Supporting Information

Two-step synthesis of a red-emissive warped nanographene derivative via a ten-fold C–H borylation

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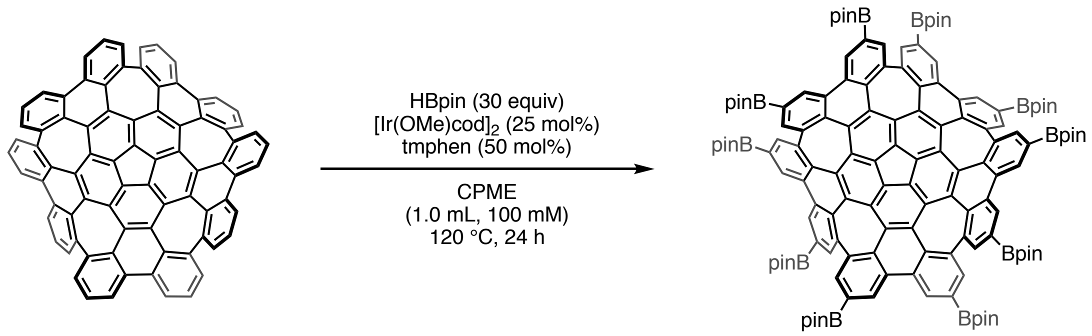
1. Experimental Section

General

Unless otherwise noted, all materials including dry solvent were obtained from commercial suppliers and used without further purification. All reactions were performed with dry solvents under an atmosphere of nitrogen in dried glassware with standard vacuum-line techniques. Work-up and purification procedures were carried out with reagent-grade solvents under air. Warped nanographene (**1**)[S1] was synthesized according to the reported procedure.

Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm). The developed chromatograms were analyzed by UV lamp (254 or 365 nm). Flash column chromatography was performed with KANTO Silica Gel 60N (spherical, neutral, 40-100 μm). The high-resolution mass spectra (HRMS) were obtained from a JEOL JMS-S3000 SpiralTOF (MALDI-TOF MS). Melting points were measured on a MPA100 Optimelt automated melting point system. Preparative recycling gel permeation chromatography (GPC) was performed with a SHIMADZU Prominence high performance liquid chromatograph instrument equipped with JAIGEL-2H-40/JAIGEL-2H-40 columns using chloroform as an eluent. Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL ECA600II spectrometer with UltraCool™ probe (^{1}H 600 MHz, ^{13}C 150 MHz) or a JEOL ECA600 (^{19}F 565 MHz). Chemical shifts for ^{1}H, ^{13}C, and ^{19}F NMR are expressed in parts per million (ppm) relative to C_2HDCl_4 (δ 5.98 ppm), $C_2D_2Cl_4$ (δ 73.79 ppm), and C_6F_6 (δ –163 ppm), respectively. Data are reported as follows: chemical shift, multiplicity (s = singlet, m = multiplet, br = broad) and integration.

Synthesis of 2



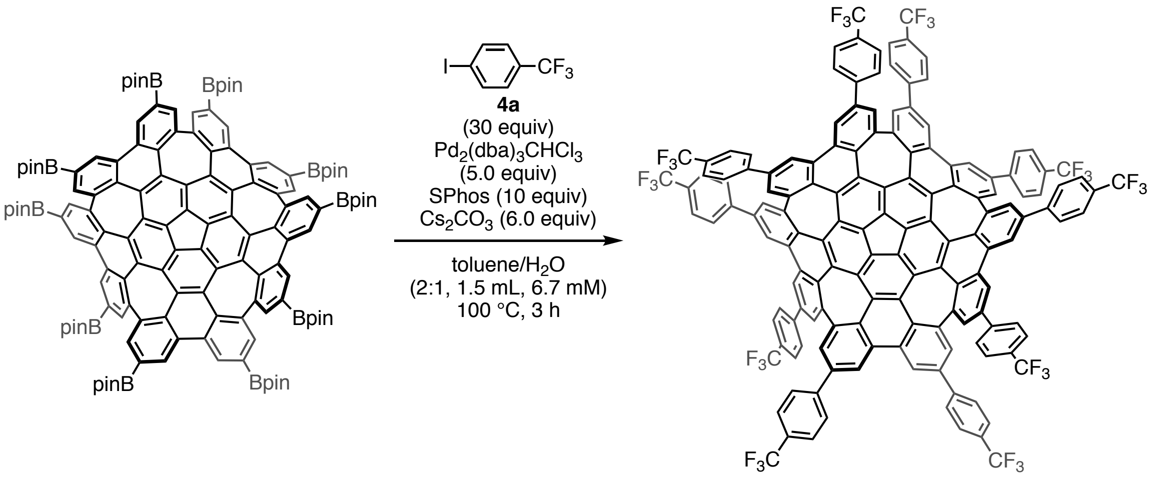
1
(99.1 mg, 100 μmol)

2
(170 mg, 75%)

To a 20 mL J-Young Schlenk equipped with a magnetic stirring bar were added a solution of **1** (99.1 mg, 100 μmol, 1.0 equiv) in dry cyclopentyl methyl ether (CPME; 1.0 mL), 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin; 384 mg, 3.00 mmol, 30 equiv), $[IrOMe(cod)]_2$ (16.6 mg, 25.0 μmol, 25 mol%), and 3,4,7,8-tetramethyl-1,10-phenanthroline (tmphen; 11.8 mg, 50.0 μmol, 50 mol%) under nitrogen atmosphere. The Schlenk was sealed with a J-Young screw tap and the resultant mixture was stirred at 120 °C for 24 h. After cooling the mixture to room temperature, the reaction mixture was diluted in chloroform and passed short-path silica gel chromatography with chloroform. The solution was removed under reduce pressure. The crude material was purified by GPC (eluent: chloroform) to afford **2** (170 mg, 75% yield) as an orange solid.

^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 140 °C) δ 9.08 (s, 10H), 7.85 (s, 10H), 1.46 (s, 120H); ^{13}C NMR (150 MHz, $C_2D_2Cl_4$, 140 °C) δ 138.2 (4°), 136.8 (CH), 136.0 (4°), 133.0 (4°), 130.8 (4°), 129.2 (CH), 126.9 (4°), 83.83 (4°), 24.74 (CH_3). HRMS (MALDI-TOF MS) *m/z* calcd for $C_{140}H_{140}B_{10}O_{20}$ $[M\cdot]^{+}$: 2251.0970, found: 2251.0963; mp: >300 ºC.

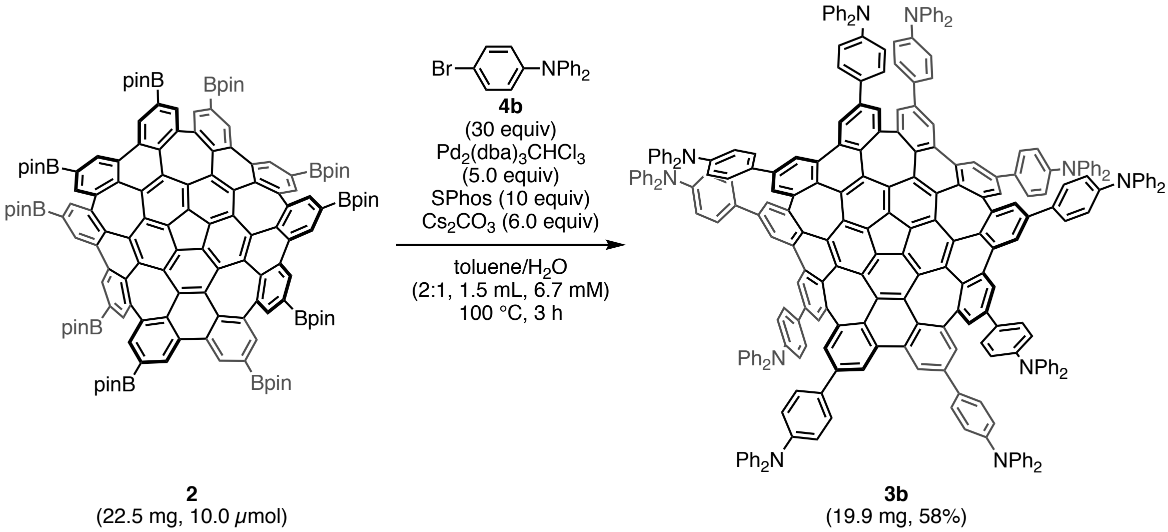
Synthesis of 3a



To a 3 mL screw-capped pressure vessel equipped with a magnetic stirring bar were added a solution of $Pd_2(dba)_3{\cdot}CHCl_3$ (51.8 mg, 50.0 µmol, 5.0 equiv), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (SPhos; 41.1 mg, 100 µmol, 5.0 equiv) in toluene (1.0 mL), **2** (22.5 mg, 10.0 µmol, 1.0 equiv), 1-iodo-4-(trifluoromethyl)benzene (**4a**; 68.7 mg, 300 µmol, 30 equiv), and a solution of Cs_2CO_3 (19.6 mg, 60.0 µmol, 6.0 equiv) in H_2O (0.50 mL) under nitrogen atmosphere. The vessel was sealed with a PTFE-coated screw cap and the resultant mixture was stirred at 100 °C for 3 h under nitrogen atmosphere. After cooling the mixture to room temperature, the reaction mixture was extracted with chloroform. The combined organic layer was dried over $MgSO_4$, and the solvent was removed under reduce pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane/EtOAc = 6:1) and GPC (eluent: chloroform) to afford **3a** (12.0 mg, 60%) as a reddish orange solid.

^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 140 °C) δ 7.80–8.00 (br m, 50H), 8.91 (br s, 10H); ^{13}C NMR (150 MHz, $C_2D_2Cl_4$, 85 °C) δ 125.9 (CH), 127.6 (CH); ^{19}F NMR (565 MHz, $C_2D_2Cl_4$, 140 °C) δ –63.7 (s, 30F); HRMS (MALDI-TOF MS) *m/z* calcd for $C_{150}H_{60}F_{30}$ $[M{\cdot}]^+$: 2430.4216, found: 2430.4290; mp: >300 ºC.

Synthesis of 3b



To a 3 mL screw-capped pressure vessel equipped with a magnetic stirring bar were added a solution of $Pd_2(dba)_3 \cdot CHCl_3$ (51.8 mg, 50.0 μmol, 5.0 equiv), SPhos (41.1 mg, 100 μmol, 5.0 equiv) in toluene (1.0 mL), **2** (22.5 mg, 10.0 μmol, 1.0 equiv), 4-bromo-*N*,*N*-diphenylaniline (**4b**; 92.3 mg, 300 μmol, 30 equiv), and a solution of Cs_2CO_3 (19.6 mg, 60.0 μmol, 6.0 equiv) in H_2O (0.50 mL) under nitrogen atmosphere. The vessel was sealed with a PTFE-coated screw cap and the resultant mixture was stirred at 100 °C for 3 h under nitrogen. After cooling the mixture to room temperature, the reaction mixture was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$, and the solvent was removed under reduce pressure. The crude material was purified by silica-gel column chromatography (eluent: hexane/EtOAc = 6:1 and chloroform) and GPC (eluent: chloroform) to afford **3b** (19.9 mg, 58%) as a red solid.

^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 140 °C) δ 7.08–7.30 (br m, 120H), 7.76–7.85 (br m, 30H), 8.87 (br s, 10H); ^{13}C NMR (150 MHz, $C_2D_2Cl_4$, 85 °C) δ 123.1 (CH), 123.4 (CH), 124.6 (CH), 129.2 (CH), 145.1 (CH), 147.4 (CH); HRMS (MALDI-TOF MS) *m/z* calcd for $C_{260}H_{160}N_{10}$ $[M\cdot]^+$: 3423.2895, found: 3423.2880; mp: >300 ºC.

2. X-ray Crystallography

Details of the crystal data and a summary of the intensity data collection parameters for **2** are listed in Table S1. A suitable crystal was mounted with mineral oil on a MiTeGen MicroMeshes and transferred to the goniometer of a Rigaku PILATUS diffractometer. Graphite-monochromated Mo Kα radiation was used. The structures were solved by direct methods with (SIR-97)[S2] and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/7)[S3] by using Yadokari-XG software package.[S4] The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions. CCDC 1893066 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. Alert A (VERY LARGE Solvent Accessible VOID(S) in Structure) is caused by the disorder of solvent molecules. Suitable solvent molecules could not be placed because of the lack of observed electron density.

Table S1. Crystallographic data and structure refinement details of **2**

	2·1.5C_4H_8O
formula	$C_{146}H_{155}B_{10}O_{21.5}$
fw	2361.79
T (K)	123(2)
λ (Å)	0.71073
cryst syst	Triclinic
space group	P-1
a (Å)	17.1883(7)
b (Å)	19.8237(8)
c (Å)	25.0041(10)
α (deg)	112.264(4)
β (deg)	93.732(3)
γ (deg)	109.808(4)
V (Å^3)	7232.6(6)
Z	2
D_{calc} (g·cm^{-3})	1.084
μ (mm^{-1})	0.070
F(000)	2506
cryst size (mm)	0.10 × 0.10 × 0.10
θ range (deg)	1.790–25.000
reflns collected	105367
indep reflns/R_{int}	25435/ 0.2479
params	1653
GOF on F^2	1.064
R_1, wR_2 [I>2σ(I)]	0.1266, 0.3072
R_1, wR_2 (all data)	0.3042, 0.4142

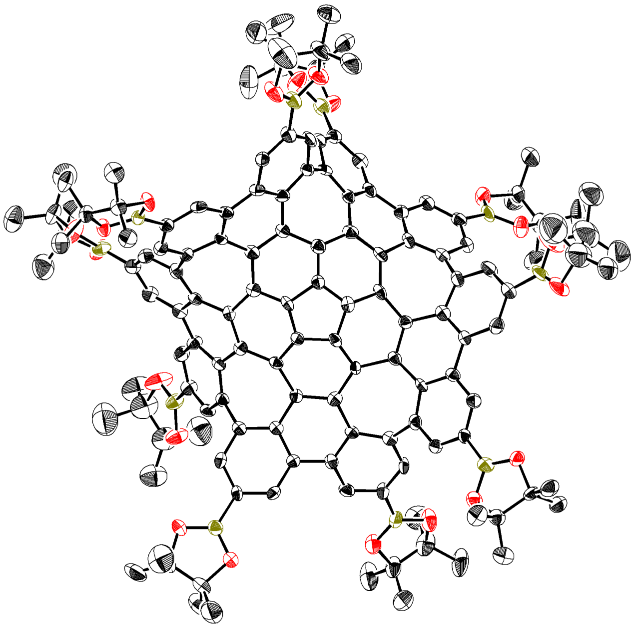


Figure S1. ORTEP drawing of **2** with 50% probability. All hydrogen atoms and solvent molecules (Et_2O) are omitted for clarity.

3. Photophysical measurement

UV–Vis absorption spectra were recorded on a Shimadzu UV-3510 spectrometer with a resolution of 0.5 nm. Emission spectra were measured on Shimadzu RF-6000 spectrometer with a resolution of 0.4 nm. Absolute fluorescence quantum yields (Φ_F) were determined on a Shimadzu RF-6000 using a calibrated integrating sphere system upon excitation at 340 nm. For FL lifetime measurements, Hamamatsu Photonics Quantaurus-Tau® fluorescence lifetime spectrometer C11367-21 with LED as a light source was used.

Table S2. The fluorescence quantum yield (Φ_F), lifetime (τ), radiative (k_r) and nonradiative (k_{nr}) decay rate constants of **1**, **2**, **3a**, and **3b**.

	Φ_F	τ (ns)	k_r (s^{-1})[a]	k_{nr} (s^{-1})[a]
1	0.26	6.86	3.8×10^7	1.1×10^8
2	0.20	6.34	3.2×10^7	1.3×10^8
3a	0.28	6.33	4.4×10^7	1.1×10^8
3b	0.47	6.61	7.1×10^7	8.0×10^7

[a] $\Phi_F = k_r \times \tau$, $k_r + k_{nr} = \tau^{-1}$

4. Computational Study

The Gaussian16 program[S5] running on a SGI Altix4700 system was used for optimization (B3LYP/6-31G(d)).[S6] Structures were optimized without any symmetry assumptions. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculation at the same level was performed to verify all stationary points as local minima (with no imaginary frequency). Visualization of the results was performed by use of GaussView 5.0.9 software.

Table S3. TD-DFT vertical one-electron excitations of **2**.

Excitation [nm]	Oscillator strength (*f*)	Description
506	0.131	H→L, H–1→L+1
492	0.004	H–2, H–1→L
		H→L+1
479	0.005	H–3, H–2, H–1→L
467	0.048	H–3, H–1, H→L
		H→L

H: HOMO, L: LUMO.

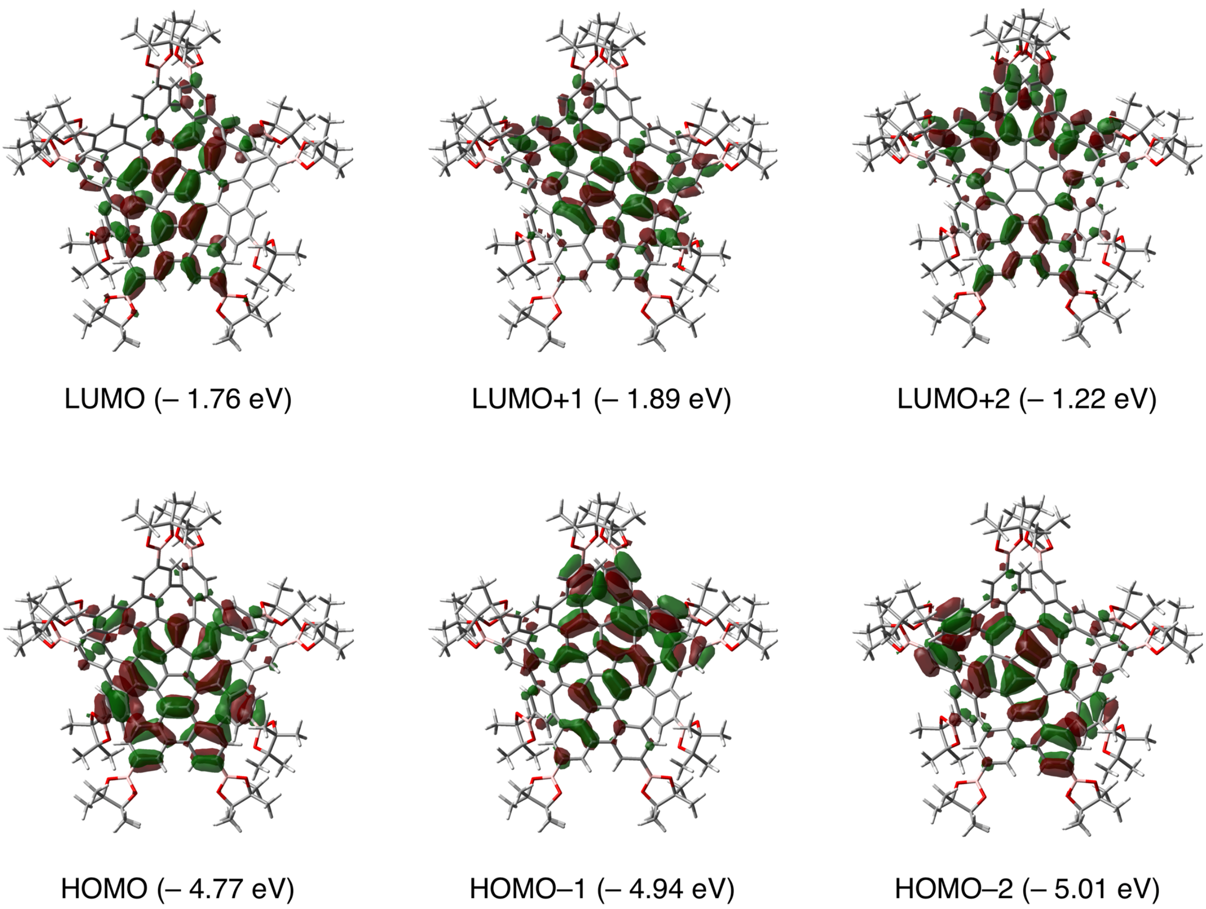


Figure S2. Distributions and energy levels of molecular orbitals of **2** (isovalue = 0.02).

Table S4. TD-DFT vertical one-electron excitations of **3a**

Excitation [nm]	Oscillator strength (*f*)	Description
515	0.180	H→L
		H–1→L+1
500	0.004	H–2, H–1→L
		H→L+1
486	0.008	H–3, H–2, H–1→L
474	0.093	H–3, H–2, H–1, H→L
		H–2, H–1→L+1

H: HOMO, L: LUMO.

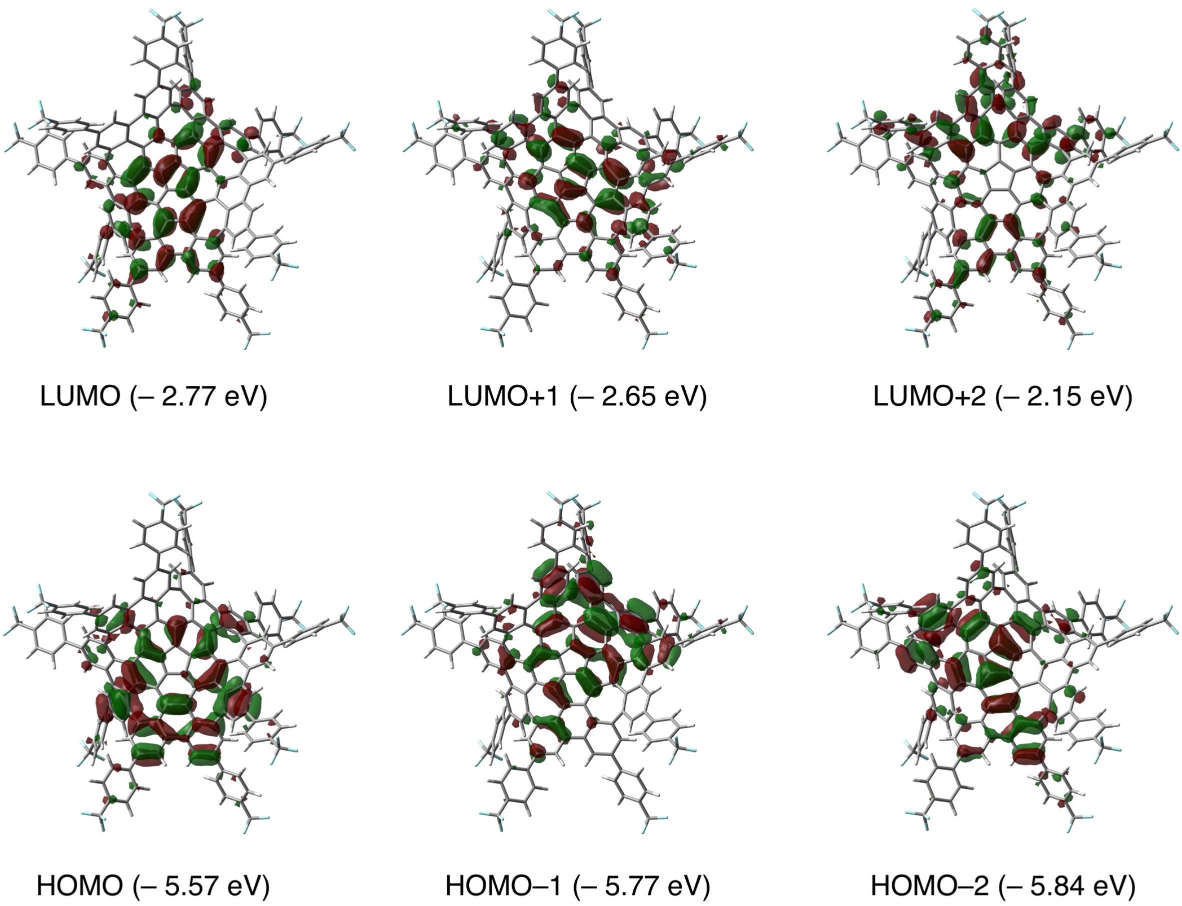


Figure S3. Distributions and energy levels of molecular orbitals of **3a** (isovalue = 0.02).

Table S5. TD-DFT vertical one-electron excitations of **3b**.

Excitation [nm]	Oscillator strength (*f*)	Description
548	0.321	H–10, H→L
		H–1→L+1
530	0.018	H–11, H–1→L
		H→L+1
524	0.011	H–12, H–3, H–2, H–1→L
515	0.033	H–13, H–3, H–2→L
		H–1→L+1

H: HOMO, L: LUMO.

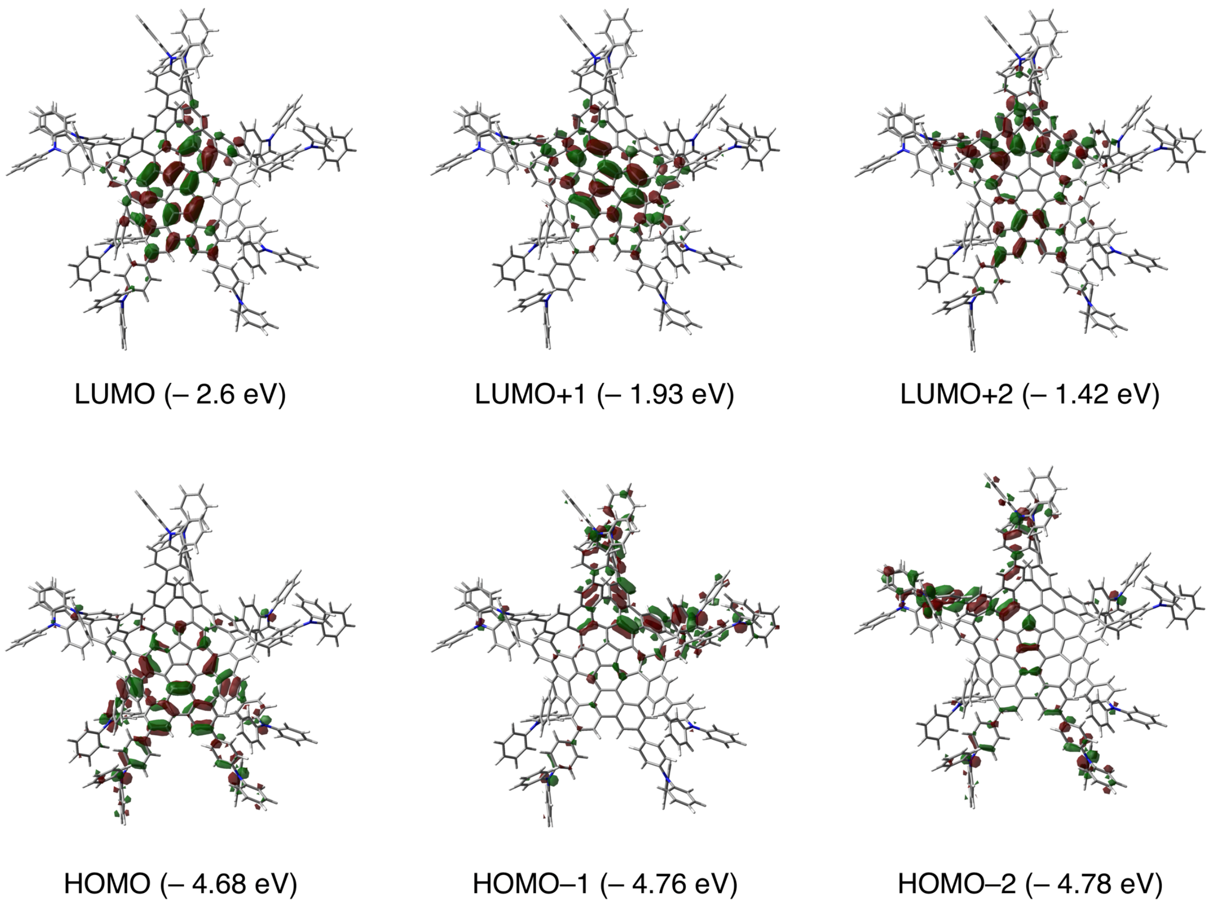


Figure S4. Distributions and energy levels of molecular orbitals of **3b** (isovalue = 0.02).

Table S6. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).[a]

	E	*E* + *ZPE*	*H*	*G*
2	-7173.63841675	-7171.085028	-7170.933750	-7171.283292
3a	-8747.66122956	-8745.979531	-8745.845710	-8746.184210
3b	-10551.7776533	-10548.364020	-10548.159908	-10548.662104

a) *E*: electronic energy; *ZPE*: zero-point energy; *H* (= $E + ZPE + E_{vib} + E_{rot} + E_{trans} + RT$): sum of electronic and thermal enthalpies; *G* (= $H - TS$): sum of electronic and thermal free energies.

Table S7. Cartesian coordinates of optimized structures.

2

C	-0.220175	-1.197262	-0.449534
C	1.031916	-0.599548	-0.582521
C	0.837904	0.790039	-0.705389
C	-0.537443	1.053270	-0.596057
C	-1.207595	-0.190553	-0.547502
C	-0.434237	-2.473379	-0.007007
C	0.792838	-3.125094	0.474618
C	2.090034	-2.520818	0.280781
C	2.230658	-1.205055	-0.331278
C	3.353715	-0.318340	-0.691629
C	3.161004	1.081274	-0.877488
C	1.838737	1.712466	-0.648381
C	1.362339	3.040204	-0.290533
C	-0.042578	3.302465	-0.032934
C	-1.094267	2.271495	-0.290425
C	-2.579599	2.177603	-0.195997
C	-3.289423	0.899729	-0.345145
C	-2.552413	-0.382545	-0.412427
C	-2.869567	-1.847160	-0.409112
C	-1.859152	-2.829111	-0.116180
C	0.673339	-4.210068	1.441149
C	1.705445	-4.400526	2.402418
C	3.249632	-3.094283	0.954511
C	3.042824	-3.894067	2.113320
C	4.145556	-4.264828	2.904962
C	5.447467	-3.909223	2.570572
C	5.642308	-3.211681	1.365732
C	4.586009	-2.819837	0.543650
C	4.563682	-0.939412	-1.203315
C	4.986439	-2.223317	-0.763691
C	5.960446	-2.898518	-1.494417
C	6.582670	-2.331975	-2.624257
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C	5.276457	-0.294966	-2.252667
C	4.140668	1.824396	-1.650143
C	5.025314	1.118152	-2.511530
C	5.675376	1.823946	-3.542277
C	5.539732	3.201152	-3.692528
C	4.809455	3.899514	-2.709272
C	4.141944	3.245191	-1.679100
C	2.368799	4.041979	0.055258
C	3.670387	4.062663	-0.526560
C	4.626017	4.948131	-0.025725
C	4.356403	5.854072	1.013346
C	3.063174	5.879173	1.519073
C	2.063940	5.004982	1.051722
C	-0.347863	4.486383	0.765867
C	0.687246	5.142584	1.496480
C	0.359404	5.984045	2.574894
C	-0.954995	6.309583	2.884991
C	7.799102	-5.087100	5.283841
O	6.523862	-5.111293	4.584329
O	8.062595	-4.390428	-3.099778
C	8.870246	-4.891923	-4.200757
C	9.325062	-3.559368	-4.917652
O	8.253889	-2.639240	-4.568394
O	6.108919	5.301426	-5.078815
C	7.049857	5.666207	-6.126397
C	7.284118	4.288315	-6.862073
O	7.016464	3.324570	-5.805603
O	5.210644	7.796057	2.483167
C	6.497945	8.328156	2.903004
C	7.434335	7.940076	1.690820
O	6.764354	6.770851	1.143624
O	-2.589298	7.516394	4.474958
C	-2.513359	8.531261	5.513866
C	-1.050935	8.327810	6.077095
O	-0.355065	7.758439	4.933325
O	-6.923808	6.979463	-1.762893
C	-7.374461	8.354254	-1.910482
C	-6.010990	9.145526	-2.018085
O	-5.093206	8.279454	-1.294229
O	-1.242802	-7.277926	5.282862
C	-1.064752	-8.061654	6.495168
C	0.097999	-7.284471	7.229055
O	0.802673	-6.662608	6.118321
C	-8.275288	8.436871	-3.141531
C	-8.177656	8.692457	-0.647075
C	-5.477643	9.249487	-3.453470
C	-6.002367	10.520821	-1.353263
C	-11.801513	2.077285	0.315956
C	-11.565678	2.496598	2.779423
C	-10.688178	-0.252304	3.285164
C	-12.109430	-0.679604	1.261171
C	-10.209628	-3.678633	-4.481456
C	-9.497107	-2.268079	-6.432134
C	-8.818016	-5.744213	-6.024594
C	-7.274411	-4.064637	-7.071952
C	-2.720553	-10.412329	-3.666161
C	-4.872334	-11.037039	-2.535452
C	-1.605076	-11.797708	-1.336539
C	-3.581916	-11.199908	0.091297
C	1.085415	-8.162331	7.995610
C	-0.404097	-6.145245	8.126610
C	-3.637878	8.279290	6.516742
C	-2.718312	9.885896	4.821564
C	-0.328171	9.608131	6.491345
C	-0.971018	7.287939	7.203223
C	6.342814	9.827317	3.152136
C	6.863380	7.611969	4.210439
H	-10.948520	2.353070	3.669045
H	-10.430127	-1.314805	3.330503
H	-11.572331	-0.084836	3.909544
H	-9.852452	0.315265	3.706284
H	-11.930851	-1.744940	1.439166
H	-13.050155	-0.406832	1.753364
H	-12.223109	-0.533353	0.184758
H	-10.666863	-2.802638	-4.011039
H	-9.888137	-4.359105	-3.686783
H	-10.971078	-4.183291	-5.085639
H	-10.089621	-1.462762	-5.986042
H	-8.658576	-1.813323	-6.963926
H	-10.129736	-2.792585	-7.157573
H	-9.305097	-6.081842	-5.107033
H	-9.572863	-5.672147	-6.816219
H	-8.090410	-6.507122	-6.319721
H	-6.527294	-4.848919	-7.228403
H	-7.898905	-3.999044	-7.969283
H	-6.744191	-3.115247	-6.947312
H	-1.753976	-9.908129	-3.568369
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H	-3.282630	-9.910944	-4.460074
H	-5.379440	-10.641080	-3.421192
H	-4.736246	-12.115479	-2.676993
H	-5.525764	-10.876968	-1.674924
H	-2.033756	-12.744961	-1.683772
H	-1.065648	-11.991910	-0.403910
H	-0.881572	-11.449166	-2.076714
H	-2.960164	-11.279664	0.988366
H	-4.369299	-10.466376	0.290836
H	-4.050417	-12.172873	-0.091738
H	1.564752	-8.894307	7.341927
H	1.869580	-7.535961	8.432936
H	0.583606	-8.696155	8.810984
H	0.449556	-5.534016	8.435469
H	-1.106115	-5.498188	7.591537
H	-0.899122	-6.527119	9.025898
H	-3.600292	7.264541	6.919208
H	-3.585023	8.989521	7.349956
H	-4.605620	8.409253	6.021690
H	-2.741661	10.709496	5.543125
H	-1.926627	10.084666	4.092316
H	-3.672604	9.868916	4.286118
H	-0.247411	10.311847	5.659978
H	-0.849014	10.102218	7.319761
H	0.685068	9.363949	6.826349
H	0.080883	7.058624	7.399937
H	-1.422890	7.658171	8.129676
H	-1.471603	6.356693	6.920349
H	7.305045	10.281041	3.416505

C	-1.947487	5.836860	2.010890
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3a

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F	2.816982	-12.974017	-3.355421
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F	10.594758	-5.582522	-6.802380
F	10.601013	-3.497571	-7.441685
F	13.752056	1.445614	1.765535
F	13.532212	-0.621483	2.396724
F	13.039881	1.000322	3.769013
F	3.606807	8.930903	8.114722
F	1.626754	9.820981	8.197997
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F	-8.214017	9.469764	4.554988
F	-7.891890	10.879652	2.933726
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F	8.973691	10.511590	-2.236381

3b

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C	4.480836	-13.269314	-0.308022
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C	-5.437865	6.254254	-10.852175
H	-5.264092	6.461952	-8.713771
C	-6.302758	6.148640	-11.943562
H	-8.367724	6.057979	-12.561824
H	-4.362205	6.264872	-11.007759
H	-5.907314	6.069046	-12.952156
C	-8.967261	7.297609	-7.759823
C	-9.053594	8.568036	-8.351687
C	-10.006144	6.866677	-6.918974
C	-10.159433	9.381545	-8.112066
H	-8.251456	8.910237	-8.997819
C	-11.099057	7.694894	-6.670687
H	-9.950170	5.882770	-6.464146
C	-11.186436	8.954383	-7.267668
H	-10.209459	10.361977	-8.578652
H	-11.893907	7.344904	-6.017123
H	-12.043404	9.594239	-7.077491
C	-8.904310	9.335646	3.905372
C	-10.222032	9.797423	3.756641
C	-8.614137	8.426157	4.935222
C	-11.221321	9.363499	4.625672
H	-10.454968	10.495668	2.959003
C	-9.624014	7.983757	5.787561
H	-7.596507	8.070354	5.061202
C	-10.931911	8.451452	5.642821
H	-12.235808	9.731405	4.495620
H	-9.381164	7.279407	6.578960
H	-11.714983	8.109759	6.313653
C	-7.814169	11.158841	2.663072
C	-8.013960	12.161026	3.626103
C	-7.552041	11.533550	1.335355
C	-7.960330	13.505454	3.263154
H	-8.210917	11.878891	4.655489
C	-7.482017	12.880764	0.985803
H	-7.404247	10.764461	0.583865
C	-7.689707	13.875289	1.943983
H	-8.117323	14.267793	4.021865
H	-7.278047	13.152354	-0.046693
H	-7.641461	14.924358	1.666308
C	2.820137	9.057391	8.476854
C	2.319369	9.850158	9.522035
C	3.250822	7.751066	8.759517
C	2.260747	9.346690	10.820181
H	1.978841	10.858618	9.309676
C	3.170899	7.250129	10.057501
H	3.645886	7.134772	7.958168
C	2.680642	8.043846	11.096722
H	1.870072	9.974374	11.616945
H	3.508414	6.236582	10.257933
H	2.626471	7.652215	12.108487
C	3.348865	10.901746	6.936163
C	4.454791	11.398759	7.644505
C	2.699593	11.738548	6.014048
C	4.892106	12.705799	7.438385
H	4.965416	10.755786	8.354337
C	3.155771	13.038038	5.801362

H	11.014459	2.003715	3.084224
H	11.829107	-1.372526	0.551454
C	6.903029	-3.790482	-4.014610
C	7.443849	-2.819417	-4.875425
C	7.313708	-5.121135	-4.206619
C	8.350954	-3.154994	-5.874291
H	4.027329	-14.524294	-3.533508
C	1.419457	-14.251785	-5.709322
H	-0.289480	-12.967791	-5.416313
H	3.236585	-15.414781	-5.701319
H	1.074886	-14.637033	-6.664745
H	1.839334	11.364023	5.468395
C	4.250490	13.532530	6.513692
H	5.749803	13.073681	7.995598
H	2.640872	13.671601	5.083792
H	4.598643	14.548477	6.350511

5. References

S1) K. Kawasumi, Q. Zhang, Y. Segawa, L. T. Scott and K. Itami, *Nat. Chem.*, 2013, **5**, 739.

S2) A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *J. Appl. Crystallogr.,* 1999, **32**, 115.

S3) G. M. Sheldrick, *Acta Crystallogr. A,* 2008, **64**, 112.

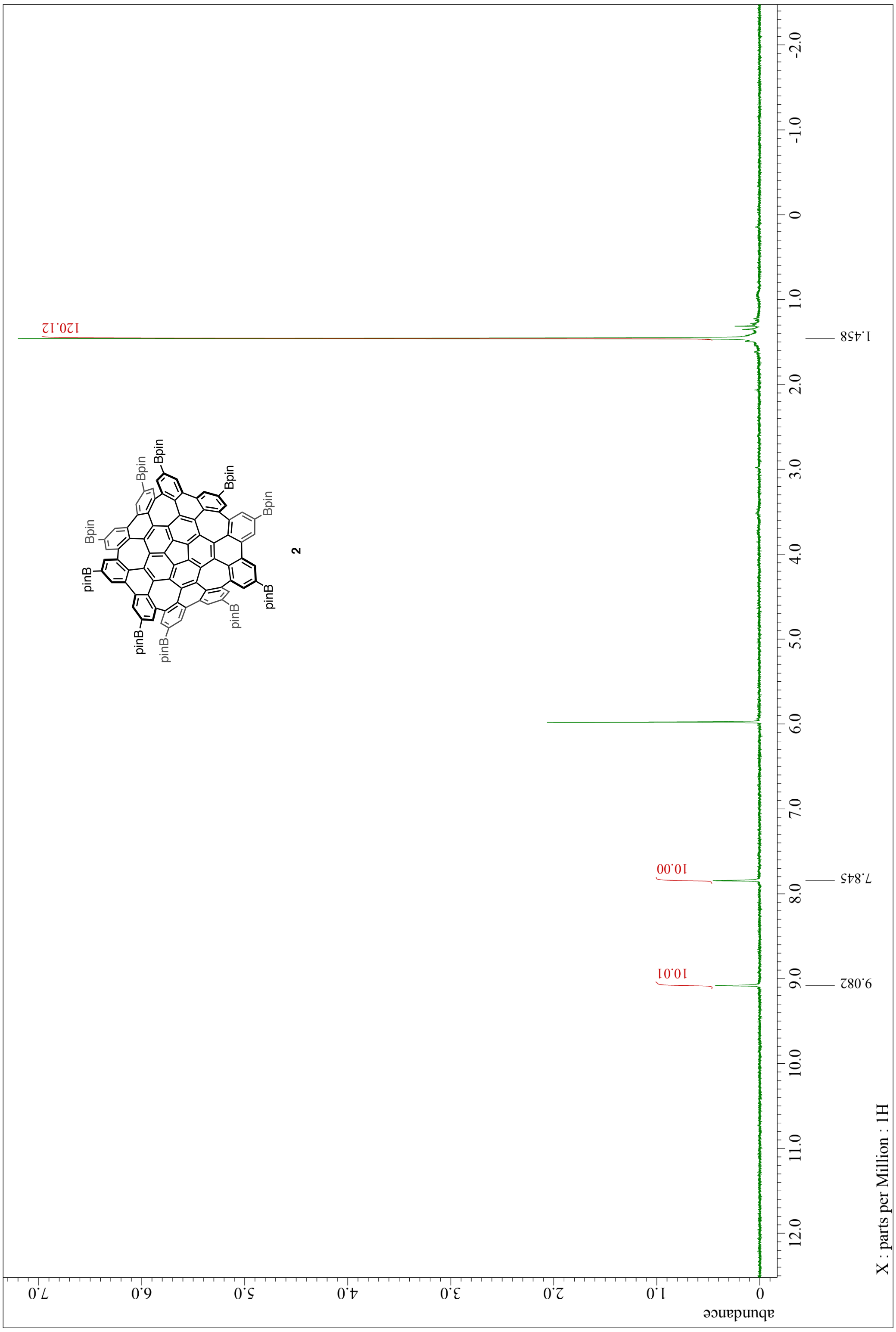
S4) (a) K. Wakita, Yadokari-XG, Software for crystal structure analyses, 2001. (b) C. Kabuto, S. Akine, T. Nemoto and E. Kwon, *J. Cryst. Soc. Jpn.,* 2009, **51**, 218.

S5) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox Gaussian 16, Revision B.01, Gaussian, Inc., Wallingford CT, 2016.

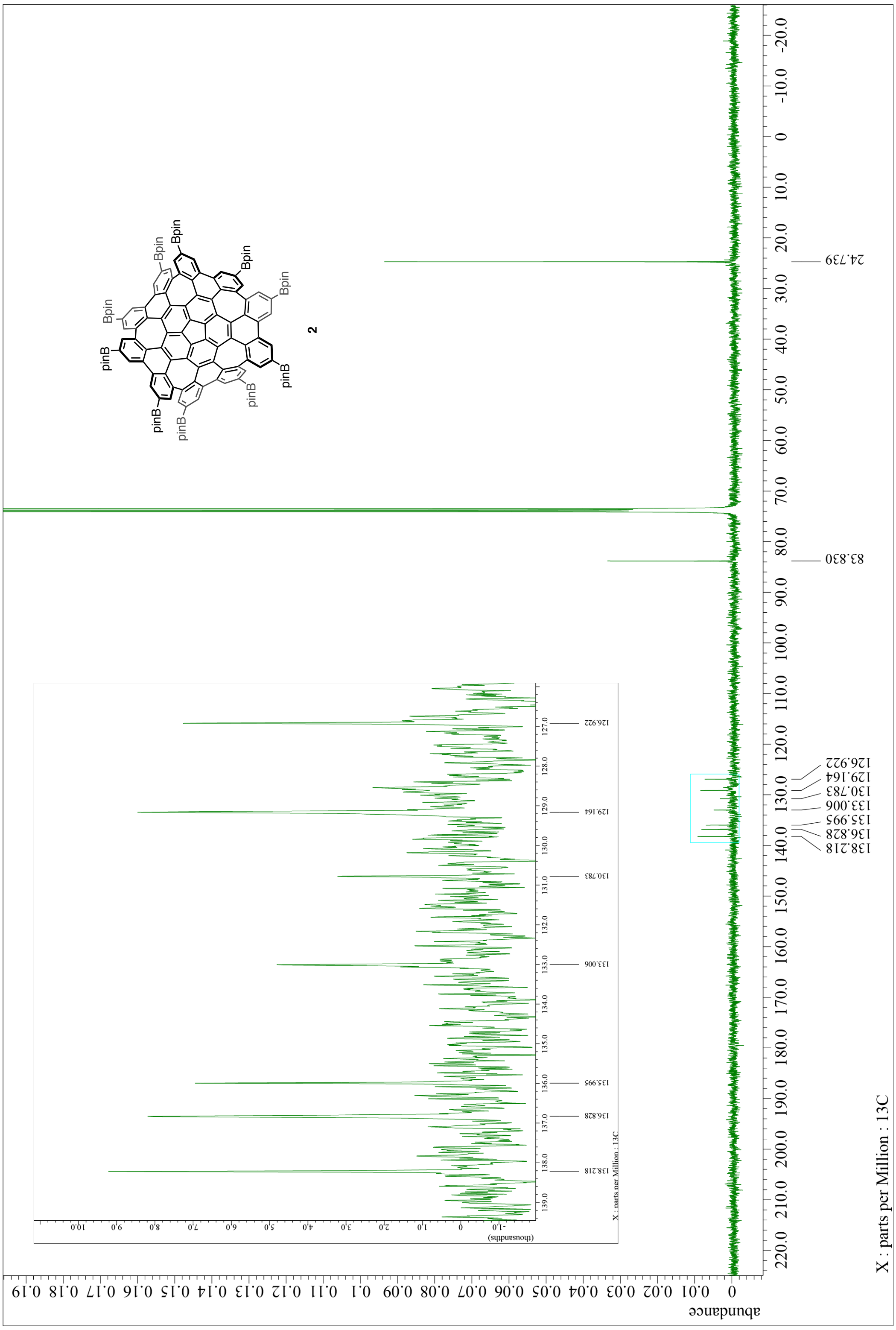
S6) (a) A. D. Becke, *J. Chem. Phys.,* 1993, **98**, 5648. (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.,* 1988, **37**, 785.

6. [1]H NMR and [13]C NMR Spectra

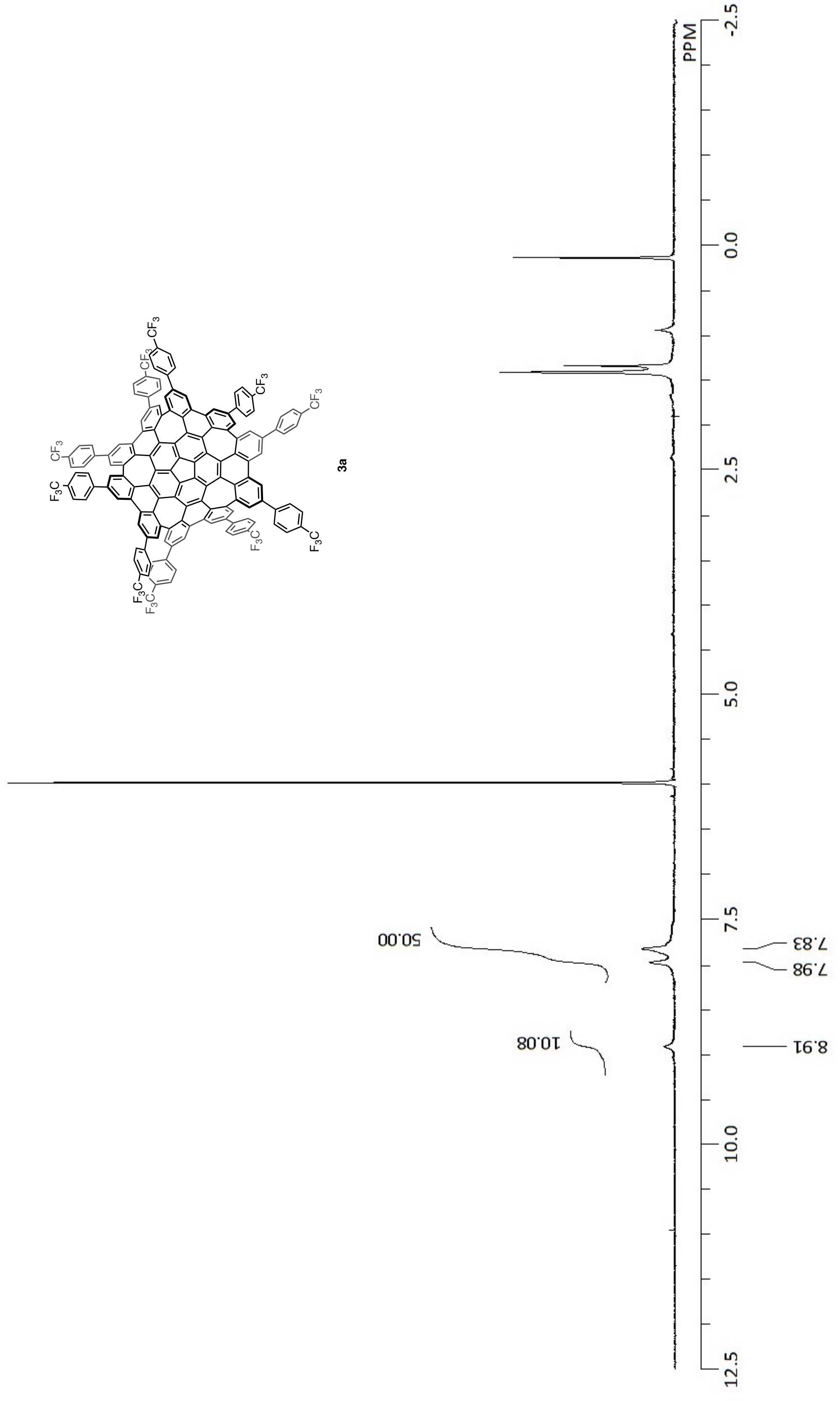
[1]H NMR spectrum of **2** (600 MHz, $C_2D_2Cl_4$, 140 °C)



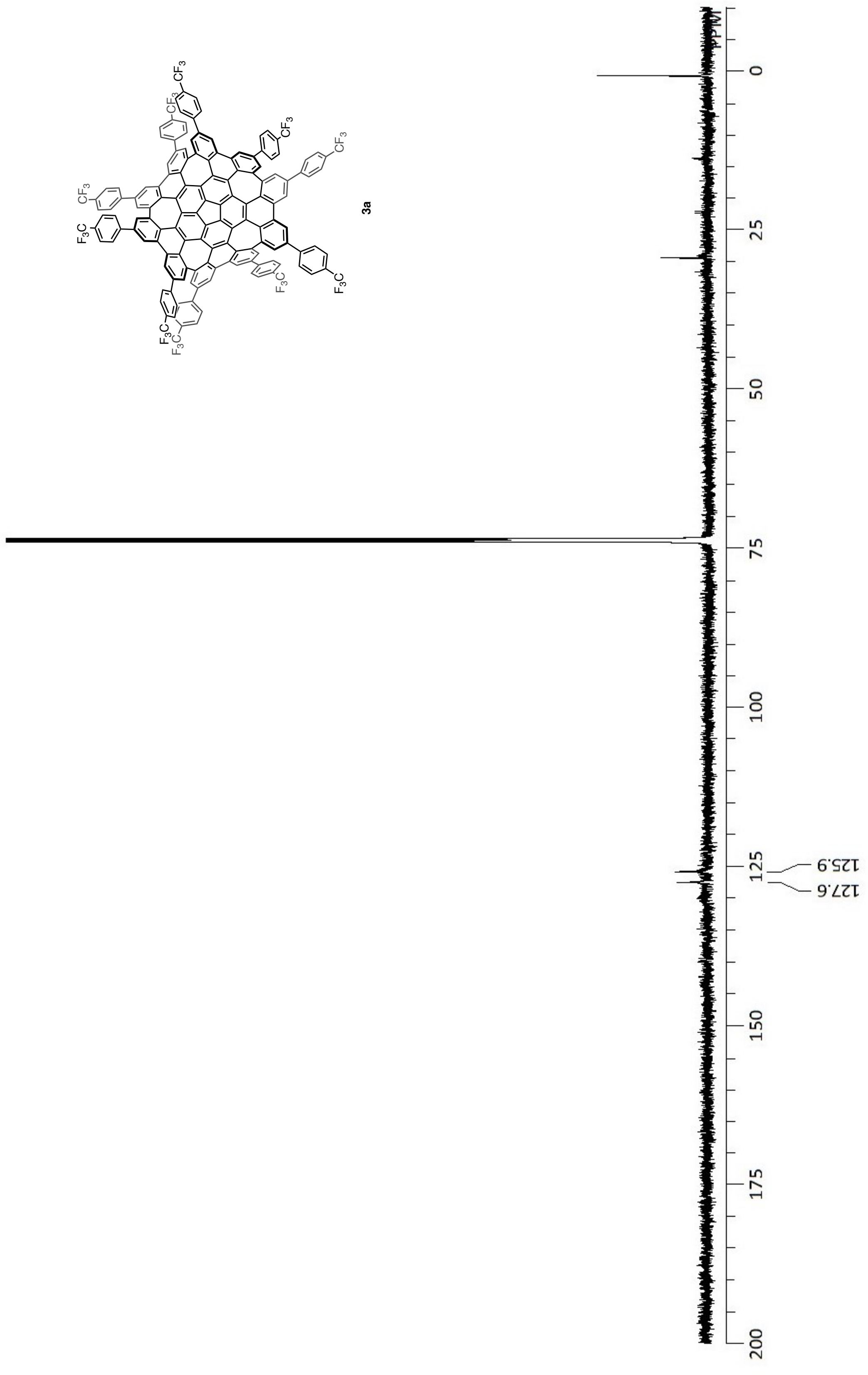
^{13}C NMR spectrum of **2** (150 MHz, $C_2D_2Cl_4$, 140 °C)



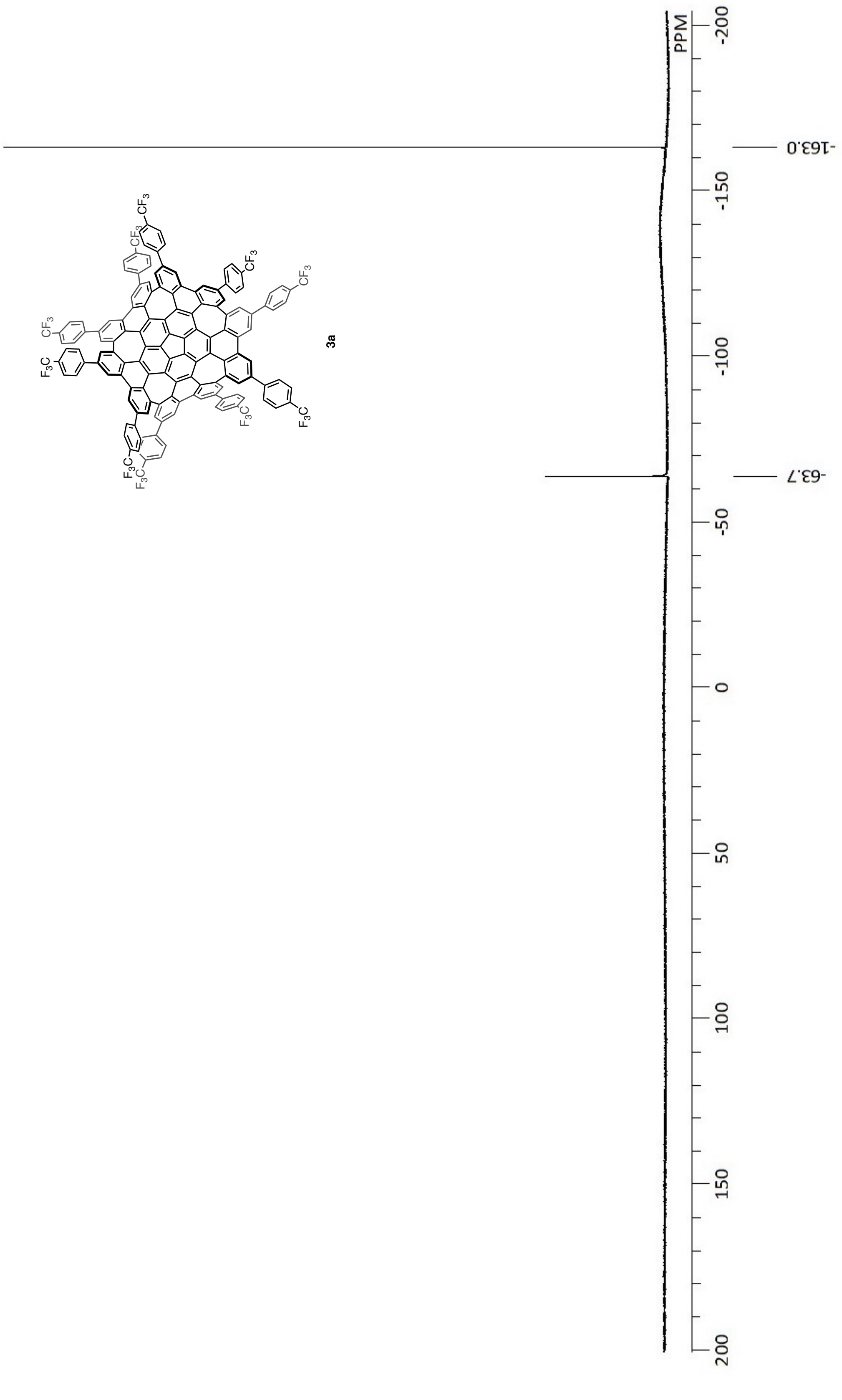
^{1}H NMR spectrum of **3a** (600 MHz, $C_2D_2Cl_4$, 140 °C)



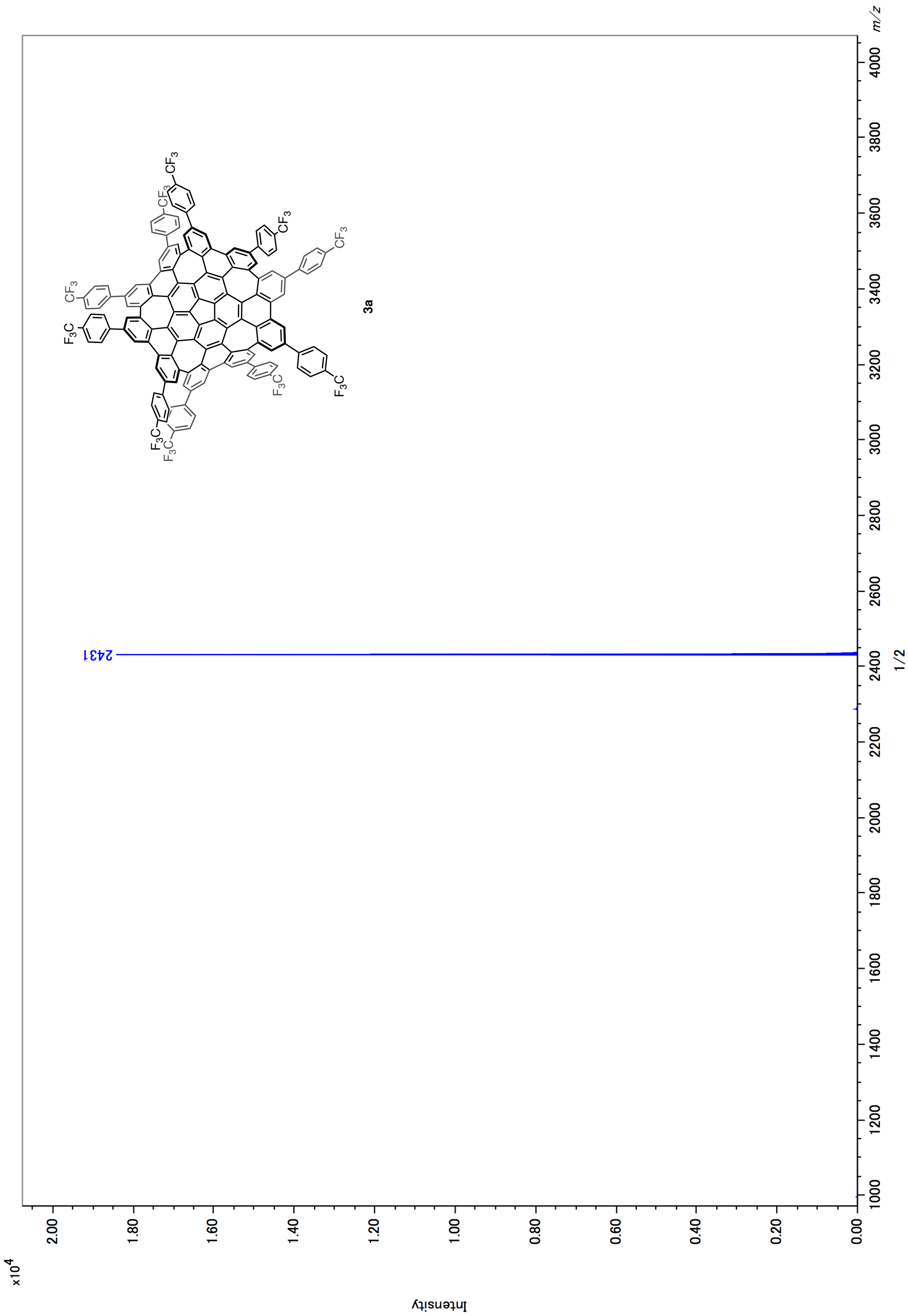
^{13}C NMR spectrum of **3a** (150 MHz, $C_2D_2Cl_4$, 85 °C)



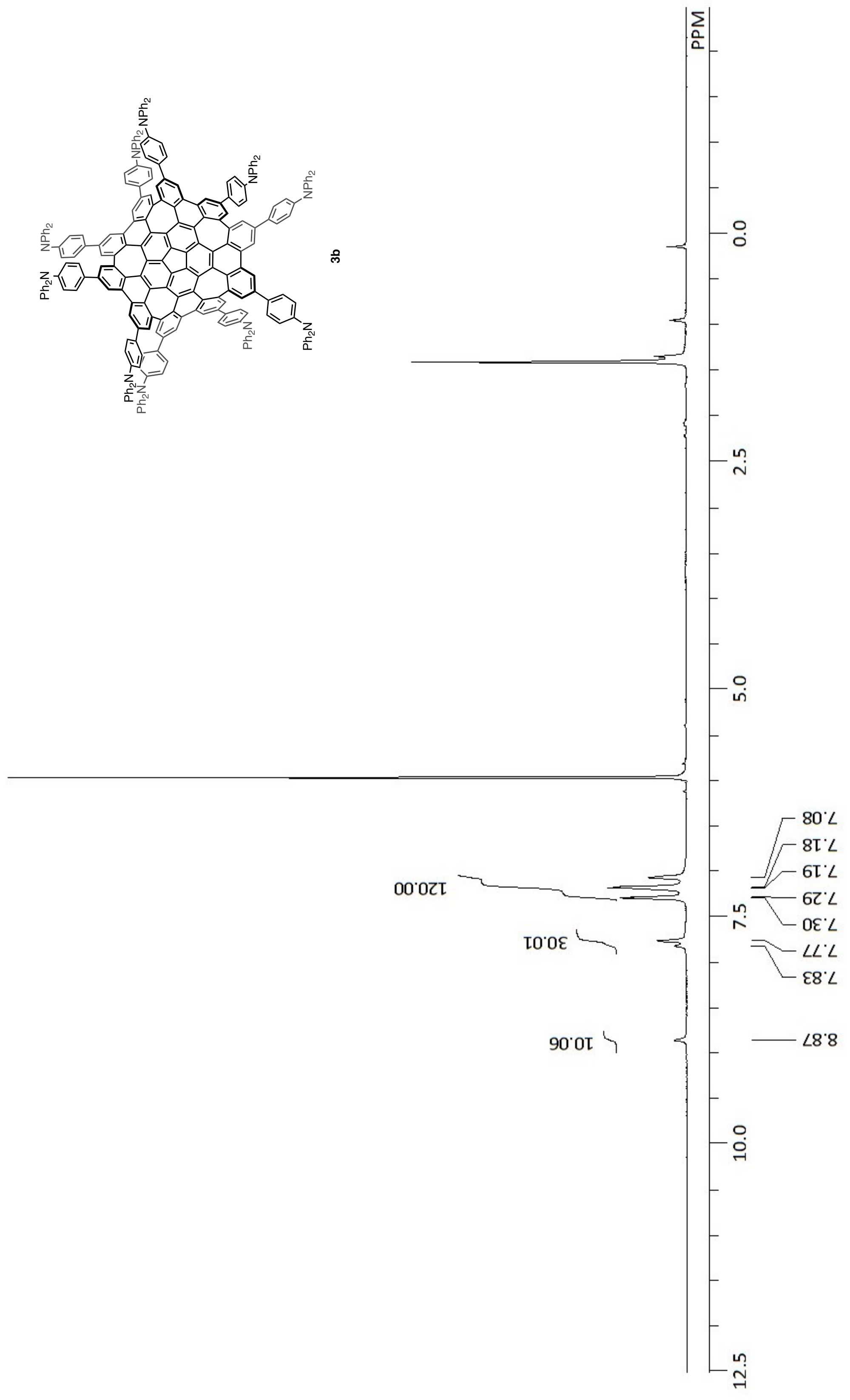
^{19}F NMR spectrum of **3a** (565 MHz, $C_2D_2Cl_4$, 140 °C)



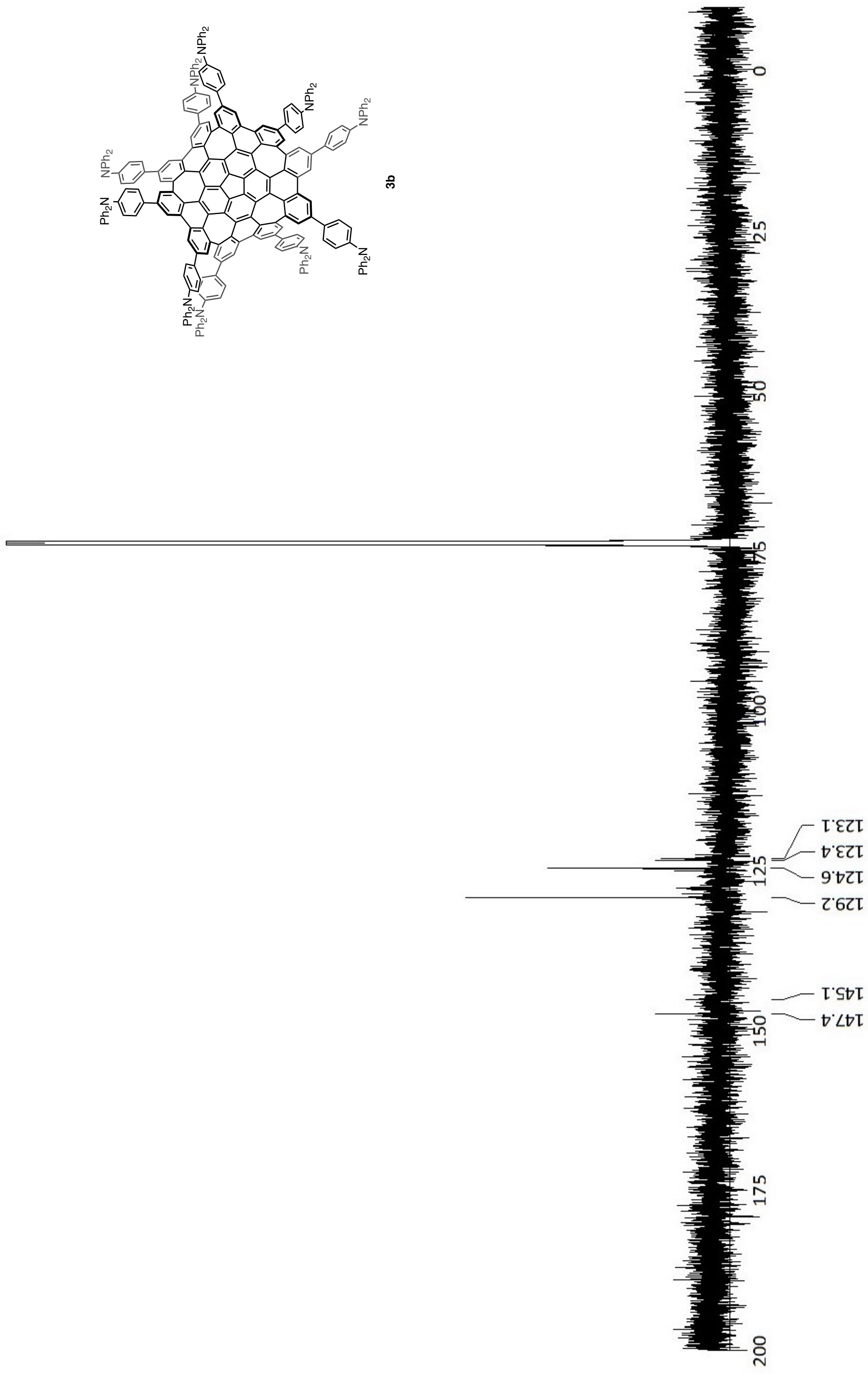
MALDI-TOF mass spectrum of **3a**



[1]H NMR spectrum of **3b** (600 MHz, $C_2D_2Cl_4$, 140 °C)



^{13}C NMR spectrum of **3b** (150 MHz, $C_2D_2Cl_4$, 85 °C)



MALDI-TOF mass spectrum of **3b**