

Supporting Information

Ring-Size Effect on Molecular Assembly Structures and Optical Properties of C_3 -Symmetrical Dehydrobenzoannulene Derivatives

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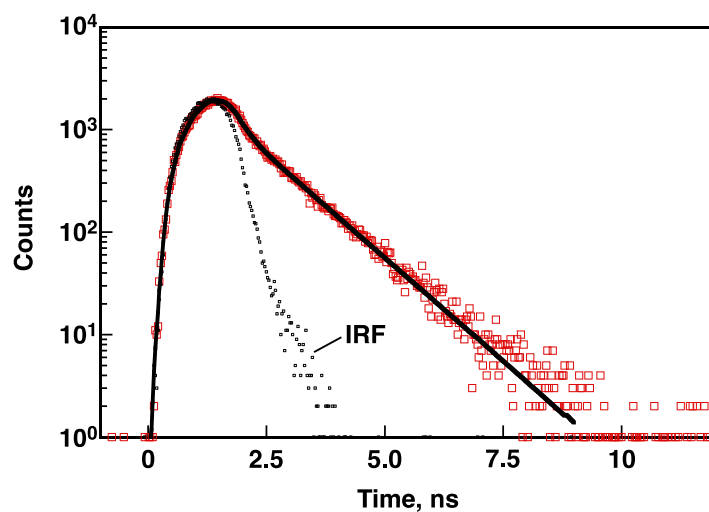
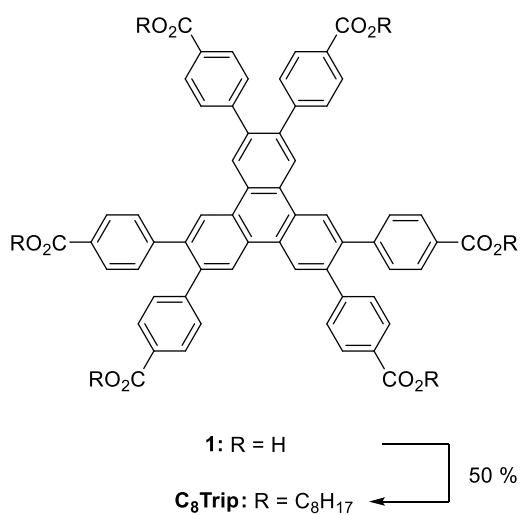
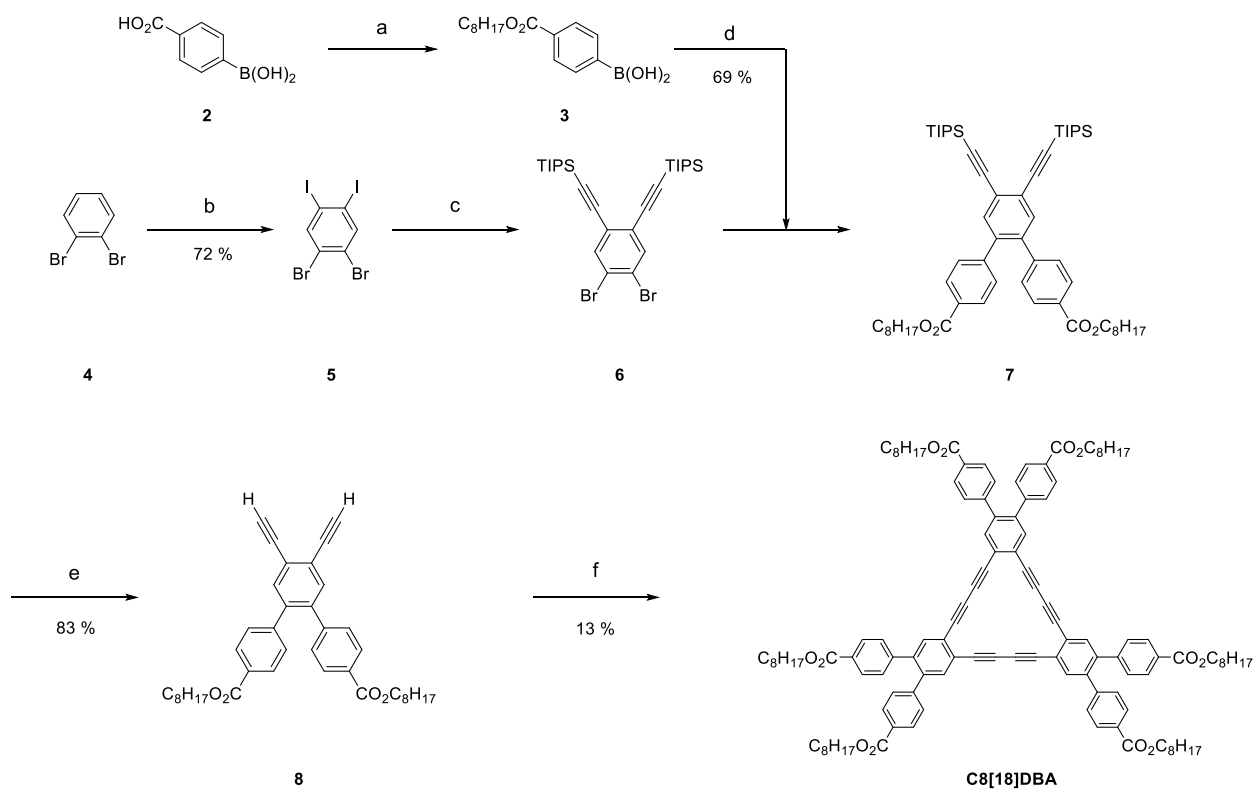


Fig. S1. Emission lifetime of Br-FL-CHO (red: 4×10^{-5} M) and instrumental response function (black: IRF) observed at 370 nm in CHCl_3 at 298 K. The solid line is a fitted line for the fluorescence emission of Br-FL-CHO. Excitation wavelength is 333 nm.



Scheme S1. Preparation of **C₈Trip**. Condition and reagents: 1) SOCl_2 , reflux, 15 h; 2) $\text{C}_8\text{H}_{17}\text{OH}$, Et_3N , CH_2Cl_2 , RT, 25 h, 50 %.



Scheme S2. Synthesis of **C8[18]DBA** a: K_2CO_3 , $C_8H_{17}Br$, dry DMF; b: I_2 , $NaIO_3$, conc. H_2SO_4 ; c: TIPS acetylene, CuI , $Pd(PPh_3)_4$, $i\text{-}Pr_2NH$, dry THF; d: Na_2CO_3 , $Pd(dppf)Cl_2$, toluene, H_2O , 1,4-dioxane; e: TBAF, THF; f: $(AcO)_2Cu$, pyridine, methanol, Et_2O .

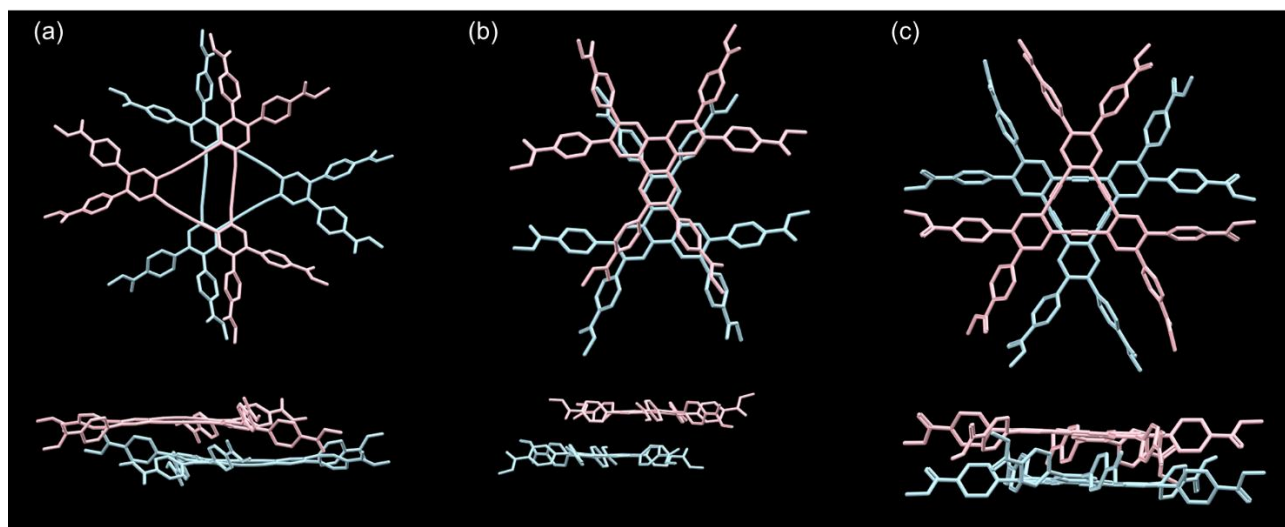


Figure S2. Estimation of the intermolecular intradimer interaction (E_{intra}). Model structures used for calculations of E_{intra} in a) **C1[18]DBA**, b) **C1Trip**, and c) **C1[12]DBA**. (Legend) Red: monomer A, blue: monomer B. Hydrogen atoms are omitted for clarity.

The interaction energy between dimers (E_{inter}) was calculated from the difference between the energy of the tetramer and the sum of the energies of the two dimers, using equation (S2) (Figure S2).

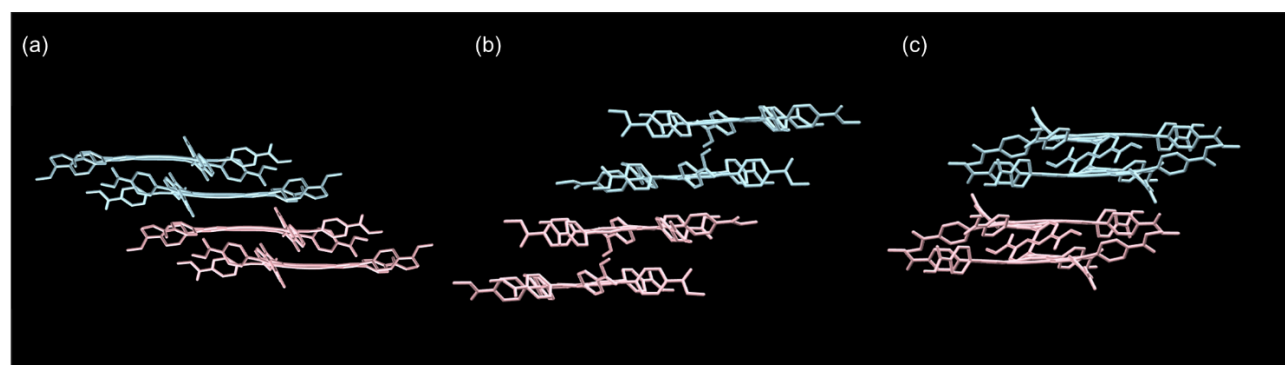


Figure S3. Estimation of the interdimer interaction (E_{inter}). Model structures using calculations of E_{inter} in a) **(C1[18]DBA)₂**, b) **(C1Trip)₂**, and c) **(C1[12]DBA)₂**. (Legend) Red: dimer A, blue: dimer B. Hydrogen atoms are omitted for clarity.

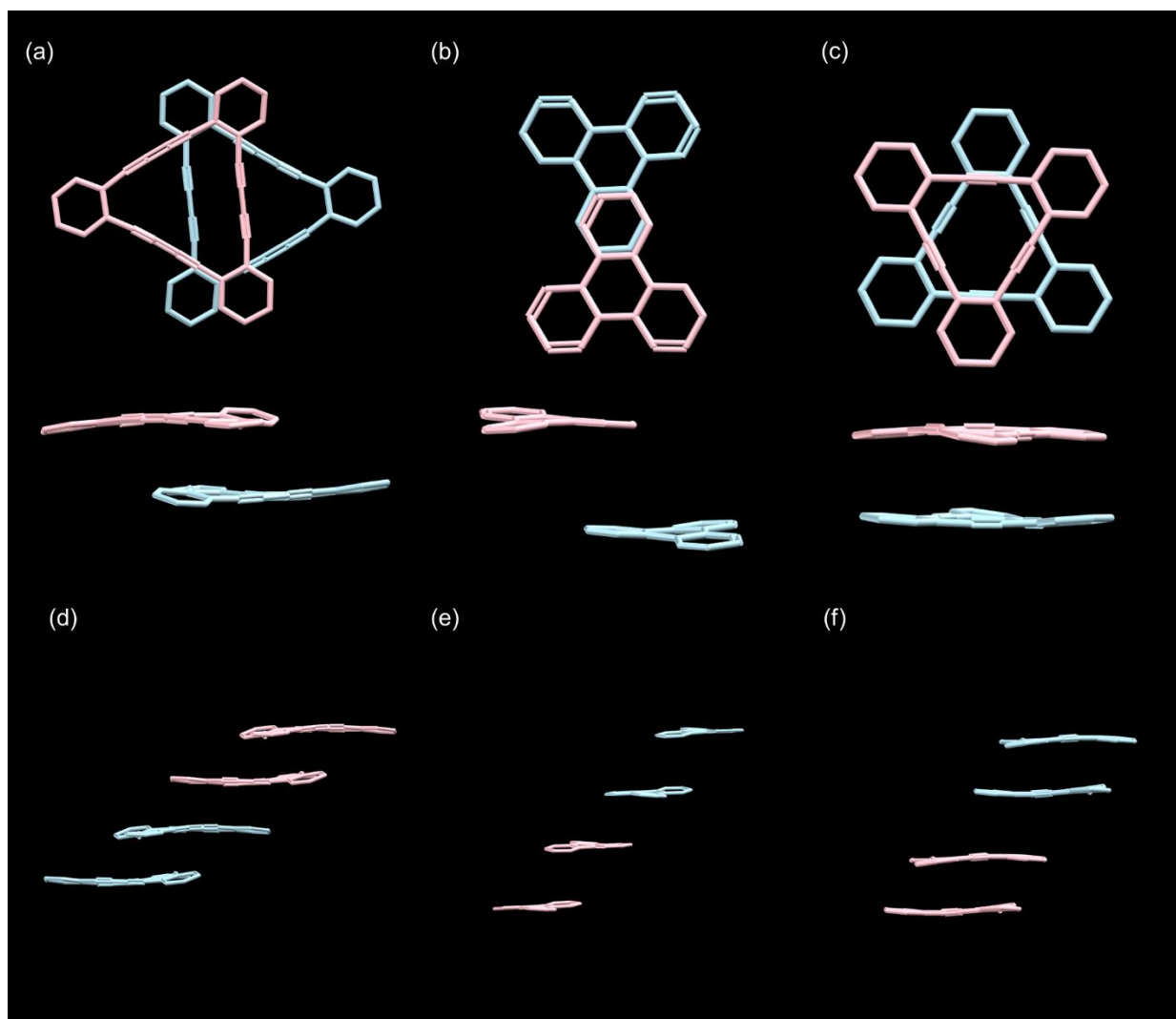


Figure S4. Estimation of intermolecular interactions of the π -electrons at the π -planar molecules. Single-point energy calculations were performed for the structures excluding the terminal methylbenzoate groups. Model structures using calculations of interaction within intradimer E^{π}_{intra} for a) **[18]DBA**, b) **Trip**, and c) **[12]DBA**. (Legend) Red: monomer A, blue: Monomer B. Model structures using calculations of interaction within interdimer E^{π}_{inter} for d) **([18]DBA)₂**, e) **(Trip)₂**, and f) **([12]DBA)₂**. (Legend) Red: dimer A, blue: dimer B. Hydrogen atoms are omitted for clarity.

Electronic structures of C1[*n*]DBA and C1Trip

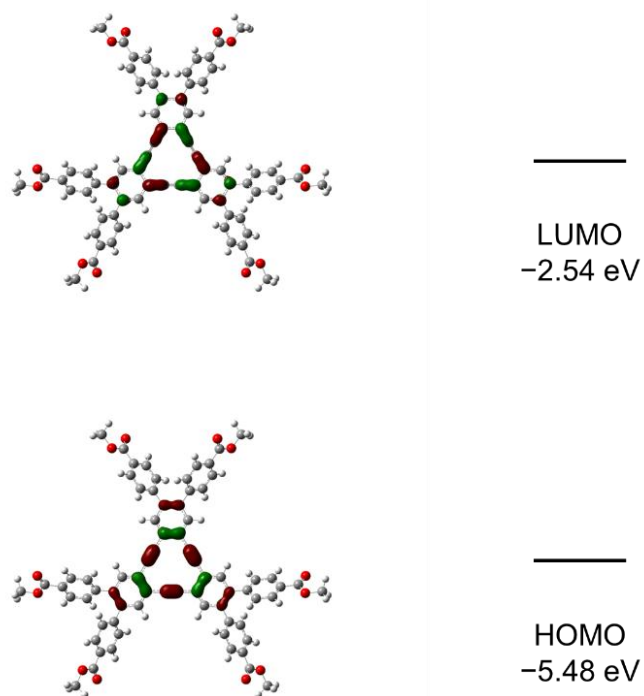


Figure S5. Frontier orbitals of C1[12]DBA estimated by B3LYP/6-31 G(d,p). Isovalue was 0.04.

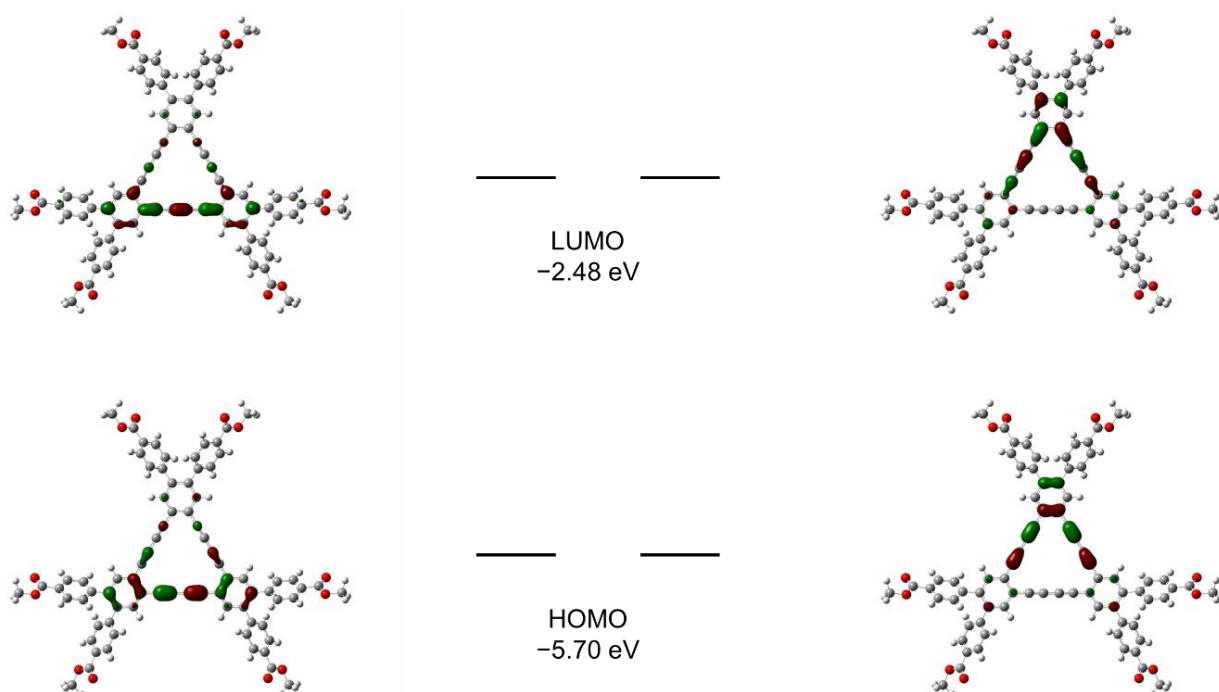


Figure S6. Frontier orbitals of C1[18]DBA estimated by B3LYP/6-31 G(d,p). Isovalue was 0.04.

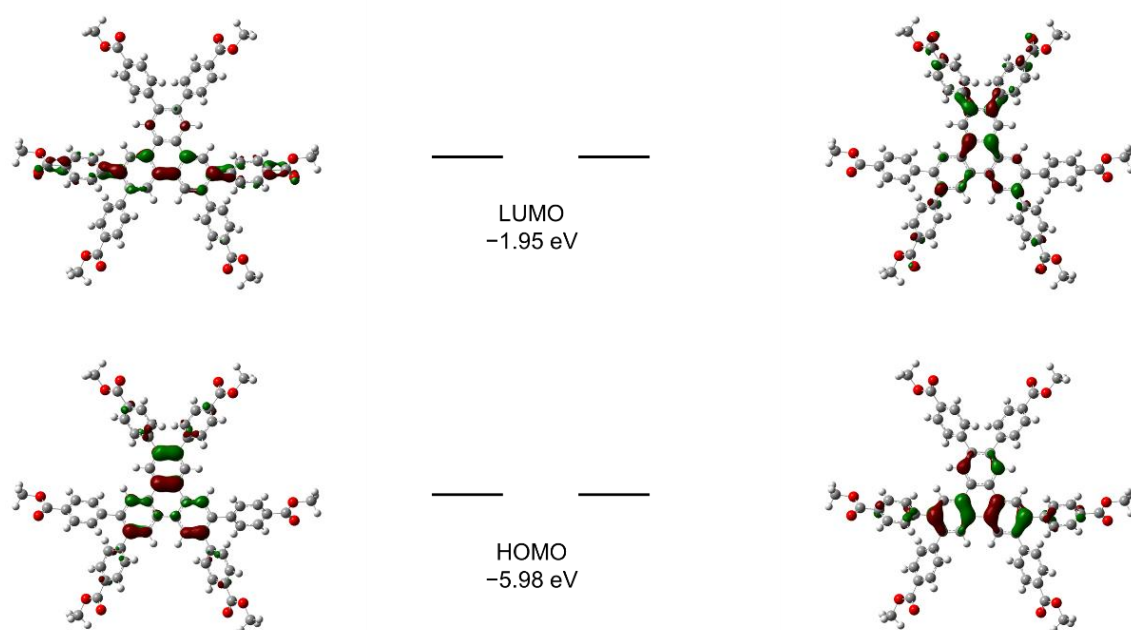


Figure S7. Frontier orbitals of **C1Trip** estimated by B3LYP/6-31 G(d,p). Isovalue was 0.04.

TG curves of C8[n]DBA and C8Trip

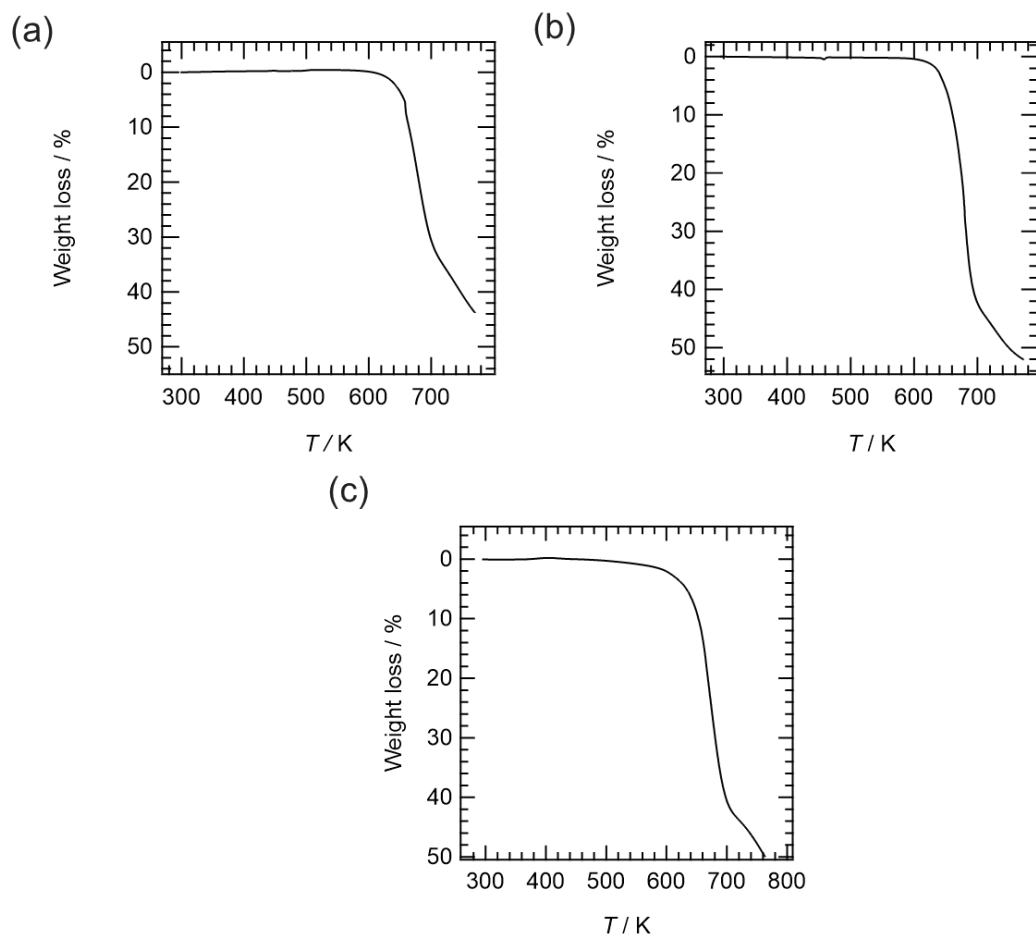


Figure S8. TG curves of a) C8[18]DBA, b) C8Trip, and c) C8[12]DBA.

PXRD pattern of C8[18]DBA after polymerization and crystal phase

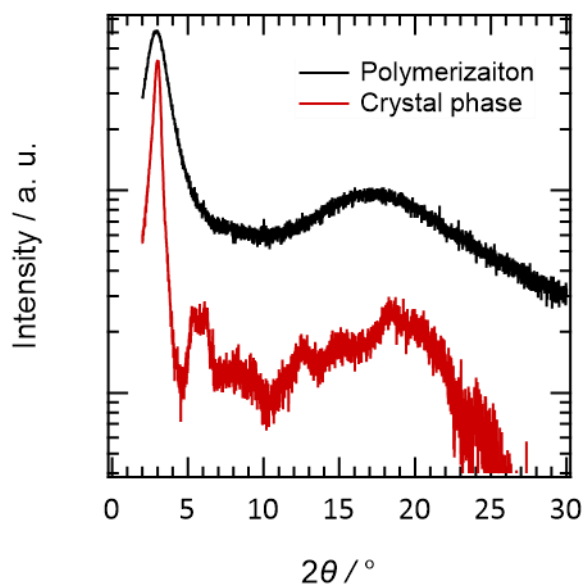


Figure S9. PXRD patterns of C8[18]DBA in crystalline phase (red) and after polymerization (black).

POM images of C8[12]DBA

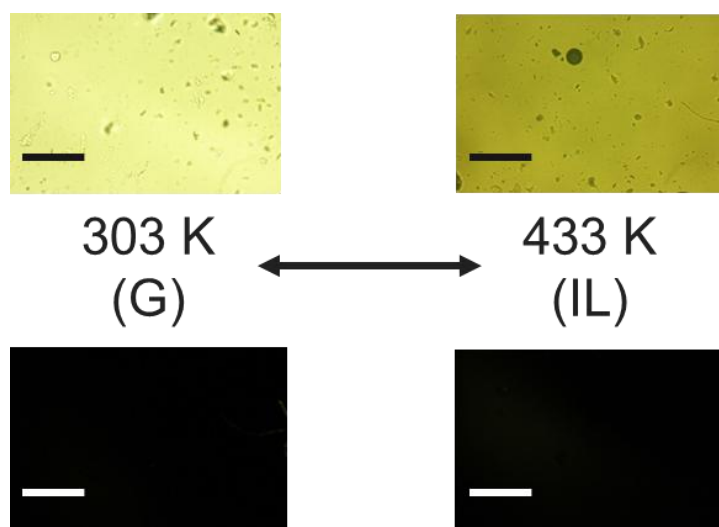


Figure S10. Variable temperature microscopic observations of C8[12]DBA.^{S1} Upper are the optical microscopic (OM) images and down are the polarized optical microscopic (POM) images. Scale bar is 300 μm .

Molecular assembly structures of C8[*n*]DBAs and C8Trip

Table S1. Molecular assembly structures, phase transition behaviors, and the transition enthalpy changes of the phase transition (ΔH) of C8[*n*]DBA and C8Trip.

Compounds	Molecular assemblies	<i>T</i> , K	ΔH , kJ/mol
C8[18]DBA	Crystal (Hexagonal columnar)	440, Polymerization	– ^[b]
C8Trip	Crystal (Dimer columnar)	450, Cr → IL	–23.8 (+16.7)
C8[12]DBA ^{S6}	Glass	320, G → IL	– ^[a]

[a] Glass transition. [b] Polymerization.

Single crystal structures of C1[*n*]DBAs and C1Trip

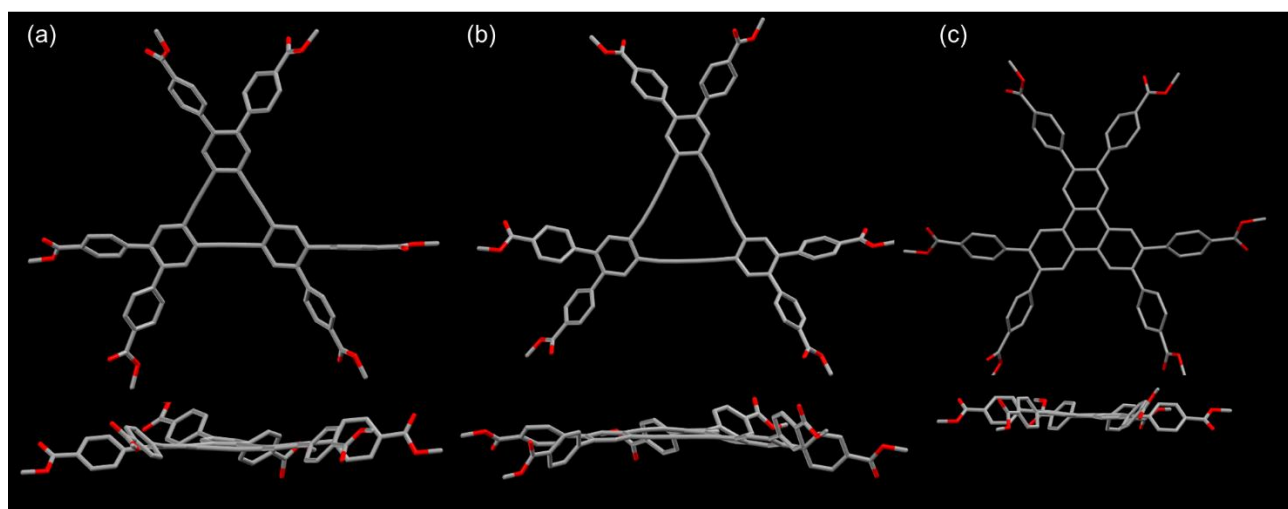


Figure S11. Single crystal structures of C1[*n*]DBA and C1Trip. Viewed from the vertical (top) and horizontal (bottom) directions of the π plane. a) C1[12]DBA^{S1}; b) C1[18]DBA^{S2}; c) C1Trip.

(Legend) Gray: carbon atoms, red: oxygen atoms. Hydrogen atoms are omitted for clarity.

PXRD patterns of C8[n]DBA and C8Trip

Table S2. The diffraction peak angle 2θ , correlation length (d), and the ratio of correlation length (d_1 / d_n) of the PXRD pattern of **C8[18]DBA**.

Hexagonal arrangement (◦)	$2\theta / ^\circ$	$d / \text{\AA}$	d_1 / d_n
Dimer columnar (•)			
◦	3.12	28.3	1.0
◦	5.41	16.3	1.7
◦	6.16	14.4	2.0
◦	8.40	10.5	2.7
◦	9.37	9.44	3.0
◦	11.7	7.59	3.7
◦	12.6	7.04	4.0
•	7.74	11.4	1.0
•	14.8	5.99	1.9

Table S3. The diffraction peak angle 2θ , correlation length (d), and the ratio of correlation length (d_1 / d_n) of the PXRD pattern of **C8Trip**.

Columnar arrangement (◦)	$2\theta / ^\circ$	$d / \text{\AA}$	d_1 / d_n
Dimer columnar (•)			
◦	3.93	22.6	1.0
◦	7.90	11.2	2.0
•	6.30	14.0	—

Dielectric constants of C8[n]DBAs and C8Trip

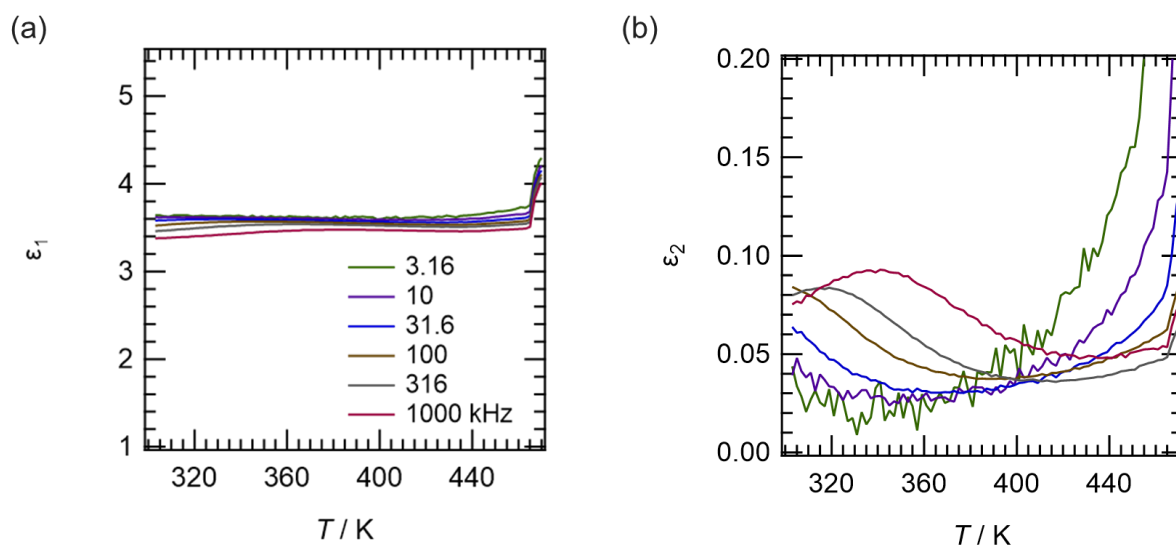


Figure S12. Real part ϵ_1 (a) and imaginary part ϵ_2 (b) of the dielectric constant of **C8Trip** measured under N₂ atmosphere.

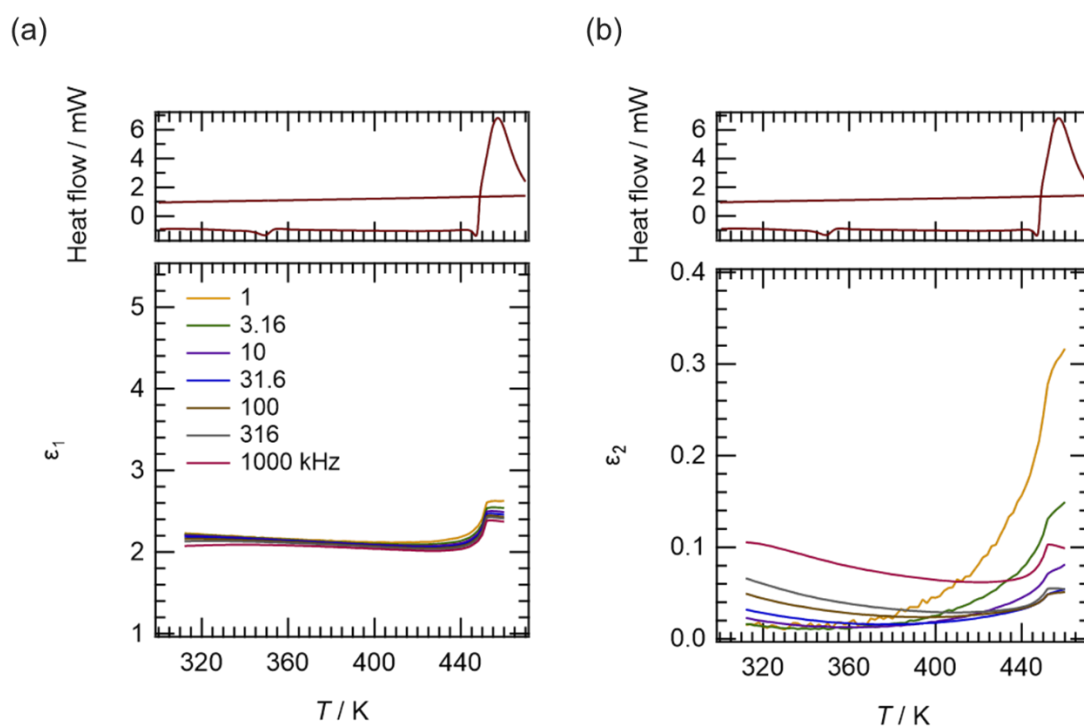


Figure S13. Real part ϵ_1 (a) and imaginary part ϵ_2 (b) of the dielectric constant of **C8[18]DBA** measured under N₂ atmosphere.

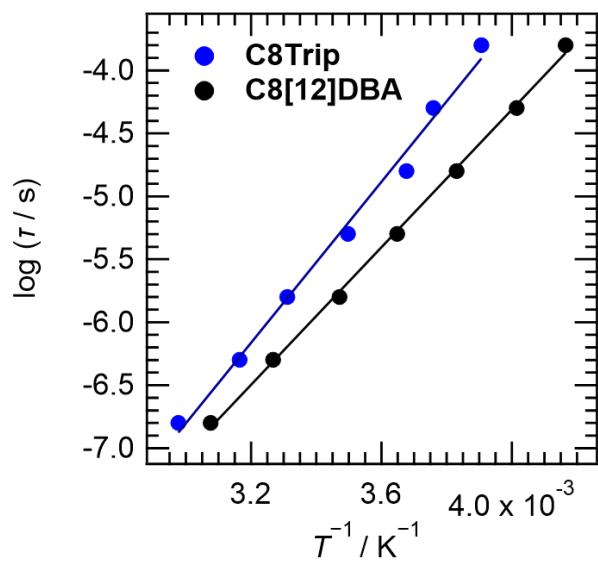


Figure S14. Temperature dependence of the dielectric relaxation time τ of **C8Trip** and **C8[12]DBA**^{S1}.

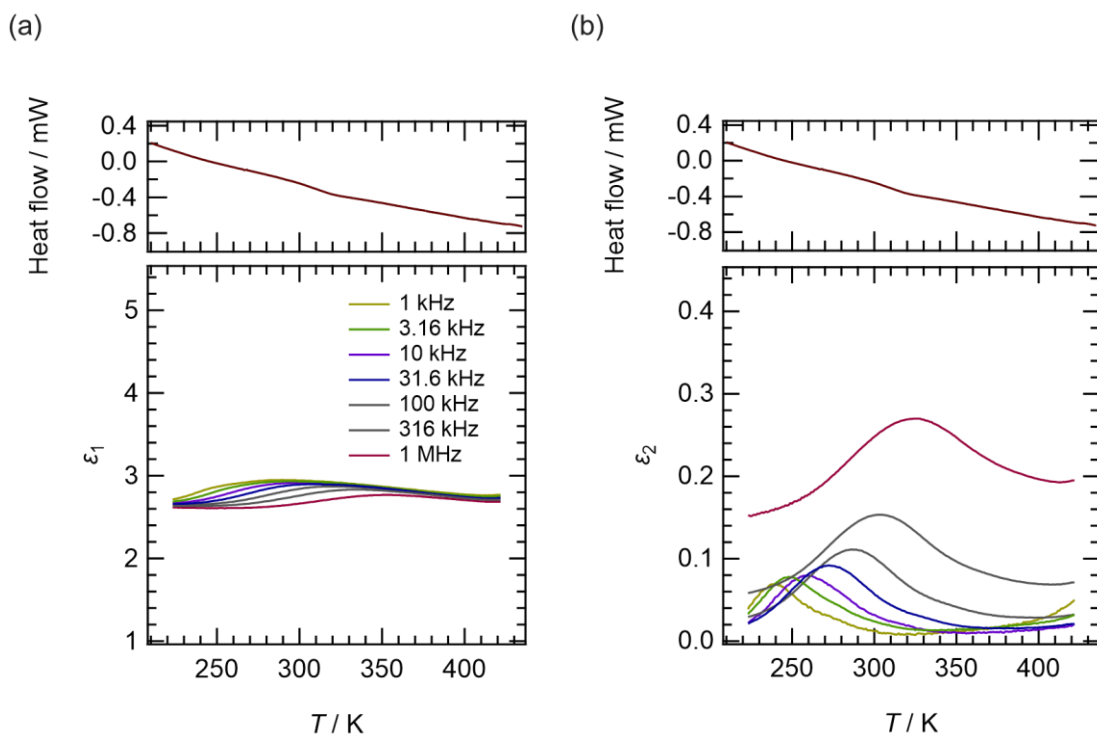


Figure S15. Real part ϵ_1 (a) and imaginary part ϵ_2 (b) of the dielectric constant of **C8[12]DBA** measured under vacuum atmosphere.^{S1}

Optical properties of C8[*n*]DBAs

Table S4. Optical properties of C8[12]DBA, C8[18]DBA, and C8Trip in CHCl₃ and solid state.

Compounds	Solution (in CHCl ₃)			Solid		
	Absorption	Fluorescent	ϕ_{FL} , %	Absorption	Fluorescent	ϕ_{FL} , %
	λ_{max} , nm	λ_{max} , nm ^a		^b λ_{max} , nm	λ_{max} , nm ^c	
C8Trip	310	391	11	313	413	5.7
C8[12]DBA^{S1}	332	511	13	332	535	10
C8[18]DBA	356	452	29	361	471	1.9

^a The excitation wavelength λ_{ex} for the fluorescence spectra of **C8[12]DBA**, **C8[18]DBA**, and **C8Trip** in CHCl₃ were 350, 395, and 310 nm, respectively. ^b Absorption spectra measured in the transmission configuration of the sample in KBr pellets. ^c The excitation wavelength λ_{ex} for the fluorescence spectra of **C8[12]DBA**, **C8[18]DBA**, and **C8Trip** in solids were 340, 395, and 310 nm, respectively.

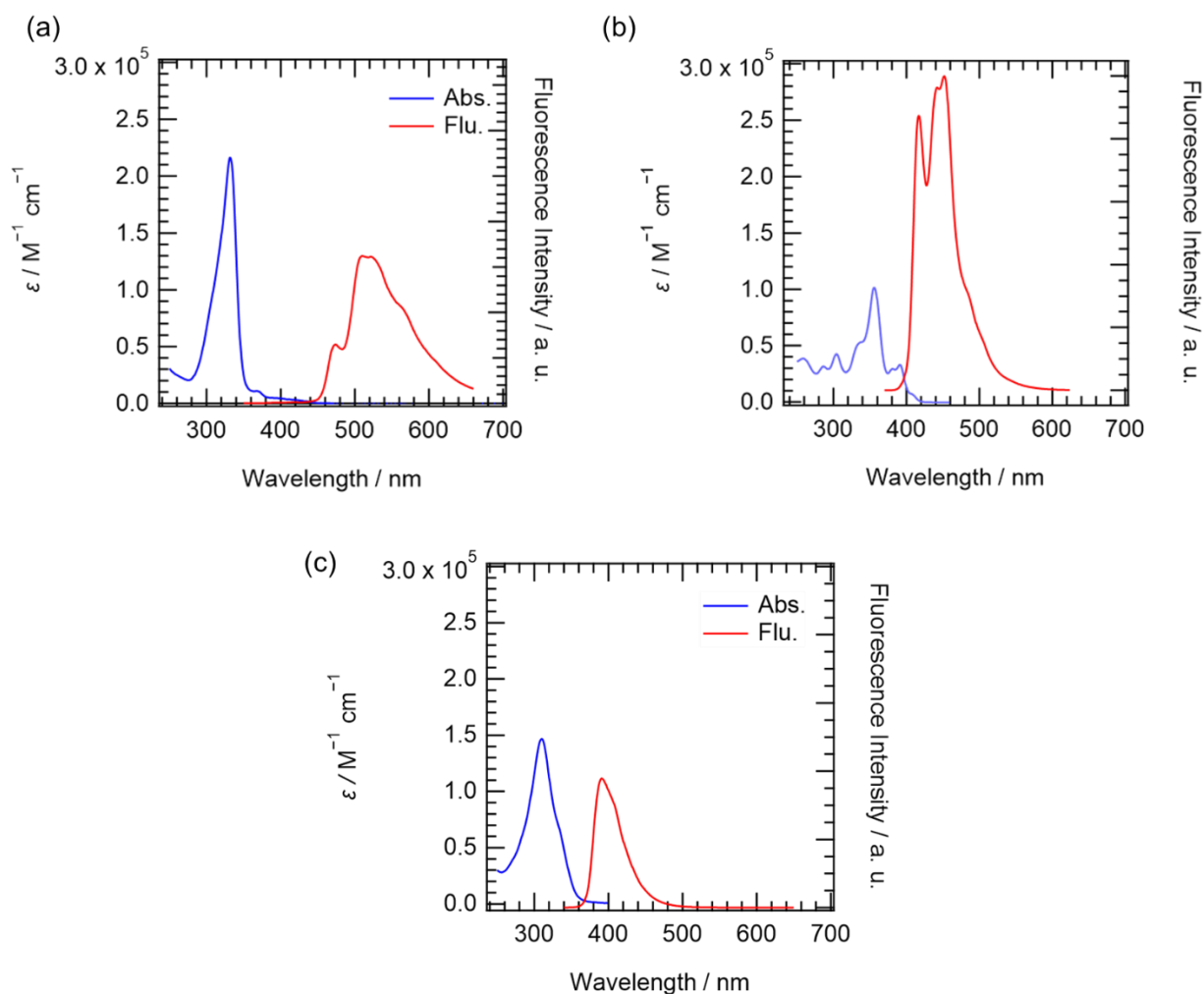


Figure S16. Optical properties of CHCl_3 solutions. a) **C8[12]DBA** ($\lambda_{\text{ex}} = 350 \text{ nm}$)^{S1}, b) **C8[18]DBA** ($\lambda_{\text{ex}} = 395 \text{ nm}$), c) Absorption-emission spectra of **C8Trip** in CHCl_3 solution and solid ($\lambda_{\text{ex}} = 310 \text{ nm}$). The vertical axis of the fluorescence spectrum is normalized based on the quantum yield (29%) of **C8[18]DBA**. In these figures, ϵ the molar absorption coefficient.

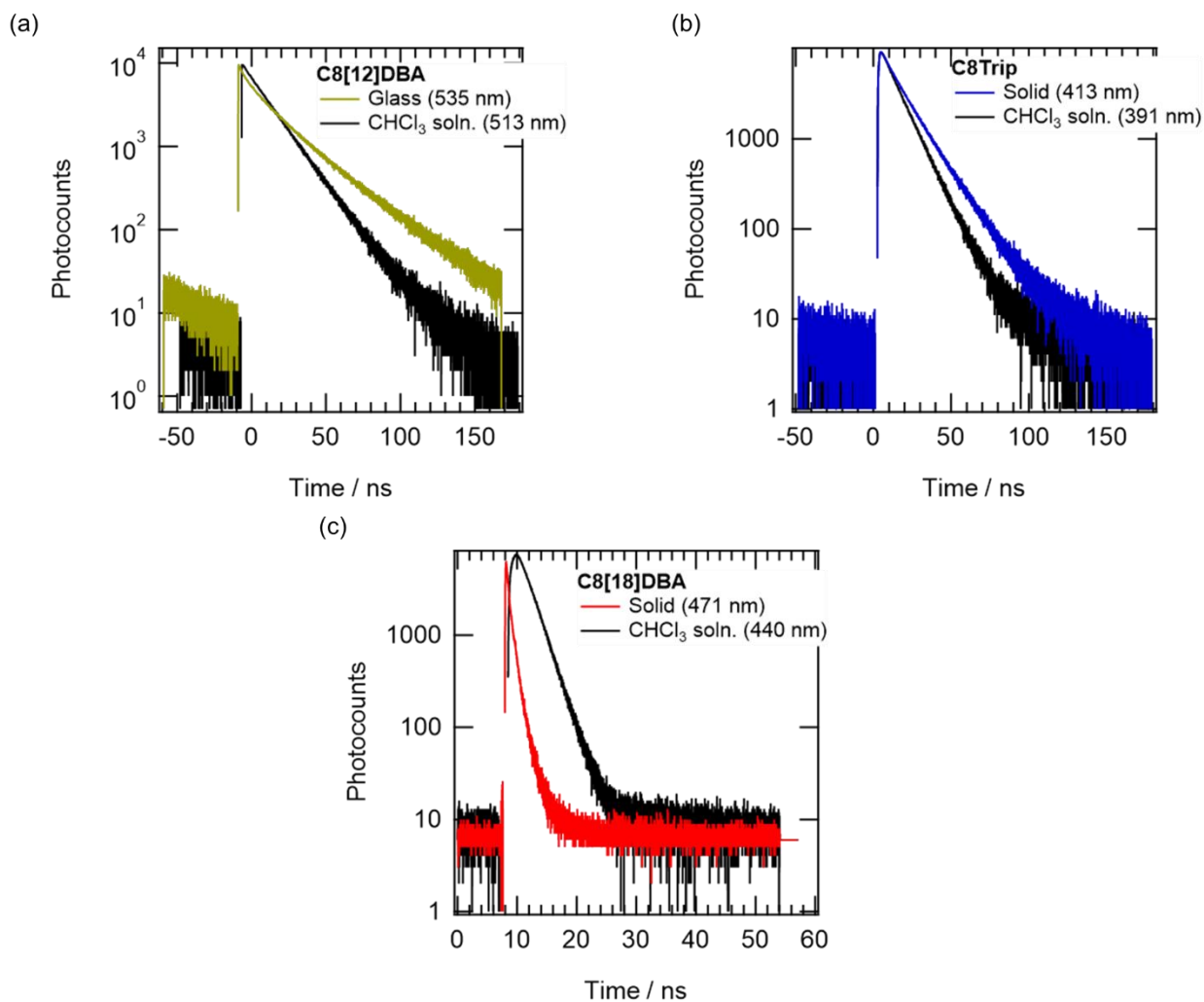


Figure S17. Fluorescence lifetime measurements of **C8[n]DBAs** and **C8Trip**. Fluorescence decay curves of a) **C8[12]DBA** (λ_{ex} : 375 nm), b) **C8Trip** (λ_{ex} : 279 nm), c) **C8[18]DBA** (λ_{ex} : 279 nm). In parentheses are the observed emission wavelengths.

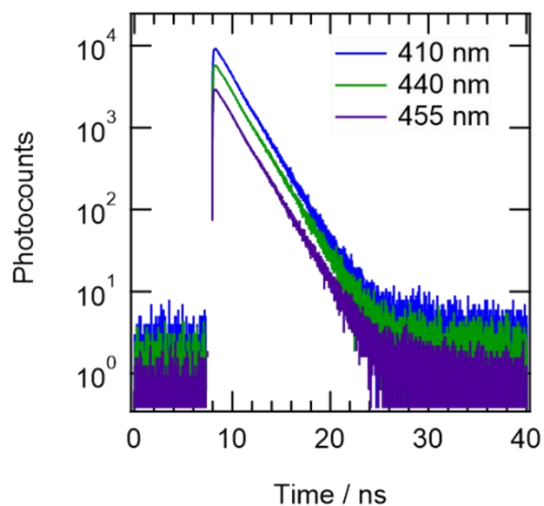


Figure S18. Observed emission wavelength-dependent fluorescence lifetime measurements of **C8[18]DBA** (λ_{ex} : 279 nm).

Table S5. Values of time constants (τ) obtained from a global multiexponential fit of the emission decays of **C8[n]DBAs** and **C8Trip** in CHCl_3 soln. and aggregated state.

Compounds	Solution (in CHCl_3) ^a			Solid		
	Excitation	Observed	τ / ns	Excitation	Observed	τ / ns
	λ_{ex} , nm	λ_{ob} , nm		λ_{ex} , nm	λ_{ob} , nm	
C8[12]DBA	375	511	7.55	375	532	6.36
			17.1			27.7
			1.43			
C8Trip	273	390	11.5	273	410	5.7
						15.3
C8[18]DBA	273	455	1.03	273	473	0.654
			2.18			1.34

^a: The concentrations of the solvents were 1.49×10^{-4} M (**C8[12]DBA**), 1.26×10^{-4} M (**C8[18]DBA**), 1.24×10^{-4} M (**C8Trip**),

Table S6. Observed emission wavelength-dependent values of time constants (τ) obtained from a global multiexponential fit of the emission decays of **C8[18]DBAs** in CHCl₃ soln.

Excitation λ_{ex} , nm	Observed λ_{ob} , nm	τ / ns
273	410	1.02
		2.20
273	440	1.03
		2.20
273	455	1.03
		2.18

a: The concentrations of the solvents was 1.26×10^{-4} M (**C8[18]DBA**).

NMR spectra.

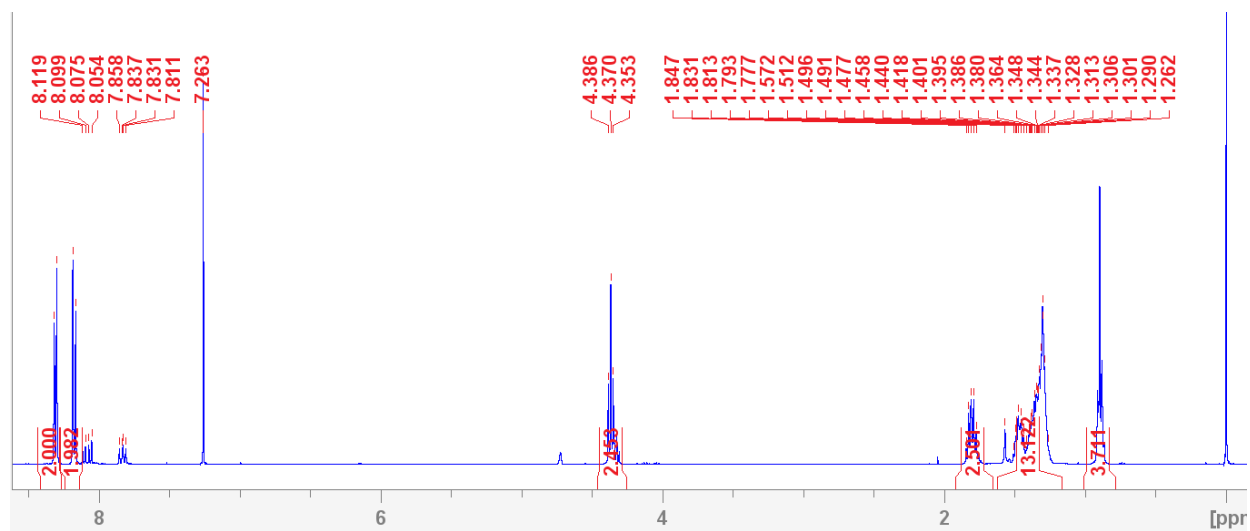


Figure S19. ¹H NMR spectrum of **3** in CDCl₃.

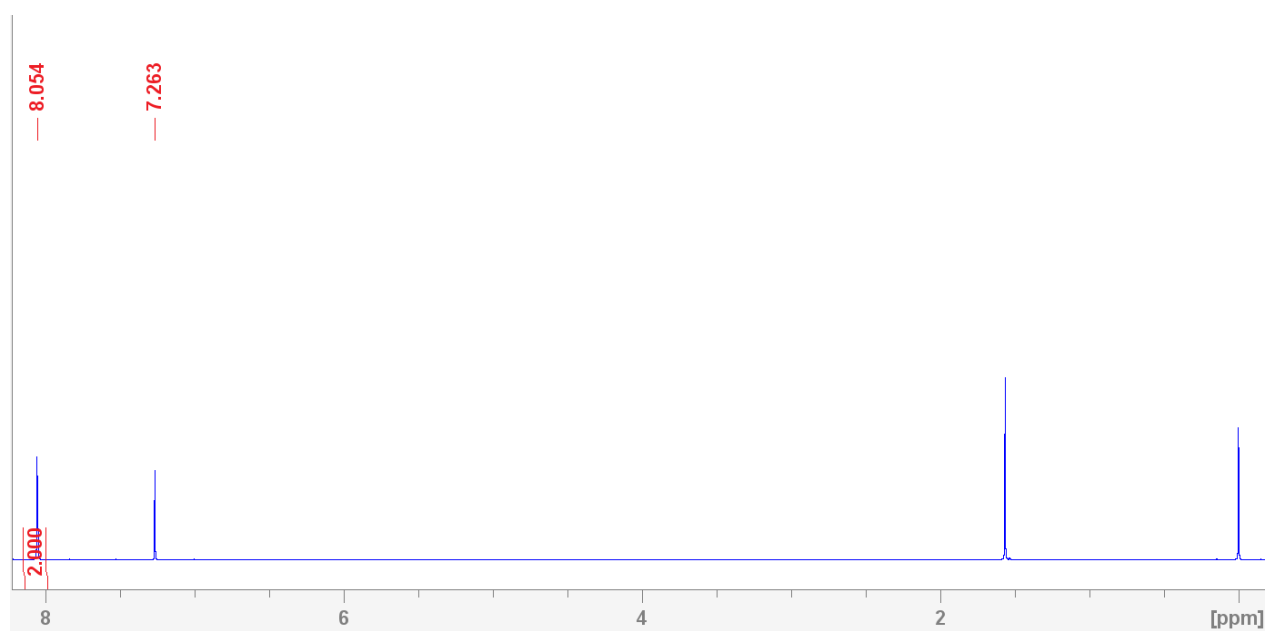


Figure S20. ¹H NMR spectrum of **5** in CDCl₃.

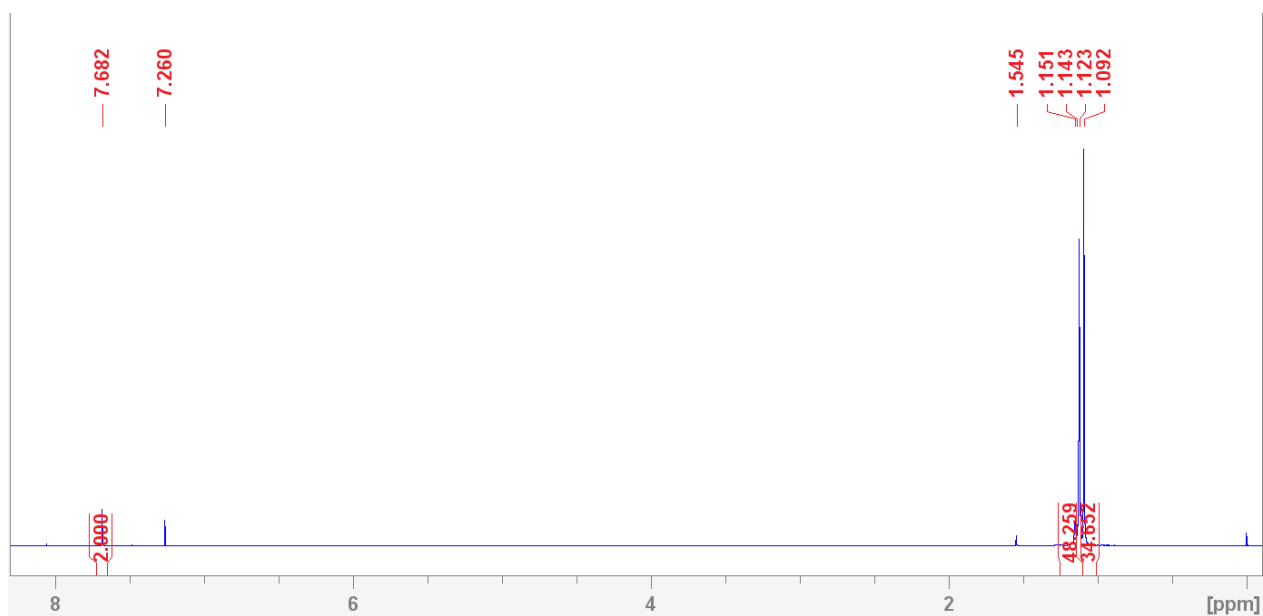


Figure S21. ¹H NMR spectrum of **6** in CDCl₃.

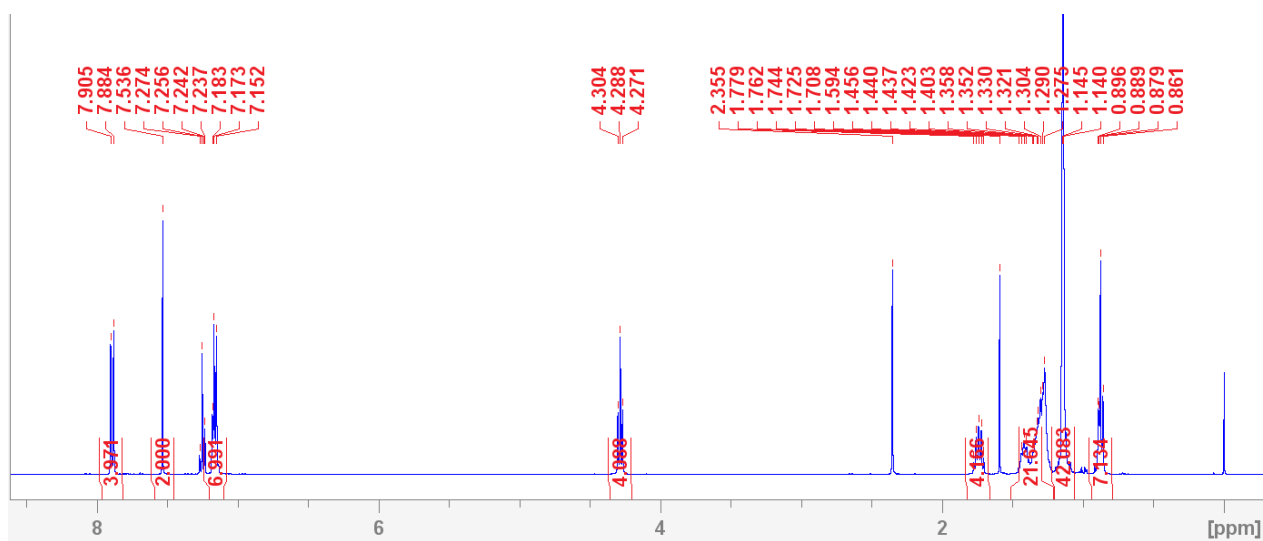


Figure S22. ¹H NMR spectrum of **7** in CDCl₃.

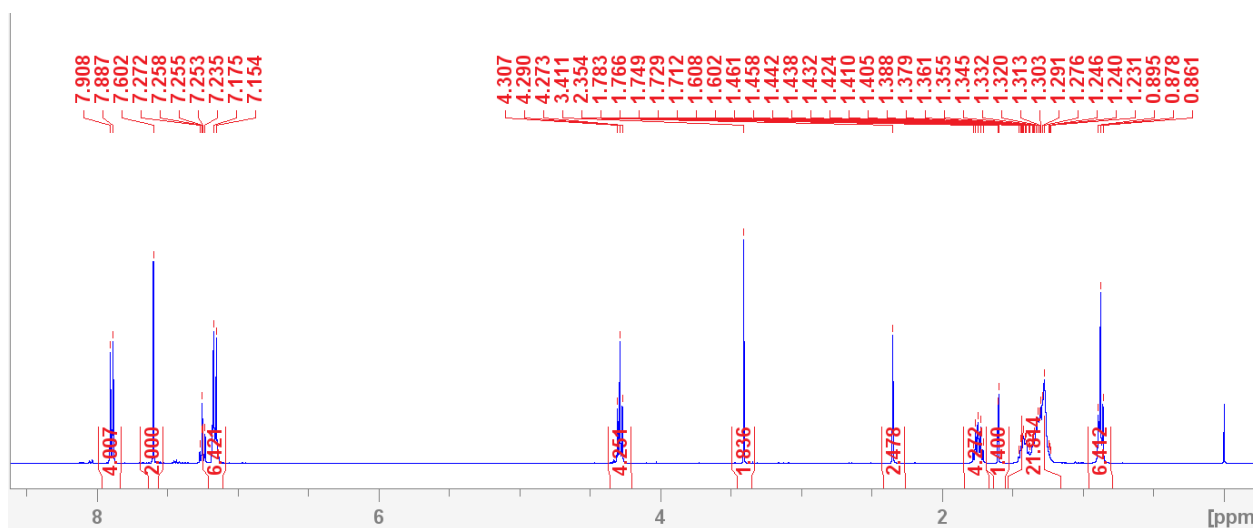


Figure S23. ¹H NMR spectrum of **8** in CDCl₃.

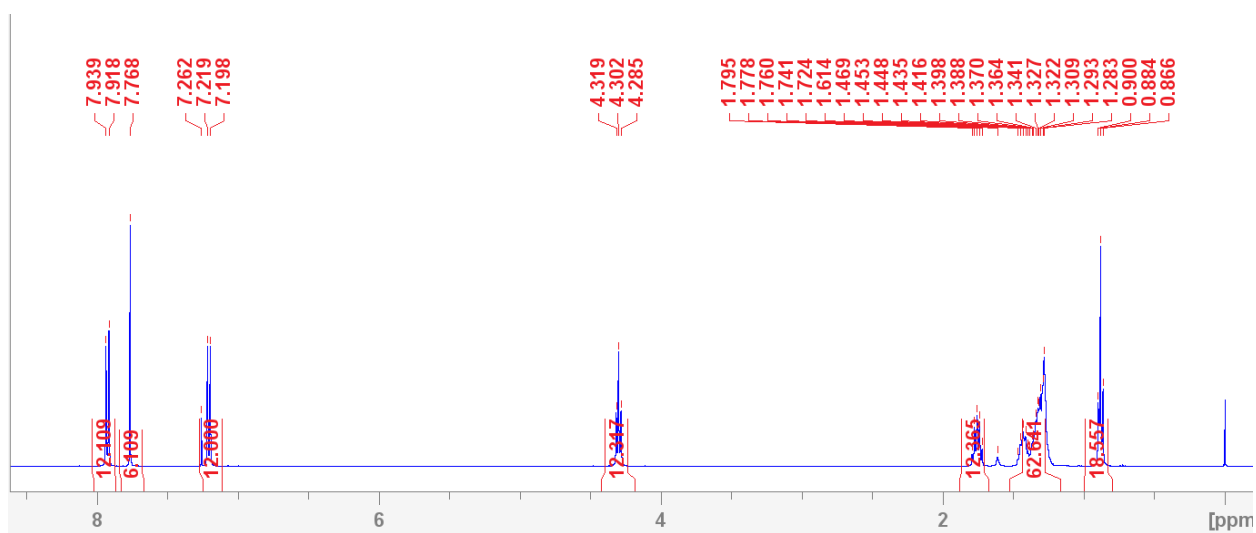


Figure S24. ¹H NMR spectrum of **C8[18]DBA** in CDCl₃.

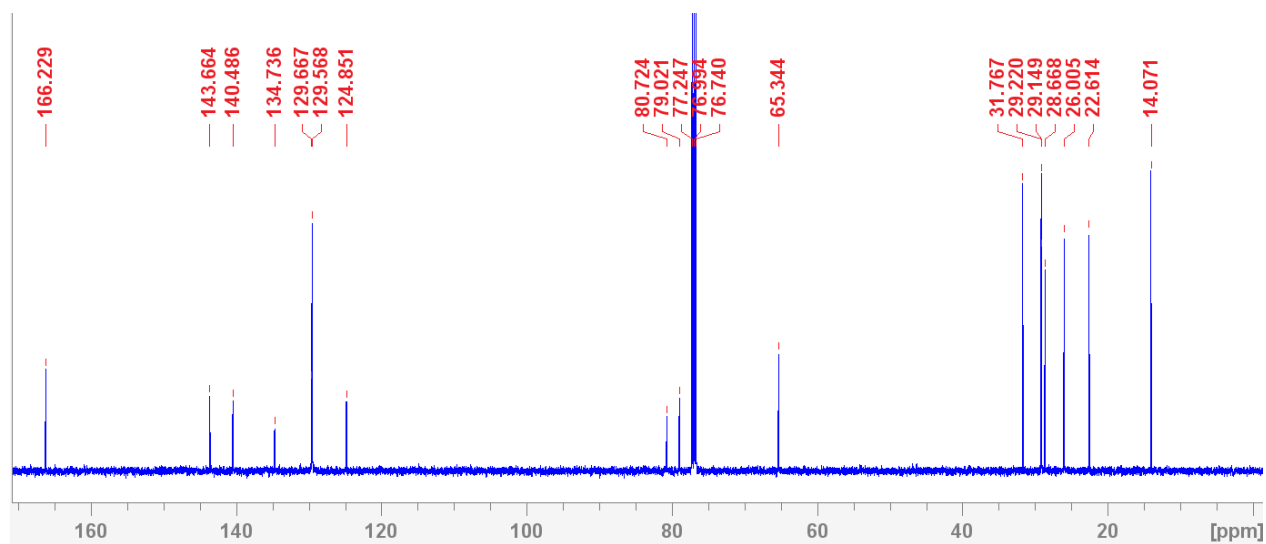


Figure S25. ¹³C NMR spectrum of C8[18]DBA in CDCl₃.

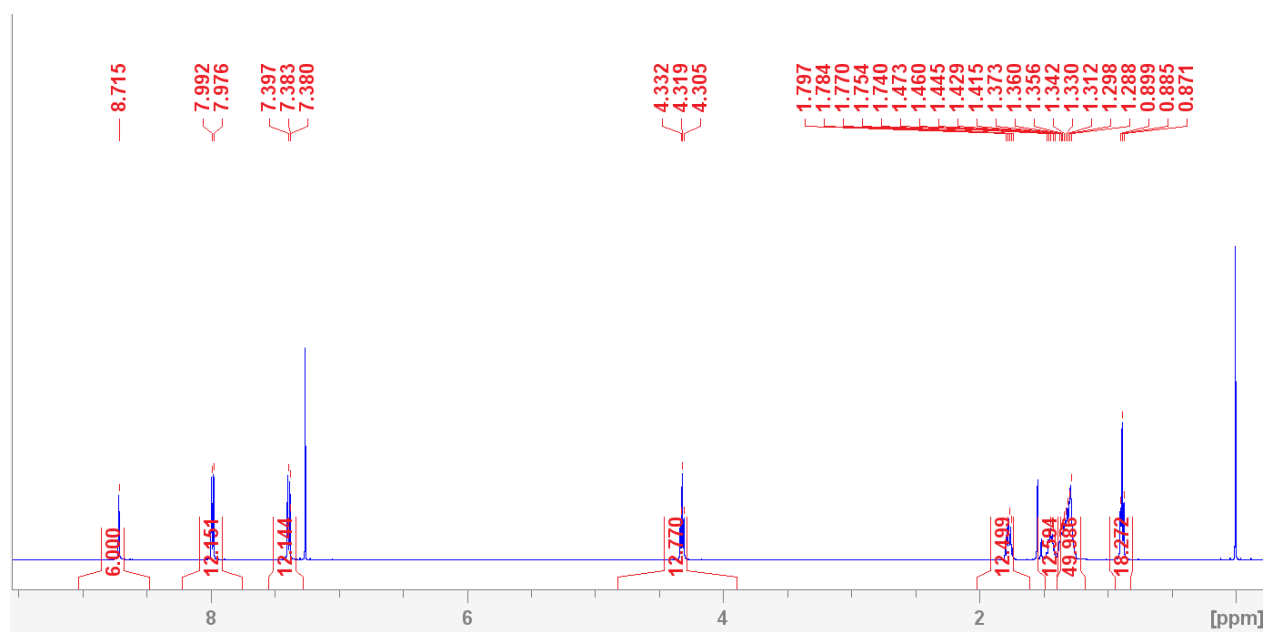


Figure S26. ¹H NMR spectrum of C8Trip in CDCl₃.

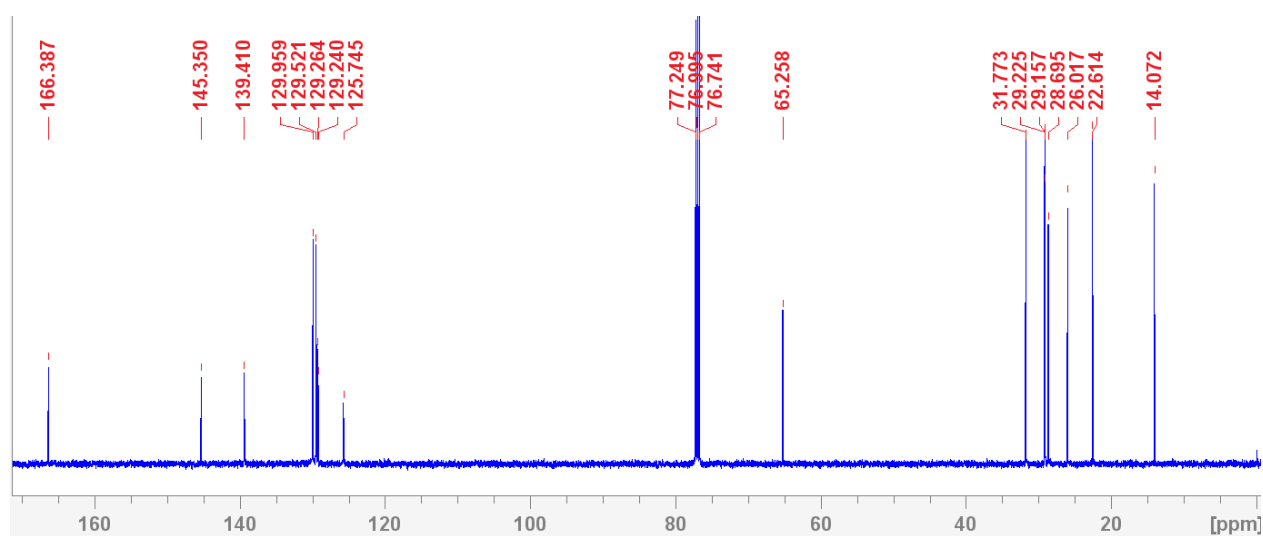
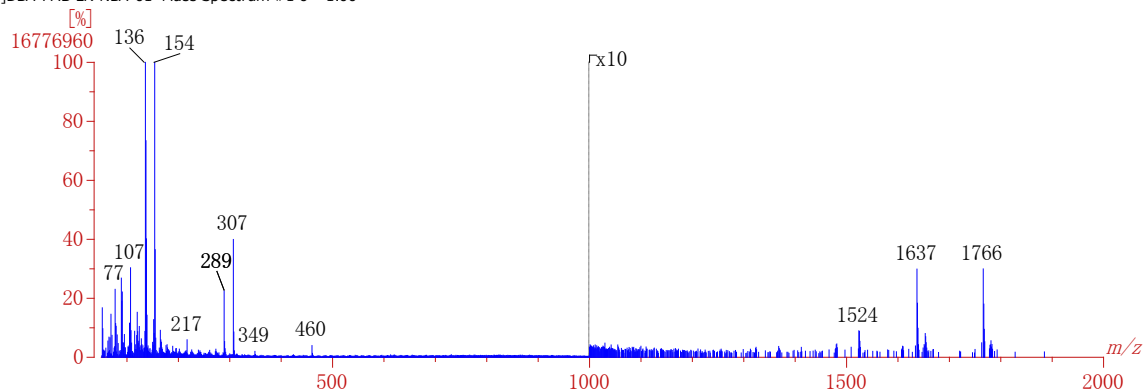


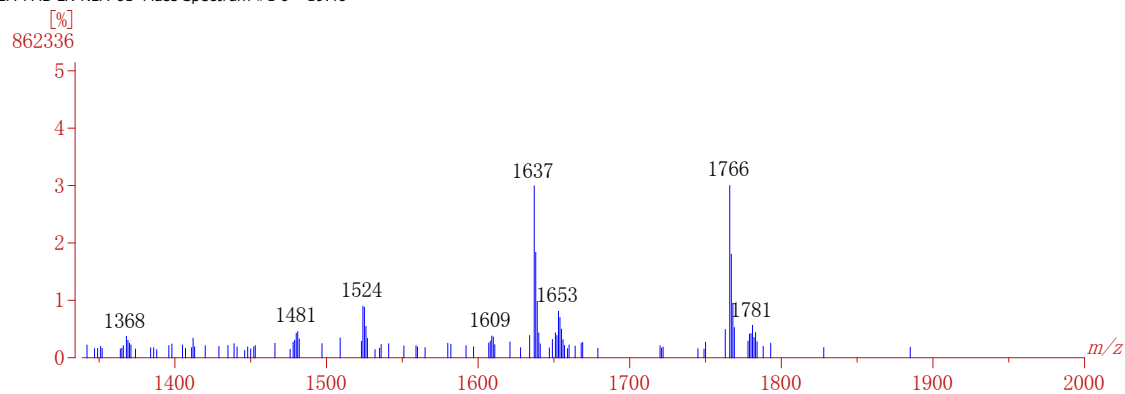
Figure S27. ¹³C NMR spectrum of C8Trip in CDCl₃.

HRMS of C8[18]DBA

C8[18]DBA-FAB-LR-NBA-01 Mass Spectrum #1 6 * 1.00



C8[18]DBA-FAB-LR-NBA-01 Mass Spectrum #1 6 * 19.46



C8[18]DBA-FAB-HR-NBA-01 Mass Spectrum #7 21 * 1.00

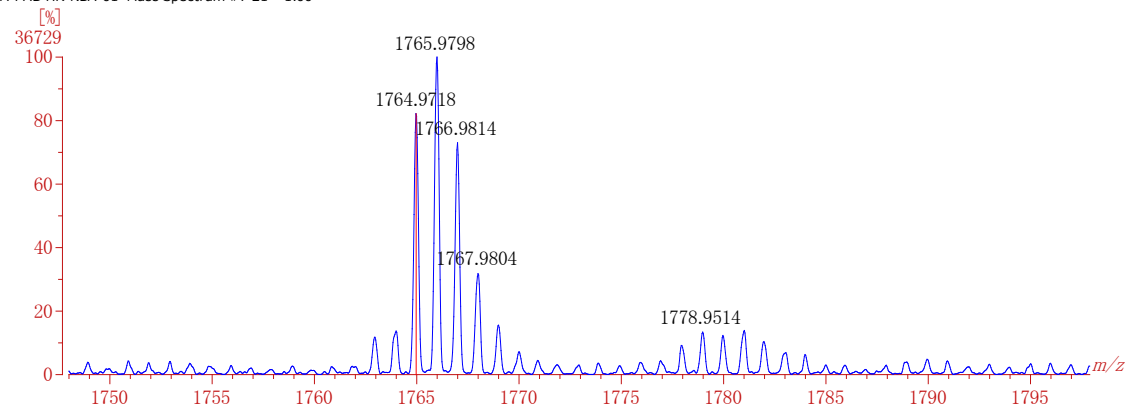


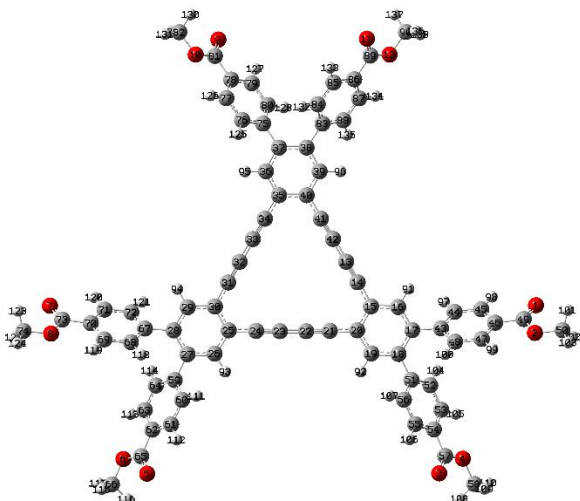
Figure S28. HRMS of C8[18]DBA (FAB in the matrix of *m*-nitrobenzylalcohol).

Cartesian coordinates for optimized structures of C8[*n*]DBA and C8Trip

C8[18]DBA

$$E(\text{B3LYP}) = -3903.788484 \text{ a. u.}$$

Number of imaginary frequencies: 0



Atom Num ber	Elem ent	<i>X</i>	<i>Y</i>	<i>Z</i>
1	O	12.547807	−1.419174	−0.387215
2	O	12.494354	−2.850572	1.360081
3	O	7.552188	−10.099969	0.513207
4	O	8.772509	−9.343948	−1.231523
5	O	−7.530046	−10.117469	0.497652
6	O	−8.752380	−9.359012	−1.244611
7	O	−12.544497	−1.444266	−0.372267
8	O	−12.486724	−2.882638	1.369151
9	O	−3.849011	12.301623	−1.398574
10	O	−5.022290	11.525736	0.369623
11	O	3.820040	12.344562	1.109309
12	O	4.994509	11.525961	−0.638734
13	C	2.748512	0.830150	−0.005018

Atom Num ber	Elem ent	<i>X</i>	<i>Y</i>	<i>Z</i>
28	C	−6.154722	−2.717392	0.047694
29	C	−5.429798	−1.522009	0.032779
30	C	−4.025497	−1.483835	0.024135
31	C	−3.343900	−0.243956	0.014456
32	C	−2.749525	0.824112	0.004202
33	C	−2.072892	1.999148	−0.008042
34	C	−1.447810	3.049526	−0.019845
35	C	−0.717255	4.261173	−0.034927
36	C	−1.388582	5.495055	−0.053986
37	C	−0.718179	6.721759	−0.077577
38	C	0.703763	6.723623	−0.064001
39	C	1.377082	5.498309	−0.056281
40	C	0.708688	4.262743	−0.044297

14	C	3.345146	-0.236654	0.006037
15	C	4.029311	-1.475105	0.017455
16	C	5.433699	-1.510331	0.024997
17	C	6.161112	-2.704165	0.042428
18	C	5.451900	-3.936678	0.033484
19	C	4.054115	-3.907557	0.038754
20	C	3.318043	-2.710961	0.033757
21	C	1.903455	-2.741334	0.032614
22	C	0.681245	-2.760298	0.032559
23	C	-0.674736	-2.761857	0.033357
24	C	-1.896984	-2.745614	0.034539
25	C	-3.311629	-2.718234	0.036860
26	C	-4.045199	-3.916371	0.039427
27	C	-5.442920	-3.948391	0.034957
55	C	6.308121	-7.556262	0.770199
56	C	5.733019	-6.292892	0.851619
57	C	7.856912	-9.200441	-0.245725
58	C	9.369004	-10.646990	-1.326296
59	C	-6.104794	-5.281351	-0.033304
60	C	-5.718734	-6.307573	0.846446
61	C	-6.291195	-7.571916	0.761556
62	C	-7.259413	-7.843827	-0.212505
63	C	-7.646818	-6.829981	-1.099589
64	C	-7.077326	-5.564775	-1.007394
65	C	-7.836878	-9.216402	-0.258605
66	C	-9.346103	-10.663046	-1.343067
67	C	-7.639621	-2.625583	0.125976
68	C	-8.364224	-3.324777	1.106343
69	C	-9.744152	-3.186382	1.207530
70	C	-10.435098	-2.345976	0.323672
71	C	-9.722647	-1.644741	-0.656571
72	C	-8.342023	-1.780458	-0.750739
73	C	-11.912234	-2.160506	0.379594
74	C	-13.912310	-2.745633	1.476768
75	C	-1.542478	7.959603	-0.166211

41	C	1.442032	3.052770	-0.029974
42	C	2.069277	2.003682	-0.017895
43	C	7.645881	-2.609006	0.119256
44	C	8.345788	-1.765414	-0.760911
45	C	9.726185	-1.626430	-0.668312
46	C	10.440882	-2.322703	0.313821
47	C	9.752422	-3.161513	1.201124
48	C	8.372720	-3.303275	1.101447
49	C	11.917651	-2.133770	0.367994
50	C	13.919665	-2.709756	1.466503
51	C	6.116546	-5.268429	-0.031289
52	C	7.089300	-5.552647	-1.004924
53	C	7.661449	-6.816905	-1.093634
54	C	7.276539	-7.828971	-0.203440
90	C	5.834900	12.688374	-0.565457
91	H	5.968820	-0.567435	0.052435
92	H	3.508025	-4.844151	0.011449
93	H	-3.497183	-4.851753	0.009293
94	H	-5.966848	-0.580290	0.062792
95	H	-2.472585	5.487124	-0.085963
96	H	2.461100	5.493775	-0.024160
97	H	7.800926	-1.229591	-1.532355
98	H	10.271727	-0.983854	-1.350784
99	H	10.301390	-3.694995	1.968127
100	H	7.849021	-3.948941	1.798129
101	H	14.190107	-1.668531	1.657985
102	H	14.408338	-3.035906	0.545187
103	H	14.215780	-3.342862	2.302533
104	H	7.388977	-4.778987	-1.703639
105	H	8.404134	-7.027188	-1.854202
106	H	6.022303	-8.347234	1.455005
107	H	4.990064	-6.087465	1.616427
108	H	8.606654	-11.406060	-1.517569
109	H	9.891368	-10.899286	-0.400291
110	H	10.070043	-10.589298	-2.158567

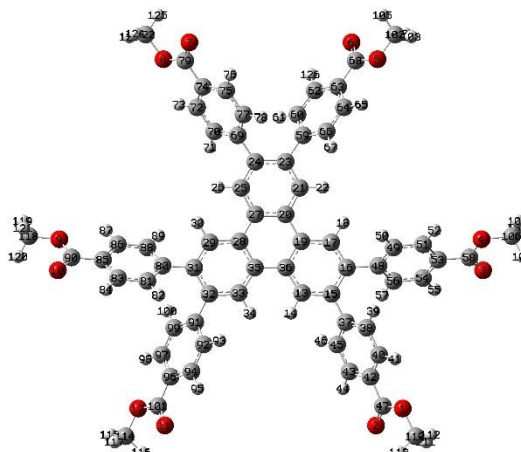
76	C	-2.623901	8.150839	0.710438
77	C	-3.437957	9.275393	0.609738
78	C	-3.190374	10.233170	-0.381427
79	C	-2.118016	10.048248	-1.264359
80	C	-1.303245	8.928335	-1.156536
81	C	-4.027222	11.454953	-0.544819
82	C	-5.866051	12.683324	0.265249
83	C	1.525015	7.965372	-0.007724
84	C	1.283441	8.959106	0.956925
85	C	2.095209	10.083660	1.035025
86	C	3.166793	10.248275	0.147148
87	C	3.416755	9.265448	-0.818567
88	C	2.605732	8.136438	-0.889406
89	C	4.000220	11.476302	0.277944
125	H	-2.815570	7.417227	1.487765
126	H	-4.263492	9.416410	1.297445
127	H	-1.943730	10.794182	-2.032056
128	H	-0.481071	8.792921	-1.850941
129	H	-6.358337	12.713940	-0.709784
130	H	-5.281803	13.597843	0.392750
131	H	-6.601484	12.583729	1.063194

111	H	-4.975875	-6.102819	1.611531
112	H	-6.003420	-8.364291	1.443917
113	H	-8.389334	-7.039614	-1.860501
114	H	-7.378896	-4.789716	-1.703740
115	H	-9.867424	-10.919321	-0.417569
116	H	-8.582206	-11.419867	-1.537076
117	H	-10.047695	-10.604325	-2.174800
118	H	-7.838618	-3.971742	1.800378
119	H	-10.291392	-3.723774	1.973038
120	H	-10.270056	-1.000985	-1.336434
121	H	-7.798978	-1.240850	-1.520821
122	H	-14.400641	-3.069497	0.554464
123	H	-14.185183	-1.705784	1.672247
124	H	-14.206525	-3.382587	2.310545
132	H	0.461774	8.839795	1.654874
133	H	1.919062	10.849033	1.782908
134	H	4.241703	9.390608	-1.510033
135	H	2.799162	7.383232	-1.647316
136	H	6.327388	12.746331	0.408229
137	H	5.247925	13.597466	-0.716992
138	H	6.570370	12.569783	-1.360767

C8Trip

$E(\text{B3LYP}) = -3446.859594$ a. u.

Number of imaginary frequencies: 0



Atom Number	Element	X	Y	Z
1	O	6.201622	-7.885557	1.339379
2	O	4.950529	-8.683298	-0.364447
3	O	9.970101	-1.401598	-1.416485
4	O	9.897768	0.059221	0.305541
5	O	5.016818	8.506580	0.367949
6	O	3.799966	9.298633	-1.363132
7	O	-3.800002	9.298599	1.363145
8	O	-5.016849	8.506543	-0.367937
9	O	-9.897761	0.059211	-0.305522
10	O	-9.970081	-1.401589	1.416520
11	O	-4.950538	-8.683291	0.364440
12	O	-6.201654	-7.885539	-1.339363
13	C	1.476864	-2.462919	0.008395
14	H	0.959990	-3.411794	0.077087
15	C	2.868044	-2.504073	-0.006979
16	C	3.578972	-1.272457	-0.056339
17	C	2.848591	-0.087547	-0.054238
18	H	3.412460	0.834873	-0.112868
19	C	1.441505	-0.039607	-0.025058
20	C	0.709019	1.229255	-0.015102
21	C	1.371310	2.471772	-0.038707

Atom Number	Element	X	Y	Z
29	C	-2.848581	-0.087548	0.054231
30	H	-3.412450	0.834871	0.112865
31	C	-3.578961	-1.272459	0.056331
32	C	-2.868032	-2.504075	0.006965
33	C	-1.476852	-2.462920	-0.008414
34	H	-0.959978	-3.411794	-0.077113
35	C	-0.732432	-1.267683	0.008020
36	C	0.732443	-1.267683	-0.008035
37	C	3.530841	-3.835444	0.081386
38	C	4.518763	-4.098228	1.045845
39	H	4.831288	-3.307719	1.719744
40	C	5.090750	-5.360821	1.156994
41	H	5.846064	-5.553278	1.909848
42	C	4.689949	-6.394486	0.299180
43	C	3.706836	-6.143891	-0.665601
44	H	3.409506	-6.950921	-1.326396
45	C	3.133587	-4.881308	-0.769995
46	H	2.381192	-4.692384	-1.529852
47	C	5.269216	-7.765132	0.365952
48	C	5.062557	-1.181256	-0.158725
49	C	5.778702	-0.322038	0.692134

22	H	2.451670	2.499124	-0.104551
23	C	0.710861	3.696929	-0.026970
24	C	-0.710847	3.696929	0.026954
25	C	-1.371298	2.471773	0.038696
26	H	-2.451658	2.499126	0.104545
27	C	-0.709008	1.229256	0.015093
28	C	-1.441495	-0.039608	0.025047
57	H	5.239685	-2.558869	-1.810592
58	C	9.331116	-0.795865	-0.578312
59	C	1.531413	4.936868	-0.122511
60	C	1.267221	5.916332	-1.095897
61	H	0.428460	5.786607	-1.771387
62	C	2.076577	7.039442	-1.211443
63	C	3.169850	7.217794	-0.353004
64	C	3.442426	6.250267	0.622052
65	H	4.283299	6.386622	1.291992
66	C	2.632435	5.123461	0.730589
67	H	2.841659	4.383349	1.497236
68	C	3.999654	8.442796	-0.523278
69	C	-1.531403	4.936867	0.122496
70	C	-2.632424	5.123457	-0.730607
71	H	-2.841641	4.383345	-1.497258
72	C	-3.442421	6.250259	-0.622070
73	H	-4.283291	6.386610	-1.292014
74	C	-3.169852	7.217785	0.352988
75	C	-2.076580	7.039435	1.211429
76	H	-1.881956	7.793209	1.966523
77	C	-1.267217	5.916330	1.095883
78	H	-0.428454	5.786611	1.771371
79	C	-3.999661	8.442782	0.523265
80	C	-5.062545	-1.181259	0.158724
81	C	-5.774304	-1.898291	1.136528
82	H	-5.239667	-2.558882	1.810584
83	C	-7.151105	-1.758834	1.258028
84	H	-7.702896	-2.303385	2.016468

50	H	5.246091	0.227975	1.462260
51	C	7.158898	-0.183111	0.576995
52	H	7.700262	0.476753	1.244836
53	C	7.856181	-0.901965	-0.401919
54	C	7.151122	-1.758827	-1.258022
55	H	7.702917	-2.303374	-2.016461
56	C	5.774320	-1.898283	-1.136530
92	C	-3.133571	-4.881312	0.769972
93	H	-2.381172	-4.692391	1.529825
94	C	-3.706821	-6.143894	0.665577
95	H	-3.409488	-6.950927	1.326367
96	C	-4.689941	-6.394485	-0.299198
97	C	-5.090747	-5.360817	-1.157006
98	H	-5.846066	-5.553270	-1.909855
99	C	-4.518758	-4.098224	-1.045856
100	H	-4.831286	-3.307713	-1.719752
101	C	-5.269208	-7.765131	-0.365972
102	C	5.853913	9.667976	0.255651
103	H	6.608041	9.563297	1.035369
104	H	6.323550	9.710257	-0.730105
105	H	5.269962	10.579283	0.405649
106	C	11.321182	0.205601	0.185288
107	H	11.586969	0.585361	-0.804245
108	H	11.610040	0.916659	0.958981
109	H	11.821343	-0.753722	0.338868
110	C	6.800328	-9.185847	1.453675
111	H	7.306614	-9.459310	0.524759
112	H	7.515986	-9.108899	2.271877
113	H	6.042007	-9.940602	1.675752
114	C	-6.800395	-9.185816	-1.453630
115	H	-7.516087	-9.108853	-2.271801
116	H	-6.042100	-9.940587	-1.675739
117	H	-7.306646	-9.459265	-0.524692
118	C	-11.321173	0.205594	-0.185260
119	H	-11.610043	0.916612	-0.958985

85	C	-7.856168	-0.901967	0.401934	120	H	-11.821334	-0.753739	-0.338783
86	C	-7.158889	-0.183108	-0.576980	121	H	-11.586948	0.585405	0.804258
87	H	-7.700257	0.476760	-1.244815	122	C	-5.853980	9.667910	-0.255608
88	C	-5.778694	-0.322035	-0.692126	123	H	-6.608127	9.563210	-1.035304
89	H	-5.246087	0.227983	-1.462253	124	H	-6.323588	9.710170	0.730163
90	C	-9.331101	-0.795863	0.578338	125	H	-5.270062	10.579237	-0.405619
91	C	-3.530830	-3.835445	-0.081403	126	H	1.881950	7.793216	-1.966535

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- (S2) Hisaki, I.; Nakagawa, S.; Tohnai, N.; Miyata, M. A C_3 -Symmetric Macrocyclic-Based, Hydrogen-Bonded, Multiporous Hexagonal Network as a Motif of Porous Molecular Crystals. *Angew. Chem. Int. Ed.* **2015**, *54*, 3008–3012.