Bending Contorted Hexabenzocoronene into a Bowl

Adam C. Whalley[1], Kyle N. Plunkett[2], Alon A. Gorodetsky[1], Christine L. Schenck[1], Chien-Yang Chiu[1], Michael L. Steigerwald[1]*, and Colin Nuckolls[1]*

[1]*Department of Chemistry, Columbia University, New York, NY*

[2]*Department of Chemistry, Southern Illinois University, Carbondale, IL*

AUTHOR EMAIL ADDRESS: cn37@columbia.edu; mls2064@columbia.edu

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1. DFT Calculated HOMO and LUMO Energies

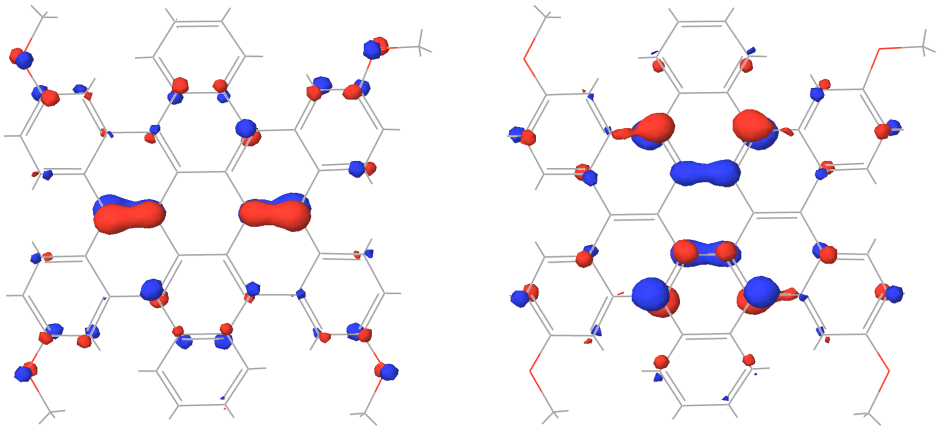


Figure 1. Tetramethoxy-HBC HOMO (left) and LUMO (right)

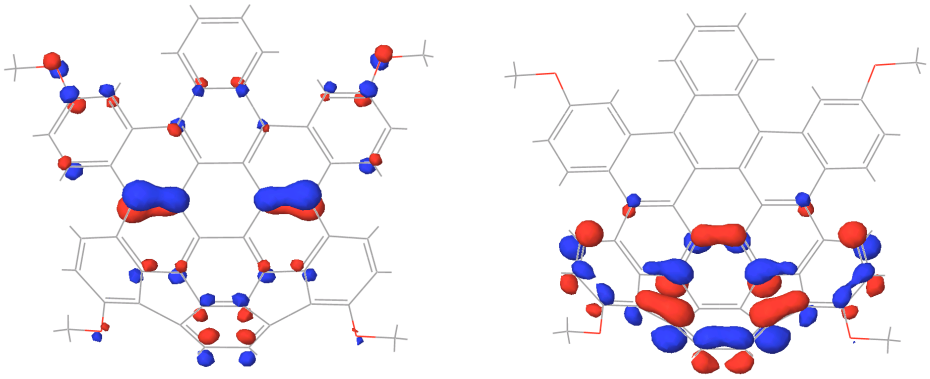


Figure 2. 2-closed tetramethoxy-HBC HOMO (left) and LUMO (right)

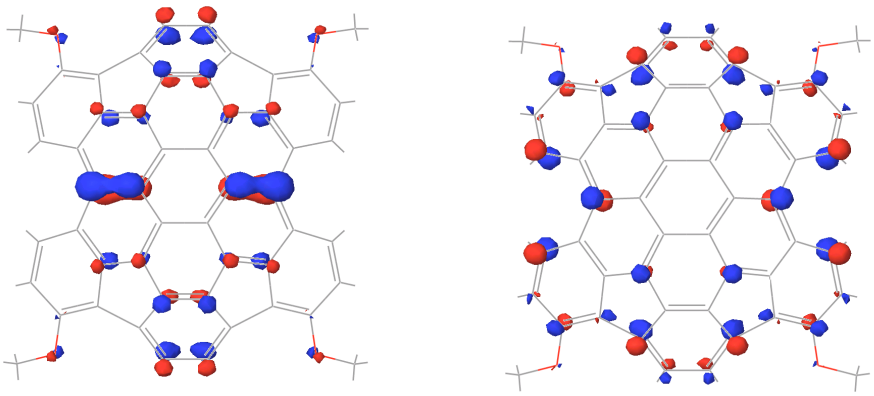
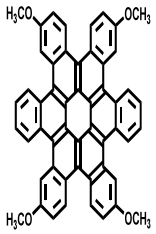


Figure 3. 4-closed tetramethoxy-HBC HOMO (left) and LUMO (right)

2. DFT state summaries and structure coordinates

B3LYP with the 631G** basis set using the Jaguar software package Version 7.0, Schrödinger, LLC, New York, NY, 2007



Tetramethoxy HBC State Summary

Excited State 1: 2.6568 eV 466.67 nm

orbitals in excitation | CI coeff.

188 => 189	0.81518
187 => 190	0.54942

Transition dipole moment (debye):
X= -0.9135 Y= 1.0194 Z= 1.5396 Tot= 2.0601

Oscillator strength, f= 0.0428

Excited State 2: 2.8410 eV 436.41 nm

orbitals in excitation | CI coeff.

187 => 189	0.62610
188 => 189	0.10443
188 => 190	-0.76229

Transition dipole moment (debye):
X= 0.8667 Y= 0.1540 Z= 0.8281 Tot= 1.2086

Oscillator strength, f= 0.0157

Excited State 3: 2.9702 eV 417.42 nm

orbitals in excitation | CI coeff.

186 => 189	0.21148
186 => 190	-0.42915
187 => 191	-0.10439
188 => 191	-0.85244

Transition dipole moment (debye):

X= -0.1755 Y= 0.0402 Z= 0.0064 Tot= 0.1801

Oscillator strength, f= 0.0004

Excited State 4: 3.0248 eV 409.90 nm

orbitals in excitation | CI coeff.

186 => 189	-0.73990
186 => 190	-0.15463
187 => 191	0.60184
188 => 191	-0.17957

Transition dipole moment (debye):
X= 0.2766 Y= 0.0349 Z= 0.2323 Tot= 0.3629

Oscillator strength, f= 0.0015

Excited State 5: 3.3089 eV 374.70 nm

orbitals in excitation | CI coeff.

187 => 189	0.72286
188 => 190	0.58699
183 => 191	-0.12506
184 => 191	-0.11807
186 => 191	0.17391

Transition dipole moment (debye):
X= -7.5281 Y= -0.6581 Z= -4.3219 Tot= 8.7054

Oscillator strength, f= 0.9509

Excited State 6: 3.3579 eV 369.23 nm

orbitals in excitation | CI coeff.

185 => 189	-0.10380
186 => 189	0.21687
188 => 189	0.33939
186 => 190	-0.49536
187 => 190	-0.57834
186 => 191	0.21113

187 => 191 0.19198
188 => 191 0.29400

Transition dipole moment (debye):
X= -2.5030 Y= 2.5371 Z= 4.3187 Tot= 5.5994

Oscillator strength, f= 0.3992

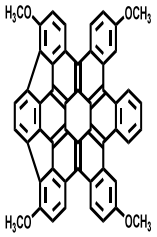
Tetramethoxy HBC DFT Summary

Final total energy = -2301.78854791482 h
final geometry:

	angstroms		
atom	x	y	z
C1	0.0371379519	0.0049513063	-0.0087638074
C2	0.0177611003	-0.0203845638	1.4072292708
C3	1.2657266490	-0.0472208330	2.0999525826
C4	2.4601878407	-0.0703966666	1.3376593353
C5	2.4431047154	-0.0828092989	-0.0418530439
C6	1.2173773643	-0.0389094880	-0.7230900844
C7	1.2845038129	0.1227871344	3.5365566010
C8	0.1475920760	0.6752111740	4.1478658927
C9	-1.1213411968	0.6483134165	3.4650333927
C10	-1.2102597530	0.1161705871	2.1663194463
C11	-2.2956985488	1.1574199063	4.1208882629
C12	-2.1964727693	1.7273238638	5.4406655951
C13	-0.9173137679	1.7930373819	6.1010130134
C14	0.2516534991	1.2618345726	5.4555475847
C15	-3.3430085381	2.2184653544	6.0847972492
C16	-3.2889461718	2.4097629799	7.5178088421
C17	-2.0195495161	2.4911058121	8.1660850540
C18	-0.8124438168	2.3665668559	7.3793227660
C19	-4.4546617640	2.3753063156	8.3236327684
C20	-4.3918691543	2.4537966063	9.6992293297
C21	-3.1442502496	2.5369985800	10.3362906121
C22	-1.9889115061	2.5380878759	9.5825736794
C23	1.4996152651	1.3156385886	6.1035838127
C24	1.6559359427	2.2586811429	7.1897361531
C25	0.4983985166	2.7871307982	7.8319387346
C26	-3.5434098693	1.0886455698	3.4761980276
C27	-4.6154021786	1.9265899182	3.9723180265
C28	-4.5149751628	2.5002260904	5.2786694404
C29	2.4148927886	-0.2118093191	4.3768728231
C30	2.5369061425	0.4136947660	5.6517669548
C31	0.6541016552	3.8017190877	8.8091932853
C32	1.9041283148	4.2818351965	9.1541840581
C33	3.0491407734	3.7687862527	8.5145444941
C34	2.9184782403	2.7934593311	7.5549728007

C35	-2.5142702225	-0.2769827290	1.6748136241
C36	-3.6799312550	0.1934007727	2.3486506942
C37	-5.4995208274	3.4190986746	5.6941708820
C38	-6.5674294430	3.7657524570	4.8829224956
C39	-6.6683227164	3.2112166820	3.5956829121
C40	-5.7033985312	2.3232191324	3.1623118218
C41	3.6037686902	-0.0026399661	6.4907434488
C42	4.4954456337	-0.9759657431	6.1095076244
C43	4.3585607004	-1.6051654361	4.8567078104
C44	3.3309520075	-1.2300052385	4.0107088186
C45	-2.6603679307	-1.2211425367	0.6253584196
C46	-3.9039938582	-1.6891500663	0.2445999200
C47	-5.0532566343	-1.2522542490	0.9309457442
C48	-4.9327785095	-0.3475640501	1.9571284863
H1	3.8030814539	2.4735864869	7.0183002230
H2	4.0159610734	4.1938199744	8.7634126091
O1	2.1276051206	5.2735048836	10.0561617508
H3	-0.2288272126	4.2582519424	9.2286794468
H4	-1.7744753899	-1.6369098397	0.1722924437
O2	-4.1182616303	-2.6028533288	-0.7382531135
H5	-6.0134270213	-1.6783243135	0.6589547845
H6	-5.8186577210	-0.0876762360	2.5210997731
H7	3.6778824731	0.3993966949	7.4925786855
H8	5.2833977676	-1.3138563053	6.7745884207
O3	5.2573906743	-2.5890375251	4.5924822352
H9	3.1745808885	-1.7587100786	3.0820312911
H10	-5.7535232298	1.9784530246	2.1376695724
H11	-7.4642645074	3.5021931408	2.9204954492
O4	-7.4402549768	4.6781711405	5.3949905718
H12	-5.4103540505	3.9408412223	6.6371484847
H13	3.4116668042	-0.0072963557	1.8506902351
H14	3.3781477108	-0.0755432211	-0.5951311423
H15	1.1951878847	0.0059761783	-1.8084331924
H16	-0.8949628947	0.1267879522	-0.5449318999
H17	-5.4164118578	2.2203399009	7.8521182093
H18	-5.3050044475	2.4049415004	10.2858148875
H19	-3.0836058192	2.5518524912	11.4210110933
H20	-1.0321503070	2.5055080434	10.0882820319
C49	-8.5121371221	5.1210646161	4.5800174229
H21	-9.0692754525	5.8424951584	5.1798634096
H22	-8.1535316610	5.6152307282	3.6677756800
H23	-9.1803135665	4.2962412465	4.3004501046
C50	-3.0007028509	-3.1014909378	-1.4518998556
H24	-3.4001523835	-3.7849463929	-2.2028469101
H25	-2.4490326960	-2.2958658094	-1.9533114108
H26	-2.3122395249	-3.6498364293	-0.7961948719
C51	1.0112288673	5.8760321966	10.6878505283
H27	1.4160618880	6.6246709233	11.3706207727
H28	0.3529260987	6.3694317528	9.9613995233

H29	0.4253936712	5.1451698287	11.2599408070
C52	5.1477939345	-3.2906756258	3.3669176356
H30	5.9628669317	-4.0159642994	3.3579218652
H31	4.1911857554	-3.8231055824	3.2895945163
H32	5.2521600002	-2.6186663196	2.5054384374



2-closed Tetramethoxy HBC State Summary

Excited State 1: 2.4235 eV 511.59 nm

orbitals in excitation | CI coeff.

186 => 187	0.95099
184 => 188	0.21165
185 => 188	0.10492

Transition dipole moment (debye):
X= 1.2643 Y= 0.1185 Z= 2.3427 Tot= 2.6647

Oscillator strength, f= 0.0653

Excited State 2: 2.5559 eV 485.10 nm

orbitals in excitation | CI coeff.

183 => 187	0.20531
184 => 187	-0.94139
185 => 187	-0.21123
186 => 188	-0.11384

Transition dipole moment (debye):
X= -0.0081 Y= 0.0060 Z= -0.0949 Tot= 0.0955

Oscillator strength, f= 0.0001

Excited State 3: 2.6354 eV 470.45 nm

orbitals in excitation | CI coeff.

184 => 187 0.15762
185 => 187 -0.88850
186 => 188 0.39859

Transition dipole moment (debye):
X= -1.2786 Y= -0.2945 Z= 0.7040 Tot= 1.4890

Oscillator strength, f= 0.0222

Excited State 4: 2.8096 eV 441.29 nm

orbitals in
excitation CI coeff.
---
186 => 187 0.10896
184 => 188 -0.14056
185 => 188 -0.58219
186 => 189 -0.77859

Transition dipole moment (debye):
X= -0.2733 Y= 0.1860 Z= 0.1726 Tot= 0.3729

Oscillator strength, f= 0.0015

Excited State 5: 2.8757 eV 431.14 nm

orbitals in
excitation CI coeff.
---
183 => 187 0.41426
184 => 187 0.22684
185 => 187 -0.25801
186 => 188 -0.74236
184 => 189 0.23415
185 => 189 0.26875

Transition dipole moment (debye):
X= -3.2004 Y= -0.9628 Z= 1.7815 Tot= 3.7872

Oscillator strength, f= 0.1564

Excited State 6: 3.0643 eV 404.60 nm

orbitals in
excitation CI coeff.
---

183 => 187 0.82648
184 => 187 0.11257
185 => 187 0.15276
186 => 188 0.33900
184 => 189 -0.32081
184 => 192 -0.10297

Transition dipole moment (debye):
X= 2.6440 Y= 0.6746 Z= -1.3580 Tot= 3.0480

Oscillator strength, f= 0.1080

Excited State 7: 3.1840 eV 389.40 nm

orbitals in
excitation CI coeff.
---
182 => 187 -0.25164
183 => 188 0.25488
184 => 188 -0.77827
185 => 188 0.44711
186 => 189 -0.15429

Transition dipole moment (debye):
X= -0.3607 Y= 0.0759 Z= -0.5292 Tot= 0.6450

Oscillator strength, f= 0.0050

Excited State 8: 3.3360 eV 371.66 nm

orbitals in
excitation CI coeff.
---
181 => 187 0.16956
183 => 187 0.18672
185 => 187 0.14462
183 => 188 -0.20471
184 => 188 0.11569
185 => 188 0.19836
184 => 189 0.69750
185 => 189 -0.48426
186 => 189 -0.18243

Transition dipole moment (debye):
X= 0.6953 Y= 0.8196 Z= -2.1309 Tot= 2.3866

Oscillator strength, f= 0.0721

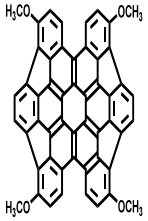
2-closed Tetramethoxy HBC DFT Summary

Final total energy = -2299.36499902024 h

final geometry:

	angstroms		
atom	x	y	z
C1	-0.1008298469	0.1070592417	0.0351178025
C2	-0.0598262327	0.1247587130	1.4387277060
C3	1.2074030069	0.0108926804	2.1048685516
C4	2.3605452215	-0.0501808007	1.2907884313
C5	2.3029741970	-0.0154664244	-0.0956275859
C6	1.0507622086	0.0543290100	-0.7325606386
C7	-1.2942699956	0.1695812016	2.2037421784
C8	-1.2691400002	-0.3786474505	3.4901387440
C9	0.0117102671	-0.5925069665	4.1326493566
C10	1.2398049700	-0.1711107083	3.5477649309
C11	-2.5179111661	-0.6033639588	4.2033015107
C12	-3.7356489053	-0.2774212522	3.5984761860
C13	-3.7337835420	0.5745005122	2.4310244629
C14	-2.5073635825	0.8028597276	1.7319469640
C15	-4.9444154947	-0.7862902943	4.2265489889
C16	-4.9479540469	-1.1161395958	5.6227500141
C17	-3.7060616538	-1.0302221045	6.3749682867
C18	-2.5245997852	-1.0357714594	5.5841874216
C19	-6.0763001210	-1.0821551504	3.4476043302
C20	-7.2022513101	-1.6790968553	3.9935373794
C21	-7.2386921462	-1.9607952574	5.3715868183
C22	-6.1284880100	-1.6782846329	6.1554919283
C23	-1.2569697108	-1.2696066764	6.1847949957
C24	-1.1954453149	-1.3769521031	7.5620108600
C25	-2.2913833820	-1.0436614075	8.3793294666
C26	-3.5786477921	-0.8978334869	7.8345998663
C27	-0.0255366125	-1.0600619613	5.4775663016
C28	-2.4982039081	1.7739974292	0.6959828188
C29	-3.6346653437	2.4674436574	0.3371374168
C30	-4.8398402387	2.2367925012	1.0196909066
C31	-4.8785482744	1.3215631834	2.0502732994
C32	1.1336863527	-0.9942084267	6.2256786225
C33	2.2744563018	-0.3091798644	5.7701887598
C34	2.3951612440	0.0876385386	4.4266051177
C35	1.1605896381	-0.9882834709	7.6388342791
C36	-0.0175113049	-1.1691963698	8.3129042884
C37	-1.8062859765	-0.5783199824	9.6442793245
C38	-2.7656836315	-0.0353038089	10.4901941621
C39	-4.1214466855	0.0152801769	10.0404415542

C40	-4.5209531523	-0.3764825397	8.7668997127
C41	-0.2966212725	-0.5871315192	9.5696257584
C42	0.7911942273	0.0991072646	10.1376231736
C43	2.0343635953	0.2782685305	9.4347152899
C44	2.2338019522	-0.2155685140	8.1334363487
C45	3.0286653642	0.1439793670	6.8996832748
C46	4.1369193058	0.9286619503	6.6078729274
C47	4.3857629027	1.2663221948	5.2421895242
C48	3.5456825513	0.8969918683	4.1957070642
H49	3.7587141934	1.2987300334	3.2121910812
H50	5.2363851857	1.8954891425	5.0070273642
O51	4.8924163242	1.3680837688	7.6518775854
H52	-6.0587055424	-0.9324058245	2.3758671715
O53	-8.1908658536	-1.9808326564	3.0995633376
H54	-8.1014897415	-2.4380477595	5.8211838304
H55	-6.1424894364	-1.9761346247	7.1978360528
H56	3.3262767795	-0.1954320302	1.7594416005
H57	3.2194664264	-0.0892300754	-0.6695493291
O58	0.8445438271	0.0476349364	-2.0834251196
H59	-1.0482226477	0.0918401484	-0.4857775980
H60	-5.5525833861	-0.2063403011	8.4793070225
H61	-4.8741395515	0.4329380237	10.6989647195
O62	-2.3460160260	0.4637181833	11.6854113192
H63	-1.5624758895	2.0259558041	0.2168953653
H64	-3.5824818586	3.2202857809	-0.4441325492
H65	-5.7296874820	2.8072536195	0.7698214788
H66	-5.7907156547	1.2130391561	2.6214522402
H67	0.6804329680	0.6151614665	11.0860596443
H68	2.7801260950	0.9159870764	9.9003269052
C69	6.0335774912	2.1743502679	7.3932702260
H70	6.4793273457	2.3793410201	8.3676834892
H71	6.7650841389	1.6492027719	6.7666845552
H72	5.7615622623	3.1232561081	6.9142805053
C73	-3.2821193553	1.1213587045	12.5288078246
H74	-2.7135830564	1.4618357201	13.3950750022
H75	-3.7377871227	1.9863340756	12.0319078213
H76	-4.0725840731	0.4394331313	12.8653421607
C77	-9.2996074973	-2.7456890142	3.5420778589
H78	-9.9185665402	-2.9152579210	2.6593698018
H79	-8.9862482897	-3.7136548885	3.9539147694
H80	-9.8918083524	-2.2102689851	4.2955837898
C81	1.9674954920	0.0028424166	-2.9466385692
H82	1.5670774865	0.0284464130	-3.9615461192
H83	2.6281887631	0.8673222721	-2.7996892138
H84	2.5488678198	-0.9187713917	-2.8133213185



4-closed Tetramethoxy HBC State Summary

Excited State 1: 2.5007 eV 495.79 nm

orbitals in
excitation CI coeff.
---
184 => 185 -0.96905
182 => 187 -0.13711

Transition dipole moment (debye):
X= -0.1072 Y= -0.1557 Z= -0.1451 Tot= 0.2383

Oscillator strength, f= 0.0005

Excited State 2: 2.5311 eV 489.85 nm

orbitals in
excitation CI coeff.
---
181 => 185 0.76468
182 => 185 -0.22413
183 => 185 0.42997
182 => 186 -0.39577

Transition dipole moment (debye):
X= -0.0322 Y= 0.0000 Z= 0.0334 Tot= 0.0464

Oscillator strength, f= 0.0000

Excited State 3: 2.5745 eV 481.59 nm

orbitals in
excitation CI coeff.
---
181 => 185 -0.17210
182 => 185 -0.68603
181 => 186 0.54179
182 => 186 -0.15385
183 => 186 0.35795

184 => 187 -0.17349

Transition dipole moment (debye):
X= -0.8287 Y= 0.0731 Z= 0.5350 Tot= 0.9891

Oscillator strength, f= 0.0096

Excited State 4: 2.6169 eV 473.77 nm

orbitals in
excitation CI coeff.
---
184 => 186 0.90100
181 => 187 -0.20856
183 => 187 -0.32060

Transition dipole moment (debye):
X= -0.9403 Y= 1.7635 Z= -1.7710 Tot= 2.6703

Oscillator strength, f= 0.0708

Excited State 5: 2.7370 eV 452.99 nm

orbitals in
excitation CI coeff.
---
183 => 185 -0.68583
180 => 186 0.11235
181 => 186 -0.14904
182 => 186 -0.66780
182 => 189 -0.10784

Transition dipole moment (debye):
X= -0.0507 Y= -0.0269 Z= 0.0209 Tot= 0.0611

Oscillator strength, f= 0.0000

Excited State 6: 2.7884 eV 444.64 nm

orbitals in
excitation CI coeff.
---
182 => 185 0.15761
183 => 186 0.72821
184 => 187 0.64828

Transition dipole moment (debye):
X= 1.3468 Y= -0.1408 Z= -0.8356 Tot= 1.5912

Oscillator strength, f= 0.0268

Excited State 7: 2.8219 eV 439.37 nm

orbitals in
excitation CI coeff.
---
181 => 185 0.35679
182 => 185 -0.44365
183 => 185 -0.42800
181 => 186 -0.42786
182 => 186 0.53860

Transition dipole moment (debye):
X= -0.4919 Y= 0.0334 Z= 0.3022 Tot= 0.5783

Oscillator strength, f= 0.0036

Excited State 8: 2.8329 eV 437.66 nm

orbitals in
excitation CI coeff.
---
181 => 185 0.48098
182 => 185 0.35570
183 => 185 -0.31014
181 => 186 0.67887
182 => 186 0.26607

Transition dipole moment (debye):
X= 0.5148 Y= -0.0631 Z= -0.3282 Tot= 0.6138

Oscillator strength, f= 0.0040

4-closed Tetramethoxy HBC DFT Summary

Final total energy = -2296.8628662726 h

final geometry:
angstroms
atom x y z

C1	-0.0012846909	-0.0024764560	-0.0017025373
C2	-0.0030736197	-0.0024621520	1.4016167140
C3	1.2795311048	-0.0017025302	1.9882651960
C4	2.4364981766	-0.1118288351	1.2656565580
C5	2.4674849997	-0.2343186438	-0.1394296042
C6	1.2149348355	-0.1161306683	-0.7605210216
C7	3.7983174358	-0.8796874177	-0.4238006574
C8	4.3771148811	-1.2379996396	0.8393853579
C9	3.5457646743	-0.7448072750	1.8661331726
C10	4.4505723601	-1.3472459100	-1.5537378424
C11	5.6051303933	-2.1598349473	-1.3690345316
C12	6.0445471933	-2.5844364897	-0.1235631317
C13	5.3944827483	-2.1835241038	1.0813665839
C14	3.5413072249	-1.2869241770	3.1312778359
C15	4.5600897561	-2.2492316656	3.4287095296
C16	5.5086278212	-2.7346700883	2.4497126270
C17	4.3793104496	-2.8537058072	4.7130655768
C18	5.2231647204	-3.8907538879	5.0397619110
C19	6.1013506381	-4.4729761026	4.1036451264
C20	6.3214197424	-3.9144740084	2.8275896516
C21	3.1471656093	-2.7326715414	5.4851201773
C22	2.0063284344	-1.9991419052	5.0283484314
C23	2.3081298559	-1.1673755729	3.9028765044
C24	1.2511106079	-0.5239719661	3.2998305442
C25	4.9663187138	-4.8425678550	6.0492271369
C26	3.8125402335	-4.7282783272	6.7742098097
C27	2.9354107195	-3.6659818101	6.4740856710
C28	1.6451942868	-4.0278853691	6.9062798604
C29	0.4919438508	-3.3310436220	6.4949033662
C30	0.6596653473	-2.2615027137	5.4862048042
C31	-0.4413217329	-1.6316382624	4.7221048050
C32	-0.0903241519	-0.8130288700	3.6278886514
C33	1.7178986279	-5.3250424559	7.5161947240
C34	3.1262816856	-5.8284286927	7.3286284297
C35	3.7878054271	-7.0563224958	7.1769761246
C36	4.9998070521	-7.1776507422	6.4112099903
C37	5.5921602036	-6.0758316662	5.7749751632
C38	6.4262189048	-5.7978423632	4.5508937014
C39	7.2031864640	-4.7185779626	2.0447068710
C40	7.6520191997	-5.9559224292	2.4852928291
C41	7.2369297886	-6.5463830235	3.7129806646
C42	0.5175439046	-5.8658245199	7.9481435184
C43	-0.6694535154	-5.1060646910	7.7393152973
C44	-0.6952660263	-3.9139863204	7.0299831652
C45	-0.9161867101	-0.4379774394	2.5163842007
C46	-2.2655216452	-0.7327858731	2.6237851595
C47	-2.7096889897	-1.4071148181	3.7961683949
C48	-1.8479874117	-1.8610208399	4.7856317093
H49	6.9017086152	-3.2410821931	-0.1151393392

H50	6.1504493177	-2.5055479441	-2.2395211833
O51	3.9355408313	-1.0282316571	-2.7696053137
O52	0.5390865465	-7.0950711264	8.5251609442
H53	-1.6109478608	-5.4863072504	8.1182248580
H54	-1.6611354682	-3.4464045589	6.9104423473
H55	7.5575681579	-4.3972157114	1.0764779268
H56	8.3214744924	-6.5086741766	1.8363689166
O57	7.5657772846	-7.8062816916	4.0995489587
H58	-2.2981134991	-2.4156304174	5.5951722834
H59	-3.7657388756	-1.6233254815	3.9097400614
O60	-3.0731065794	-0.3955094951	1.5847233816
H61	5.3820653216	-8.1795117688	6.2425887238
H62	3.3325197242	-7.9736414775	7.5389529306
H63	-0.9379211262	-0.0372940518	-0.5504909926
H64	1.1242728223	-0.2297251932	-1.8369619642
C65	-4.4569111195	-0.7028035199	1.6564475623
H66	-4.8906704875	-0.3472551932	0.7207477154
H67	-4.6295101165	-1.7823299561	1.7468327112
H68	-4.9421630389	-0.1874030324	2.4945196713
C69	4.6025675509	-1.4810595185	-3.9383006269
H70	4.0263253339	-1.0957489246	-4.7805157361
H71	5.6260215278	-1.0900463207	-3.9956988193
H72	4.6313113637	-2.5764171553	-3.9920728707
C73	8.4098077677	-8.5862852911	3.2666740216
H74	8.5360991896	-9.5408111773	3.7795077423
H75	7.9594393712	-8.7627478843	2.2821049985
H76	9.3930121142	-8.1174883826	3.1358662657
C77	-0.6806507527	-7.6645154569	8.9762629065
H78	-0.4207445204	-8.6396496277	9.3901255411
H79	-1.1449386497	-7.0547108942	9.7612547477
H80	-1.3946077373	-7.7997812403	8.1544635162

3. Cyclic Voltammetry – See General Procedures for detailed experimental protocol.

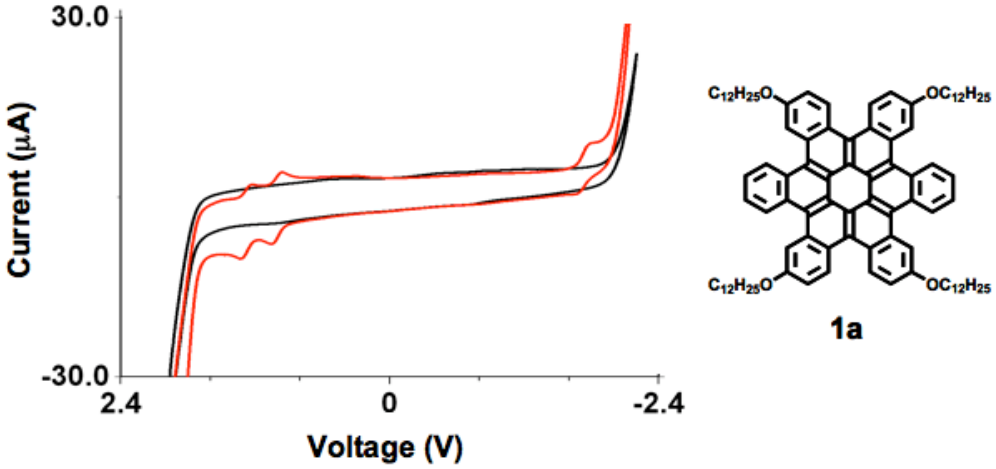


Figure 4. Cyclic voltammetry of compound **1a** (red)**.** The background scan is shown in black.

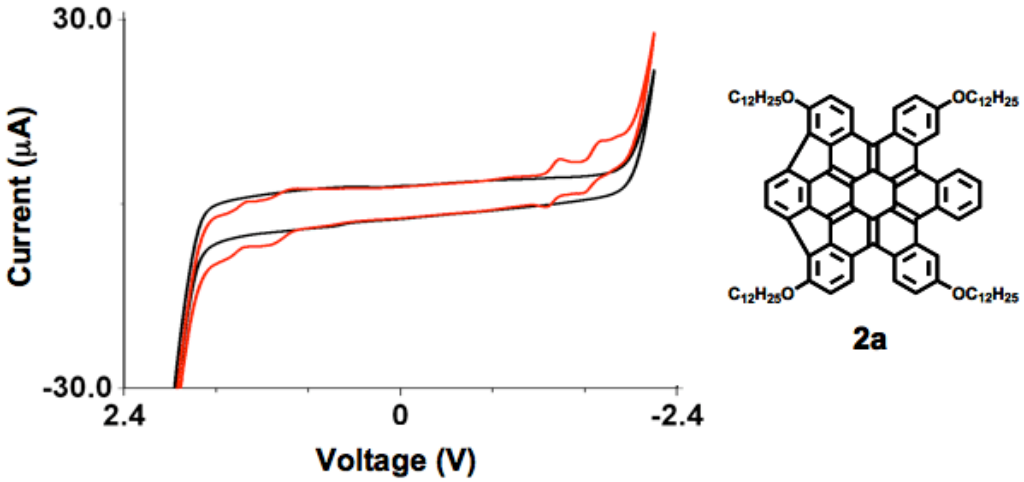


Figure 5. Cyclic voltammetry of compound **2a** (red)**.** The background scan is shown in black.

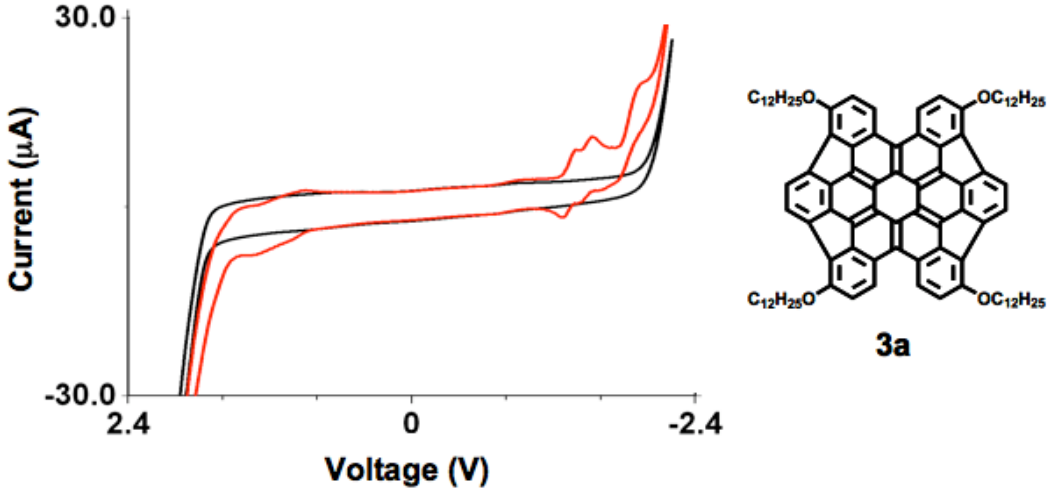


Figure 6. Cyclic voltammetry of compound **3a** (red)**.** The background scan is shown in black.

4. Fluorescence Quenching Data

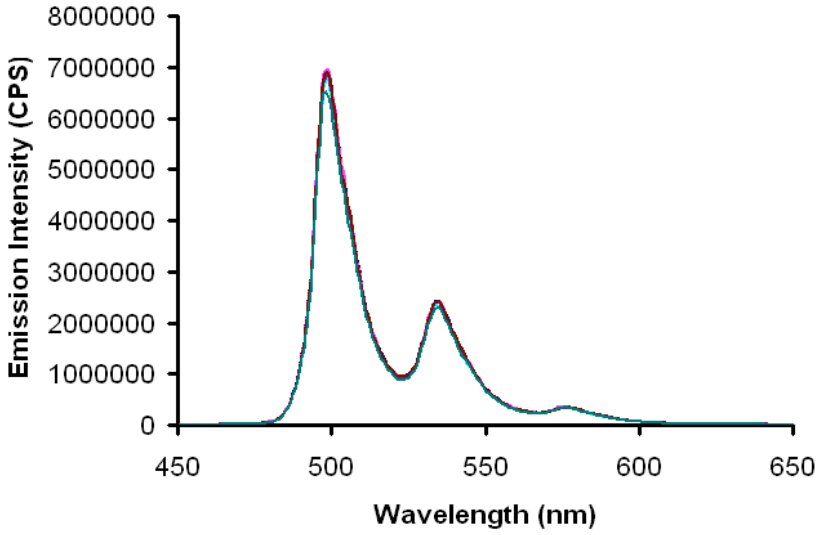


Figure 7. Emission spectra of **1a** ($1.00X10^{-6}$ M) excited at 379 nm with: (a) 0, (b) 0.25, (c) 0.50, (d) 0.75, (e) 1.0, and (f) 2.0 equivalents of C_{70} added. There is minimal difference between all spectra.

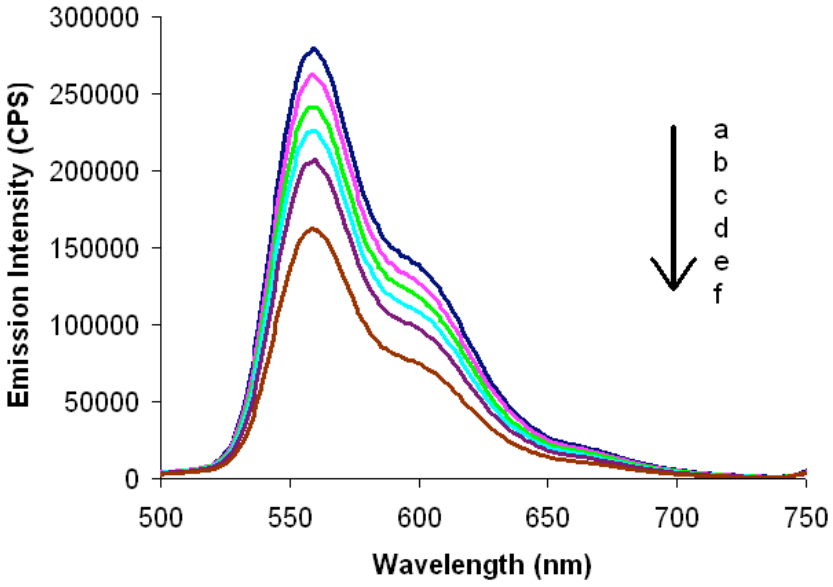
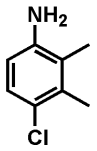


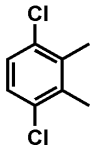
Figure 8. Emission spectra of **2a** ($1.00X10^{-6}$ M) excited at 377 nm with: (a) 0, (b) 0.25, (c) 0.5, (d) 0.75, (e) 1.0, and (f) 2.0 equivalents of C_{70} added.

5. General Procedures

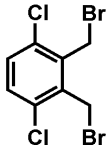
Unless otherwise noted, all reagents were used as received and all reactions were carried out under an argon atmosphere. Column chromatography was performed on a CombiFlash® Rf system with Redisep normal phase silica columns (Teledyne ISCO Inc., Lincoln, NE). Microwave reactions were performed in a CEM Discover Labmate with Teflon capped tubes. An IR sensor and pressure sensor regulated the temperature and pressure, respectively. Millipore filtrations were accomplished with a 47 mm Millipore vacuum filter. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker DRX-300 or Bruker DRX-400 spectrometers at room temperature, unless otherwise noted. High resolution mass spectra were recorded on a JEOL JMSHX110A/110A tandem mass spectrometer. A CH Instruments electrochemical workstation was used for the electrochemical measurements. Cyclic voltammetry experiments were performed in a single-compartment cell using a platinum wire auxiliary (BAS), a Ag/AgCl reference (BAS), and a glassy carbon working electrode (BAS). The supporting electrolyte was 0.1 M tetratbutylammonium tetrafluoroborate (Fluka) in anhydrous dichloromethane (Fluka). The working electrodes were polished on PSA microcloth (Buehler) with 1.0 μm alumina micropolish and with 0.05 μm alumina micropolish. The electrodes were then thoroughly sonicated in water, isopropanol, and dichloromethane to remove residual alumina particles. Prior to measurements, the electrochemical cell was degassed with argon. For experimental consistency, all reference electrodes were frequently standardized against the ferrocene/ferrocenium couple. POAV angles were measured using Mol2mol (http://www.gunda.hu/mol2mol/index.html). Inversion barriers were calculated using the formula $\Delta G_c = 4.57\ T_c\{9.97 + \log_{10}(T_c/\Delta\nu)\}$, where T_c is the coalescence temperature measured where the two signals have merged, and $\Delta\nu$ is the line width at half maximum of that signal in Hz. IUPAC naming was accomplished using the ACD/I-Lab Web service (ACD/IUPAC Name 8.05). All calculations were performed using Jaguar, version 7.0, Schrodinger, LLC, New York, NY, 2007. The B3LYP functional and 6-31G** basis sets were used throughout.



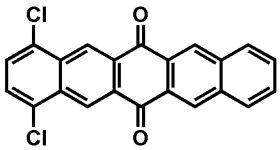
4-chloro-2,3-dimethylaniline (S1). In a 500 mL roundbottom flask, 2,3-dimethylaniline (40.0 g, 330 mmol) was added to 200 mL of anhydrous DMF. The mixture was cooled to 0 °C with an ice/water bath and N-chlorosuccinimide (44.1 g, 330 mmol) was added in one shot. The mixture was allowed to slowly warm to room temperature and was stirred at that temperature for 24 h. The mixture was diluted with water and extracted with CH_2Cl_2. The organic layer was then washed with water, dried over $MgSO_4$, and the solvent was removed under reduced pressure. The crude mixture was chromatographed on silica gel (1:1 hexane:CH_2Cl_2) to produce pure **1** (26.3 g, 51 %) as a clear liquid that browned quickly upon standing. ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.06 (d, J = 8.7 Hz, 1H), 6.53 (d, J = 8.4 Hz, 1H), 3.59 (bs, 2H), 2.36 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm). δ 143.7, 134.9, 127.1, 124.6, 123.1, 114.3, 17.35, 14.25. HRMS (EI+): calcd. for $C_8H_{10}NCl$: 155.0502, found: 155.0510.



1,4-dichloro-2,3-dimethylbenzene (S2). In a 1000 mL Erlenmeyer flask, a mixture of conc. HCl (35 mL) and **S1** (25.3 g, 163 mmol) was cooled to 0 °C by the addition of ice water. Sodium nitrite (11.2 g, 163 mmol) in water (26 mL) was cautiously added to the mixture while the temperature was kept below 10 °C by the addition of ice. In a separate 1000 mL Erlenmeyer flask, copper (I) chloride (16.1 g, 163 mmol) was dissolved in conc. HCl (15 mL). The solution of the diazonium salt was poured slowly into the copper (I) chloride solution and the resulting mixture was allowed to stir for 1 h. The solution was extracted with CH_2Cl_2 and the combined organic layers were dried over $MgSO_4$ and the solvent was removed under reduced pressure. Chromatography on silica gel eluting with hexane produced the desired product **2** (7.86 g, 28 %) as a clear oil that solidified on standing. ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.14 (s, 2H), 2.37 (s, 6H), 3.59 (bs, 2H), 2.36 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 136.6, 133.3, 127.7, 17.9. HRMS (EI+): calcd. for $C_8H_8Cl_2$: 174.0003, found: 173.9994.

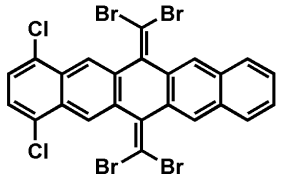


1,4-dichloro-2,3-bis(dibromomethyl)benzene (S3). In a flame dried 250 mL roundbottom flask equipped with a reflux condenser, CCl_4 (100 mL) was degassed by bubbling with argon for 15 minutes. **S2** (4.50 g, 25.7 mmol), NBS (13.7 g, 77.1 mmol) and benzoyl peroxide (311 mg, 1.29 mmol) were added and the reaction was refluxed overnight. After cooling, water (100 mL) was added and the mixture was extracted with CH_2Cl_2 (3 x 75 mL). The organic layers were combined, dried with $MgSO_4$, and the solvent was removed under reduced pressure. The crude mixture was purified by flash chromatography on silica gel. Eluting with hexane afforded the desired product as a crystalline white solid (7.56 g, 80 %). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.34 (s, 2H), 4.77 (s, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.73, 134.49, 131.32, 26.43. HRMS (EI+): calcd. for $C_8H_6Cl_2Br_2$: 331.8191, found: 329.8215.

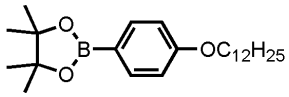


1,4-dichloropentacene-6,13-dione (S4). In a 250 mL roundbottom flask, 1,4-anthraquinone (2.00 g, 9.61 mmol), **S3** (3.19 g, 9.61 mmol), potassium iodide (11.16 g, 67.2 mmol), were added to 150 mL of anhydrous DMF. The flask was closed with a rubber septum and then flushed with argon for five minutes. The mixture was stirred at 110 °C for 16 h, cooled to 0 °C and then filtered. The solid was washed with methanol to provide a yellow solid (2.91 g, 80 %) that was analytically pure. ^{1}H NMR (300 MHz,

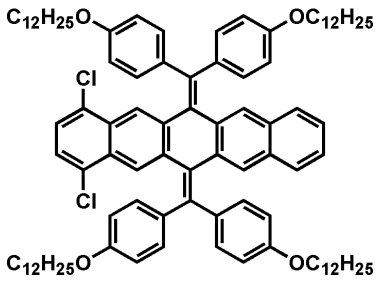
$CDCl_3$, ppm) δ. 9.43 (s, 2H), 9.02 (s, 2H), 8.12 (m, 2H), 7.74 (m, 4H). Too insoluble for carbon and mass.



1,4-dichloro-6,13-bis(dibromomethylene)-6,13-dihydropentacene (S5). In a 100 mL roundbottom flask, **S4** (1.18 g, 3.13 mmol), CBr_4 (4.15 g, 12.5 mmol), and PPh_3 (6.56 g, 25.0 mmol) were added to 100 mL of toluene. The mixture was heated to 100 °C and stirred for 16 h under an argon atmosphere. The reaction was cooled to room temperature and the solvent was removed under reduced pressure revealing a white solid. The solid was suspended in 5 mL of CH_2Cl_2 and isolated by vacuum filtration to provide product that was analytically pure (1.42 g, 66 %). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 8.85 (s, 2H), 8.35 (s, 2H), 7.89 (m, 2H), 7.57 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 139.4, 135.7, 133.2, 132.2, 131.6, 130.5, 129.0, 128.5, 127.8, 127.3, 125.0, 92.34. MS did not show molecular ion.

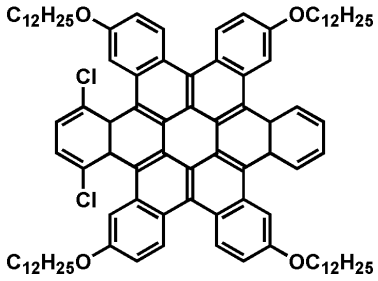


2-(4-(dodecyloxy)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (S6). Prepared as previously described.[1]

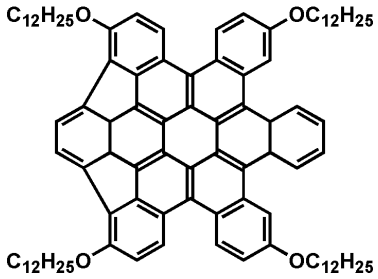


6,13-bis(bis(4-(dodecyloxy)phenyl)methylene)-1,4-dichloro-6,13-dihydropentacene (S7). In a 2-necked roundbottom flask equipped with a stirbar and a reflux condensor, 24 mL of toluene and 12 mL of water was degassed by bubbling with argon for 15 minutes. **S5** (500 mg, 0.726 mmol), **S6** (1.69 g, 4.36 mmol), $Pd(PPh_3)_4$ (336 mg, 0.290 mmol), and K_2CO_3 (3.21 g, 23.2 mmol) were added and the reaction was stirred at 110°C for 16 h. The reaction was cooled to room temperature and saturated $NH_4Cl_{(aq)}$ (10 mL) was added. The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 x 30 mL). The organic fractions were combined, dried over $MgSO_4$, and the solvent was removed under reduced pressure. Purification of the crude material by silica gel chromatography (5:1 hexane:CH_2Cl_2) produced pure compound as an off-white solid (832 mg, 81 %). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.95 (s, 2H), 7.58 (s, 2H), 7.43 (m,

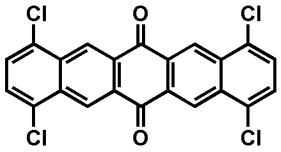
2H), 7.33 (m, 8H), 7.23 (m, 2H), 7.19 (s, 2H), 6.79 (m, 8H), 3.89 (m, 8H), 1.72 (m, 8H), 1.26 (m, 72H), 0.88 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm). δ 158.4, 158.3, 141.9, 138.8, 136.5, 135.0, 134.9, 132.0, 131.2, 131.2, 131.0, 129.7, 128.2, 127.5, 125.9, 125.6, 124.5, 114.8, 114.7, 68.42, 68.33, 32.33, 30.05, 29.82, 29.77, 29.70, 26.44, 23.11, 14.54. MS (FAB+): calcd. for $C_{96}H_{126}Cl_2O_4$: 1414.93, found: 1415.87. Anal. calcd. for $C_{96}H_{126}Cl_2O_4$: C, 81.49; H, 8.98, Found: C, 81.53; H, 8.97.



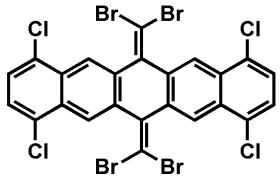
1,4,-dichloro-6,11,18,23-tetrakis(dodecyloxy)trinaphtho[1,2,3,4-fgh:1',2',3',4'-pqr:1'',2'',3'',4''-za1b1]trinaphthylene (2-Chloro-HBC, S8). The photocyclization setup has been previously described.[2] A mixture of compound **S7** (240 mg, 0.17 mmol), iodine (259 mg, 1.02 mmol) and propylene oxide (20 mL) in 300 mL of anhydrous benzene were irradiated with UV light (Hanovia 450 W high-pressure quartz Hg-vapor lamp) in an immersion well. Argon was bubbled through the reaction vessel during the photocyclization. To maintain a constant temperature, the whole apparatus was submerged in a large bath of circulating water. After 3 h of irradiation, the solvent was removed under reduced pressure. The resulting material was half-closed HBC. The material was quickly purified with a silica plug and a 2:1 hexane:CH_2Cl_2 wash. The fractions were concentrated and the resulting material was taken up into 300 mL CH_2Cl_2 and bubbled with argon while $FeCl_3$ (182 mg, 1.1 mmol) in 0.5 mL CH_3NO_2 was added. The resulting mixture was stirred for 2 h and then quenched by the addition of 300 mL methanol. The CH_2Cl_2 was removed by rotary evaporation and led to a yellow precipitate. This solid was filtered with a Millipore vacuum filtration apparatus to give 184 mg of a yellow solid (77 %). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 9.40 (m, 2H), 9.12 (d, J = 8.7 Hz, 2H), 8.93 (d, J = 9.0 Hz, 2H), 8.71 (s, 2H), 7.85 (s, 2H), 7.80 (m, 2H), 7.71 (s, 2H), 7.48 (d, J = 8.1 Hz, 2H), 7.35 (d, J = 8.7 Hz, 2H), 4.23 (bm, 8H), 1.93 (bm, 8H), 1.27 (bs, 44H), 0.874 (bs, 12H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm). δ 158.1, 156.7, 132.2, 132.0, 131.8, 131.5, 130.6, 130.3, 129.6, 128.7, 128.5, 126.5, 125.6, 125.4, 125.1, 123.4, 122.0, 121.7, 118.2, 117.4, 117.3, 113.0, 111.9, 68.9, 68.7, 32.3, 30.1, 29.9, 29.8, 26.6, 23.1, 14.5. MS (FAB+): calcd. for $C_{96}H_{118}Cl_2O_4$: 1406.87, found: 1407.16. Anal. calcd. for $C_{96}H_{118}Cl_2O_4$: C, 81.96; H, 8.45, Found: C, 81.99; H, 8.44.



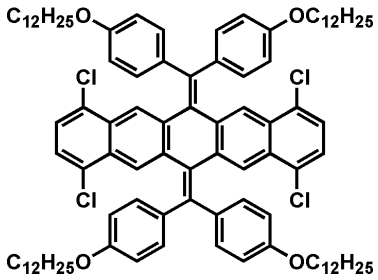
3,8,15,20-tetrakis(dodecyloxy)-9c,13a,20c,20d-tetrahydrobenzo[1,8]-*as*-indaceno[2,3,4,5,6,7-*defghij*]dinaphtho[1,2,3,4-*pqr*:1',2',3',4'-za_1b_1]trinaphthylene (2-closed HBC, S9). In an oven dried 10 mL microwave vial were added **S8** (10.0 mg, 7.10 μmol), $Pd(PCy_3)_2Cl_2$ (10.5 mg, 14.2 μmol), DBU (100 μL, 1.34 mmol), and DMA (2 mL). The vial was capped and the mixture was degassed by bubbling with argon for 15 minutes. In a microwave reactor the sample was heated at 150°C for 3 h. After cooling, the crude reaction mixture was added to 5 mL of H_2O and the mixture was extracted with CH_2Cl_2 (3 x 10 mL). The organic layers were combined, dried over $MgSO_4$, and the solvent was removed under reduced pressure. Purification by preparative TLC on neutral alumina eluting with CS_2 yielded 7.8 mg of the product as a reddish-orange solid (82 %). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 9.26 (m, 2H), 8.83 (d, *J* = 9.0 Hz, 2H) 8.63 (s, 2H), 8.02 (d, *J* = 9.0 Hz, 2H), 7.66 (m, 2H), 7.49 (d, *J* = 9.0 Hz, 2H), 7.28 (s, 2H), 6.75 (d, *J* = 9.0 Hz, 2H), 4.45-4.15 (m, 6H), 3.97 (m, 2H), 2.02 (m, 8H), 1.80 (m, 16H), 1.35 (m, 56H), 0.88 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 157.2, 155.0, 140.5, 140.0, 138.7, 137.6, 131.6, 130.8, 130.0, 128.4, 127.9, 126.4, 124.2, 121.9, 121.5, 117.0, 116.7, 113.13, 69.46, 68.88, 32.26, 30.09, 29.91, 29.80, 28.13, 27.05, 26.67, 26.40, 23.11, 14.29. MS (FAB+): calcd. for $C_{96}H_{116}O_4$: 1333.95, found: 1334.36. Anal. calcd. for $C_{96}H_{116}O_4$: C, 86.44; H, 8.77, Found: C, 86.51; H, 8.84.



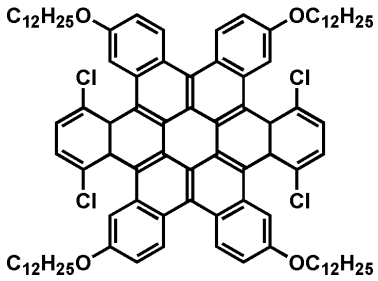
1,4,8,11-tetrachloropentacenequinone (S10). In a 1000 mL roundbottom flask were added **S3** (12.0 g, 36.1 mmol), benzoquinone (1.95 g, 18.0 mmol), potassium iodide (90.0 g, 54.2 mmol) and 500 mL of anhydrous DMF. The flask was closed with a rubber septum and then flushed with argon for five minutes. The mixture was stirred at 110 °C for 16 h then cooled to 0 °C and filtered. The solid was washed with methanol to provide a yellow solid (7.07 g, 88 %). This material proved to be too insoluble for characterization so was carried on without further manipulation.



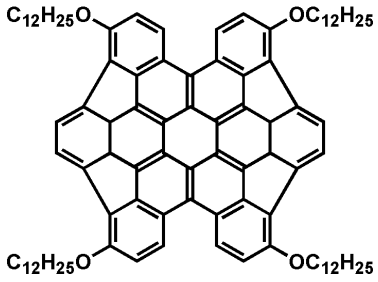
1,4,8,11-tetrachloro-6,13-bis(dibromomethylene)-6,13-dihydropentacene (S11). In a 100 mL roundbottom flask, **S10** (250 mg, 0.560 mmol), CBr_4 (929 mg, 2.80 mmol), and PPh_3 (1.47 g, 5.60 mmol) were added to 30 mL of toluene. The mixture was heated to 100 °C and stirred for 16 h under an argon atmosphere. The reaction was cooled to room temperature and the solvent was removed under reduced pressure revealing a white solid. The solid was suspended in 5 mL of CH_2Cl_2 and isolated by vacuum filtration to provide product that was pure enough for further use (203 mg, 48%). Purification with silica gel chromatography (19:1 hexane:CH_2Cl_2) produced analytically pure product as a white crystalline solid. ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 8.73 (s, 4H), 7.44 (s, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) 138.7, 135.1, 131.7, 130.6, 127.5, 125.2, 93.9. MS did not show molecular ion. Carried forward.



6,13-bis(bis(4-(dodecyloxy)phenyl)methylene)-1,4,8,11-tetrachloro-6,13-dihydropentacene (S12). In a 2-necked roundbottom flask equipped with a stirbar and a reflux condensor, 12 mL of toluene and 6 mL of water was degassed by bubbling with argon for 15 minutes. **S11** (250 mg, 0.330 mmol), **S6** (769 mg, 1.98 mmol), $Pd(PPh_3)_4$ (152 mg, 0.132 mmol), and K_2CO_3 (1.46 g, 10.56 mmol) were added and the reaction was stirred at 110°C for 16 h. The reaction was cooled to room temperature and saturated $NH_4Cl_{(aq)}$ (10 mL) was added. The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 x 15 mL). The organic fractions were combined, dried over $MgSO_4$, and the solvent was removed under reduced pressure. Purification of the crude material by silica gel chromatography (5:1 hexane:CH_2Cl_2) produced pure compound as an off white solid (323 mg, 66%). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.99 (s, 4H), 7.33 (d, J = 8.7 Hz, 8H), 7.21 (s, 4H), 6.81 (d, J = 8.7 Hz, 8H), 3.91 (t, J = 6.6 Hz, 8H), 1.74 (m, 8H), 1.27 (m, 72H), 0.88 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 158.13, 143.01, 137.81, 134.22, 133.90, 130.64, 129.42, 125.28, 124.38, 68.013, 31.879, 29.590, 29.355, 29.309, 29.210, 25.977, 22.645, 14.070, MS (FAB+): calcd. For $C_{96}H_{124}Cl_4O_4$: 1483.82, found: 1483.10. Anal. calcd. for $C_{96}H_{124}Cl_4O_4$: C, 77.71; H, 8.42, Found: C, 77.66; H, 8.48.

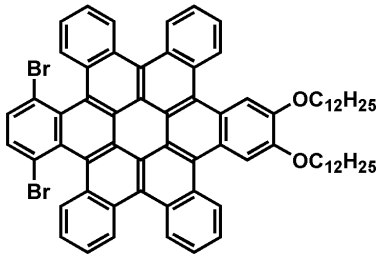


1,4,13,16-tetrachloro-6,11,18,23-tetrakis(dodecyloxy)trinaphtho[1,2,3,4-fgh:1',2',3',4'-pqr:1'',2'',3'',4''-za1b1]trinaphthylene (4-Chloro-HBC, S13). A mixture of compound **S12** (229 mg, 0.15 mmol), iodine (662 mg, 2.5 mmol) and propylene oxide (20 mL) in 300 mL of anhydrous benzene were irradiated with UV light (Hanovia 450 W high-pressure quartz Hg-vapor lamp) in an immersion well. Argon was bubbled through the reaction vessel during the photocyclization. To maintain a constant temperature, the whole apparatus was submerged in a large bath of circulating water. After 3 h of irradiation, the solvent was removed under reduced pressure. The resulting material was half-closed HBC. The material was quickly purified with a silica plug and a 2:1 hexane:CH_2Cl_2 as an eluent. The fractions were concentrated and the resulting material was taken up into 250 mL CH_2Cl_2 and bubbled with argon while $FeCl_3$ (200 mg, 1.2 mmol) in 0.5 mL CH_3NO_2 was added. The resulting mixture was stirred for 2 h and then quenched by the addition of 300 mL methanol. The CH_2Cl_2 was removed by rotary evaporation and led to a yellow precipitate. This solid was filtered with a Millipore vacuum filtration apparatus to give 169 mg of a yellow solid (74 %). ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 9.02 (d, J = 9.0 Hz, 4H), 7.90 (s, 4H), 7.78 (s, 4H), 7.46 (d, J = 9.0 Hz, 4H), 4.34 (m, 4H), 4.17 (m, 4H), 1.94 (m, 8H), 1.29 (m, 72H), 0.88 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 156.8, 132.1, 130.8, 130.5, 130.1, 129.5, 124.4, 123.6, 122.4, 117.8, 113.9, 68.7,2, 32.31, 30.03, 29.86, 29.75, 23.08, 14.50. MS (FAB+): calcd. for $C_{96}H_{116}Cl_4O_4$: 1475.76, found:. 1475.24. Anal. calcd. for $C_{96}H_{116}Cl_4O_4$: C, 78.13; H, 7.92, Found: C, 78.19; H, 7.86.

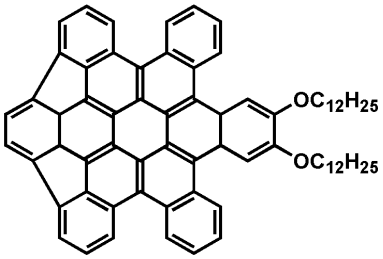


4-closed (S14). In an oven dried 10 mL microwave vial were added **S13** (10.0 mg, 6.78 μmol), $Pd(PCy_3)_2Cl_2$ (20.0 mg, 27.1 μmol), DBU (200 μL, 1.34 mmol), and DMA (2 mL). The vial was capped and the mixture was degassed by bubbling with argon for 15 minutes. In a microwave reactor the sample was heated at 150 °C for 3 h. Three more reactions were performed (4 X 10 mg total) and the solutions were combined. After cooling, the crude reaction mixture was added to 5 mL of H_2O and the mixture was extracted with CH_2Cl_2 (3 x 10 mL). The organic layers were combined, dried over $MgSO_4$, and the solvent was removed under reduced pressure. The above procedure was repeated 4 times and the crude material from each reaction was combined. Multiple

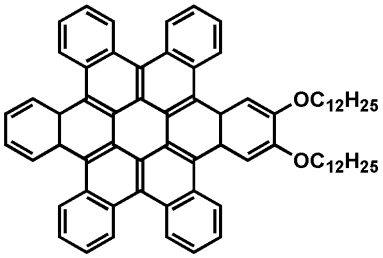
purifications by preparative TLC on neutral alumina eluting with CS_2 eventually yielded the product as a reddish-orange solid (7 mg, 16%). ^{1}H NMR (300 MHz, CD_2Cl_2, ppm) δ 8.34 (d, *J* = 9.3 Hz, 4H), 7.32 (s, 4H), 6.89 (d, *J* = 9.0 Hz, 4H), 4.36 (m, 4H), 4.11 (m, 4H), 1.93 (m, 8H), 1.60 (m, 8H), 1.38 (m, 64H), 0.91 (m, 12H). ^{13}C NMR (75 MHz, CD_2Cl_2, ppm) δ 154.2, 139.6, 139.5, 138.5, 137.6, 131.0, 130.8, 128.1, 126.7, 126.2, 125.2, 123.1, 116.6, 69.37, 32.33, 30.15, 30.04, 29.79, 26.58, 23.08, 14.26, . HRMS (FAB+): calcd. for $C_{96}H_{113}O_4$: 1329.8639, found: 1329.8616.



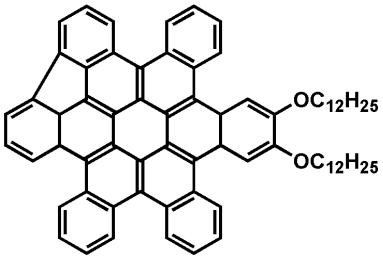
1,4-dibromo-14,15-bis(dodecyloxy)trinaphtho[1,2,3,4-fgh:1',2',3',4'-pqr:1'',2'',3'',4''-za1b1]trinaphthylene (HBC, S15). Prepared as described previously.[3]



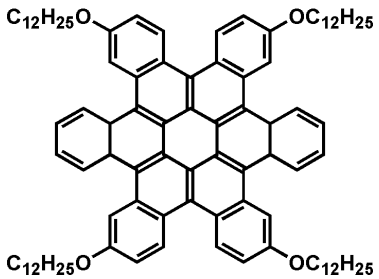
11,12-bis(dodecyloxy)-9c,13a,20c,20d-tetrahydrobenzo[1,8]-*as*-indaceno[2,3,4,5,6,7-*defghij*]dinaphtho[1,2,3,4-*pqr*:1',2',3',4'-za_1b_1]trinaphthylene (2-closed-2chain-HBC, S16). In the glove box, **S15** (21.5 mg, 0.021 mmol), $Pd(PCy_3)_2Cl_2$ (14.0 mg, 0.019 mmol), DBU (0.150 mL, 1.00 mmol), and DMA (3 mL) were added to a 10 mL microwave vial and the vial was capped. The vessel was removed from the glove box and placed into a microwave reactor where it was heated at 140 °C for 3 h. After cooling, the solvent was removed under reduced pressure and the crude material was chromatographed on silica gel (4:1 hexane:CH_2Cl_2). The first product off the column was completely debrominated **S17** as a yellow solid (4.4 mg, 24%) followed by the desired product **S16** as a red solid (1.8 mg, 10%) and finally **S18** as a yellow solid (10.5 mg, 57%). Often multiple columns were required to afford pure product. ^{1}H NMR (300MHz, $C_2D_2Cl_4$, ppm): δ 8.69 (d, *J* = 7.5 Hz, 2H), 8.62 (d, *J* = 7.8 Hz, 2H), 7.98 (s, 2H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.40-7.20 (m, 4H), 6.97 (d, *J* = 6.9 Hz, 2H), 6.89 (s, 2H), 6.81 (t, *J* = 7.8 Hz, 2H), 3.65 (m, 2H), 3.50 (m, 2H), 1.30 (m, 4H), 1.2-0.1 (m, 42H). ^{13}C NMR (75 MHz, $C_2D_2Cl_4$, ppm): δ 148.9, 142.1, 136.7, 131.4, 130.1, 129.3, 129.0, 127.8, 127.7, 127.4, 127.1, 127.0, 126.1, 125.5, 125.4, 124.9, 122.3, 121.8, 120.2, 111.5, , 31.79, 29.57, 29.39, 29.25, 36.03, 22.60, 14.11. HRMS (FAB+): calcd. for $C_{72}H_{68}O_2$: 964.5219, found 964.5205.



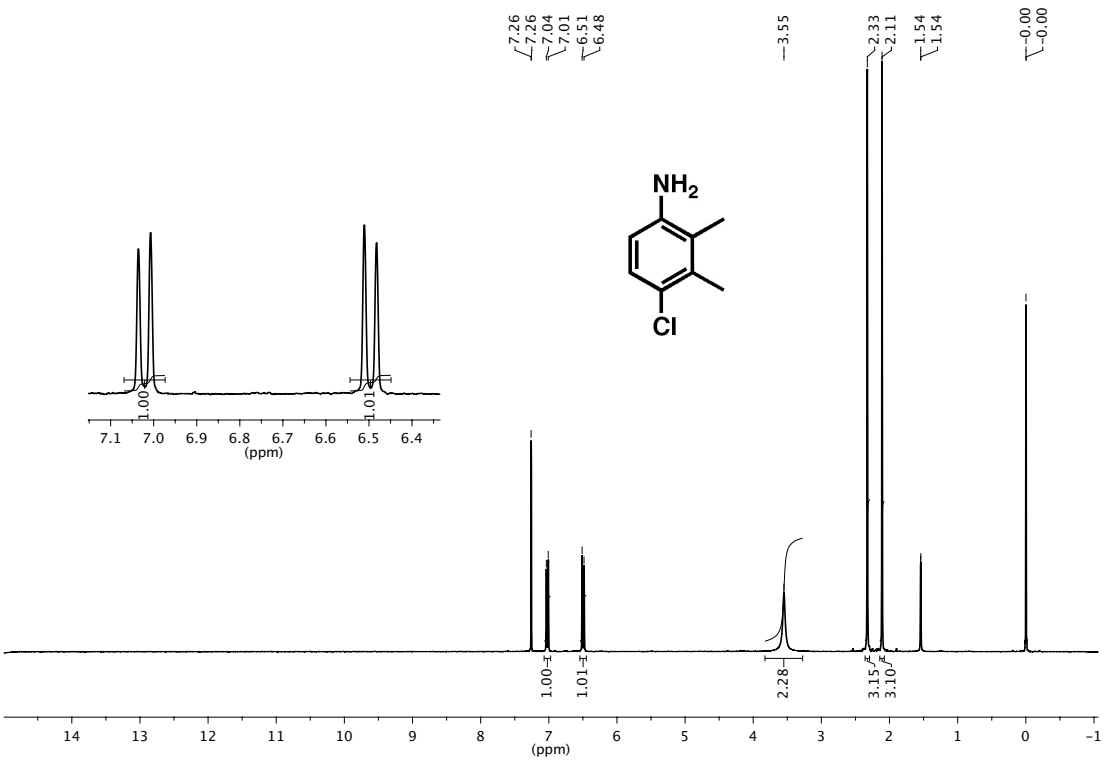
2,3-bis(dodecyloxy)-4a,12c,16a,24c-tetrahydrotrinaphtho[1,2,3,4-*fgh*:1',2',3',4'-*pqr*:1'',2'',3'',4''-*za*$_1$*b*$_1$]trinaphthylene (2-chain-HBC, S17). Isolated from the reaction to form **S16**. ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 9.29 (m, 10H), 8.73 (s, 2H), 7.84 (m, 10H), 4.42 (m, 4H), 4.28 (m, 4H), 2.02 (m, 4H), 1.28 (m, 32H), 0.88 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 149.3, 130.5, 130.3, 129.6, 129.4, 129.3, 128.5, 126.7, 126.5, 126.3, 125.8, 120.9, 111.81, 69.74, 32.33, 30.09, 29.95, 29.74, 26.58, 23.09, 14.51. HRMS (FAB+): calcd. for $C_{72}H_{72}O_2$: 968.5532, found: 968.5507.



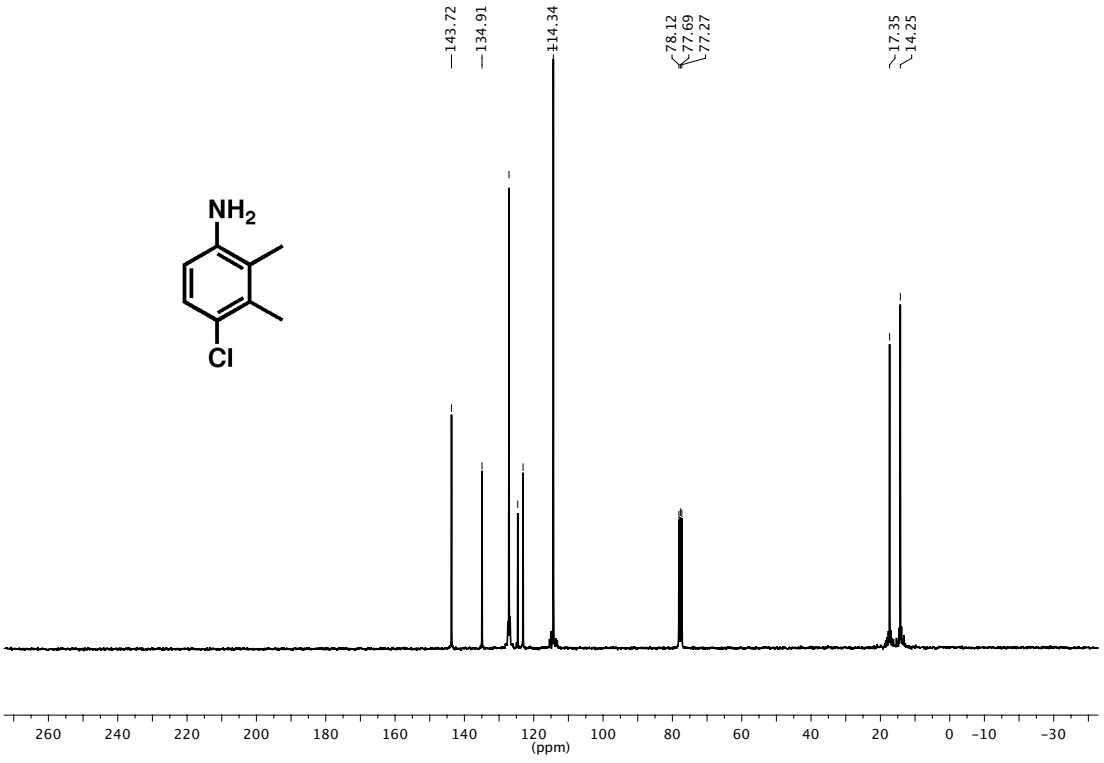
16,17-bis(dodecyloxy)-3c,6a,14c,18a-tetrahydroacenaphtho[1,2,3,4,5-*defgh*]dinapht ho[1,2,3,4-*pqr*:1',2',3',4'-*za*$_1$*b*$_1$]trinaphthylene (1-closed-2-chain-HBC, S18). Isolated from the reaction to form **S16**. ^{1}H NMR (300MHz, $CDCl_3$, ppm): δ 9.26 (d, J = 7.5 Hz, 2H), 9.17 (d, J = 8.4 Hz, 1H), 9.02 (m, 2H), 8.94 (d, J = 7.8 Hz, 1H), 8.66 (s, 1H), 8.53 (s, 1H), 8.39 (d, J = 8.4 Hz, 1H), 8.29 (d, J = 8.4 Hz), 7.87-7.62 (m, 6H), 7.45-7.26 (m, 4H), 4.36 (m, 4H), 2.07 (quint, J = 6.9 Hz, 4H), 1.80-1.20 (m, 36H), 0.88 (m, 6H). ^{13}C NMR (75MHz, $CDCl_3$, ppm): δ 149.0, 138.2, 132.6, 132.4, 132.0, 131.8, 129.9, 129.5, 129.2, 128.8, 128.4, 127.5, 126.5, 126.5, 126.1, 125.4, 125.2, 125.0, 123.2, 122.2, 117.7, 112.4, 29.8, 32.4, 30.1, 30.0, 29.8, 26.7, 23.1, 14.5. HRMS (FAB+) calcd. for $C_{72}H_{70}O_2$: 966.5376, found 966.5347.



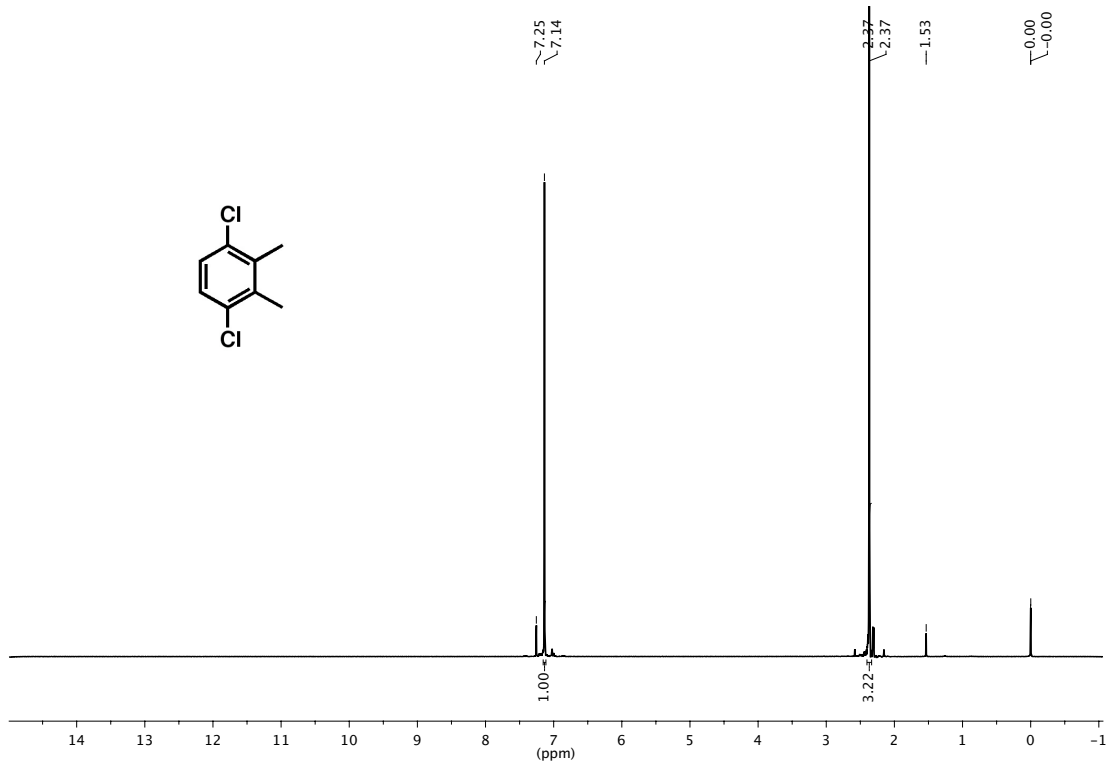
6,11,18,23-tetrakis(dodecyloxy)-4a,12c,16a,24c-tetrahydrotrinaphtho[1,2,3,4-*fgh*: 1',2',3',4'-*pqr*:1'',2'',3'',4''-*za*$_1$*b*$_1$]trinaphthylene (S19). Prepared as previously described.[4]



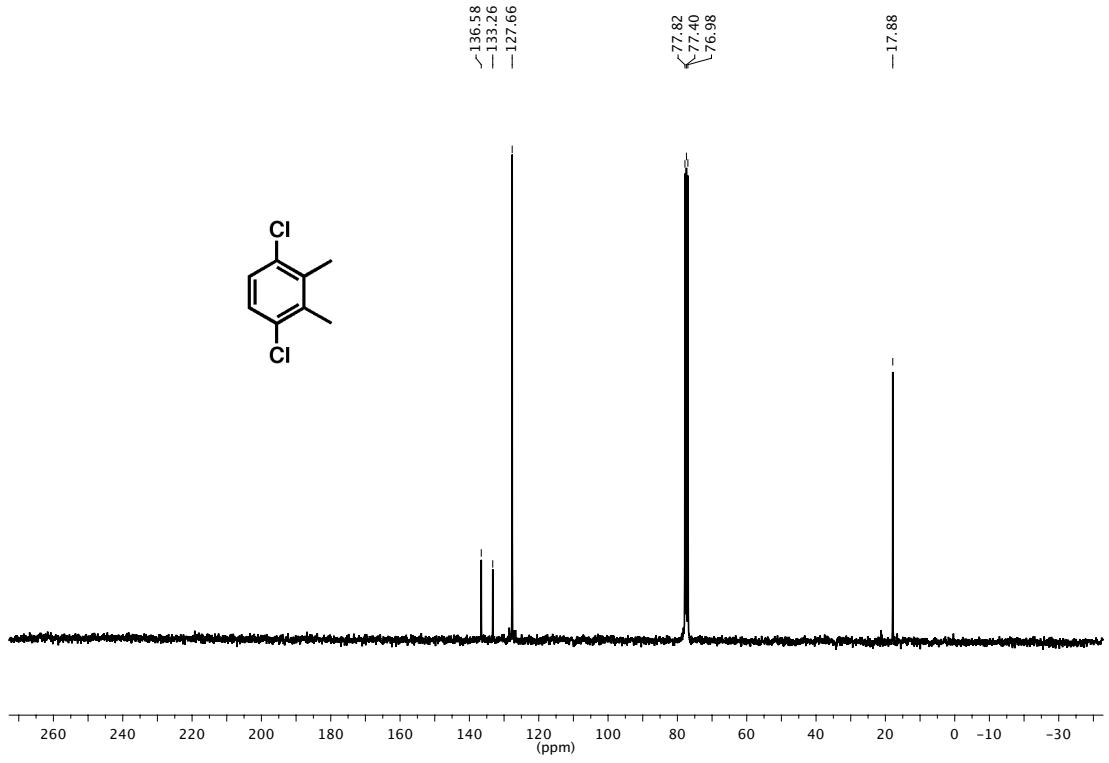
^{1}H NMR ($CDCl_3$) of S**1**.



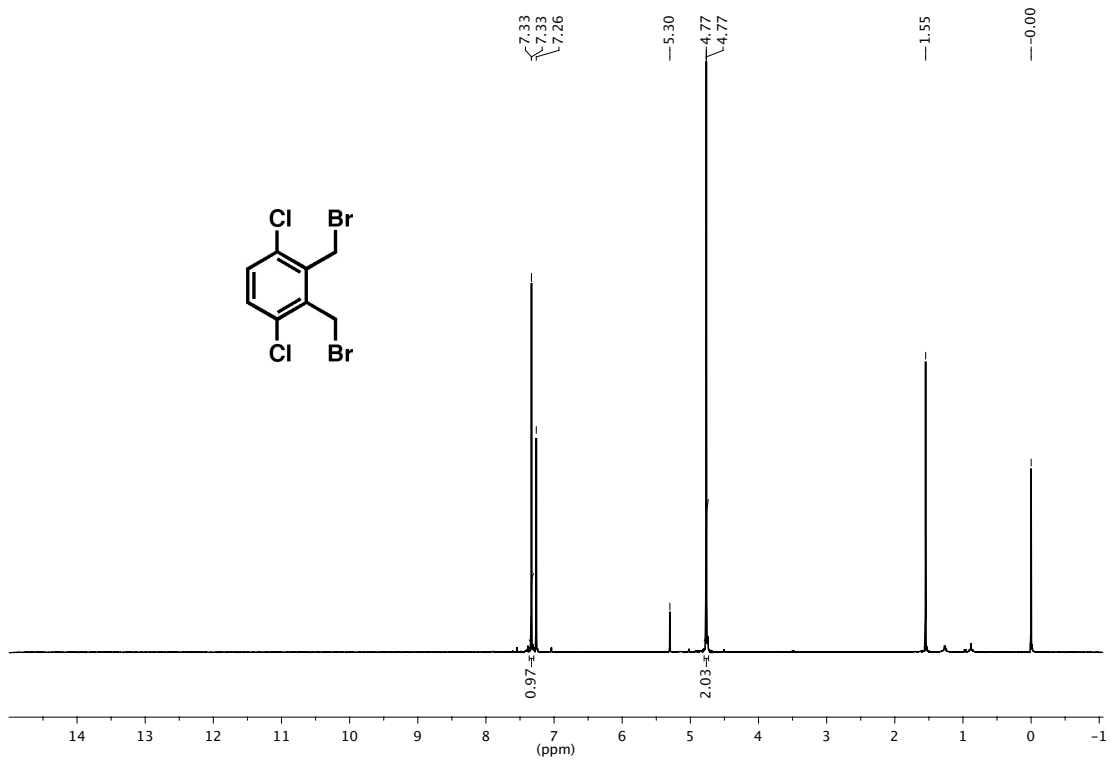
^{13}C NMR ($CDCl_3$) of S**1**.



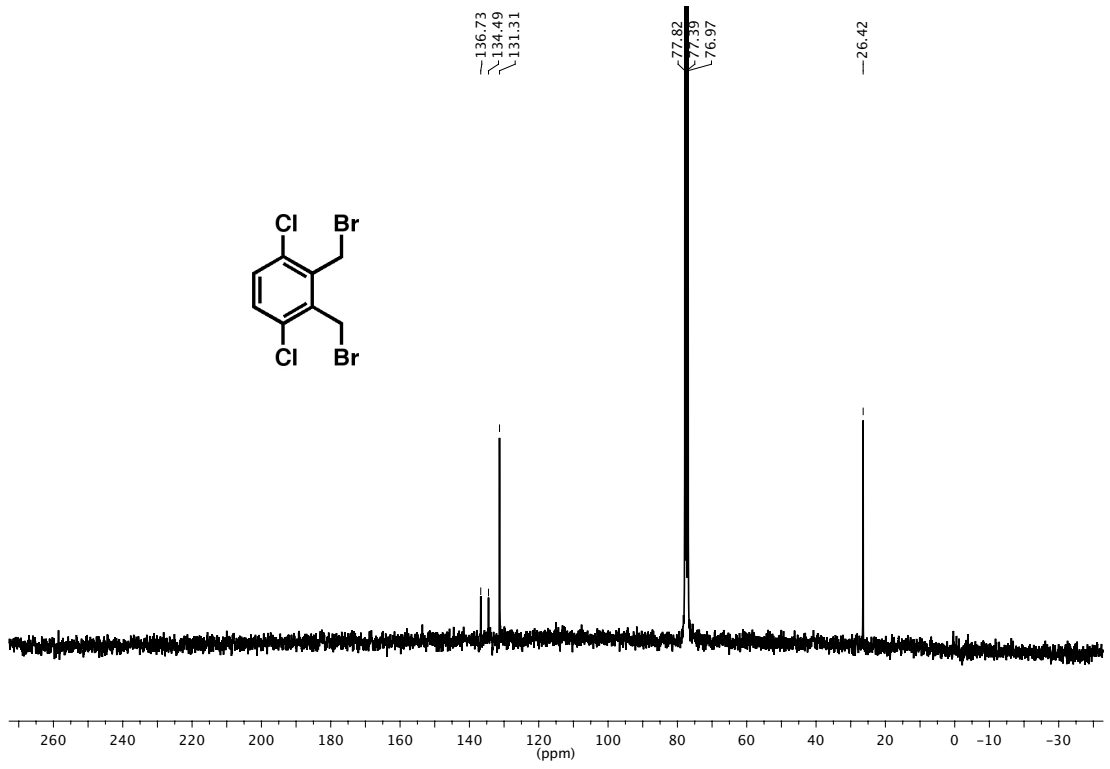
^{1}H NMR ($CDCl_3$) of S**2**.



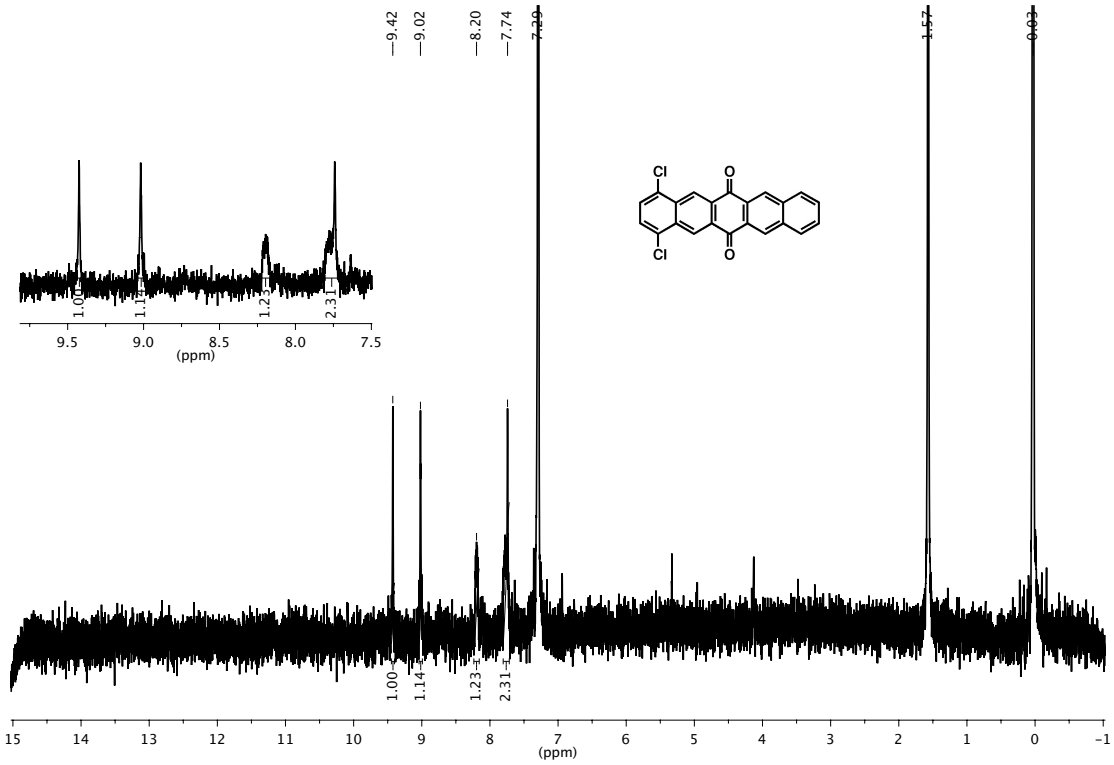
^{13}C NMR ($CDCl_3$) of S**2**.



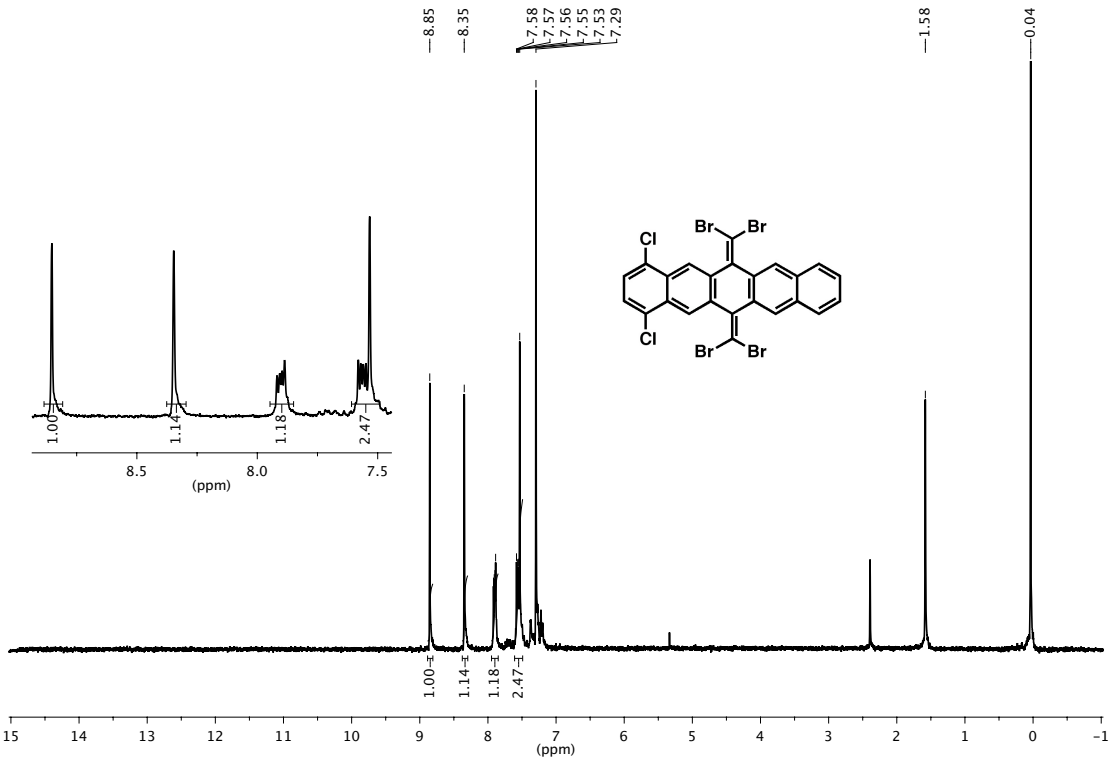
^{1}H NMR ($CDCl_3$) of S**3**.



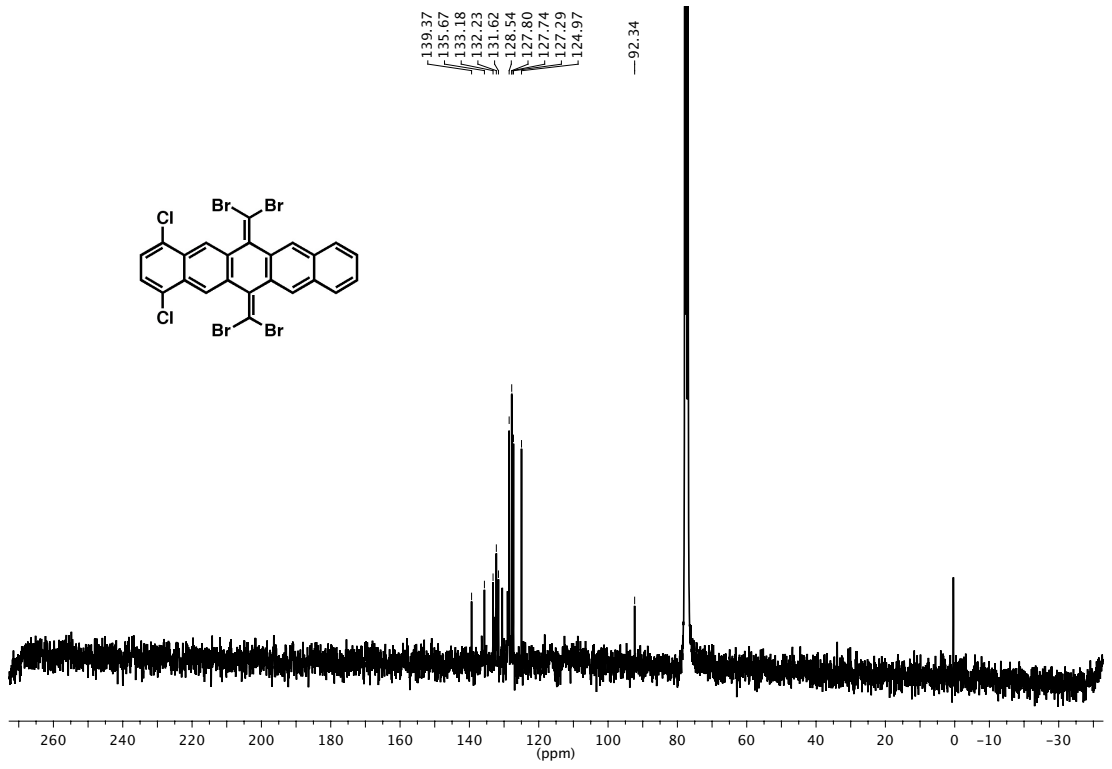
^{13}C NMR ($CDCl_3$) of S**3**.



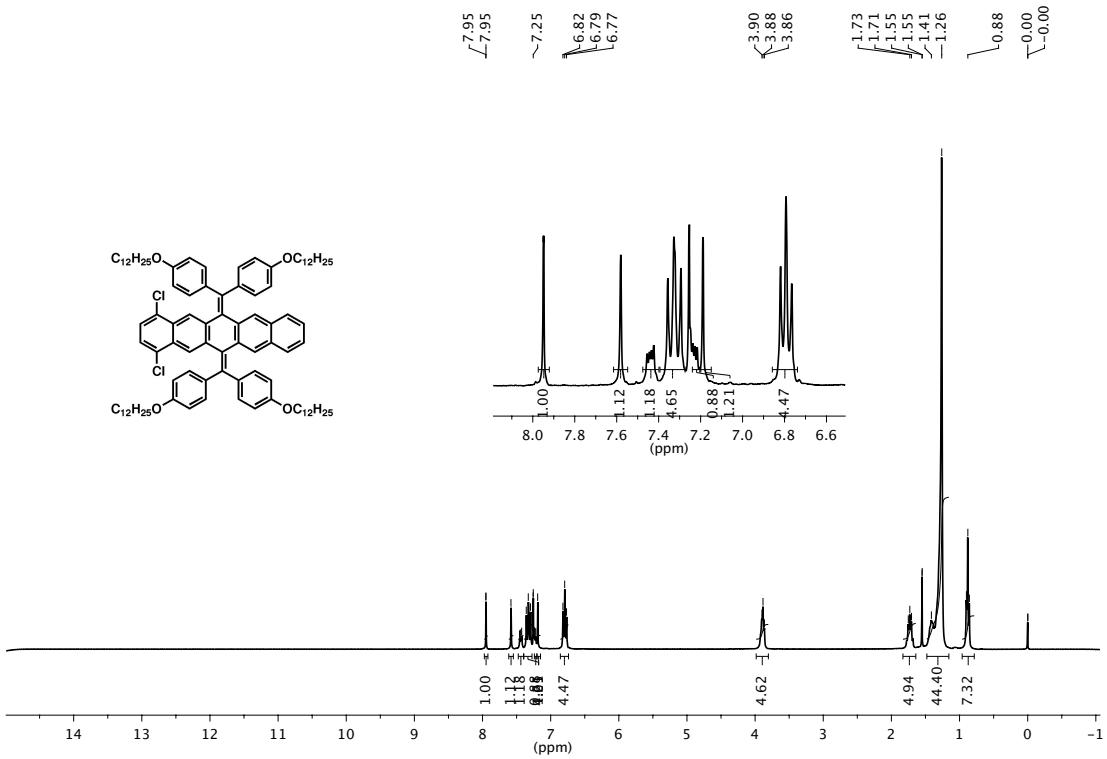
^{1}H NMR ($CDCl_3$) of S**4**.



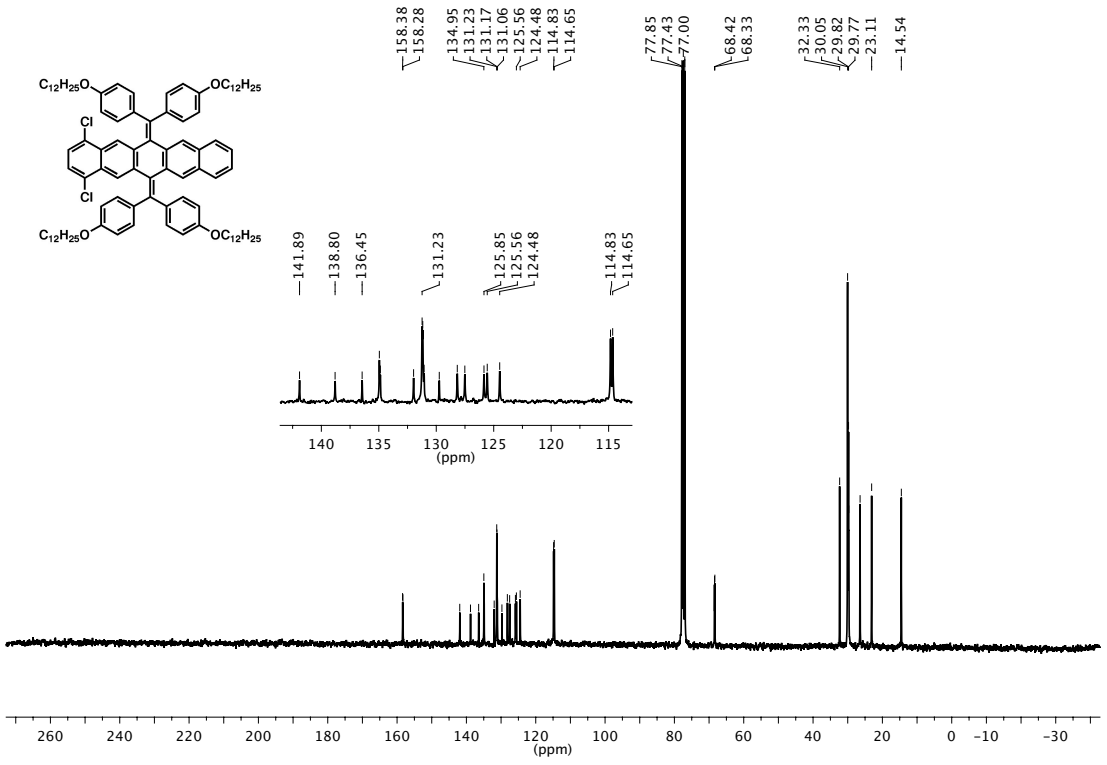
^{1}H NMR ($CDCl_3$) of S**5**.



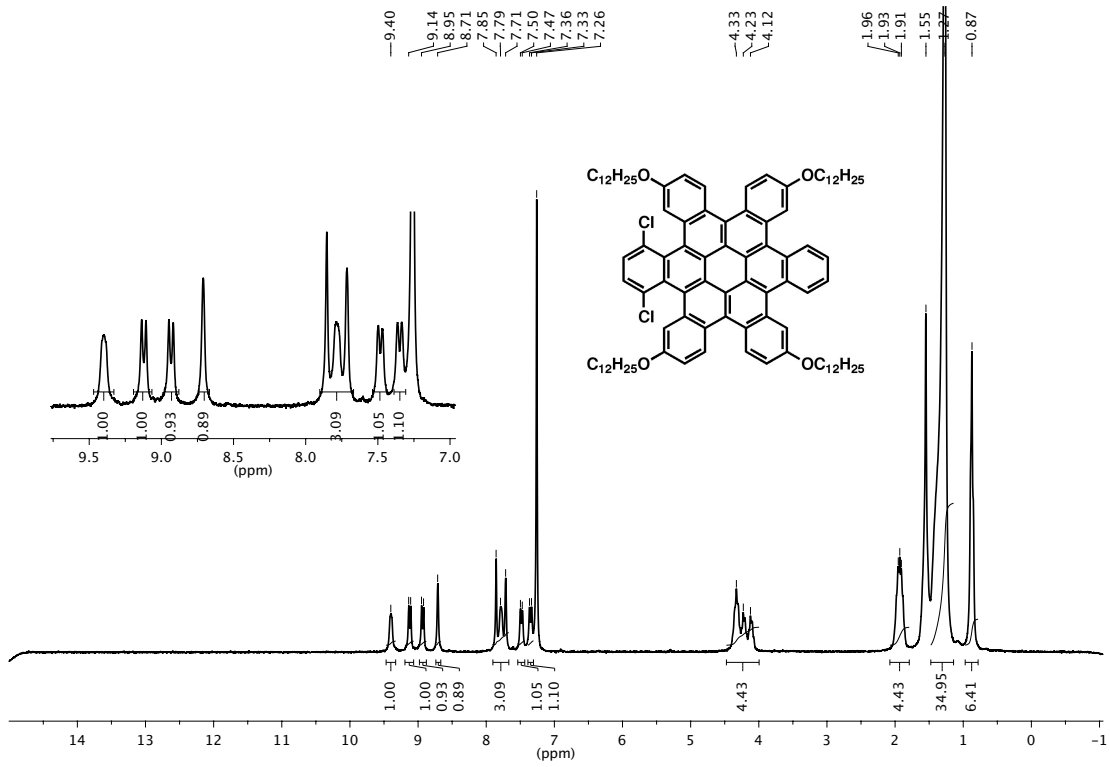
^{13}C NMR ($CDCl_3$) of S**5**.



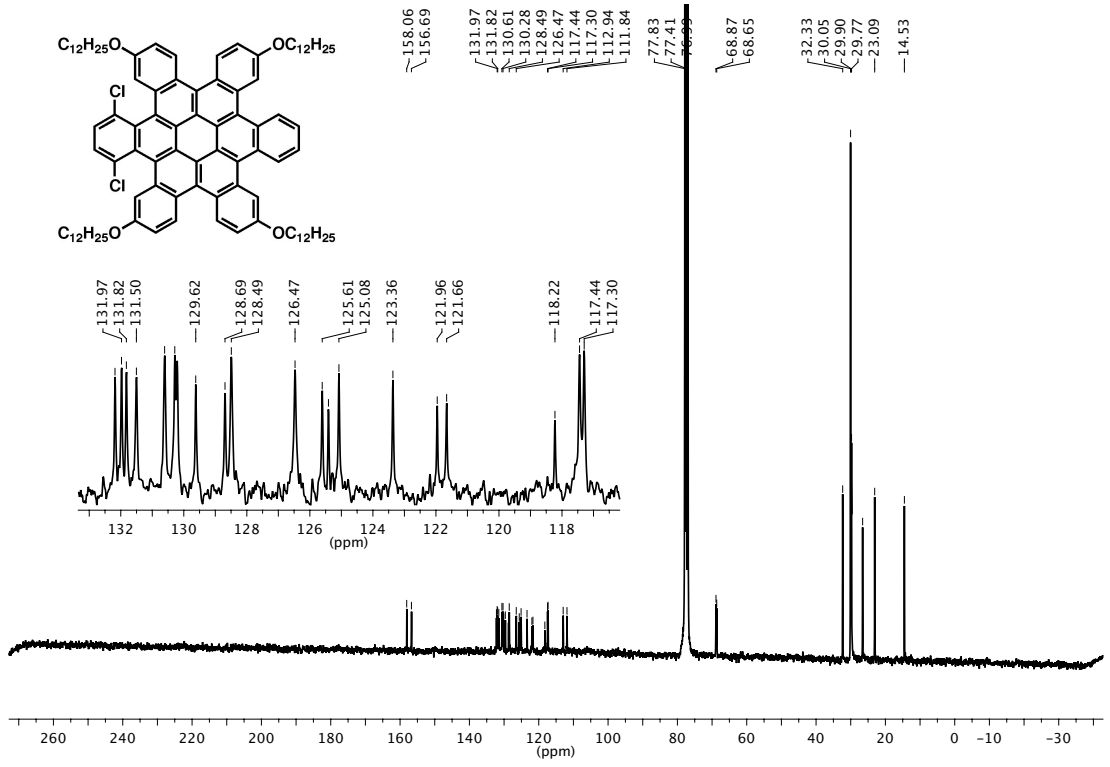
^{1}H NMR ($CDCl_3$) of S**7**.



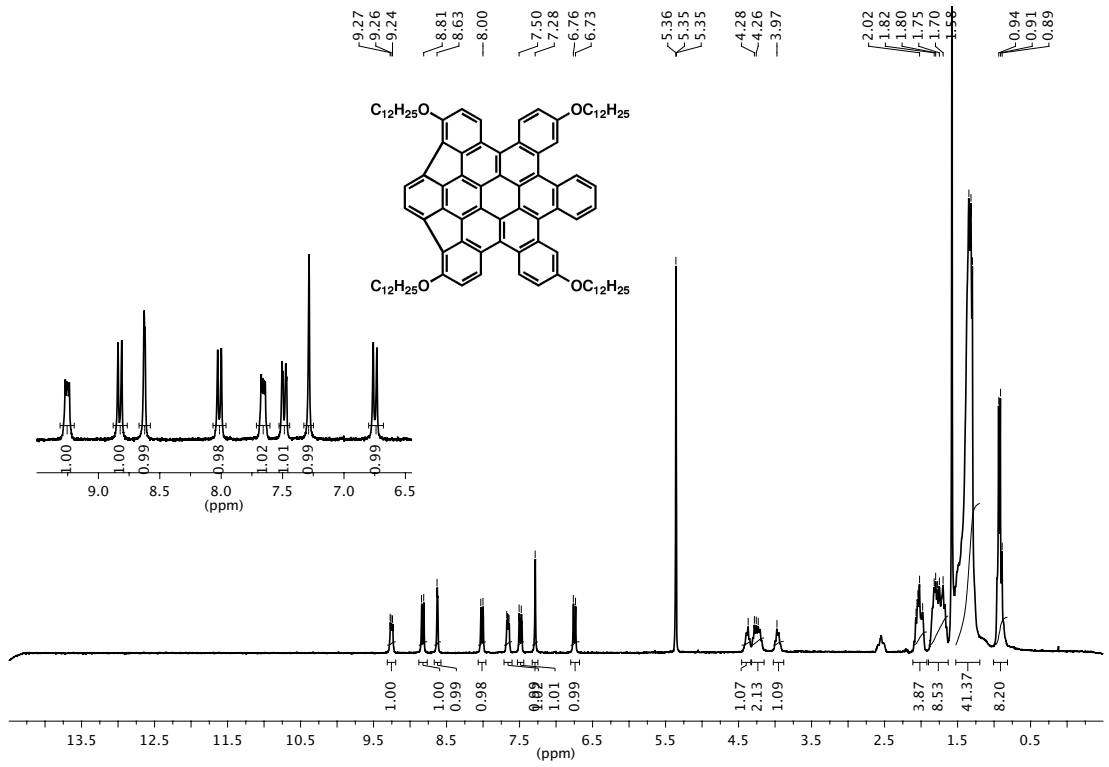
^{13}C NMR ($CDCl_3$) of S**7**.



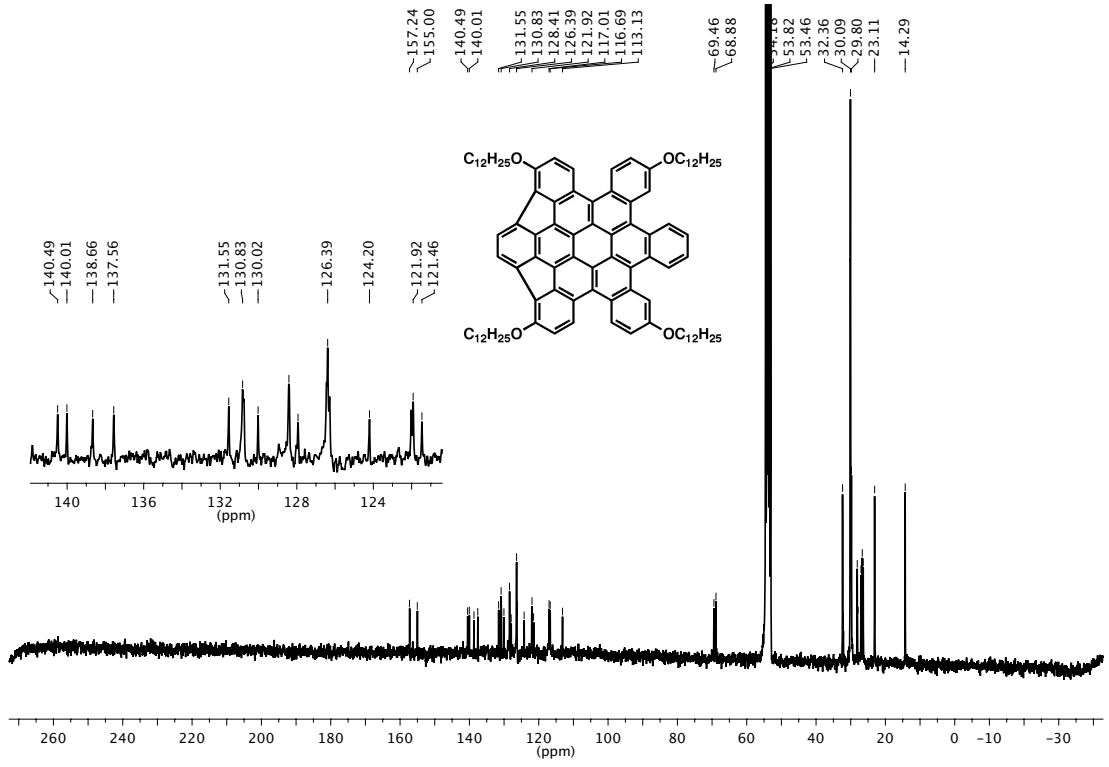
^{1}H NMR ($CDCl_3$) of S**8**.



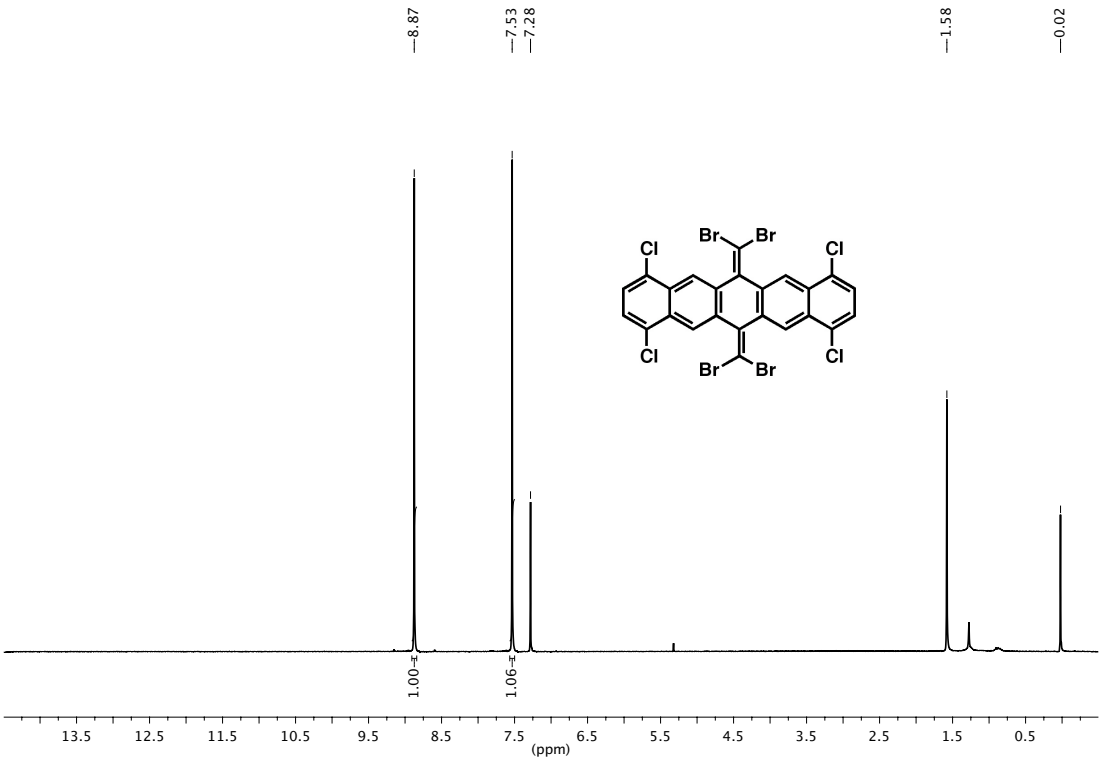
^{13}C NMR ($CDCl_3$) of S**8**.



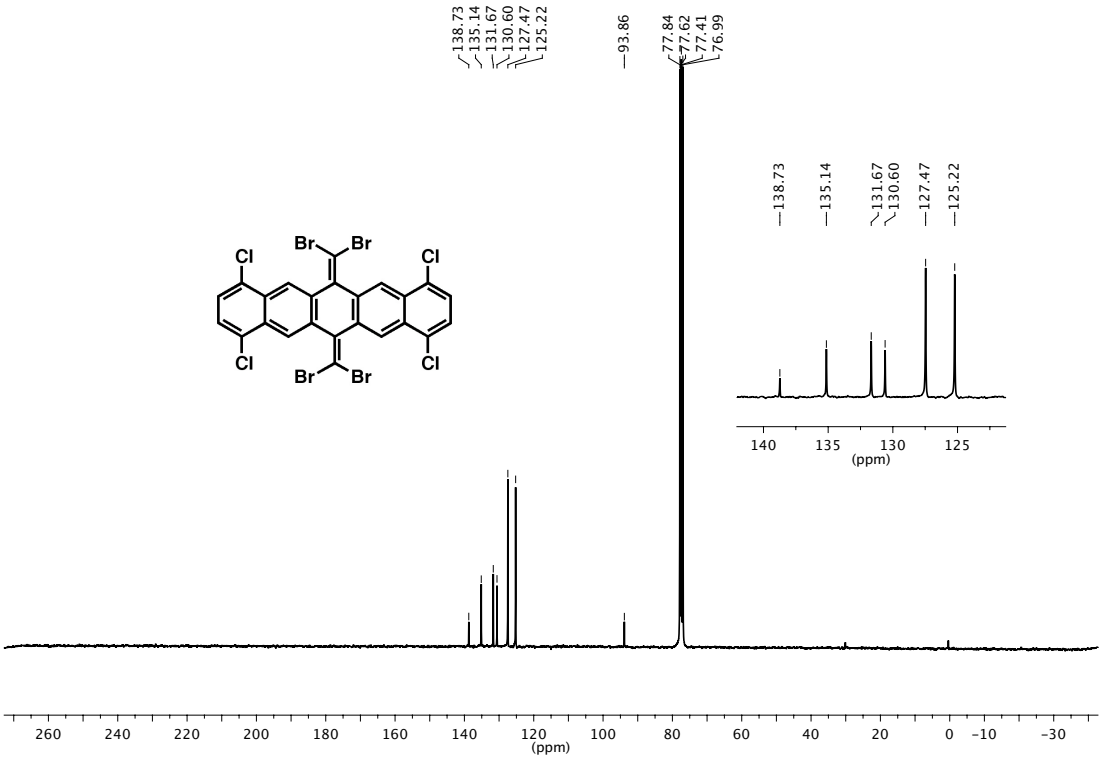
^{1}H NMR ($CDCl_3$) of S**9**.



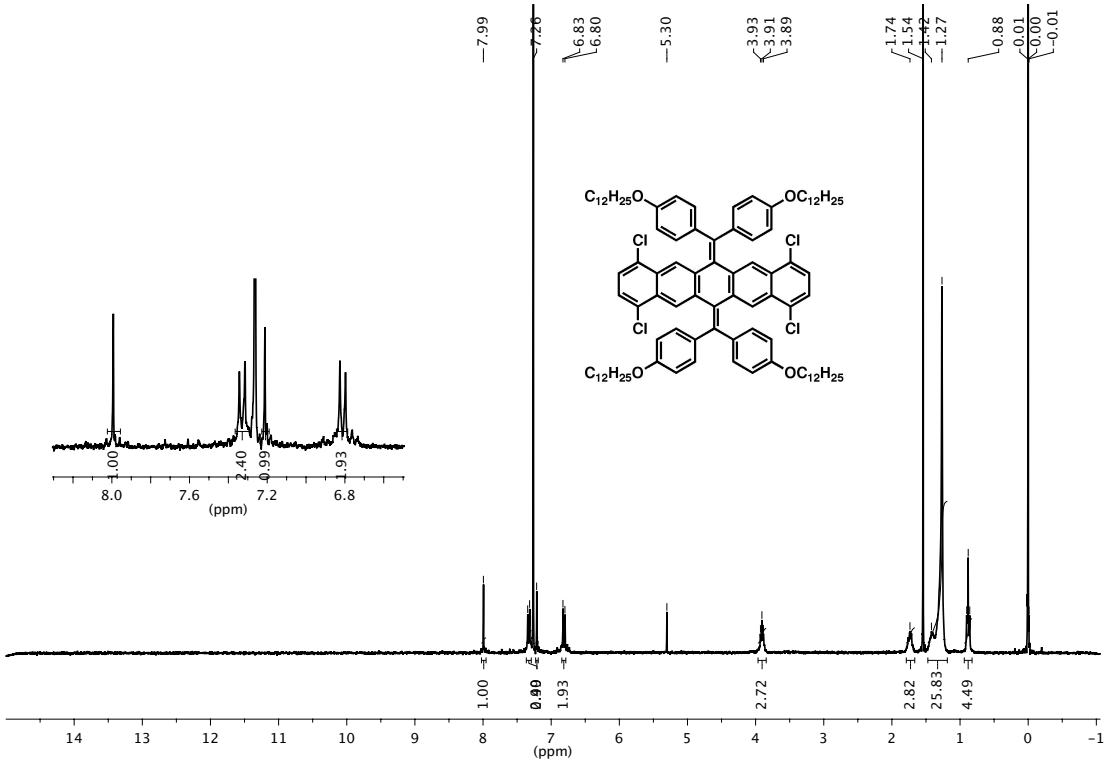
^{13}C NMR ($CDCl_3$) of S**9**.



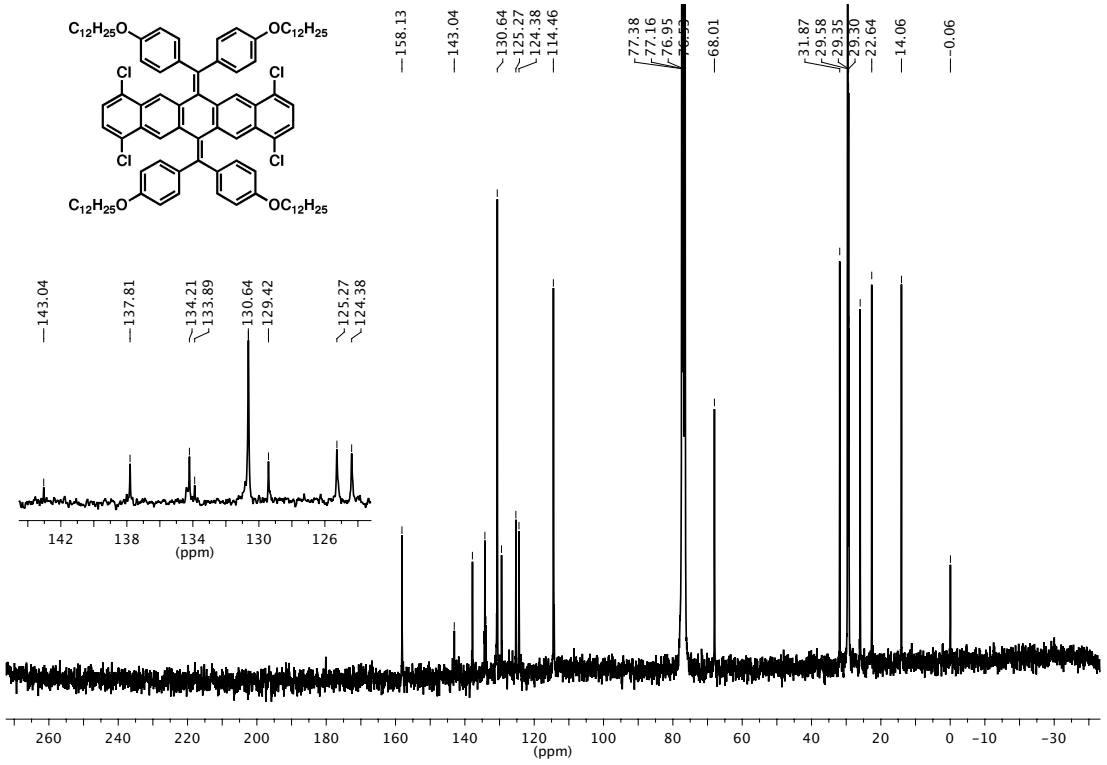
^{1}H NMR ($CDCl_3$) of S**11**.



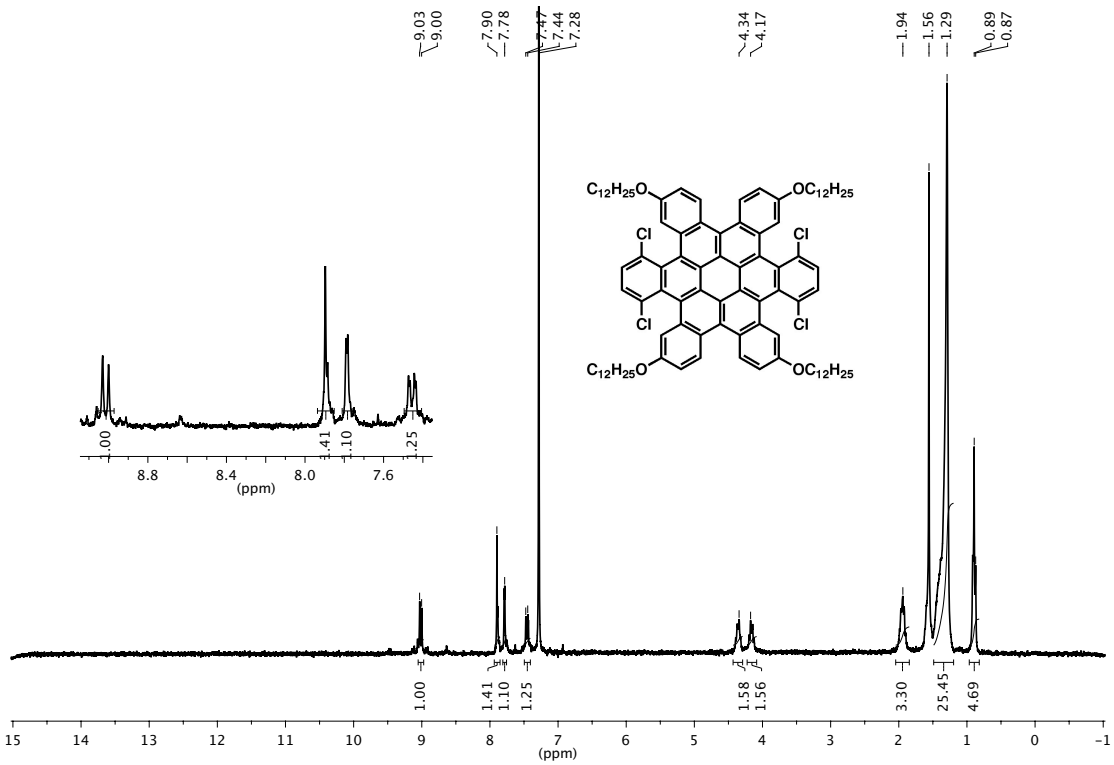
^{13}C NMR ($CDCl_3$) of S**11**.



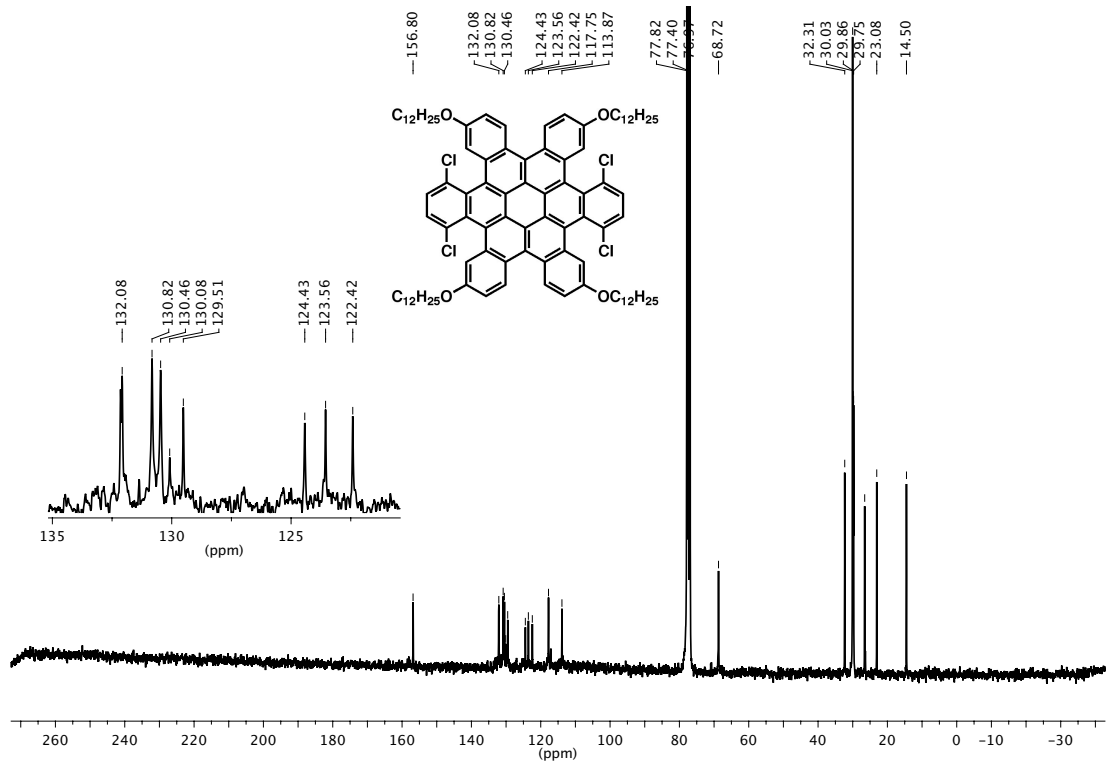
^{1}H NMR ($CDCl_3$) of S**12**.



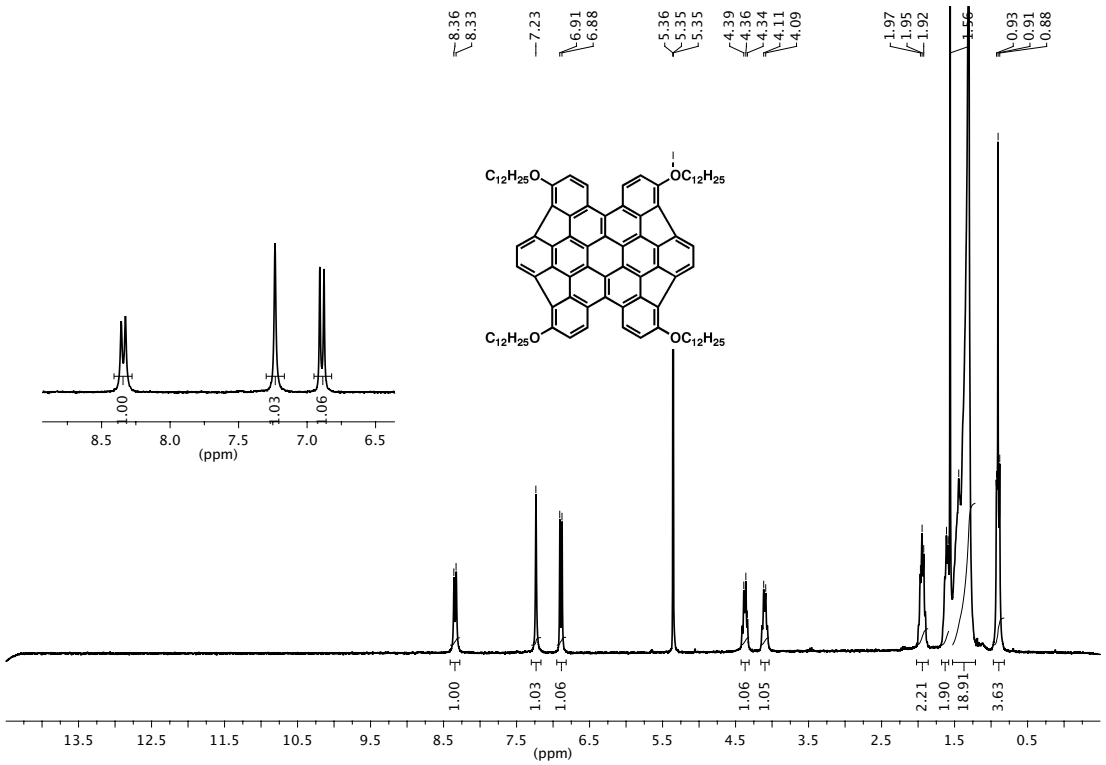
^{13}C NMR ($CDCl_3$) of S**12** .



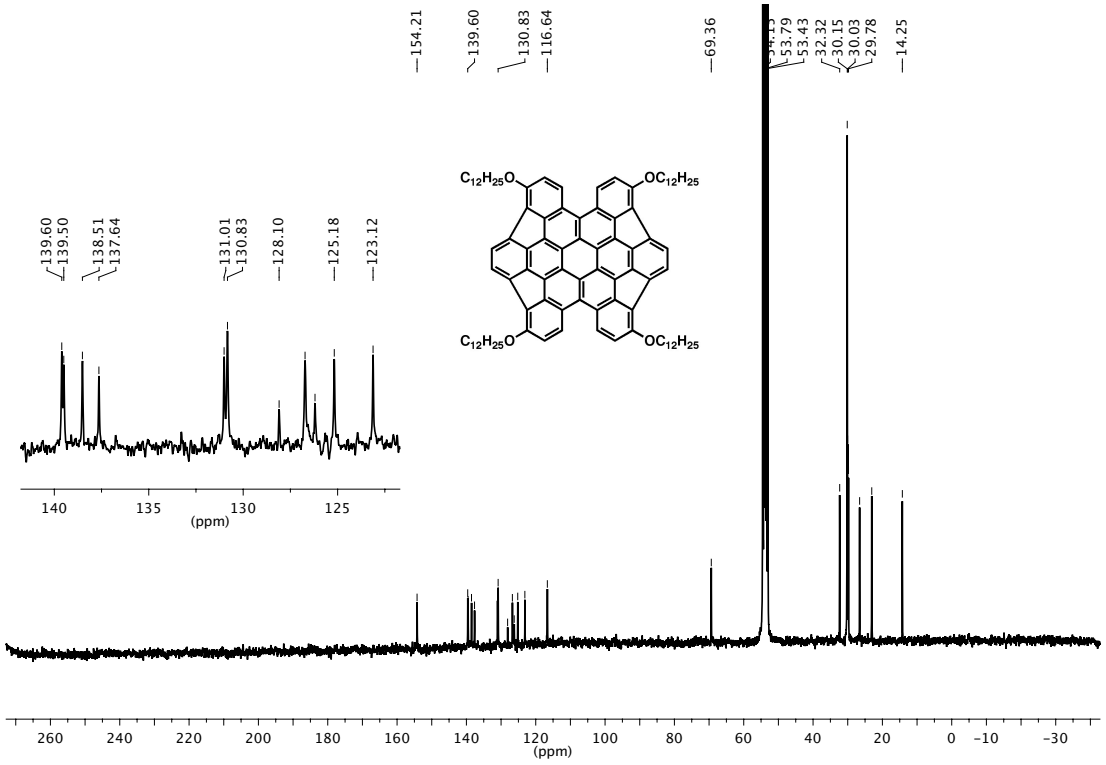
^{1}H NMR ($CDCl_3$) of S**13**.



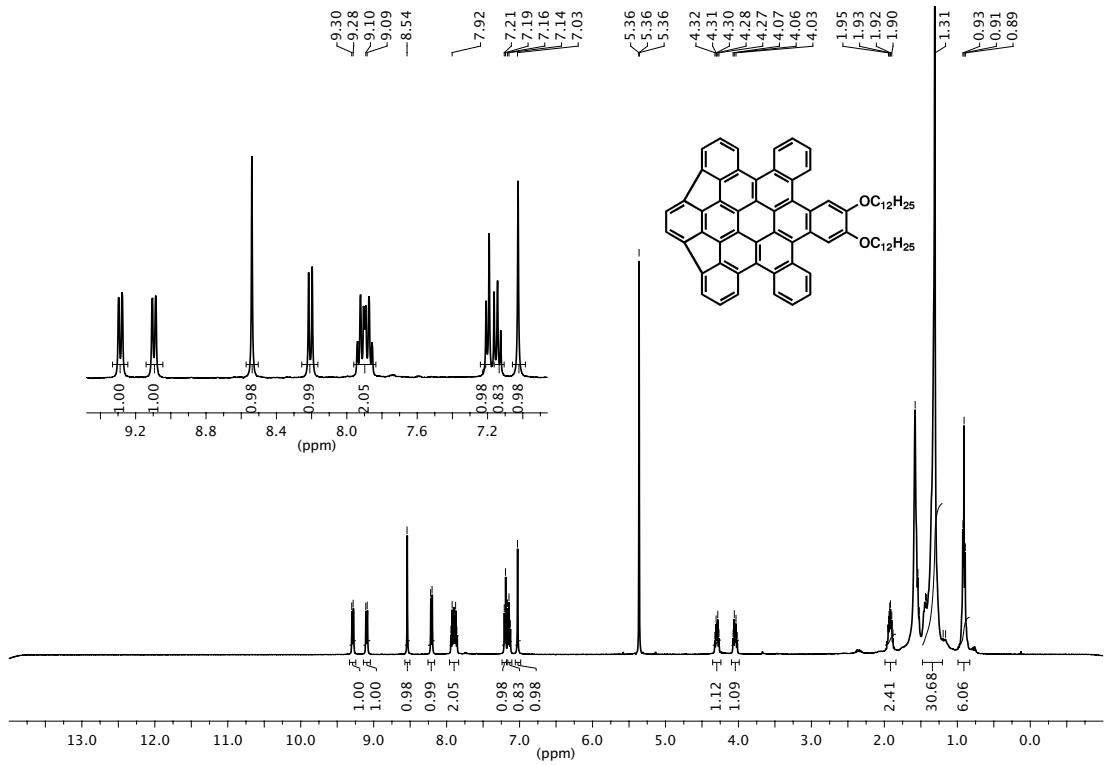
^{13}C NMR ($CDCl_3$) of S**13**.



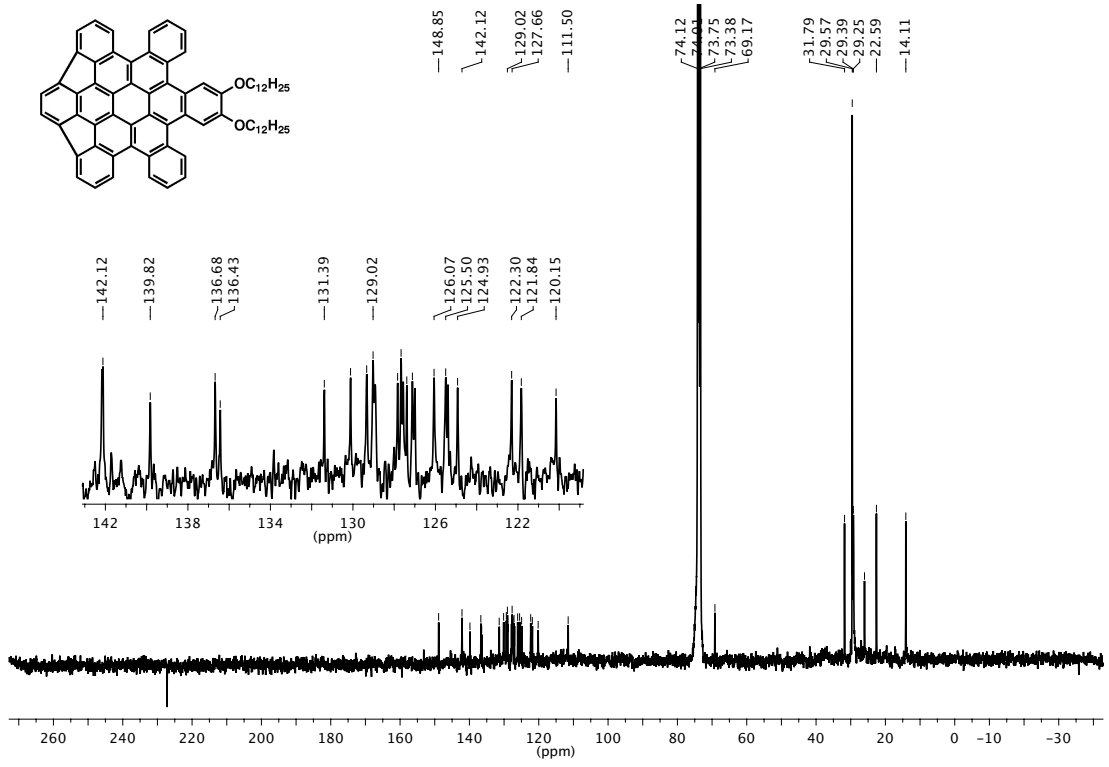
^{1}H NMR (CD_2Cl_2) of S**14**.



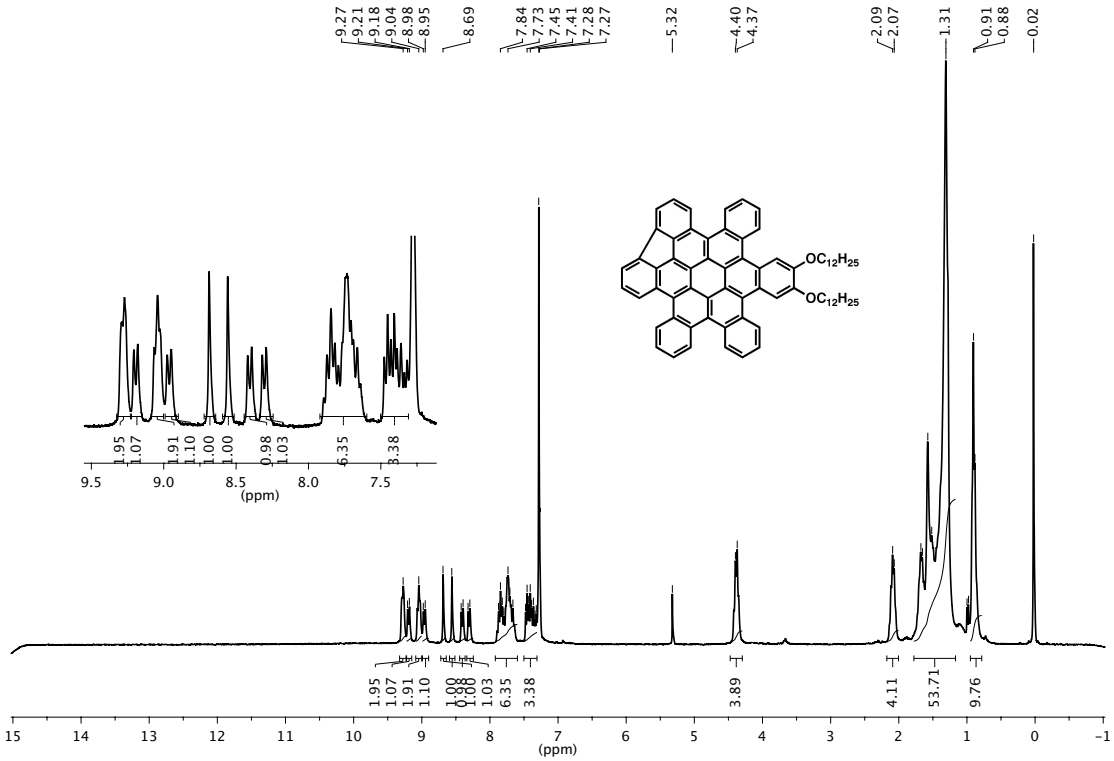
^{13}C NMR (CD_2Cl_2) of S**14**.



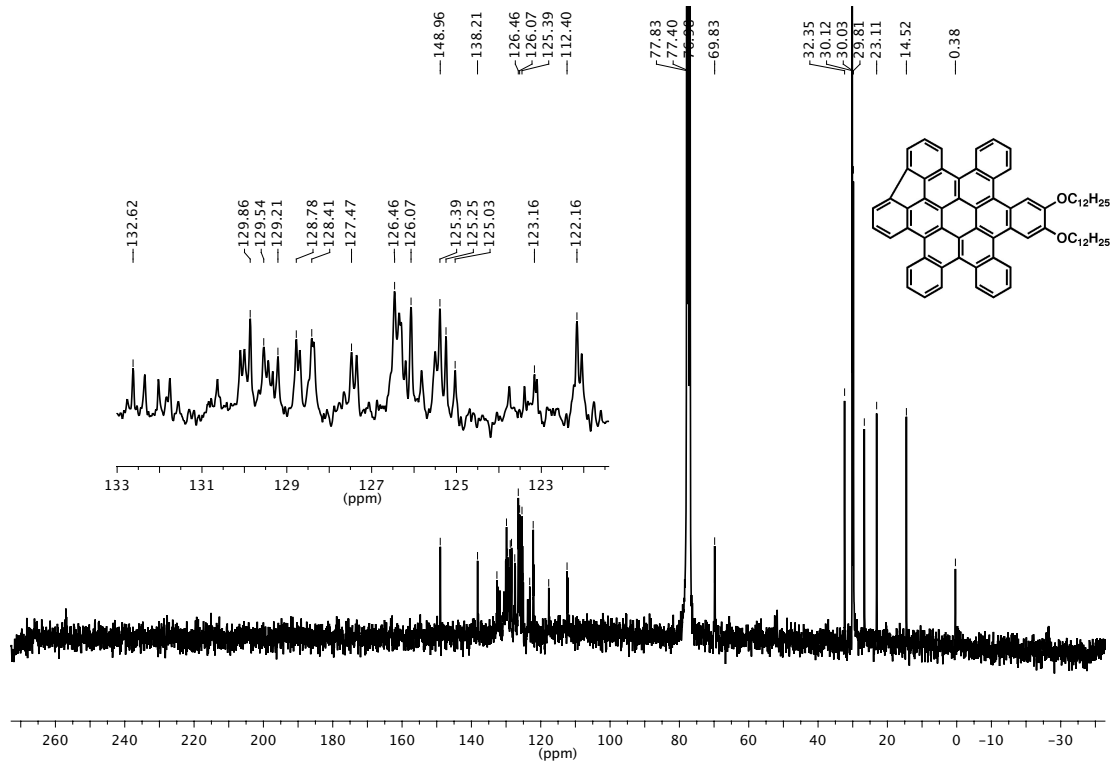
^{1}H NMR (CD_2Cl_2) of S**16**.



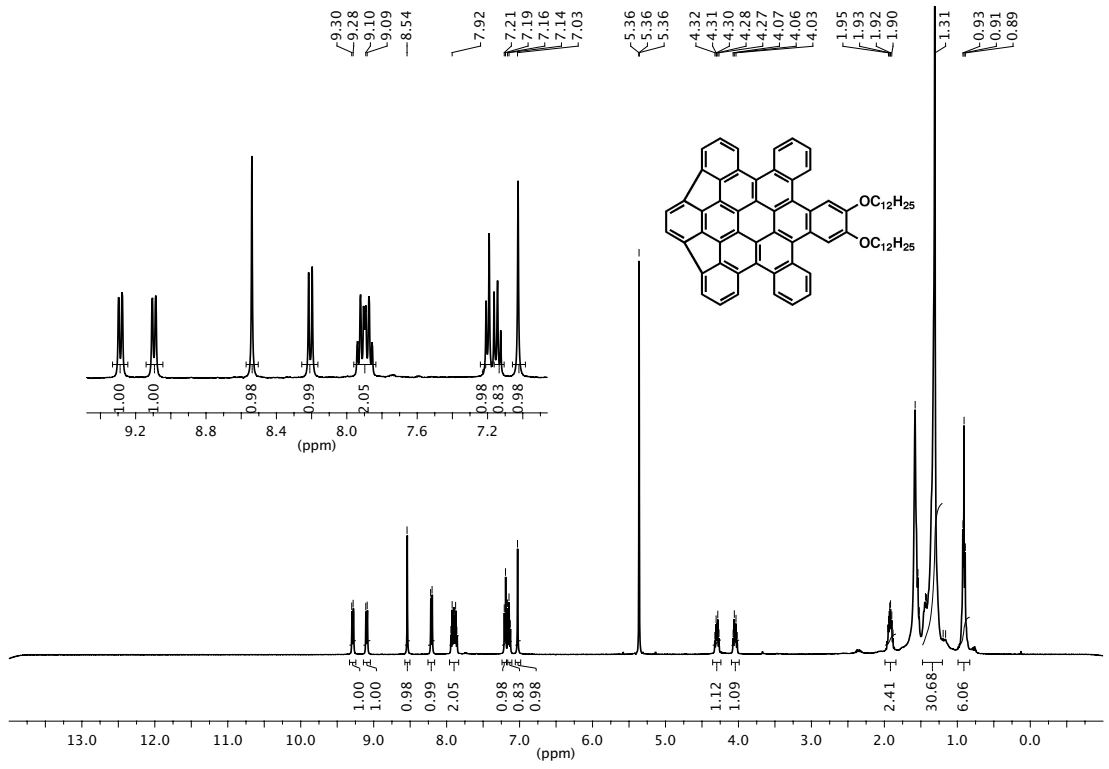
^{13}C NMR (CD_2Cl_2) of S**16**.



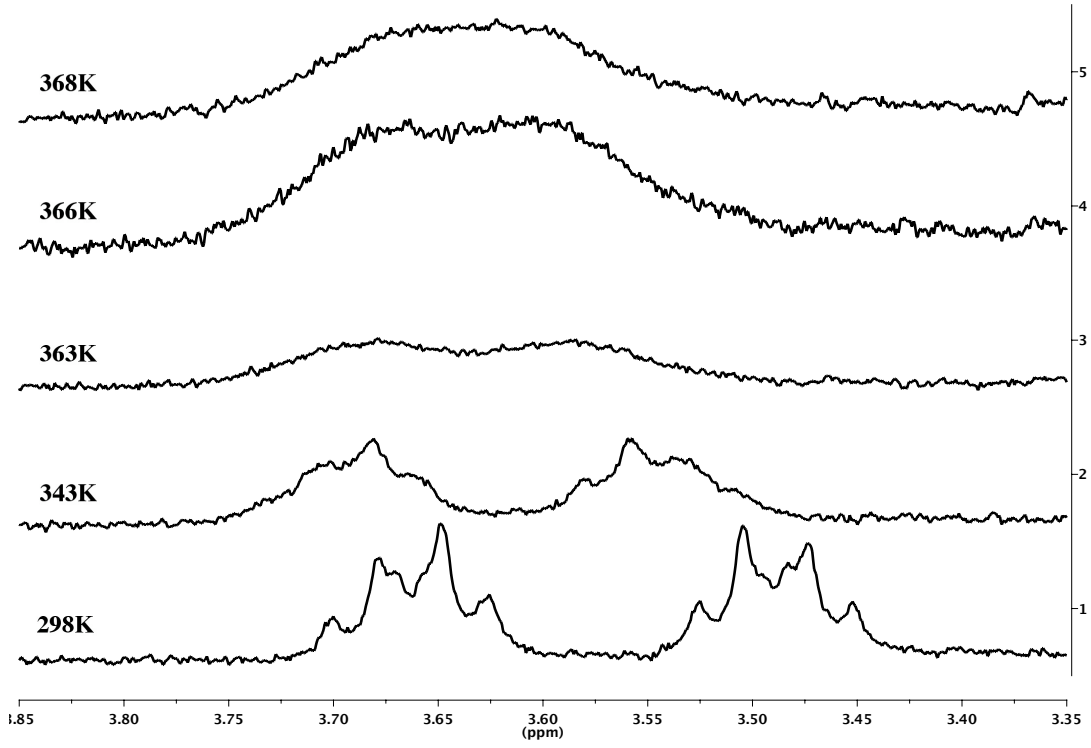
^{1}H NMR ($CDCl_3$) of S**18**.



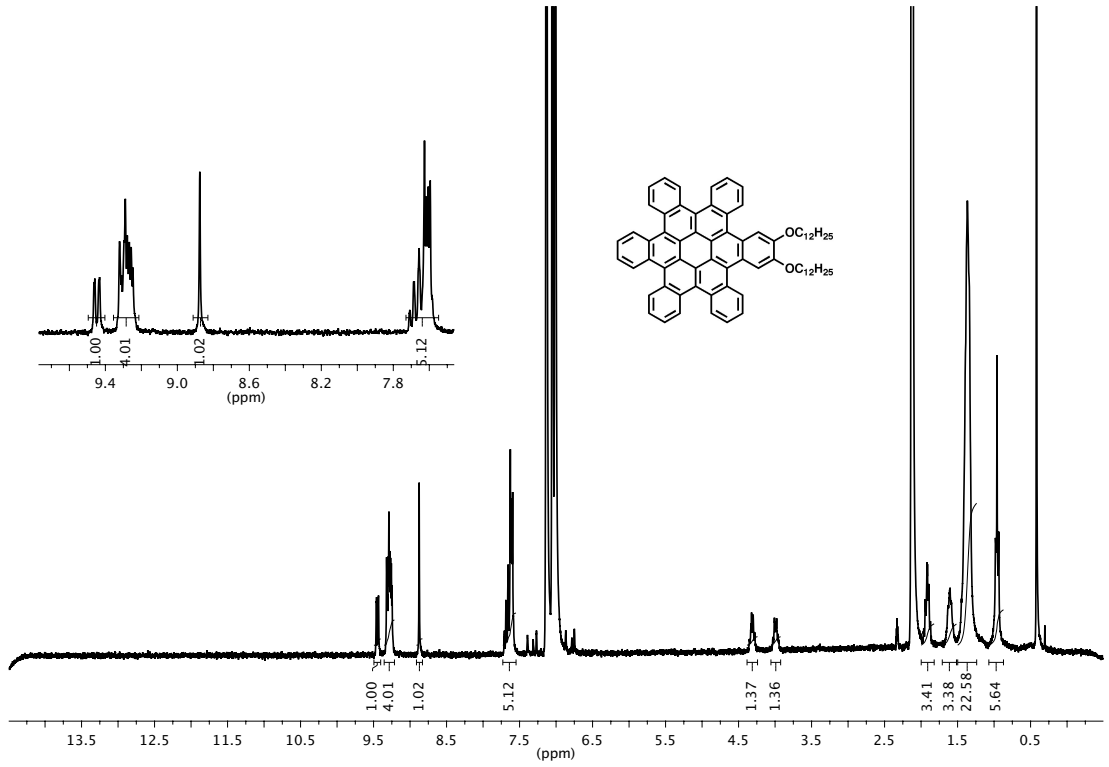
^{13}C NMR ($CDCl_3$) of S**18**.



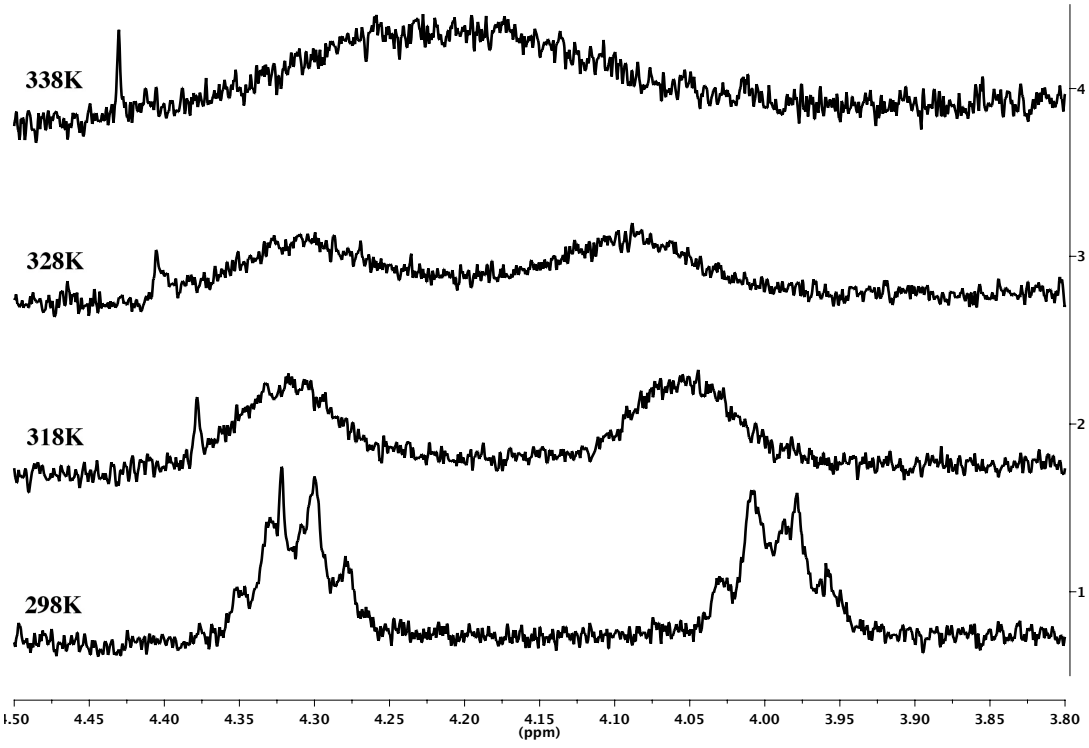
^{1}H NMR (CD_2Cl_2) of S**16**.



Variable Temperature Experiment (Cl_2CCDCl_2) of S**16**.



^{1}H NMR ($Cl_2CDCDCl_2$) of S**17**.



Variable Temperature Experiment (Cl_2CCDCl_2) of S**17**.

7. References

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