

# ***Supporting Information***

## **Development of fluorinated benzils and bisbenzils as room-temperature phosphorescent molecules**

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### **Contents**

1. Experimental procedure	..... S-2
2. NMR spectra	..... S-6
3. Cartesian coordinates	..... S-15

## 1. Experimental procedure

### 1-1. General

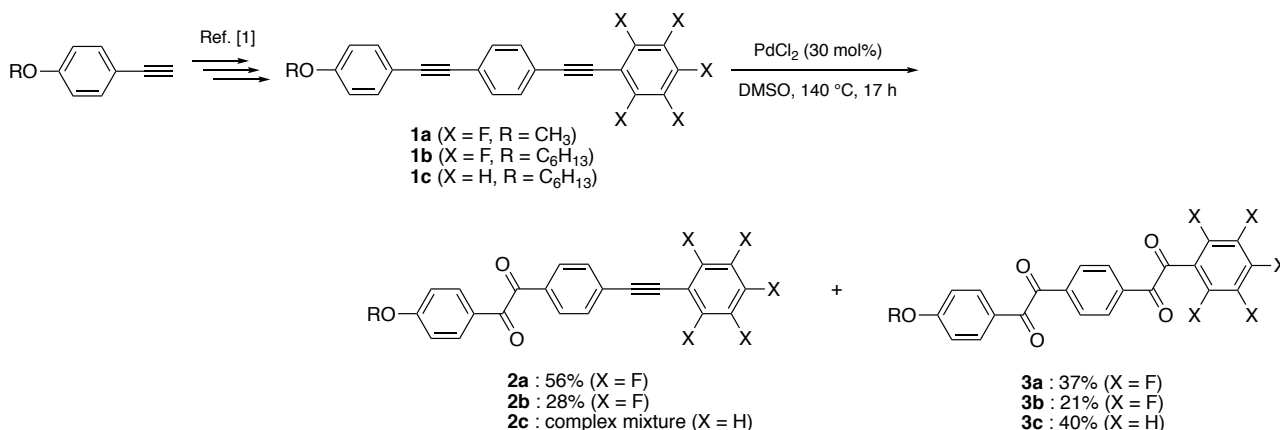
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were obtained with a Bruker AVANCE III 400 NMR spectrometer ( $^1\text{H}$ : 400 MHz and  $^{13}\text{C}$ : 100 MHz) in chloroform-*d* ( $\text{CDCl}_3$ ) solution and the chemical shifts are reported in parts per million (ppm) using the residual proton in the NMR solvent.  $^{19}\text{F}$  NMR (376 MHz) spectra were obtained with a Bruker AVANCE III 400 NMR spectrometer in  $\text{CDCl}_3$  solution with  $\text{CFCl}_3$  ( $\delta_{\text{F}} = 0$  ppm) as an internal standard. Infrared spectra (IR) were recorded in a KBr method with a JASCO FT/IR-4100 type A spectrometer; all spectra were reported in wavenumber ( $\text{cm}^{-1}$ ). High resolution mass spectra (HRMS) were recorded on a JEOL JMS700MS spectrometer using fast atom bombardment (FAB) methods. All chemicals including solvent were of reagent grade and where necessary were purified in the usual manner prior to use. Column chromatography was carried out on silica gel (Wakogel® 60N, 38–100  $\mu\text{m}$ ) and thin-layer chromatography (TLC) analysis was performed on silica gel TLC plates (Merck, Silica gel 60F<sub>254</sub>).

### 1-2. Photophysical properties

UV-vis absorption spectra were recorded on a JASCO V-500 absorption spectrometer. Samples for the absorption measurements were prepared by dissolving the pristine powder solid sample of **2** and **3** in toluene to a concentration of  $1.0 \times 10^{-5}$  M, and the solution was transferred into quartz cuvettes with an optical path length 1.0 cm. The steady-state PL spectra and quantum yields in solution, and pristine powder solid states were acquired using a JASCO FP-6600 fluorescence spectrometer and an absolute PL quantum yield measurement system (Hamamatsu Photonics, C11347-01). A solution-phase sample with a concentration of  $1.0 \times 10^{-3}$  mol L<sup>-1</sup> was used for PL measurements using quartz cuvettes (1.0 cm path length). The excitation wavelength ( $\lambda_{\text{ex}}$ ) corresponded to the maximum absorption wavelength.

### 1-3. Synthesis

Pentafluorinated benzils **2a** and **2b** and bisbenzils **3a** and **3b** were synthesized from the corresponding pentafluorinated bistolanenes **1a** and **1b**, which were prepared according to the reported procedure [1] (Scheme S1). The non-fluorinated bisbenzil **3c** was also prepared from the corresponding **1c** in a similar manner.



**Scheme S1.** Synthetic pathway for benzils **2a**, **2b** and bisbenzils **3a–c**.

#### Typical procedure for PdCl<sub>2</sub>-catalyzed DMSO-oxidation of bistolane 1

In a two-necked round-bottomed flask equipped with a teflon®-coated magnetic stirrer bar were placed pentafluorinated bistolane (**1a**, 0.47 g, 1.2 mmol), freshly prepared according to our previous reports [1], in dimethyl sulfoxide (DMSO, 12 mL). To the solution was added PdCl<sub>2</sub> (63 mg, 1.2 mmol) at room temperature, and the whole was heated at 140 °C for 17 h. The resultant was poured into H<sub>2</sub>O (30 mL), and extracted with diethyl ether (30 mL, three times). The combined extracts were washed with H<sub>2</sub>O (20 mL), brine (20 mL) and dried over anhydrous sodium sulfate (Na<sub>2</sub>SO<sub>4</sub>), filtered and concentrated under reduced pressure using a rotary evaporator. The residue was purified by silica gel column chromatography (eluent: hexane/EtOAc = 10/1 → 5/1), followed by recrystallization from hexane, providing the corresponding benzil (**2a**, 0.29 g, 0.67 mmol) in 56% yield as a white solid and bisbenzil (**3a**, 0.20 g, 0.44 mmol) in 37% yield as a white solid.

#### 1-(4-Methoxyphenyl)-2-[3-{2-(2,3,4,5,6-pentafluorophenyl)ethyn-1-yl}phenyl]-1,2-ethanedione (**2a**)

Yield: 56% (White solid); R<sub>f</sub> = 0.42 (hexane/EtOAc = 5/1); M.p.: 138.2–139.4 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ 3.90 (s, 3H), 6.99 (d, *J* = 9.2 Hz, 2H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.95 (d, *J* = 9.2 Hz, 2H), 8.00 (d, *J* = 8.8 Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ 55.7, 77.0–77.5 (one carbon was overlapped with CDCl<sub>3</sub>), 99.6 (td, *J* = 18.9, 2.9 Hz), 100.0 (d, *J* = 2.9 Hz), 114.4, 125.9, 127.7, 129.8, 132.3, 132.5, 133.4, 136.0–139.2 (dm, *J* = 252.5 Hz), 140.4–143.8 (dm, *J* = 263.5 Hz), 145.8–148.7 (dm, *J* = 254.7 Hz), 165.2, 192.4, 193.6; <sup>19</sup>F NMR (CDCl<sub>3</sub>): δ –135.6 to –135.9 (m, 2F), –151.53 (t, *J* = 20.3 Hz, 1F), –161.6 to –161.9 (m, 2F); IR

[1] (a) Yamada, S.; Miyano, K.; Konno, T.; Agou, T.; Kubota, T.; Hosokai, T. *Org. Biomol. Chem.* **2017**, *15*, 5949; (b) Yamada, S.; Morita, M.; Konno, T. *J. Fluorine Chem.* **2017**, *202*, 54; (c) Yamada, S.; Morita, M.; Agou, T.; Kubota, T.; Ichikawa, T.; Konno, T. *Org. Biomol. Chem.* **2018**, *16*, 5609; (d) Yamada, S.; Miyano, K.; Agou, T.; Kubota, T.; Konno, T. *Crystals* **2019**, *9*, 195; (e) Morita, M.; Yamada, S.; Agou, T.; Kubota, T.; Konno, T. *Appl. Sci.* **2019**, *9*, 1905.

(KBr):  $\nu$  3075, 3016, 2971, 2845, 2360, 2345, 2225, 1678, 1600, 1522, 1504, 1266, 1168, 993  $\text{cm}^{-1}$ ; HRMS (FAB+)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>23</sub>H<sub>12</sub>F<sub>5</sub>O<sub>3</sub>: 431.0707, found 431.0709.

**1-(4-Hexyloxyphenyl)-2-[4-{2-(2,3,4,5,6-pentafluorophenyl)ethyn-1-yl}phenyl]-1,2-ethanedione (2b)**

Yield: 28% (Yellow solid); R<sub>f</sub> = 0.57 (hexane/EtOAc = 5/1); M.p.: 114.0–114.5 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  0.90 (t,  $J$  = 6.8 Hz, 3H), 1.30–1.38 (m, 4H), 1.46 (quin.,  $J$  = 8.0 Hz, 2H), 1.81 (quin.,  $J$  = 6.8 Hz, 2H), 4.04 (t,  $J$  = 6.8 Hz, 2H), 6.97 (d,  $J$  = 8.8 Hz, 2H), 7.69 (d,  $J$  = 8.8 Hz, 2H), 7.94 (d,  $J$  = 8.8 Hz, 2H), 7.99 (d,  $J$  = 8.8 Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  14.0, 22.5, 25.6, 28.9, 31.5, 68.6, 77.0–77.5 (one carbon was overlapped with CDCl<sub>3</sub>), 99.6 (td,  $J$  = 17.6, 2.9 Hz), 100.0 (d,  $J$  = 2.9 Hz), 114.9, 125.6, 127.7, 129.8, 132.3, 132.4, 133.4, 136.2–139.3 (dm,  $J$  = 250.1 Hz), 140.4–143.7 (dm,  $J$  = 262.6 Hz), 145.7–148.8 (dm,  $J$  = 254.5 Hz), 164.8, 192.4, 193.6; <sup>19</sup>F NMR (CDCl<sub>3</sub>):  $\delta$  –135.6 to –135.9 (m, 2F), –151.56 (t,  $J$  = 20.3 Hz, 1F), –161.6 to –161.9 (m, 2F); IR (KBr):  $\nu$  3073, 2937, 2857, 2364, 2329, 2217, 1670, 1600, 1522, 1502, 1261, 1170, 992  $\text{cm}^{-1}$ ; HRMS (FAB+)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>28</sub>H<sub>22</sub>F<sub>5</sub>O<sub>3</sub>: 501.1490, found 501.1491.

**1,1'-(1,4-phenylene)-2-(4-methoxyphenyl)-2'-(2,3,4,5,6-pentafluorophenyl)bis(1,2-ethanedione) (3a)**

Yield: 37% (Yellow solid); R<sub>f</sub> = 0.42 (hexane/EtOAc = 10/1); M.p.: 113.7–114.8 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  3.91 (s, 3H), 7.01 (d,  $J$  = 8.8 Hz, 2H), 7.97 (d,  $J$  = 8.8 Hz, 2H), 8.15 (ABq,  $J$  = 8.8 Hz, 2H), 8.17 (ABq,  $J$  = 8.8 Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  55.7, 114.5, 125.6, 128.8, 130.3, 130.7, 132.5, 135.0, 136.5–139.8 (dm,  $J$  = 247.2 Hz), 137.8, 143.2–146.3 (dm,  $J$  = 271.3 Hz), 144.5–148.0 (dm,  $J$  = 254.4 Hz), 165.4, 184.3, 187.8, 191.7, 193.3; <sup>19</sup>F NMR (CDCl<sub>3</sub>):  $\delta$  –137.8 to –138.0 (m, 2F), –143.97 (t,  $J$  = 20.7 Hz, 1F), –159.4 to –159.7 (m, 2F); IR (KBr):  $\nu$  3056, 2980, 2851, 1735, 1700, 1686, 1602, 1498, 1425, 1257, 1172, 1001, 888  $\text{cm}^{-1}$ ; HRMS (FAB+)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>28</sub>H<sub>22</sub>F<sub>5</sub>O<sub>5</sub>: 533.1388, found 533.1380.

**1,1'-(1,4-phenylene)-2-(4-hexyloxyphenyl)-2'-(2,3,4,5,6-pentafluorophenyl)bis(1,2-ethanedione) (3b)**

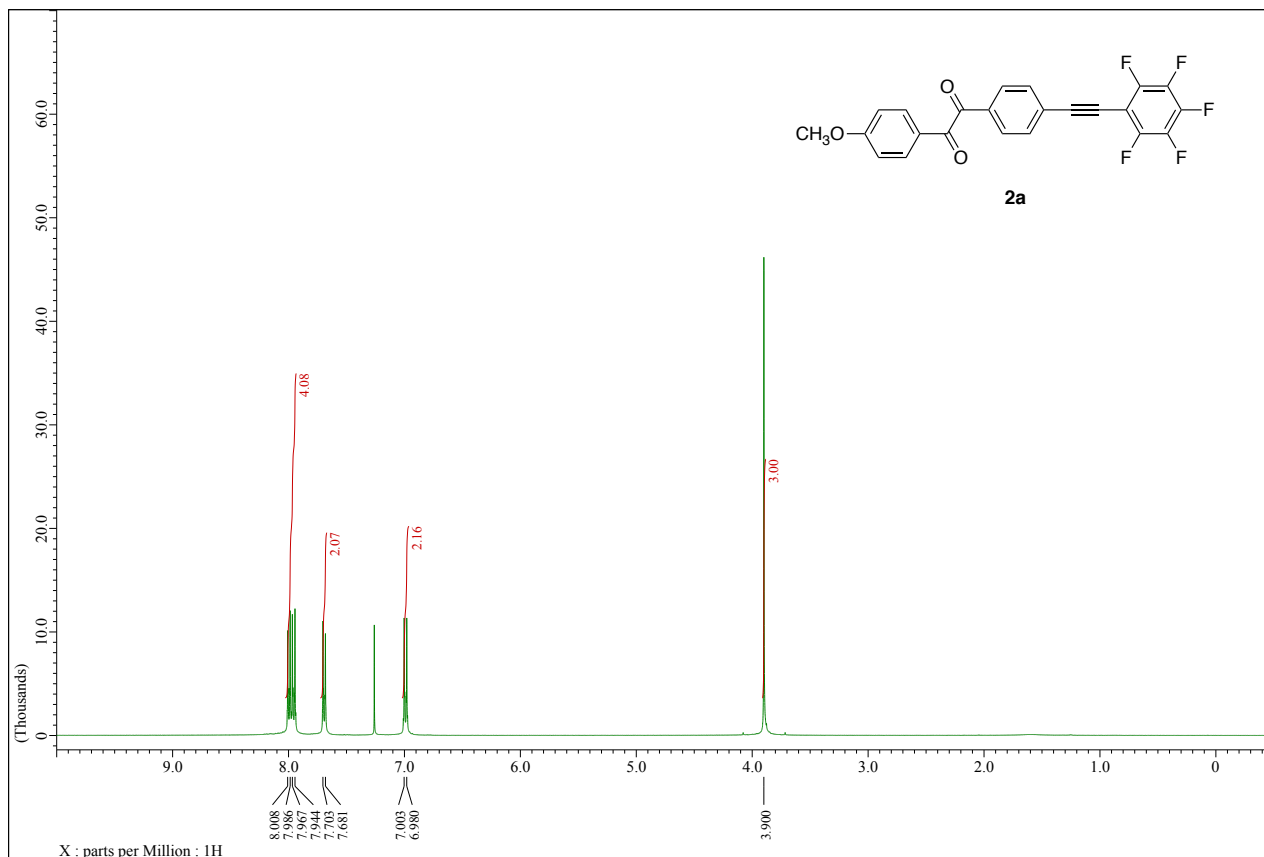
Yield: 21% (Yellow solid); R<sub>f</sub> = 0.34 (hexane/EtOAc = 10/1); M.p.: 94.3–95.9 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  0.91 (t,  $J$  = 6.4 Hz, 3H), 1.30–1.52 (m, 6H), 1.81 (quin.,  $J$  = 6.8 Hz, 2H), 4.05 (t,  $J$  = 6.8 Hz, 2H), 6.98 (d,  $J$  = 8.8 Hz, 2H), 7.94 (d,  $J$  = 8.8 Hz, 2H), 8.14 (ABq,  $J$  = 8.8 Hz, 2H), 8.17 (ABq,  $J$  = 8.8 Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  14.0, 22.5, 25.6, 28.9, 31.5, 68.6, 115.0, 125.4, 128.8, 130.3, 130.7, 132.5, 134.9, 136.2–139.3 (dm,  $J$  = 250.1 Hz), 137.8, 140.4–143.7 (dm,  $J$  = 262.6 Hz), 145.7–148.8 (dm,  $J$  = 254.5 Hz), 165.0, 184.4 (d,  $J$  = 11.1 Hz), 187.8, 191.8, 193.4, three sp<sup>2</sup> carbons attached with fluorine atom cannot be detected due to low solubility; <sup>19</sup>F NMR (CDCl<sub>3</sub>):  $\delta$  –137.8 to –138.0 (m, 2F), –143.97 (tt,  $J$  = 20.7, 5.6 Hz, 1F), –159.4 to –159.7 (m, 2F); IR (KBr):  $\nu$  3098, 2939, 2857, 1684, 1603, 1498, 1255, 1172, 991, 896  $\text{cm}^{-1}$ ; HRMS (FAB+)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>28</sub>H<sub>22</sub>F<sub>5</sub>O<sub>3</sub>: 501.1490, found 501.1491.

**1,1'-(1,4-phenylene)-2-(4-hexyloxyphenyl)-2'-phenylbis(1,2-ethanedione) (3c)**

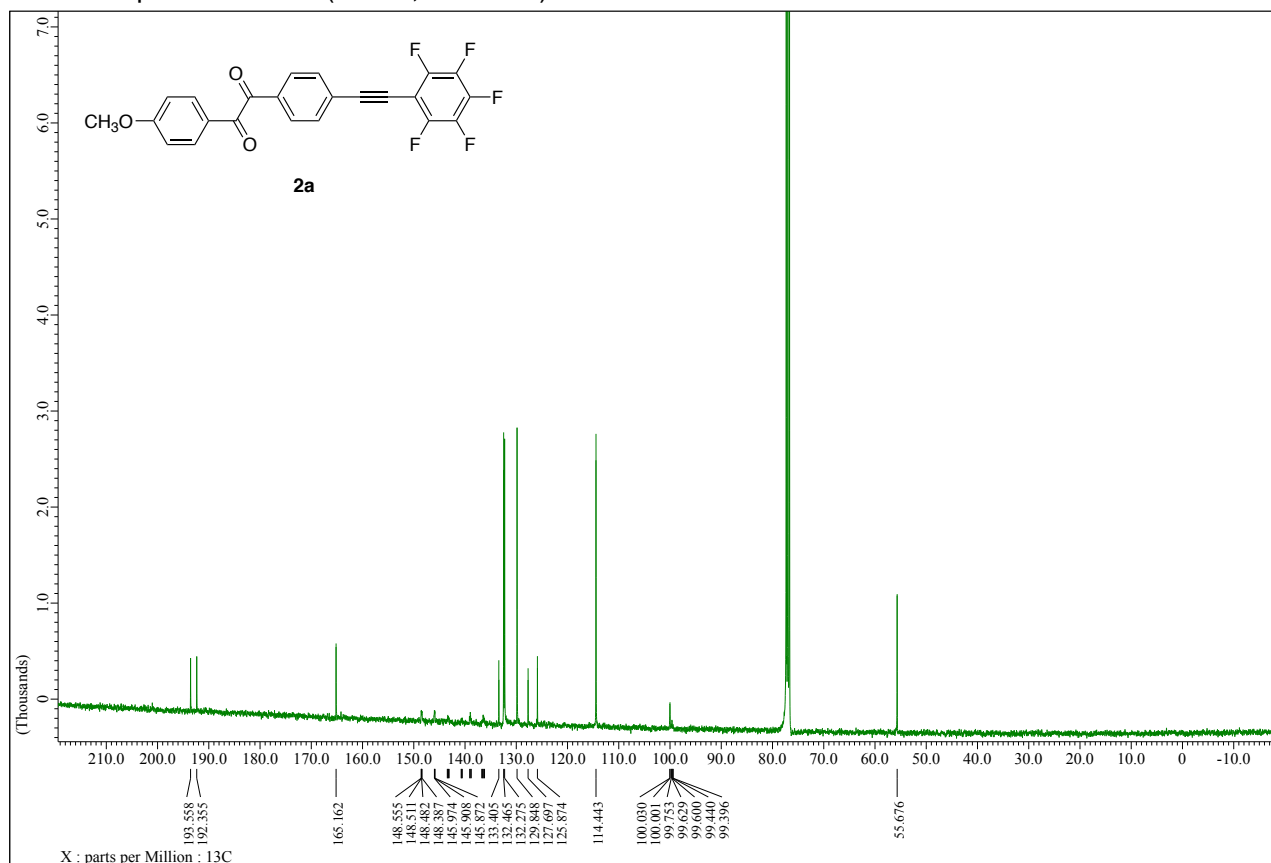
Yield: 40% (Yellow solid); R<sub>f</sub> = 0.45 (hexane/EtOAc = 5/1); M.p.: 115.6–116.8 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ 0.90 (t, *J* = 7.6 Hz, 3H), 1.30–1.37 (m, 4H), 1.46 (quin., *J* = 8.0 Hz, 2H), 1.80 (quin., *J* = 7.6 Hz, 2H), 4.04 (t, *J* = 6.4 Hz, 2H), 6.97 (d, *J* = 9.2 Hz, 2H), 7.53 (t, *J* = 8.0 Hz, 2H), 7.68 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.96 (dd, *J* = 8.4 Hz, 1.2 Hz, 2H), 8.10 (s, 4H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ 14.0, 22.5, 25.6, 28.9, 31.4, 68.6, 114.9, 125.3, 129.1, 129.9, 130.16, 130.22, 132.5, 132.6, 135.2, 136.9, 137.4, 164.9, 191.9, 193.3, 193.5, 193.6; IR (KBr): ν 3069, 2951, 2857, 2361, 2332, 1675, 1663, 1601, 1572, 1263, 1210, 1169, 887 cm<sup>-1</sup>; HRMS (FAB+) *m/z* [M+H]<sup>+</sup> calcd for C<sub>28</sub>H<sub>27</sub>O<sub>5</sub>: 443.1859, found 443.1869.

## 2. NMR spectra

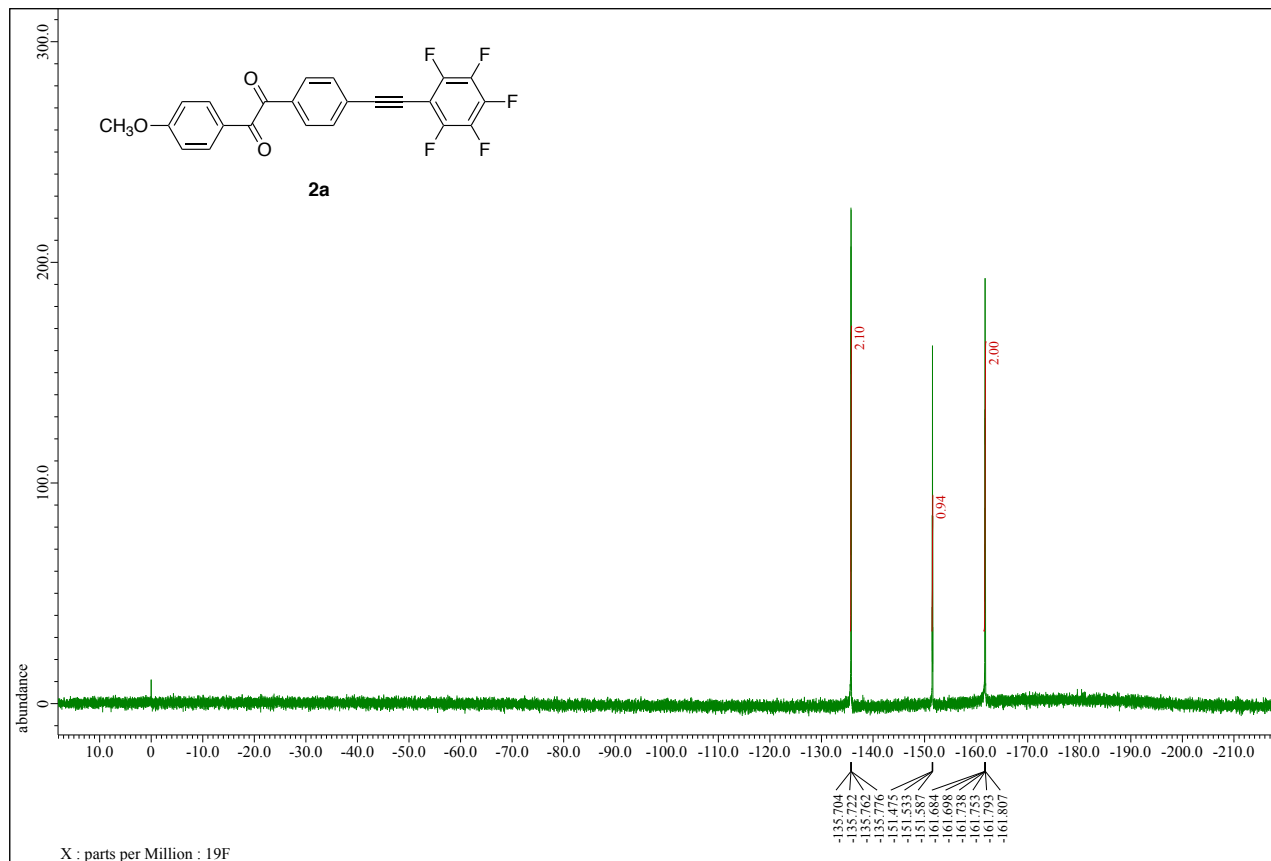
<sup>1</sup>H NMR spectrum for **2a** (CDCl<sub>3</sub>, 400 MHz)



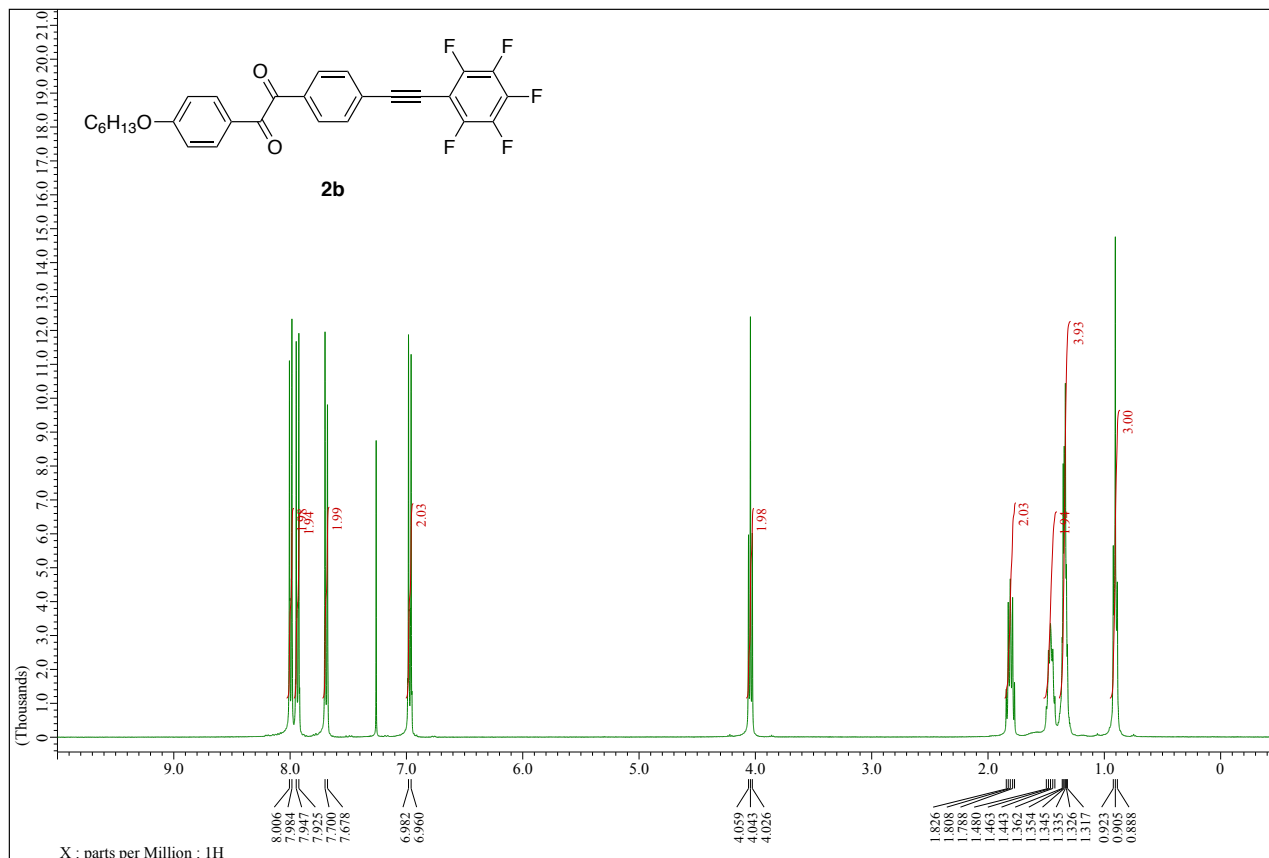
<sup>13</sup>C NMR spectrum for **2a** (CDCl<sub>3</sub>, 100 MHz)



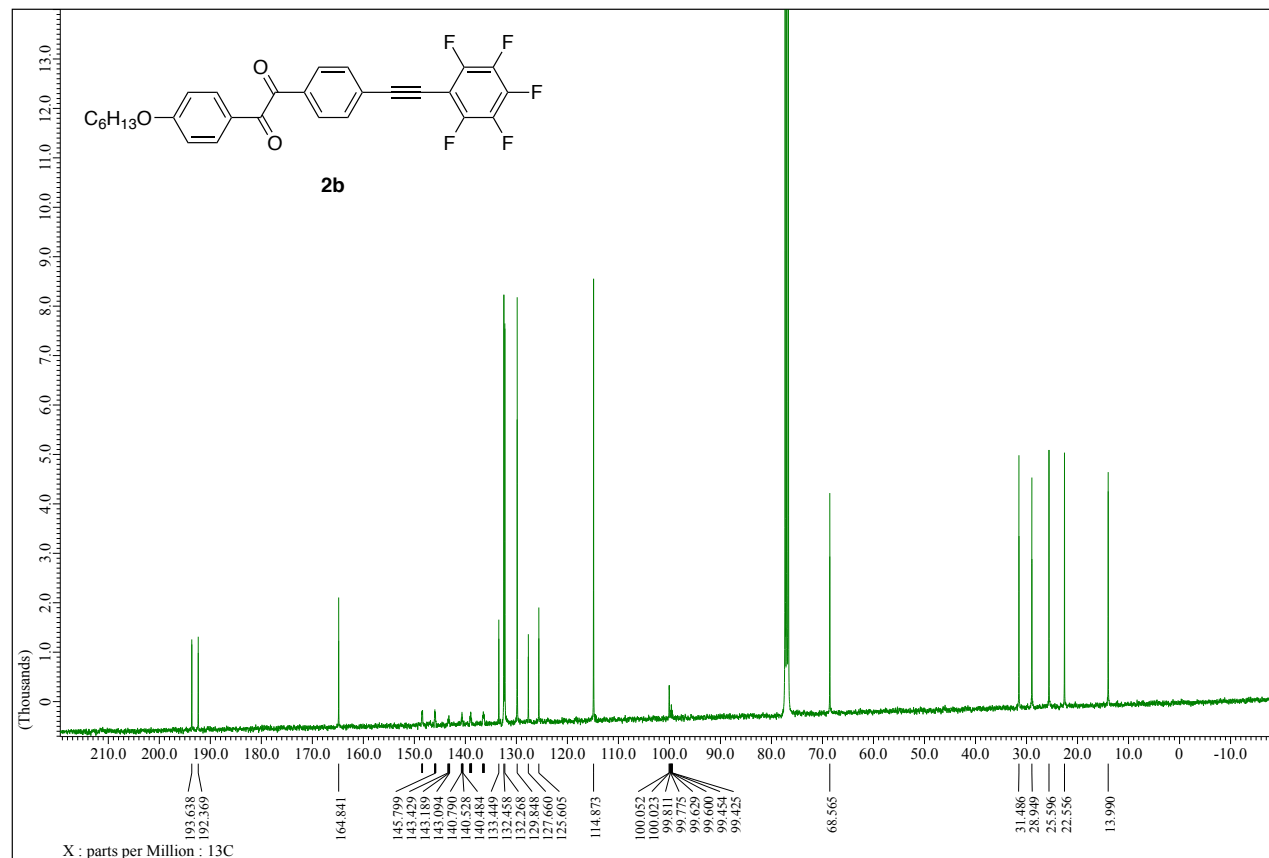
$^{19}\text{F}$  NMR spectrum for **2a** ( $\text{CDCl}_3$ , 376 MHz)



<sup>1</sup>H NMR spectrum for **2b** (CDCl<sub>3</sub>, 400 MHz)

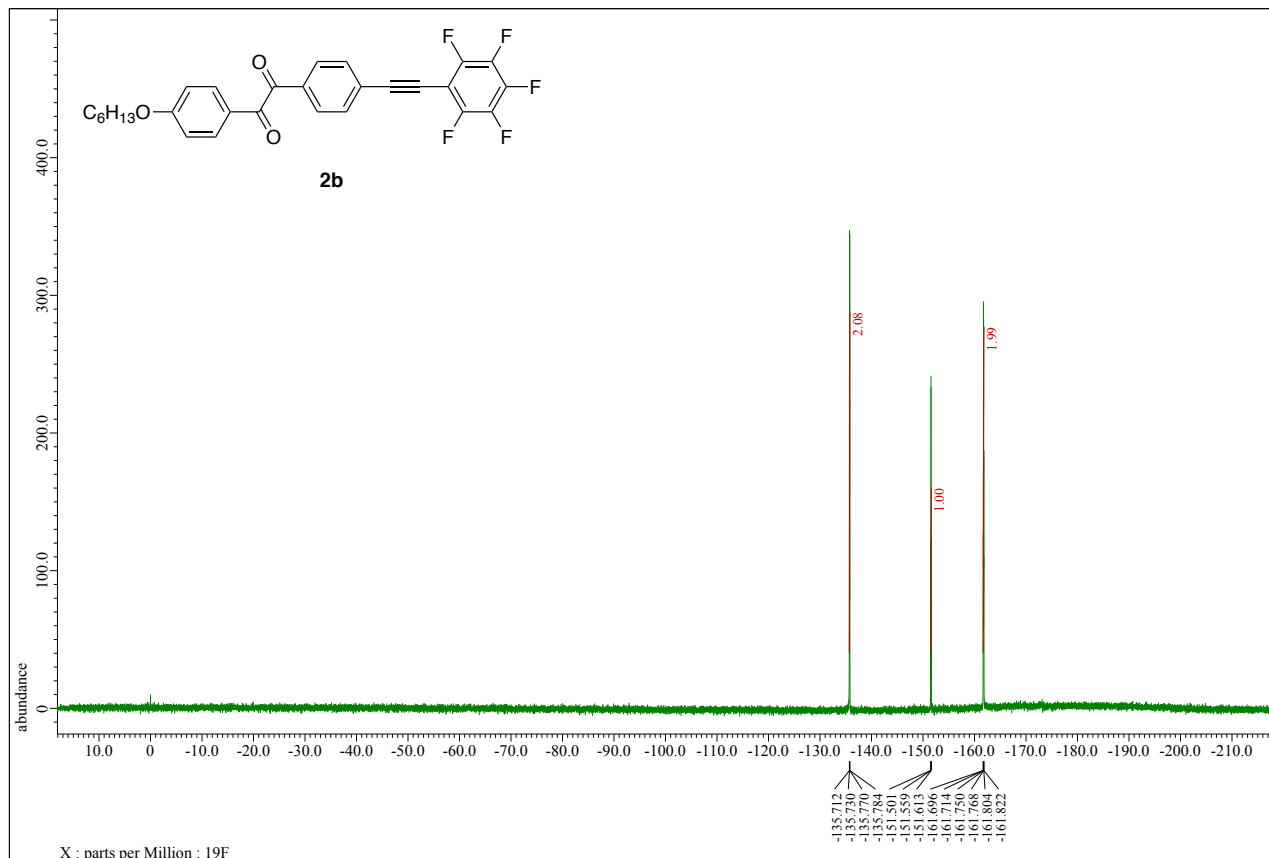


<sup>13</sup>C NMR spectrum for **2b** (CDCl<sub>3</sub>, 100 MHz)

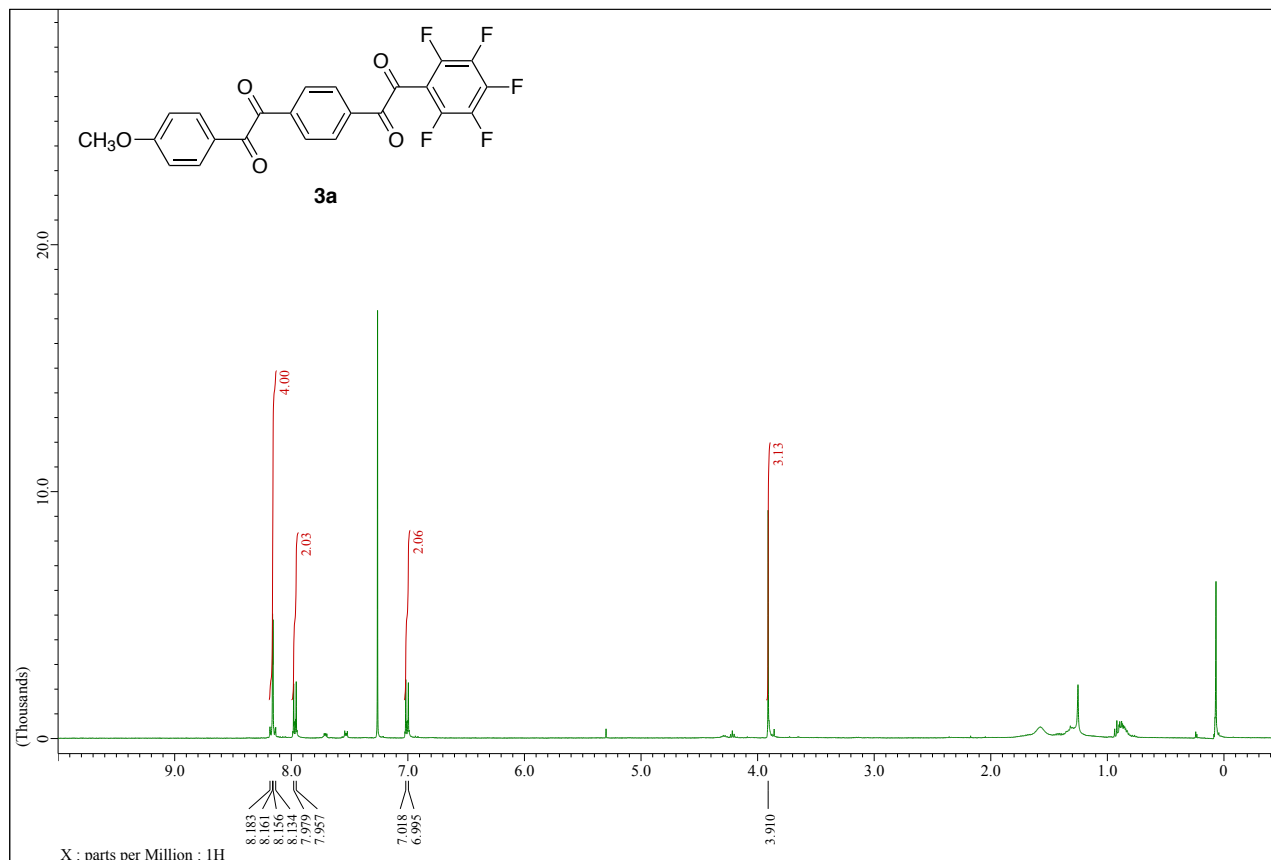




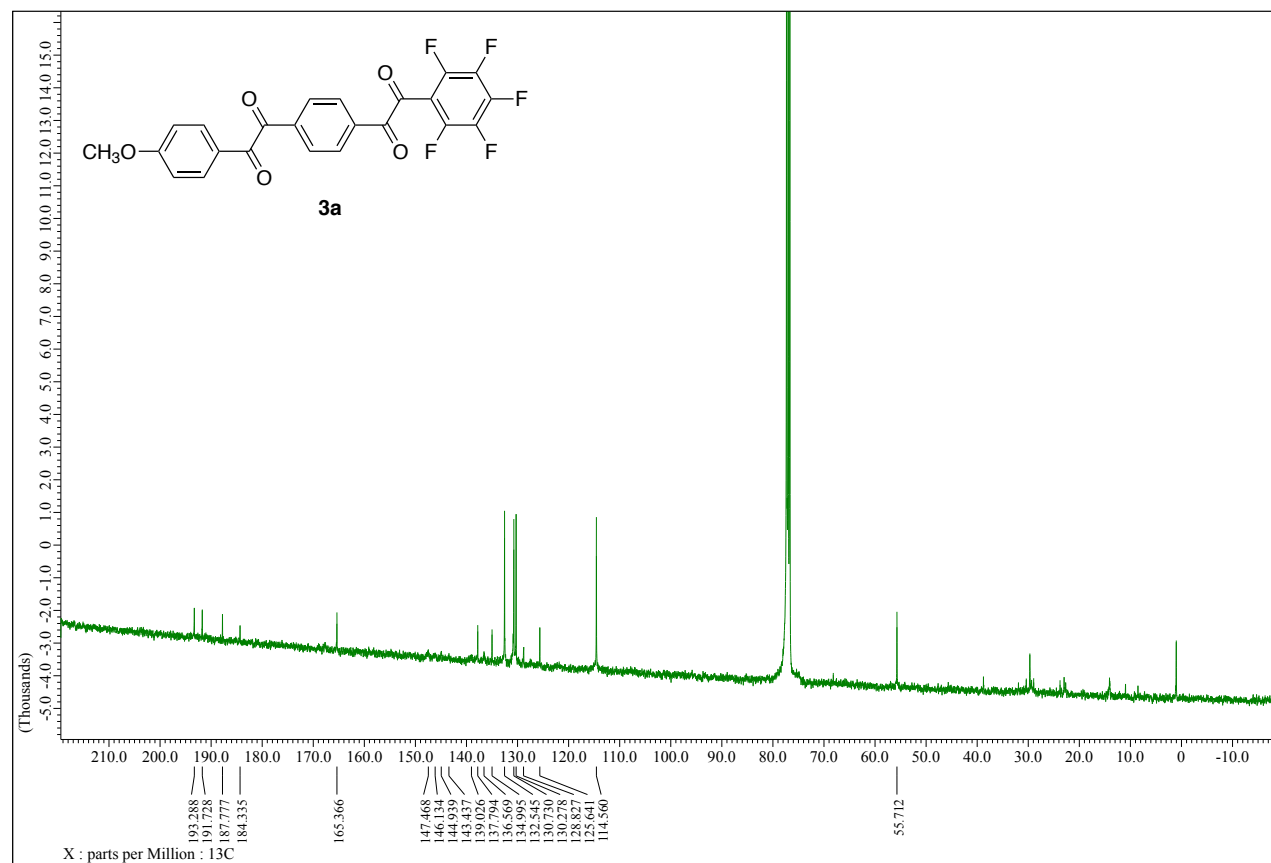
$^{19}\text{F}$  NMR spectrum for **2b** ( $\text{CDCl}_3$ , 376 MHz)



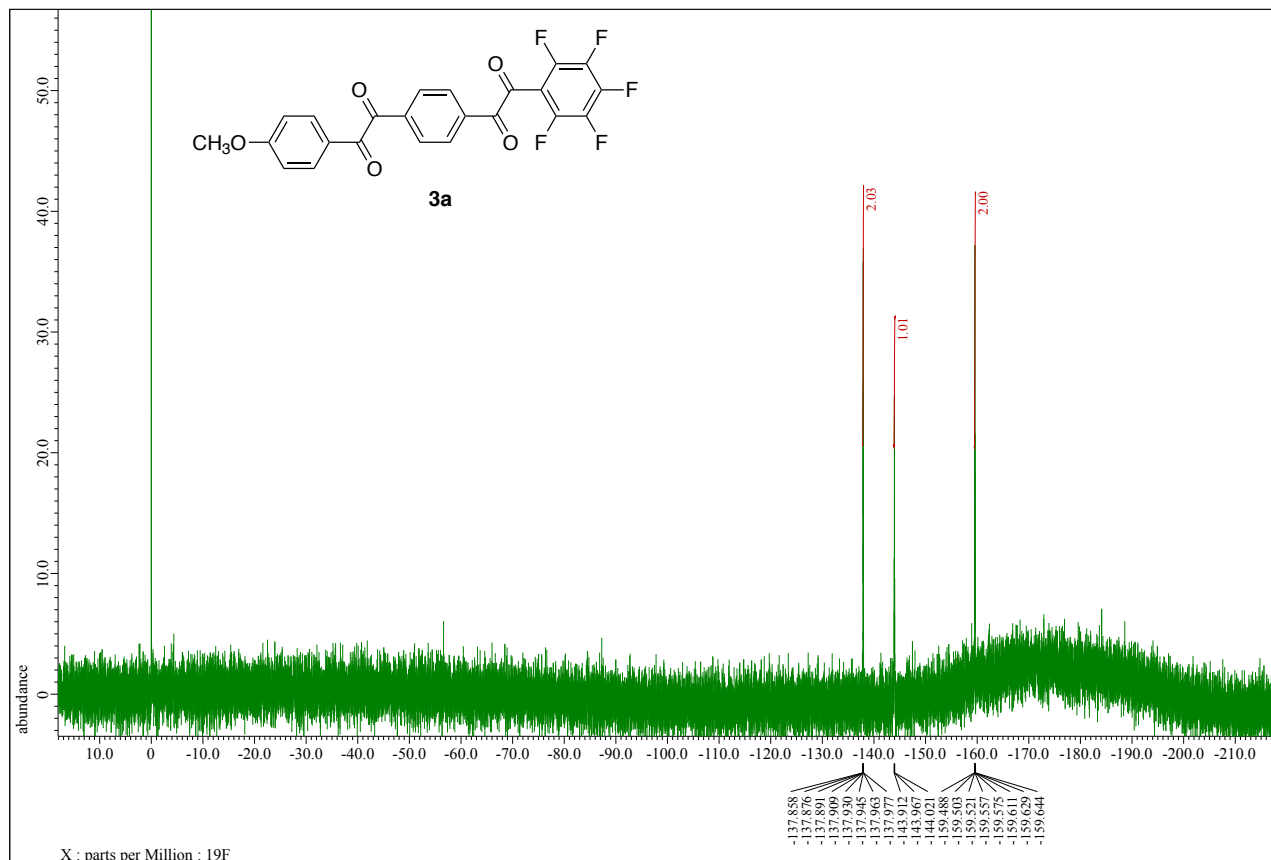
<sup>1</sup>H NMR spectrum for **3a** (CDCl<sub>3</sub>, 400 MHz)



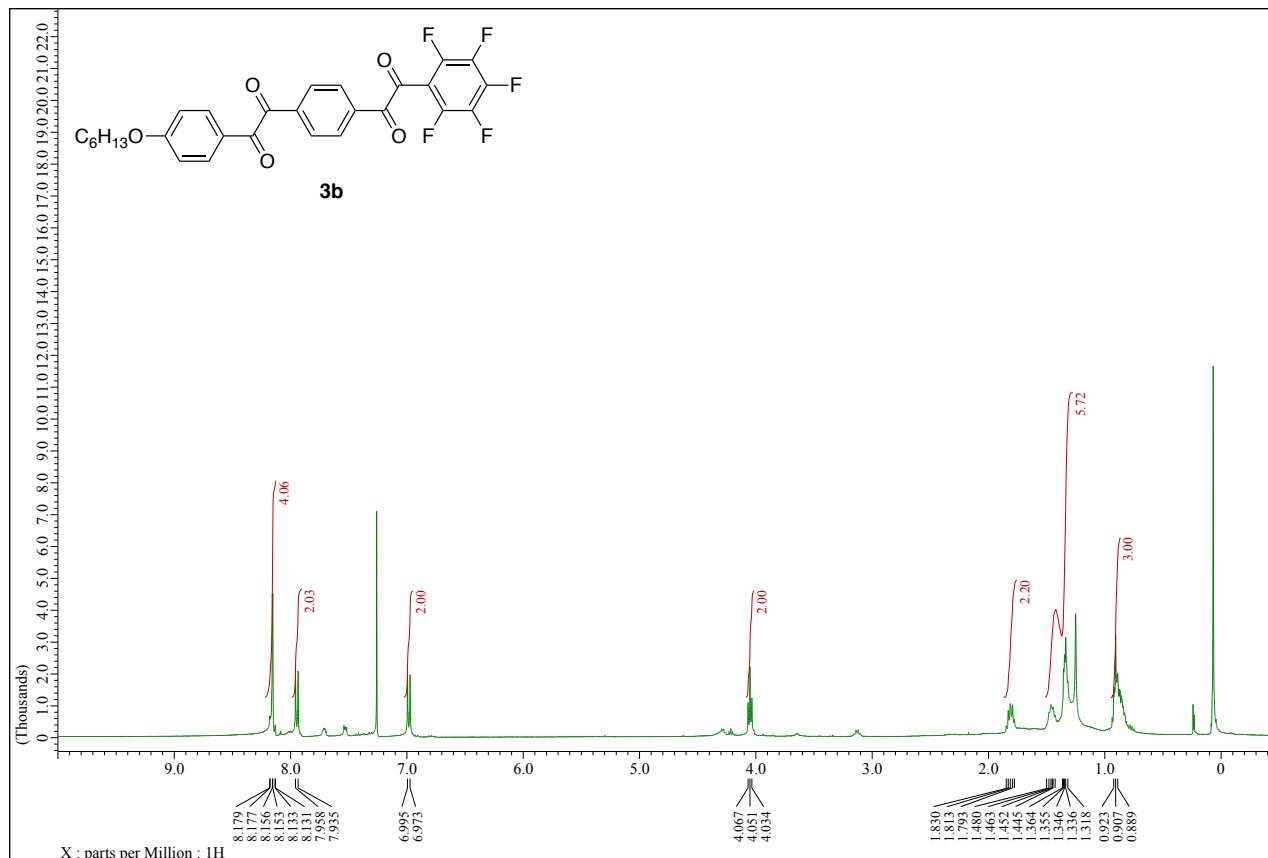
<sup>13</sup>C NMR spectrum for **3a** (CDCl<sub>3</sub>, 100 MHz)



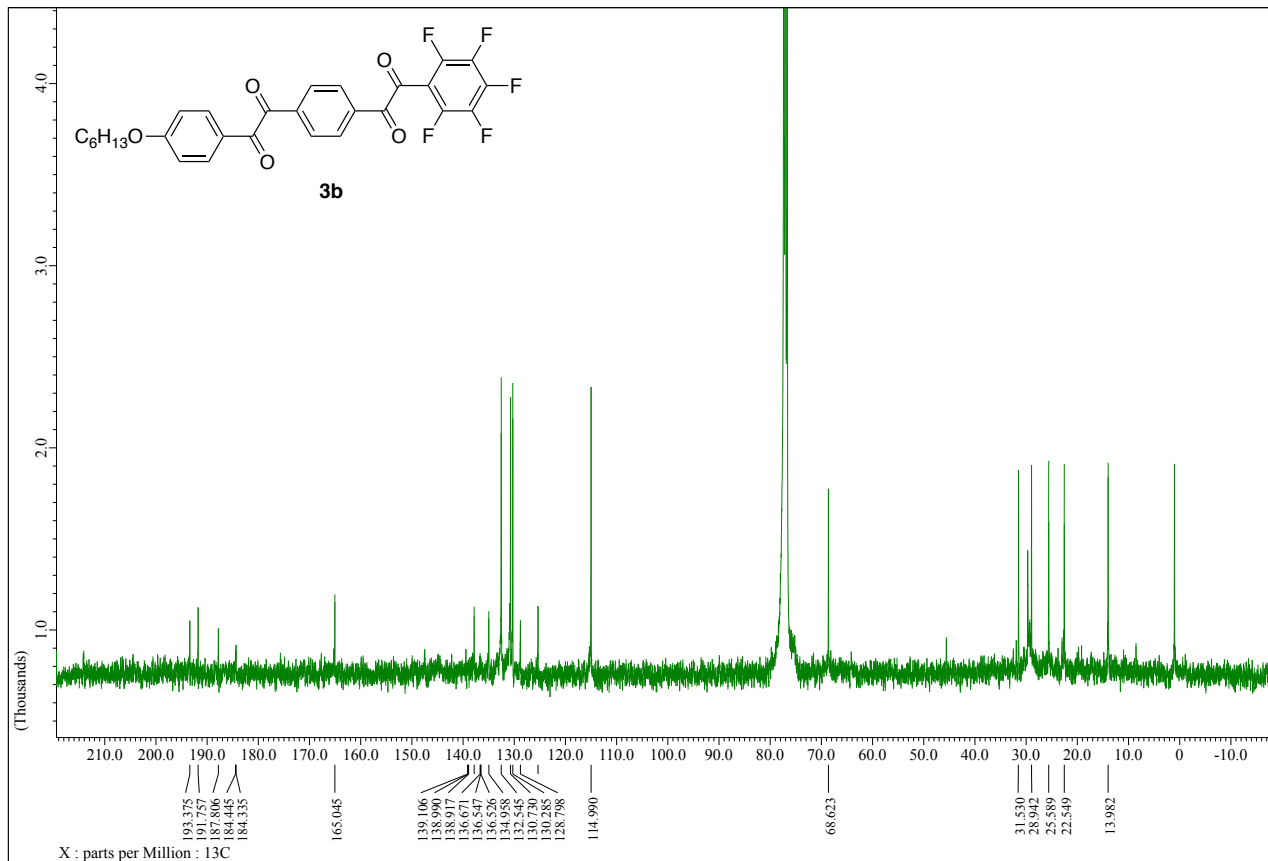
$^{19}\text{F}$  NMR spectrum for **3a** ( $\text{CDCl}_3$ , 376 MHz)



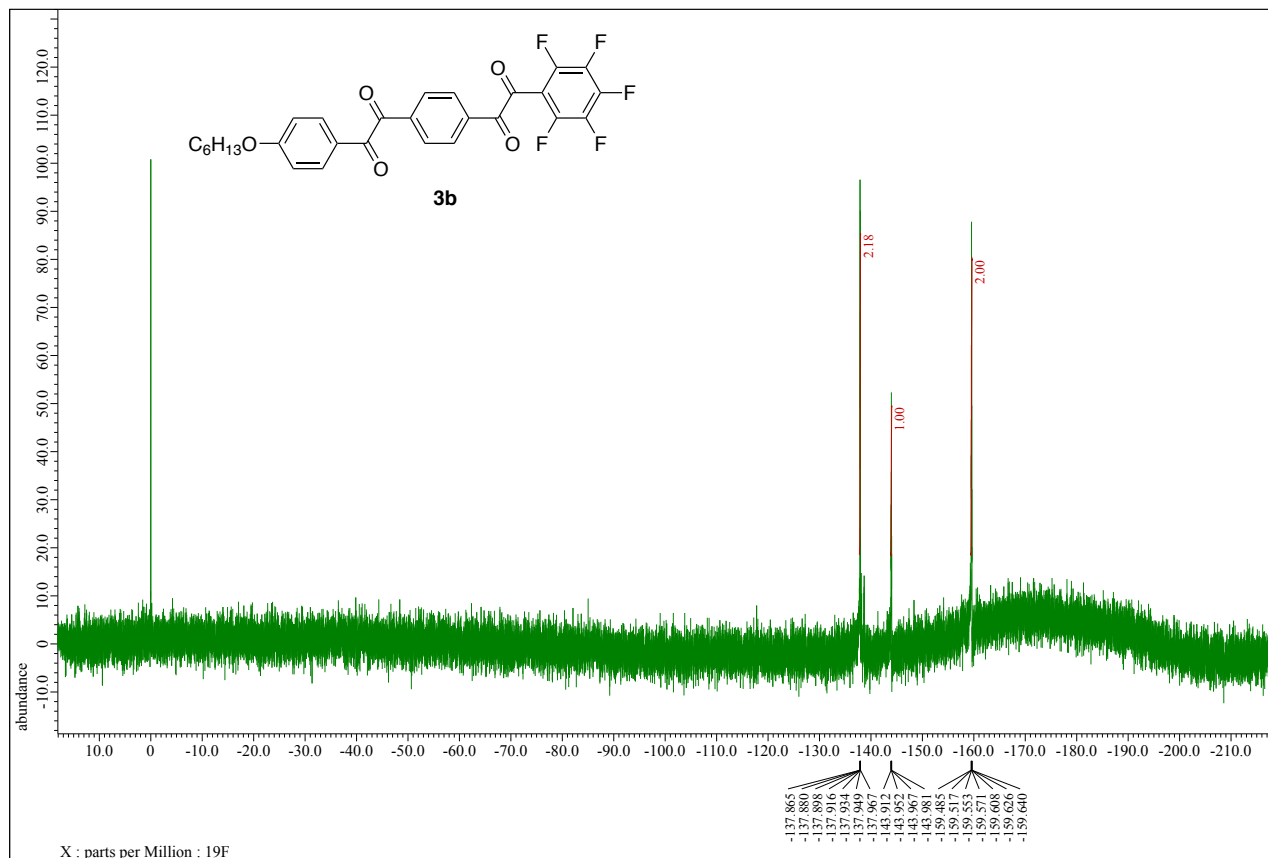
<sup>1</sup>H NMR spectrum for **3b** (CDCl<sub>3</sub>, 400 MHz)



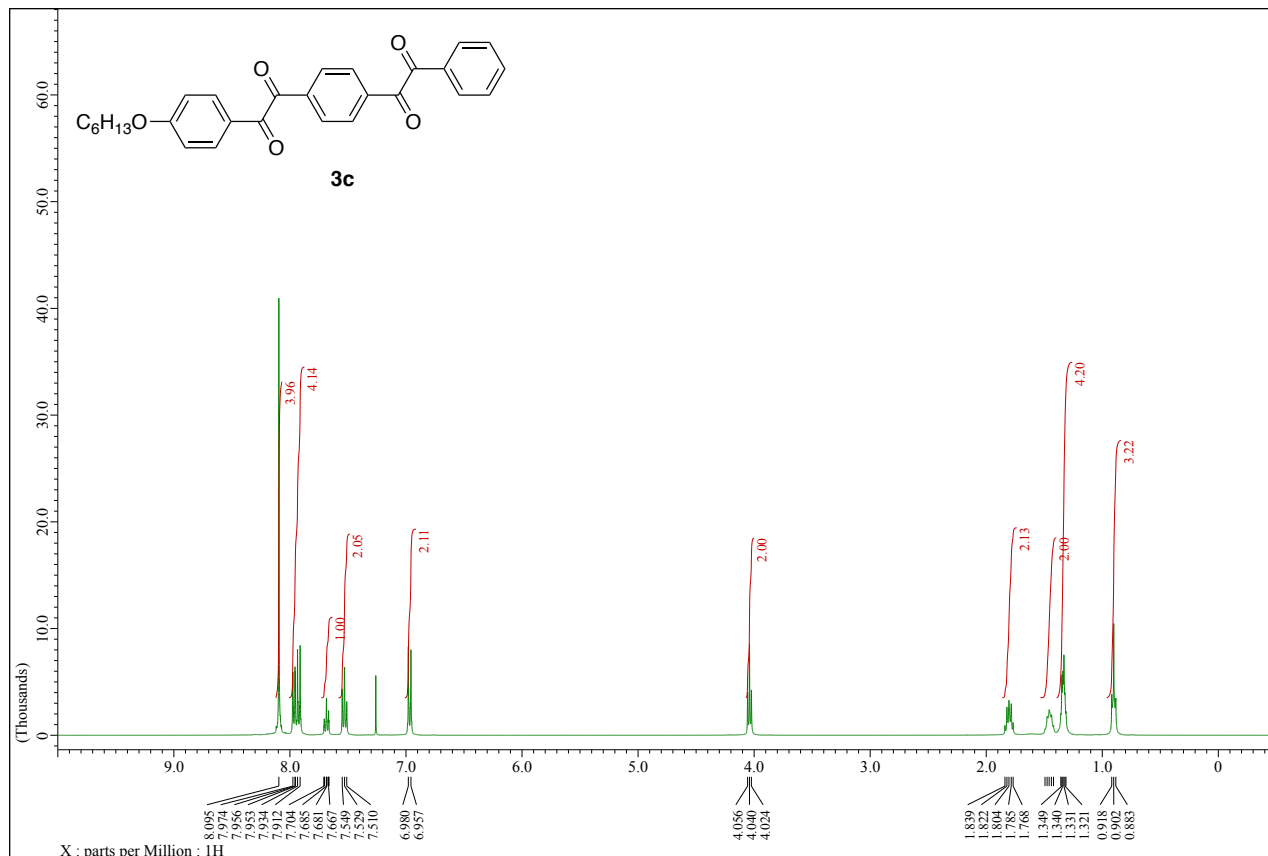
<sup>13</sup>C NMR spectrum for **3b** (CDCl<sub>3</sub>, 100 MHz)



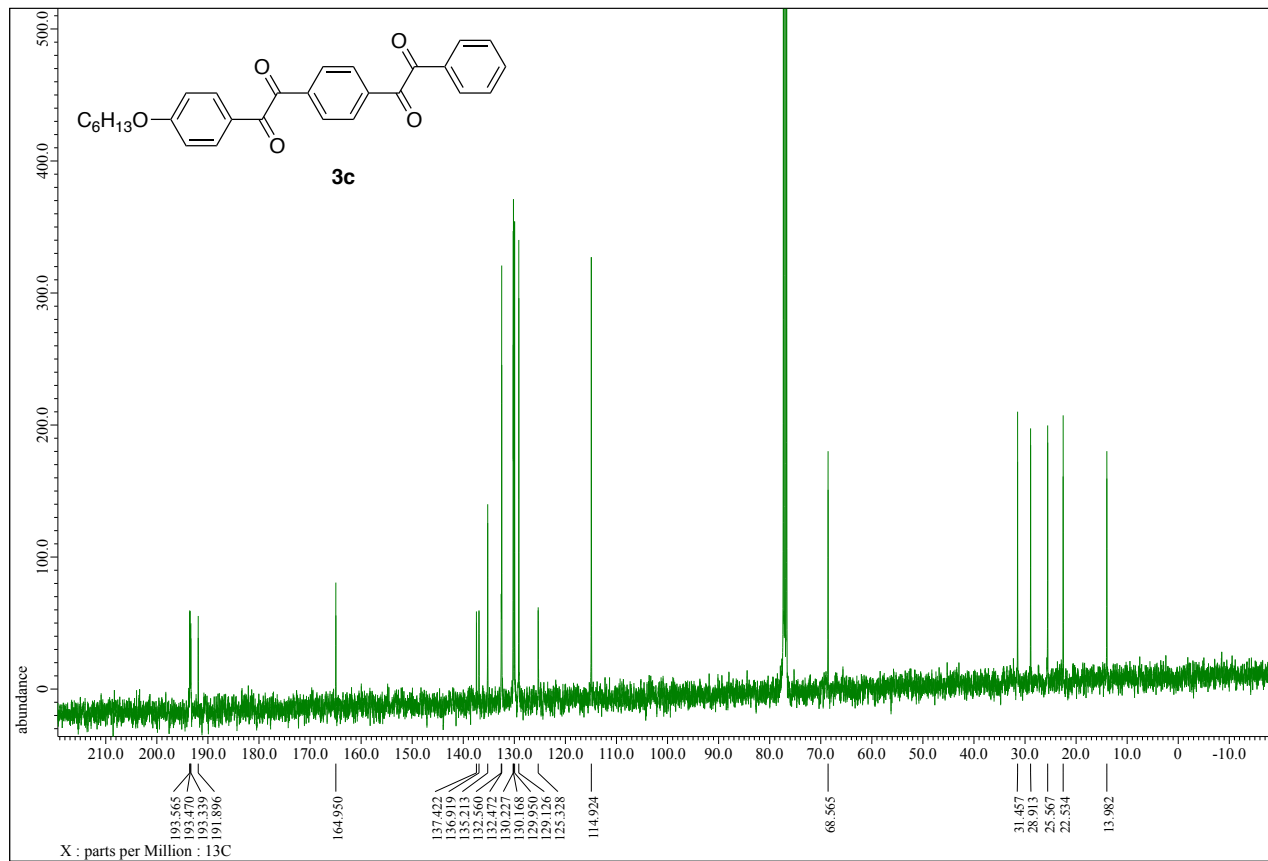
$^{19}\text{F}$  NMR spectrum for **3b** ( $\text{CDCl}_3$ , 376 MHz)



<sup>1</sup>H NMR spectrum for **3c** (CDCl<sub>3</sub>, 400 MHz)



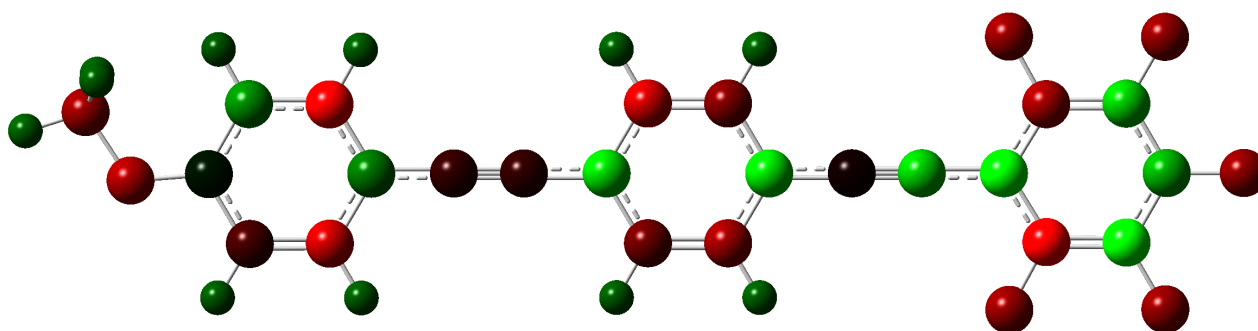
<sup>13</sup>C NMR spectrum for **3c** (CDCl<sub>3</sub>, 100 MHz)



### 3. Computation

All computations were performed by a density functional theory (DFT) using the Gaussian 16 (Rev. B.01) suite of programs. Geometry optimizations were executed at the CAM-B3LYP/6-31G(d) level of theory with the implicit solvation model, namely, the conductor-like polarizable continuum model (CPCM), for heptane. The vertical electronic transitions were calculated using a time-dependent (TD)-DFT method at the same level of theory.

### 3-1. Optimized structure (charge distribution) of 1a



SCF Done: E (RCAM-B3LYP) = -1456.76520762 hartree

Dipole moment (field-independent basis, Debye-Ang):

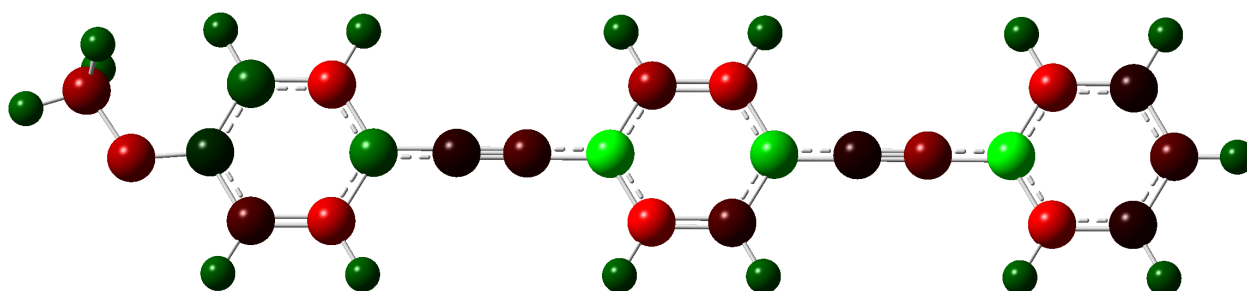
X = -4.9568, Y = 1.2690, Z = 0.0001, Tot = 5.1167

### 3-2. Cartesian coordinates

No.	Atom	Type	Coordinates (Angstroms)			20	6	0	0.037781	-1.25508	-0.000108
	No.		X	y	z						
1	6	0	-11.09	0.873484	0.000009	22	6	0	0.73295	-0.037224	0.000029
2	1	0	-10.9045	1.47744	0.895991	23	6	0	0.006753	1.1624	0.000186
3	1	0	-12.1259	0.534657	-0.000058	24	1	0	0.539664	2.10758	0.000301
4	1	0	-10.9044	1.47761	-0.895852	25	6	0	-1.37767	1.14371	0.000192
5	8	0	-10.299	-0.299563	-0.000073	26	1	0	-1.93413	2.07501	0.000314
6	6	0	-8.94753	-0.173342	-0.000049	27	6	0	-2.07656	-0.073287	0.000041
7	6	0	-8.22376	-1.37095	-0.000137	28	6	0	2.15988	-0.018659	0.000017
8	1	0	-8.77109	-2.30767	-0.000225	29	6	0	3.36832	-0.002205	0.000013
9	6	0	-6.84285	-1.34824	-0.000111	30	6	0	4.78789	0.017019	0.000002
10	1	0	-6.28671	-2.28009	-0.000185	31	6	0	5.53557	-1.16517	0.000052
11	6	0	-6.14231	-0.129029	0.000003	32	6	0	6.92003	-1.15512	0.000042
12	6	0	-6.8783	1.05909	0.0001	33	6	0	7.59898	0.05526	-0.000027
13	1	0	-6.35331	2.00894	0.000194	34	6	0	6.88737	1.24673	-0.000074
14	6	0	-8.26954	1.04603	0.000075	35	6	0	5.50315	1.2191	-0.000064
15	1	0	-8.80717	1.98632	0.000159	36	9	0	4.90939	-2.34385	0.000118
16	6	0	-4.71431	-0.107056	0.000031	37	9	0	7.60473	-2.30023	0.000093
17	6	0	-3.50376	-0.091643	0.000049	38	9	0	8.93022	0.073351	-0.000037
18	6	0	-1.3467	-1.27198	-0.000102	39	9	0	7.5407	2.41005	-0.000135
19	1	0	-1.87907	-2.21724	-0.000211	40	9	0	4.84515	2.38037	-0.000112



### 3-3. Optimized structure (charge distribution) of 1c



SCF Done: E (RCAM-B3LYP) = -960.681573201 hartree

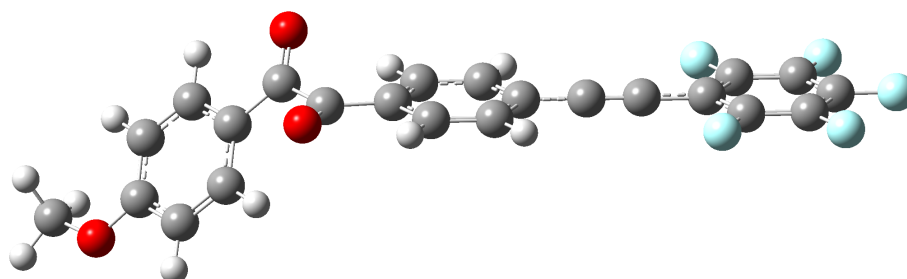
Dipole moment (field-independent basis, Debye-Ang):

X = 1.2195, Y = -1.3069, Z = 0.0007, Tot = 1.7875

### 3-4. Cartesian coordinates

No.	Atom No.	Type	Coordinates (Angstroms)								
			x	y	z						
						20	6	0	-1.71362	1.237	-0.000185
						21	1	0	-2.27185	2.1675	-0.000296
1	6	0	9.42305	-0.861537	0.000486	22	6	0	-2.41004	0.019411	-0.000021
2	1	0	9.23864	-1.46564	0.896729	23	6	0	-1.67617	-1.17598	0.000119
3	1	0	10.4586	-0.521509	0.00005	24	1	0	-2.20529	-2.12334	0.000252
4	1	0	9.23827	-1.46682	-0.894881	25	6	0	-0.291357	-1.15448	0.0001
5	8	0	8.63057	0.309972	-0.000127	26	1	0	0.266841	-2.08498	0.000207
6	6	0	7.27837	0.180508	-0.000069	27	6	0	0.405539	0.063136	-0.000065
7	6	0	6.55168	1.376	-0.001034	28	6	0	-3.83837	-0.002775	-0.000003
8	1	0	7.09649	2.31424	-0.001769	29	6	0	-5.04852	-0.02163	0.000011
9	6	0	5.17054	1.34986	-0.001039	30	6	0	-6.4785	-0.043963	0.000028
10	1	0	4.6122	2.2804	-0.001799	31	6	0	-7.20843	1.15328	0.001269
11	6	0	4.47232	0.129399	-0.000084	32	6	0	-8.5972	1.12791	0.001289
12	6	0	5.21173	-1.0565	0.000869	33	6	0	-9.27725	-0.087711	0.000071
13	1	0	4.6891	-2.00766	0.001617	34	6	0	-8.55955	-1.28148	-0.001169
14	6	0	6.60324	-1.04012	0.000887	35	6	0	-7.17066	-1.26342	-0.001195
15	1	0	7.14291	-1.97929	0.001664	36	1	0	-6.67571	2.09878	0.002219
16	6	0	3.04395	0.104069	-0.000089	37	1	0	-9.15149	2.06177	0.002261
17	6	0	1.83344	0.085372	-0.000087	38	1	0	-10.363	-0.104668	0.000089
18	6	0	-0.328792	1.25857	-0.000206	39	1	0	-9.08437	-2.23221	-0.002122
19	1	0	0.200247	2.20592	-0.000333	40	1	0	-6.60867	-2.19182	-0.002169

### 3-5. Optimized geometry of 2a



SCF Done: E (RCAM-B3LYP) = -1607.22472657 hartree

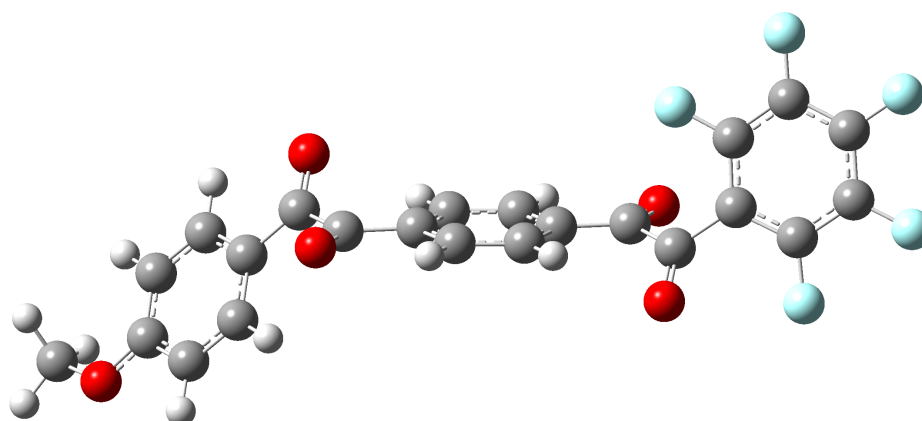
Dipole moment (field-independent basis, Debye-Ang):

X = -3.5454, Y = 2.5640, Z = -1.8632, Tot = 4.7556

### 3-6. Cartesian coordinates of 2a

No.	Atom No.	Type	Coordinates (Angstroms)								
			x	y	z						
						21	1	0	0.983298	-2.73583	-0.179698
						22	1	0	0.345439	1.36266	0.940614
1	6	0	-7.79207	0.664165	-0.994869	23	8	0	-4.0912	0.107549	2.34942
2	6	0	-6.90737	-0.291934	-1.50785	24	8	0	-3.80291	-2.59381	0.53562
3	6	0	-5.78984	-0.660464	-0.784976	25	8	0	-8.85667	0.957871	-1.77382
4	6	0	-5.5279	-0.081481	0.467166	26	6	0	-9.79951	1.91235	-1.31661
5	6	0	-6.41794	0.872884	0.966864	27	1	0	-9.33225	2.89364	-1.17722
6	6	0	-7.54476	1.24949	0.251881	28	1	0	-10.5567	1.97812	-2.0974
7	1	0	-7.12504	-0.733508	-2.47431	29	1	0	-10.2673	1.58831	-0.380287
8	1	0	-5.12542	-1.41617	-1.18747	30	6	0	2.21457	-0.395005	0.205293
9	1	0	-6.21086	1.31903	1.93411	31	6	0	3.39485	-0.173679	0.074391
10	1	0	-8.21739	1.9904	0.666081	32	6	0	4.78163	0.092074	-0.077609
11	6	0	-4.33521	-0.407147	1.26976	33	6	0	5.30998	1.36543	0.158716
12	6	0	-3.36131	-1.48477	0.775139	34	6	0	5.67901	-0.906616	-0.469528
13	6	0	-1.91294	-1.16366	0.666698	35	6	0	6.66031	1.63423	0.013795
14	6	0	-1.04407	-2.18769	0.27329	36	6	0	7.03212	-0.65435	-0.619128
15	6	0	-1.40528	0.116985	0.90568	37	6	0	7.52435	0.620533	-0.376503
16	6	0	0.308851	-1.94175	0.122795	38	9	0	4.50128	2.35751	0.534676
17	1	0	-1.45256	-3.17572	0.089802	39	9	0	7.13536	2.8585	0.246275
18	6	0	-0.050233	0.370268	0.752844	40	9	0	8.82336	0.870681	-0.517928
19	1	0	-2.06331	0.91447	1.2293	41	9	0	7.86441	-1.62652	-0.994148
20	6	0	0.819222	-0.655787	0.360874	42	9	0	5.23221	-2.14048	-0.709095

### 3-7. Optimized geometry of 3a



SCF Done: E (RCAM-B3LYP) = -1757.67288894 hartree

Dipole moment (field-independent basis, Debye-Ang):

X = -4.5783, Y = -0.3793, Z = -1.3769, Tot = 4.7959

### 3-8. Cartesian coordinates of 3a

No.	Atom No.	Type	Coordinates (Angstroms)								
			x	y	z						
						22	1	0	0.019385	0.652454	-2.11013
						23	6	0	2.08139	-0.331576	-0.796345
1	6	0	-8.1024	-0.641623	-0.29745	24	6	0	3.15365	-1.07878	0.015177
2	6	0	-7.12931	-1.33762	0.429992	25	6	0	4.54114	-0.523154	-0.029653
3	6	0	-5.90044	-0.757427	0.67426	26	6	0	5.65414	-1.35575	-0.146371
4	6	0	-5.61212	0.530561	0.194632	27	6	0	4.77192	0.847111	0.063814
5	6	0	-6.59058	1.21297	-0.533514	28	6	0	6.94097	-0.840206	-0.182485
6	6	0	-7.82969	0.642788	-0.781878	29	6	0	6.04774	1.38207	0.043413
7	1	0	-7.36778	-2.33001	0.796913	30	6	0	7.13633	0.530059	-0.083177
8	1	0	-5.16553	-1.30207	1.25561	31	8	0	-4.03344	2.29066	-0.047694
9	1	0	-6.36287	2.20704	-0.904306	32	8	0	-3.52549	0.180274	2.39061
10	1	0	-8.56937	1.19672	-1.34654	33	8	0	2.89217	-2.13207	0.548802
11	6	0	-4.30934	1.18695	0.394667	34	8	0	2.40816	0.011586	-1.91504
12	6	0	-3.23841	0.501852	1.2536	35	9	0	3.73844	1.68348	0.214222
13	6	0	-1.86361	0.318343	0.700827	36	9	0	6.23839	2.69582	0.154553
14	6	0	-0.893374	-0.228165	1.54437	37	9	0	8.36723	1.02785	-0.105861
15	6	0	-1.53696	0.634569	-0.622263	38	9	0	7.99014	-1.65078	-0.313828
16	6	0	0.391148	-0.459862	1.07781	39	9	0	5.51022	-2.67207	-0.268834
17	1	0	-1.16568	-0.470715	2.56578	40	8	0	-9.2733	-1.28958	-0.481151
18	6	0	-0.252552	0.404761	-1.08986	41	6	0	-10.3126	-0.642756	-1.19633
19	1	0	-2.27685	1.07672	-1.27853	42	1	0	-10.0064	-0.422147	-2.22499
20	6	0	0.717376	-0.143974	-0.245947	43	1	0	-11.1454	-1.34526	-1.20794
21	1	0	1.1301	-0.896578	1.73862	44	1	0	-10.6206	0.281333	-0.694747

