Electronic Supplementary Information

Fluorine-containing bistolanes as light-emitting liquid crystalline molecules

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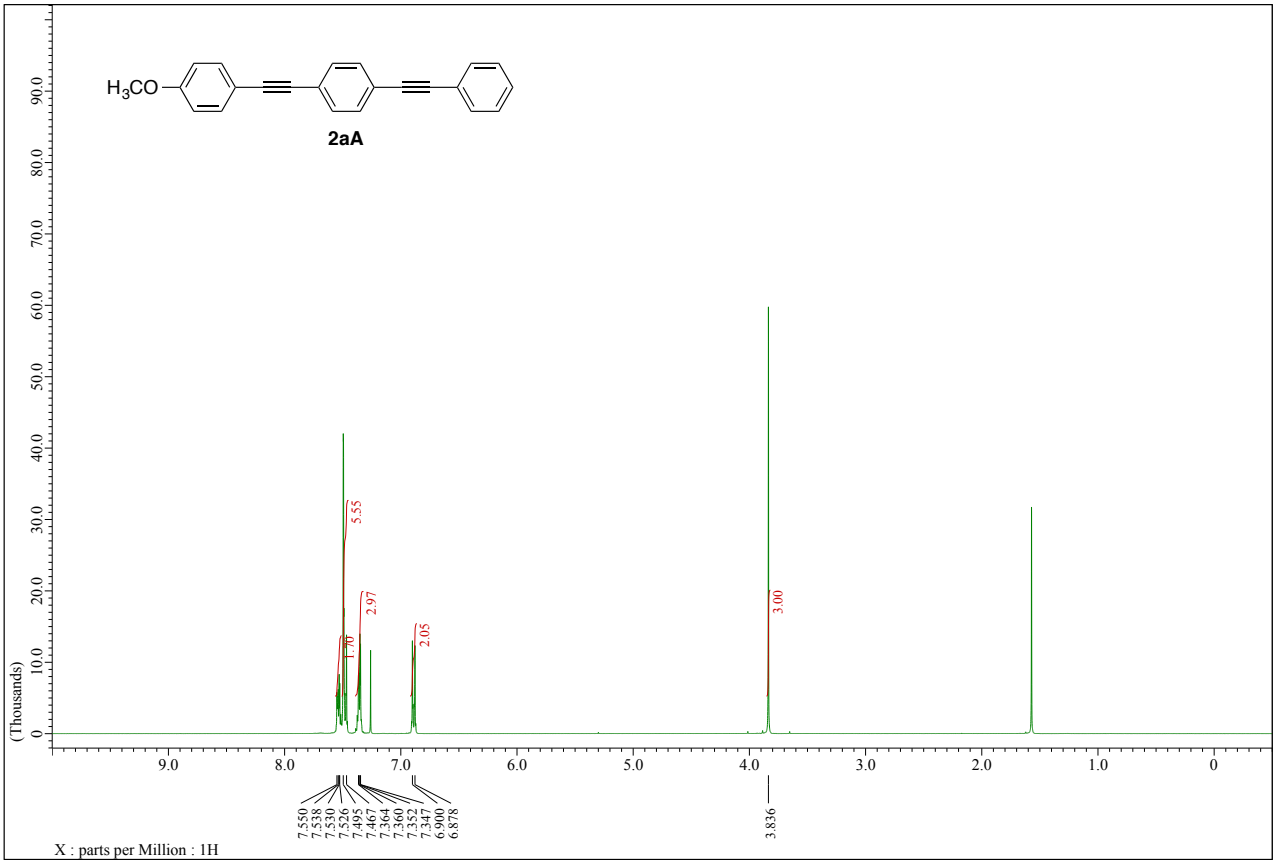
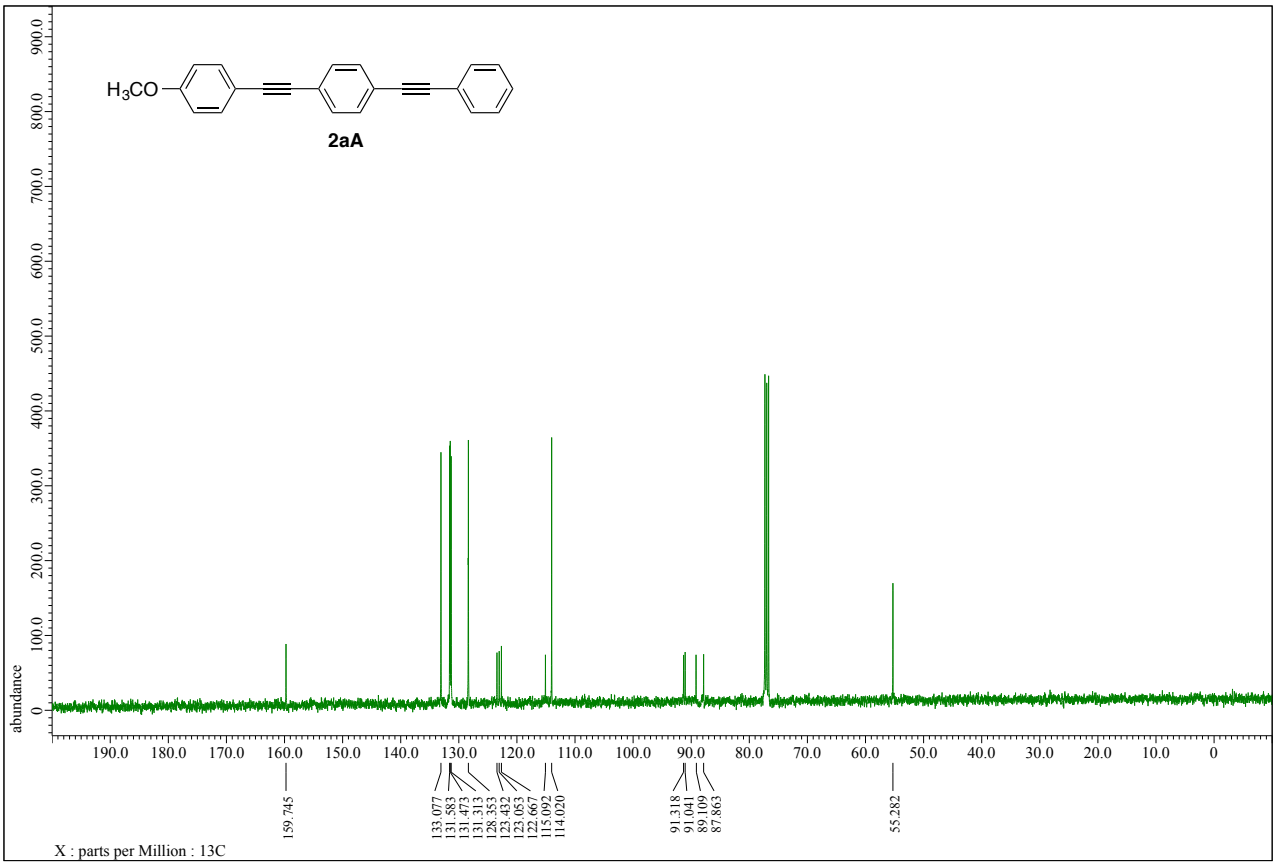


^{12}C NMR spectrum of **2aA** (Solvent: $CDCl_3$)



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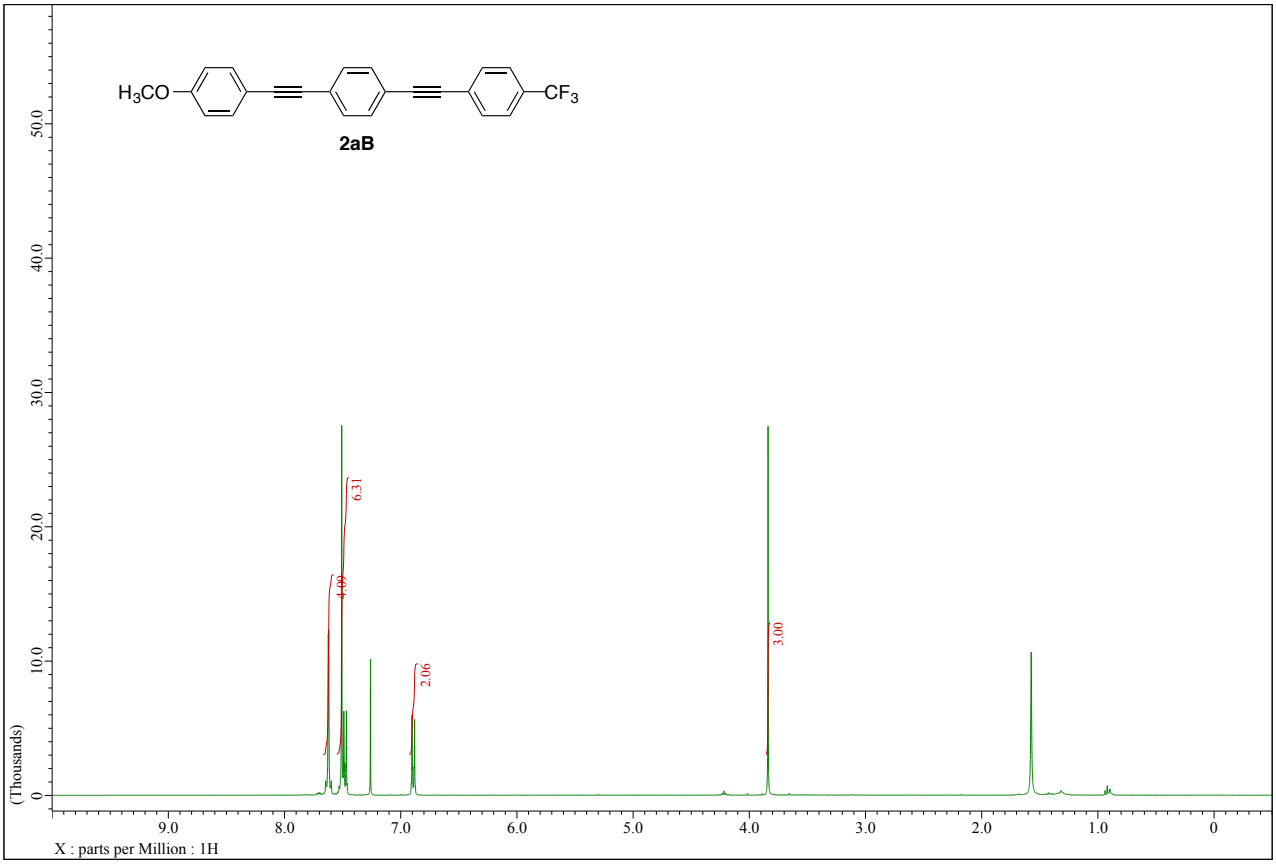

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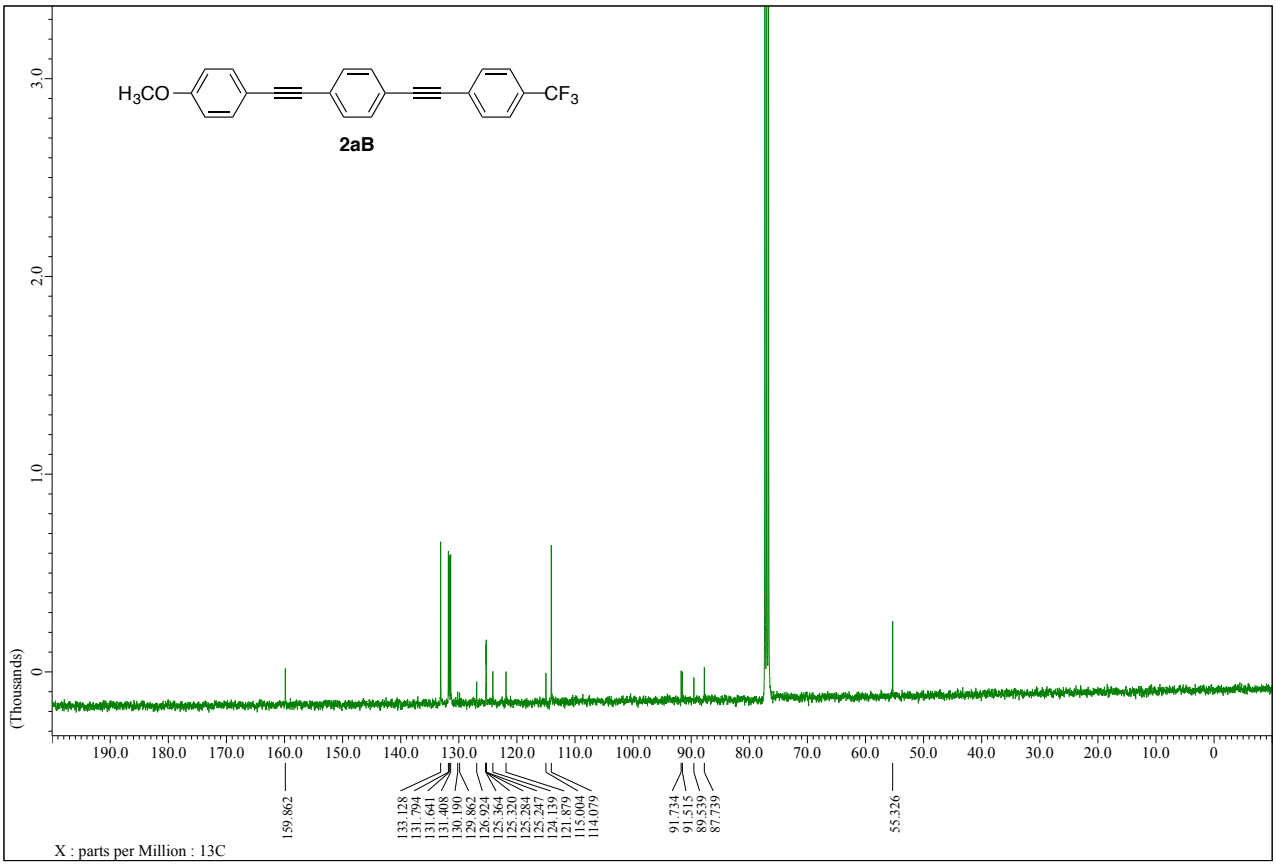

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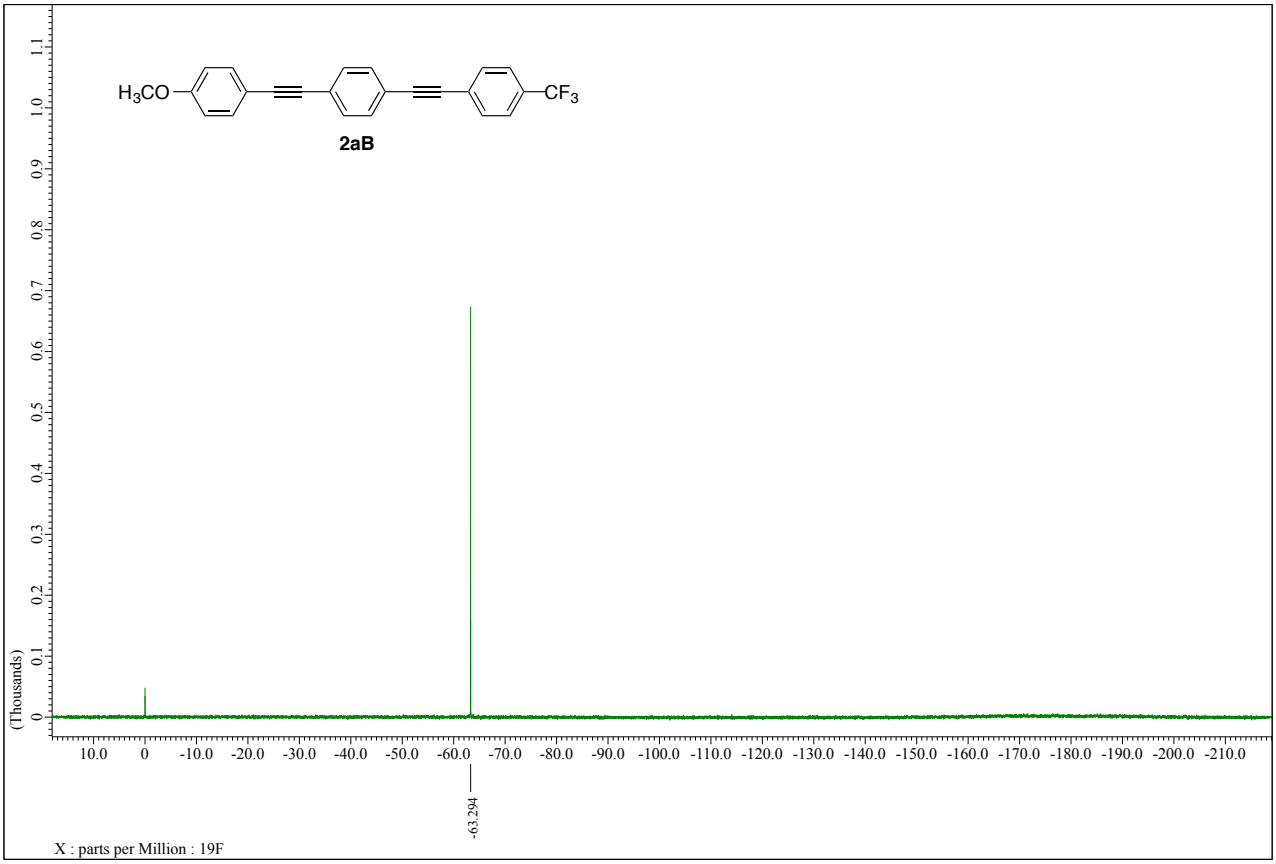

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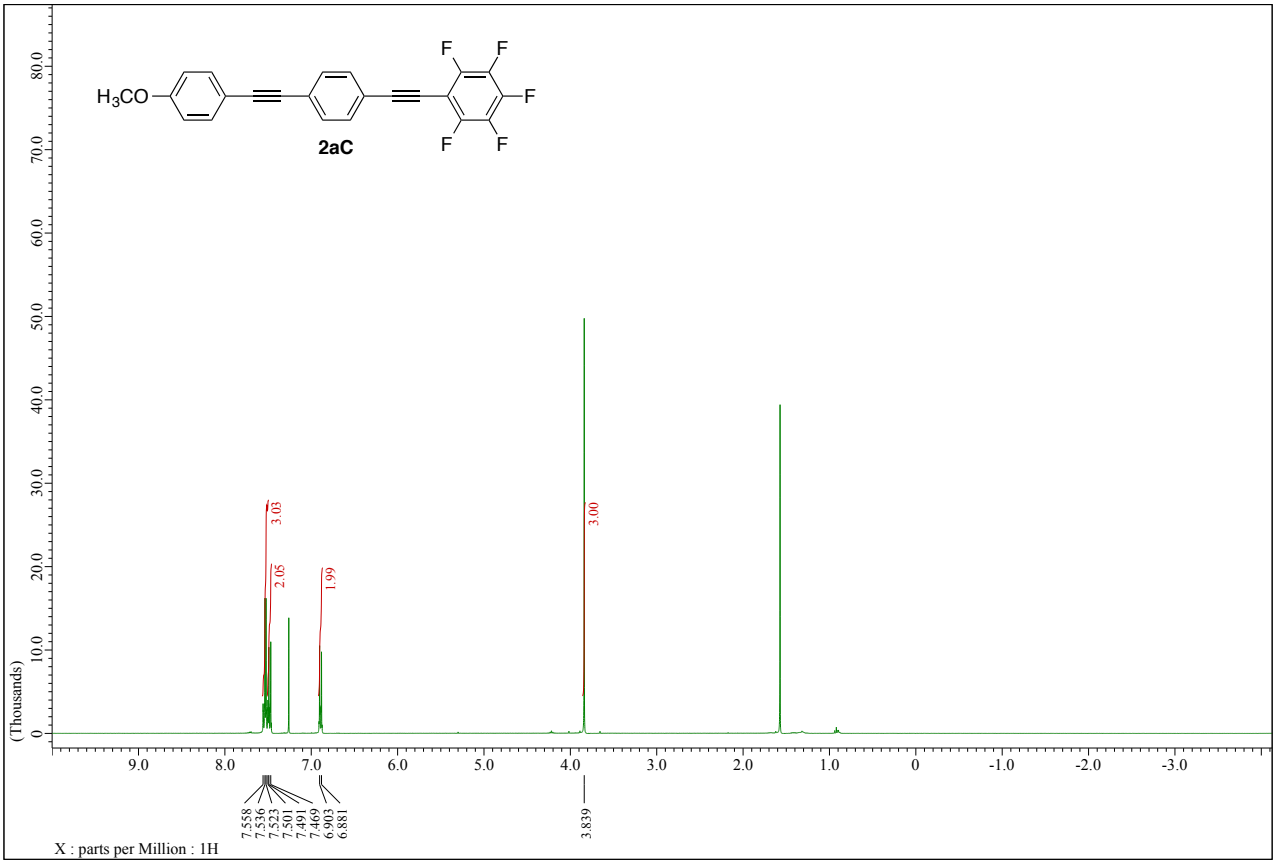

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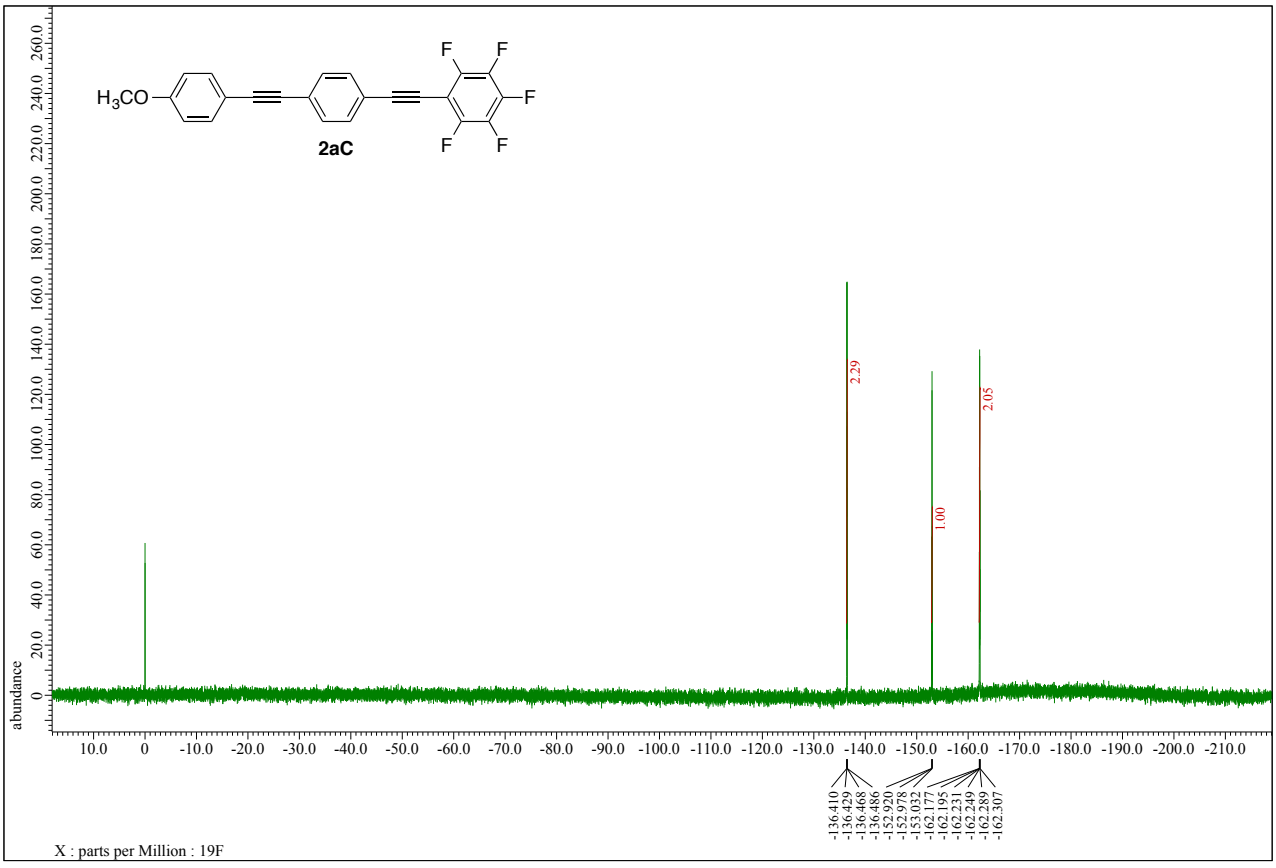

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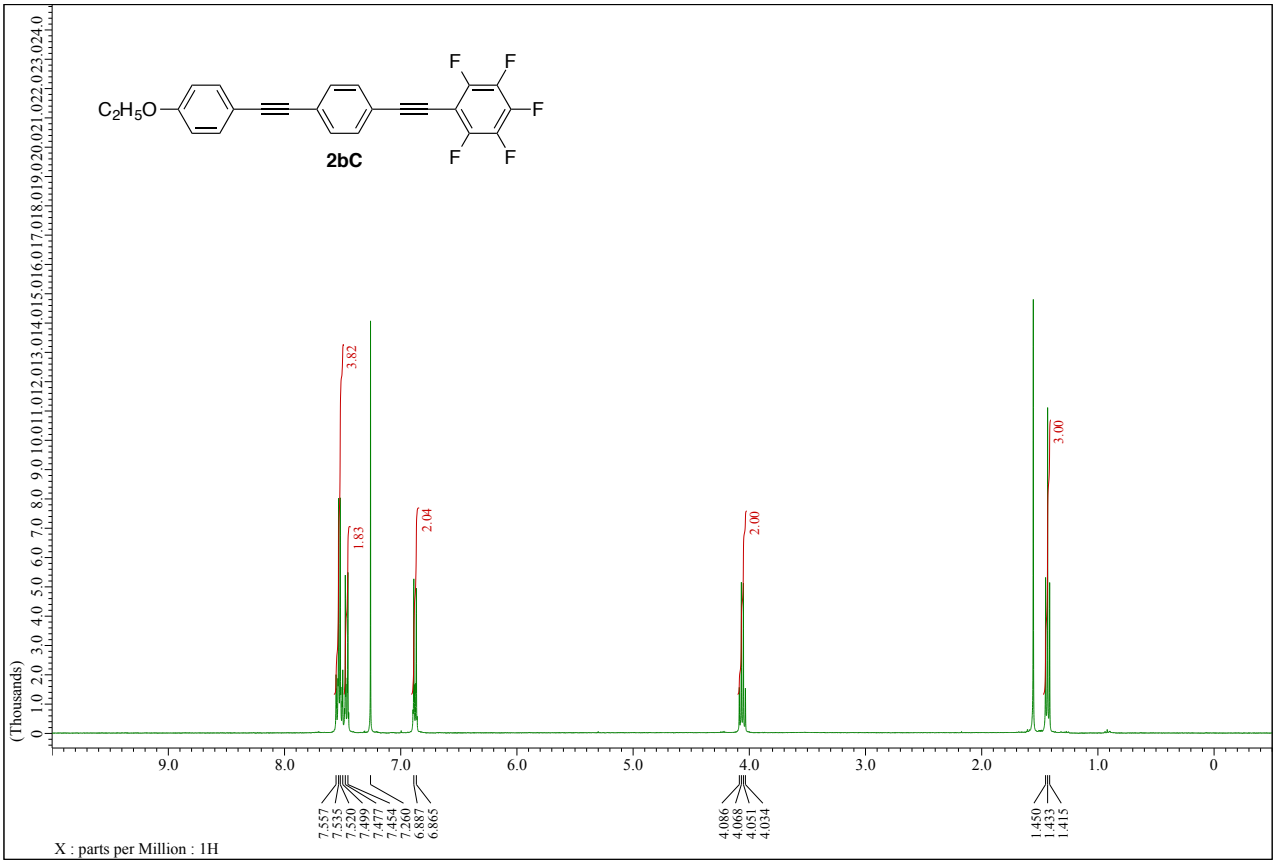

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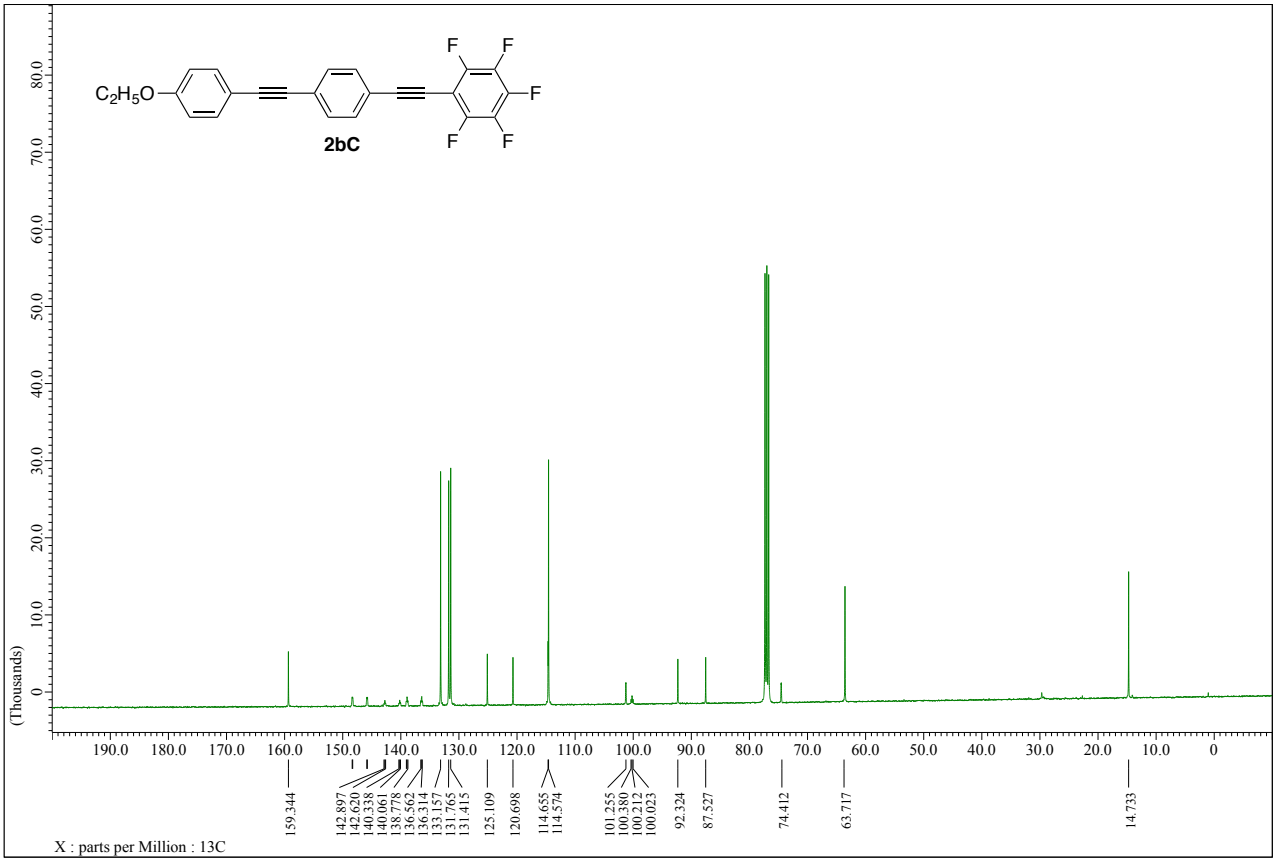

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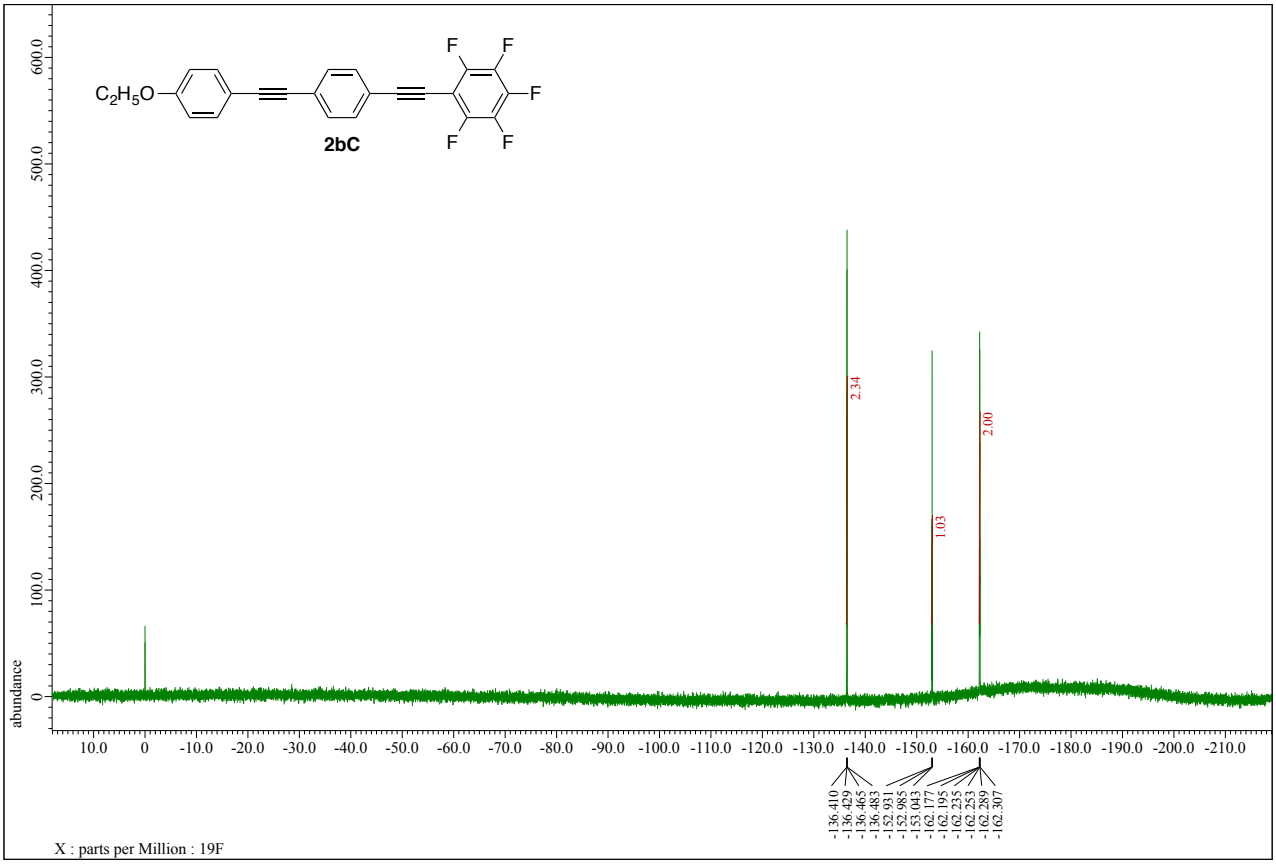

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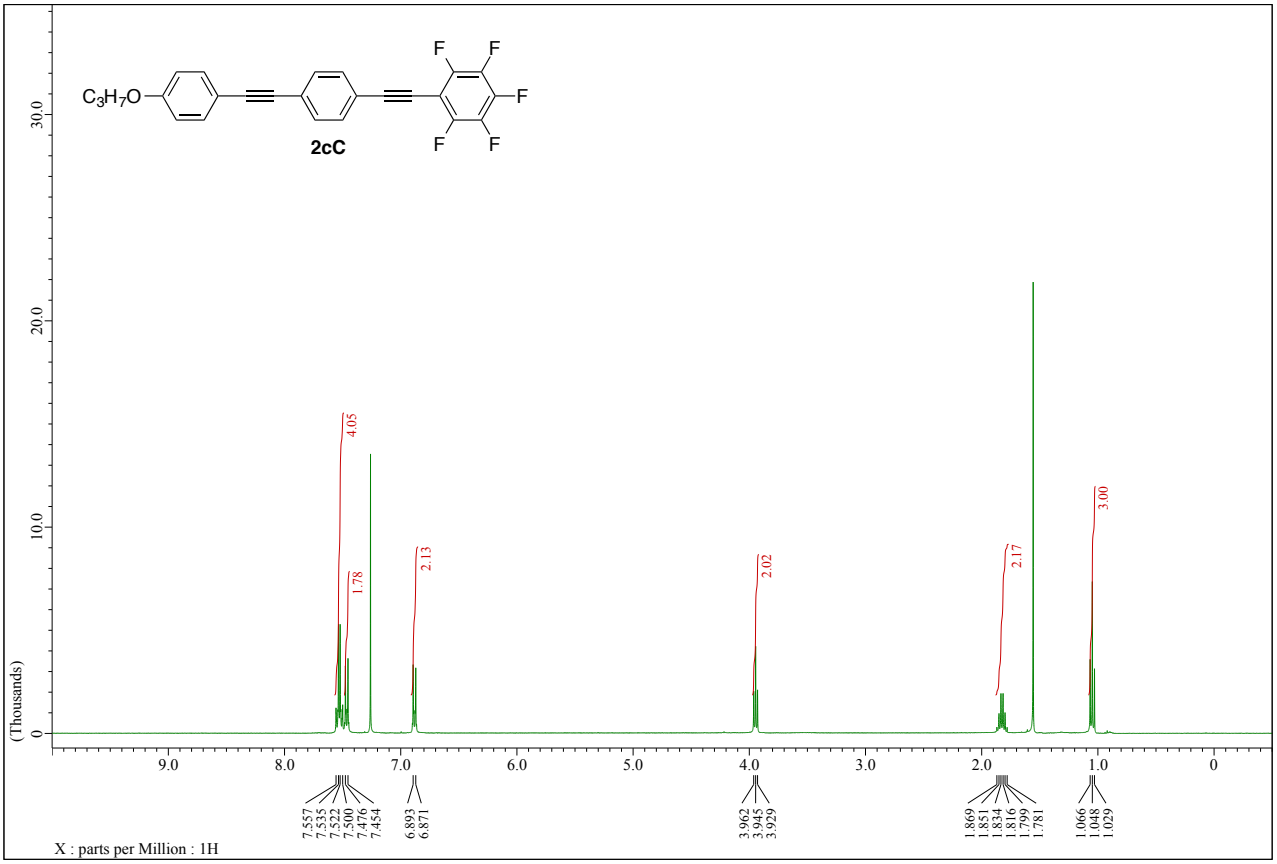

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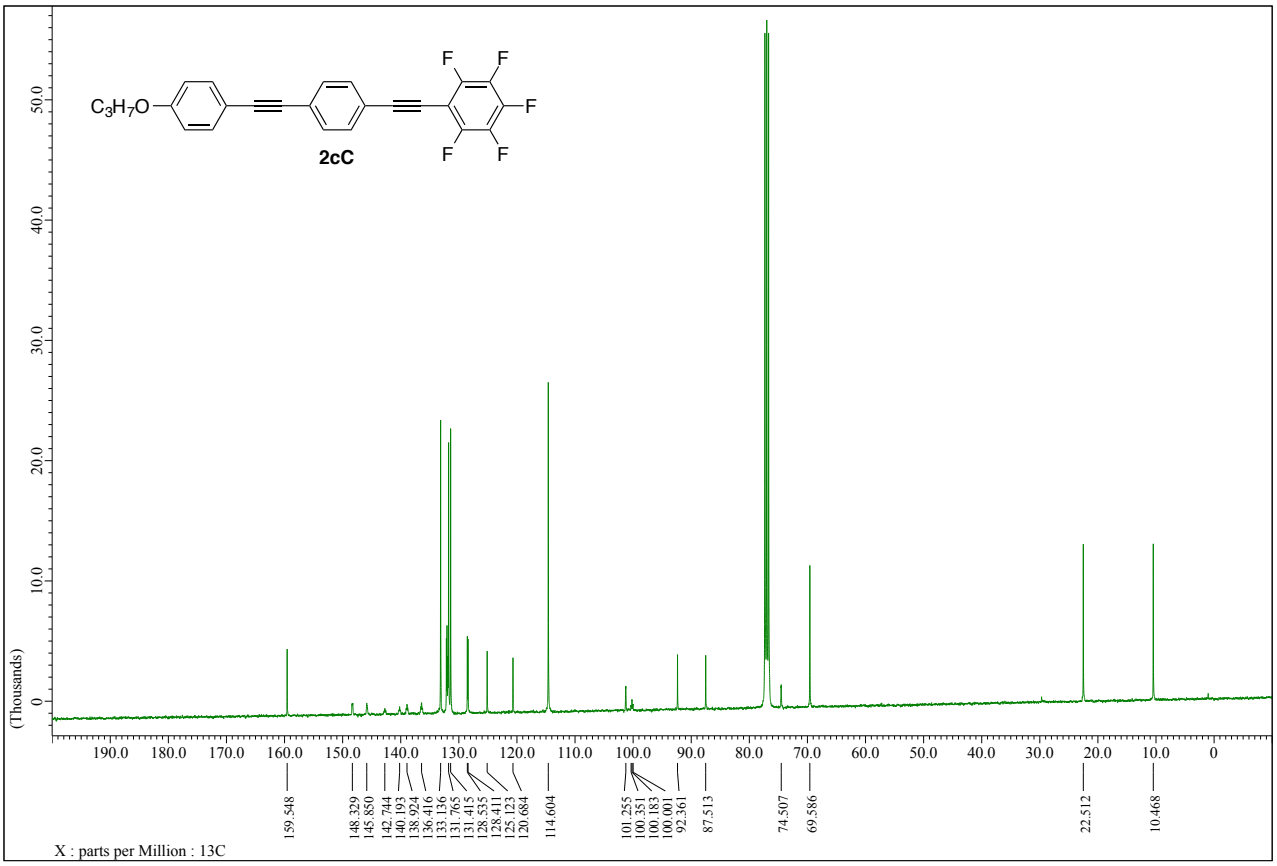

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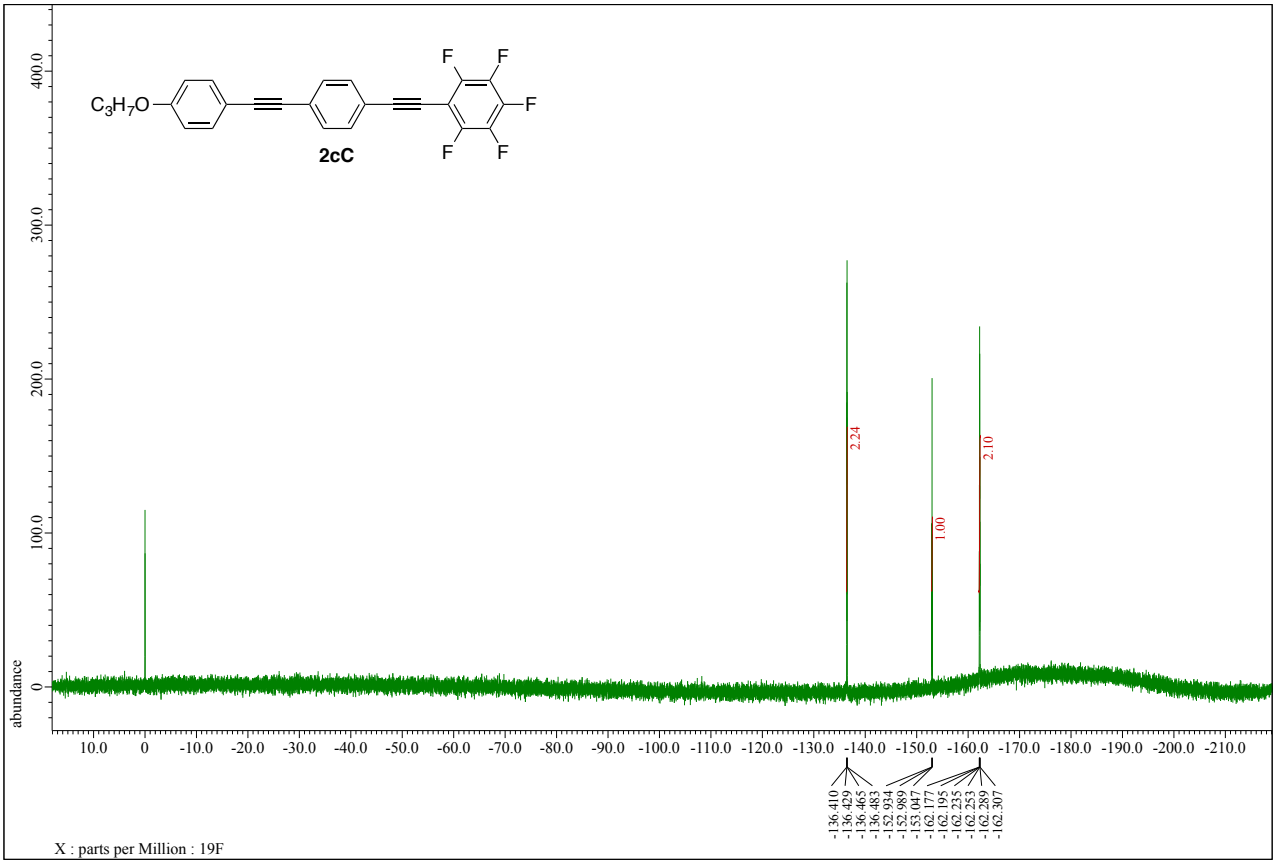

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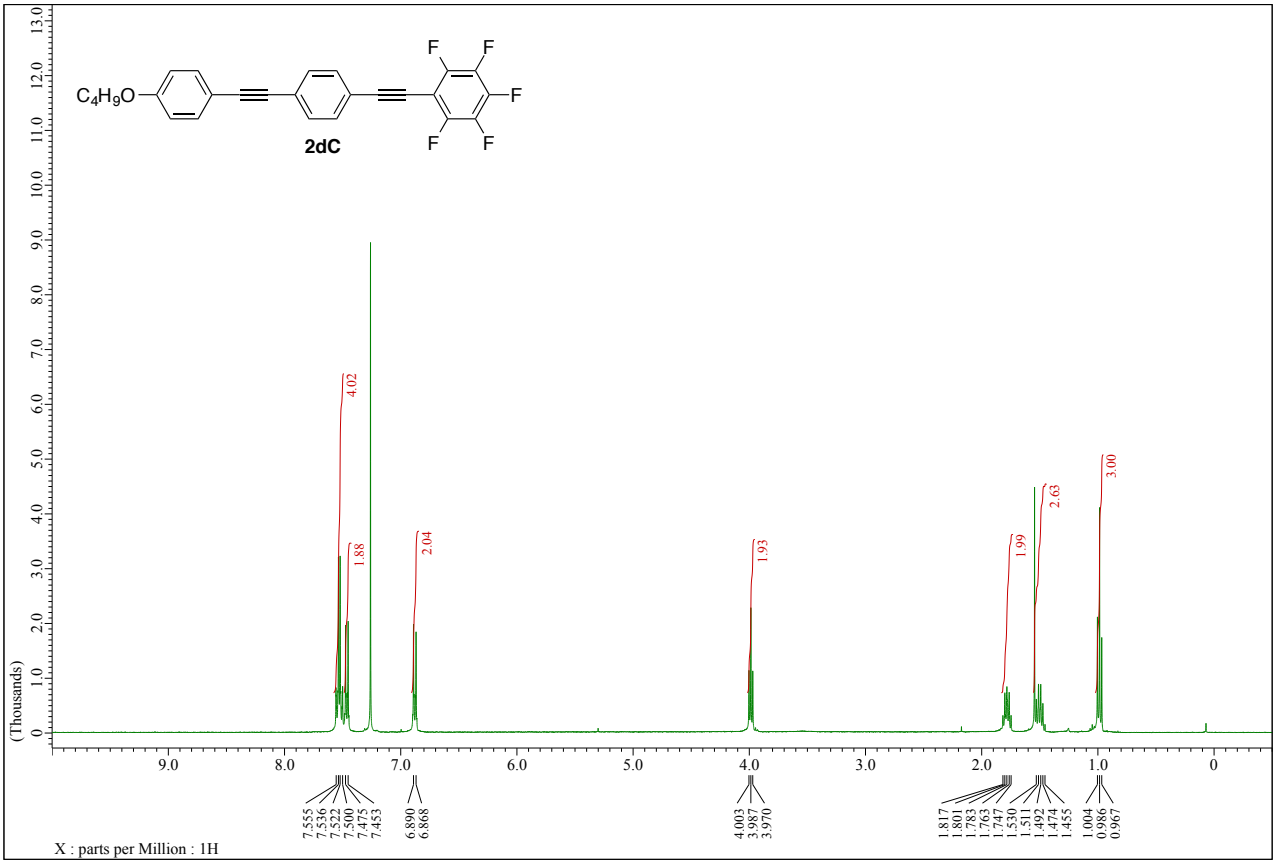

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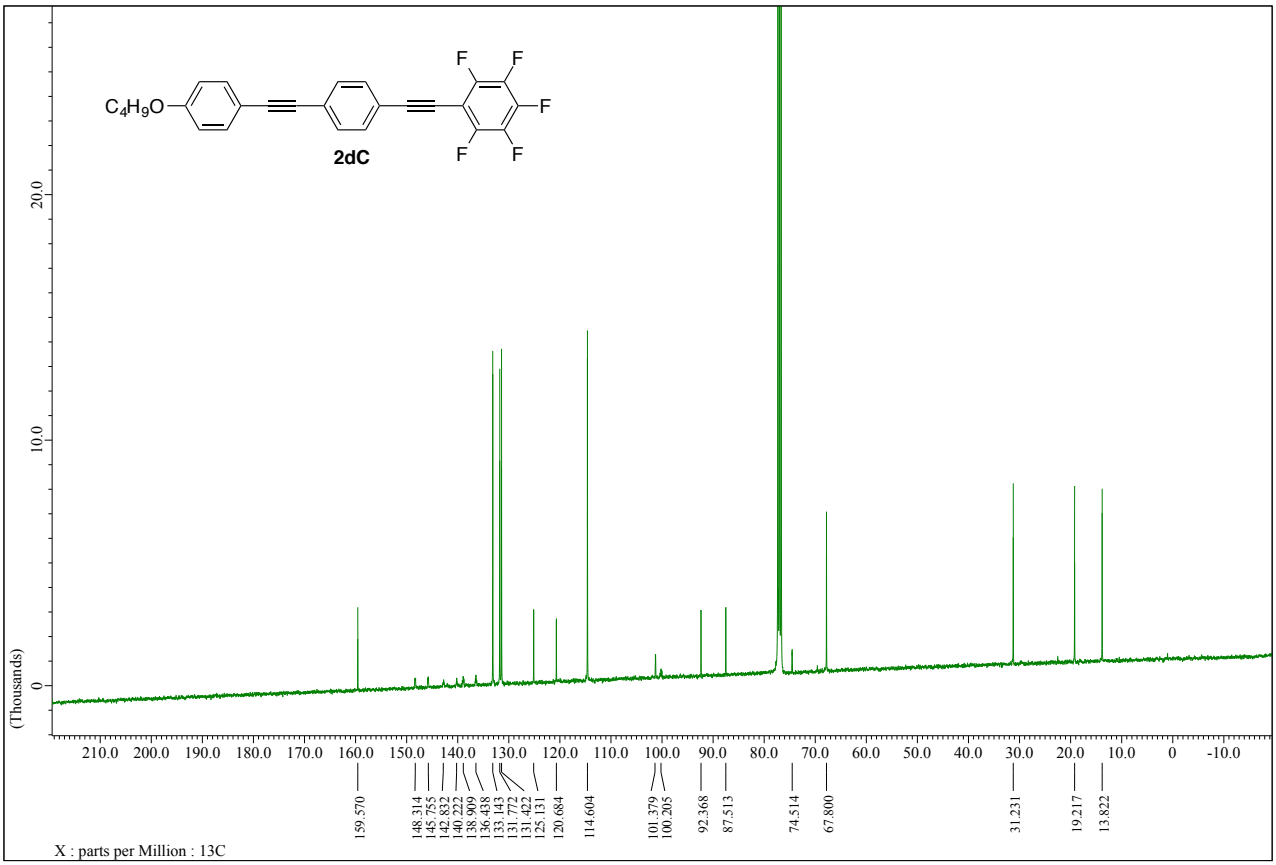

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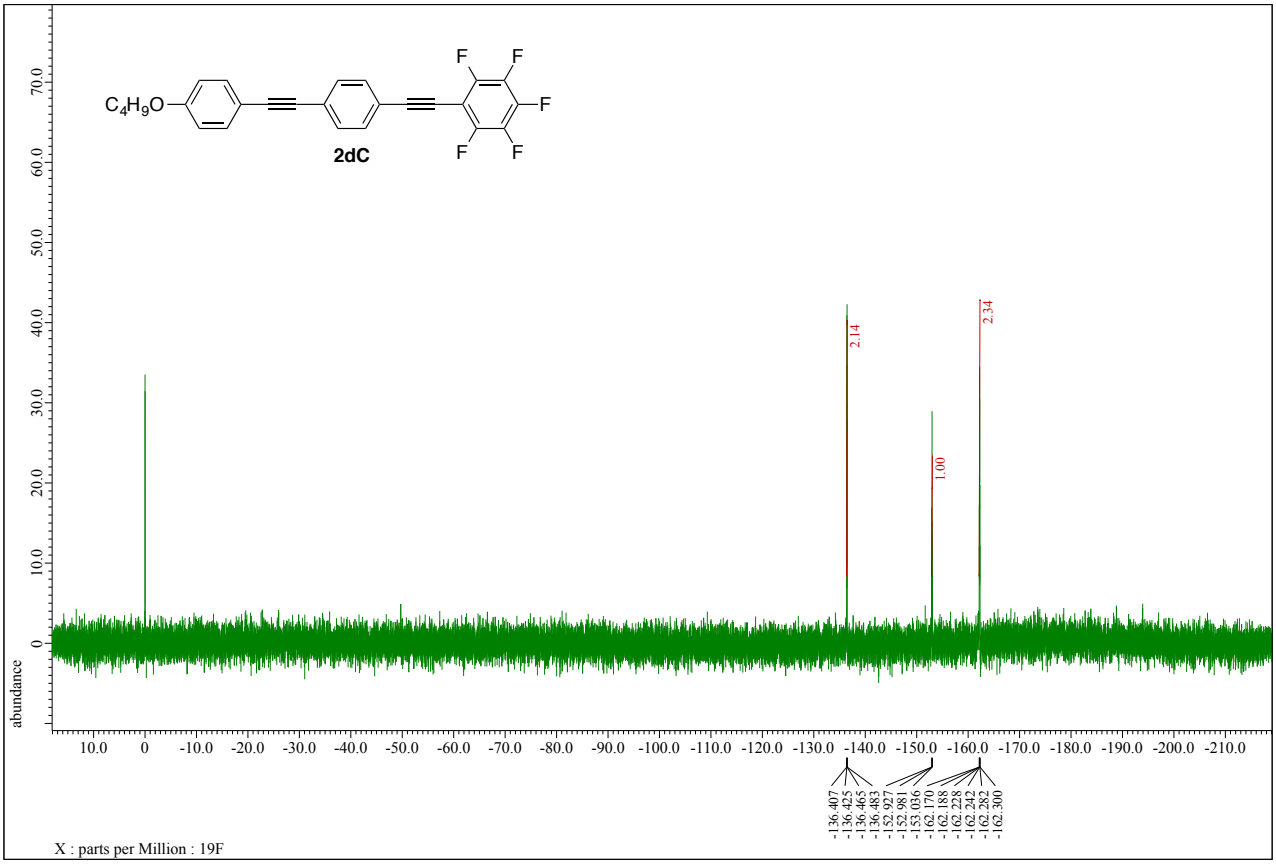

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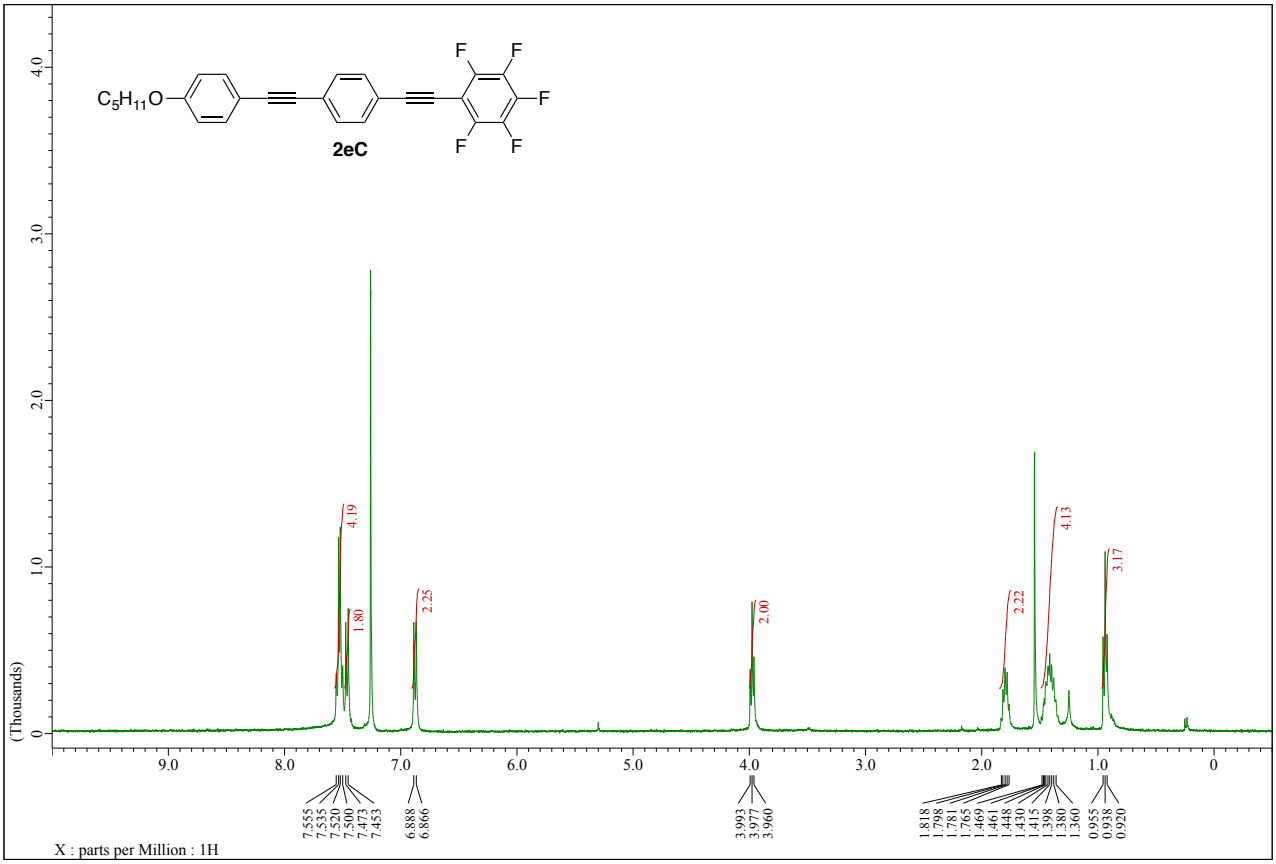

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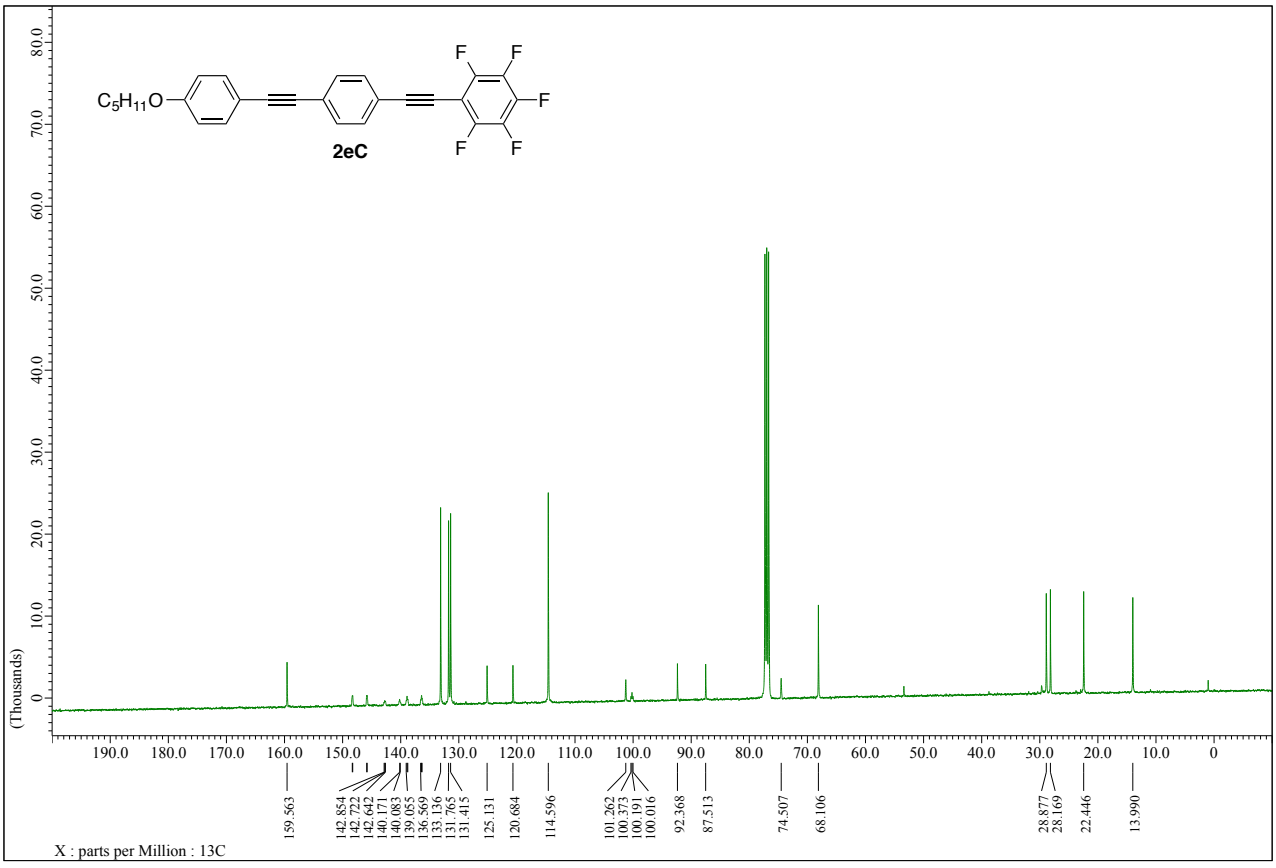

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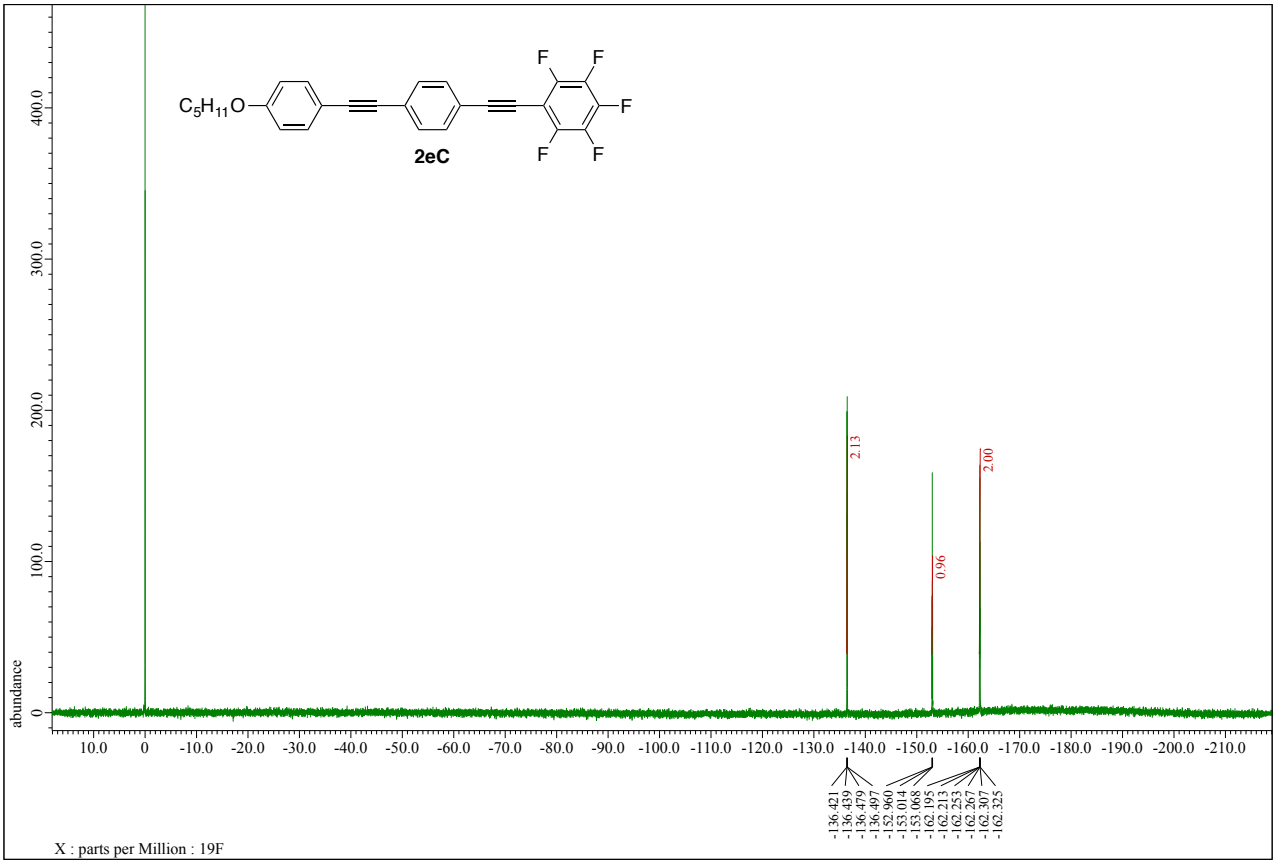

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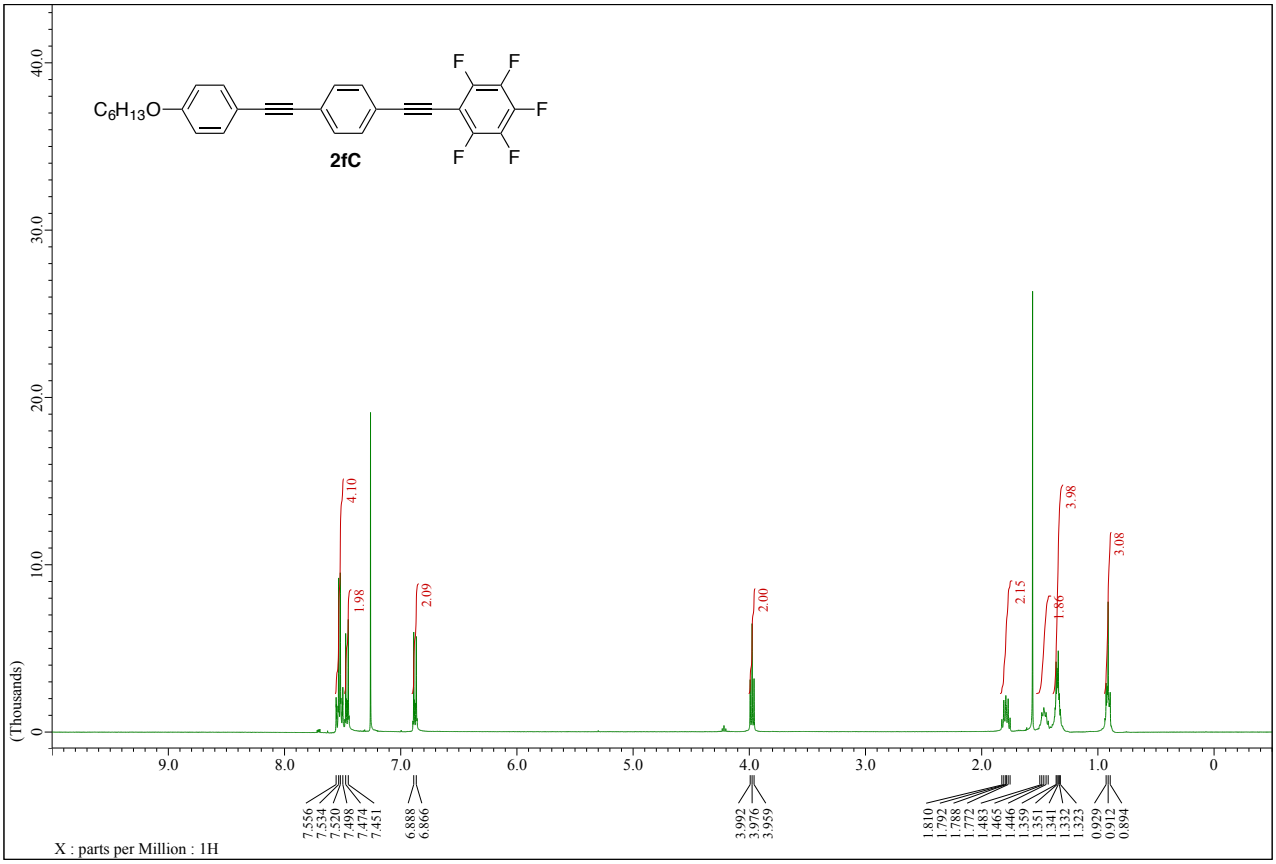

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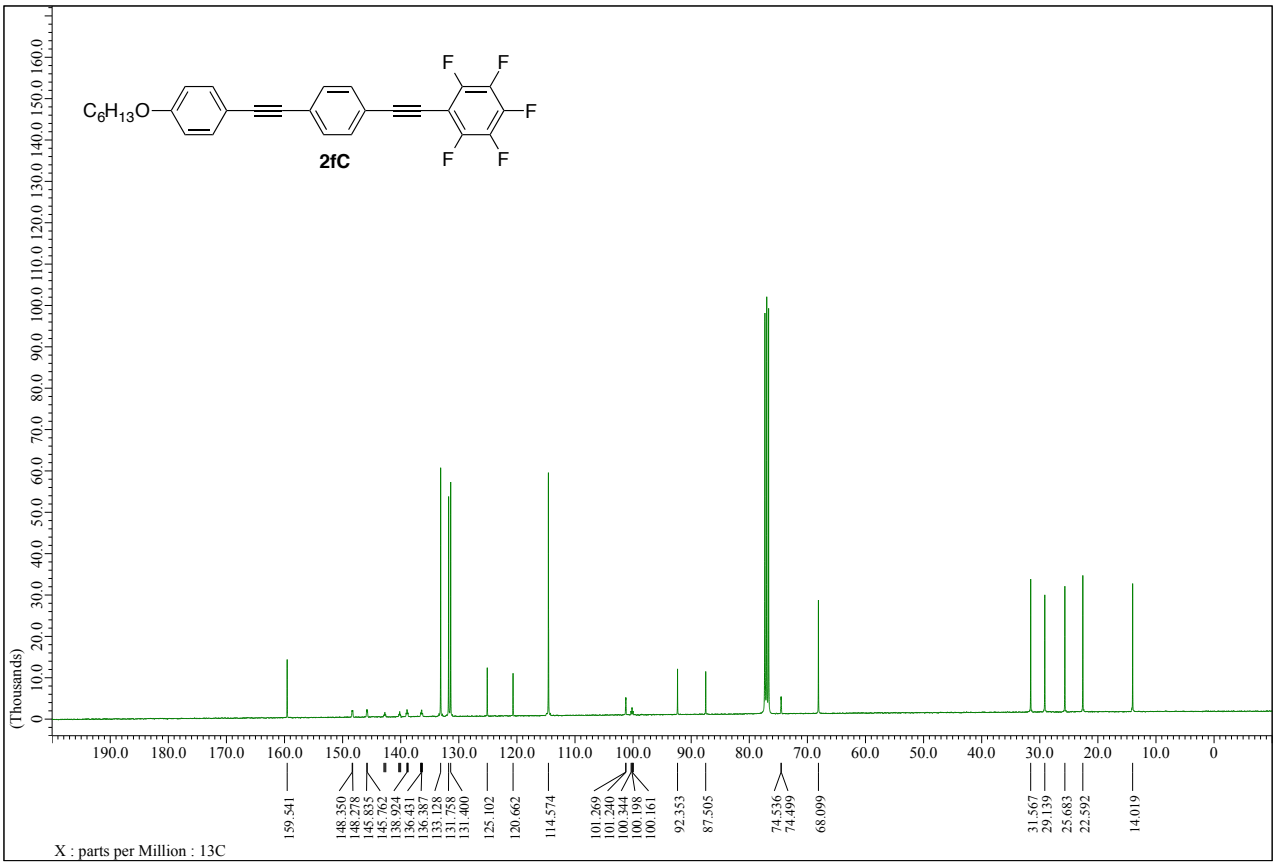

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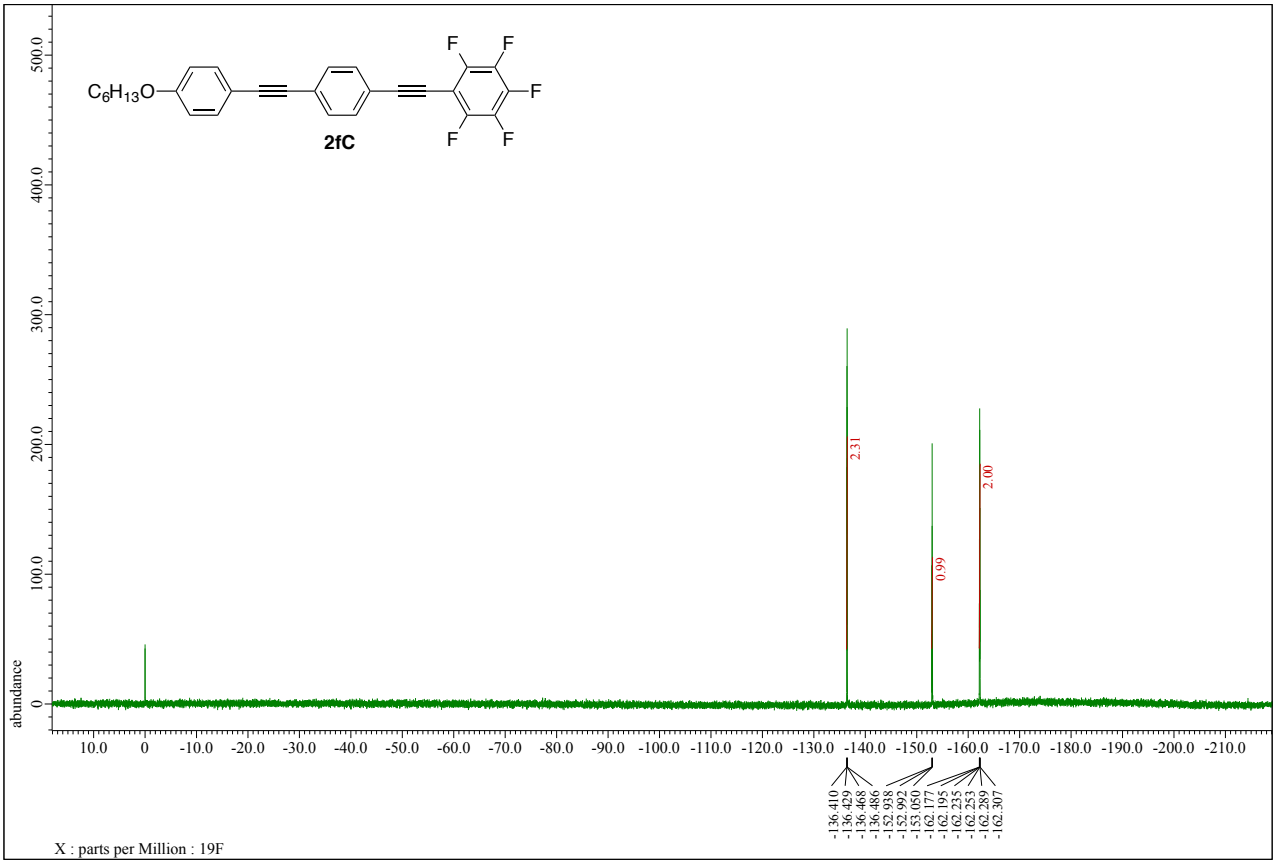


2. X-ray crystallographic analysis

Single crystals were obtained by iterative purification technique of column chromatography and recrystallization (solvent system: CH_2Cl_2/methanol = 1/1). The X-ray diffraction measurement was carried out at room temperature (296 K). Crystal structures of **2aC** and **2eC** obtained and their packing structures are shown in Fig. S1. For a comparison, crystal structure of non-substituted **1** (CCDC 162387), which was reported in *Angew. Chem. Int. Ed.* **2004**, *43*, 3061, are also described here. The crystal data of the **1**, **2aC** and **2bC** disclosed in Table 1 have been indexed, and are included in the Cambridge Crystallographic Center (CCDC) database with the following numbers: CCDC 1552781 for **2aC** and 1552782 for **2eC**. The indexed database contains additional supplementary crystallographic data for this paper and may be accessed without charge at http://www.ccdc.cam.ac.uk/conts/retrieving.html. The CCDC may be contacted by mail at 12 Union Road, Cambridge CB2 1EZ, U.K., by fax at (44) 1223-336-033, or by e-mail at deposit@ccdc.cam.ac.uk.

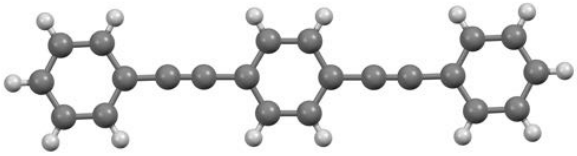
Table S1. Crystallographic data for bistolanes **1**, **2aC** and **2eC**.

Bistolane	**1**	**2aC**	**2eC**
CCDC #	162387	1552781	1552782
Empirical Formula	$C_{22}H_{24}$	$C_{23}H_{11}F_5O$	$C_{27}H_{19}F_5O$
Formula Weight	278.33	398.32	454.43
Temperature [K]	160(2)	298	298
Crystal Colour / Habit	Colourless / Block	Colourless / Block	Pale yellow / Plate
Crystal Size [mm]	0.78 x 0.28 x 0.18	0.22 x 0.21 0.18	0.54 x 0.20 x 0.05
Crystal System	*P*-1	*P* $2_1/n$	C_1c_1
Space group	triclinic	monoclinic	monoclinic
a [Å]	6.0202(10)	5.9797(2)	37.637(3)
b [Å]	9.662(2)	7.5043(3)	4.9401(5)
c [Å]	13.692(2)	40.9251(14)	11.5774(11)
α [°]	90.719(4)	90	90
β [°]	94.732(4)	92.350(3)	94.936(3)
γ [°]	103.859(4)	90	90
V [Å^3]	770.2(2)	1834.91(11)	2144.6(3)
Z	2	4	4
R [$F^2 > 2s(F^2)$]	0.0415	0.0409	0.0395
wR (F^2)	0.1173	0.1064	0.1265

[a] $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR = \{[\Sigma w(|F_o| - |F_c|)]/\Sigma w|F_o|\}^{1/2}$.

(a) Prototypical bistolane **1**

Top view

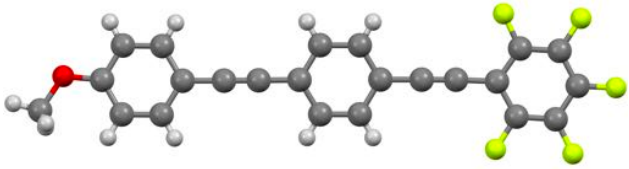


Side view

Packing structure

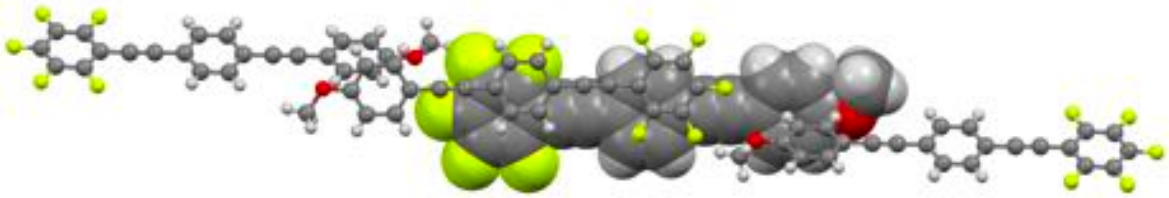
(b) disymmetric bistolane **2aC**

Top view



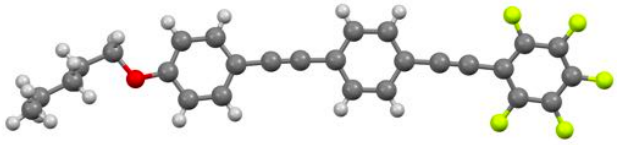
Side view

Packing structure

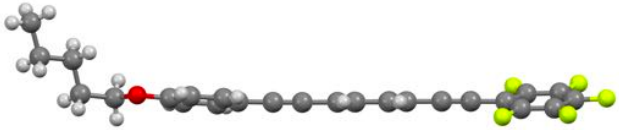


(c) disymmetric bistolane **2eC**

Top view



Side view



Packing structure

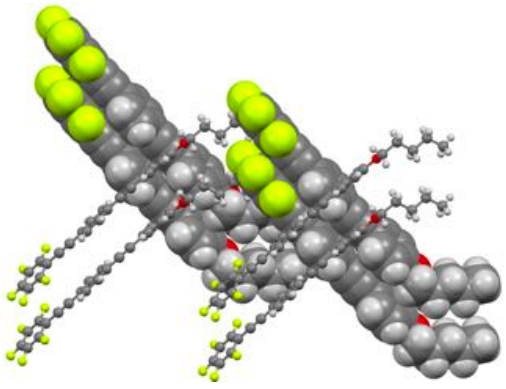
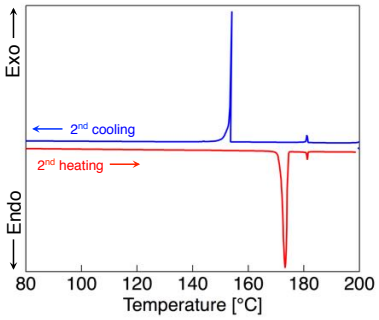


Fig. S1 Crystal and packing structures of prototypical **1**, bistolanes **2aC** and **2eC**

3. Phase transition behaviour

Phase transition behaviour of the bistolane derivatives were assessed using DSC (SII, X-DSC7000) at heating and cooling rates of 5.0 °C min^{-1}. The obtained thermograms were shown in Fig. S3. At least three scans were conducted to obtain the reproducibility. In Table S2 are summarized the phase transition sequence and thermodynamic parameters.

(A) **2aA**



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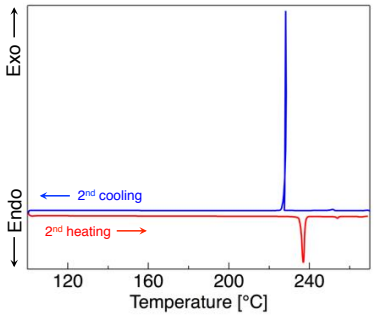
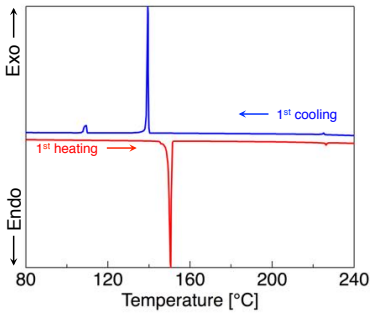
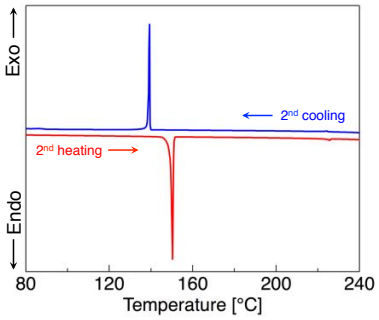


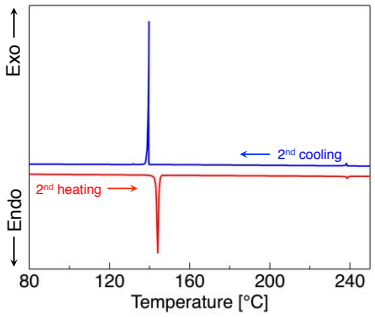
(C) **2aC** (1st cycle)



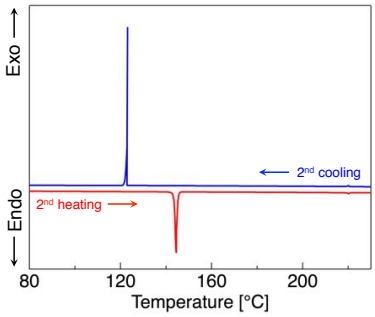
(D) **2aC** (2nd cycle)



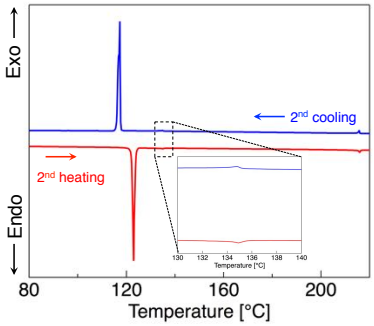
(E) **2bC**



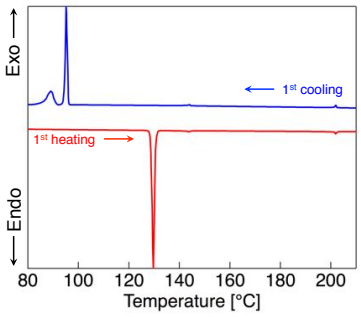
(F) **2cC**



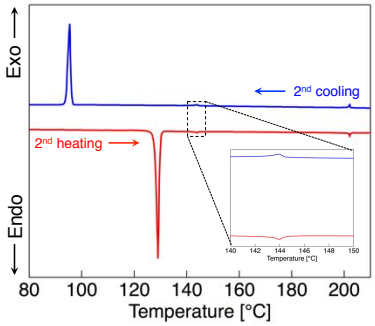
(G) **2dC**



(H) **2eC** (1st cycle)



(I) **2eC** (2nd cycle)



(J) **2fC**

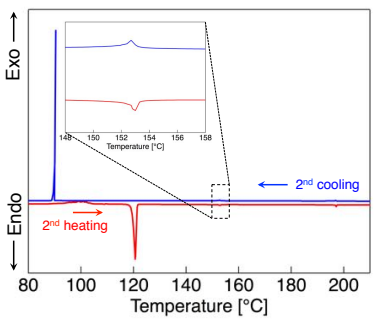


Fig. S3 DSC thermograms of dissymmetric bistolane derivatives under N_2 atmosphere. Scan rate: 5.0 °C min^{-1}. Unless other mentioned, the thermograms were taken in the 2nd cycles.

Table S2. Phase transition behaviours and thermodynamic parameters.

Bistolanes	Phase transition sequence and temperature [°C]			ΔH [kJ mol^{-1}]	ΔS [J mol^{-1} K^{-1}]
2aA	Heating	Cr – N	171	41.3	93.1
		N – Iso	181	0.69	1.51
	Cooling	Cr – N	154	–31.4	–73.7
		N – Iso	181	–0.57	–1.27
2aB	Heating	Cr – N	235	38.8	76.3
		N – Iso	253	1.14	2.16
	Cooling	Cr – N	228	–34.7	–69.2
		N – Iso	253	–1.10	–2.10
2aC	Heating	Cr – N	149	26.0	61.6
		N – Iso	225	0.45	0.91
	Cooling	Cr – N	140	–14.1	–34.4
		N – Iso	225	–0.24	–0.47
2bC	Heating	Cr – N	143	31.3	75.2
		N – Iso	238	0.88	1.72
	Cooling	Cr – N	140	–29.3	–70.9
		N – Iso	239	–0.67	–1.32
2cC	Heating	Cr – N	144	38.3	91.9
		N – Iso	220	0.84	1.69
	Cooling	Cr – N	123	–33.2	–84.0
		N – Iso	221	–0.72	–1.47
2dC	Heating	Cr – SmA	122	31.9	80.8
		SmA – N	134	0.30	0.76
		N – Iso	215	0.73	1.50
	Cooling	Cr – SmA	117	–29.7	–76.1
		SmA – N	136	–0.24	–0.58
		N – Iso	216	–0.76	–1.55
2eC	Heating	Cr – SmA	128	52.3	130.4
		SmA – N	143	0.69	1.68
		N – Iso	201	0.94	1.97
	Cooling	Cr – SmA	96	–32.2	–87.3
		SmA – N	144	–0.60	–1.42
		N – Iso	202	–0.76	–1.60
2fC	Heating	Cr – SmA	120	52.0	132.4
		SmA – N	152	0.86	2.02
		N – Iso	197	0.92	1.96
	Cooling	Cr – SmA	90	–29.1	–80.4
		SmA – N	153	–0.95	–2.23
		N – Iso	197	–0.89	–1.89

Abbreviations: Cry, crystalline; SmA, smectic A phase; N, nematic; Iso, isotropic phases.

4. Polarized optical microscopy (POM)

Polarized optical microscopy was carried out using an Olympus BX51 microscope equipped with a temperature-controlled stage (Instec HCS302 microscope hot/cold stage and mK1000 temperature controller). The observed optical texture images were shown in Fig. S2.

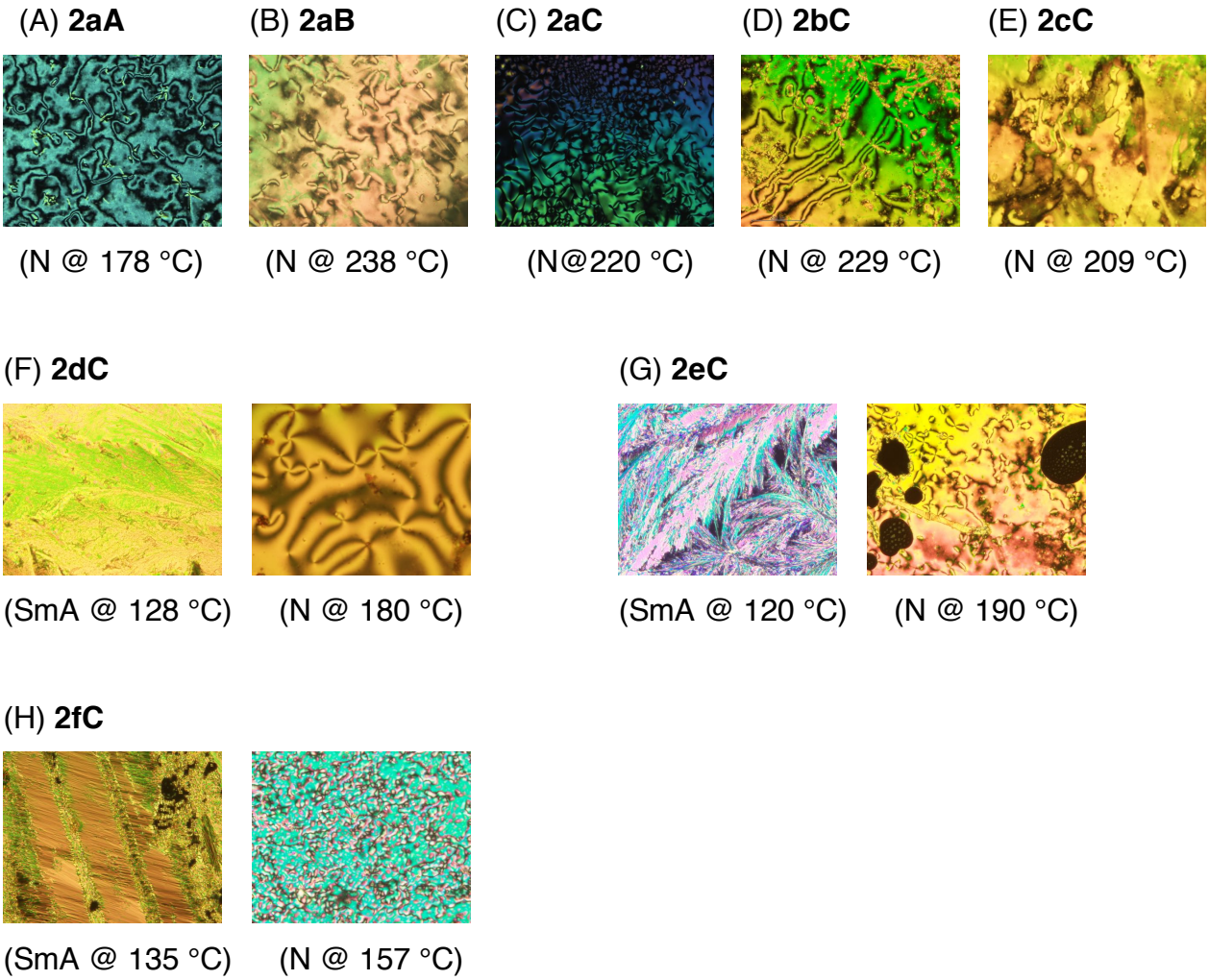
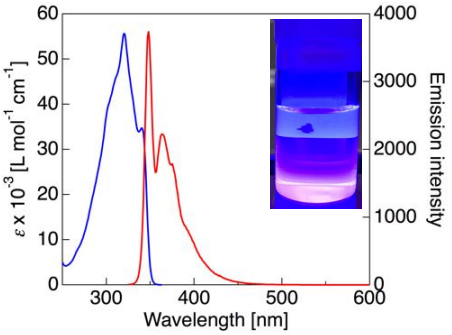


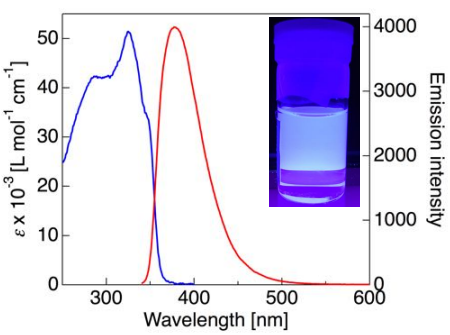
Fig. S2 POM texture images of dissymmetric bistolane derivatives **2** in the LC phases.

5. Absorption and photoluminescence spectra in solution

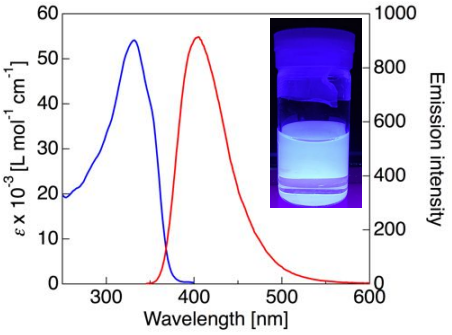
(A) **2aA**



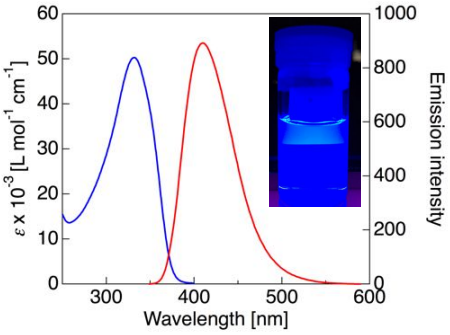
(B) **2aB**



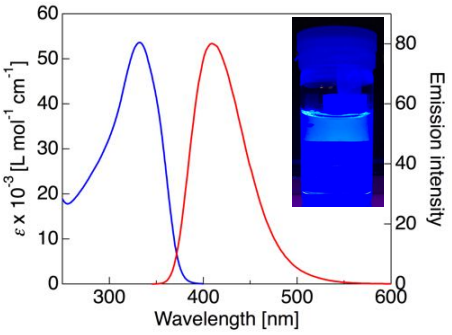
(C) **2aC**



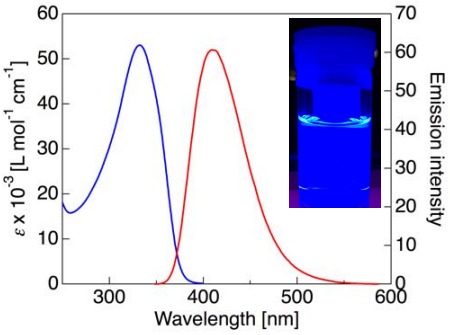
(D) **2bC**



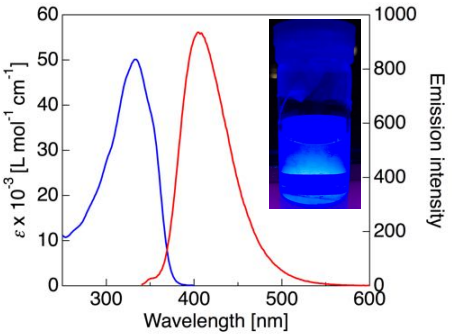
(E) **2cC**



(F) **2dC**



(G) **2eC**



(H) **2fC**

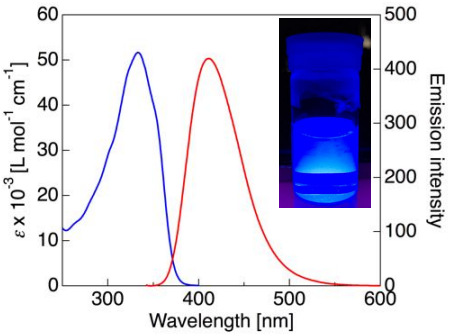
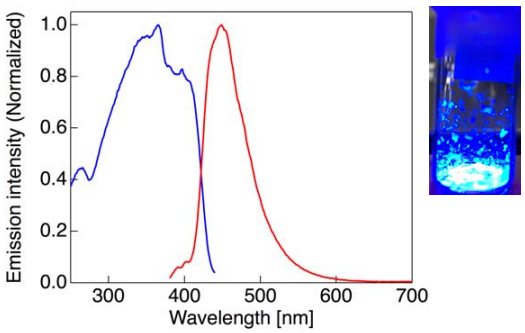


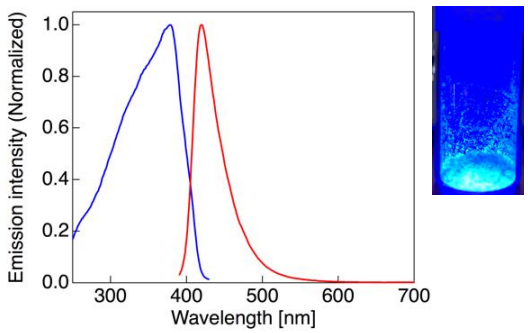
Fig. S4 Absorption (blue line) and corrected photoluminescence spectra (red line) for the dissymmetric bistolanes **2** in dilute CH_2Cl_2 solution. Absorption spectra were measured in 10^{-5} mol L^{-1} and photoluminescence measurement were carried out using 10^{-6} mol L^{-1} concentration.

6. Excitation and photoluminescence spectra in crystal

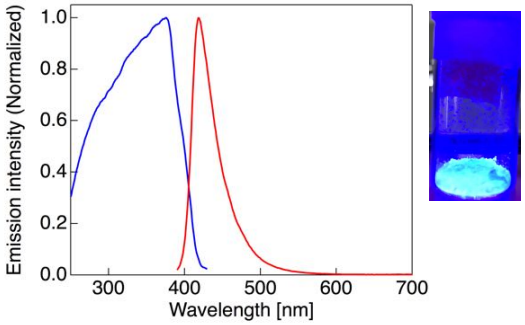
(A) **2aA**



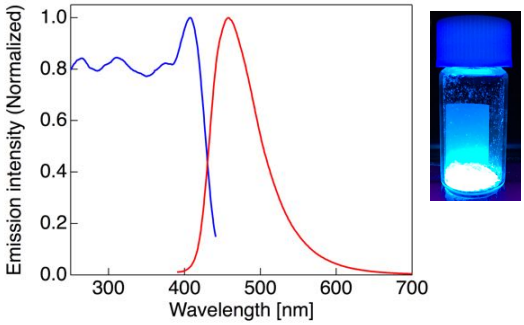
(B) **2aB**



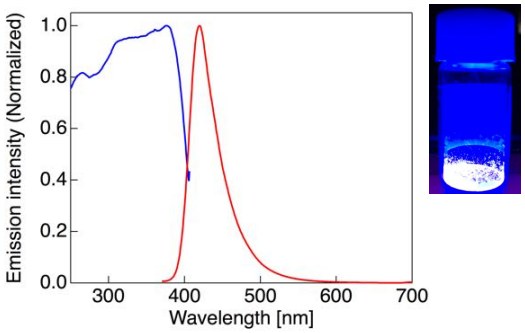
(C) **2aC**



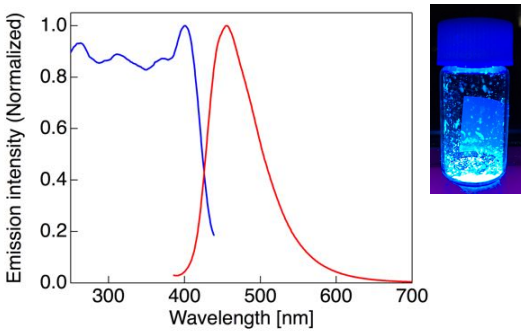
(D) **2bC**



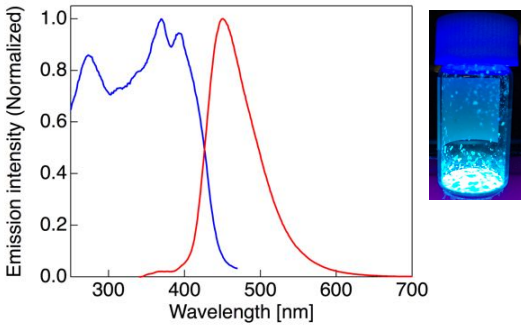
(E) **2cC**



(F) **2dC**



(G) **2eC**



(H) **2fC**

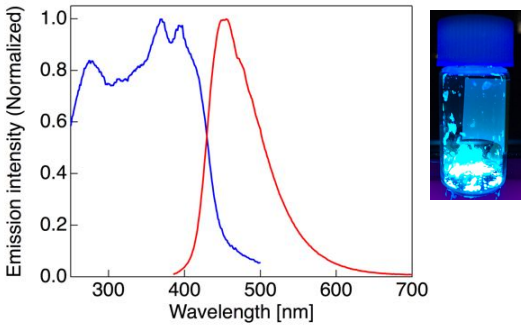
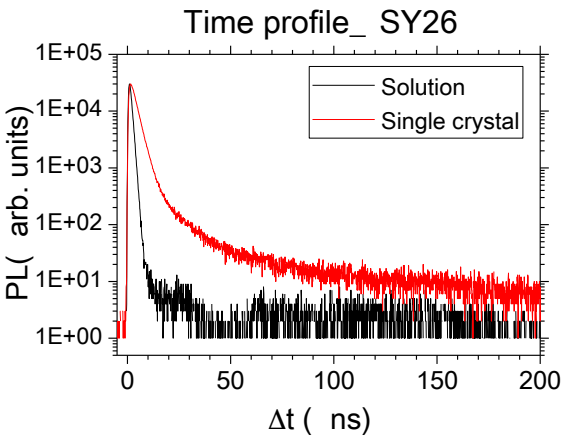


Fig. S5 Excitation (blue line) and photoluminescence spectra (Red line) corrected for the dissymmetric bistolanes **2** in crystal.

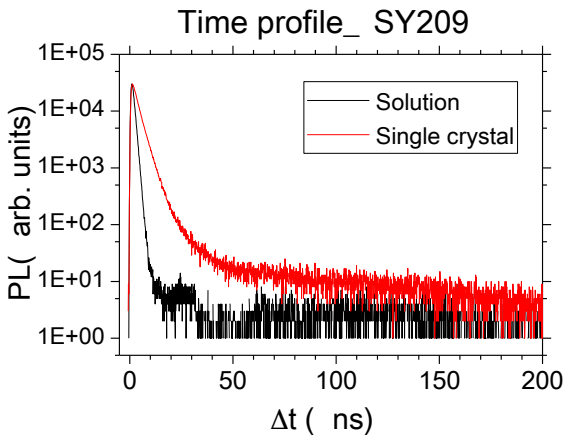
7. Transient emission measurement

Transient emission measurement was performed using a Fluorocube fluorescence lifetime system (HORIBA, λ_{ex} = 342 nm, pulse width = 1.1 nm).

(a) **2aA**



(b) **2aB**



(c) **2aC**

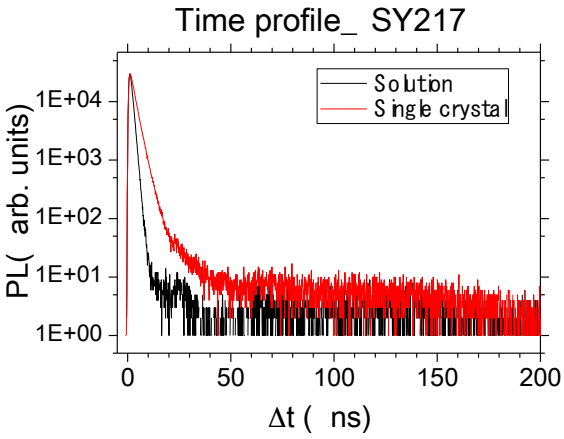
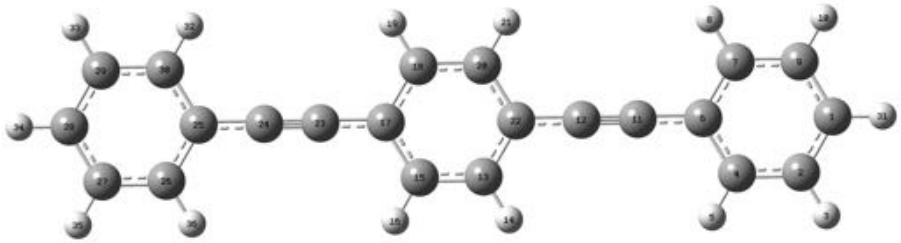


Fig. S6 Decay profile obtained from transient emission measurement of dissymetric bistolanes, **2aA**, **2aB** and **2aC** as a selected example.

Table S3. Photophysical data obtained from transient emission measurement.

Bistolane		Time constant [ns]	Φ_{em}	k_r (x10^8) [s^{-1}]	k_{nr} (x10^8) [s^{-1}]
2aA (SY26)	solution	1.14	0.85	8.8	1.6
	crystal	3.15	0.88	3.2	0.43
2aB (SY209)	solution	1.22	0.77	8.2	2.4
	crystal	3.19	0.72	3.1	1.2
2aC (SY217)	solution	1.29	0.79	7.8	2.1
	crystal	2.47	0.66	4.0	2.1

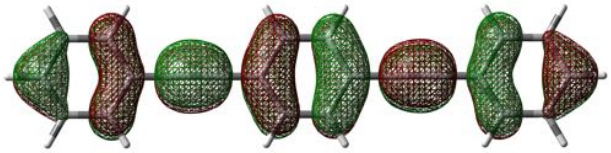
8. Cartesian coordinates for prototypical bistolane **1**[a]



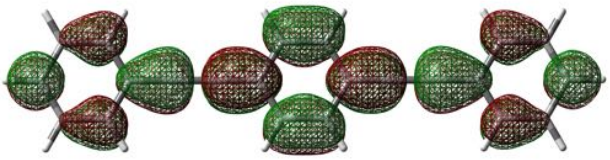
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–8.275718	0.000587	0.000008
2	6	0	–7.575474	–1.206042	0.000083
3	1	0	–8.114714	–2.146622	0.000155
4	6	0	–6.185443	–1.211124	0.000067
5	1	0	–5.640625	–2.147489	0.000125
6	6	0	–5.468266	–0.000020	–0.000026
7	6	0	–6.184920	1.211393	–0.000102
8	1	0	–5.639698	2.147523	–0.000176
9	6	0	–7.574953	1.206913	–0.000085
10	1	0	–8.113787	2.147726	–0.000145
11	6	0	–4.045728	–0.000330	–0.000047
12	6	0	–2.834247	–0.000538	–0.000059
13	6	0	–0.692429	–1.210043	0.000067
14	1	0	–1.234066	–2.148151	0.000118
15	6	0	0.692553	–1.209971	0.000094
16	1	0	1.234287	–2.148022	0.000167
17	6	0	1.414027	–0.000314	0.000028
18	6	0	0.692429	1.209269	–0.000065
19	1	0	1.234066	2.147376	–0.000117
20	6	0	–0.692554	1.209197	–0.000092
21	1	0	–1.234287	2.147248	–0.000165
22	6	0	–1.414028	–0.000460	–0.000027
23	6	0	2.834246	–0.000242	0.000060
24	6	0	4.045728	–0.000162	0.000079
25	6	0	5.468263	0.000049	0.000039
26	6	0	6.185360	–1.211101	0.000103
27	6	0	7.575392	–1.206116	0.000069
28	6	0	8.275720	0.000464	–0.000030
29	6	0	7.575036	1.206837	–0.000093
30	6	0	6.185003	1.211411	–0.000060
31	1	0	–9.359698	0.000821	0.000021
32	1	0	5.639849	2.147582	–0.000110
33	1	0	8.113931	2.147615	–0.000169
34	1	0	9.359701	0.000624	–0.000056
35	1	0	8.114564	–2.146735	0.000120
36	1	0	5.640483	–2.147433	0.000180

SCF Done: E(RB3LYP) = –846.728045409 a.u.
Imaginary frequency number: 0

HOMO (–5.62 eV)

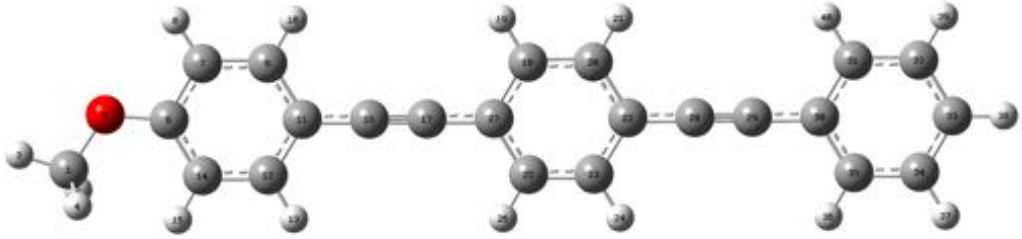


LUMO (–1.96 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

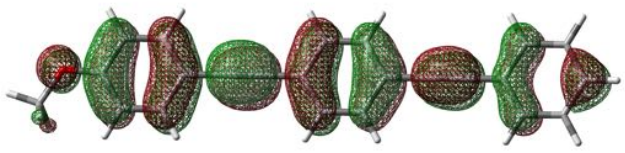
Cartesian coordinates for dissymmetric bistolane **2aA**[a]



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.437785	–0.857110	0.000898
2	1	0	9.257963	–1.462292	0.895709
3	1	0	10.469445	–0.509864	0.001362
4	1	0	9.259024	–1.463010	–0.893645
5	8	0	8.634316	0.316802	–0.000042
6	6	0	7.279345	0.182910	–0.000011
7	6	0	6.547741	1.378847	–0.000013
8	1	0	7.088819	2.317314	0.000034
9	6	0	5.165504	1.351185	–0.000106
10	1	0	4.608109	2.280101	–0.000109
11	6	0	4.463340	0.127314	–0.000156
12	6	0	5.210409	–1.060431	–0.000122
13	1	0	4.691344	–2.011372	–0.000157
14	6	0	6.602359	–1.040777	–0.000055
15	1	0	7.142828	–1.977646	–0.000067
16	6	0	3.042774	0.100467	–0.000249
17	6	0	1.830953	0.081077	–0.000306
18	6	0	–0.329467	1.257430	–0.000849
19	1	0	0.197614	2.203810	–0.001355
20	6	0	–1.714255	1.236423	–0.000802
21	1	0	–2.269842	2.166407	–0.001278
22	6	0	–2.417927	0.016328	–0.000170
23	6	0	–1.677629	–1.181880	0.000380
24	1	0	–2.204860	–2.128231	0.000844
25	6	0	–0.292808	–1.161045	0.000322
26	1	0	0.262660	–2.091072	0.000746
27	6	0	0.411417	0.059133	–0.000279
28	6	0	–3.838026	–0.005025	–0.000086
29	6	0	–5.049444	–0.022928	–0.000018
30	6	0	–6.471801	–0.043294	0.000088
31	6	0	–7.206209	1.157519	0.000928
32	6	0	–8.596045	1.133073	0.001018
33	6	0	–9.279544	–0.083128	0.000293
34	6	0	–8.561771	–1.279413	–0.000534
35	6	0	–7.171778	–1.264493	–0.000649
36	1	0	–6.613572	–2.192958	–0.001336
37	1	0	–9.087321	–2.227748	–0.001121
38	1	0	–10.363423	–0.098521	0.000368
39	1	0	–9.148260	2.066131	0.001673
40	1	0	–6.674585	2.101445	0.001539

SCF Done: E(RB3LYP) = –961.256949364 a.u.
Imaginary frequency number: 0

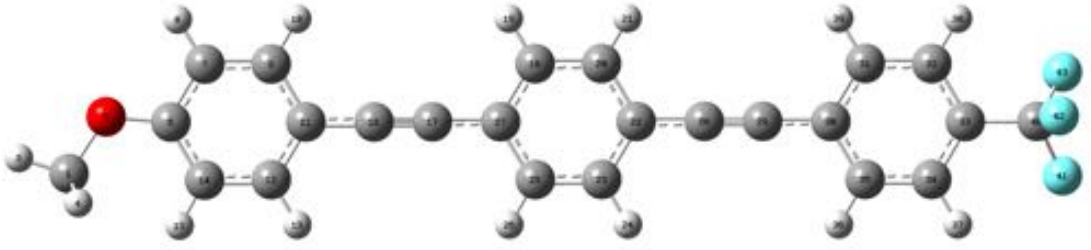
HOMO (–5.39 eV)



LUMO (–1.82 eV)

[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

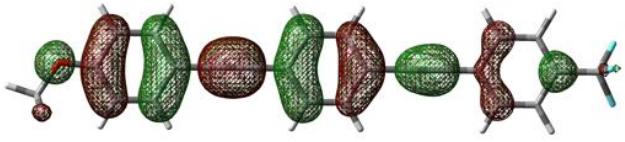
Cartesian coordinates for dissymmetric bistolane **2aB**[a]



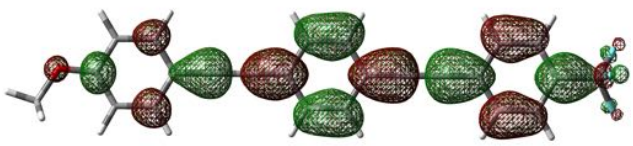
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–11.281194	–0.886650	0.007012
2	1	0	–11.100598	–1.487592	–0.890409
3	1	0	–12.314154	–0.543499	0.009901
4	1	0	–11.097933	–1.494631	0.899133
5	8	0	–10.482435	0.290948	0.010452
6	6	0	–9.127721	0.163959	0.007843
7	6	0	–8.402276	1.363943	0.011360
8	1	0	–8.948369	2.299447	0.015920
9	6	0	–7.020153	1.343441	0.009024
10	1	0	–6.467484	2.275153	0.011784
11	6	0	–6.312145	0.122888	0.003138
12	6	0	–7.052708	–1.069012	–0.000244
13	1	0	–6.528668	–2.017200	–0.004797
14	6	0	–8.444491	–1.056515	0.002040
15	1	0	–8.980321	–1.995993	–0.000769
16	6	0	–4.891811	0.103210	0.000660
17	6	0	–3.679862	0.089919	–0.001517
18	6	0	–1.525485	1.276359	–0.003678
19	1	0	–2.056881	2.220198	–0.001051
20	6	0	–0.140872	1.261359	–0.006594
21	1	0	0.410844	2.193613	–0.006217
22	6	0	0.566617	0.043607	–0.010002
23	6	0	–0.167244	–1.158455	–0.010305
24	1	0	0.364125	–2.102453	–0.012881
25	6	0	–1.551841	–1.143414	–0.007497
26	1	0	–2.103625	–2.075502	–0.007884
27	6	0	–2.260825	0.074325	–0.004181
28	6	0	1.986355	0.027763	–0.013328
29	6	0	3.197733	0.013315	–0.016359
30	6	0	4.618257	–0.005057	–0.020441
31	6	0	5.352410	1.196148	–0.029082
32	6	0	6.739637	1.176450	–0.034375
33	6	0	7.421567	–0.042221	–0.034048
34	6	0	6.707891	–1.241919	–0.023940
35	6	0	5.320255	–1.224921	–0.019190
36	1	0	4.766111	–2.155177	–0.016171
37	1	0	7.237124	–2.186448	–0.027814
38	1	0	7.293167	2.107131	–0.046415
39	1	0	4.822920	2.140642	–0.033777
40	6	0	8.923489	–0.059233	0.015352
41	9	0	9.442857	–1.180327	–0.534123
42	9	0	9.388801	–0.004796	1.291212
43	9	0	9.469424	0.993901	–0.635096

SCF Done: E(RB3LYP) = –1298.31741834 a.u.
Imaginary frequency number: 0

HOMO (–5.56 eV)

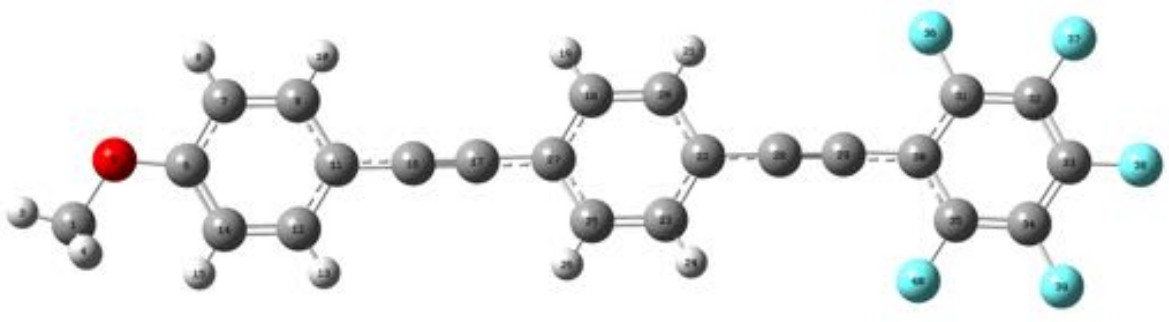


LUMO (–2.12 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

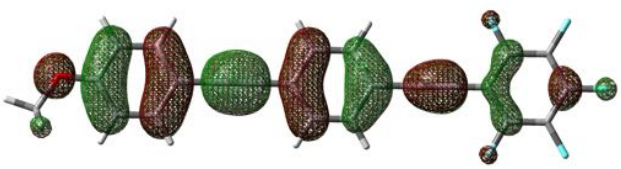
Cartesian coordinates for dissymmetric bistolane **2aC**[a]



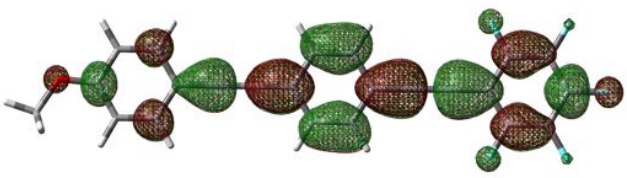
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–11.054141	0.912290	0.026519
2	1	0	–10.857563	1.342812	0.884389
3	1	0	–12.007142	0.677336	–0.009110
4	1	0	–10.840820	1.530062	–0.704302
5	8	0	–10.267408	–0.270156	–0.104206
6	6	0	–8.913332	–0.143176	–0.035450
7	6	0	–8.196614	–1.328090	–0.163762
8	1	0	–8.655303	–2.149714	–0.288243
9	6	0	–6.825495	–1.313977	–0.113355
10	1	0	–6.346784	–2.130647	–0.192536
11	6	0	–6.125878	–0.117163	0.054755
12	6	0	–6.856944	1.062883	0.182407
13	1	0	–6.396191	1.886118	0.301677
14	6	0	–8.240583	1.055888	0.136536
15	1	0	–8.725522	1.868613	0.224122
16	6	0	–4.693289	–0.108481	0.058925
17	6	0	–3.495769	–0.119196	0.037714
18	6	0	–1.352315	–1.323730	0.081183
19	1	0	–1.819547	–2.148443	0.148315
20	6	0	0.024625	–1.317100	0.055773
21	1	0	0.498008	–2.138591	0.096014
22	6	0	0.729157	–0.119753	–0.027531
23	6	0	0.016376	1.080290	–0.105247
24	1	0	0.484550	1.905322	–0.172483
25	6	0	–1.361099	1.072480	–0.088282
26	1	0	–1.834998	1.893219	–0.145081
27	6	0	–2.067612	–0.125899	0.012343
28	6	0	2.162509	–0.111725	–0.018464
29	6	0	3.354135	–0.100557	0.002757
30	6	0	4.774823	–0.031689	0.006614
31	6	0	5.577746	–1.168004	0.028983
32	6	0	6.950641	–1.086657	0.013167
33	6	0	7.567093	0.135082	–0.004970
34	6	0	6.803829	1.287708	–0.021948
35	6	0	5.435539	1.189440	–0.016255
36	9	0	5.006082	–2.376362	0.061122
37	9	0	7.692894	–2.203581	0.006951
38	9	0	8.899241	0.213101	–0.005899
39	9	0	7.394592	2.484741	–0.031216
40	9	0	4.713877	2.319875	–0.022467

SCF Done: E(RB3LYP) = –1457.24697154 a.u.
Imaginary frequency number: 0

HOMO (–5.62 eV)

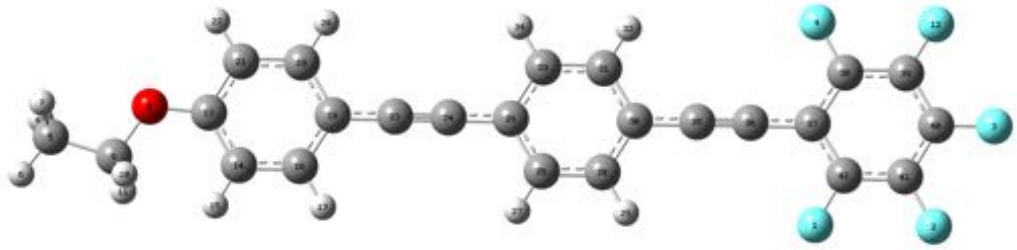


LUMO (–2.18 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

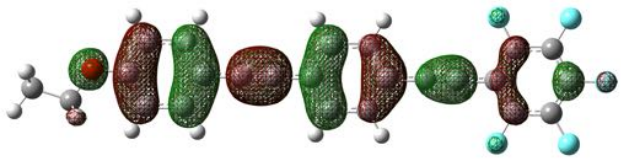
Cartesian coordinates for dissymmetric bistolane **2bC**[a]



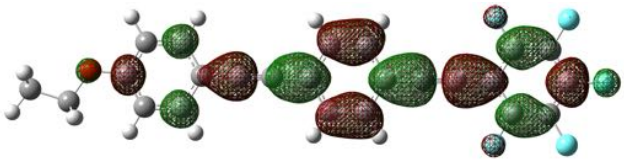
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	–7.314593	–2.249927	0.516432
2	9	0	–10.022691	–2.177800	0.641321
3	9	0	–11.343471	0.185919	0.300596
4	9	0	–7.238707	2.423881	–0.292949
5	6	0	10.178986	–1.008118	–0.668314
6	1	0	10.769425	–1.940995	–0.708155
7	1	0	10.327951	–0.500262	–1.637583
8	8	0	7.932861	–0.199481	–0.658733
9	6	0	8.712284	–1.395277	–0.549522
10	1	0	8.425119	–2.098689	–1.352160
11	1	0	8.511586	–1.883039	0.423119
12	9	0	–9.947271	2.482739	–0.165782
13	6	0	6.579065	–0.278653	–0.573598
14	6	0	5.854830	–1.465525	–0.375507
15	1	0	6.363699	–2.423426	–0.275724
16	6	0	4.461999	–1.425030	–0.304358
17	1	0	3.905161	–2.350840	–0.150130
18	6	0	3.756638	–0.212605	–0.427958
19	6	0	4.502253	0.973424	–0.627616
20	1	0	3.974860	1.923675	–0.726317
21	6	0	5.886332	0.940308	–0.698767
22	1	0	6.466196	1.851742	–0.853174
23	6	0	2.333875	–0.178717	–0.355374
24	6	0	1.113567	–0.144852	–0.294418
25	6	0	–0.307820	–0.104538	–0.224130
26	6	0	–1.055407	–1.283010	0.001479
27	1	0	–0.528793	–2.230845	0.122573
28	6	0	–2.441795	–1.243823	0.069799
29	1	0	–3.008533	–2.159769	0.244344
30	6	0	–3.135845	–0.023381	–0.085376
31	6	0	–2.391657	1.155860	–0.310688
32	1	0	–2.919380	2.103203	–0.431833
33	6	0	–1.005277	1.115464	–0.378545
34	1	0	–0.439718	2.031978	–0.553168
35	6	0	–4.557222	0.016568	–0.016918
36	6	0	–5.775569	0.049458	0.041024
37	6	0	–7.191739	0.084838	0.107668
38	6	0	–7.904531	1.287164	–0.063165
39	6	0	–9.293745	1.327382	0.000472
40	6	0	–10.010213	0.153273	0.239071
41	6	0	–9.332555	–1.054757	0.412914
42	6	0	–7.943149	–1.081811	0.346943
43	1	0	10.529477	–0.386290	0.128797

SCF Done: E(RB3LYP) = –1496.74631964 a.u.
Imaginary frequency number: 0

HOMO (–5.60 eV)

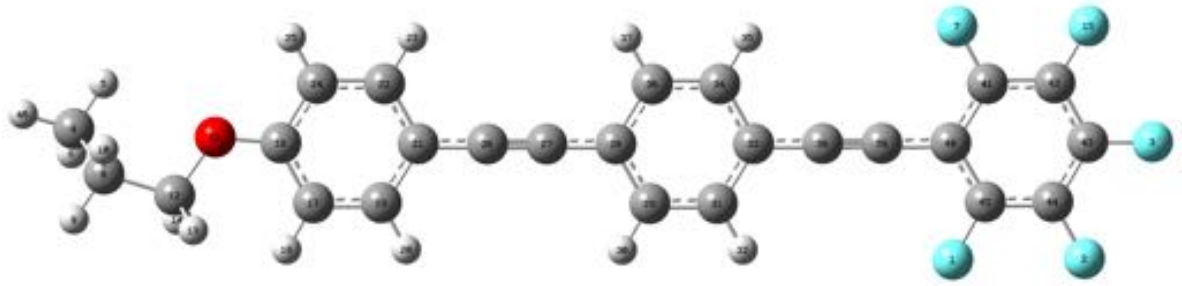


LUMO (–2.17 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

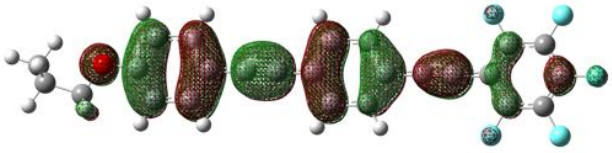
Cartesian coordinates for dissymmetric bistolane **2cC**[a]



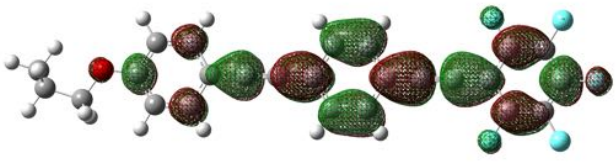
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	–7.314593	–2.249927	0.516432
2	9	0	–10.022691	–2.177800	0.641321
3	9	0	–11.343471	0.185919	0.300596
4	6	0	10.680913	–0.117618	0.473204
5	1	0	10.045185	0.782452	0.531025
6	1	0	10.548155	–0.650017	1.434255
7	9	0	–7.238707	2.423881	–0.292949
8	6	0	10.178986	–1.008118	–0.668314
9	1	0	10.769425	–1.940995	–0.708155
10	1	0	10.327951	–0.500262	–1.637583
11	8	0	7.932861	–0.199481	–0.658733
12	6	0	8.712284	–1.395277	–0.549522
13	1	0	8.425119	–2.098689	–1.352160
14	1	0	8.511586	–1.883039	0.423119
15	9	0	–9.947271	2.482739	–0.165782
16	6	0	6.579065	–0.278653	–0.573598
17	6	0	5.854830	–1.465525	–0.375507
18	1	0	6.363699	–2.423426	–0.275724
19	6	0	4.461999	–1.425030	–0.304358
20	1	0	3.905161	–2.350840	–0.150130
21	6	0	3.756638	–0.212605	–0.427958
22	6	0	4.502253	0.973424	–0.627616
23	1	0	3.974860	1.923675	–0.726317
24	6	0	5.886332	0.940308	–0.698767
25	1	0	6.466196	1.851742	–0.853174
26	6	0	2.333875	–0.178717	–0.355374
27	6	0	1.113567	–0.144852	–0.294418
28	6	0	–0.307820	–0.104538	–0.224130
29	6	0	–1.055407	–1.283010	0.001479
30	1	0	–0.528793	–2.230845	0.122573
31	6	0	–2.441795	–1.243823	0.069799
32	1	0	–3.008533	–2.159769	0.244344
33	6	0	–3.135845	–0.023381	–0.085376
34	6	0	–2.391657	1.155860	–0.310688
35	1	0	–2.919380	2.103203	–0.431833
36	6	0	–1.005277	1.115464	–0.378545
37	1	0	–0.439718	2.031978	–0.553168
38	6	0	–4.557222	0.016568	–0.016918
39	6	0	–5.775569	0.049458	0.041024
40	6	0	–7.191739	0.084838	0.107668
41	6	0	–7.904531	1.287164	–0.063165
42	6	0	–9.293745	1.327382	0.000472
43	6	0	–10.010213	0.153273	0.239071
44	6	0	–9.332555	–1.054757	0.412914
45	6	0	–7.943149	–1.081811	0.346943
46	1	0	11.705327	0.172145	0.365905

SCF Done: E(RB3LYP) = –1536.06109118 a.u.
Imaginary frequency number: 0

HOMO (–5.60 eV)

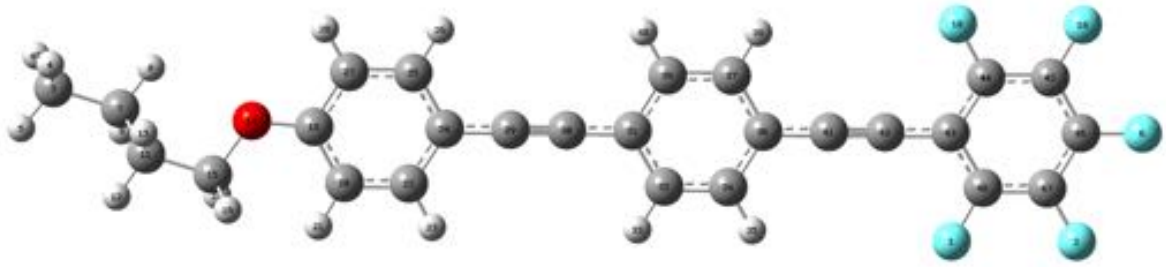


LUMO (–2.17 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

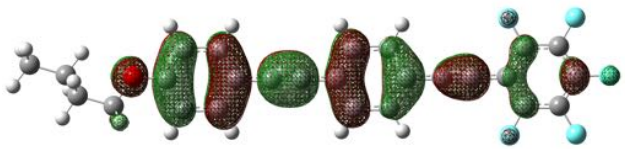
Cartesian coordinates for dissymmetric bistolane **2dC**[a]



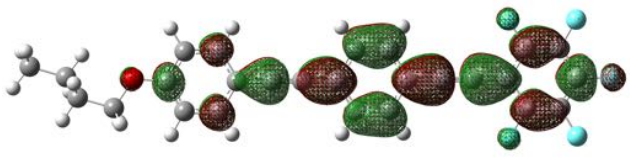
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	–7.314593	–2.249927	0.516432
2	9	0	–10.022691	–2.177800	0.641321
3	6	0	12.147152	0.297119	0.319627
4	1	0	12.276171	0.830706	–0.641213
5	1	0	12.781803	–0.607084	0.249915
6	9	0	–11.343471	0.185919	0.300596
7	6	0	10.680913	–0.117618	0.473204
8	1	0	10.045185	0.782452	0.531025
9	1	0	10.548155	–0.650017	1.434255
10	9	0	–7.238707	2.423881	–0.292949
11	6	0	10.178986	–1.008118	–0.668314
12	1	0	10.769425	–1.940995	–0.708155
13	1	0	10.327951	–0.500262	–1.637583
14	8	0	7.932861	–0.199481	–0.658733
15	6	0	8.712284	–1.395277	–0.549522
16	1	0	8.425119	–2.098689	–1.352160
17	1	0	8.511586	–1.883039	0.423119
18	9	0	–9.947271	2.482739	–0.165782
19	6	0	6.579065	–0.278653	–0.573598
20	6	0	5.854830	–1.465525	–0.375507
21	1	0	6.363699	–2.423426	–0.275724
22	6	0	4.461999	–1.425030	–0.304358
23	1	0	3.905161	–2.350840	–0.150130
24	6	0	3.756638	–0.212605	–0.427958
25	6	0	4.502253	0.973424	–0.627616
26	1	0	3.974860	1.923675	–0.726317
27	6	0	5.886332	0.940308	–0.698767
28	1	0	6.466196	1.851742	–0.853174
29	6	0	2.333875	–0.178717	–0.355374
30	6	0	1.113567	–0.144852	–0.294418
31	6	0	–0.307820	–0.104538	–0.224130
32	6	0	–1.055407	–1.283010	0.001479
33	1	0	–0.528793	–2.230845	0.122573
34	6	0	–2.441795	–1.243823	0.069799
35	1	0	–3.008533	–2.159769	0.244344
36	6	0	–3.135845	–0.023381	–0.085376
37	6	0	–2.391657	1.155860	–0.310688
38	1	0	–2.919380	2.103203	–0.431833
39	6	0	–1.005277	1.115464	–0.378545
40	1	0	–0.439718	2.031978	–0.553168
41	6	0	–4.557222	0.016568	–0.016918
42	6	0	–5.775569	0.049458	0.041024
43	6	0	–7.191739	0.084838	0.107668
44	6	0	–7.904531	1.287164	–0.063165
45	6	0	–9.293745	1.327382	0.000472
46	6	0	–10.010213	0.153273	0.239071
47	6	0	–9.332555	–1.054757	0.412914
48	6	0	–7.943149	–1.081811	0.346943
49	1	0	12.501702	0.916365	1.116953

SCF Done: E(RB3LYP) = –1575.37573672 a.u.
Imaginary frequency number: 0

HOMO (–5.59 eV)

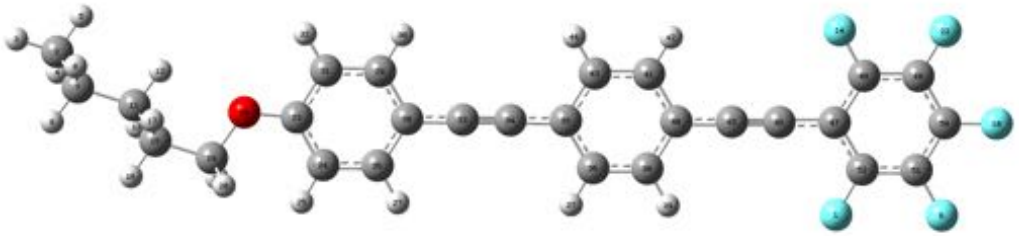


LUMO (–2.17 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

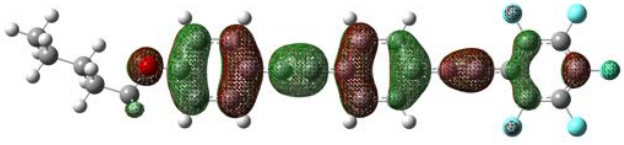
Cartesian coordinates for dissymmetric bistolane **2eC**[a]



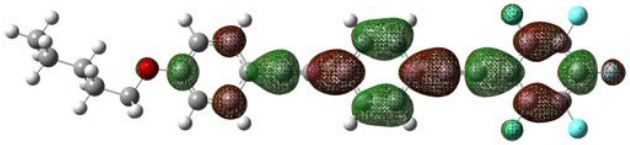
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	–6.967397	–2.240303	0.671119
2	6	0	12.848657	1.162088	2.252950
3	1	0	13.624610	1.725193	2.203962
4	1	0	13.068556	0.360209	2.734429
5	1	0	12.143834	1.624702	2.709605
6	9	0	–9.617089	–1.905150	0.929248
7	6	0	12.400921	0.806466	0.872419
8	1	0	12.388262	1.612509	0.332956
9	1	0	13.049073	0.202063	0.479628
10	9	0	–10.735930	0.506847	0.427325
11	6	0	11.052599	0.168106	0.815499
12	1	0	10.394377	0.797542	1.151054
13	1	0	11.045852	–0.604197	1.401298
14	9	0	–6.518621	2.278594	–0.528866
15	6	0	10.650478	–0.268643	–0.576289
16	1	0	11.280255	–0.937138	–0.888281
17	1	0	10.711189	0.492974	–1.172797
18	8	0	8.349155	0.249450	–0.477688
19	6	0	9.248574	–0.843403	–0.656382
20	1	0	9.104872	–1.263283	–1.517872
21	1	0	9.116564	–1.508695	0.038935
22	9	0	–9.170650	2.588551	–0.292108
23	6	0	7.012748	–0.009166	–0.536839
24	6	0	6.437985	–1.259744	–0.691394
25	1	0	6.976020	–2.012223	–0.795098
26	6	0	5.051126	–1.382366	–0.688898
27	1	0	4.667946	–2.222068	–0.800118
28	6	0	4.225409	–0.276058	–0.526966
29	6	0	4.836935	0.981298	–0.402436
30	1	0	4.304666	1.741640	–0.324402
31	6	0	6.201444	1.112496	–0.396691
32	1	0	6.586412	1.953803	–0.300003
33	6	0	2.800977	–0.384237	–0.480022
34	6	0	1.609287	–0.416532	–0.419733
35	6	0	0.175917	–0.418422	–0.333394
36	6	0	–0.563945	–1.590520	–0.308388
37	1	0	–0.128652	–2.408581	–0.361723
38	6	0	–1.944224	–1.559087	–0.208605
39	1	0	–2.422167	–2.355911	–0.175654
40	6	0	–2.621493	–0.345233	–0.154835
41	6	0	–1.877491	0.837066	–0.189421
42	1	0	–2.317690	1.655624	–0.158034
43	6	0	–0.500533	0.807764	–0.267911
44	1	0	–0.019667	1.604576	–0.278003
45	6	0	–4.054441	–0.266687	–0.064174
46	6	0	–5.234355	–0.163835	–0.000591
47	6	0	–6.653575	0.007916	0.071568
48	6	0	–7.263155	1.227910	–0.166544
49	6	0	–8.622413	1.407663	–0.065690
50	6	0	–9.420849	0.336657	0.292091
51	6	0	–8.851916	–0.882036	0.529887
52	6	0	–7.491398	–1.041325	0.414314

SCF Done: E(RB3LYP) = –1614.69030462 a.u.
Imaginary frequency number: 0

HOMO (–5.59 eV)

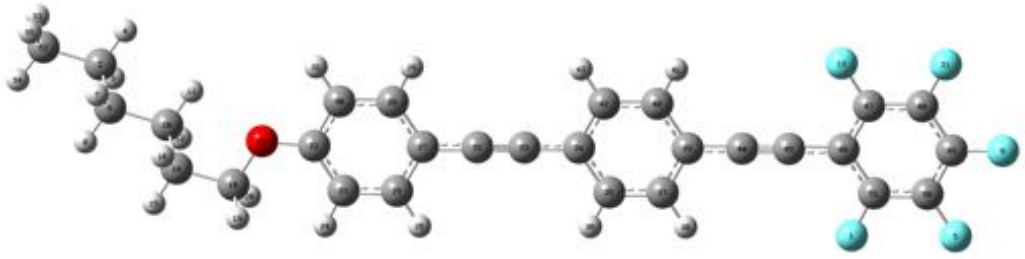


LUMO (–2.17 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theory.

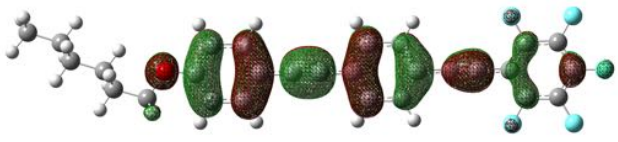
Cartesian coordinates for dissymmetric bistolane **2fC**[a]



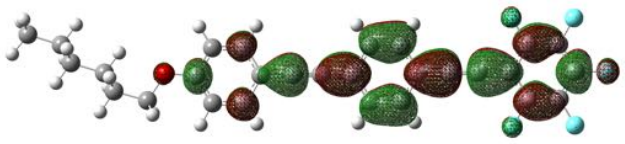
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-7.329416	-2.250419	0.491204
2	6	0	12.640925	1.256864	1.418714
3	1	0	12.554518	0.788043	2.413849
4	1	0	12.050247	2.188417	1.441062
5	9	0	-10.036867	-2.161373	0.618310
6	6	0	12.148187	0.316158	0.316836
7	1	0	12.283568	0.798733	-0.668714
8	1	0	12.777651	-0.593040	0.297211
9	9	0	-11.342224	0.213644	0.298241
10	6	0	10.679238	-0.086281	0.480847
11	1	0	10.046712	0.817988	0.493945
12	1	0	10.539863	-0.573246	1.464982
13	9	0	-7.223062	2.429594	-0.277926
14	6	0	10.181233	-1.026384	-0.621711
15	1	0	10.773212	-1.959185	-0.619380
16	1	0	10.332479	-0.560858	-1.611693
17	8	0	7.933624	-0.221574	-0.645562
18	6	0	8.714952	-1.410984	-0.490475
19	1	0	8.430536	-2.144684	-1.266493
20	1	0	8.513237	-1.862175	0.499444
21	9	0	-9.930945	2.505325	-0.149255
22	6	0	6.579825	-0.300327	-0.559487
23	6	0	5.857380	-1.481708	-0.325366
24	1	0	6.367791	-2.435112	-0.194774
25	6	0	4.464346	-1.441580	-0.257868
26	1	0	3.908904	-2.363130	-0.075544
27	6	0	3.757070	-0.234822	-0.419944
28	6	0	4.500945	0.945773	-0.655150
29	1	0	3.972047	1.891587	-0.783987
30	6	0	5.885170	0.912895	-0.723524
31	1	0	6.463676	1.820093	-0.905575
32	6	0	2.334176	-0.200811	-0.350084
33	6	0	1.113784	-0.166117	-0.291432
34	6	0	-0.307657	-0.123717	-0.223551
35	6	0	-1.057664	-1.300895	0.000682
36	1	0	-0.532900	-2.249683	0.122430
37	6	0	-2.444119	-1.259343	0.066867
38	1	0	-3.012658	-2.174361	0.240522
39	6	0	-3.135783	-0.037627	-0.088876
40	6	0	-2.389150	1.140310	-0.312996
41	1	0	-2.915062	2.088612	-0.434646
42	6	0	-1.002782	1.097507	-0.378979
43	1	0	-0.435381	2.013069	-0.552689
44	6	0	-4.557105	0.005842	-0.021511
45	6	0	-5.775328	0.043628	0.035960
46	6	0	-7.191265	0.086989	0.102766
47	6	0	-7.896268	1.295373	-0.057572
48	6	0	-9.285160	1.344209	0.006862
49	6	0	-10.009246	0.172831	0.235687
50	6	0	-9.339428	-1.041065	0.398869
51	6	0	-7.950243	-1.076725	0.332109
52	6	0	14.117044	1.644581	1.212926
53	1	0	14.428095	2.296152	2.002611
54	1	0	14.721907	0.761974	1.219643
55	1	0	14.226744	2.145004	0.273542

SCF Done E(RB3LLYP) = –1654.00485480 a.u.
Imaginary frequency number: 0

HOMO (–5.59 eV)



LUMO (–2.17 eV)



[a] Computation was conducted by using Gaussian 09 (rev. D01) with B3LYP/cc-pVDZ levels of theor