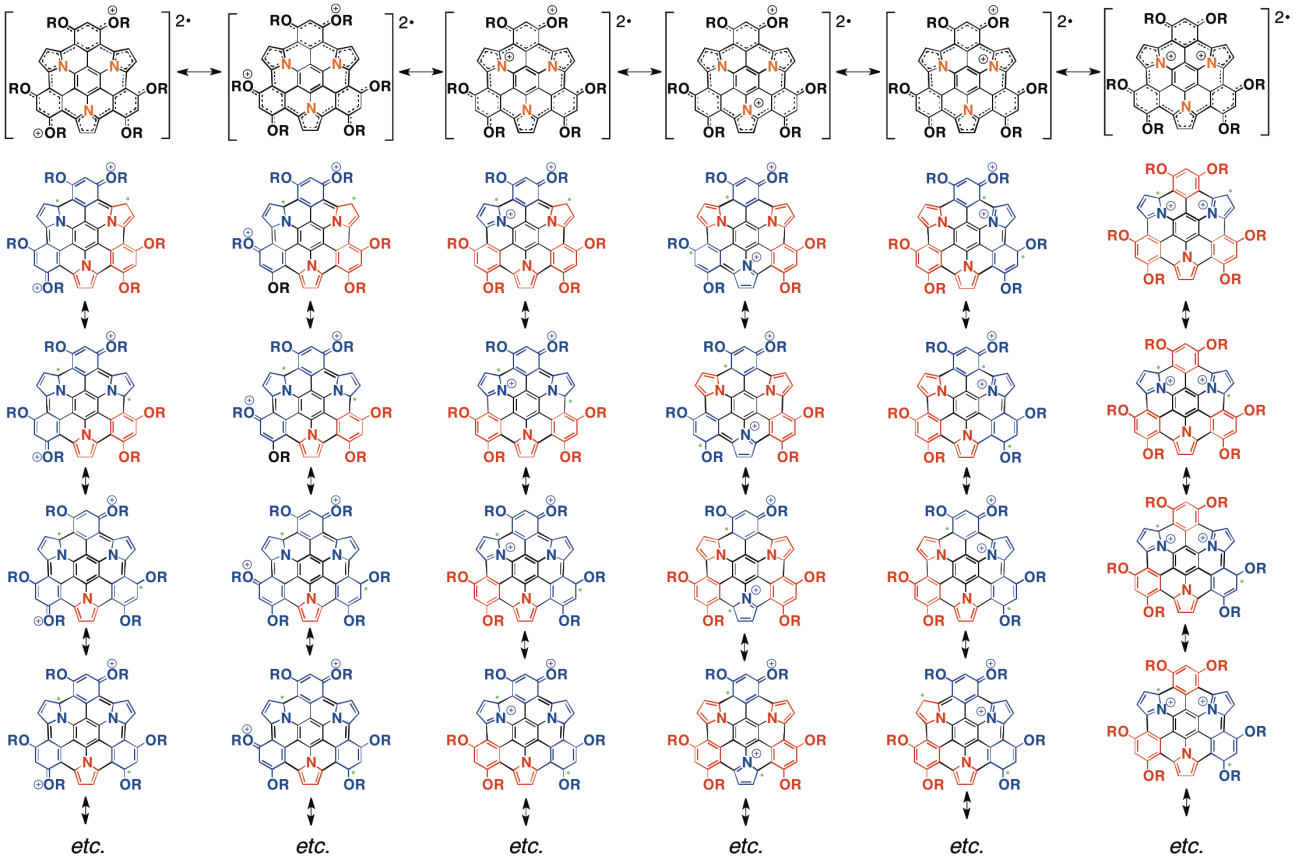
Spin density map MO for α-spin MO for β-spin

Spin density maps of **4c**$^{2+}$ in triplet state.



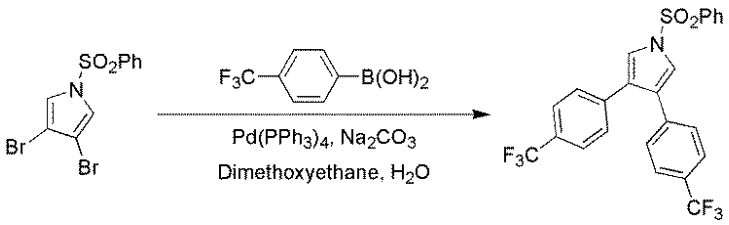
Spin density map of triplet

Possible resonance structures of **4c**$^{2+}$



S21. Synthetic procedures

1. *N*-Benzenesulfonyl-3,4-bis(4-trifluoromethylphenyl)pyrrole



In a double-neck round-bottom flask, were added *N*-benzenesulfonyl-3,4-dibromopyrrole (6.40 g, 17.5 mmol), 4-trifluoromethylphenylboronic acid (9.95 g, 52.4 mmol), Na_2CO_3 (12.25 g, 115.6 mmol), and $Pd(PPh_3)_4$ (0.93 g, 0.8 mmol), and then evacuated and backfilled with N_2 three times. Then, degassed dimethoxyethane (140 ml) and H_2O (38 ml) were added. The reaction mixture was stirred at reflux for overnight. After addition of H_2O, the aqueous phase was extracted with CH_2Cl_2. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/AcOEt 4:1) to give *N*-benzenesulfonyl-3,4-bis(4-trifluoromethylphenyl)pyrrole (7.66 g, 15.5 mmol) as white solid, yield: 88%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.99 (d, *J* = 7.5 Hz, 2H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 4H), 7.34 (s, 2H), 7.27 (d, *J* = 8.2 Hz, 4H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 138.48, 136.72, 134.43, 129.73, 129.50, 129.24, 128.69, 127.20, 127.14, 125.49 (q, *J* = 3.6 Hz, -CF_3), 119.79.

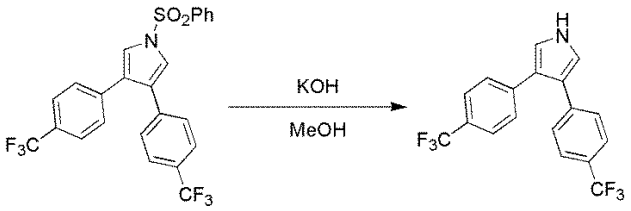
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.71.

EI-MS *m/z* 495 (M^+)

Anal. Calcd for $C_{24}H_{15}F_6NO_2S$: C, 58.18%; H, 3.05%; N, 2.83%. Found: C, 58.53%; H, 3.06%; N, 2.66%.

Melting point: 125.4 – 127.3 °C

2. 3,4-Bis(4-trifluoromethylphenyl)-*1H*-pyrrole



In a round-bottom flask, was added MeOH (1000 ml) to *N*-benzenesulfonyl-3,4-bis(4-trifluoromethylphenyl)pyrrole (7.66 g, 15.5 mmol) and KOH (9.15 g, 163.0 mmol). The reaction mixture was stirred at room temperature for 4 h. The reaction was quenched by adding 2N-HCl aq. until the solution to be pH 7. The aqueous phase was extracted with CH_2Cl_2. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:2) to give 3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrole (5.26 g, 14.8 mmol) as white solid, yield: 96%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 8.44 (s, br, 1H), 7.52 (d, *J* = 8.0 Hz, 4H), 7.34 (d, *J* = 8.0 Hz, 4H), 6.99 (s,

2H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 139.03, 128.52, 128.16, 125.49, 125.3 (q, J = 3.7 Hz, -CF_3), 122.53, 118.44.

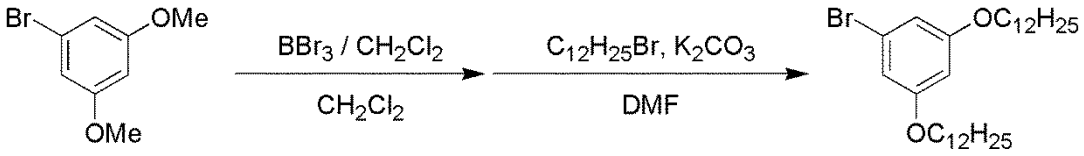
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.47.

EI-MS *m/z* 356 (M^+)

Anal. Calcd for $C_{18}H_{11}F_6N$: C, 60.85%; H, 3.12%; N, 3.94%. Found: C, 60.89%; H, 3.38%; N, 3.99%.

Melting point: 139.8 – 145.3 °C

3. 3,5-Bisdodecyloxybromobenzene



In a three-necked round-bottom flask equipped with a thermometer, was added CH_2Cl_2 (100 ml) to 3,5-dimethoxybromobenzene (10.0 g, 46.2 mmol). The solution of 3,5-dimethoxybromobenzene was cooled to -78 °C, and 1 M-CH_2Cl_2 solution of BBr_3 (100 ml, 100.0 mmol) was added slowly. The reaction mixture was allowed to warm up to room temperature for overnight. The stirred solution was again cooled to 0 °C, and then quenched with H_2O. The aqueous phase was extracted with Et_2O. The combined organic layers were washed with H_2O, dried over $MgSO_4$, and evaporated under reduced pressure. Resulting white solids were used to the next reaction without further purification.

In a double-neck round-bottom flask, was added 3,5-dihydroxybromobenzene (8.73 g, 46.2 mmol), K_2CO_3 (47.2 g, 341.5 mmol) and DMF (200 ml). The reaction mixture was stirred at room temperature for 30 min. Then dodecylbromide (45 ml, 187.8 mmol) was added and stirred at 60 °C for overnight. Resulting suspension was passed through celite, and the filtrate was evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane) to afford 3,5-bisdodecyloxybromobenzene (19.5 g, 37.1 mmol) as white solid, yield: 80% (2-steps).

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 6.62 (d, J = 2.2 Hz, 2H), 6.35 (t, J = 2.2 Hz, 1H), 3.88 (t, J = 6.6 Hz, 4H), 1.77-1.72 (m, 4H), 1.44-1.39 (m, 4H), 1.33-1.21 (m, 32H), 0.88 (t, J = 7.1 Hz, 6H).

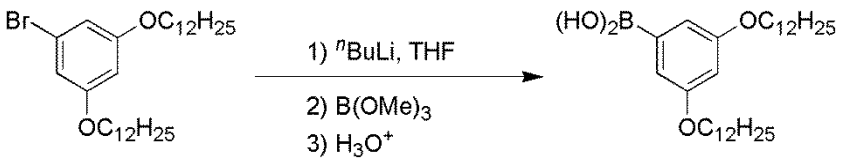
^{13}C NMR ($CDCl_3$, 125 MHz) δ 160.76, 122.82, 110.23, 100.60, 68.31, 31.94, 29.67, 29.65, 29.60, 29.57, 29.36, 29.13, 25.99 (2C), 22.71, 14.13.

EI-MS *m/z* 524 (M^+)

Anal. Calcd for $C_{30}H_{53}BrO_2$: C, 68.55%; H, 10.16%. Found: C, 68.19%; H, 9.86%.

Melting point: 32.9 – 34.8 °C

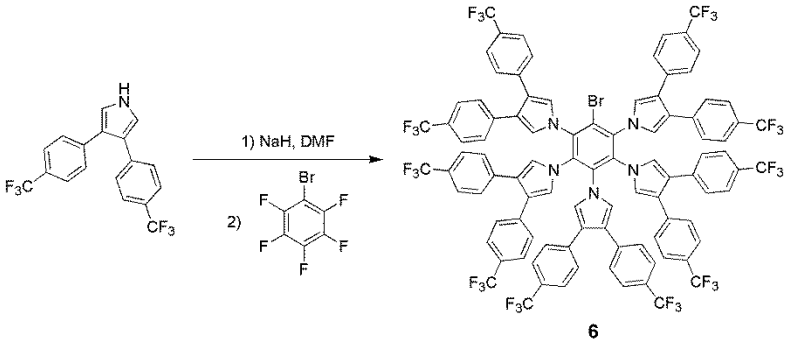
4. 3,5-Bisdodecyloxyphenylboronic acid



In a double-neck round-bottom flask, was added THF (10 ml) to 3,5-bisdodecyloxybromobenzene (531 mg,

1.01 mmol). The solution was cooled to -5 °C, and then ^{n}BuLi (1.61 M in hexane, 0.7 ml, 1.13 mmol) was added dropwise. After completion of the addition, the reaction mixture was further cooled to -78 °C, and stirred for 30 min. Then, $B(OMe)_3$ (0.2 ml, 1.79 mmol) was added in one portion. After stirring at room temperature for 2 h, the reaction was quenched with 2N-HCl and stirred for 30 min. The aqueous phase extracted with Et_2O, and the combined organic layers were washed with sat-NaCl aq., dried over $MgSO_4$, and evaporated under reduced pressure. Resulting solids were used to the next reaction without further purification.

5. Pentakis[3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrolo]bromobenzene (**6**)



In a double-neck round-bottom flask, was added DMF (4 ml) to 3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrole (402 mg, 1.13 mmol) and sodium hydride (60% in mineral oil, 55 mg, 1.37 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 20 min. And then pentafluorobromobenzene (28 μl, 0.22 mmol) was added in one portion. After stirring at room temperature for overnight, the reaction was quenched with H_2O, and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 2:1) to afford pentakis[3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrolo]bromobenzene (**6**, 340 mg, 0.18 mmol) as white solid, yield: 82%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.57 (d, *J* = 8.3 Hz, 8H), 7.52-7.47 (m, 12H), 7.31 (d, *J* = 8.2 Hz, 8H), 7.13-7.09 (m, 12H), 6.96 (s, 4H), 6.56 (s, 4H), 6.55 (s, 2H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 137.35, 137.13, 136.99, 135.26, 132.68, 129.48, 129.35, 129.22, 129.09, 128.51, 128.23, 128.19, 125.88-125.69 (m, $-CF_3$, 3C), 125.60, 125.26, 125.20, 125.07, 123.24, 123.04, 122.91, 122.16, 120.92, 120.75.

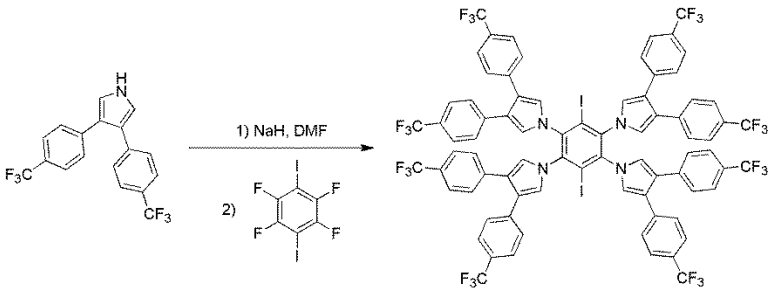
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.56, -65.63, -65.65.

APCI-MS calcd. for $C_{96}H_{50}BrF_{30}N_5$: 1921.2770, Found: 1921.2782.

Anal. Calcd for $C_{96}H_{50}BrF_{30}N_5$: C, 59.95%; H, 2.62%; N, 3.64%. Found: C, 59.95%; H, 2.72%; N, 3.61%.

Melting Point: 298.5 – 300.2 °C

6. 2,3,5,6-Tetrakis[3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrolo]-1,4-diiodobenzene (**7**)



7

In a double-neck round-bottom flask, was added DMF (4 ml) to 3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrole (397 mg, 1.12 mmol) and sodium hydride (60% in mineral oil, 47 mg, 1.17 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 20 min. And then 1,4-diiodotetrafluorobenzene (108 mg, 0.48 mmol) was added in one portion. After stirring at room temperature for overnight, the reaction was quenched with H_2O, and the aqueous phase extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was dispersed in a small amount of CH_2Cl_2, and insoluble solids were collected by filtration to afford 2,3,5,6-tetrakis[3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrolo] -1,4-diiodobenzene (**7**, 330 mg, 0.19 mmol) as white solid, yield: 70%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.49 (d, J = 8.1 Hz, 16H), 7.21 (d, J = 8.1 Hz, 16H), 6.80 (s, 8H).

^{13}C NMR peaks were not able to be observed due to quite low solubility.

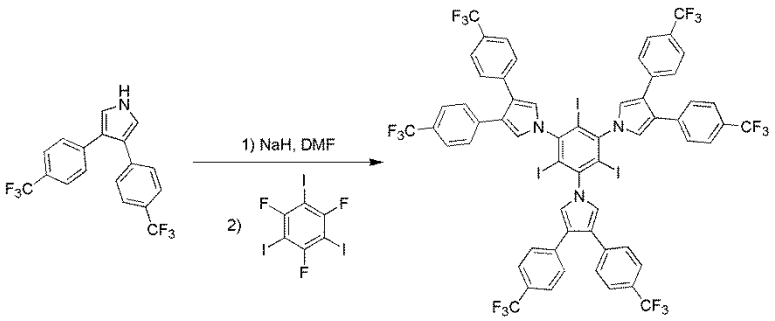
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.63.

APCI-MS calcd. for $C_{78}H_{40}F_{24}I_2N_4$: 1742.0949, Found: 1742.0950.

Anal. Calcd for $C_{78}H_{40}F_{24}I_2N_4$: C, 53.75%; H, 2.31%; N, 3.21%. Found: C, 53.76%; H, 2.25%; N, 3.21%.

Melting Point: > 300 °C

7. 2,4,6-Tris[3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrolo]-1,3,5-triiodobenzene (**8**)



8

In a double-neck round-bottom flask, was added DMF (5 ml) to 3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrole (591 mg, 1.66 mmol) and sodium hydride (60% in mineral oil, 70 mg, 1.75 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 20 min. And then 2,4,6-trifluoro-1,3,5-triiodobenzene (278 mg, 0.55 mmol) was added in one portion. After stirring at room temperature for overnight, the reaction was quenched with H_2O, and the aqueous phase extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq.,

and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 2:1) to afford 2,4,6-tris[3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrolo]-1,3,5-tri iodobenzene (**8**, 746 mg, 0.49 mmol) as white solid, yield: 90%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.57 (d, *J* = 8.2 Hz, 12H), 7.42 (d, *J* = 8.2 Hz, 12H), 6.89 (s, 6H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 148.01, 138.10, 128.63, 125.45 (q, *J* = 3.7 Hz, -CF_3), 125.35, 124.58, 123.18, 120.57, 103.32.

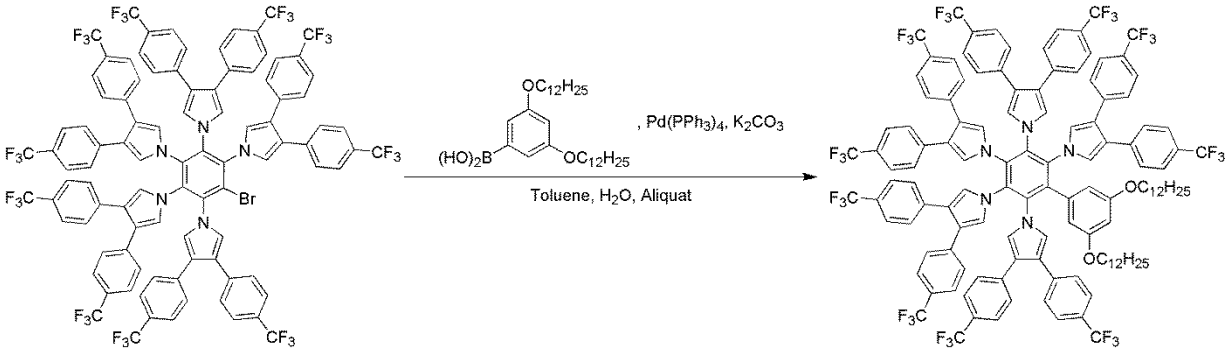
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.54.

APCI-MS calcd. for $C_{60}H_{30}F_{18}I_3N_3$: 1514.9287, Found: 1514.9276.

Anal. Calcd for $C_{60}H_{30}F_{18}I_3N_3$: C, 47.55%; H, 2.00%; N, 2.77%. Found: C, 48.00%; H, 2.21%; N, 2.71%.

Melting Point: 189.4 – 192.5 °C

8. 5AC($OC_{12}H_{25}$)-prefused (**9a**)



6 **9a**

In a double-neck round-bottom flask, were added **6** (313 mg, 0.16 mmol), 3,5-bisdodecyloxyphenylboronic acid (493 mg, 1.00 mmol), K_2CO_3 (142 mg, 1.03 mmol), toluene (5 ml), H_2O (2 ml), aliquat336 (3 drops). Then evacuated and backfilled with N_2 three times. $Pd(PPh_3)_4$ (48 mg, 42 μmol) was added to the reaction mixture. After stirring at reflux for overnight. The reaction mixture was cooled to room temperature and quenched with H_2O, and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:1) to afford **9a** (240 mg, 0.10 mmol) as white solid, yield: 64%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.55 - 7.51 (m, 20H), 7.22 - 7.18 (m, 12H), 7.10 (d, *J* = 8.1 Hz, 8H), 6.68 (s, 2H), 6.66 - 6.64 (m, 5H), 6.62 (s, 4H), 6.31 (d, *J* = 2.1 Hz, 2H), 3.77 (t, *J* = 6.5 Hz, 4H), 1.66 (p, *J* = 6.5 Hz, 4H), 1.28 - 1.19 (m, 36H), 0.86 (t, *J* = 6.8 Hz, 6H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 161.14, 137.76, 137.59, 137.35, 137.29, 135.62, 133.46, 133.07, 132.64, 129.40, 129.18, 129.14, 128.93, 128.39, 128.33, 128.30, 125.84-125.63 (m, -CF_3, 3C), 125.55, 125.25, 125.19, 124.83, 123.09, 123.02, 121.87, 121.06, 106.75, 103.11, 68.74, 31.91, 29.65, 29.62, 29.60(2C), 29.35, 29.06, 26.07(2C), 22.69, 14.06.

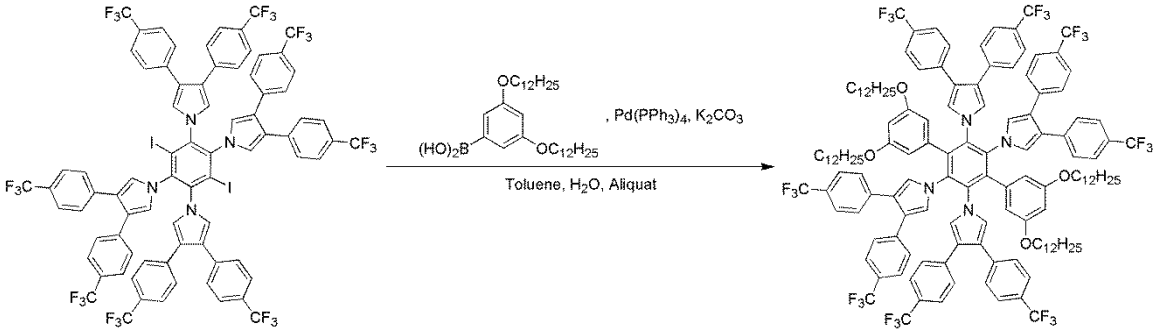
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.49, -65.52, -65.53.

APCI-MS calcd. for $C_{126}H_{103}F_{30}N_5O_2$: 2287.7633, Found: 2287.7636.

Anal. Calcd for $C_{126}H_{103}F_{30}N_5O_2$: C, 66.11%; H, 4.54%; N, 3.06%. Found: C, 65.90%; H, 4.54%; N, 2.97%.

Melting Point: 121.2 – 124.7 °C

9. 4AC($OC_{12}H_{25}$)-prefused (**11a**)



7 **11a**

In a double-neck round-bottom flask, were added **7** (310 mg, 0.18 mmol), 3,5-bisdodecyloxyphenylboronic acid (493 mg, 1.00 mmol), K_2CO_3 (181 mg, 1.31 mmol), toluene (5 ml), H_2O (2 ml), aliquat336 (3 drops). Then evacuated and backfilled with N_2 three times. $Pd(PPh_3)_4$ (48 mg, 42 μmol) was added to the reaction mixture. After stirring at reflux for overnight. The reaction mixture was cooled to room temperature and quenched with H_2O, and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:1) to afford **11a** (397 mg, 0.17 mmol) as white solid, yield: 94%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.46 (d, *J* = 8.2 Hz, 16H), 7.02 (d, *J* = 8.2 Hz, 16H), 6.58 (t, *J* = 2.1 Hz, 2H), 6,53 (s, 8H), 6.24 (d, *J* = 2.1 Hz, 4H), 3.71 (t, *J* = 6.5 Hz, 8H), 1.61 (p, *J* = 6.5 Hz, 8H), 1.29 - 1.15 (m, 72H), 0.86 (t, *J* = 7.2 Hz, 12H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 160.90, 137.83, 136.88, 135.45, 134.09, 128.28, 125.49 (q, *J* = 3.6 Hz, -CF_3), 125.22, 124.14, 123.06, 122.07, 106.79, 102.88, 68.65, 31.87, 29.60, 29.57 (2C), 29.55 (2C), 29.31, 29.03, 26.01, 22.66, 14.07.

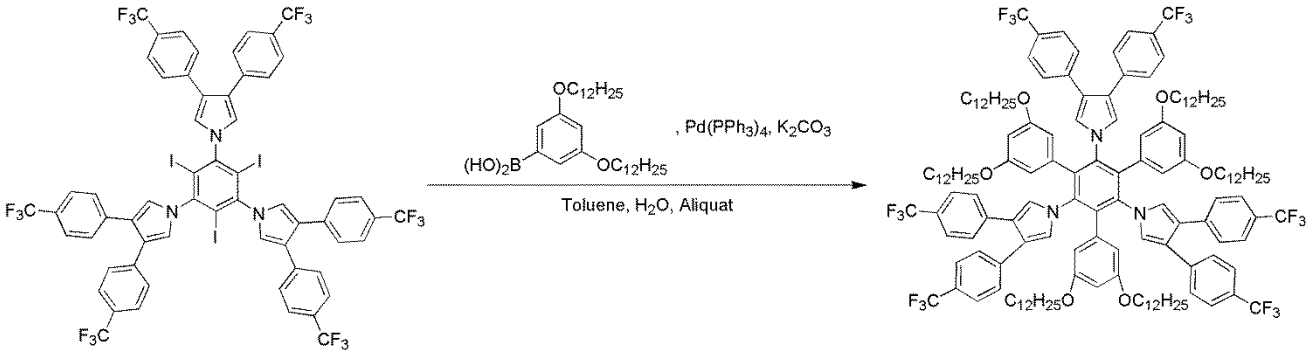
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.61.

APCI-MS calcd. for $C_{138}H_{146}F_{24}N_4O_4$: 2379.0961, Found: 2379.0941.

Anal. Calcd for $C_{138}H_{146}F_{24}N_4O_4$: C, 69.62%; H, 6.18%; N, 2.35%. Found: C, 69.89%; H, 6.30%; N, 2.27%.

Melting Point: 140.6 – 142.9 °C

10. 3AC($OC_{12}H_{25}$)-prefused (**12a**)



8 **12a**

In a double-neck round-bottom flask, were added **8** (384 mg, 0.25 mmol), 3,5-bisdodecyloxyphenyl boronic acid (987 mg, 2.00 mmol), K_2CO_3 (382 mg, 2.76 mmol), toluene (10 ml), H_2O (4 ml), aliquat336 (3 drops). Then evacuated and backfilled with N_2 three times. $Pd(PPh_3)_4$ (29 mg, 25 μmol) was added to the reaction mixture. After stirring at reflux for overnight. The reaction mixture was cooled to room temperature and quenched with H_2O, and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:1) to afford **12a** (431 mg, 0.17 mmol) as white solid, yield: 69%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.43 (d, *J* = 7.9 Hz, 12H), 6.94 (d, *J* = 7.9 Hz, 12H), 6.48 (s, 6H), 6.47 (m, 3H), 6.22 (m, 6H), 3.65 (t, *J* = 6.0 Hz, 12H), 1.57-1.55 (m, 12H), 1.27-1.16 (m, 108H), 0.87 (t, *J* = 6.9 Hz, 18H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 160.48, 138.37, 137.71, 136.86, 135.37, 128.33, 128.10, 125.32, 125.19 (q, *J* = 3.3 Hz, -CF_3), 123.15, 122.92, 106.77, 102.47, 68.54, 31.87, 29.58, 29.56, 29.53 (2C), 29.30 (2C), 29.07, 25.96, 22.65, 14.06.

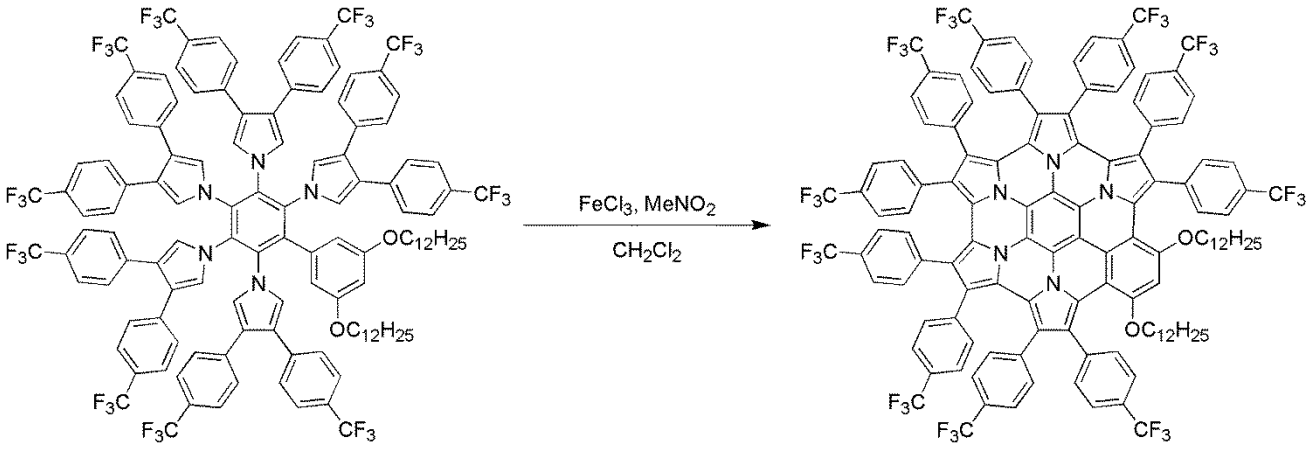
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.56.

APCI-MS calcd. for $C_{150}H_{189}F_{18}N_3O_6$: 2470.4289, Found: 2470.4293.

Anal. Calcd for $C_{150}H_{189}F_{18}N_3O_6$: C, 72.88%; H, 7.71%; N, 1.70%. Found: C, 72.62%; H, 7.72%; N, 1.74%.

Melting Point: 105.2 – 106.3 °C

11. 5AC($OC_{12}H_{25}$) (**2a**)



9a **2a**

In a double-neck round-bottom flask, was added CH_2Cl_2 (120 ml) to **9a** (125 mg, 55 μmol). Then Ar gas was bubbled to the solution for 30min. Under light shielding with foil, $FeCl_3$ (322 mg, 1.98 mmol) in $MeNO_2$ (6 ml) was added dropwise. After stirring at room temperature for overnight, the reaction mixture was quenched with Na_2CO_3 aq. and Na_2SO_3 aq., and then the aqueous phase was extracted with CH_2Cl_2. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:1), and recrystallization from CH_2Cl_2-MeOH to afford **2a** (97 mg, 42 μmol) as orange solid, yield: 78%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.33 (d, *J* = 7.7 Hz, 4H), 7.02 (d, *J* = 7.7 Hz, 4H), 6.97-6.86 (m, 8H), 6.85-6.78 (m, 8H), 6.77-6.69 (m, 4H), 6.66-6.50 (m, 12H), 6.23 (s, br, 1H), 3.22 (m, 4H), 1.30-1.09 (m, 32H), 1.05-0.94 (m, 8H), 0.87(t, *J* = 7.2 Hz, 6H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 142.00, 139.18, 138.14, 137.28, 136.94, 136.74, 131.35, 131.00, 130.70, 130.62, 128.95, 128.68, 128.12, 127.85, 125.41, 125.31, 124.80, 124.77, 124.64, 124.62, 124.44, 124.33-124.13 (m, -CF_3, 5C), 124.12, 123.54, 123.52, 123.14, 122.76, 122.64, 122.60, 122.59, 122.48, 118.38, 116.89, 116.17, 115.00, 110.56, 108.81, 107.21, 103.09, 67.78, 31.91, 29.62, 29.61, 29.49, 29.47, 29.34, 29.14, 27.78, 25.59, 22.68, 14.09.

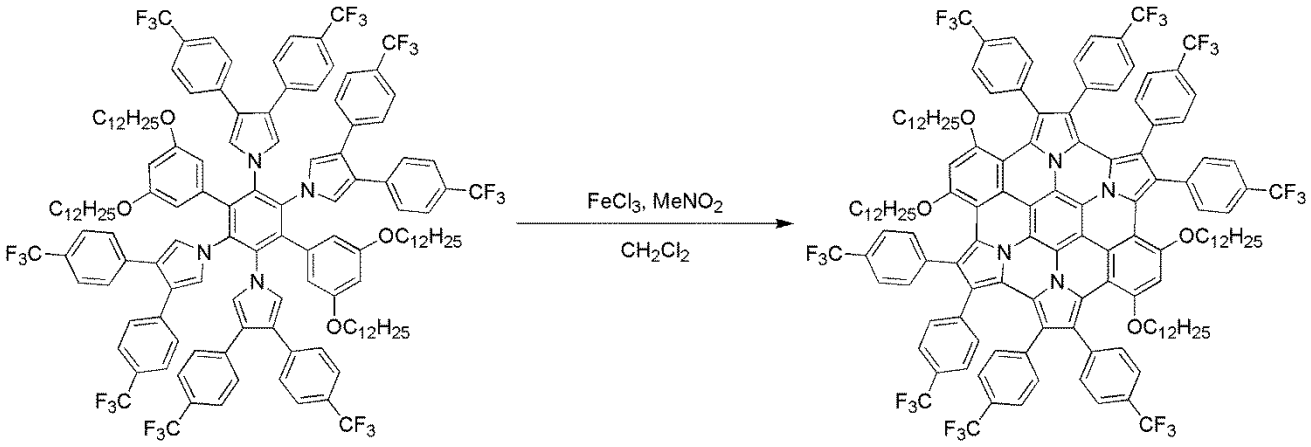
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.73, -66.39, -66.43, -66.52, -66.53.

APCI-MS calcd. for $C_{126}H_{91}F_{30}N_5O_2$: 2275.6694, Found: 2275.6676.

Anal. Calcd for $C_{126}H_{91}F_{30}N_5O_2$: C, 66.46%; H, 4.03%; N, 3.08%. Found: C, 66.74%; H, 4.05%; N, 3.05%.

Melting Point: > 300 °C

12. 4AC($OC_{12}H_{25}$) (**3a**)



11a **3a**

In a double-neck round-bottom flask, charged with **11a** (106 mg, 45 μmol) and CH_2Cl_2 (100 ml). Then Ar gas was bubbled to the solution for 30min. Under light shielding with foil, $FeCl_3$ (274 mg, 1.69 mmol) in $MeNO_2$ (5 ml) was added dropwise. After stirring at room temperature for overnight, the reaction mixture was quenched with Na_2CO_3 aq. and Na_2SO_3 aq., and then the aqueous was phase extracted with CH_2Cl_2. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:1), and recrystallization from CH_2Cl_2-MeOH to afford **3a** (86 mg, 36 μmol) as red solid, yield: 82%.

^{1}H-NMR (CD_2Cl_2, 500 MHz) δ 7.30 (d, *J* = 8.0 Hz, 8H), 7.05 (d, *J* = 8.0 Hz, 8H), 6.98 (d, *J* = 7.8 Hz, 8H), 6.79 (d, *J* = 7.8 Hz, 8H), 6.17 (s, 2H), 3.23-3.16 (m, 8H), 1.32-1.06 (m, 64H), 1.05-0.94 (m, 16H), 0.86 (t, *J* = 7.0 Hz, 12H).

^{13}C NMR (CD_2Cl_2, 125 MHz) δ 154.29, 142.83, 139.35, 132.06, 130.77, 127.49, 127.01, 125.81, 125.57, 125.48, 124.58, 124.35-124.22 (m, -CF_3), 123.64 (q, *J* = 3.4 Hz, -CF_3), 123.31, 123.08, 122.89, 120.71, 116.89, 116.09, 109.60, 67.82, 32.16, 29.87, 29.86, 29.74, 29.72, 29.59, 29.36, 28.01, 25.80, 22.92, 14.09.

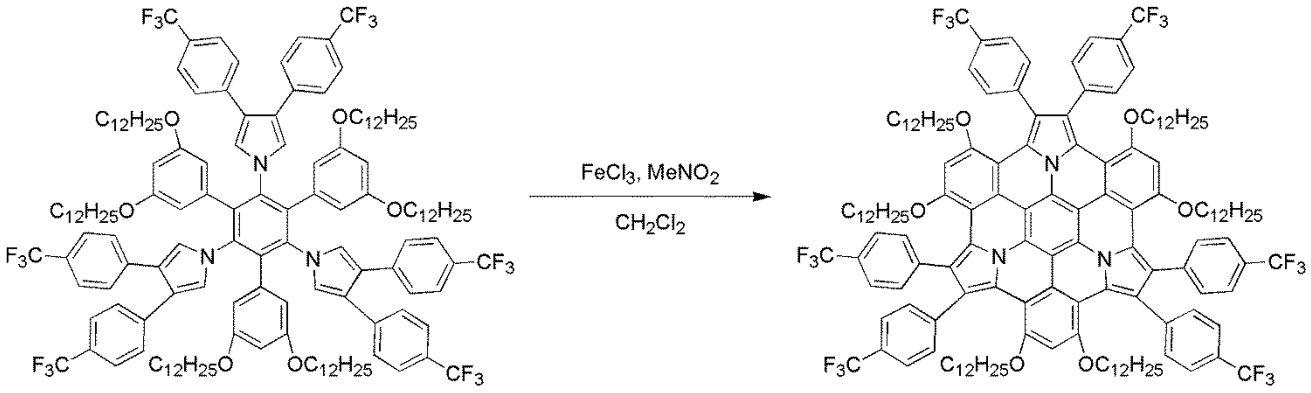
^{19}F NMR (CD_2Cl_2, 470.5 MHz) δ -64.95, -65.45.

APCI-MS calcd. for $C_{138}H_{134}F_{24}N_4O_4$: 2367.0022, Found: 2367.0026.

Anal. Calcd for $C_{138}H_{134}F_{24}N_4O_4$: C, 69.98%; H, 5.70%; N, 2.37%. Found: C, 70.14%; H, 5.54%; N, 2.31%.

Melting Point: > 300 °C

13. 3AC($OC_{12}H_{25}$) (**4a**)



12a **4a**

In a double-neck round-bottom flask, charged with **12a** (176 mg, 71 μmol) and CH_2Cl_2 (100 ml). Then Ar gas was bubbled to the solution for 30min. Under light shielding with foil, $FeCl_3$ (433 mg, 2.67 mmol) in $MeNO_2$ (5 ml) was added dropwise. After stirring at room temperature for overnight, the reaction mixture was quenched with Na_2CO_3 aq. and Na_2SO_3 aq., and then the aqueous phase was extracted with CH_2Cl_2. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 3:1), and recrystallization from CH_2Cl_2-MeOH to afford **4a** (151 mg, 61 μmol) as yellow needle, yield: 86%.

^{1}H-NMR (CD_2Cl_2, 500 MHz) δ 7.40 (d, J = 8.2 Hz, 12H), 7.22 (d, J = 8.2 Hz, 12H), 6.28 (s, 3H), 3.23 (t, J = 7.1 Hz, 12H), 1.32-0.99 (m, 120H), 0.86 (t, J = 7.2 Hz, 18H).

^{13}C NMR (CD_2Cl_2, 125 MHz) δ 153.07, 144.63, 131.57, 127.69, 127.43, 126.98, 126.14, 125.35, 124.78, 123.98, 123.80 (q, J = 3.6 Hz, -CF_3), 120.12, 107.90, 67.73, 32.34, 30.07, 30.01, 29.99, 29.78, 29.68 (2C), 28.40, 26.07, 23.10, 14.27.

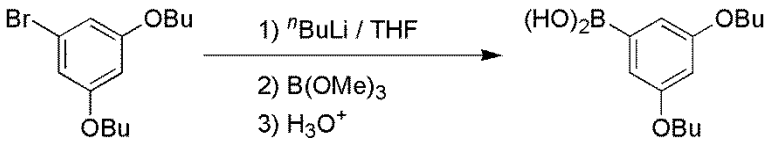
^{19}F NMR (CD_2Cl_2, 470.5 MHz) δ -64.79.

APCI-MS calcd. for $C_{150}H_{177}F_{18}N_3O_6$: 2458.3350, Found: 2458.3294.

Anal. Calcd for $C_{150}H_{177}F_{18}N_3O_6$: C, 73.24%; H, 7.25%; N, 1.71%. Found: C, 73.02%; H, 7.33%; N, 1.73%.

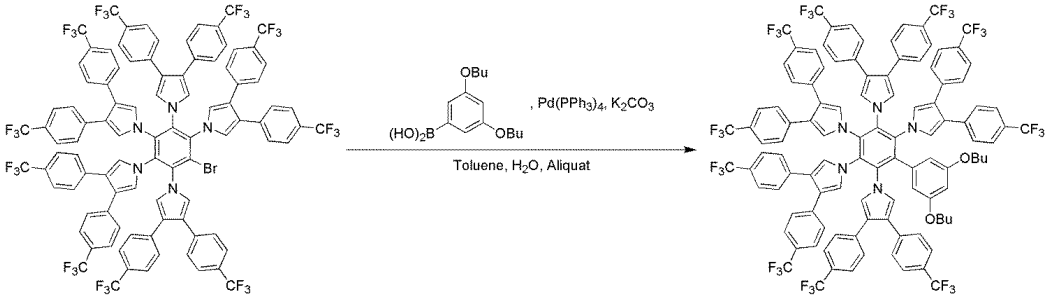
Melting Point: 148.2 – 151.2 °C

14. 3,5-Bisbuthoxyphenylboronic acid



This compound was synthesized following the procedure of 3,5-Bisdodecyloxyphenylboronic acid.

15. 5AC(OBu)-prefused (**9b**)



6 **9b**

This compound was synthesized following the procedure of **9a**.

White solid, yield: 37%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.56-7.46 (m, 20H), 7.21-7.12 (m, 12H), 7.07 (d, *J* = 8.1 Hz, 8H), 6.65 (s, 2H), 6.64-6.60 (m, 5H), 6.59 (s, 4H), 6.28 (d, *J* = 2.0 Hz, 2H), 3.76 (t, *J* = 6.5 Hz, 4H), 1.67-1.57 (m, 4H), 1.35-1.22 (m, 4H), 0.82 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 161.09, 137.83, 137.54, 137.30, 137.24, 135.60, 133.45, 133.07, 132.61, 129.49, 129.41, 129.16, 128.90, 128.34, 128.29, 128.26, 126.03-125.54 (m, -CF_3, 3C), 125.51, 125.22, 125.15, 124.78, 123.06, 122.99, 121.87, 121.03, 106.77, 102.88, 68.32, 30.96, 19.13, 13.61.

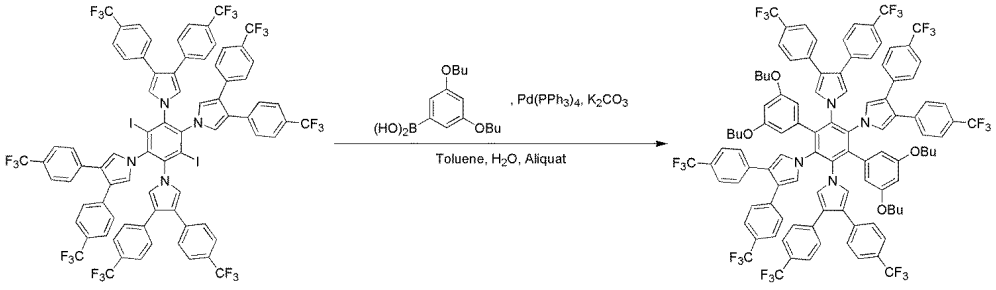
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.89, -65.90, -65.91.

APCI-MS calcd. for $C_{110}H_{71}F_{30}N_5O_2$: 2063.5129, Found: 2063.5130.

Anal. Calcd for $C_{110}H_{71}F_{30}N_5O_2$: C, 63.99%; H, 3.47%; N, 3.39%. Found: C, 64.06%; H, 3.11%; N, 3.31%.

Melting Point: 179.2 – 183.7 °C

16. 4AC(OBu)-prefused (**11b**)



7 **11b**

This compound was synthesized following the procedure of **11a**.

White solid, yield: 60%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.46 (d, *J* = 8.3 Hz, 16H), 7.03 (d, *J* = 8.3 Hz, 16H), 6.58 (t, *J* = 2.2 Hz, 2H), 6.26 (d, *J* = 2.2 Hz, 4H), 3.74 (t, J = 6.5 Hz, 8H), 1.64-1.56 (m, 8H), 1.32-1.21 (m, 8H), 0.80 (t, *J* = 7.5 Hz, 12H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 160.92, 137.89, 137.03, 135.55, 134.18, 128.30, 125.51 (q, *J* = 3.5 Hz, -CF_3), 125.28, 124.15, 123.11, 122.16, 106.90, 102.74, 68.28, 30.98, 19.12, 13.61.

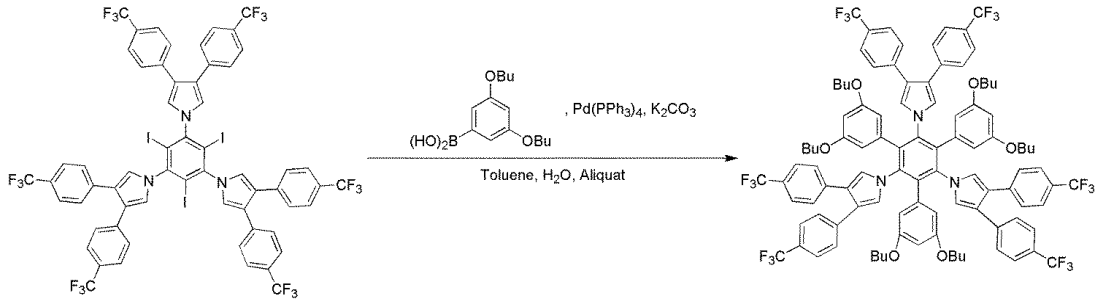
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.58.

APCI-MS calcd. for $C_{108}H_{82}F_{24}N_4O_4$: 1930.5953, Found: 1930.5963.

Anal. Calcd for $C_{108}H_{82}F_{24}N_4O_4$: C, 65.91%; H, 4.28%; N, 2.90%. Found: C, 66.14%; H, 4.17%; N, 2.89%.

Melting Point: 231.2 – 232.3 °C

17. 3AC(OBu)-prefused (**12b**)



This compound was synthesized following the procedure of **12a**.

Colorless needle, yield: 33%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.43 (d, *J* = 8.1 Hz, 12H), 6.94 (d, *J* = 8.1 Hz, 12H), 6.49 (s, 6H), 6.47-6.44 (m, 3H), 6.24-6.21 (m, 6H), 3.67 (t, *J* = 6.5 Hz, 12H), 1.62-1.49 (m, 12H), 1.29-1.17 (m, 12H), 0.79 (t, *J* = 4.9 Hz, 18H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 160.47, 138.41, 137.74, 137.06, 135.40, 128.32, 128.08, 125.37, 125.20 (q, *J* = 3.5 Hz, -CF_3), 123.24, 122.90, 106.84, 102.31, 68.15, 31.02, 19.07, 13.59.

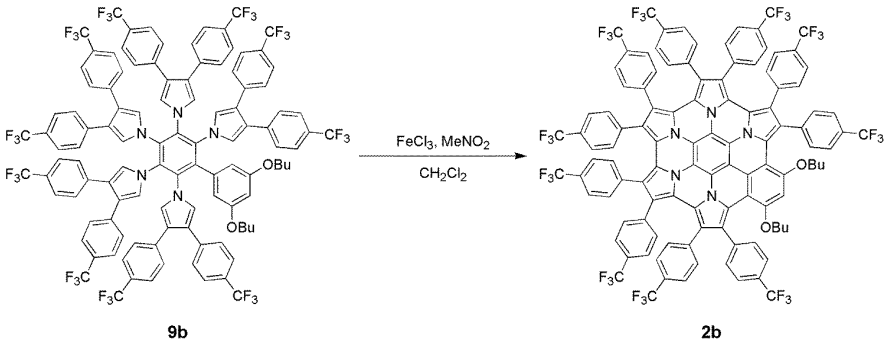
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.80.

APCI-MS calcd. for $C_{102}H_{93}F_{18}N_3O_6$: 1797.6777, Found: 1797.6777.

Anal. Calcd for $C_{102}H_{93}F_{18}N_3O_6$: C, 68.11%; H, 5.21%; N, 2.34%. Found: C, 68.07%; H, 5.04%; N, 2.33%.

Melting Point: 212.7 – 216.3 °C

18. 5AC(OBu) (**2b**)



This compound was synthesized following the procedure of **2a**.

Orange solid, yield: 64%.

^{1}H-NMR (CD_2Cl_2, 500 MHz) δ 7.35 (d, *J* = 7.8 Hz, 4H), 7.07 (d, *J* = 7.8 Hz, 4H), 7.00-6.88 (m, 8H), 6.86-6.77 (m, 12H), 6.69-6.60 (m, 12H), 6.27 (s, 1H), 3.31-3.22 (m, 4H), 1.10-0.95 (m, 8H), 0.75 (t, *J* = 5.2 Hz, 6H).

^{13}C NMR (CD_2Cl_2, 125 MHz) δ 155.06, 142.78, 138.91, 138.23, 137.85, 137.62, 136.84, 132.03, 131.66, 131.38, 131.19, 128.88, 128.62, 128.15, 127.90, 127.49, 125.96, 125.84, 125.48, 125.45, 125.33, 124.96,

124.69-124.44 (m, -CF_3, 4C), 124.44, 123.90 (q, J = 4.1 Hz, -CF_3), 123.79, 123.32, 123.28, 123.17, 123.01, 122.99, 121.90, 118.92, 117.43, 116.73, 115.50, 111.07, 110.60, 109.20, 107.70, 67.89, 30.17, 19.23, 13.74.

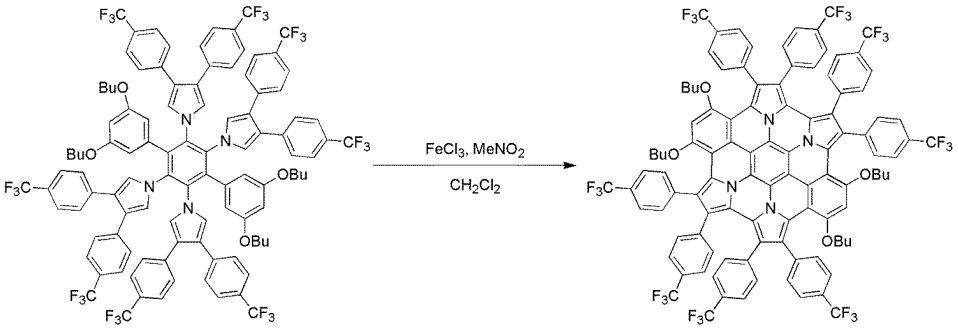
^{19}F NMR (CD_2Cl_2, 470.5 MHz) δ -65.02, -65.57, -65.60, -65.69, -65.69.

APCI-MS calcd. for $C_{110}H_{59}F_{30}N_5O_2$: 2051.4190, Found: 2051.4187.

Anal. Calcd for $C_{138}H_{134}F_{24}N_4O_4$: C, 64.37%; H, 2.90%; N, 3.41%. Found: C, 64.63%; H, 2.82%; N, 3.39%.

Melting Point: > 300 °C

19. 4AC(OBu) (**3b**)



11b **3b**

This compound was synthesized following the procedure of **3a**.

Thin red plate, yield: 41%.

^{1}H-NMR ($C_2D_2Cl_4$, 80 °C, 500 MHz) δ 7.27 (d, J = 8.0 Hz, 8H), 7.00 (d, J = 7.9 Hz, 8H), 6.93 (d, J = 8.0 Hz, 8H), 6.73 (d, J = 7.9 Hz, 8H), 6.16 (s, 2H) 3.22-3.12 (m, 8H), 1.05-0.95 (m, 16H), 0.77-0.67 (m, 12H).

^{13}C NMR ($C_2D_2Cl_4$, 80 °C, 125 MHz) δ 154.43, 147.31, 142.83, 139.19, 132.01, 130.82, 125.71, 125.55, 125.31, 125.21, 124.90, 124.25-124.15 (m, -CF_3), 123.58 (q, J = 4.2 Hz, -CF_3), 123.50, 123.14, 123.03, 120.61, 116.79, 116.17, 110.00, 67.83, 30.23, 18.99, 13.63.

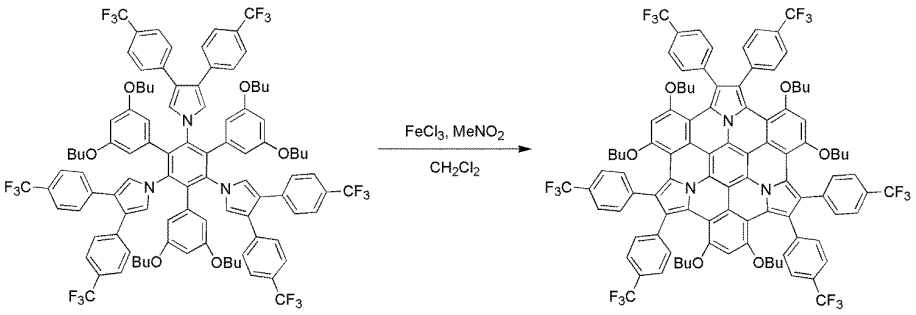
^{19}F NMR ($C_2D_2Cl_4$, 80 °C, 470.5 MHz) δ -65.53, -66.03.

APCI-MS calcd. for $C_{108}H_{70}F_{24}N_4O_4$: 1918.5014, Found: 1918.5009.

Anal. Calcd for $C_{108}H_{70}F_{24}N_4O_4$: C, 66.32%; H, 3.68%; N, 2.92%. Found: C, 66.42%; H, 3.57%; N, 2.89%.

Melting Point: > 300 °C

20. 3AC(BuO) (**4b**)



12b **4b**

This compound was synthesized following the same procedure for **4a**.

Yellow solid, yield: 62%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.42 (d, *J* = 7.6 Hz, 12H), 7.24 (d, *J* = 7.6 Hz, 12H), 6.32 (s, 3H), 3.38-3.16 (m, 12H), 1.19-1.05 (m, 24H), 0.80 (t, *J* = 7.1 Hz, 18H).

^{13}C NMR spectrum could not be record due to low solubility, seriously broadened signals and quite low thermal stability of this compound.

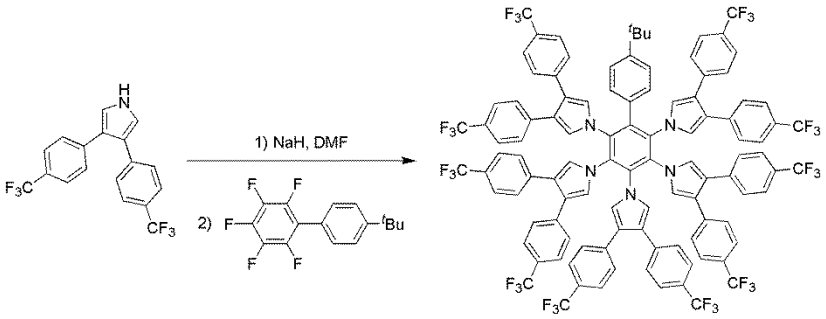
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -64.69.

APCI-MS calcd. for $C_{102}H_{81}F_{18}N_3O_6$: 1785.5838, Found: 1785.5818.

Anal. Calcd for $C_{102}H_{81}F_{18}N_3O_6$: C, 68.57%; H, 4.57%; N, 2.35%. Found: C, 68.49%; H, 4.27%; N, 2.36%.

Melting Point: > 300 °C

21. 5AC(^{t}Bu)-prefused (**10**)



10

In a double-neck round-bottom flask, was added DMF (7 ml) to 3,4-bis(4-trifluoromethylphenyl)-*1H*-pyrrole (1.01 g, 2.84 mmol) and sodium hydride (60% in mineral oil, 119 mg, 2.97 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 20 min. And then, pentafluoro-4'-*tert*-butyl-1,1'-biphenyl (90 mg, 0.30 mmol) was added in one portion. After stirring at room temperature for overnight, the reaction was quenched with H_2O, and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with sat-NaCl aq., and dried over $MgSO_4$, and evaporated under reduced pressure. The residue was purified by column chromatography over silica gel (hexane/CH_2Cl_2 2:1) to afford **10** (542 mg, 0.27 mmol) as white solid, yield: 92%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.55-7.44 (m, 22H), 7.21-7.14 (m, 12H), 7.10 (d, *J* = 8.3 Hz, 2H), 7.01 (d, *J* = 8.1 Hz, 8H), 6.66 (s, 2H), 6.62 (s, 4H), 6.50 (s, 4H), 1.44 (s, 9H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 153.03, 137.68, 137.59, 137.33, 137.29, 135.80, 132.69, 129.38, 129.12, 129.08, 129.06, 128.82, 128.34, 128.30, 128.26, 128.17, 126.25, 125.84 – 125.49 (m, -CF_3, 3C), 125.31, 125.22, 125.16, 124.57, 123.06, 123.00, 121.84, 121.05, 121.00, 35.06, 31.37.

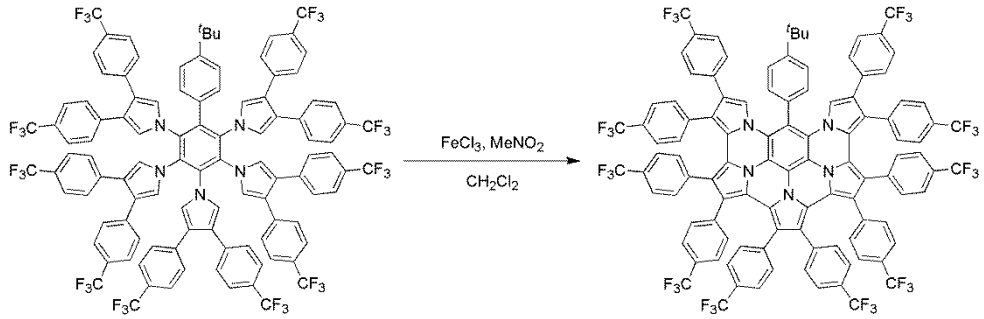
^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.57, -65.60, -65.61.

APCI-MS calcd. for $C_{106}H_{63}F_{30}N_5$: 1975.4604, Found: 1975.4692.

Anal. Calcd for $C_{106}H_{63}F_{30}N_5$: C, 64.41%; H, 3.21%; N, 3.54%. Found: C, 64.38%; H, 3.17%; N, 3.56%.

Melting Point: > 300 °C

22. Partially-fused 5AC(^{t}Bu) (**5**)



10 **5**

This compound was synthesized following the procedure of **2a**.

Recrystallization from hexane-CH_2Cl_2. Orange crystal, yield: 91%.

^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 7.0 Hz, 4H), 7.15 (d, *J* = 7.8 Hz, 4H), 7.00 (d, *J* = 7.8 Hz, 4H), 6.95-6.88 (m, 12H), 6.82 (d, *J* = 7.8 Hz, 4H), 6.73 (d, *J* = 7.8 Hz, 4H), 6.64 (d, *J* = 7.8 Hz, 4H), 6.57 (d, *J* = 7.8 Hz, 4H), 6.45 (s, 2H), 1.58 (s, 9H).

^{13}C NMR ($CDCl_3$, 125 MHz) δ 155.17, 137.86, 137.28, 137.20, 137.09, 136.77, 132.69, 131.44, 131.39, 131.06, 130.82, 129.17, 129.07, 128.90, 128.81, 128.65, 128.39, 127.75, 127.68, 125.97, 125.28 (q, *J* = 3.4 Hz, -CF_3), 124.97 (q, *J* = 3.0 Hz, -CF_3), 124.60 (q, *J* = 3.4 Hz, -CF_3), 124.50 (q, *J* = 3.3 Hz, -CF_3), 124.31 (q, *J* = 3.4 Hz, -CF_3), 123.76, 123.31, 122.95, 122.82, 122.70, 122.68, 122.55, 122.22, 121.97, 120.21, 120.11, 118.65, 118.13, 117.60, 116.72, 115.01, 113.29, 112.71, 35.39, 31.50.

^{19}F NMR ($CDCl_3$, 470.5 MHz) δ -65.73, -66.08, -66.12, -66.30, -66.30.

APCI-MS calcd. for $C_{106}H_{55}F_{30}N_5$: 1967.3978, Found: 1967.3994.

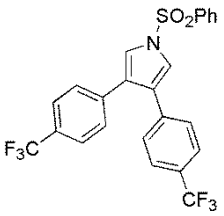
Anal. Calcd for $C_{106}H_{55}F_{30}N_5$: C, 64.67%; H, 2.82%; N, 3.56%. Found: C, 64.55%; H, 2.89%; N, 3.55%.

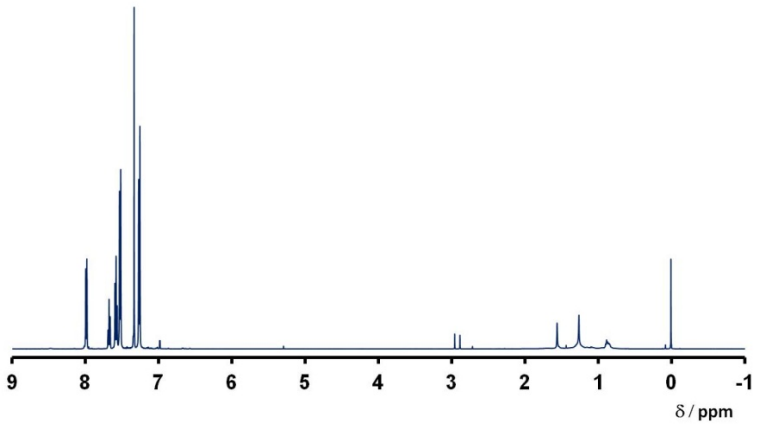
Melting Point: > 300 °C

S22. ^{1}H-, ^{13}C- and ^{19}F- NMR spectra

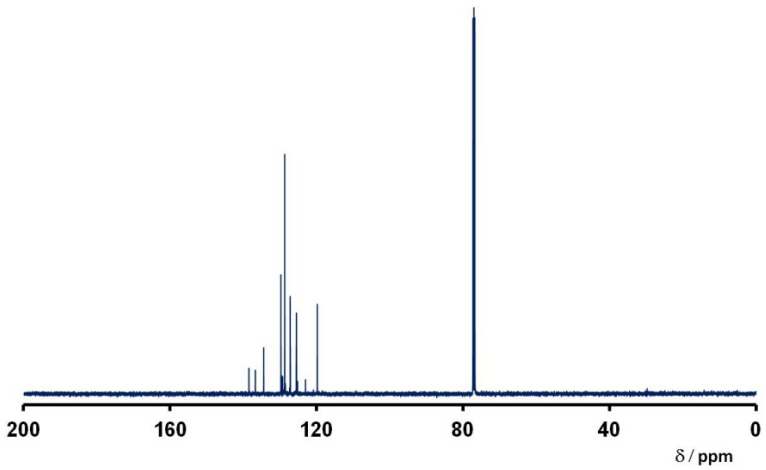
1. *N*-Benzenesulfonyl- 3,4-bis(4-trifluoromethylphenyl)pyrrole in $CDCl_3$

^{1}H-NMR

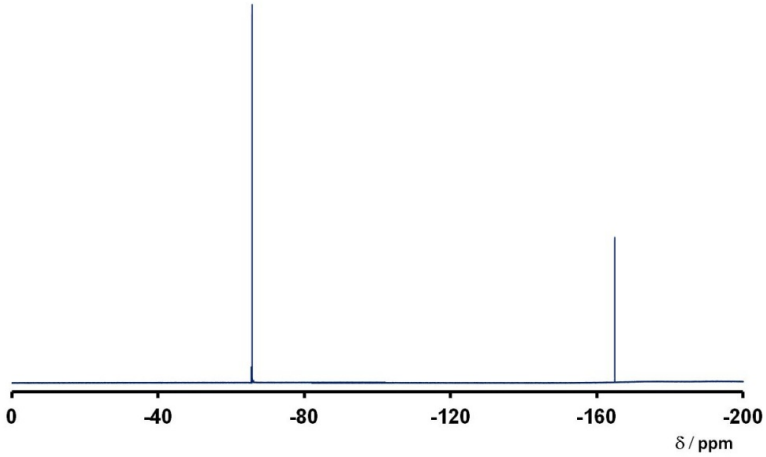




^{13}C-NMR

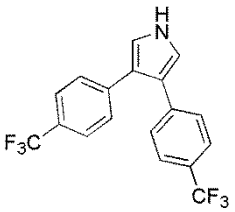


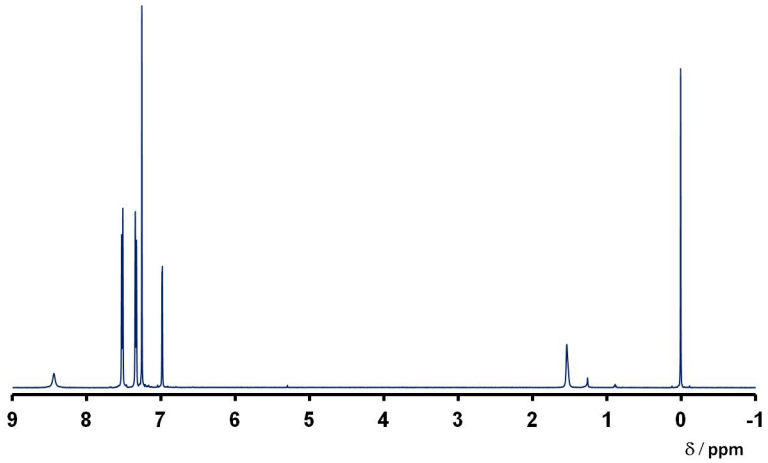
^{19}F-NMR



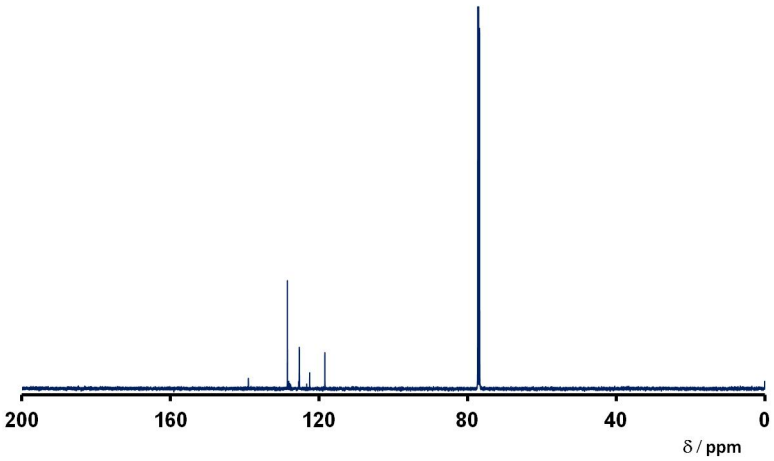
2. 3,4-Bis(4-trifluoromethylphenyl)-*1H*-pyrrole in $CDCl_3$

^{1}H-NMR

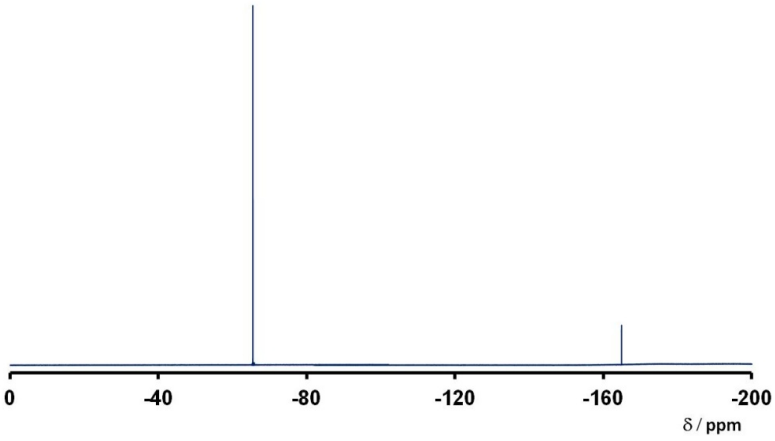




^{13}C-NMR

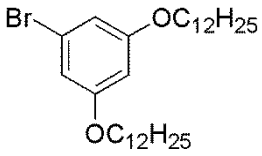


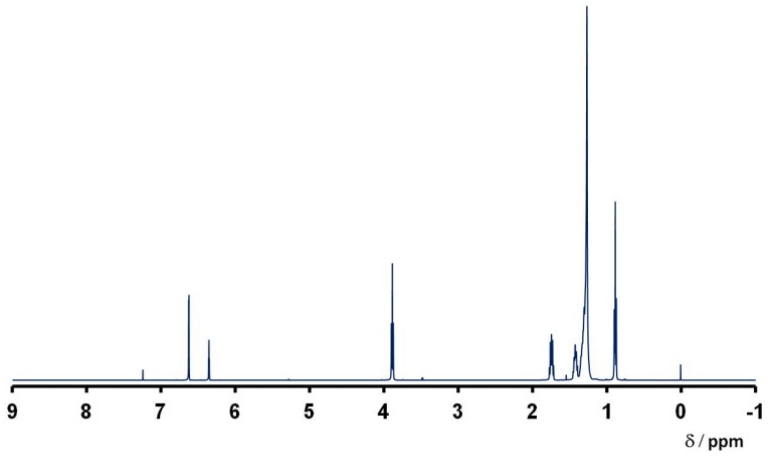
^{19}F-NMR



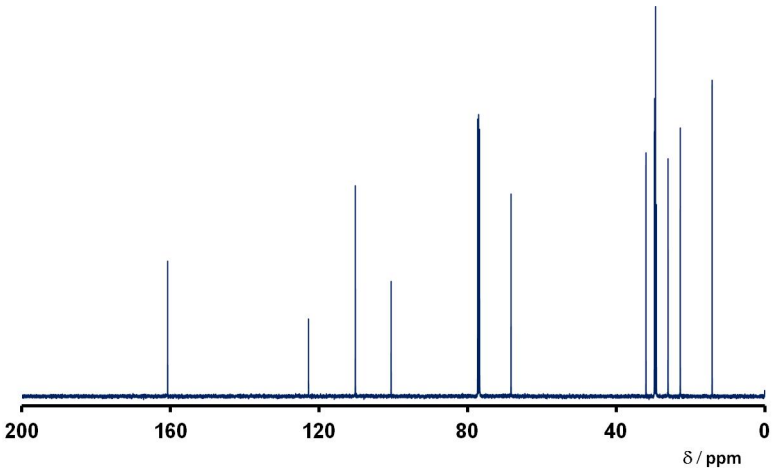
3. 3,5-Bisdodecyloxybromobenzene in $CDCl_3$

^{1}H-NMR



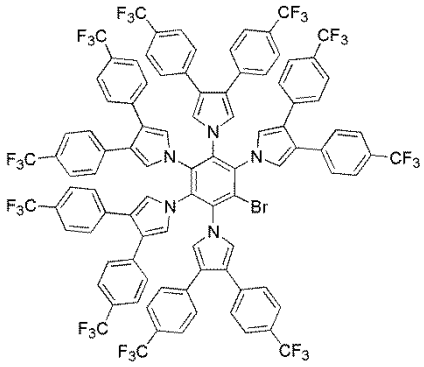


^{13}C-NMR

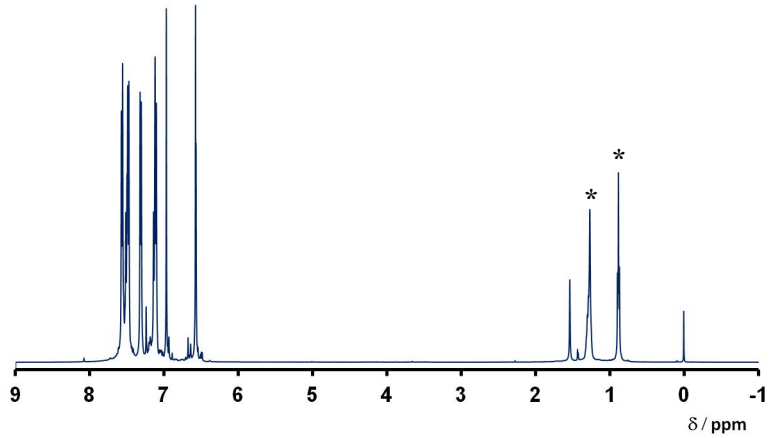


5. **6** in $CDCl_3$

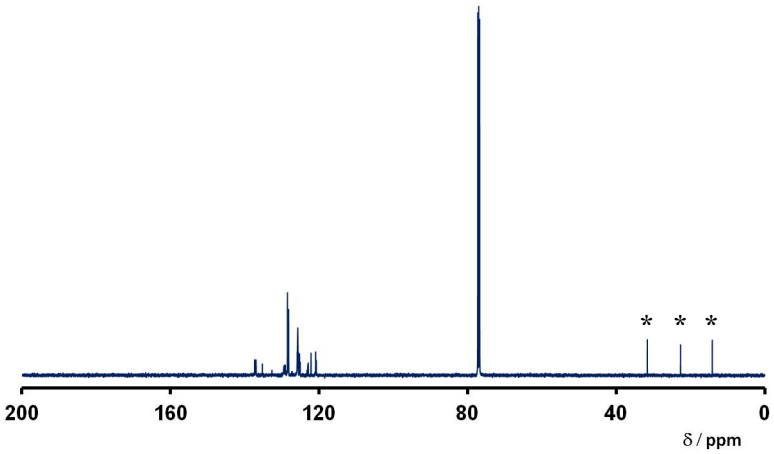
^{1}H-NMR



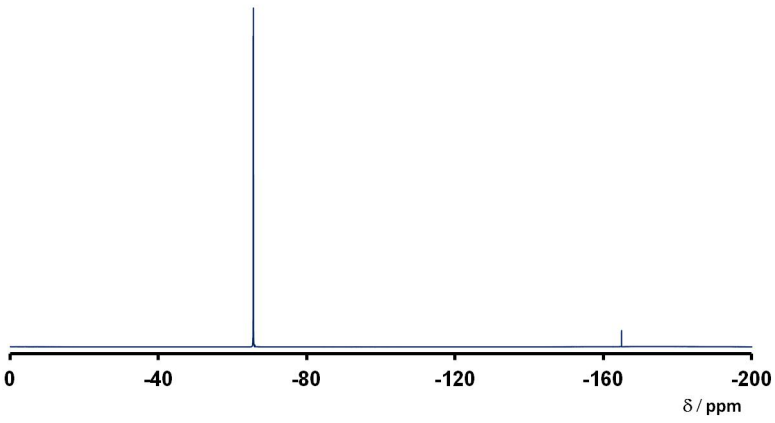
6



^{13}C-NMR

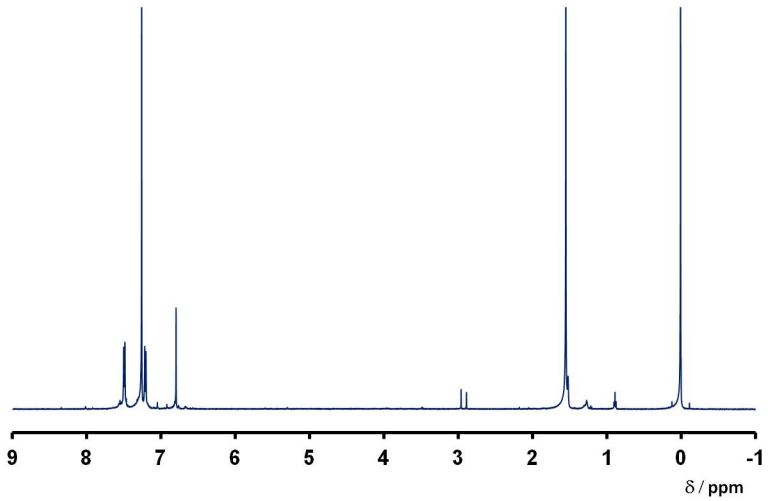


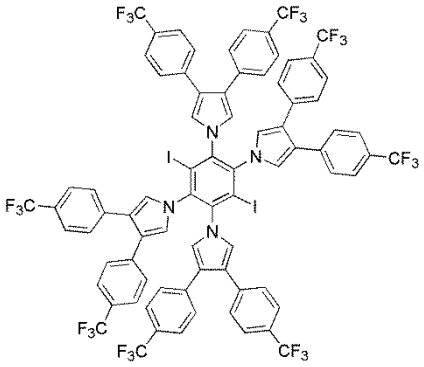
^{19}F-NMR



6. **7** in $CDCl_3$

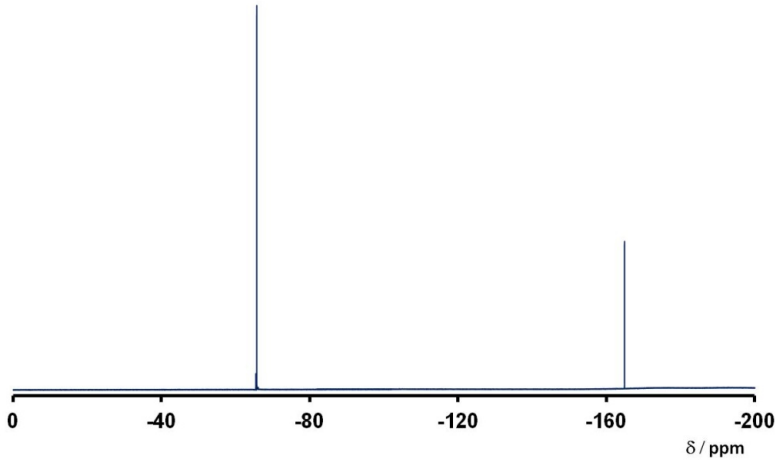
^{1}H-NMR





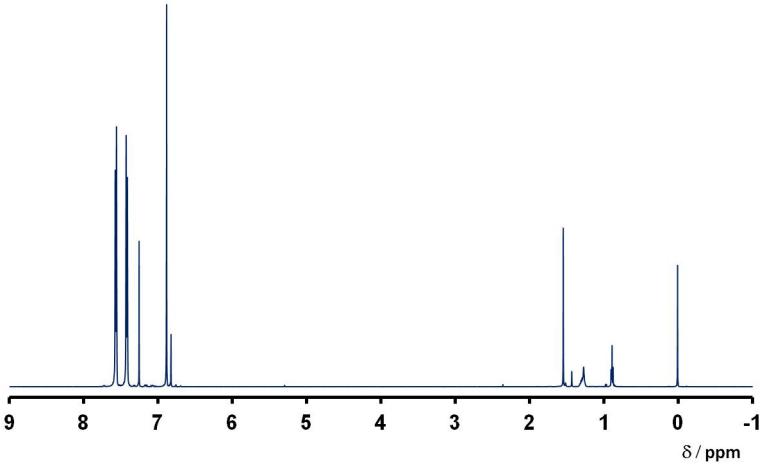
7

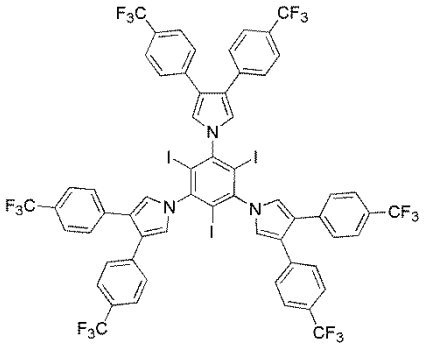
^{19}F-NMR



7. **8** in $CDCl_3$

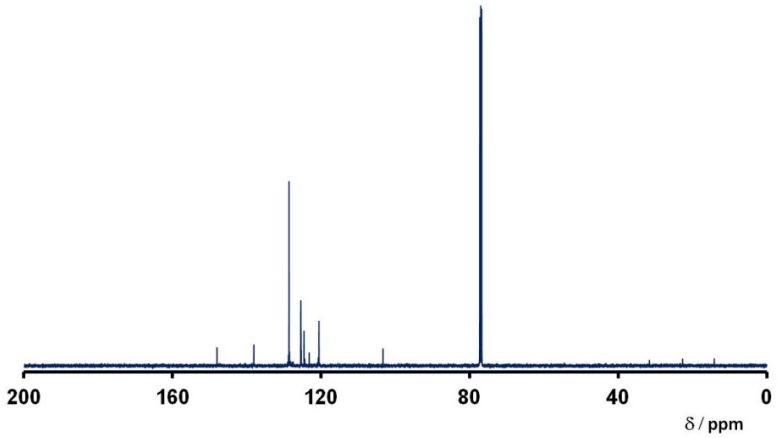
^{1}H-NMR



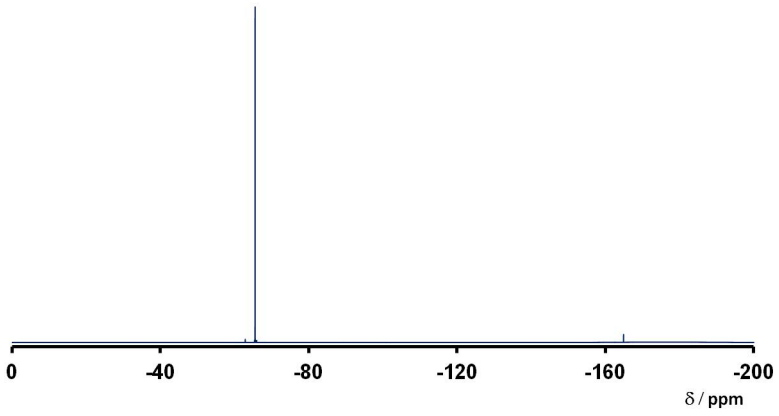


8

^{13}C-NMR

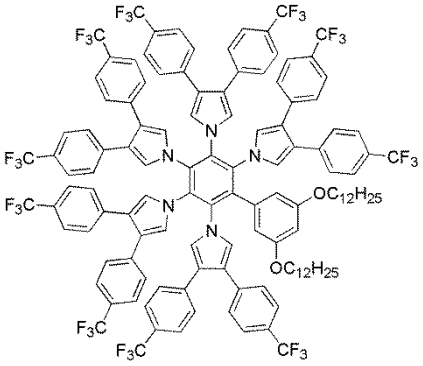


^{19}F-NMR

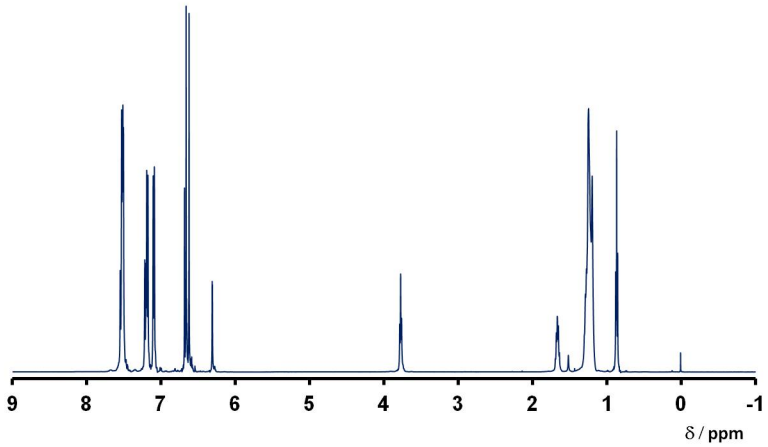


8. **9a** in $CDCl_3$

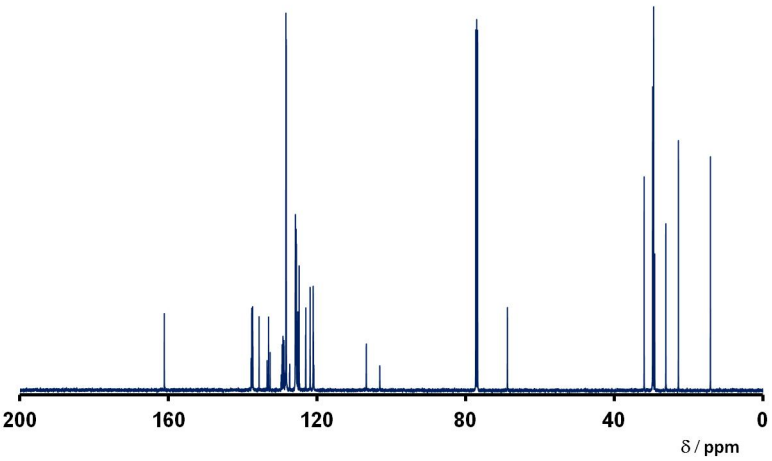
^{1}H-NMR



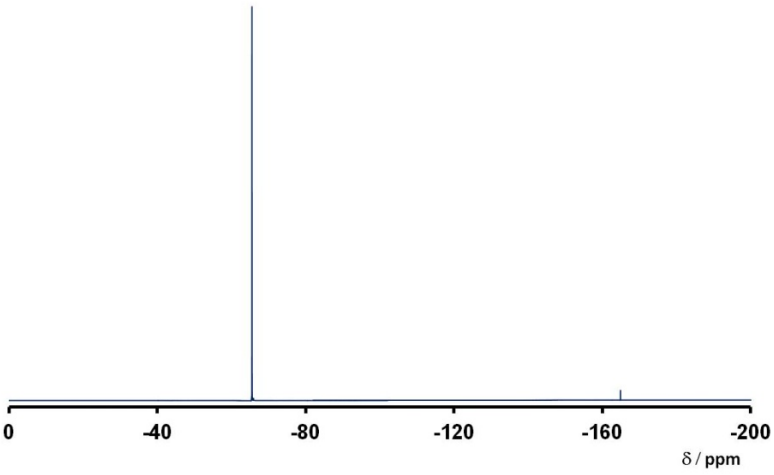
9a



^{13}C-NMR

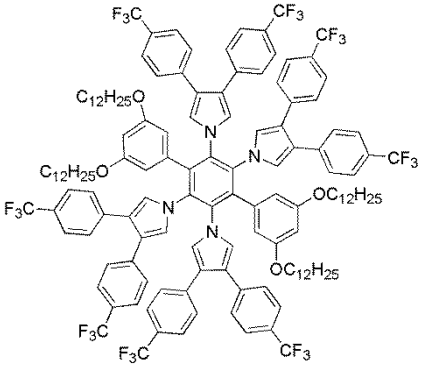


^{19}F-NMR

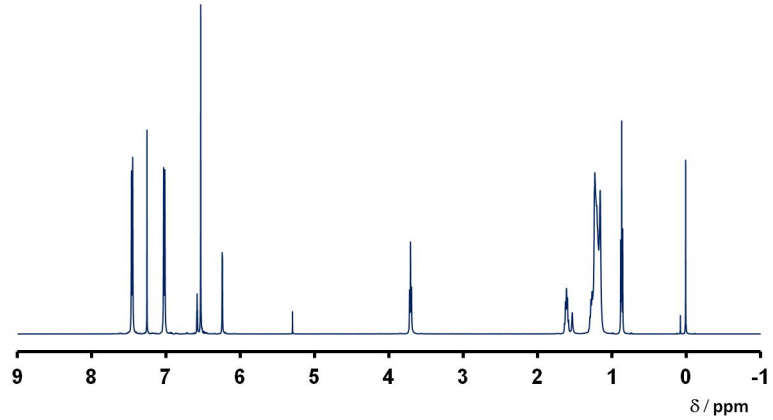


9. **11a** in $CDCl_3$

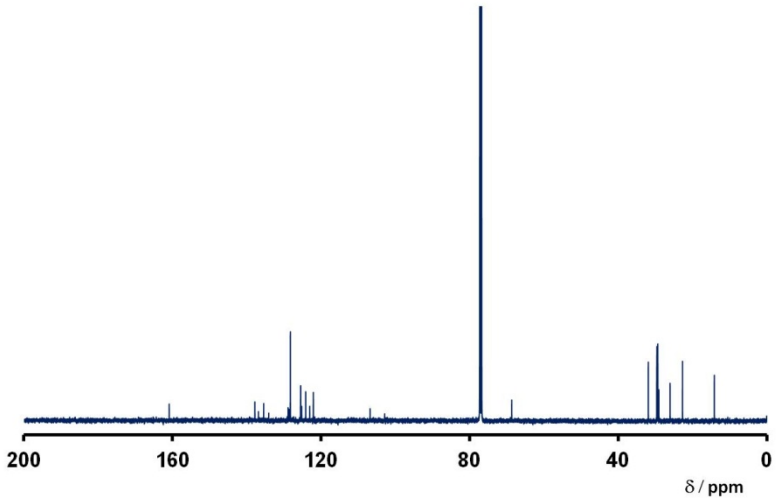
^{1}H-NMR



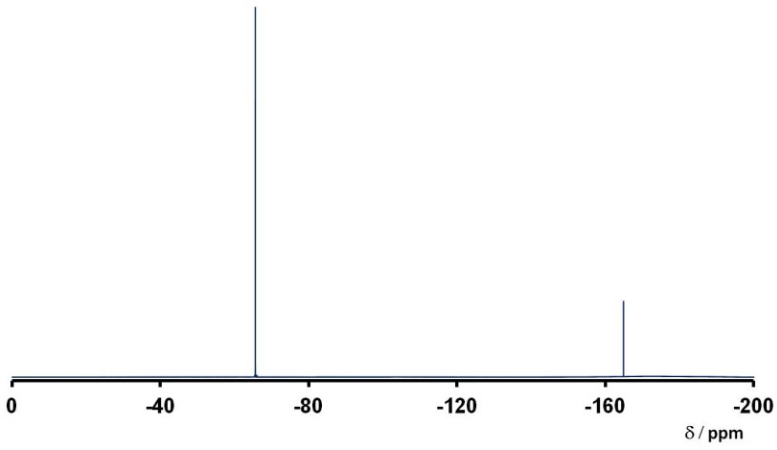
11a



^{13}C-NMR

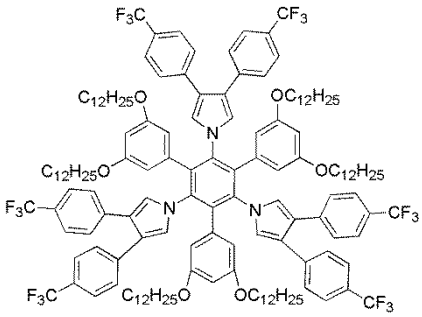


^{19}F-NMR

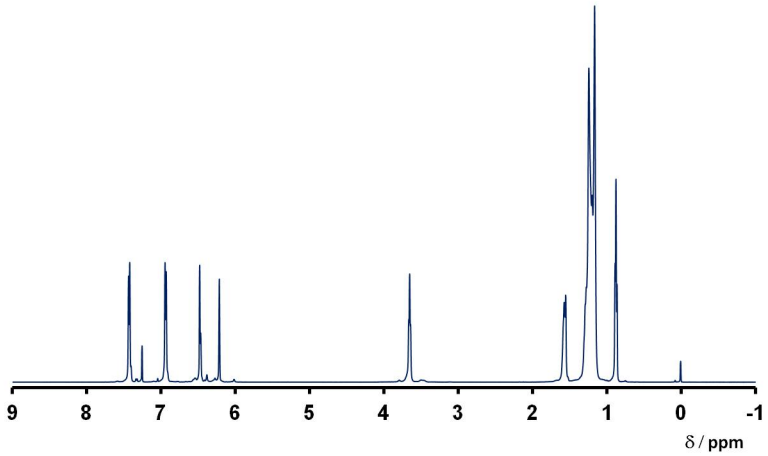


10. **12a** in $CDCl_3$

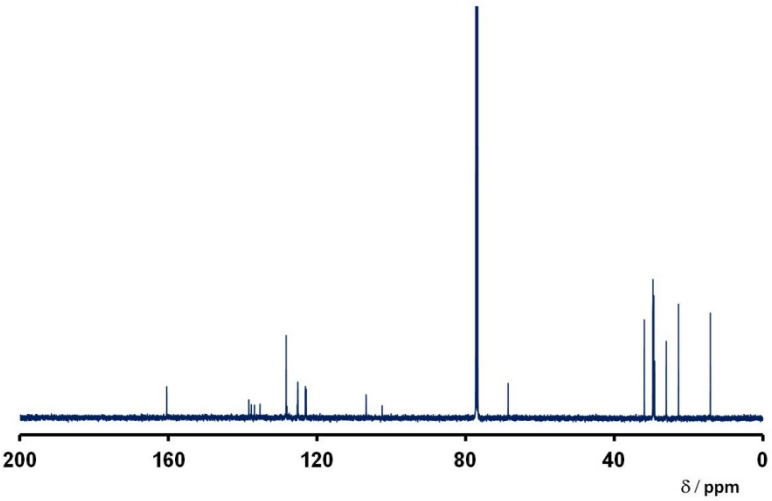
^{1}H-NMR



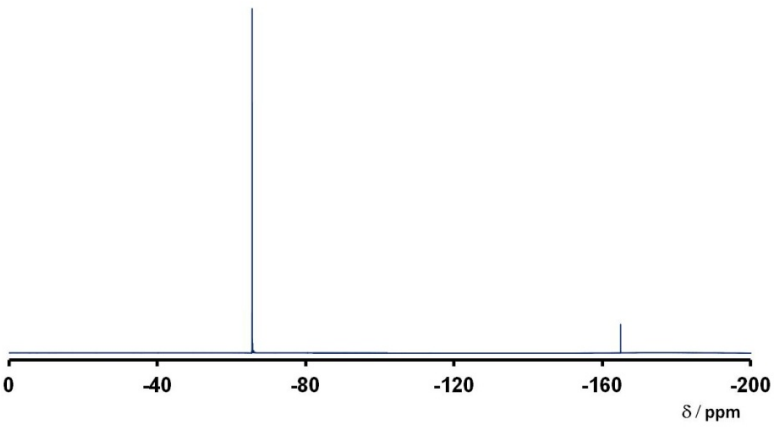
12a



^{13}C-NMR

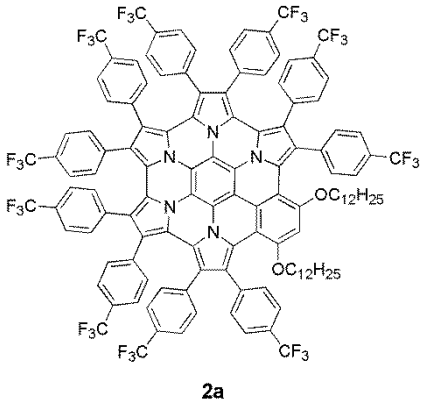


^{19}F-NMR

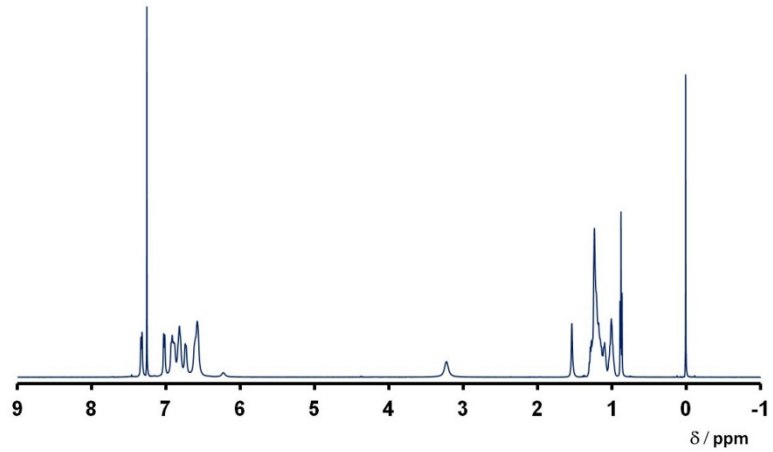


11. **2a** in $CDCl_3$

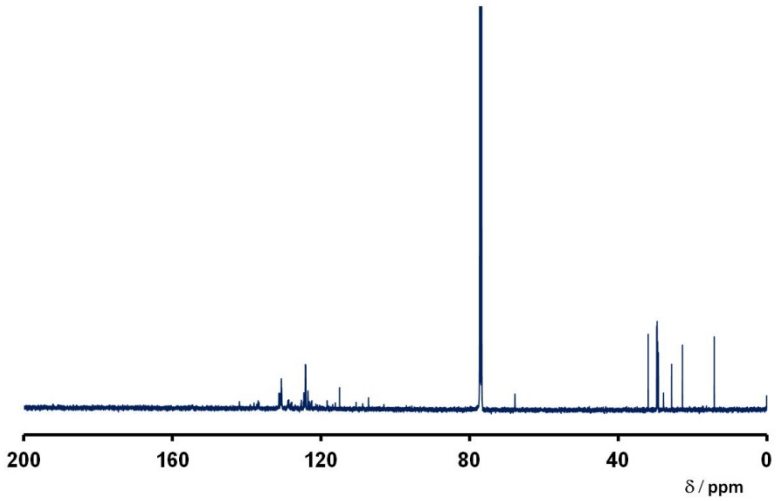
^{1}H-NMR



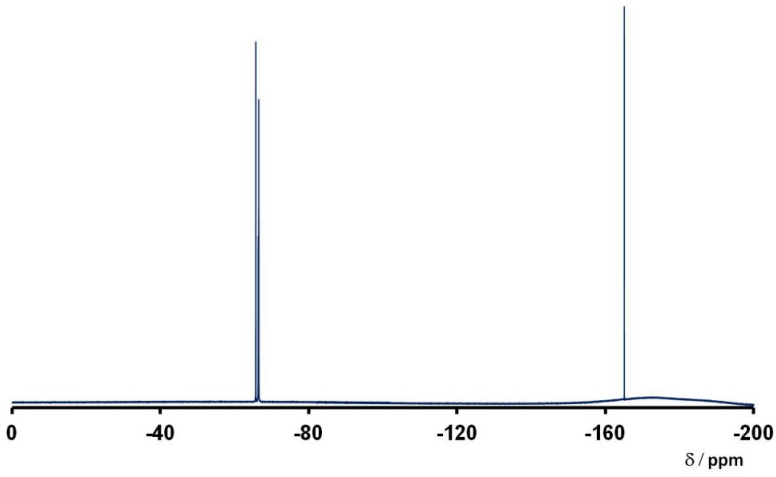
2a



^{13}C-NMR

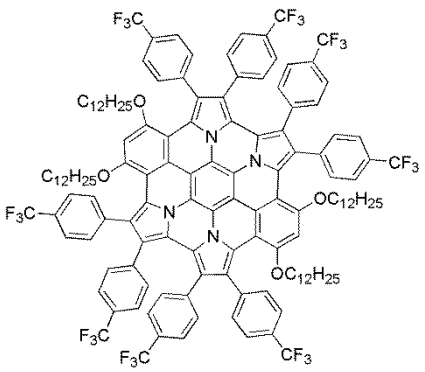


^{19}F-NMR

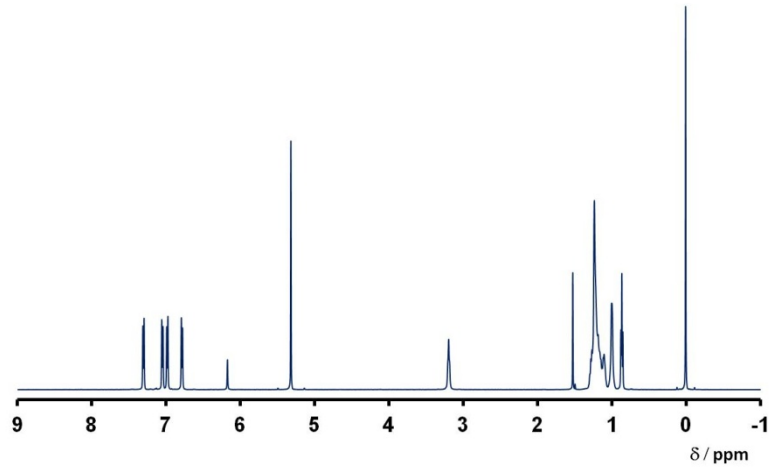


12. **3a** in CD_2Cl_2

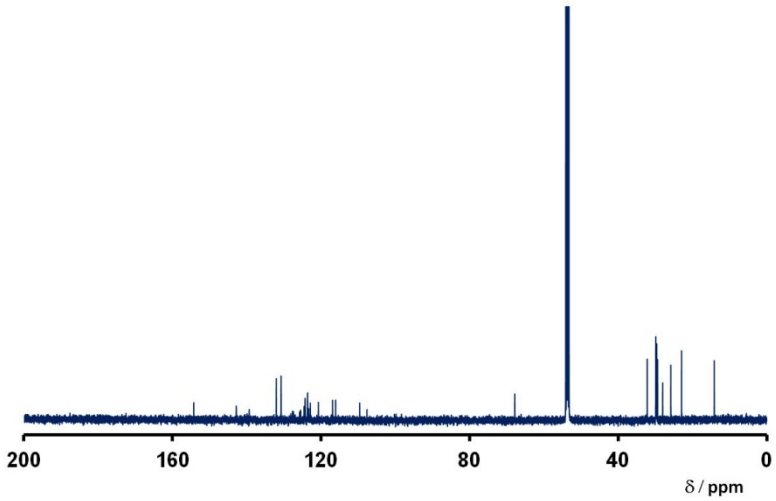
^{1}H-NMR



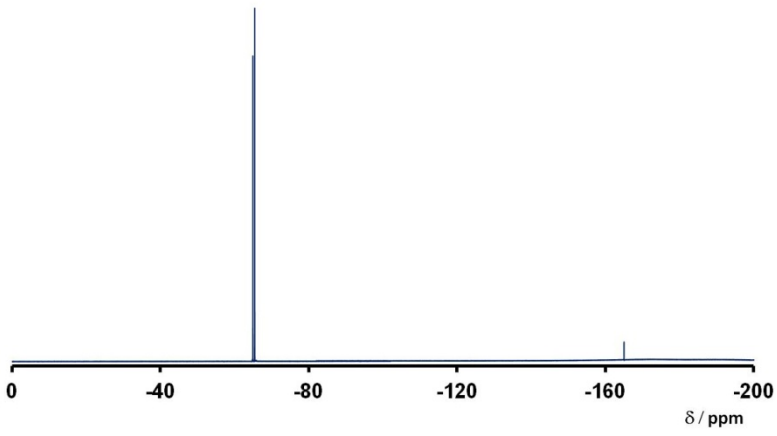
3a



^{13}C-NMR

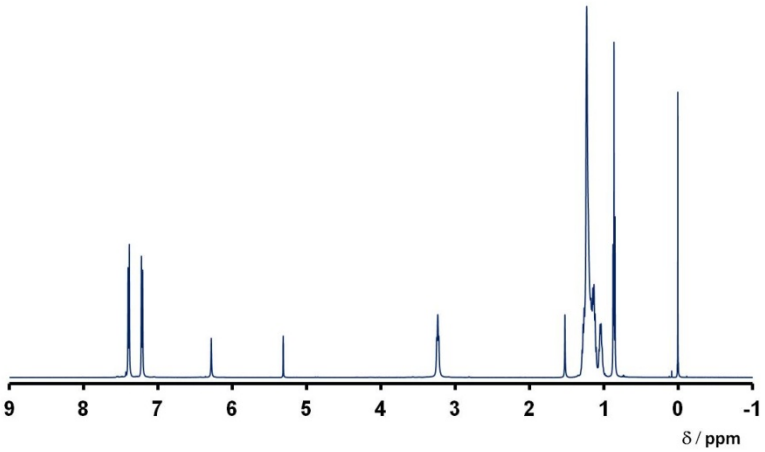


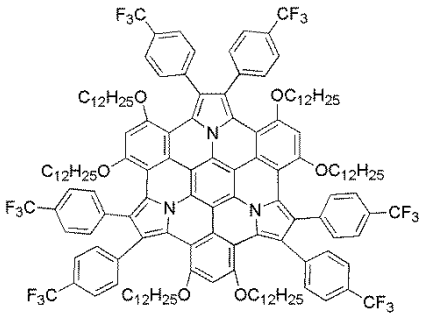
^{19}F-NMR



13. **4a** in CD_2Cl_2

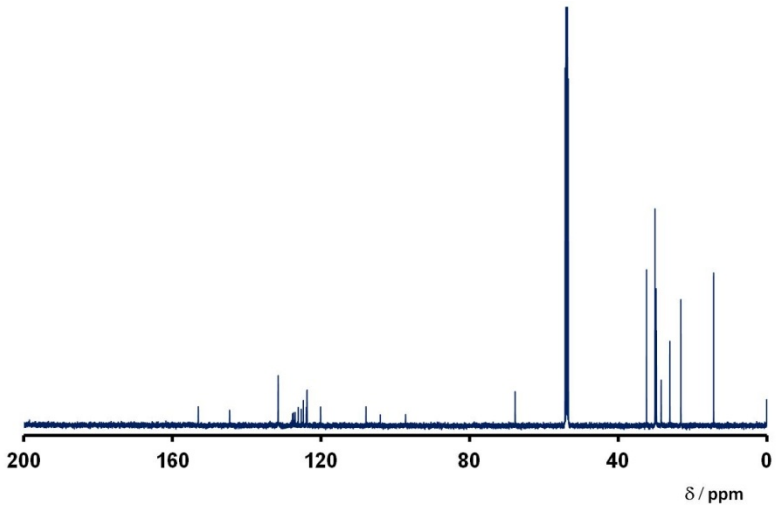
^{1}H-NMR



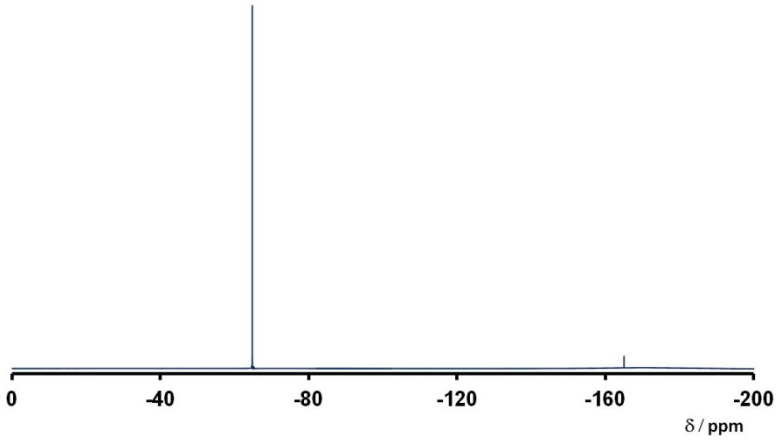


4a

^{13}C-NMR

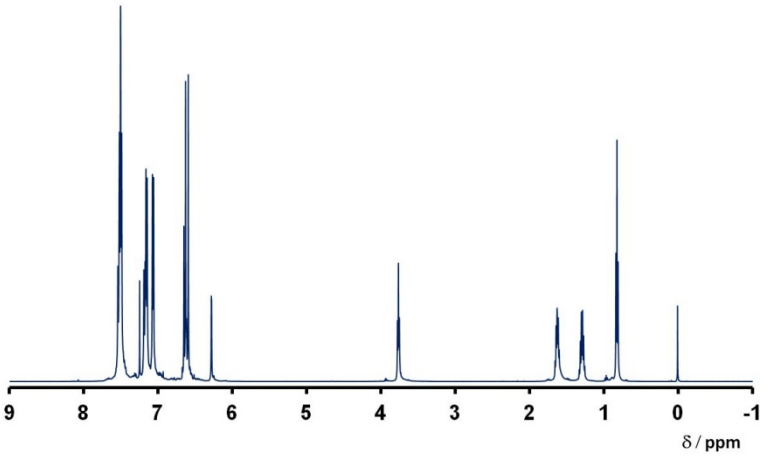


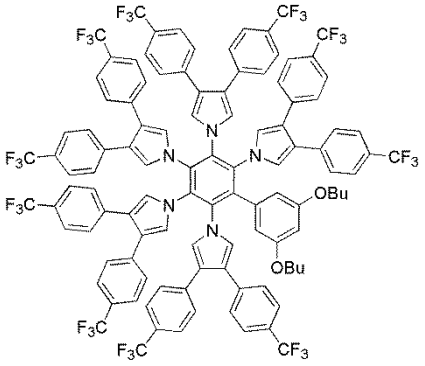
^{19}F-NMR



14. **9b** in $CDCl_3$

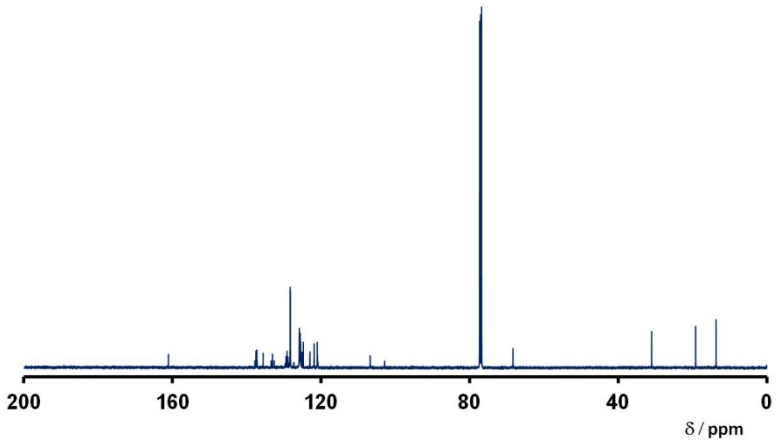
^{1}H-NMR



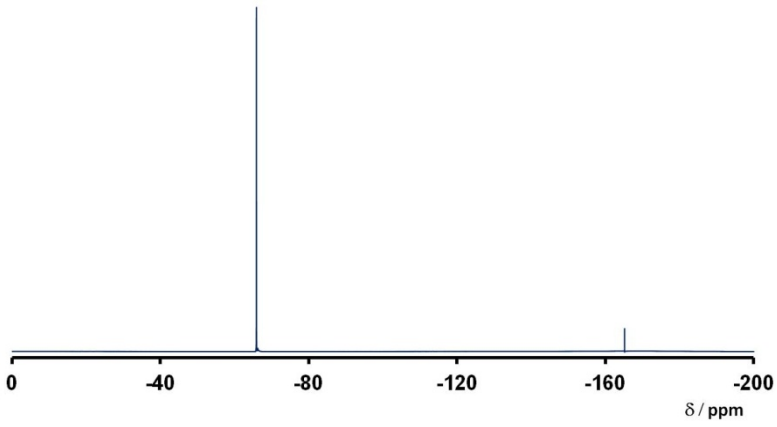


9b

^{13}C-NMR

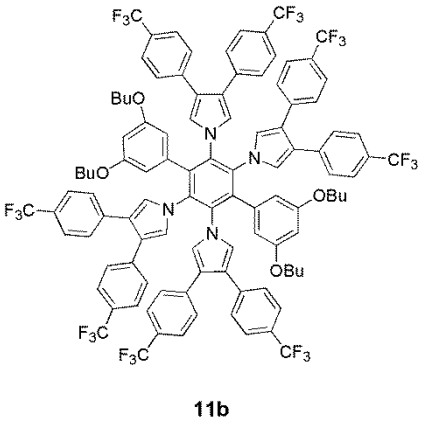


^{19}F-NMR

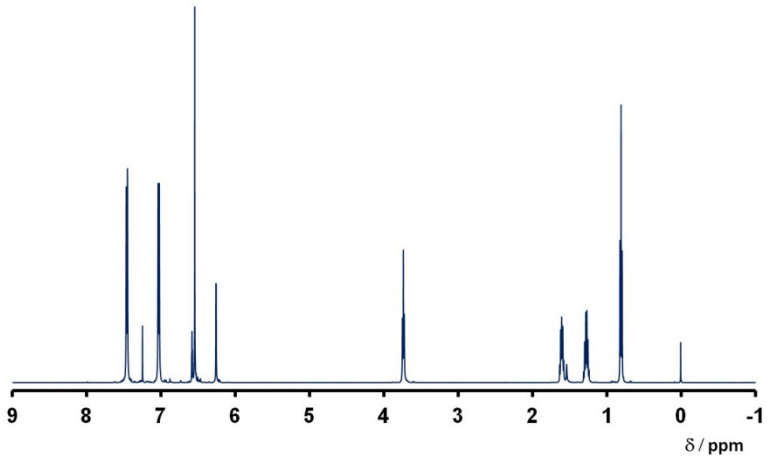


15. **11b** in $CDCl_3$

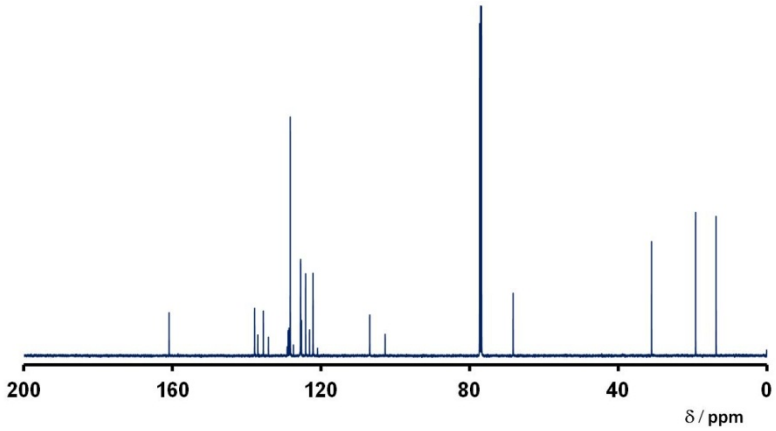
^{1}H-NMR



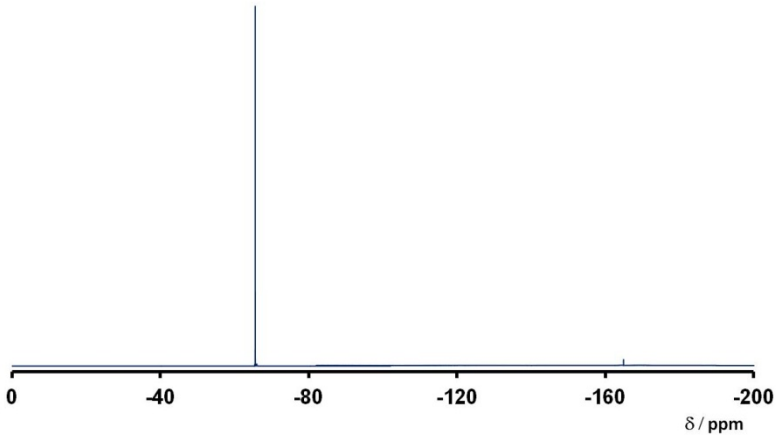
11b



^{13}C-NMR

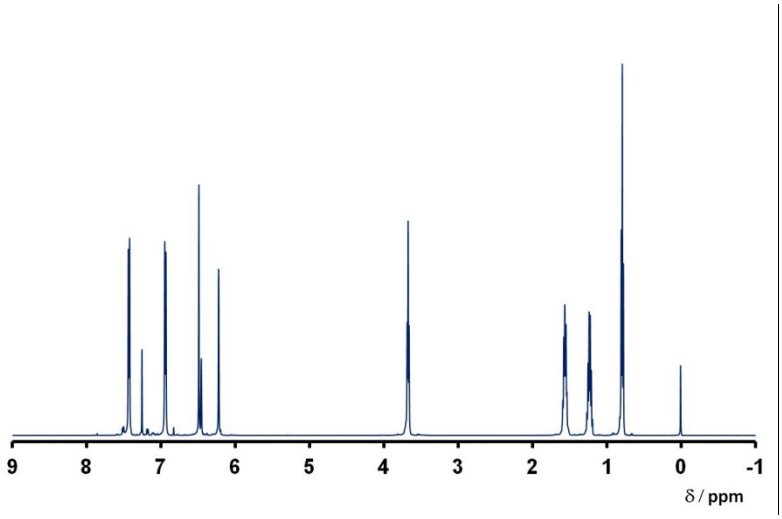


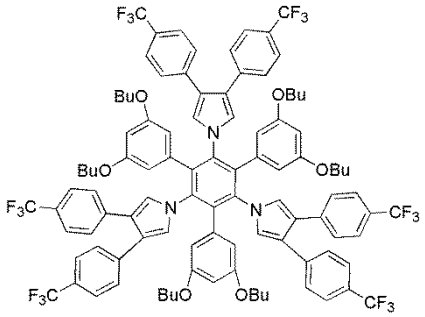
^{19}F-NMR



16. **12b** in $CDCl_3$

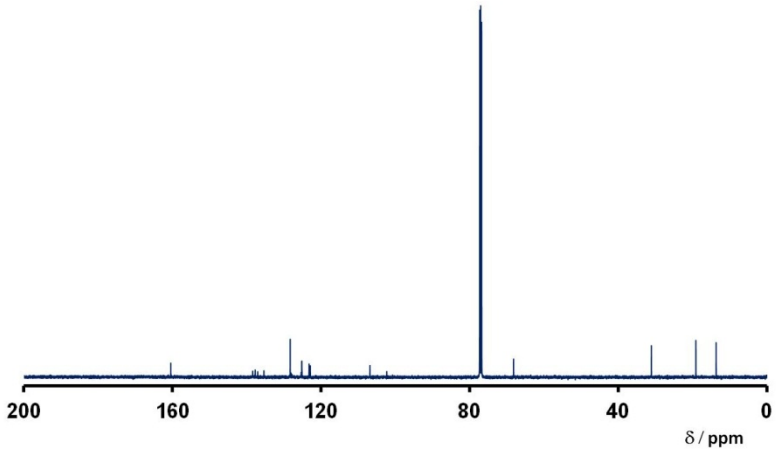
^{1}H-NMR



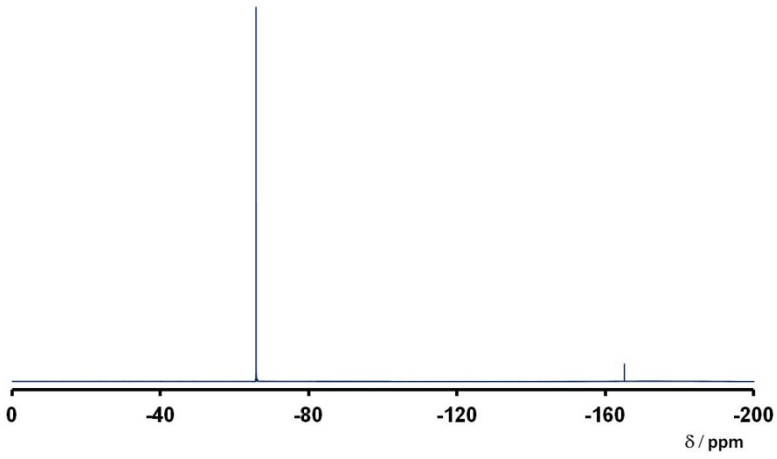


12b

^{13}C-NMR

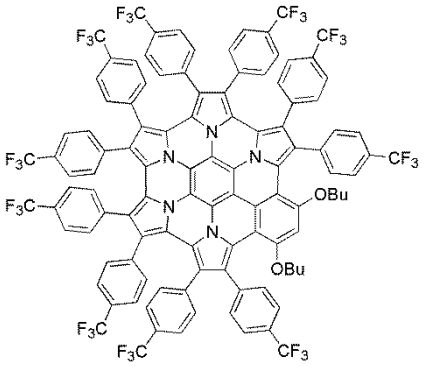


^{19}F-NMR

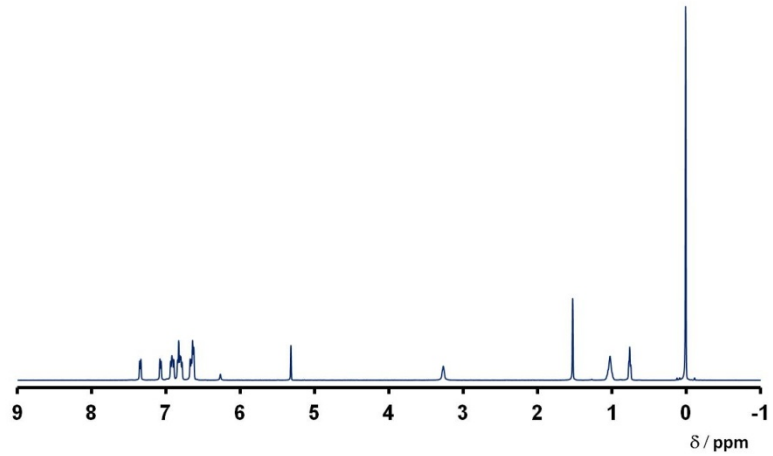


17. **2b** in CD_2Cl_2

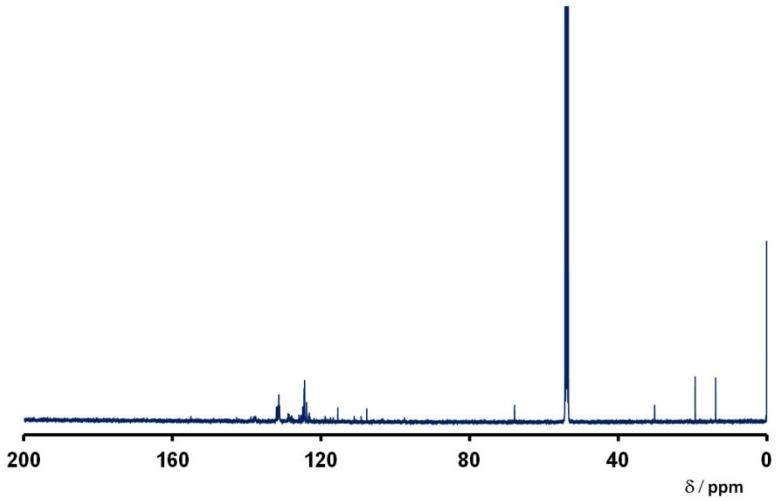
^{1}H-NMR



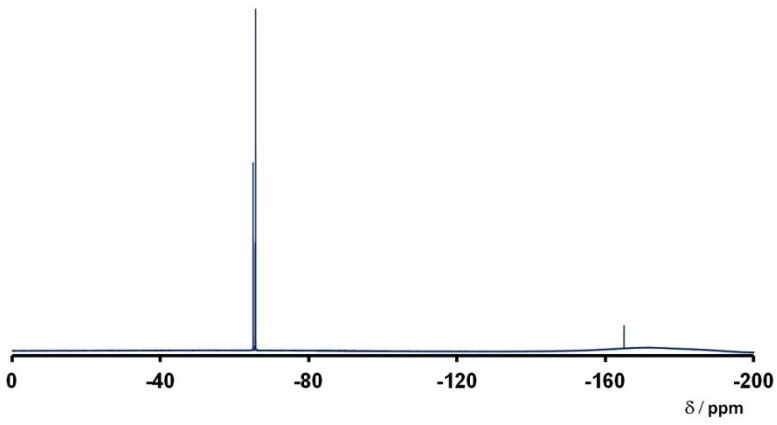
2b



^{13}C-NMR

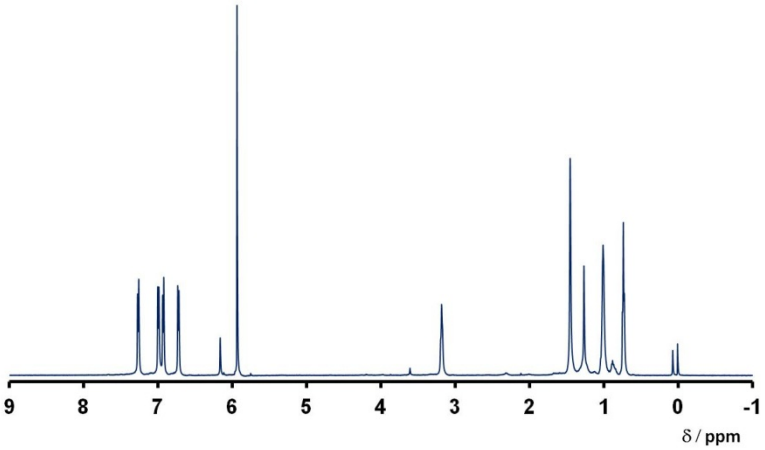


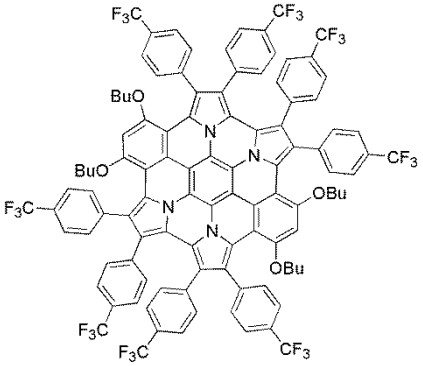
^{19}F-NMR



18. **3b** in CD_2Cl_2

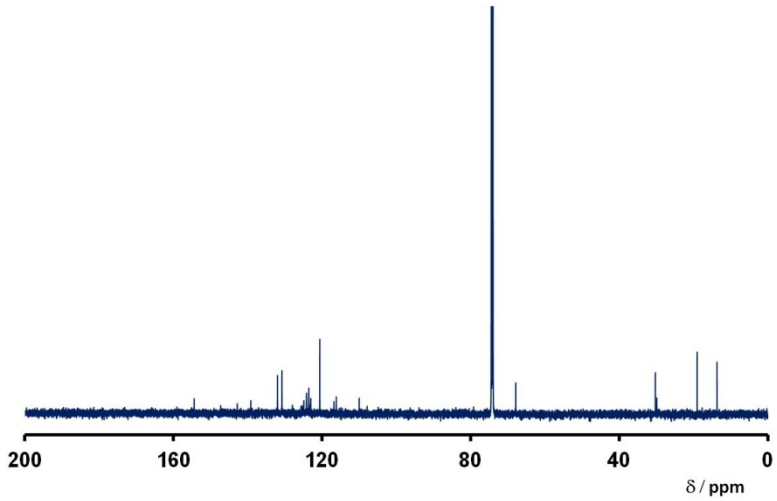
^{1}H-NMR



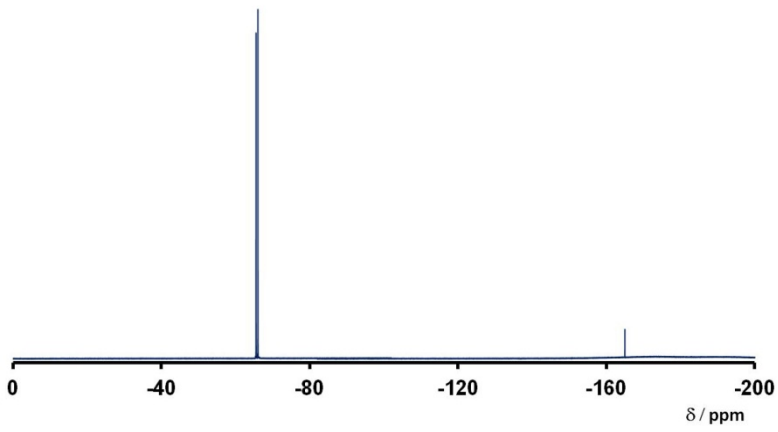


3b

^{13}C-NMR

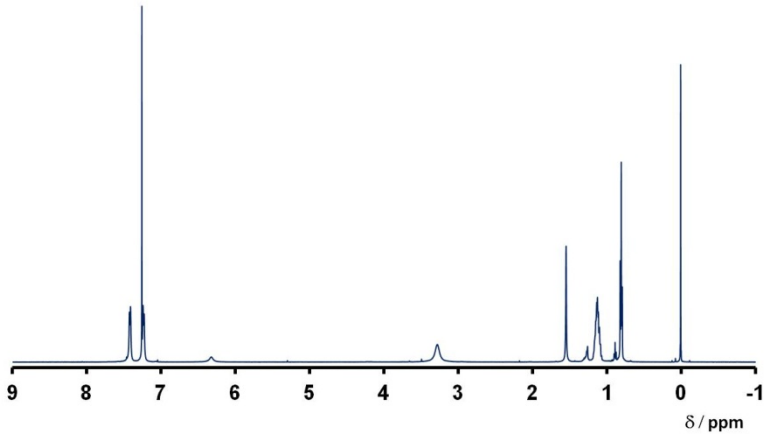


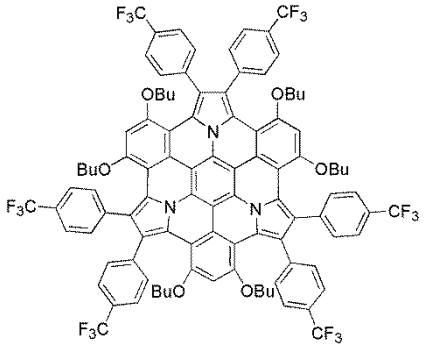
^{19}F-NMR



19. **4b** in CD_2Cl_2

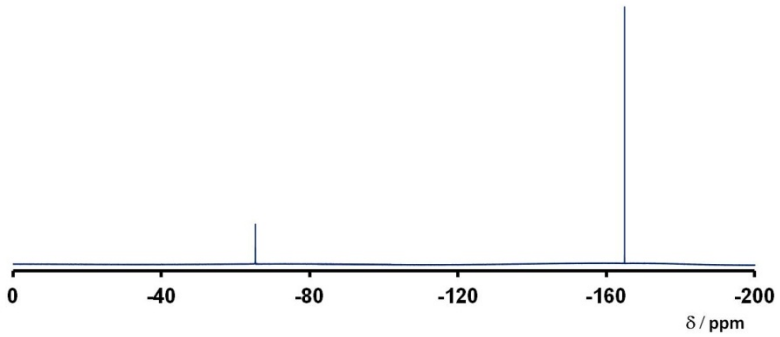
^{1}H-NMR





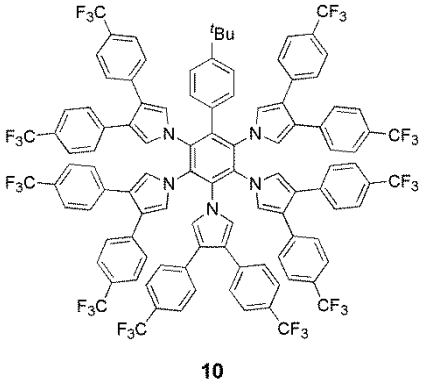
4b

^{19}F-NMR

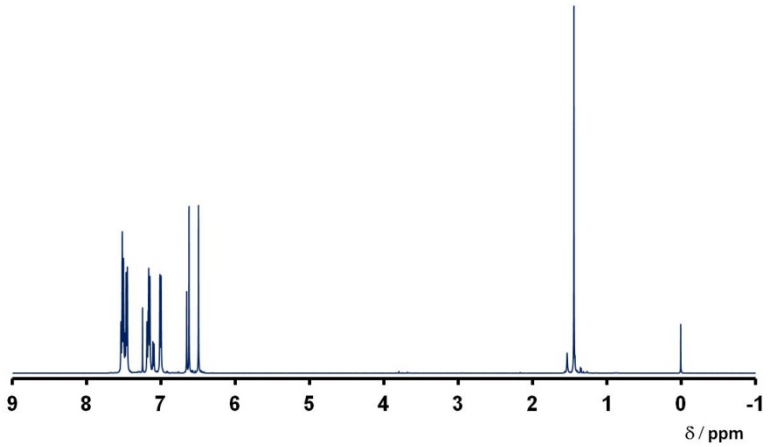


20. **10** in $CDCl_3$

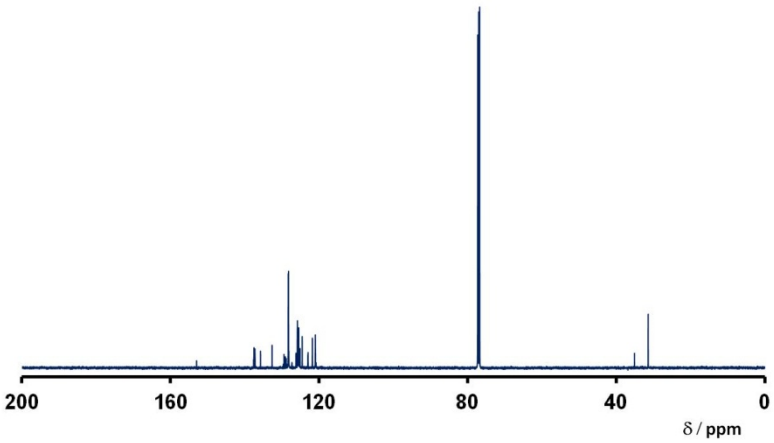
^{1}H-NMR



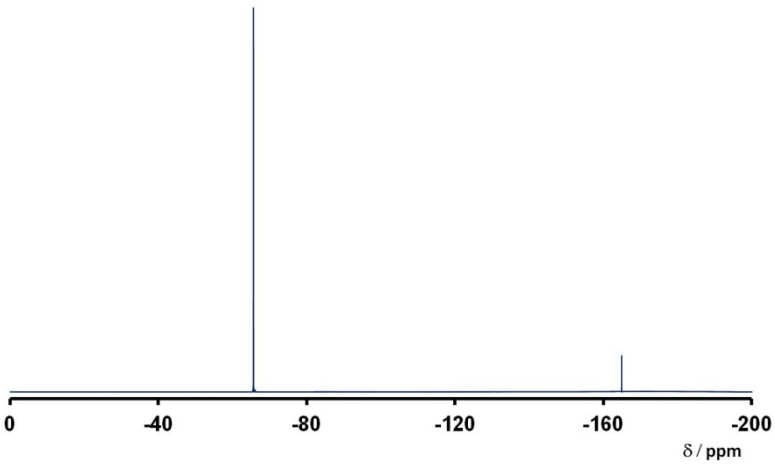
10



^{13}C-NMR

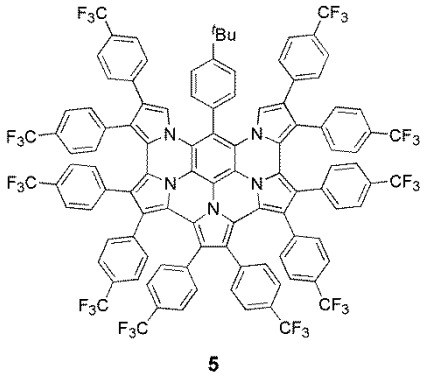


^{19}F-NMR

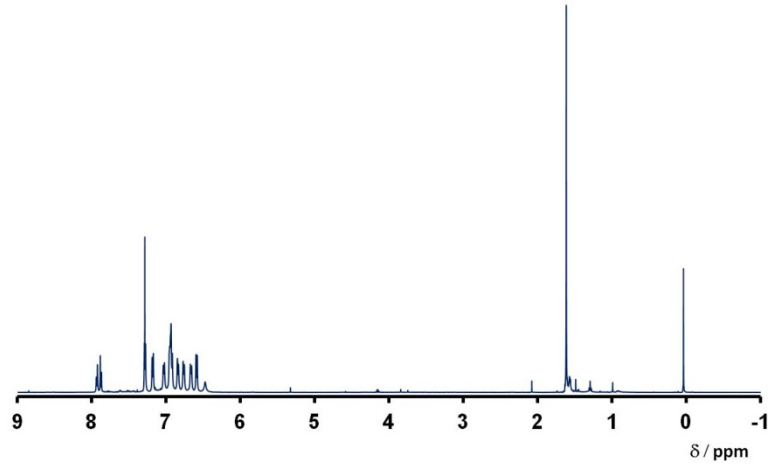


21. **5** in $CDCl_3$

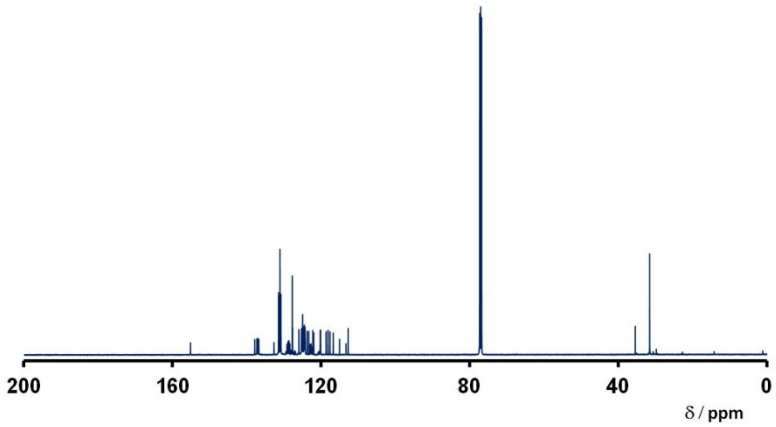
^{1}H-NMR



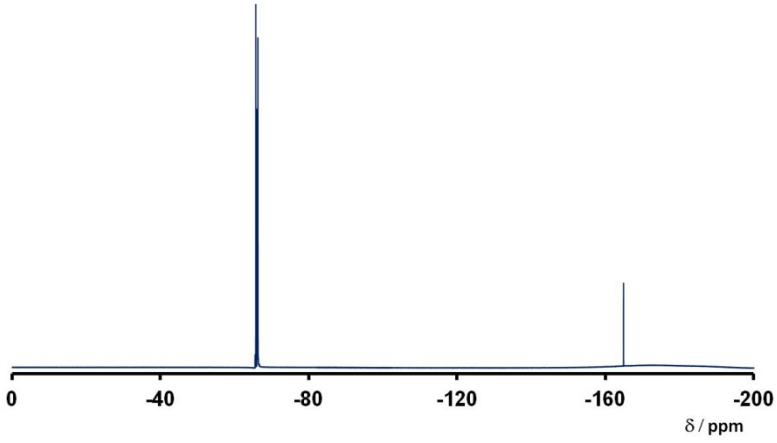
5



^{13}C-NMR



^{19}F-NMR



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