Supporting Information

Cycloparaphenylene Nanoring with Graphenic Hexabenzocoronene Sidewalls

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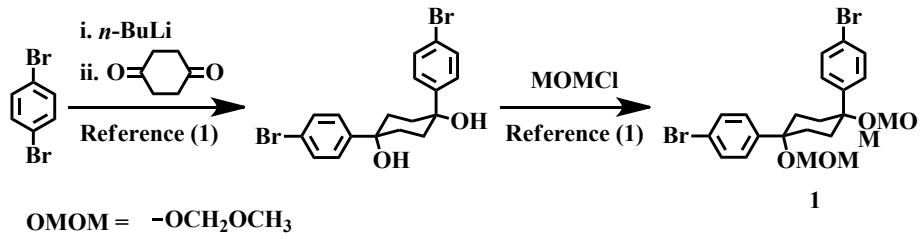
1. General information

All solvents for syntheses were dried by distillation under nitrogen prior to use (diethyl ether (Et_2O), tetrahydrofuran (THF), methyl *tert*-butyl ether, *m*-xylene and mesitylene were distilled after reflux with sodium under nitrogen; dichloromethane (DCM) and dimethylsulfoxide (DMSO) were dried with CaH_2.). Other chemicals were obtained from commercial suppliers (Aldrich or Acros) and used without further purification. Air-sensitive reactions were all carried out under nitrogen or argon. The starting materials *cis*-1,4-bis(4-bromophenyl)-1,4-bis(methoxymethoxy)cyclohexane (**1**)[1] and 2,11-diboryl-5,8,14,17-tetramesitylhexabenzo[*bc,ef,hi,kl,no,qr*]coronene (**2**)[2] were synthesized according to the reported procedures.

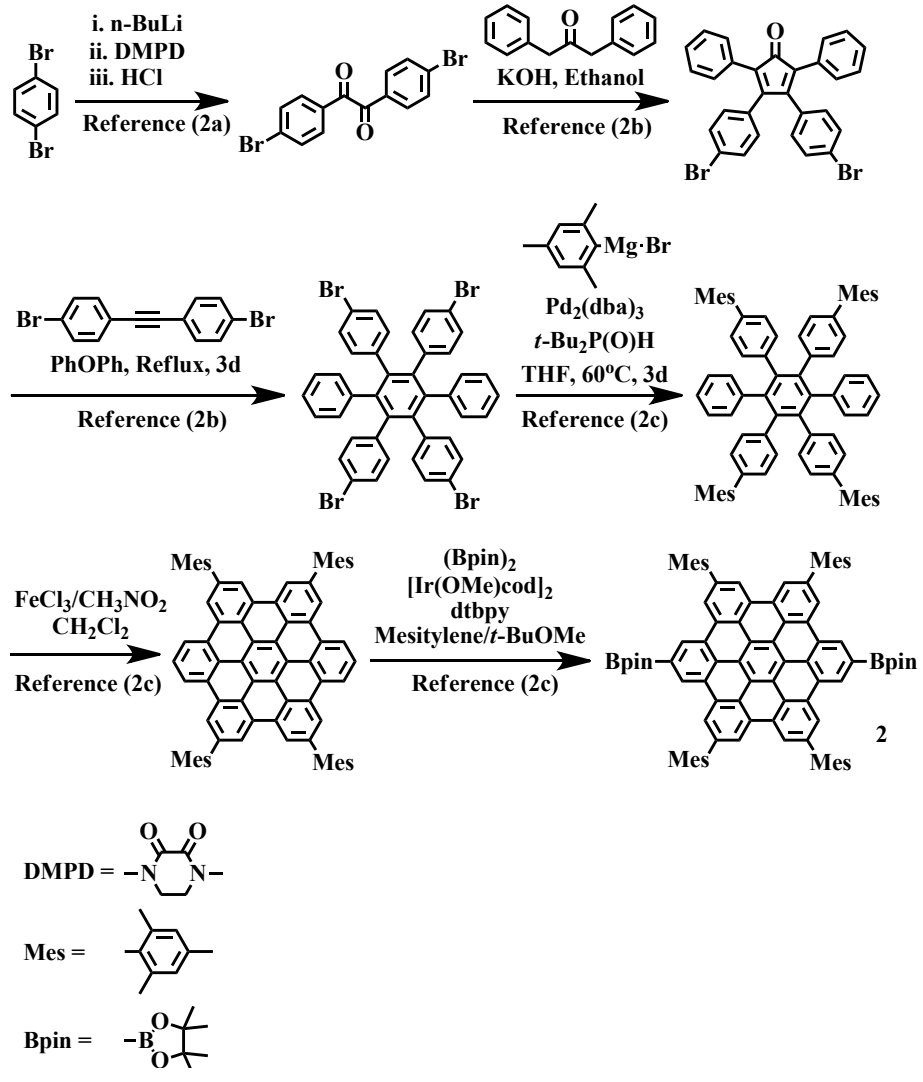
High resolution mass spectrometry (HR-MS) analyses were carried out using MALDI-TOF-MS techniques. NMR spectra were recorded on Bruker BioSpin (^{1}H 400 MHz, ^{13}C 100 MHz) spectrometer. Chemical shifts for ^{1}H NMR are shown in parts per million (ppm) relative to $CDCl_3$ (δ 7.26 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm). Coupling constants (*J*) are given in Hz. The apparent resonance multiplicity is described as s (singlet), br s (broad singlet), d (doublet), t (triplet), q (quartet), sept (septuplet), and m (multiplet). Flash chromatography was performed on silica gel (300～400 mesh). Preparative thin-layer chromatography (PTLC) experiments were performed using silica gel GF 254 coated plates. UV-vis absorption spectra were performed on a UNIC-3802 spectrophotometer.

2. Synthetic procedures

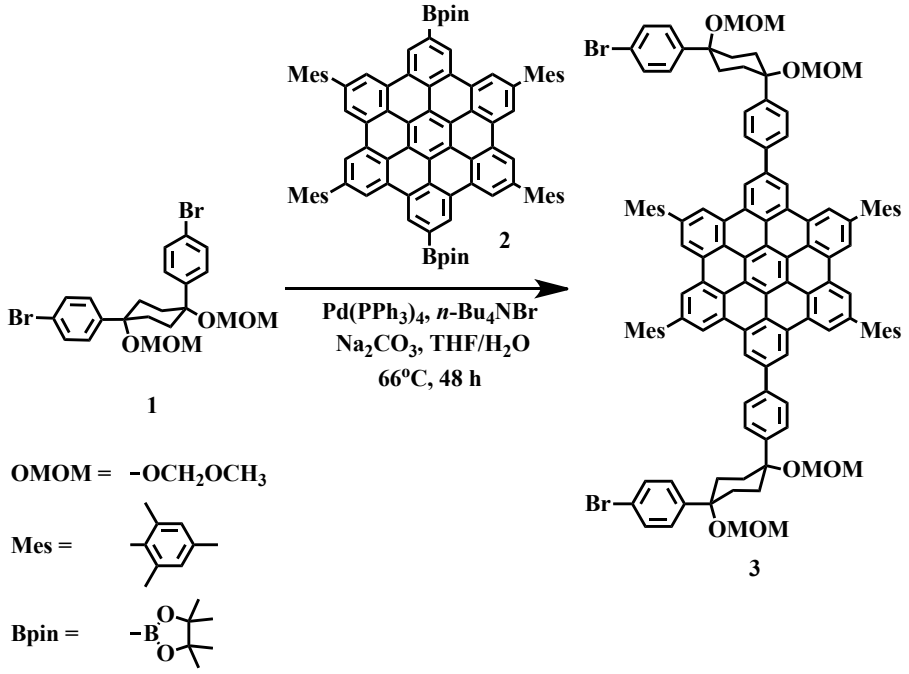
2.1 Synthesis of *cis*-1,4-bis(4-bromophenyl)-1,4-bis(methoxymethoxy)cyclohexane (1)



2.2 Synthesis of 2,11-diboryl-5,8,14,17-tetramesitylhexabenzo[*bc,ef,hi,kl,no,qr*]coronene (2)



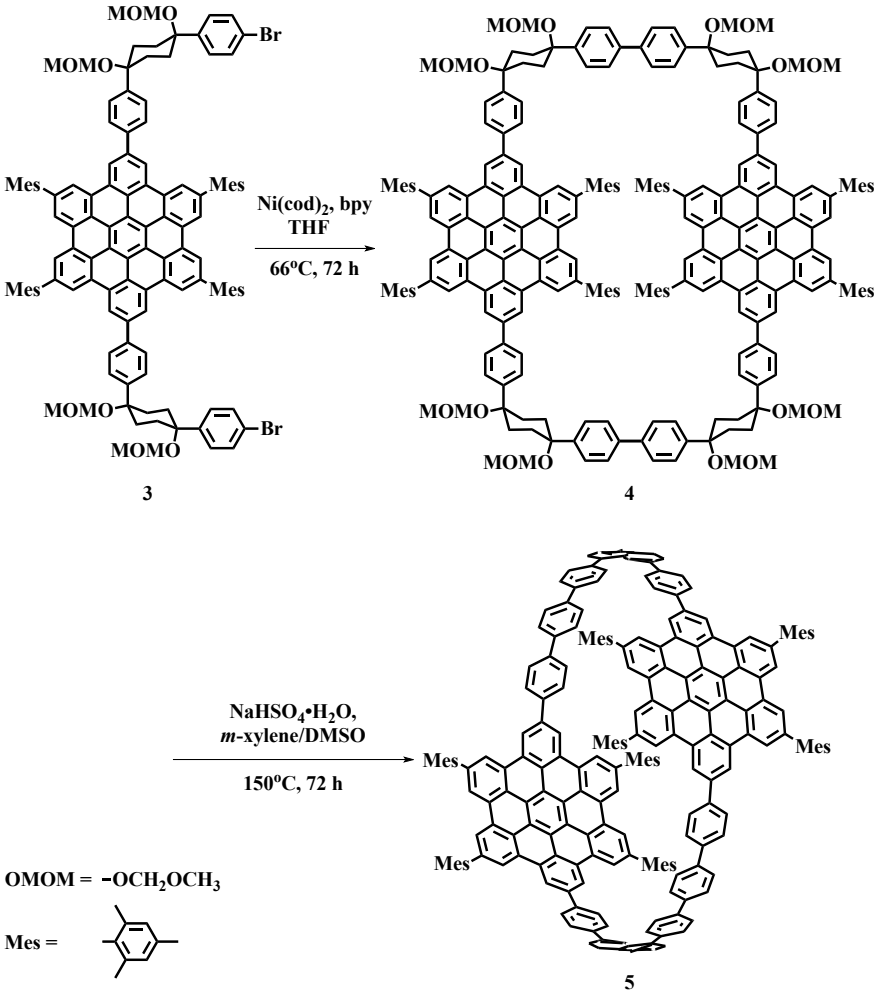
2.3 Synthesis of compound 3



To a degassed suspension of **2** (400 mg, 0.32 mmol), **1** (1.7 g, 3.3 mmol), Na_2CO_3 (270 mg, 2.55 mmol), and *n*-Bu_4NBr (132 mg, 0.41 mmol) in THF (44 mL) and H_2O (6 mL) was added $Pd(PPh_3)_4$ (31 mg, 0.027 mmol), then the mixture was degassed for 10 min. The mixture was then heated at 66 °C for 48 h under nitrogen atmosphere. After cooling down to room temperature, water was added and the mixture was extracted with DCM. The combined organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography using DCM/EtOAc (*v/v*, 20:1 to 5:1) as the eluent to give **3** as a yellow solid (406 mg, 68 %).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.32 (36H, s), 2.52 (16H, s), 3.51 (6H, s), 3.55 (6H, s), 4.49 (4H, s), 4.64 (4H, s), 7.20 (8H, s), 7.41 (4H, d, *J* = 6.0 Hz), 7.51 (4H, d, *J* = 6.8 Hz), 7.76 (4H, d, *J* = 6.8 Hz), 8.10 (4H, d, *J* = 7.6 Hz), 9.13 (4H, s), 9.25 (4H, s), 9.50 (4H, s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.3, 21.4, 33.2, 56.2, 77.4, 78.0, 78.3, 78.40, 78.44, 92.3, 92.4, 121.3, 121.4, 121.5, 121.7, 123.6, 123.8, 124.8, 125.3, 126.9, 127.8, 128.2, 128.5, 128.6, 128.7, 131.1, 131.2, 131.4, 131.6, 133.6, 136.5, 137.45, 137.48, 139.3, 139.4, 140.3, 141.0. HR-MS (MALDI-TOF) (with sulfur as matrix) *m/z* calcd. for $C_{122}H_{108}Br_2O_8$ $[M]^+$: 1861.6400, Found 1862.0550.

2.4 Synthesis of compound 5



A 100-mL Schlenk flask containing **3** (96 mg, 0.05 mmol), 2,2'-bipyridyl (bpy) (22 mg, 0.14 mmol), and a magnetic stirring bar (oven dried) was evacuated and refilled with nitrogen for 3 cycles. Then, $Ni(cod)_2$ (36 mg, 0.13 mmol) was added under nitrogen, and the flask was evacuated and refilled with nitrogen for another 3 cycles. Freshly-distilled THF (52 mL) was transferred to the flask *via* syringe under nitrogen at room temperature. The resultant mixture was allowed to stir for 1 h at room temperature and then heated at 66 °C for 72 h. After the reaction mixture was cooled to room temperature, it was passed through a short silica gel column with DCM as the eluent. The solvents were removed under reduced pressure. The residue was used for the next step without further purification.

To a 25-mL flask containing a magnetic stirring bar were added the above crude product, $NaHSO_4 \cdot H_2O$ (188 mg, 1.36 mmol), dry DMSO (1.6 mL) and dry *m*-xylene

(8 mL). The mixture was heated with stirring at 150 °C for 72 h under air. After cooling down to room temperature, water was added and the reaction mixture was extracted with DCM, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified initially by silica gel column chromatography and then by preparative thin-layer chromatography with hexane/DCM as the eluent (*v/v*, 2:1) to afford **5** as a yellow solid (3.0 mg, 2 % over two steps). Due to the highly insoluble nature in solvents and high molecular weight of the product, we could not obtain the ^{13}C NMR spectrum.

^1H NMR ($CDCl_3$, 400 MHz): δ 2.23 (48H, br s), 2.46 (24H, s), 7.13 (16H, s), 7.67 (16H, d, *J* = 8.4 Hz), 7.70 (16H, s), 7.76 (8H, d, *J* = 8.8 Hz), 8.04 (8H, d, *J* = 8.0 Hz), 8.99 (8H, s), 9.04 (8H, s), 9.24, (8H, s); HR-MS (MALDI-TOF) (without matrix) *m/z* calcd. for $C_{228}H_{160}$ $[M]^+$: 2899.2600; Found 2899.2872.

3. HR-MS spectra for compound 5

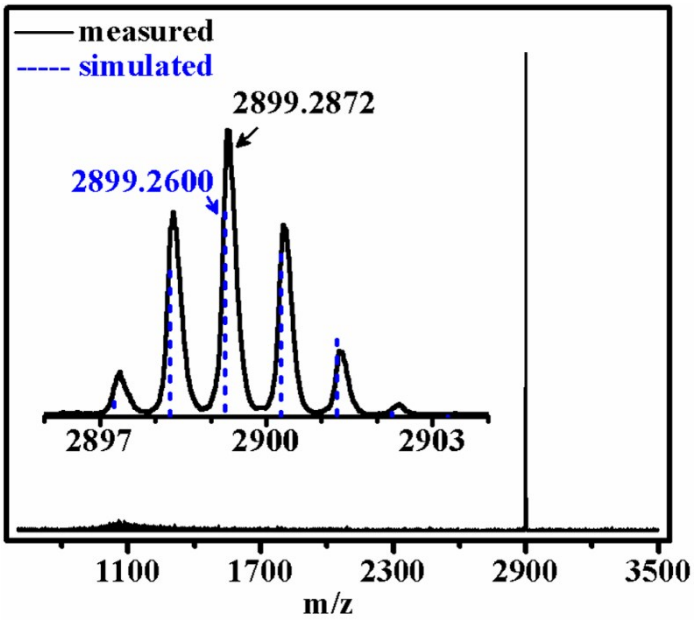


Figure S1. HR-MS (MALDI-TOF) and simulated data for compound **5.**

4. Methods for STM measurements

All STM experiments were performed using Createc LT-STM in an ultrahigh vacuum (UHV) chamber with base pressure of 1×10^{-10} mbar. Atomically flat Au(111)/mica film was used as the substrate which was cleaned by repeated cycles of Ar^+ sputtering (2 keV) and annealing at 700 K for 10 min. The sample was then deposited onto the freshly-prepared Au(111) surface by casting a small drop (~2 μL) of the solution in CH_2Cl_2 (1×10^{-5} M) and then transferred back into the UHV chamber immediately after the solvent evaporated. Before subjected to scanning, the sample was further annealed at ~600 K for 15 min in order to desorb the contaminations possibly introduced from the solution. All STM images were acquired at liquid-nitrogen temperature using an electrochemically etched tungsten tip in the constant-current mode.

5. Photophysical measurements

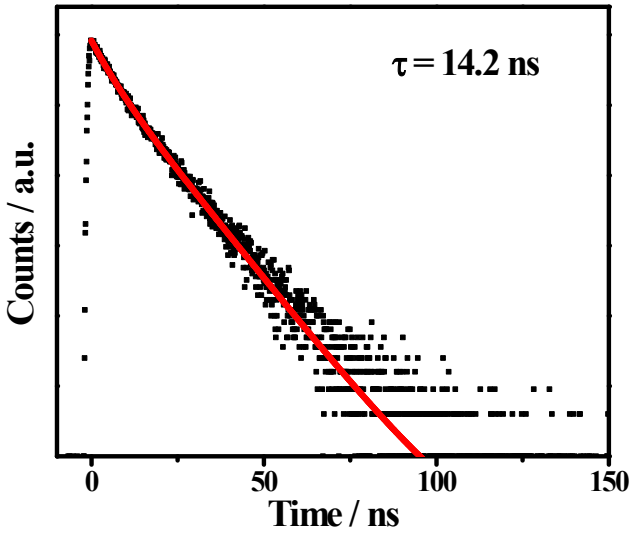


Figure S2. Emission lifetime for compound **5**.

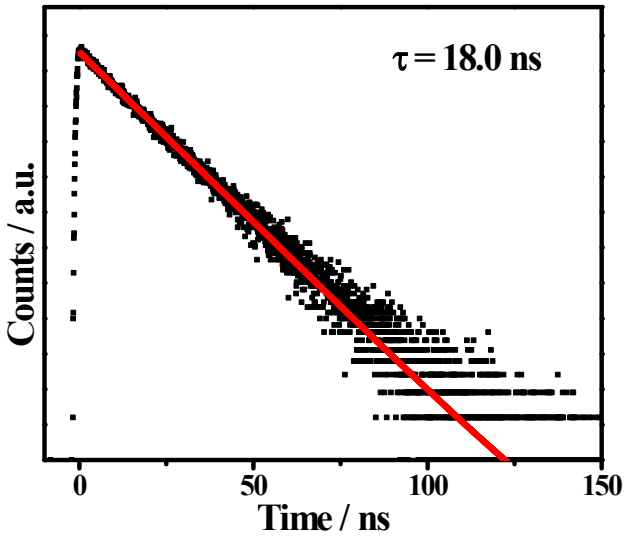


Figure S3. Emission lifetime for tetramesityl HBC.

6. Computational studies

Density functional theory with the B3LYP hybrid exchange correlation functional was used for all calculations in this work.[3] The split-valance double-zeta basis set 6-31G were employed to optimize the structure of molecule.[4] The Berny algorithm based on energy minimization was used for geometry optimization.[5] Time dependent DFT (TDDFT)[6] method was carried out for the UV-Vis absorption of the carbon nanoring molecule and the CAM-B3LYP[7] is used to improve the accuracy. The Gaussian 09 package[8] was used throughout this study.

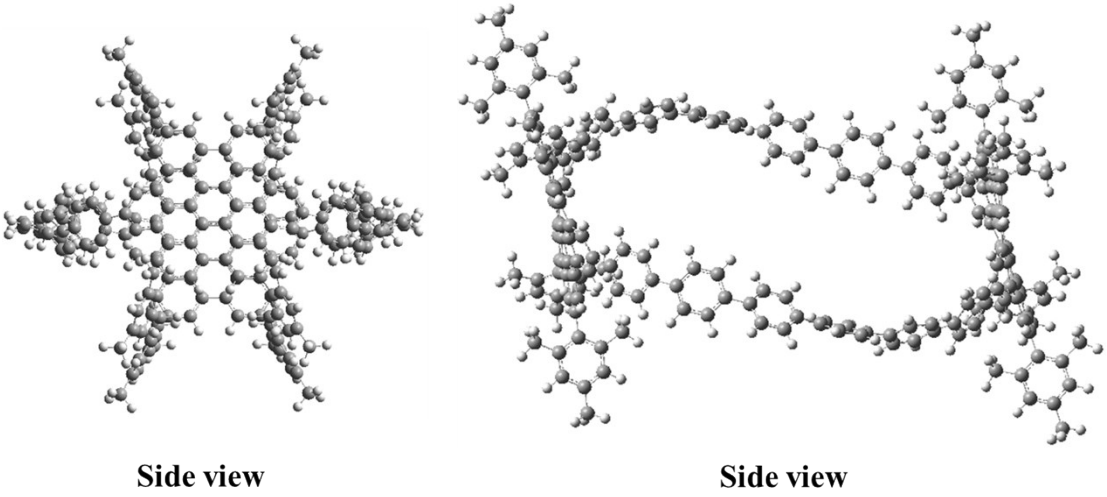


Figure S4. Side view of the optimized structure of **5**.

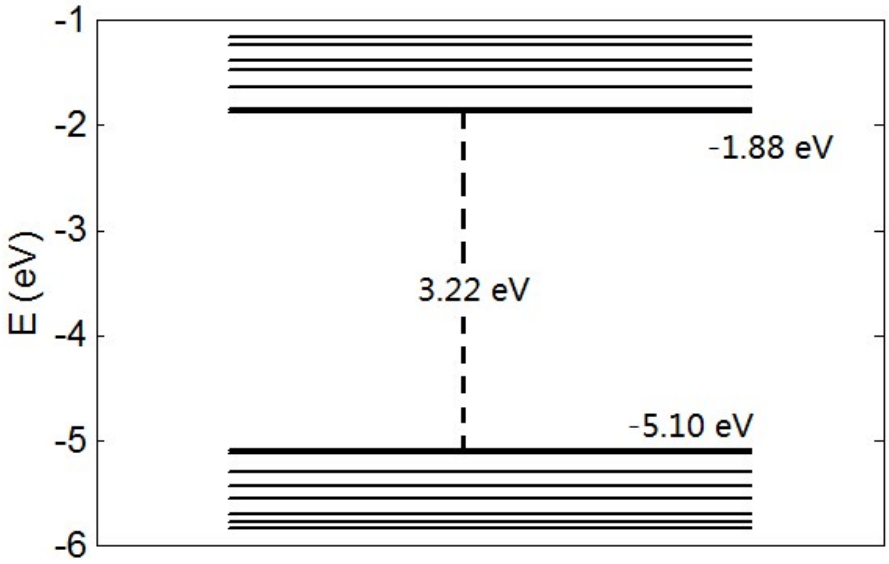


Figure S5. Energy diagrams of the frontier MOs of **5.**

Table S1. Cartesian coordinates for the optimized structure of **5**.

C1	-11.061000	-6.738000	0.097900
C2	-10.563200	-7.552200	1.136200
C3	-9.551100	-8.483200	0.907000
C4	-9.000900	-8.669500	-0.378400
C5	-9.615900	-7.973600	-1.439800
C6	-10.608300	-7.023600	-1.206800
C7	9.550900	-8.483100	-0.907000
C8	10.563000	-7.552100	-1.136200
C9	11.060900	-6.737900	-0.098000
C10	10.608100	-7.023500	1.206700
C11	9.615700	-7.973500	1.439700
C12	9.000800	-8.669400	0.378300
C13	7.717900	-9.397400	0.564900
C14	6.840900	-9.012700	1.601000
C15	5.528000	-9.469800	1.648100
C16	5.012000	-10.322000	0.651100
C17	5.916300	-10.799800	-0.318300
C18	7.239500	-10.352800	-0.356000
C19	-2.969300	-11.738400	-0.056700
C20	-1.587100	-11.843600	0.139400
C21	-0.728900	-10.763600	-0.144500
C22	-1.306200	-9.596900	-0.685000
C23	-2.677700	-9.492800	-0.880200
C24	-3.547900	-10.552400	-0.551000
C25	-5.012200	-10.322100	-0.651200
C26	0.728800	-10.763600	0.144500
C27	1.586900	-11.843600	-0.139400
C28	2.969200	-11.738400	0.056700
C29	3.547800	-10.552300	0.551000
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C31	1.306000	-9.596900	0.685000
C32	-5.528200	-9.469900	-1.648100
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C35	-7.239700	-10.352900	0.355900
C36	-5.916500	-10.799900	0.318300
C37	11.060900	6.737800	-0.097900
C38	10.563000	7.552100	-1.136200
C39	9.550900	8.483100	-0.906900
C40	9.000700	8.669300	0.378400
C41	9.615700	7.973500	1.439800
C42	10.608100	7.023500	1.206800

C43	-9.550900	8.483100	0.906900
C44	-10.562900	7.552100	1.136100
C45	-11.060800	6.737800	0.097900
C46	-10.608000	7.023400	-1.206800
C47	-9.615700	7.973500	-1.439900
C48	-9.000800	8.669400	-0.378400
C49	-7.717900	9.397500	-0.565100
C50	-6.840900	9.013000	-1.601300
C51	-5.528100	9.470100	-1.648200
C52	-5.012200	10.322300	-0.651200
C53	-5.916500	10.800100	0.318200
C54	-7.239700	10.353000	0.355800
C55	2.969200	11.738500	0.056800
C56	1.587000	11.843700	-0.139300
C57	0.728800	10.763700	0.144600
C58	1.306000	9.597000	0.685100
C59	2.677500	9.492900	0.880400
C60	3.547800	10.552400	0.551100
C61	5.012000	10.322000	0.651200
C62	-0.728900	10.763700	-0.144400
C63	-1.587100	11.843800	0.139500
C64	-2.969300	11.738600	-0.056700
C65	-3.547900	10.552600	-0.551000
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C67	-1.306200	9.597100	-0.684900
C68	5.528000	9.469800	1.648200
C69	6.840800	9.012700	1.601100
C70	7.717800	9.397300	0.565000
C71	7.239500	10.352800	-0.355900
C72	5.916300	10.799800	-0.318200
C73	-12.523200	0.709200	1.959100
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C75	-12.941400	-1.417900	0.799300
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C87	-11.855500	-5.510100	0.375500
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C113	-11.632800	-3.545900	4.260800
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C116	13.436300	-0.709800	0.329200
C117	12.941500	-1.417800	-0.799300
C118	12.523400	-0.709200	-1.959100
C119	12.523400	0.709200	-1.959100
C120	12.941500	1.417800	-0.799300
C121	12.769700	2.847300	-0.730600
C122	13.926800	1.435100	1.477600
C123	13.926800	-1.435100	1.477600
C124	12.769700	-2.847300	-0.730600
C125	12.087300	-1.431000	-3.131500
C126	12.087300	1.431000	-3.131500
C127	13.081600	-3.556300	0.465400
C128	12.618400	-4.873000	0.618400
C129	11.855400	-5.510000	-0.375600
C130	11.700700	-4.850100	-1.606400

C131	12.166800	-3.545500	-1.814200
C132	11.961000	-2.849900	-3.087400
C133	11.632900	-3.545900	-4.260900
C134	11.389400	-2.876800	-5.467000
C135	11.452800	-1.478300	-5.484400
C136	11.786400	-0.734000	-4.339300
C137	11.786400	0.734000	-4.339300
C138	11.452800	1.478300	-5.484400
C139	11.389400	2.876900	-5.466900
C140	11.632900	3.545900	-4.260800
C141	11.961000	2.849900	-3.087300
C142	12.166800	3.545500	-1.814200
C143	11.700700	4.850100	-1.606300
C144	11.855400	5.510000	-0.375500
C145	12.618400	4.872900	0.618500
C146	13.081500	3.556300	0.465500
C147	13.809700	2.857000	1.530700
C148	14.379600	3.548800	2.610600
C149	15.029900	2.876300	3.653100
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C151	14.537200	0.734800	2.561000
C152	14.537200	-0.734900	2.560900
C153	15.084700	-1.477700	3.621600
C154	15.030000	-2.876400	3.653000
C155	14.379700	-3.548800	2.610500
C156	13.809800	-2.857100	1.530700
C157	11.060500	-3.643700	-6.713800
C158	9.715300	-3.950200	-7.025300
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C161	11.770000	-4.789400	-8.735800
C162	12.097100	-4.068600	-7.578100
C163	13.548000	-3.760500	-7.269400
C164	8.582700	-3.515100	-6.117900
C165	10.112300	-5.851300	-10.334700
C166	15.650300	3.640000	4.785800
C167	16.983101	4.102000	4.682800
C168	17.545700	4.812800	5.753500
C169	16.823400	5.081700	6.923500
C170	15.505500	4.612400	7.008200
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C173	17.809299	3.835900	3.441100
C174	17.439501	5.876500	8.054300

C175	15.650500	-3.640100	4.785700
C176	14.906000	-3.898300	5.960800
C177	15.505900	-4.612500	7.008000
C178	16.823799	-5.081900	6.923100
C179	17.546000	-4.813000	5.753100
C180	16.983299	-4.102200	4.682400
C181	17.809299	-3.836100	3.440700
C182	13.477500	-3.414000	6.104500
C183	17.440001	-5.876700	8.053900
C184	11.060500	3.643800	-6.713700
C185	12.097100	4.068800	-7.578000
C186	11.770000	4.789600	-8.735600
C187	10.443100	5.099100	-9.063900
C188	9.431100	4.673000	-8.193700
C189	9.715300	3.950200	-7.025300
C190	8.582700	3.515000	-6.117900
C191	13.548000	3.760800	-7.269300
C192	10.112300	5.851400	-10.334700
C193	-11.060000	3.643700	6.713600
C194	-9.714900	3.950700	7.024800
C195	-9.430600	4.673400	8.193200
C196	-10.442400	5.098900	9.063800
C197	-11.769300	4.788700	8.736000
C198	-12.096600	4.068000	7.578400
C199	-13.547400	3.759300	7.270300
C200	-8.582400	3.516200	6.116800
C201	-10.111500	5.851200	10.334600
C202	-11.060200	-3.643800	6.713600
C203	-12.096800	-4.068000	7.578400
C204	-11.769600	-4.788800	8.736100
C205	-10.442700	-5.099100	9.063800
C206	-9.430800	-4.673700	8.193200
C207	-9.715100	-3.950900	7.024800
C208	-8.582600	-3.516600	6.116800
C209	-13.547600	-3.759200	7.270300
C210	-10.111800	-5.851400	10.334600
C211	-15.650600	3.640100	-4.785600
C212	-14.906400	3.897500	-5.961100
C213	-15.506400	4.611800	-7.008300
C214	-16.823999	5.081800	-6.923000
C215	-17.545900	4.813600	-5.752700
C216	-16.983200	4.102900	-4.682000
C217	-17.808800	3.837500	-3.439900
C218	-13.478300	3.412400	-6.105200

C219	-17.440201	5.876700	-8.053800
C220	-15.650600	-3.640000	-4.785700
C221	-16.983500	-4.101900	-4.682500
C222	-17.546200	-4.812700	-5.753200
C223	-16.823999	-5.081600	-6.923200
C224	-15.506100	-4.612400	-7.008000
C225	-14.906100	-3.898300	-5.960800
C226	-13.477600	-3.414100	-6.104400
C227	-17.809500	-3.835700	-3.440800
C228	-17.440201	-5.876500	-8.054000
H229	-10.930300	-7.421100	2.148600
H230	-9.130900	-9.013400	1.754700
H231	-9.277400	-8.133600	-2.457800
H232	-10.975400	-6.441200	-2.044800
H233	9.130700	-9.013300	-1.754800
H234	10.930100	-7.421000	-2.148700
H235	10.975200	-6.441100	2.044700
H236	9.277300	-8.133400	2.457800
H237	7.164200	-8.288200	2.339600
H238	4.878500	-9.126400	2.446300
H239	5.563700	-11.472500	-1.094100
H240	7.893000	-10.720500	-1.140600
H241	-3.605300	-12.584600	0.185600
H242	-1.176100	-12.759200	0.554400
H243	-0.666800	-8.760200	-0.945700
H244	-3.088600	-8.559600	-1.249000
H245	1.176000	-12.759200	-0.554400
H246	3.605200	-12.584600	-0.185600
H247	3.088400	-8.559600	1.249100
H248	0.666700	-8.760200	0.945800
H249	-4.878600	-9.126400	-2.446300
H250	-7.164400	-8.288300	-2.339700
H251	-7.893200	-10.720700	1.140400
H252	-5.563800	-11.472600	1.094000
H253	10.930100	7.421000	-2.148600
H254	9.130700	9.013300	-1.754700
H255	9.277200	8.133400	2.457900
H256	10.975200	6.441100	2.044800
H257	-9.130700	9.013300	1.754700
H258	-10.930000	7.421000	2.148600
H259	-10.975200	6.441000	-2.044800
H260	-9.277300	8.133400	-2.457900
H261	-7.164200	8.288500	-2.339900
H262	-4.878500	9.126700	-2.446500

H263	-5.563900	11.472800	1.093900
H264	-7.893200	10.720700	1.140300
H265	3.605200	12.584600	-0.185500
H266	1.176000	12.759300	-0.554300
H267	0.666600	8.760400	0.945900
H268	3.088400	8.559700	1.249200
H269	-1.176100	12.759300	0.554500
H270	-3.605300	12.584800	0.185600
H271	-3.088600	8.559800	-1.249100
H272	-0.666800	8.760400	-0.945700
H273	4.878400	9.126400	2.446400
H274	7.164200	8.288200	2.339700
H275	7.893000	10.720500	-1.140400
H276	5.563700	11.472500	-1.094000
H277	-11.101400	-5.316800	2.376300
H278	-12.790300	-5.388100	-1.555100
H279	-14.343500	-4.631600	-2.641900
H280	-15.569900	-0.974500	-4.448600
H281	-15.569900	0.974500	-4.448600
H282	-14.343400	4.631600	-2.641800
H283	-12.790200	5.388100	-1.555000
H284	-11.101100	5.316600	2.376300
H285	-11.585900	4.628600	4.254000
H286	-11.234600	0.976000	6.418600
H287	-11.234600	-0.976100	6.418600
H288	-11.586100	-4.628700	4.254000
H289	12.790200	-5.388100	1.555000
H290	11.101300	-5.316700	-2.376400
H291	11.586200	-4.628600	-4.254100
H292	11.234800	-0.976000	-6.418700
H293	11.234800	0.976100	-6.418600
H294	11.586200	4.628600	-4.254000
H295	11.101300	5.316700	-2.376300
H296	12.790100	5.388000	1.555100
H297	14.343300	4.631500	2.642000
H298	15.569800	0.974500	4.448700
H299	15.569800	-0.974500	4.448600
H300	14.343400	-4.631600	2.641800
H301	8.395500	-4.908300	-8.426300
H302	12.571200	-5.116600	-9.393900
H303	13.857300	-4.186700	-6.307500
H304	13.727300	-2.680600	-7.204600
H305	14.205100	-4.165500	-8.044900
H306	8.555700	-2.425500	-5.996800

H307	8.683800	-3.938100	-5.111100
H308	7.616800	-3.833500	-6.521400
H309	9.164700	-6.393000	-10.244000
H310	10.894100	-6.576400	-10.586100
H311	10.016600	-5.167800	-11.189700
H312	18.572100	5.161400	5.670100
H313	14.928700	4.804700	7.909600
H314	12.838300	3.793100	5.297900
H315	13.049800	3.741100	7.057100
H316	13.412900	2.319700	6.064600
H317	18.819300	4.241900	3.551500
H318	17.359301	4.289200	2.549600
H319	17.896200	2.762300	3.235500
H320	18.531401	5.792600	8.053600
H321	17.074400	5.535400	9.029400
H322	17.194300	6.944400	7.971500
H323	14.929200	-4.804800	7.909500
H324	18.572300	-5.161500	5.669600
H325	18.819401	-4.242000	3.551000
H326	17.359200	-4.289400	2.549200
H327	17.896299	-2.762500	3.235100
H328	12.838600	-3.793100	5.298000
H329	13.050300	-3.741200	7.057200
H330	13.413300	-2.319700	6.064800
H331	18.531900	-5.791600	8.053900
H332	17.073999	-5.536600	9.028900
H333	17.195999	-6.944800	7.970300
H334	12.571200	5.116900	-9.393800
H335	8.395500	4.908300	-8.426300
H336	8.555800	2.425500	-5.996900
H337	8.683700	3.938100	-5.111100
H338	7.616800	3.833400	-6.521500
H339	13.857400	4.187300	-6.307500
H340	14.205100	4.165500	-8.044900
H341	13.727300	2.680900	-7.204000
H342	9.164700	6.393000	-10.243900
H343	10.894100	6.576700	-10.585900
H344	10.016800	5.168000	-11.189700
H345	-8.395000	4.909100	8.425400
H346	-12.570400	5.115600	9.394600
H347	-13.856900	4.184000	6.307800
H348	-14.204500	4.165200	8.045300
H349	-13.726600	2.679200	7.207000
H350	-7.616500	3.834200	6.520500

H351	-8.683600	3.940100	5.110400
H352	-8.555600	2.426800	5.994900
H353	-9.163600	6.392200	10.244000
H354	-10.016600	5.167800	11.189700
H355	-10.892900	6.576900	10.585600
H356	-12.570700	-5.115600	9.394600
H357	-8.395300	-4.909500	8.425400
H358	-7.616700	-3.834500	6.520600
H359	-8.683700	-3.940700	5.110400
H360	-8.555800	-2.427200	5.994600
H361	-13.857100	-4.183800	6.307800
H362	-14.204800	-4.165100	8.045300
H363	-13.726700	-2.679100	7.207100
H364	-9.164000	-6.392500	10.244000
H365	-10.016800	-5.168000	11.189700
H366	-10.893300	-6.577000	10.585600
H367	-14.929900	4.803500	-7.910100
H368	-18.572001	5.162700	-5.668900
H369	-17.896000	2.764000	-3.233800
H370	-17.358299	4.291100	-2.548800
H371	-18.818800	4.243700	-3.550000
H372	-12.839100	3.790100	-5.298200
H373	-13.050700	3.740400	-7.057500
H374	-13.414800	2.318000	-6.066800
H375	-18.532101	5.791800	-8.053700
H376	-17.195999	6.944700	-7.970200
H377	-17.074301	5.536500	-9.028900
H378	-18.572599	-5.161200	-5.669700
H379	-14.929300	-4.804800	-7.909500
H380	-12.838700	-3.793400	-5.298000
H381	-13.050400	-3.741300	-7.057200
H382	-13.413200	-2.319900	-6.064600
H383	-17.897200	-2.762000	-3.235800
H384	-17.358999	-4.288100	-2.549100
H385	-18.819401	-4.242400	-3.550700
H386	-18.532101	-5.791100	-8.054200
H387	-17.196501	-6.944600	-7.970100
H388	-17.073900	-5.536600	-9.029000

Table S2. Excitation energies and oscillator strengths for the optimized structure of **5**.

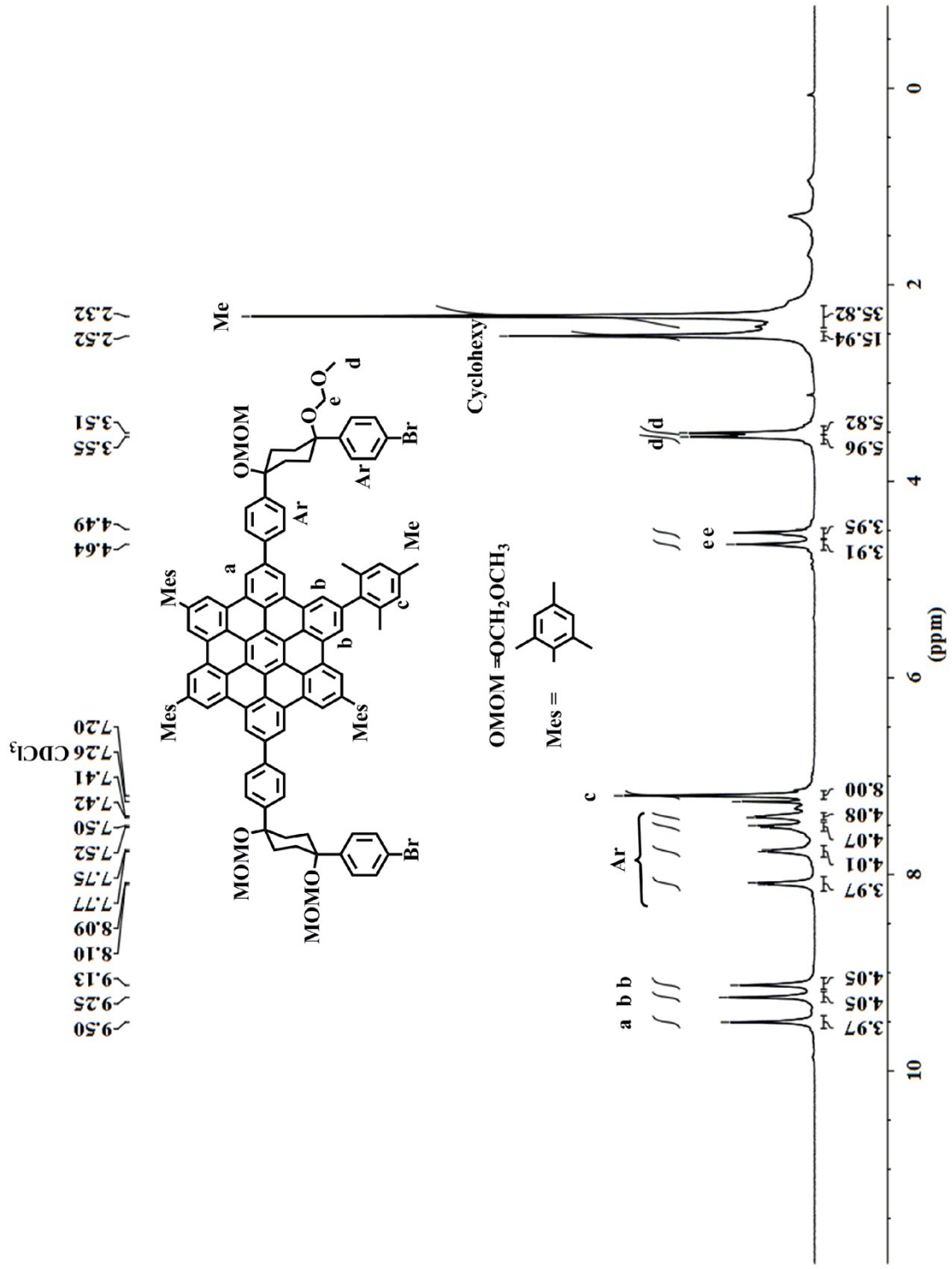
Excited state	Description				Energy	Wavelength	Oscillator strength (*f*)
1	HOMO 4	->	LUMO 2	-0.35364	2.8068eV	441.73nm	0.0019
	HOMO 3	->	LUMO 1	0.35777			
	HOMO 2	->	LUMO 4	0.33391			
	HOMO 1	->	LUMO 3	-0.3358			
2	HOMO 4	->	LUMO 1	0.35798	2.8068eV	441.72nm	0.0000
	HOMO 3	->	LUMO 2	-0.35359			
	HOMO 2	->	LUMO 3	0.33363			
	HOMO 1	->	LUMO 4	-0.33582			
3	HOMO 4	->	LUMO 4	0.12881	2.8226eV	439.26nm	0.0000
	HOMO 3	->	LUMO 3	0.12839			
	HOMO 2	->	LUMO 2	0.42398			
	HOMO 1	->	LUMO 1	0.52186			
4	HOMO 4	->	LUMO 3	-0.16712	2.8536eV	434.48nm	1.0120
	HOMO 3	->	LUMO 4	-0.16713			
	HOMO 2	->	LUMO 1	0.4651			
	HOMO 1	->	LUMO 2	0.46868			
5	HOMO 4	->	LUMO 4	0.16102	3.1209eV	397.28nm	0.0000
	HOMO 3	->	LUMO 3	0.1614			
	HOMO 2	->	LUMO 2	0.46839			
	HOMO 1	->	LUMO 1	-0.44621			
6	HOMO 2	->	LUMO 1	-0.49764	3.1294eV	396.19nm	0.0001
	HOMO 1	->	LUMO 2	0.49991			
7	HOMO 9	->	LUMO 1	0.17425	3.1692eV	391.21nm	0.0000
	HOMO 8	->	LUMO 2	0.17248			
	HOMO 2	->	LUMO 7	-0.43388			
	HOMO 1	->	LUMO 6	0.4588			
8	HOMO 9	->	LUMO 2	-0.17407	3.1697eV	391.16nm	0.0109
	HOMO 8	->	LUMO 1	-0.17654			
	HOMO 2	->	LUMO 6	-0.43951			
	HOMO 1	->	LUMO 7	0.46497			
9	HOMO 10	->	LUMO 2	0.10547	3.2104eV	386.19nm	0.0000

	HOMO 6	->	LUMO 1	-0.20396			
	HOMO 5	->	LUMO 5	-0.17301			
	HOMO 4	->	LUMO 4	0.35178			
	HOMO 3	->	LUMO 3	0.35187			
	HOMO 2	->	LUMO 2	-0.27833			
	HOMO 2	->	LUMO 10	-0.11265			
	HOMO 1	->	LUMO 8	-0.20824			
10	HOMO 10	->	LUMO 1	-0.11257	3.2706eV	379.09nm	2.4562
	HOMO 6	->	LUMO 2	0.1791			
	HOMO 4	->	LUMO 3	0.41244			
	HOMO 3	->	LUMO 4	0.41255			
	HOMO 2	->	LUMO 1	0.16799			
	HOMO 2	->	LUMO 8	0.1714			
	HOMO 1	->	LUMO 2	0.15312			
	HOMO 1	->	LUMO 10	0.12025			
11	HOMO 7	->	LUMO 2	-0.15278	3.2766eV	378.4nm	2.3971
	HOMO 6	->	LUMO 5	0.11908			
	HOMO 5	->	LUMO 1	0.54245			
	HOMO 5	->	LUMO 8	0.10349			
	HOMO 4	->	LUMO 7	-0.10138			
	HOMO 3	->	LUMO 1	-0.12967			
	HOMO 3	->	LUMO 6	-0.10257			
	HOMO 1	->	LUMO 5	0.31349			
12	HOMO 4	->	LUMO 1	0.4759	3.2923eV	376.59nm	0.0000
	HOMO 3	->	LUMO 2	-0.13434			
	HOMO 2	->	LUMO 3	-0.21126			
	HOMO 1	->	LUMO 4	0.43515			
13	HOMO 5	->	LUMO 1	0.10864	3.2953eV	376.24nm	1.5944
	HOMO 4	->	LUMO 2	-0.11444			
	HOMO 3	->	LUMO 1	0.46921			
	HOMO 2	->	LUMO 4	-0.18925			
	HOMO 1	->	LUMO 3	0.43865			
	HOMO 1	->	LUMO 5	0.10164			
14	HOMO 4	->	LUMO 1	0.36864	3.3249eV	372.9nm	0.0000
	HOMO 3	->	LUMO 2	0.55231			
	HOMO 1	->	LUMO 4	-0.19496			
15	HOMO 4	->	LUMO 2	0.55761	3.3259eV	372.79nm	0.1639
	HOMO 3	->	LUMO 1	0.35461			

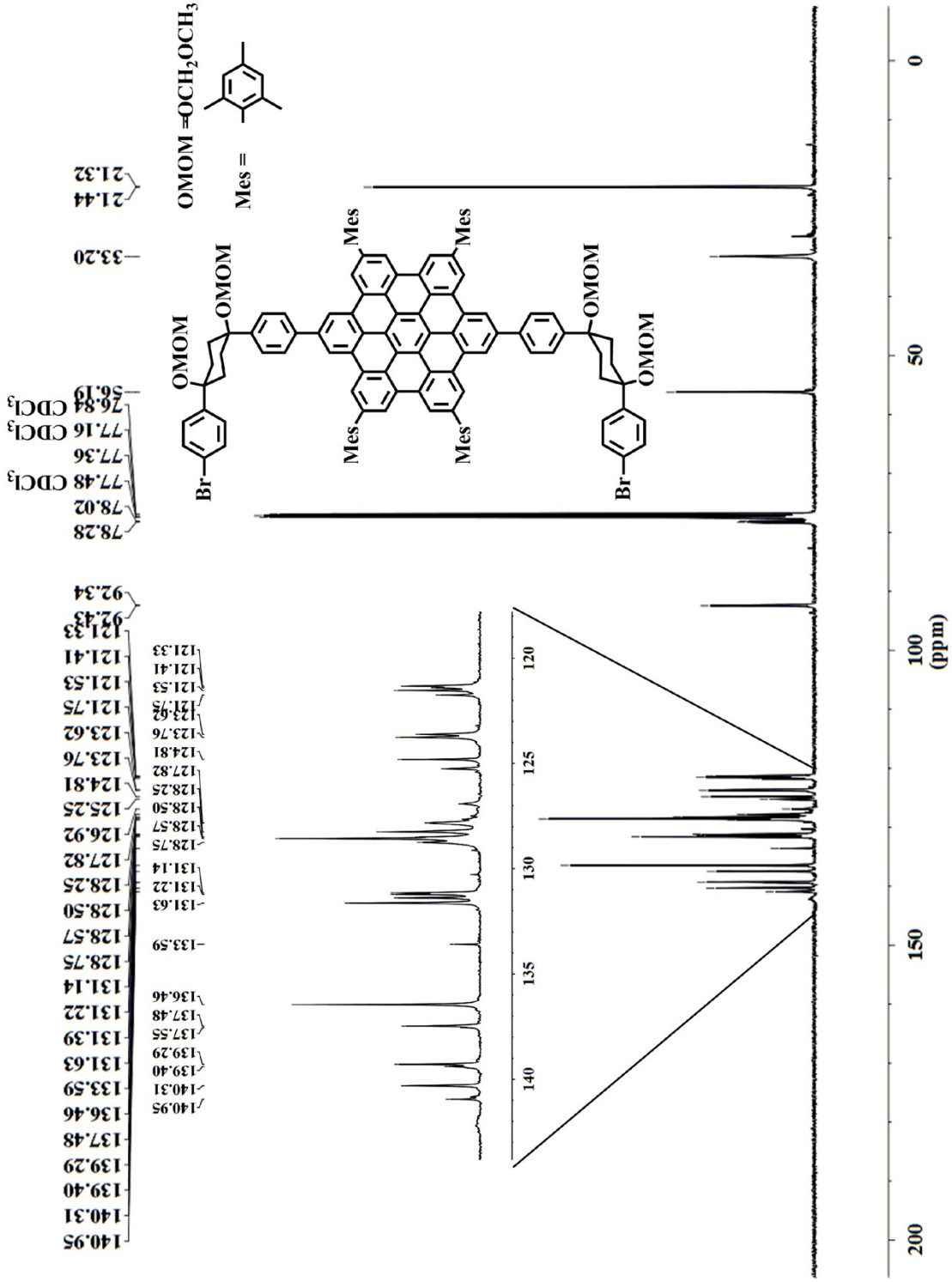
	HOMO 1	->	LUMO 3	-0.23			
16	HOMO 9	->	LUMO 4	0.13776	3.3391eV	371.31nm	0.0000
	HOMO 8	->	LUMO 3	-0.13375			
	HOMO 5	->	LUMO 2	0.22514			
	HOMO 4	->	LUMO 6	0.3948			
	HOMO 3	->	LUMO 7	0.39453			
	HOMO 2	->	LUMO 3	-0.14204			
	HOMO 2	->	LUMO 5	-0.10356			
	HOMO 1	->	LUMO 4	-0.21405			
17	HOMO 9	->	LUMO 3	0.15283	3.3431eV	370.86nm	0.0426
	HOMO 8	->	LUMO 4	-0.15001			
	HOMO 4	->	LUMO 7	0.42511			
	HOMO 3	->	LUMO 6	0.42501			
	HOMO 1	->	LUMO 3	-0.14281			
	HOMO 1	->	LUMO 5	0.20659			
18	HOMO 4	->	LUMO 2	0.19178	3.3507eV	370.03nm	0.2338
	HOMO 2	->	LUMO 4	0.56788			
	HOMO 1	->	LUMO 3	0.33107			
19	HOMO 4	->	LUMO 6	0.15279	3.3507eV	370.02nm	0.0026
	HOMO 3	->	LUMO 2	0.17769			
	HOMO 3	->	LUMO 7	0.15188			
	HOMO 2	->	LUMO 3	0.54718			
	HOMO 1	->	LUMO 4	0.3241			
20	HOMO 7	->	LUMO 1	-0.16642	3.3635eV	368.62nm	0.0000
	HOMO 5	->	LUMO 2	0.61036			
	HOMO 4	->	LUMO 6	-0.16878			
	HOMO 3	->	LUMO 7	-0.16925			
	HOMO 2	->	LUMO 5	-0.12571			

7. NMR spectra for new compounds

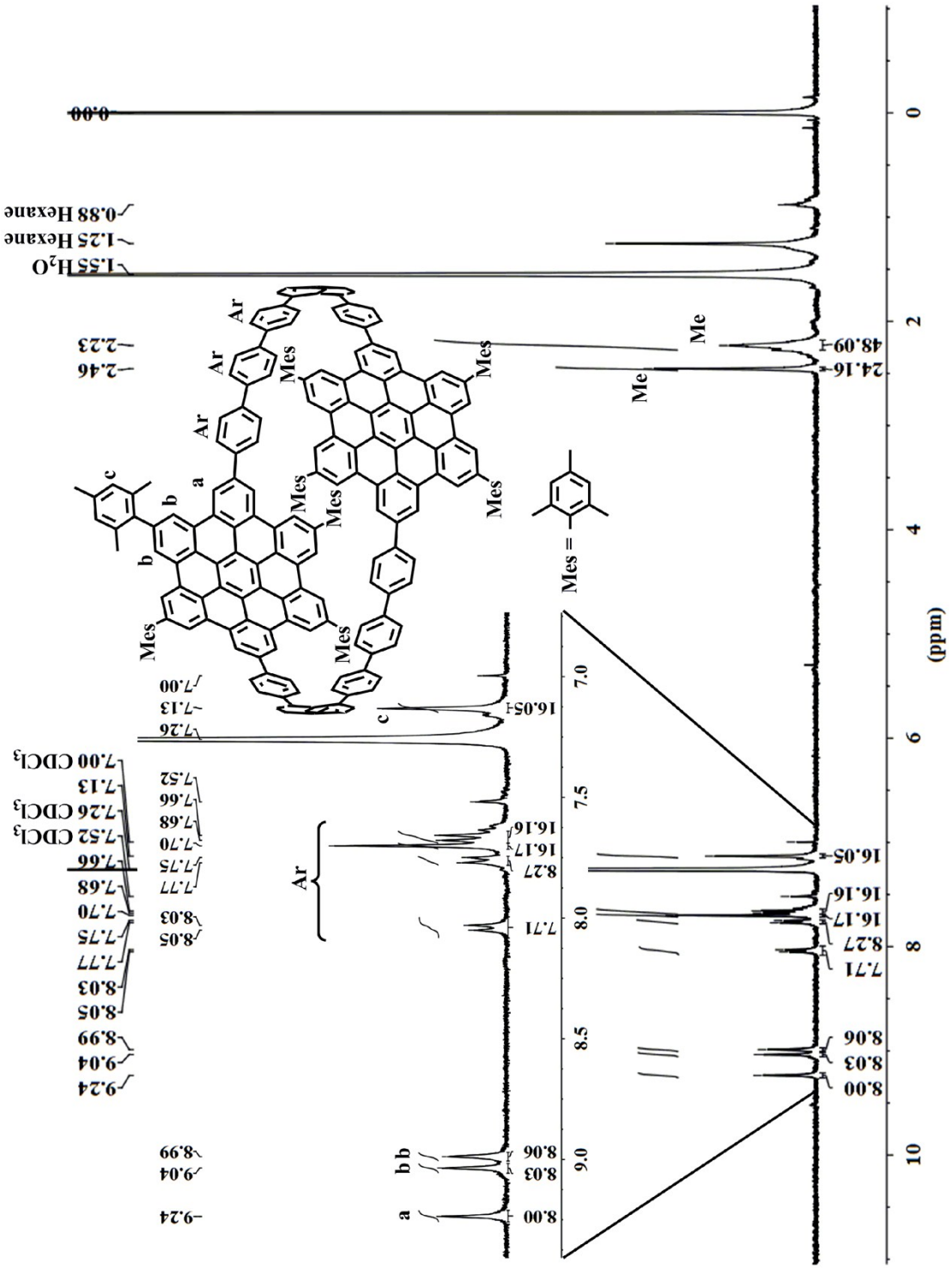
^{1}H NMR spectrum of **3** in $CDCl_3$



^{13}C NMR spectrum of **3** in $CDCl_3$



^{1}H NMR spectrum of **5** in $CDCl_3$



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