Electronic Supplementary Information (ESI)

Aryl-Fused Tetrathianaphthalene (TTN): Synthesis, Structures, Properties, and Cocrystals with Fullerenes

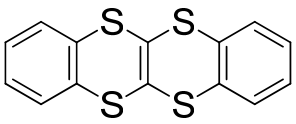
Yantao Sun, Zili Cui, Lichuan Chen, Xiaofeng Lu, Yuewei Wu, Hao-Li Zhang, and Xiangfeng Shao*

State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Tianshui Southern Road 222, Lanzhou 730000, Gansu Province, China. Fax: (+86) 0931 8915557; Tel: (+86) 0931 8912500;
E-mail: shaoxf@lzu.edu.cn (X. Shao)

Contents

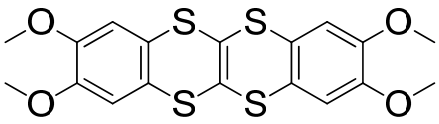
I. Characterization of the compounds

The following are the appearance, yield, melting point (Mp), ^{1}H NMR, ^{19}F NMR, ^{13}C NMR, and high-resolution mass spectra (HRMS) for the compounds reported in this work.



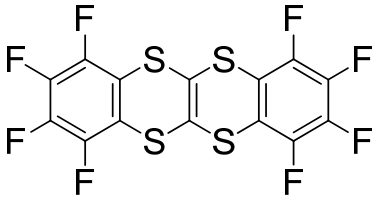
TTN-1

White solid(Yield = 63%); Mp: 249.5-251.0 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.38 (m, 4H), 7.30-7.28 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.65, 128.64, 128.38, 124.48. HRMS ($C_{14}H_8S_4$ + H): Calc. 304.9582, found 304.9583.



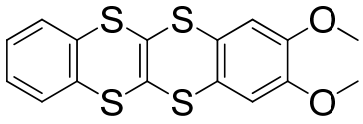
TTN-2

White solid(Yield = 73%); Mp: 309.7-311.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 (s, 4H), 3.87 (s, 12H). HRMS ($C_{18}H_{16}O_4S_4$): Calc. 423.9926, found 423.9916.



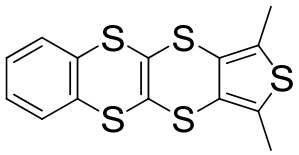
TTN-4

White solid (Yield = 70%); Mp: 226.8-228.6 °C. ^{19}F NMR (376 MHz, $CDCl_3$) δ -132.60--132.65 (m,4F), -152.19--152.24 (m, 4F). HRMS ($C_{14}F_8S_4$): Calc. 447.8750, found 447.8749.



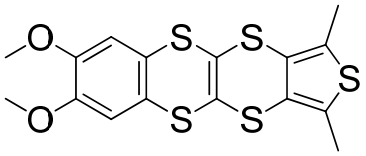
TTN-5

White solid(Yield = 78%). Mp: 222.0-224.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (dd, J = 5.8, 3.4 Hz, 1H), 7.28 (dd, J = 5.8, 3.3 Hz, 1H), 6.90 (s, 1H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.37 (s), 135.72 (s), 128.61 (s), 128.36 (s), 126.96 (s), 125.46 (s), 111.53 (s), 56.23 (s). HRMS ($C_{16}H_{12}O_2S_4$): Calc. 363.9715, found 363.9706.



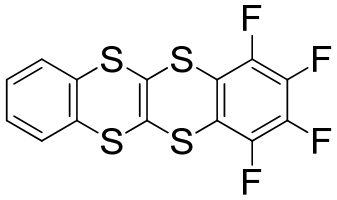
TTN-6

White solid(Yield = 81%); Mp: 251.0-252.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, J = 5.8, 3.4 Hz, 2H), 7.29 (dd, J = 5.8, 3.3 Hz, 4H), 2.33 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.12, 129.72, 128.54, 128.34, 127.41, 124.78, , 13.66. HRMS ($C_{14}H_{10}S_5$): Calc. 337.9381, found 337.9372.



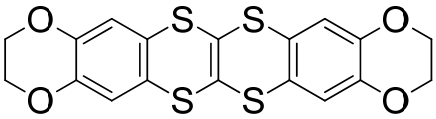
TTN-7

White solid(Yield = 61%). Decompositon point: 273°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.88 (s, 1H), 3.87 (s, 3H), 2.31 (s, 3H).^{13}C NMR (100 MHz, CDCl3) δ 149.36, 129.62, 127.47, 127.45, 125.66, 111.39, 56.23, 13.65. HRMS ($C_{16}H_{14}O_2S_5$): Calc. 397.9592, found 397.9581.



TTN-8

White solid (Yield = 71%); Mp 237.7-238.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.38 (m, 2H), 7.32-7.30 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -133.27--133.32 (m, 2F), -153.33--153.38(m, 2F). HRMS ($C_{14}H_4F_4S_4$): Calc. 375.9126, found 375.9119.



TTN-9

White solid (Yield = 71%); Mp > 310 °C. ^{1}H NMR (400 MHz, $CDCl_3$) 6.89 (s, 1H), 4.24 (s, 2H). HRMS ($C_{18}H_{12}O_4S_4$): Calc. 419.9613, found 419.9623.

II. UV/Vis absorption spectra and cyclic voltammograms (CV) of TTNs

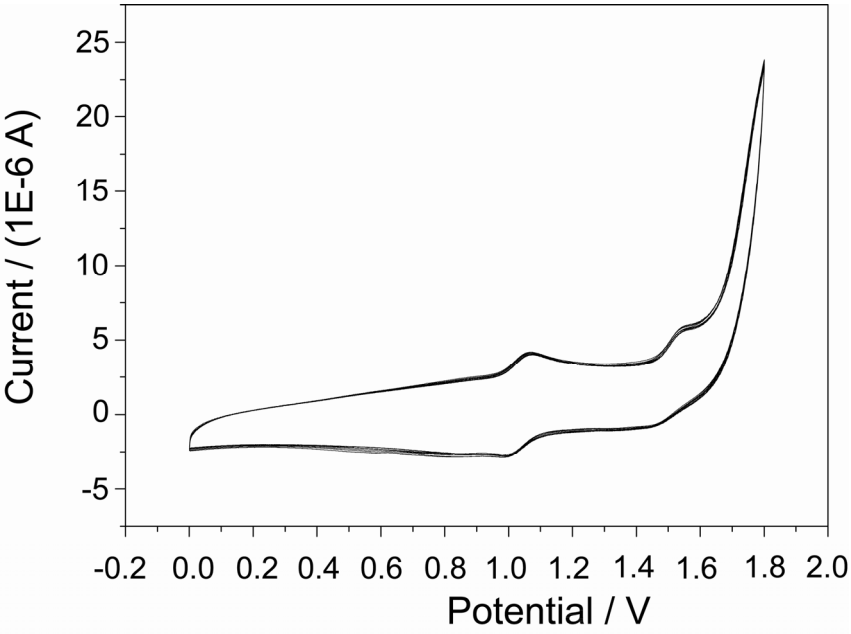


Fig. S1 Repeated cyclic voltammograms (20 times) of **TTN3**

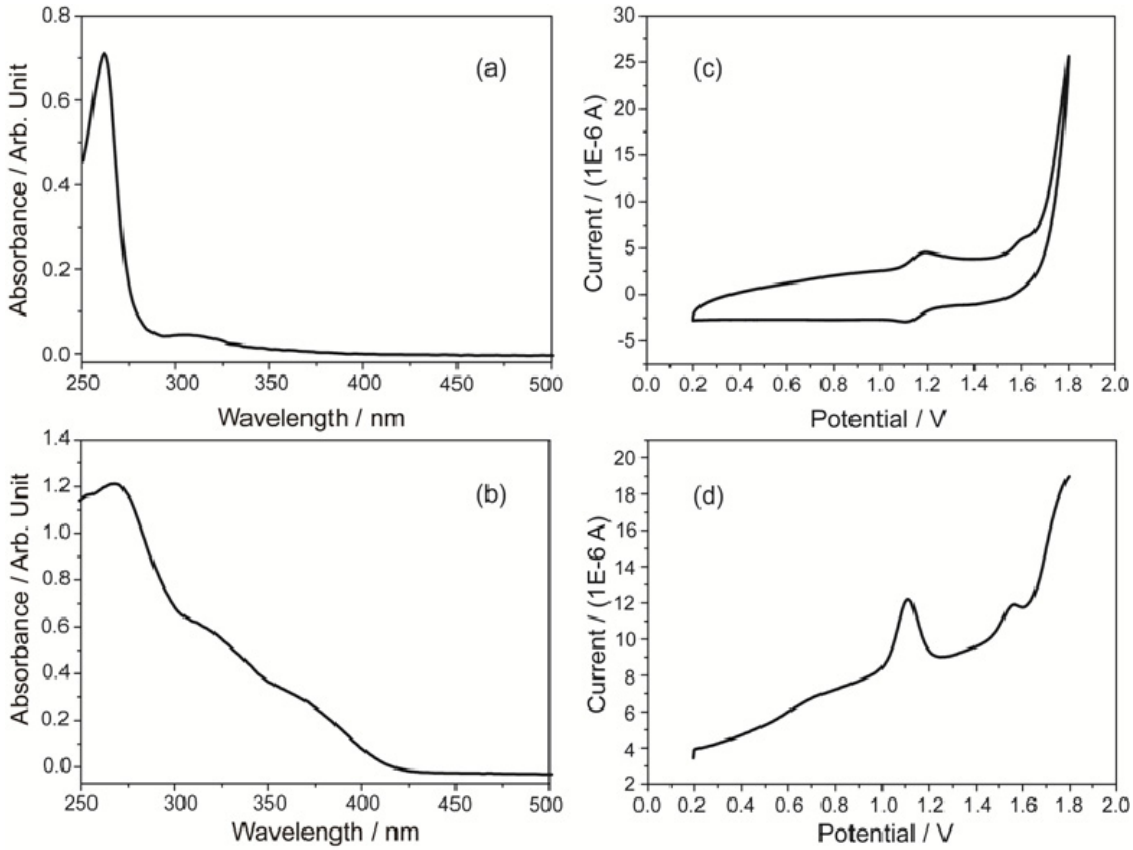


Fig. S2 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN1**

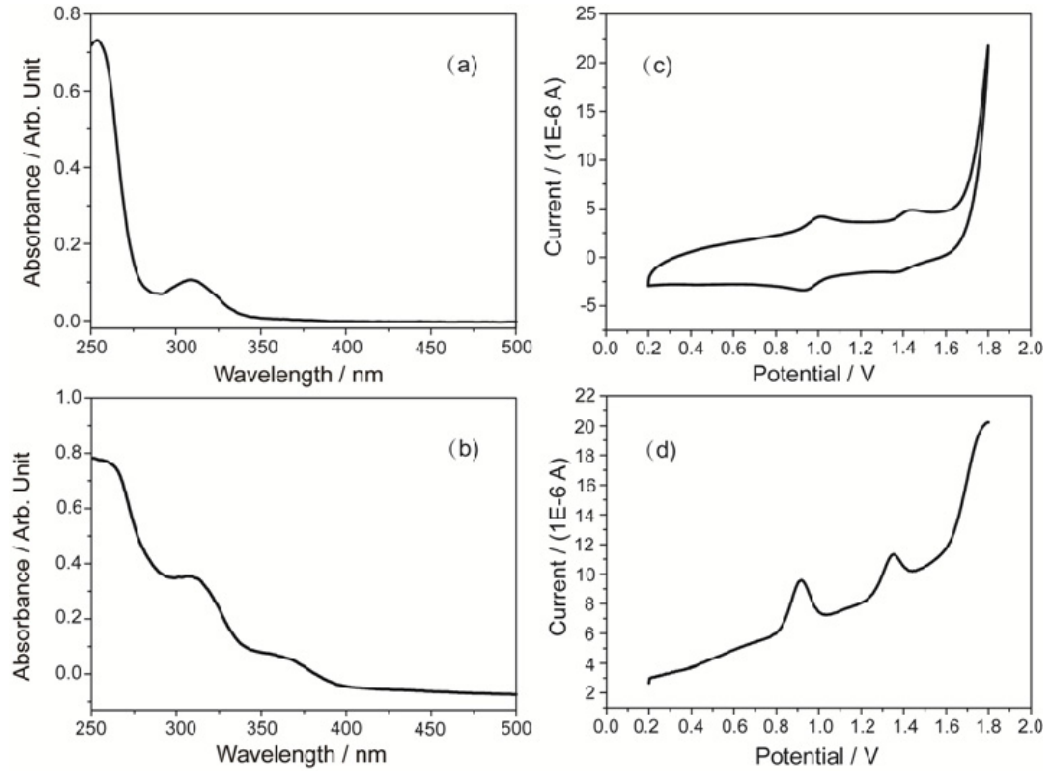


Fig. S3 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN2**

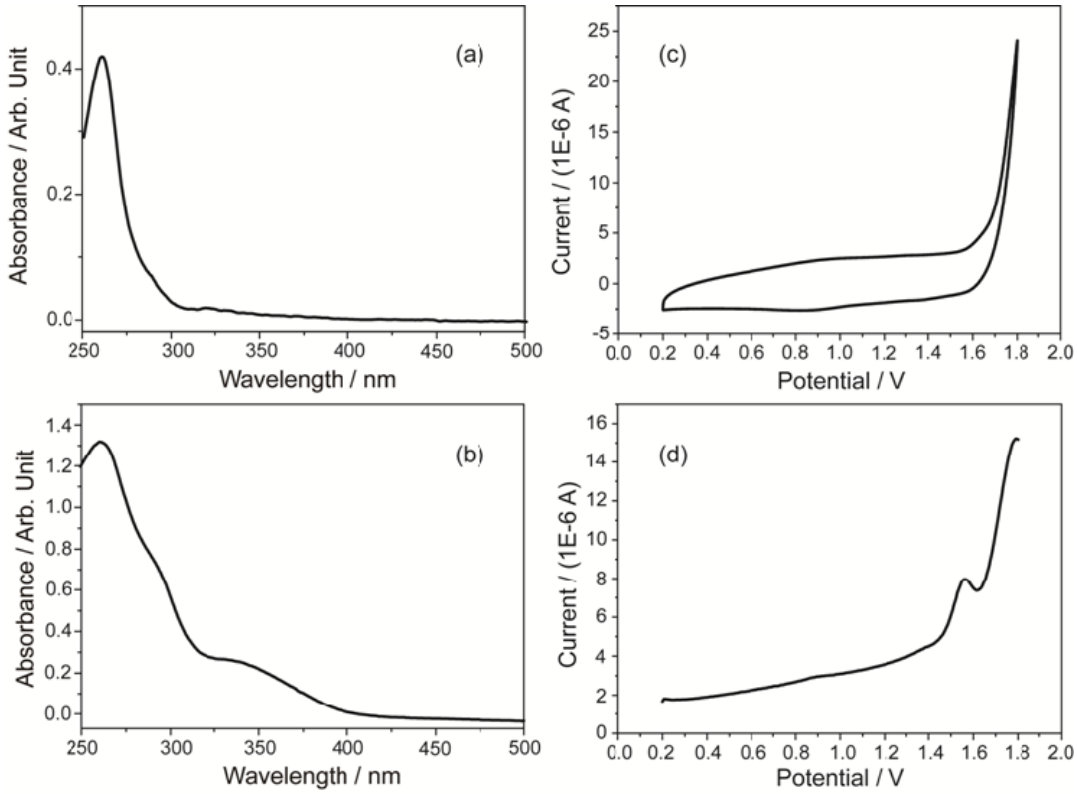


Fig. S4 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN4**

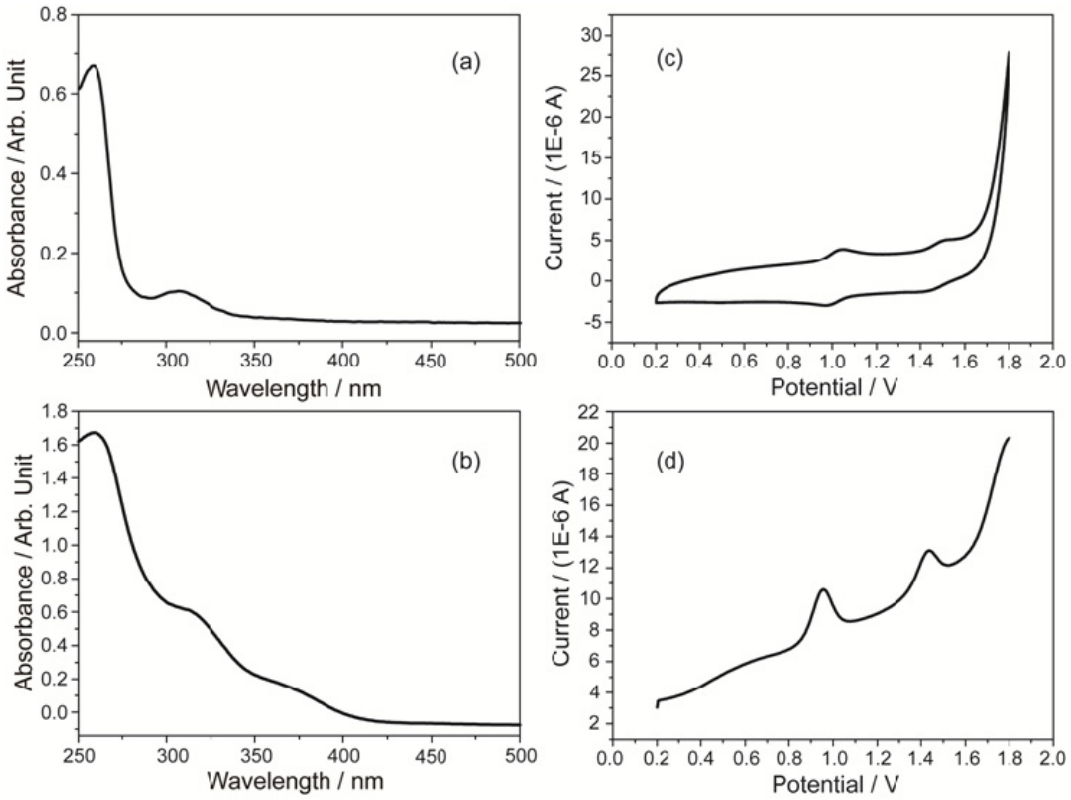


Fig. S5 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN5**

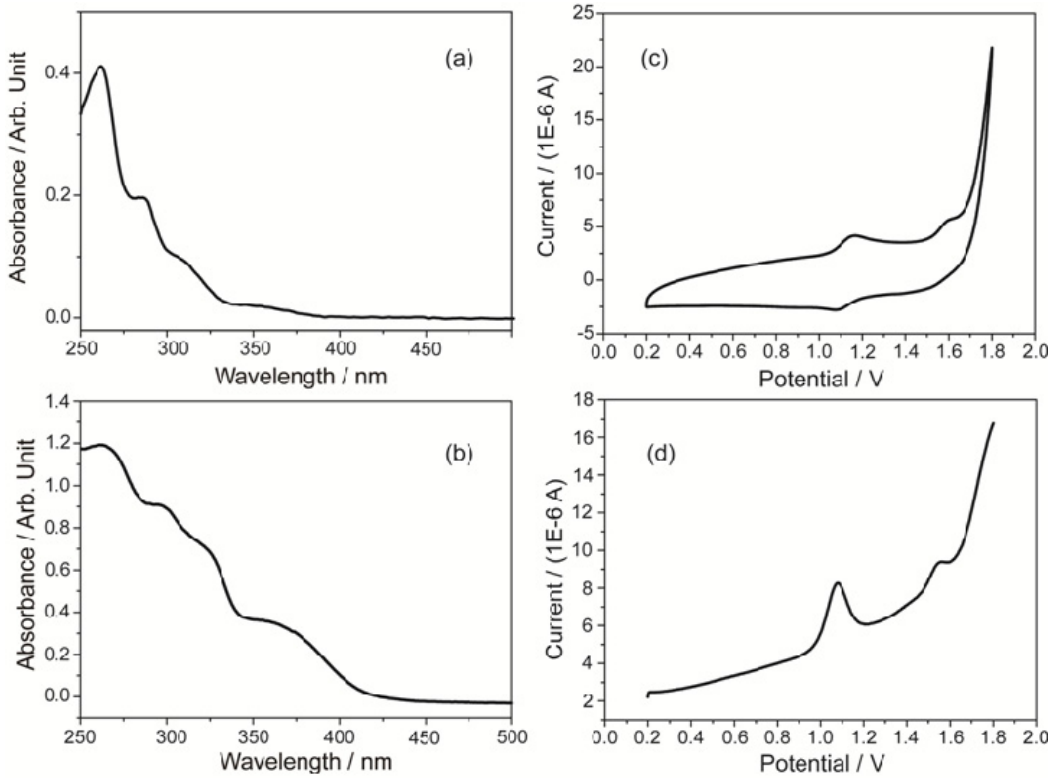


Fig. S6 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN6**

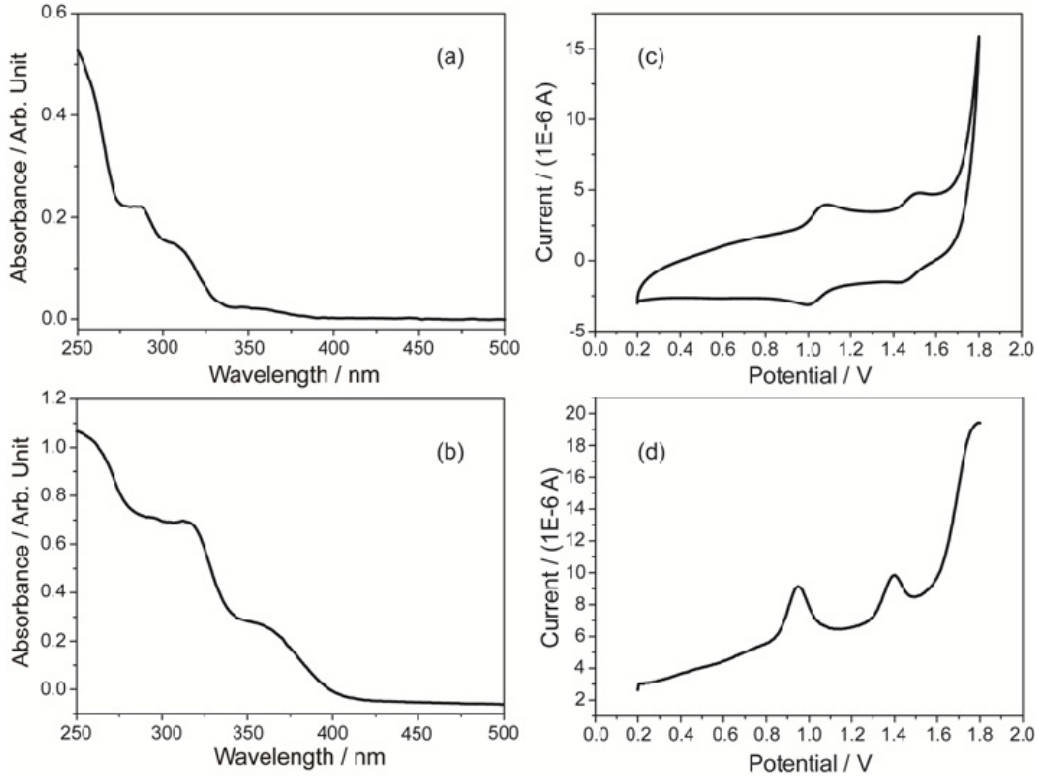


Fig. S7 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN7**

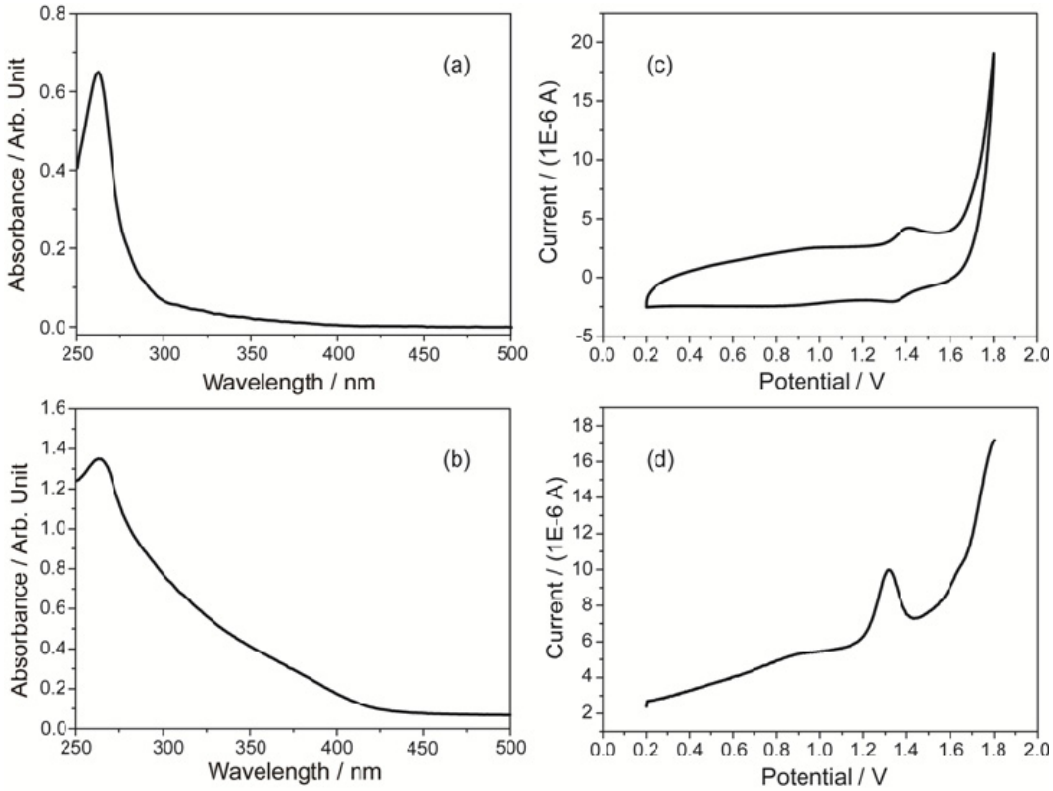


Fig. S8 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN8**

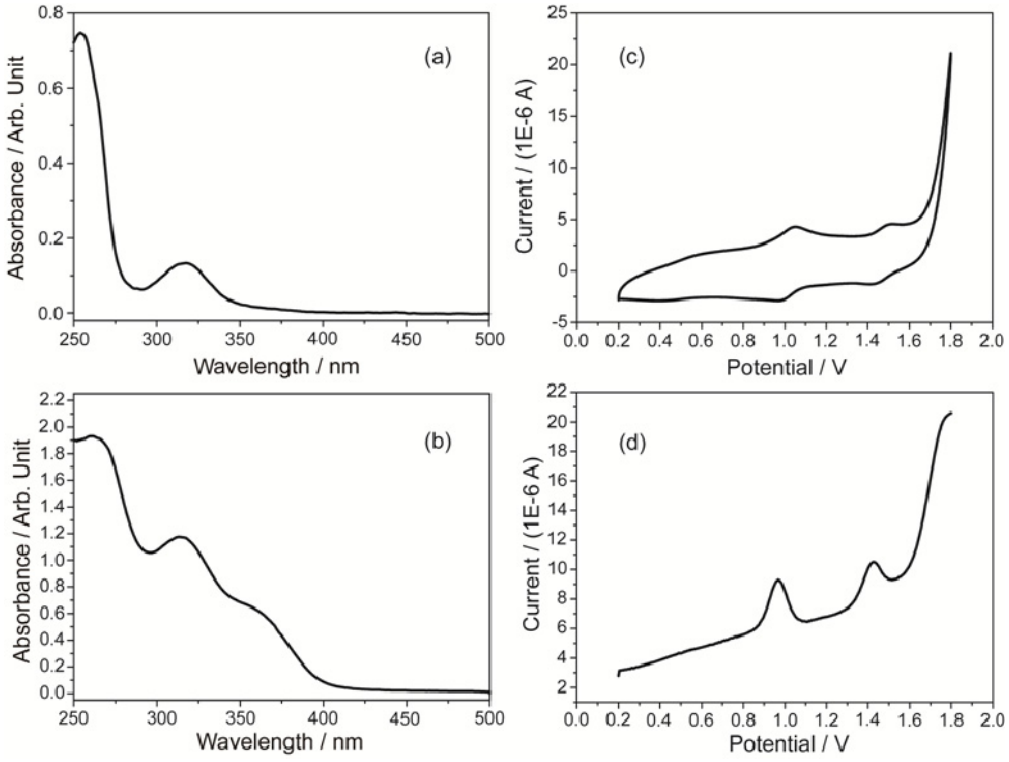
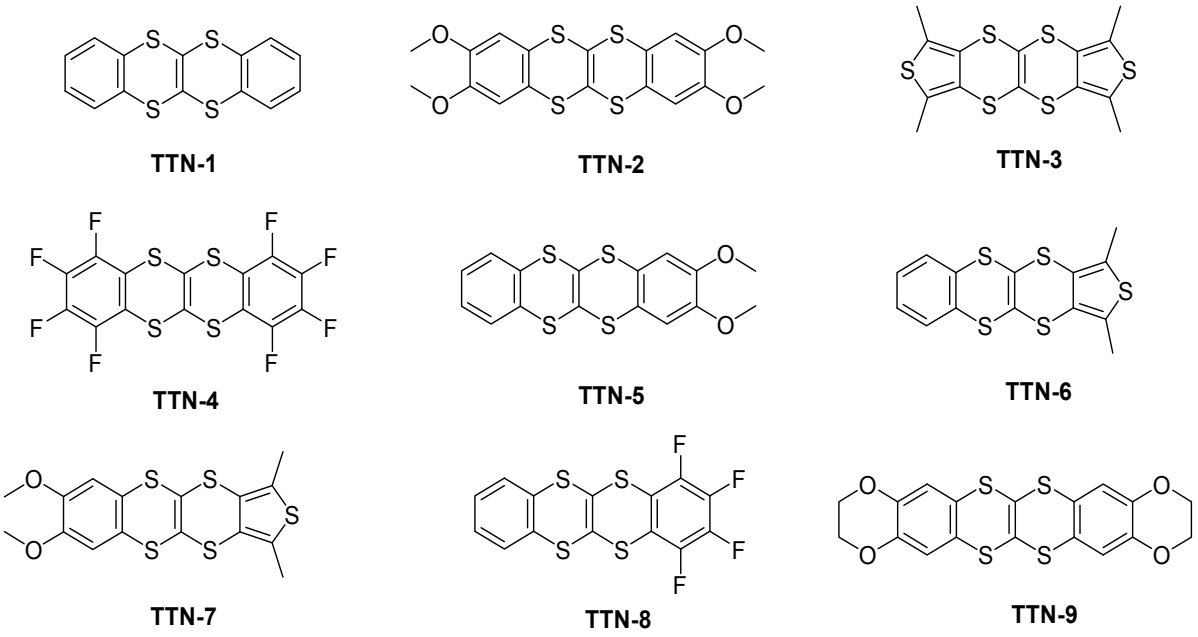


Fig. S9 UV-Vis spectra in DCM solution (a), solid state absorption spectra (b), cyclic voltammogram (c) and differential pulse voltammetry (d) of **TTN9**

III. Calculated frontier orbitals for TTNs

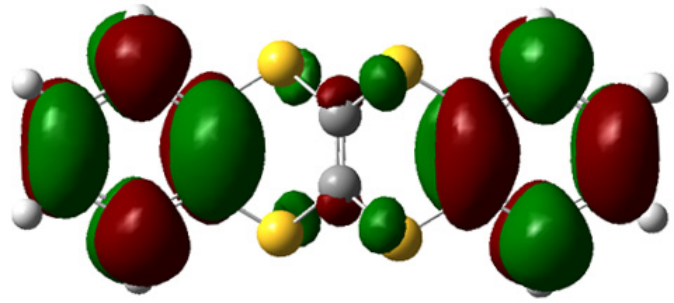


Scheme S1. Chemical structures of TTNs for theoretical calculation.

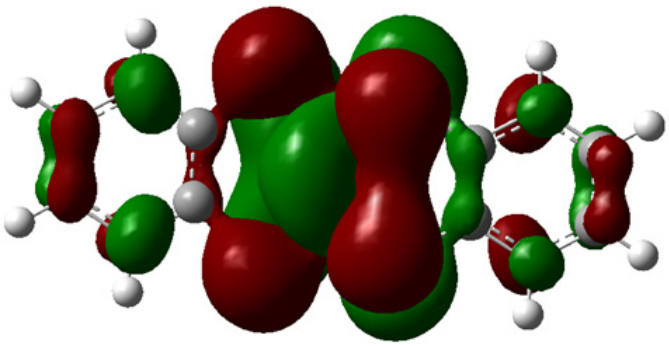
Table S1 Calculated energy levels

	Energy / eV		
	LUMO	HOMO	ΔE[b]
TTN1[a]	-0.955	-5.349	4.394
TTN2[a]	-0.607	-4.949	4.342
TTN3[a]	-0.868	-5.264	4.396
TTN4[a]	-1.724	-6.061	4.337
TTN5[c]	-0.853[c]	-5.120[c]	4.267
TTN6[a]	-0.975	-5.304	4.329
TTN7[c]	-0.828[c]	-5.183[c]	4.355
TTN8[c]	-1.417[c]	-5.702[c]	4.285
TTN9[a]	-0.646	-5.046	4.400
TTF3[a]	-1.000	-4.811	3.811

[a] Calculation was conducted on the basis of the molecular geometry in the crystal structures. [b] HOMO–LUMO energy gap $\Delta E = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}$. [c] Calculation was conducted on the basis of optimized molecular geometry.

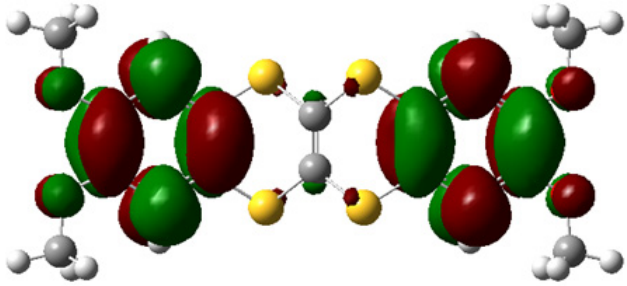


LUMO: –0.955 eV

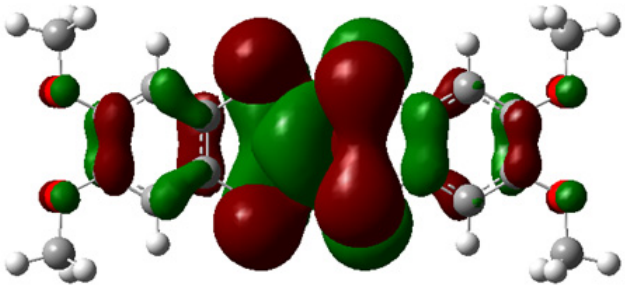


HOMO: –5.349 eV

Fig. S10 HOMO and LUMO orbitals of **TTN1**

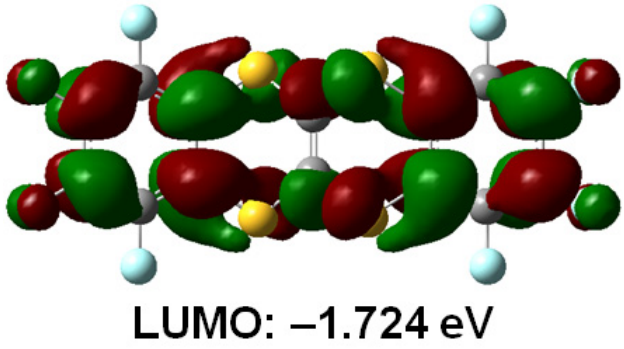


LUMO: –0.607 eV



HOMO: –4.949 eV

Fig. S11 HOMO and LUMO orbitals of **TTN2**



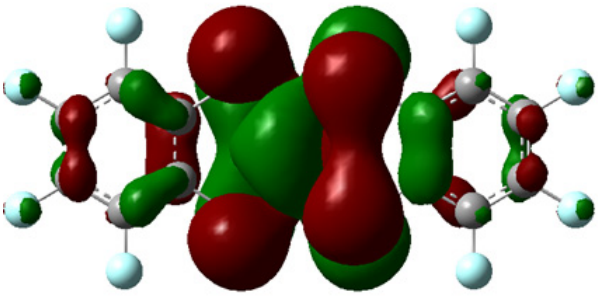
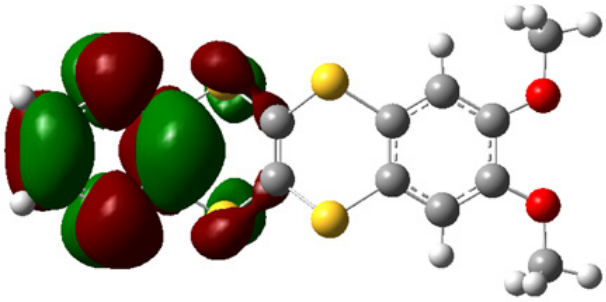


Fig. S12 HOMO and LUMO orbitals of **TTN4**



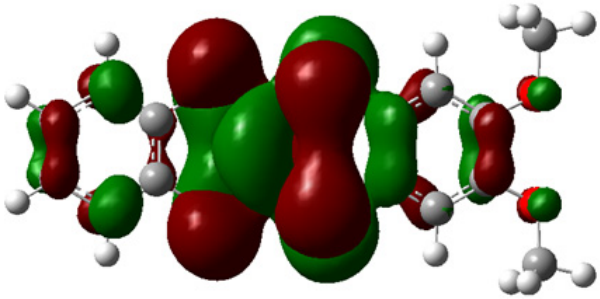
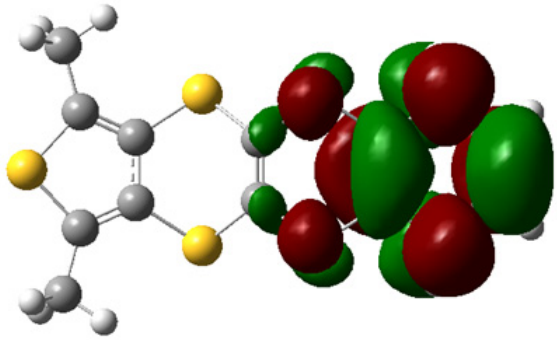
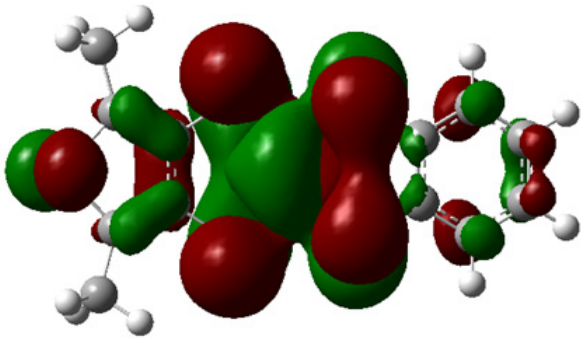


Fig. S13 HOMO and LUMO orbitals of **TTN5**

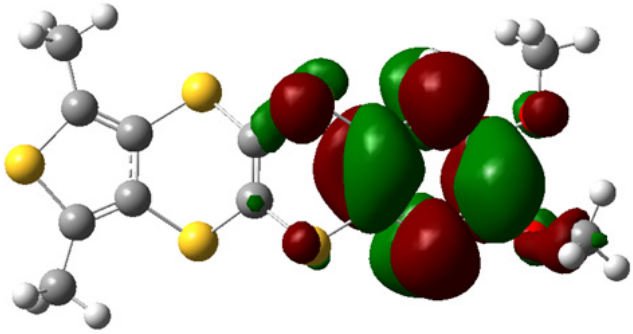


LUMO: –0.975 eV

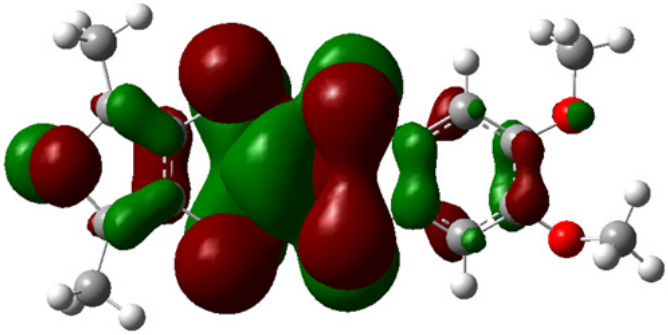


HOMO: –5.304 eV

Fig. S14 HOMO and LUMO orbitals of **TTN6**

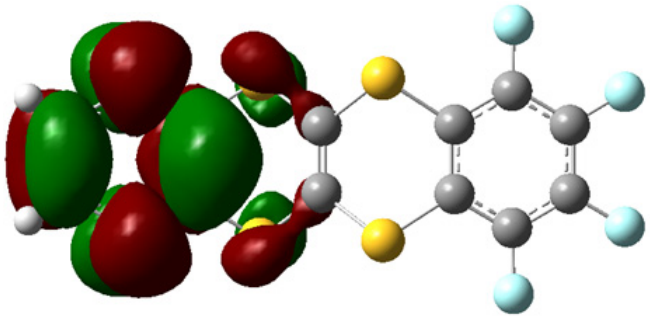


LUMO: –0.828 eV

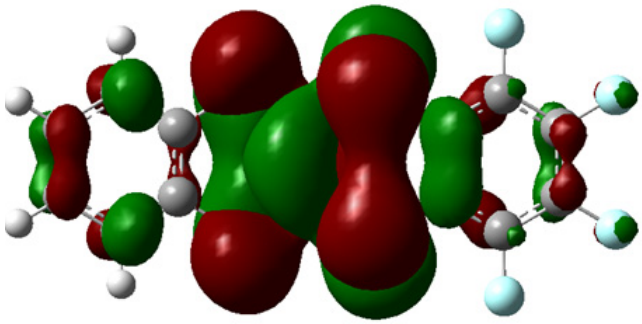


HOMO: –5.183 eV

Fig. S15 HOMO and LUMO orbitals of **TTN7**

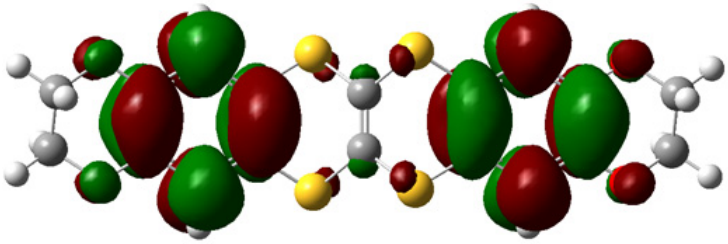


LUMO: –1.417 eV

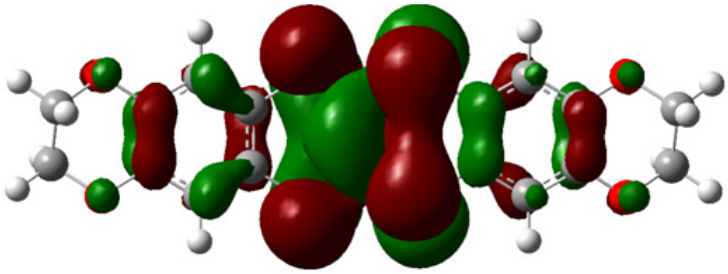


HOMO: –5.702 eV

Fig. S16 HOMO and LUMO orbitals of **TTN8**



LUMO: –0.646 eV



HOMO: –5.046 eV

Fig. S17 HOMO and LUMO orbitals of **TTN9**

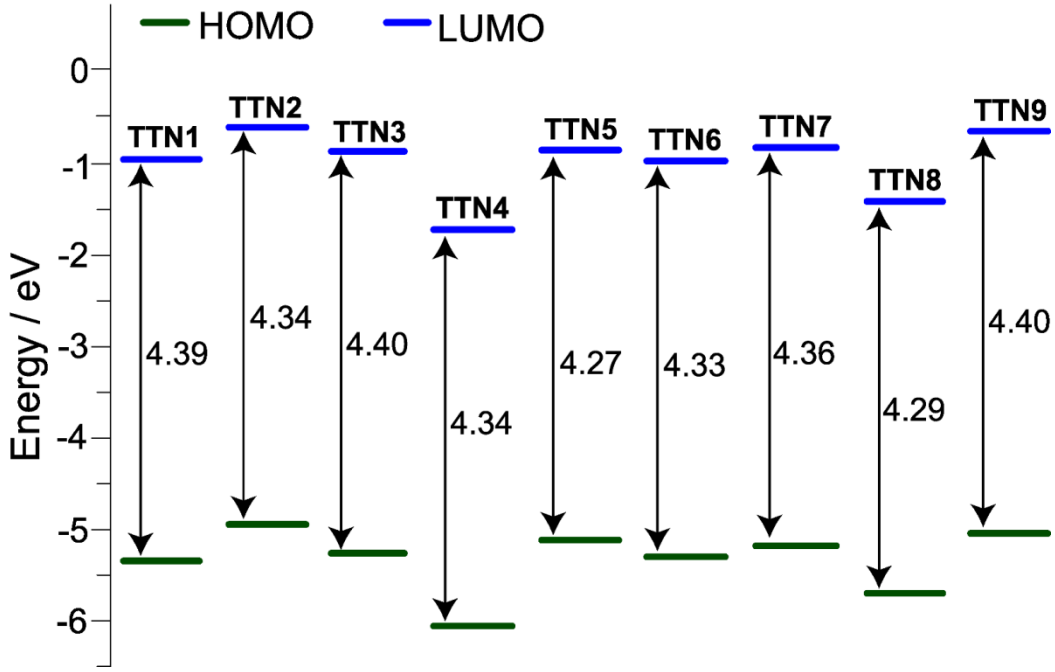


Fig. S18 Comparison of energy levels for **TTN1–TTN9**.

IV. Selected crystallographic data of TTNs

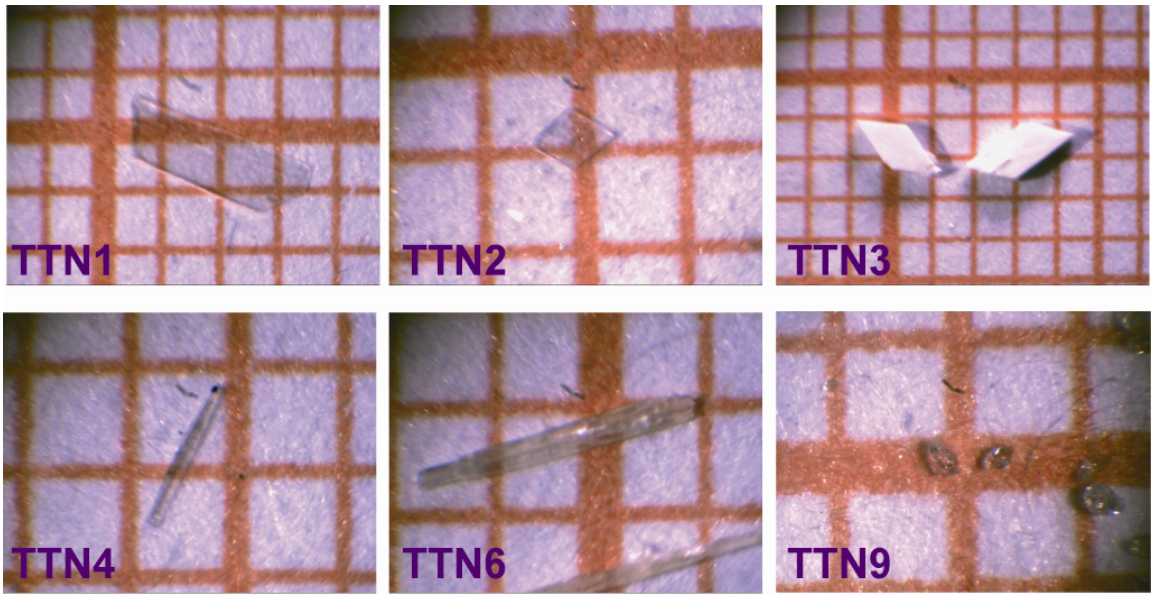


Fig. S19 Photographs for the single crystals of **TTNs**. The grid for the background of each figure is 1 mm × 1mm.

Table 2 Selected crystallographic data for **TTNs** and **TTF3**

	TTN1	**TTN2**	**TTN3•CS_2**	**TTN4**	**TTN6**	**TTN9**	**TTF3**
CCDC number	1492704	1492705	1492706	1492707	1492708	1492710	1492709
Empirical formula	$C_{14}H_8S_4$	$C_{18}H_{16}O_4S_4$	$C_{15}H_{12}S_8$	$C_{14}F_8S_4$	$C_{14}H_{10}S_5$	$C_{18}H_{12}O_4S_4$	$C_{14}H_{12}S_6$
Formula weight	304.44	424.54	448.72	448.38	338.52	420.52	372.60
Temperature / K	293(2)	293(2)	293(2)	296(2)	293(2)	293(2)	289.9
λ / Å	0.71073	0.71073	1.54184	0.71073	0.71073	0.71073	1.5418
Crystal size / mm^3	0.37×0.34×0.23	0.36×0.26×0.24	0.33×0.24×0.11	0.28×0.16×0.07	0.27×0.08×0.06	0.14×0.11×0.05	0.27×0.09×0.07
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
space group	*P2/n*	*$P2_1/c$*	*$P2_1/c$*	*$P2_1/c$*	*P-1*	*$P2_1/n$*	*I2/a*
a / Å	7.4504(9)	12.6610(5)	8.8305(6)	12.361(19)	7.4016(9)	7.8871(15)	17.1106(5)
b / Å	8.4459(9)	10.1047(5)	7.1569(6)	3.954(6)	7.7951(9)	11.518(2)	7.1272(2)
c / Å	10.8382(13)	7.3307(3)	15.0030(9)	15.050(2)	12.6647(11)	18.586(3)	13.5589(4)
α / °	90	90	90	90	83.801(8)	90	90
β / °	106.345(13)	96.481(4)	91.764(6)	97.159(15)	83.450(9)	90	104.115(3)
γ / °	90	90	90	90	77.253(10)	90	90
V / $Å^3$	654.43(13)	928.18(7)	947.73(11)	729.9(19)	705.88(14)	1688.5(5)	1603.58(8)
Z	2	2	2	2	2	4	4
d_{calc} / $g·cm^{-3}$	1.545	1.519	1.572	2.040	2.389	1.654	1.543
μ / mm^{-1}	0.701	0.533	8.677	0.740	1.202	0.586	0.838
$2\theta_{max}$ / °	57.16	56.7	141.56	51.3	56.9	57.26	51.22
Data / restraints / parameters	1484 / 0 / 82	2093 / 0 / 120	1803 / 0 / 108	1373 / 0 / 118	3189 / 0 / 174	3737 / 0 / 235	1495/0/94
GooF	1.076	1.044	1.036	1.024	1.071	1.029	1.094
R [$I>2\sigma(I)$]	0.0505	0.0369	0.0547	0.0428	0.0472	0.0598	0.0528
wR_2	0.1097	0.0874	0.1416	0.0976	0.1016	0.1292	0.1535

The following are the crystal structures of **TTN1**, **TTN2**, **TTN4**, **TTN6**, and **TTN9**. In these figures, panels (a), (b), and (c) depict the side view, top view, and packing structure of the corresponding TTN, respectively. In general, the grey, green, pink, and pale cyan balls represent carbon, sulfur, fluorine, and hydrogen atoms, respectively.

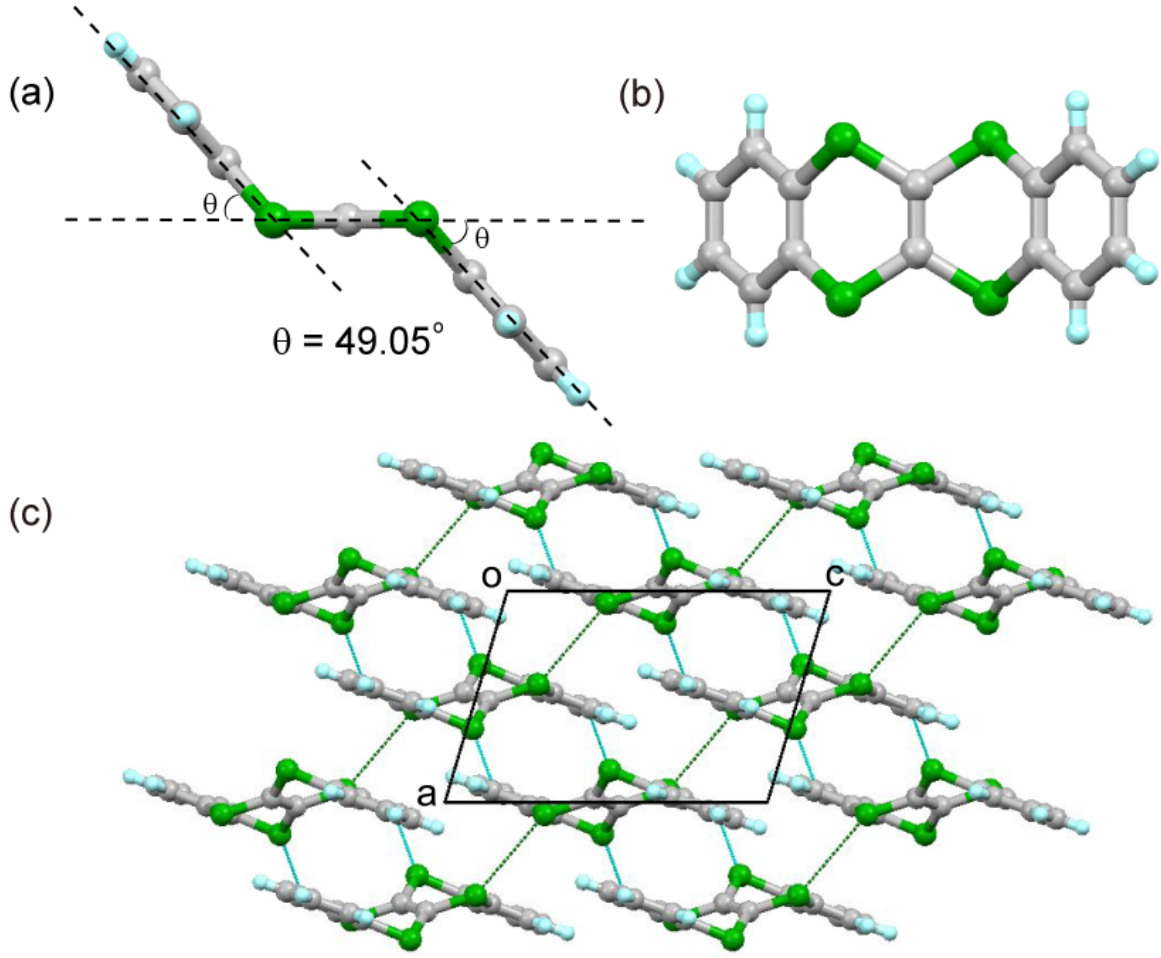


Fig. S20 Crystal structure of **TTN1**: (a), (b), and (c) depict the side view, top view, and packing structures, respectively.

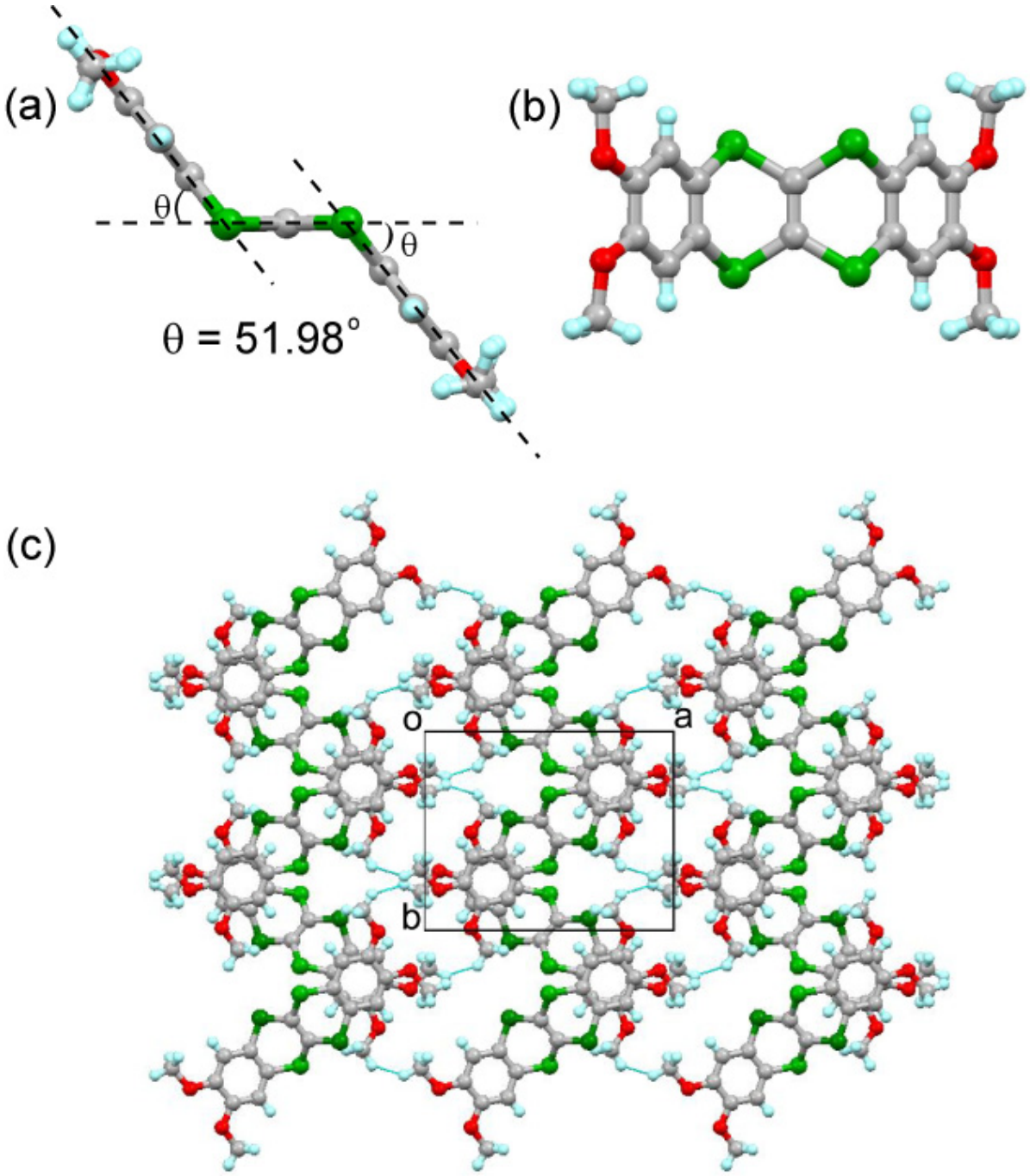


Fig. S21 Crystal structure of **TTN2**: (a), (b), and (c) depict the side view, top view, and packing structures, respectively.

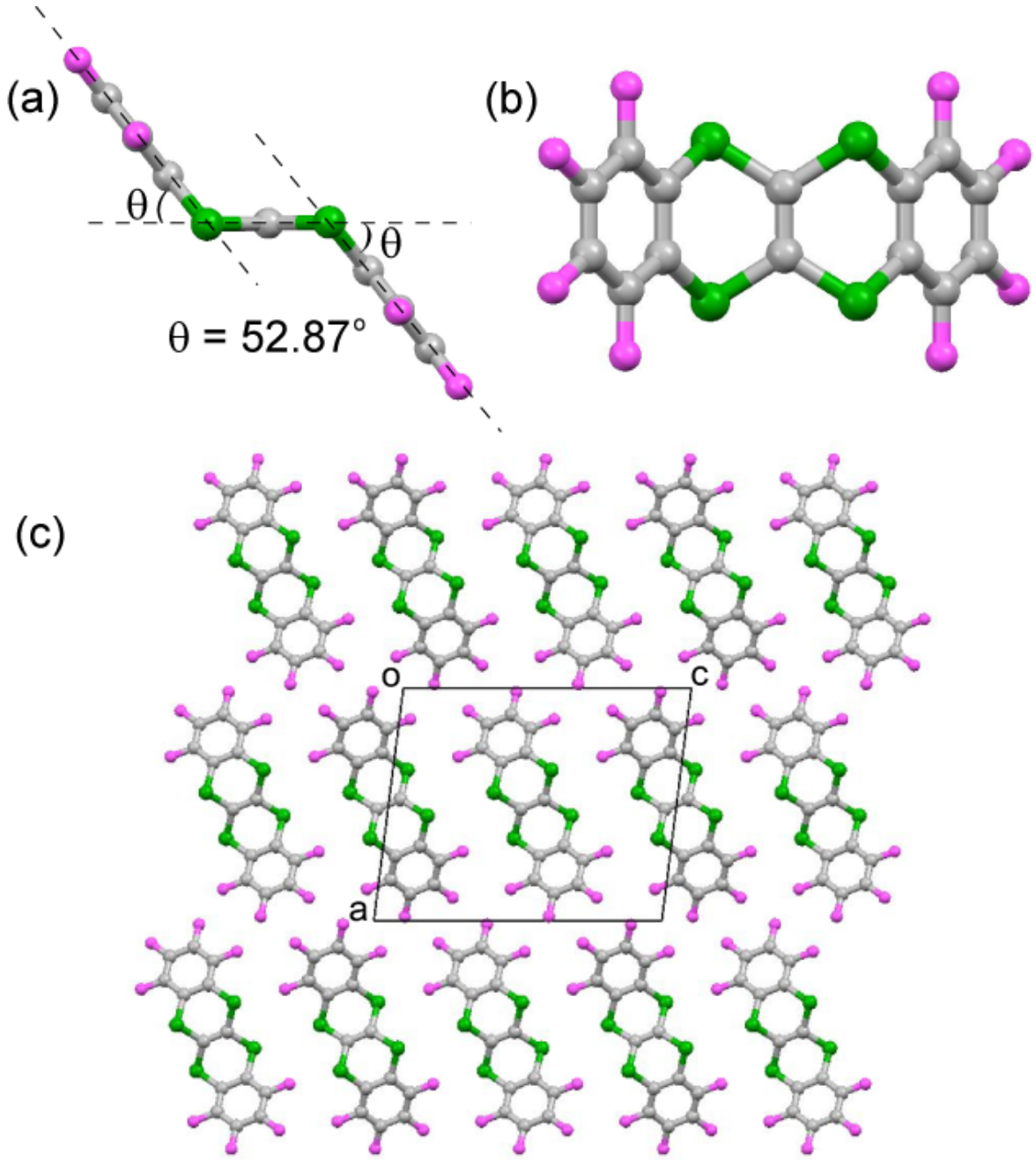


Fig. S22 Crystal structure of **TTN4**: (a), (b), and (c) depict the side view, top view, and packing structures, respectively.

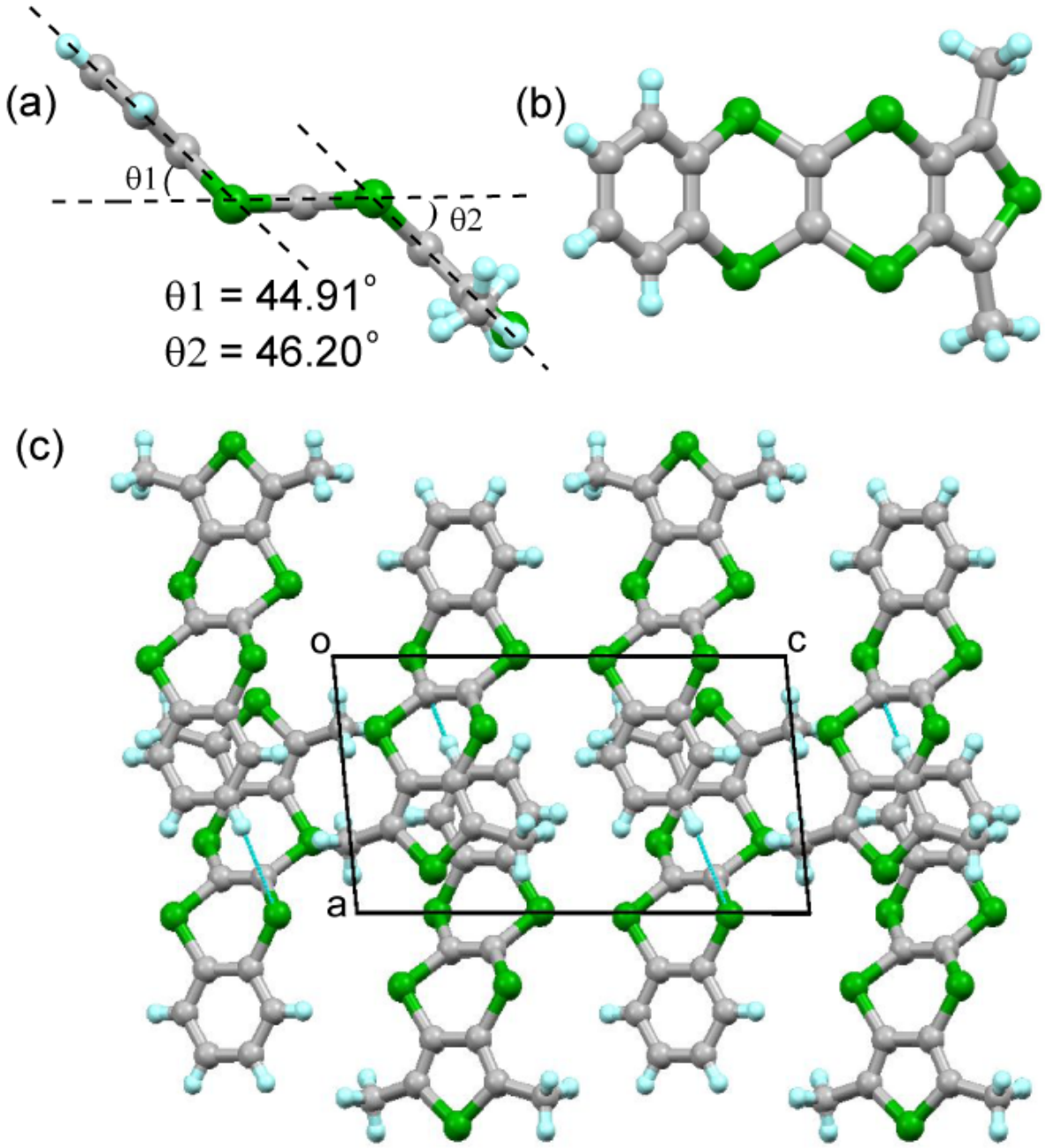


Fig. S23 Crystal structure of **TTN6**: (a), (b), and (c) depict the side view, top view, and packing structures, respectively.

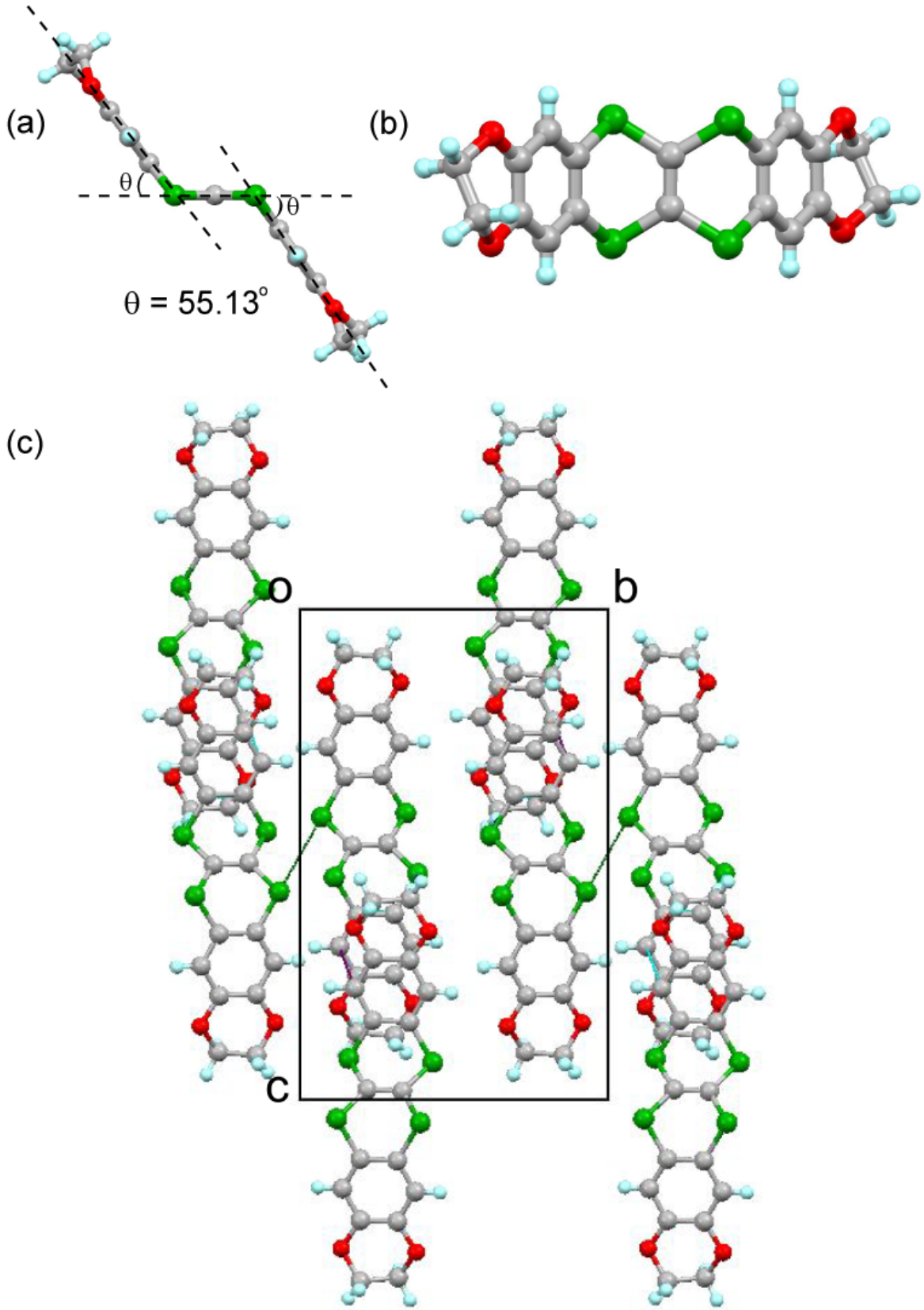


Fig. S24 Crystal structure of **TTN9**: (a), (b), and (c) depict the side view, top view, and packing structures, respectively.

V. Crystallographic data of "TTN•fullerene" cocrystals

The samples for the crystallographic analyses of the complexes were obtained by slow evaporation of the solvent. **TTN3•C_{60}•CS_2** was selected as an example. It was prepared by slow evaporation of the mixed solution of **1** (7.4 mg mg) and C_{60} (7.2 mg) in CS_2 (10 ml) at room temperature (RT). After 5 days, the black block single crystals were formed.

Table S3 Experimental conditions for the preparation of "**TTN•fullerene**" cocrystals

TTN	Fullerene	Solvent	Appearance	Composition
TTN3, 7.4 mg	C_{60}, 7.2 mg	CS_2, 10 mL	Black block	(TTN3)•(C_{60})•(CS_2)
TTN3, 7.4 mg	C_{60}, 7.2 mg	PhCl, 10 mL	Black block	(TTN3)•(C_{60})
TTN3, 7.4 mg	C_{70}, 8.4 mg	CS_2, 10 mL	Black block	(TTN3)•(C_{70})•(CS_2)
TTN3, 7.4 mg	C_{70}, 8.4 mg	$PhCH_3$, 10 mL	Black block	Not determined
TTN3, 14.4 mg	C_{70}, 16.8 mg	PhCl, 16 mL	Black block	(TTN3)•(C_{70})
TTN2, 8.5 mg	C_{60}, 7.2 mg	PhCl, 10 mL	Black block	(TTN2)•(C_{60})
TTN4, 8.8 mg	C_{60}, 7.2 mg	PhCl, 10 mL	Black block	Not determined
TTN5, 7.2 mg	C_{60}, 7.2 mg	PhCl, 10 mL	Black block	Not determined
TTN6, 6.8 mg	C_{60}, 7.2 mg	PhCl, 10 mL	Black block	$(TTN6)_2$•(C_{60})

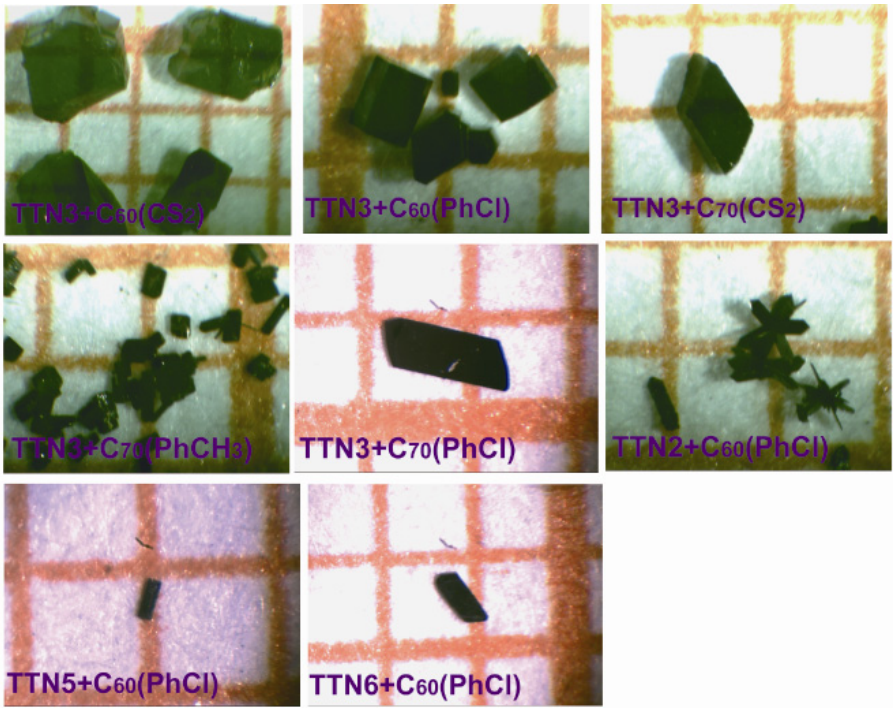


Fig. S25 Photographs for the single crystals of "**TTN•fullerene**" cocrystals. The grid for the background of each figure is 1 mm × 1mm.

Table 4 Selected crystallographic data for "**TTN•fullerene**" cocrystals

	(TTN3)•(C_{60})•(CS_2)	**(TTN3)•(C_{60})**	**(TTN3)•(C_{70})•(CS_2)**	**(TTN3)•(C_{70})**	**(TTN2)•(C_{60})**	**(TTN6)$_2$•(C_{60})**
CCDC number	1492711	1492712	1492713	1492714	1492715	1492716
Empirical formula	$C_{75}H_{12}S_8$	$C_{74}H_{12}S_6$	$C_{85}H_{12}S_8$	$C_{84}H_{12}S_6$	$C_{78}H_{16}O_4S_4$	$C_{88}H_{20}S_{10}$
Formula weight	1169.32	1093.20	1289.43	1213.30	1145.15	1397.64
Temperature / K	110(2)	110(2)	110(2)	77(1)	110(2)	110(2)
λ / Å	0.71073	0.71073	1.5418	0.95382	1.5418	1.5418
Crystal size / mm^3	0.38×0.35×0.34	0.19×0.17×0.14	0.42×0.35×0.32	0.25×0.19×0.17	0.30×0.20×0.07	0.33×0.26×0.16
Crystal system	Triclinic	Orthorhombic	Triclinic	Triclinic	Monoclinic	Monoclinic
space group	*P-1*	*Pnma*	*P-1*	*P-1*	*I2/a*	*P2$_1$/c*
a / Å	9.9766(4)	17.5533(19)	10.0905(3)	10.1580(9)	14.7684(5)	17.97(4)
b / Å	10.6457(6)	24.604(3)	13.6277(3)	12.6980(9)	13.5962(4)	9.81(2)
c / Å	10.9297(6)	9.7837（6）	18.3146(6)	19.1600(13)	22.7333(10)	17.28(6)
α / °	77.433(5)	90	86.280(2)	93.18	90	90
β / °	81.220(4)	90	77.027(3)	99.488(12)	103.105(4)	116.4(3)
γ / °	80.005(4)	90	87.191(2)	104.98	90	90
V / Å^3	1107.82(10)	4225.3（8）	2447.46(12)	2342.(3)	4445.8(3)	2729(13)
Z	1	4	2	2	4	2
d_{calc} / g·cm^{-3}	1.753	1.718	1.750	1.720	1.711	1.701
μ / mm^{-1}	0.463	0.383	3.874	0.409	2.53	4.224
$2\theta_{max}$ / °	57.2	56.92	141.52	59.6	141.38	142.3
Data / restraints / parameters	4986/0/378	4835/0/369	9358/0/845	10169/0/816	4201/0/390	4291/222/384
GooF	1.107	1.046	1.038	1.112	1.138	1.074
R [$I>2\sigma(I)$]	0.0526	0.0559	0.0516	0.0688	0.0681	0.1064
wR_2	0.1243	0.1136	0.1380	0.2102	0.1877	0.2869

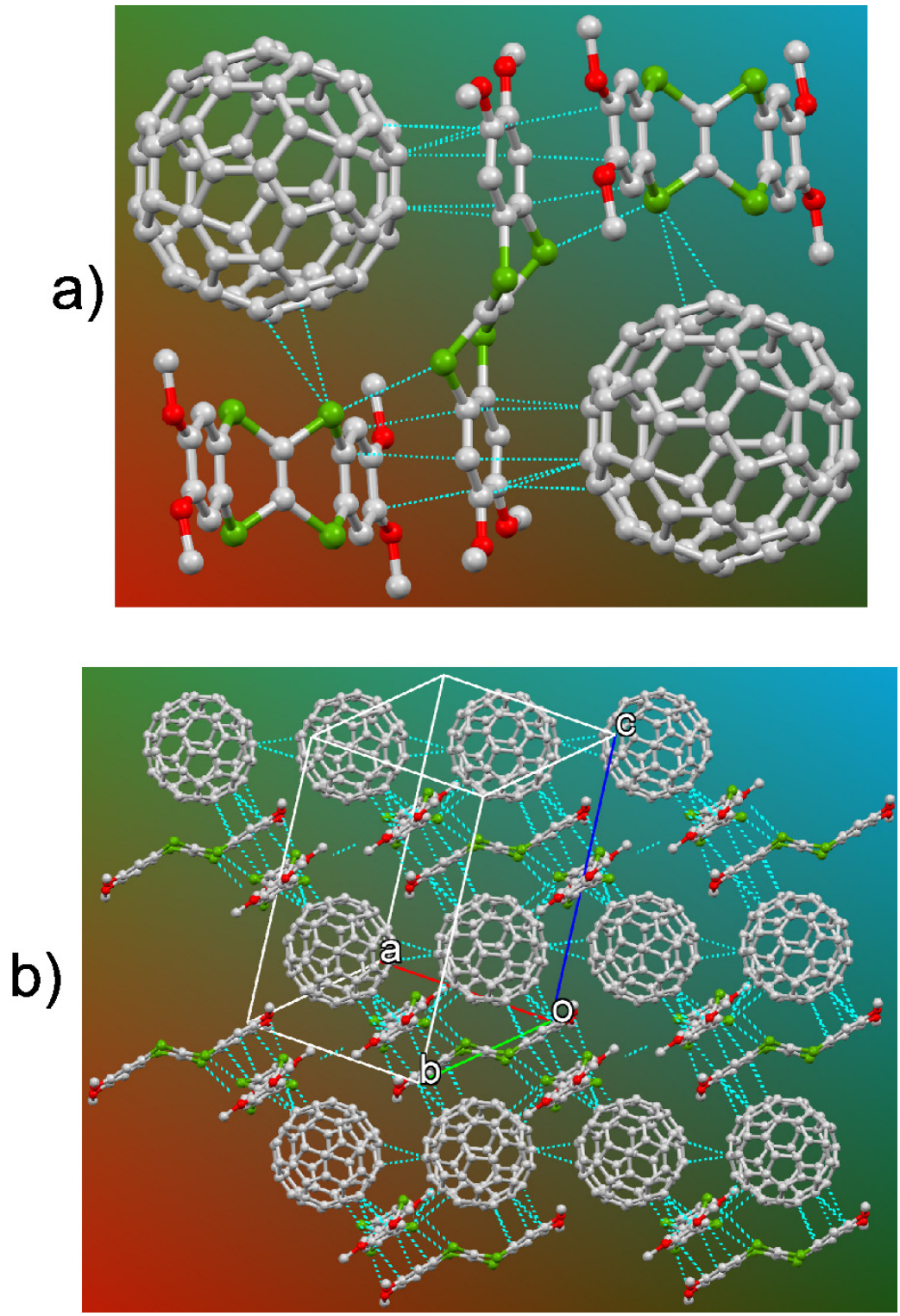


Fig. S26 Crystal structure of **(TTN2)•(C_{60})**: a) intermolecular interactions between **TTN2** and C_{60}; b) packing structures. The dashed lines shows the intermolecular interactions and the hydrogen atoms are omitted for clarity

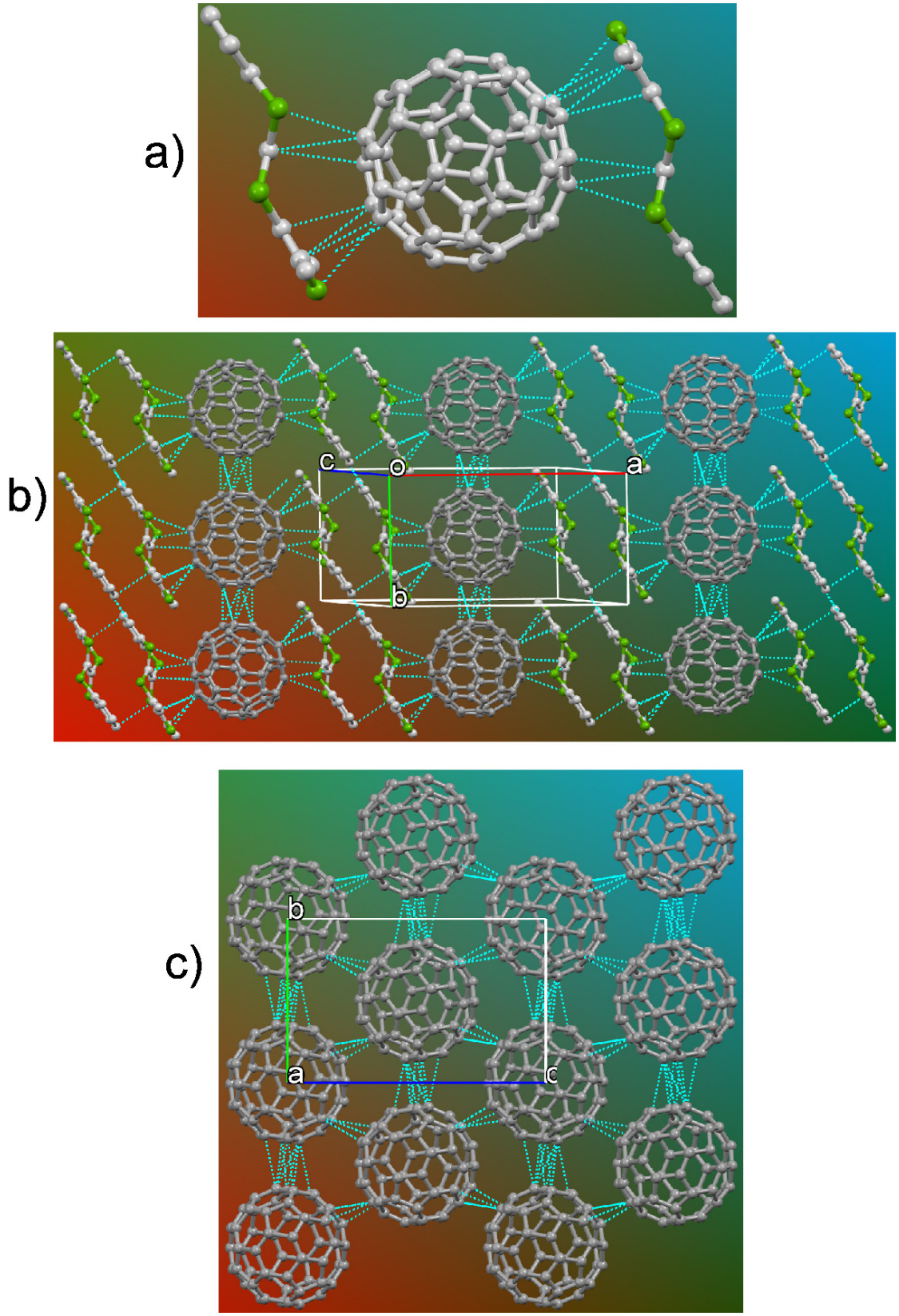


Fig. S27 Crystal structure of **(TTN6)$_2$•(C_{60})**: a) intermolecular interactions between **TTN6** and C_{60}; b) packing structures; c) packing structure of C_{60} molecules. The dashed lines shows the intermolecular interactions and the hydrogen atoms are omitted for clarity

VI. Optical spectra of the representative "TTN•fullerene" cocrystals

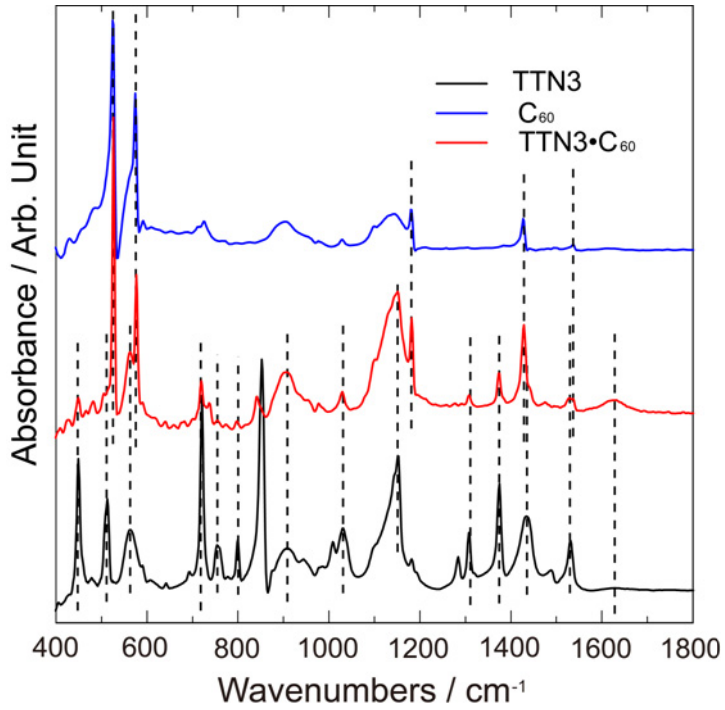


Fig. S28 IR spectra of **(TTN3)•(C_{60})** cocrystal, along with those of **TTN3** and **C_{60}** for comparison. The spectra were measured on the dispersed samples in KBr pellet, and the black dashed lines are guides for the eye.

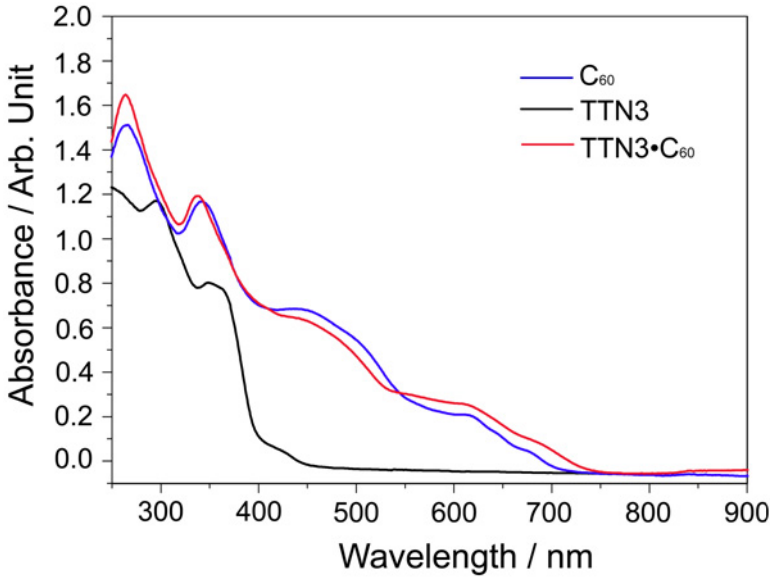


Fig. S29 Solid state absorption spectra of **(TTN3)•(C_{60})** cocrystal, along with those of **TTN3** and **C_{60}** for comparison. The spectra were measured on the dispersed samples in KBr pellet.

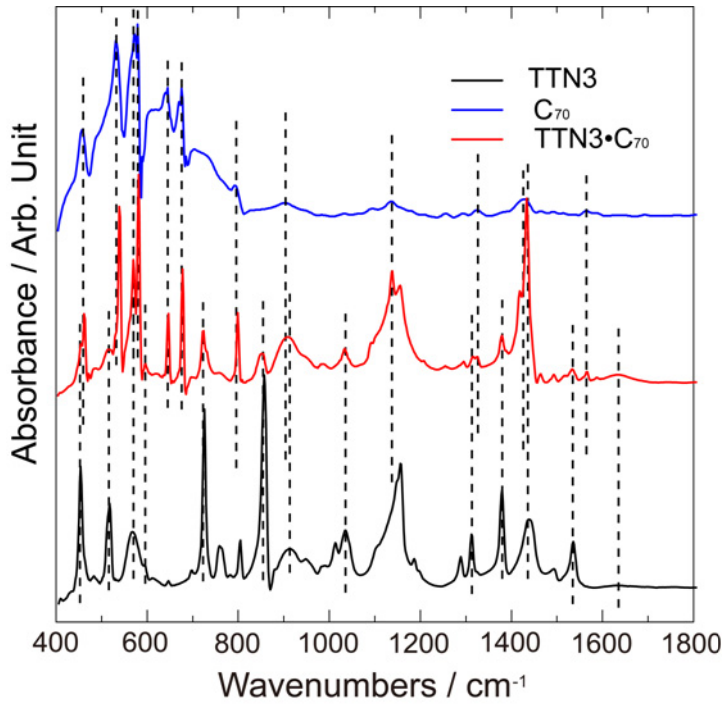


Fig. S30 IR spectra of (**TTN3**)•(**C$_{70}$**) cocrystal, along with those of **TTN3** and **C$_{70}$** for comparison. The spectra were measured on the dispersed samples in KBr pellet, and the black dashed lines are guides for the eye.

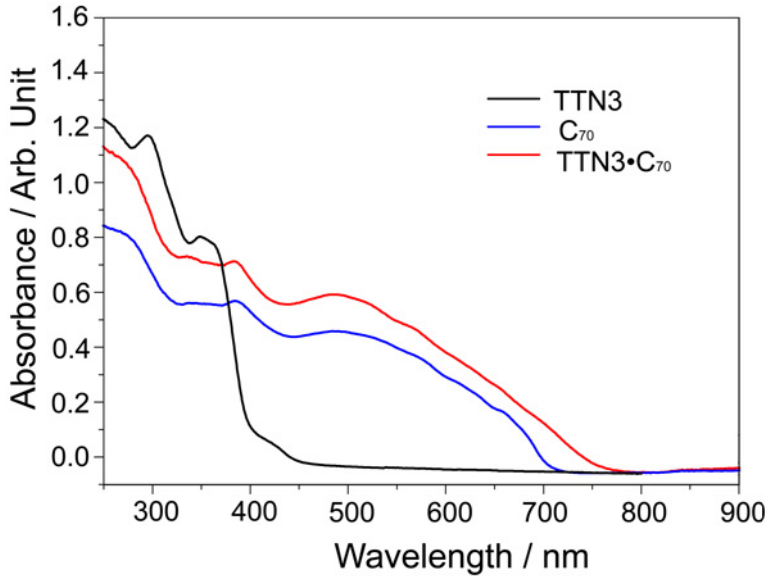
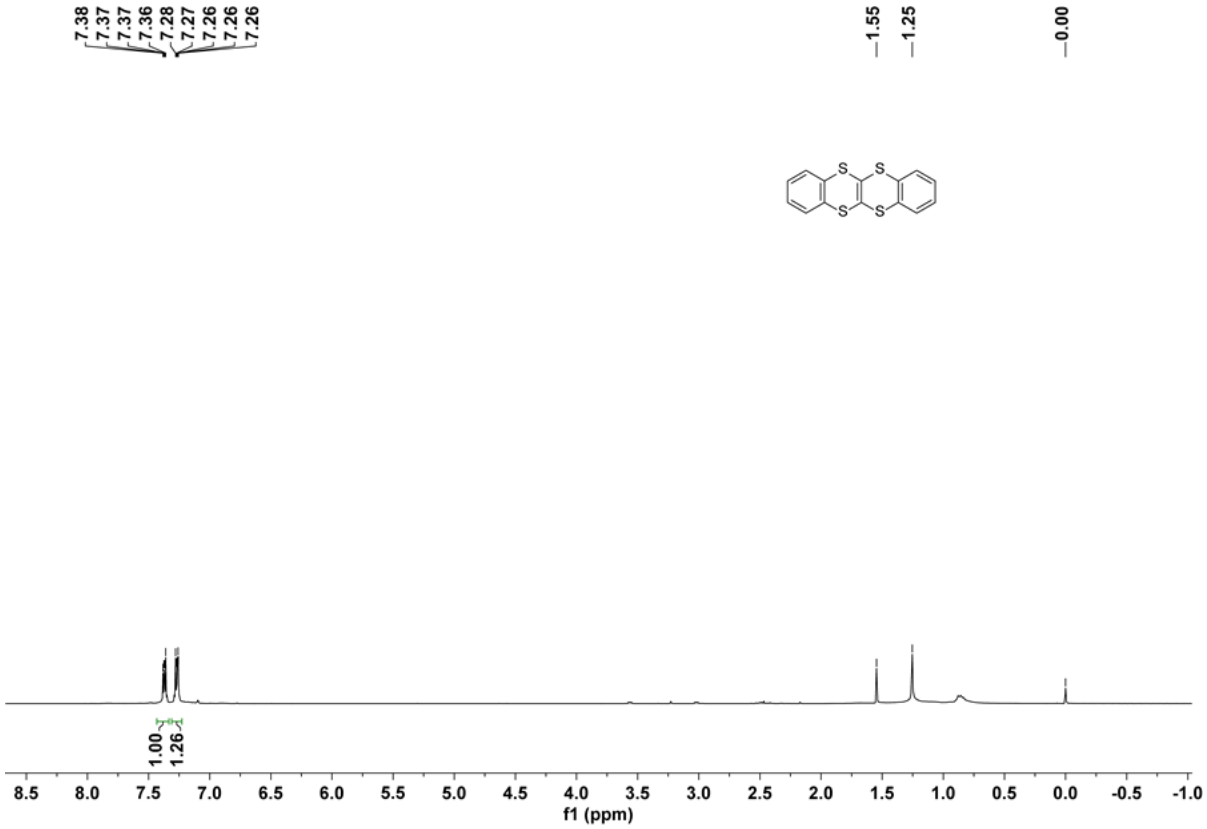
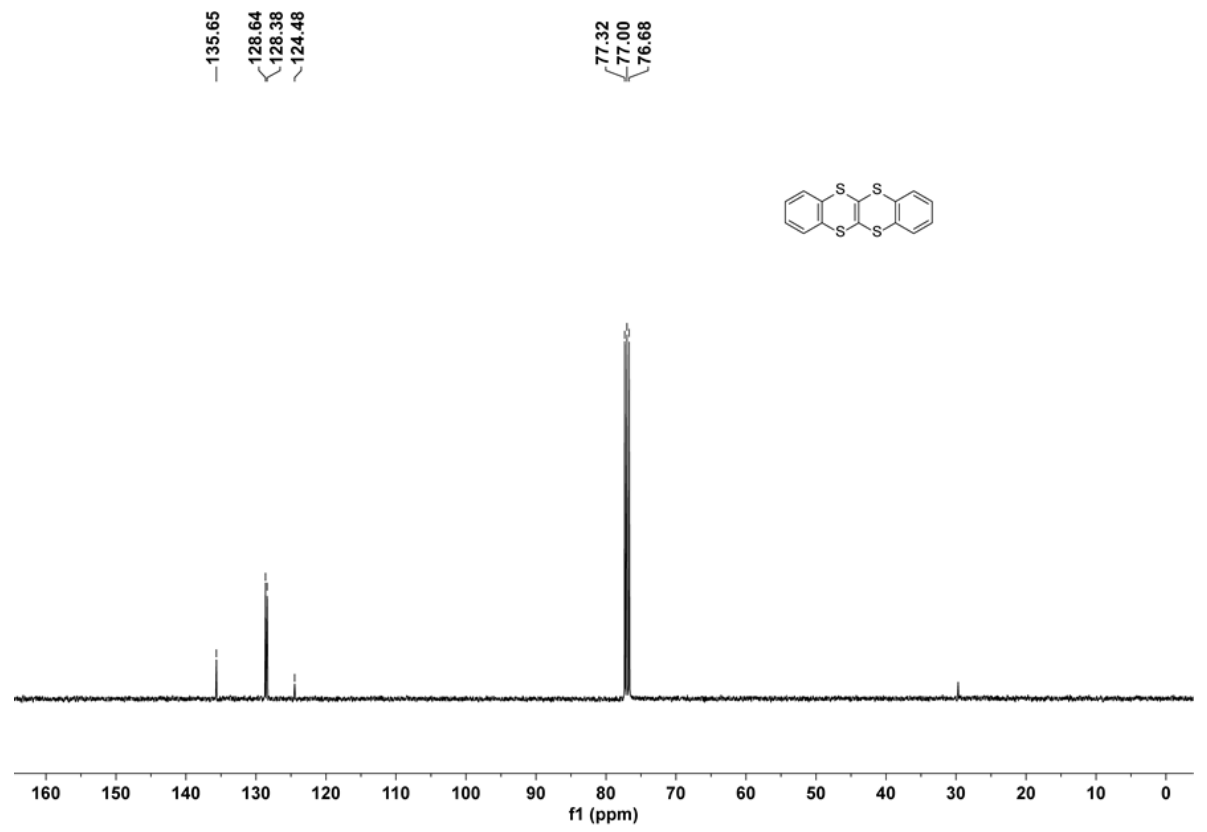
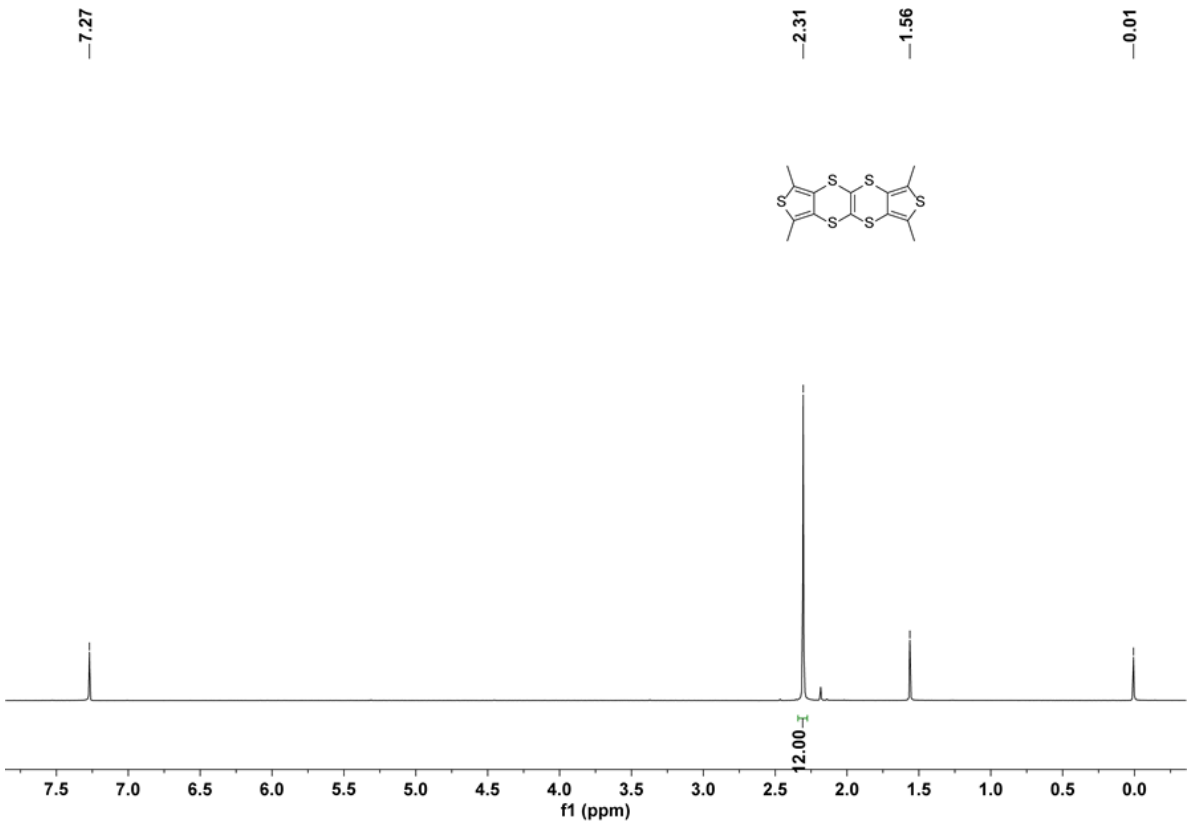


Fig. S31 Solid state absorption spectra of (**TTN3**)•(**C$_{70}$**) cocrystal, along with those of **TTN3** and **C$_{70}$** for comparison. The spectra were measured on the dispersed samples in KBr pellet.

VII. Original NMR and Mass Spectra for TTNs



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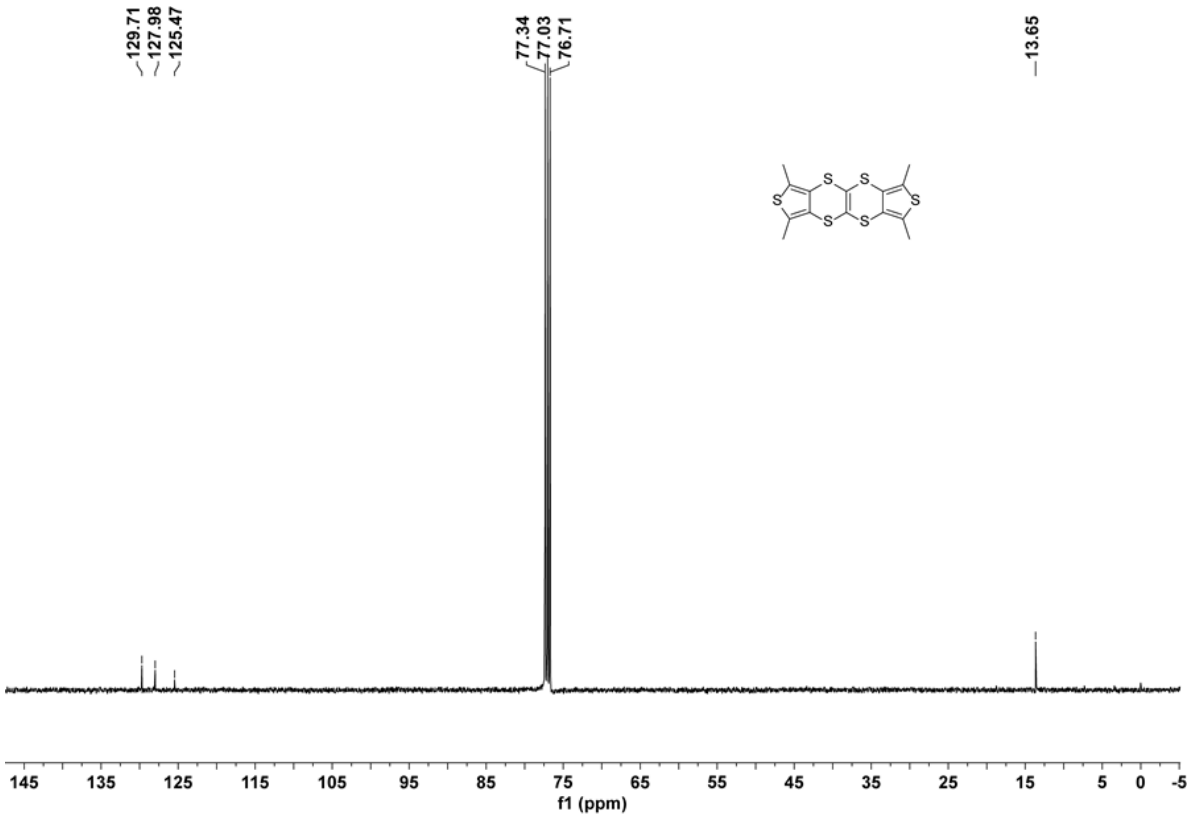
2.31
1.56
0.01
12.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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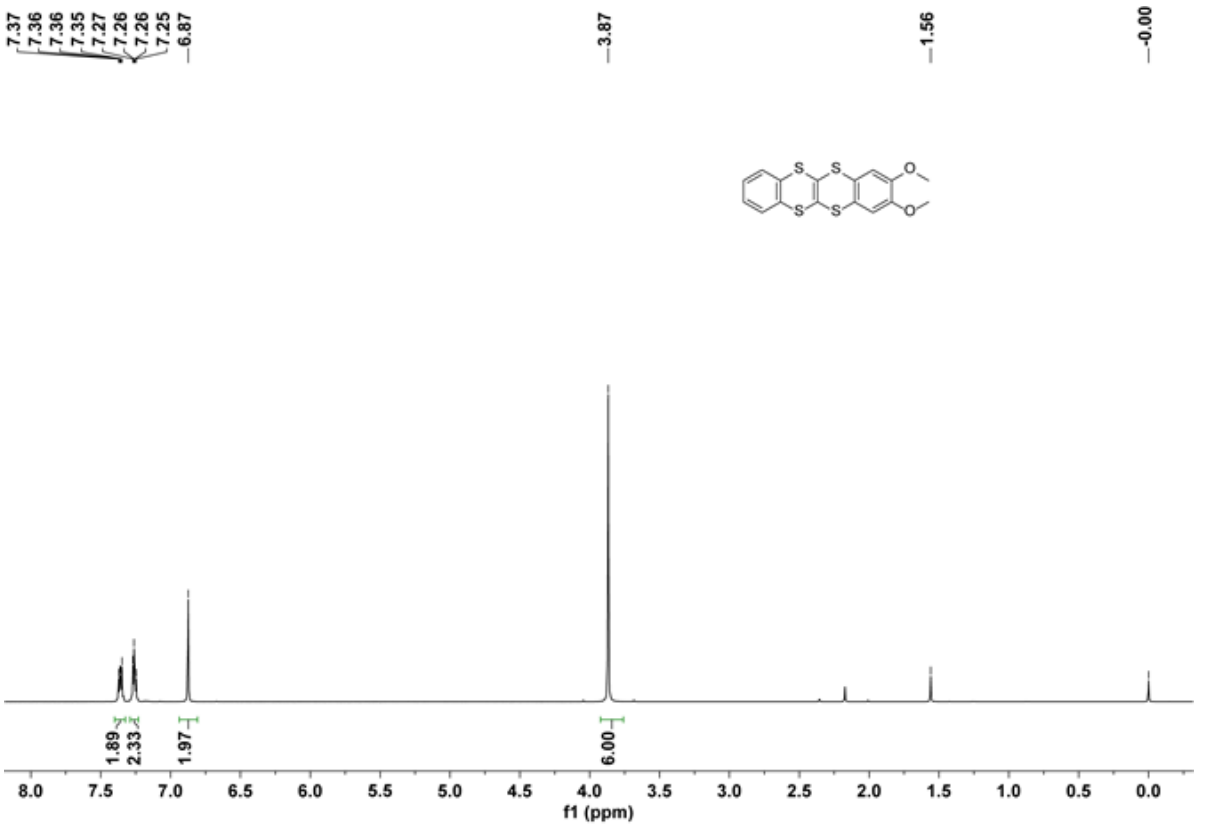
127.98
125.47
77.34
77.03
76.71
13.65
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0 -5
f1 (ppm)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7.36
7.35
7.27
7.26
7.26
7.25
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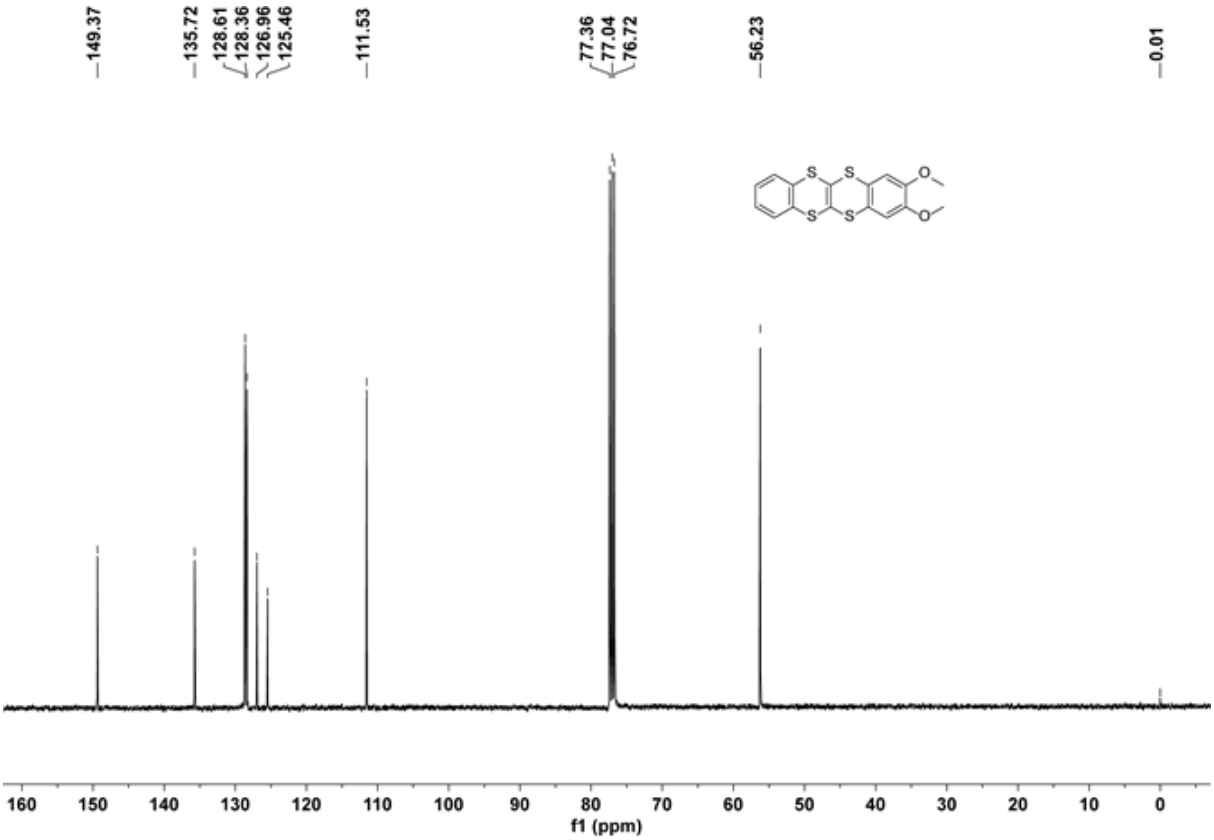
3.87
1.56
0.00
1.89
2.33
1.97
6.00
f1 (ppm)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76.72
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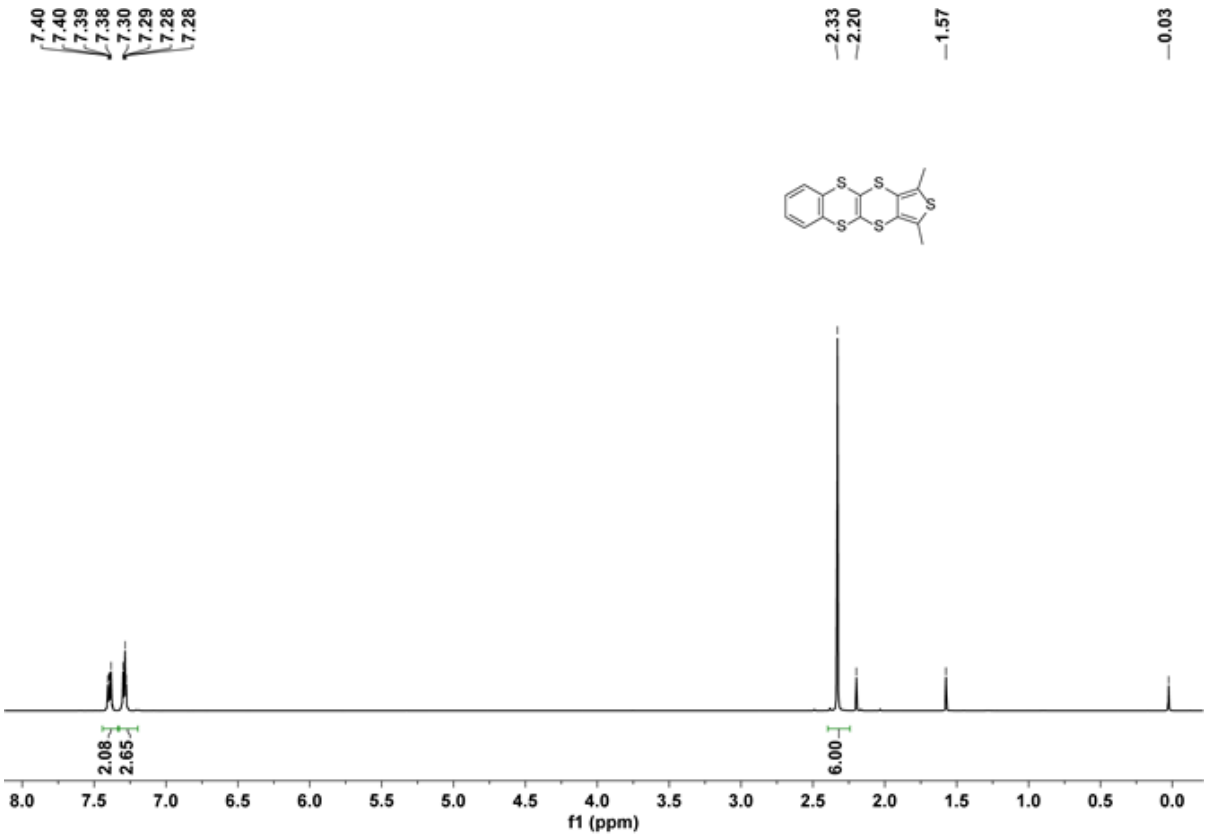
0.01
f1 (ppm)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7.28
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2.20
1.57
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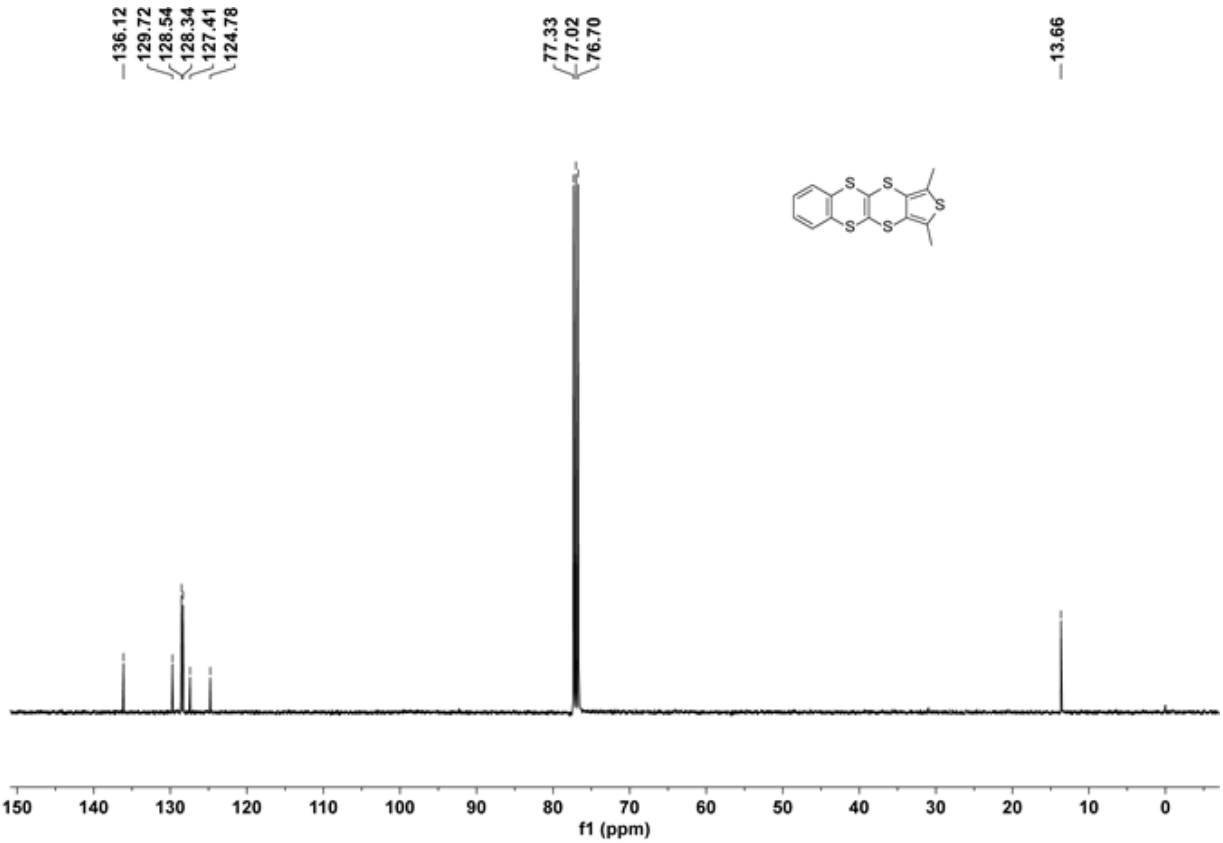
2.65
6.00
f1 (ppm)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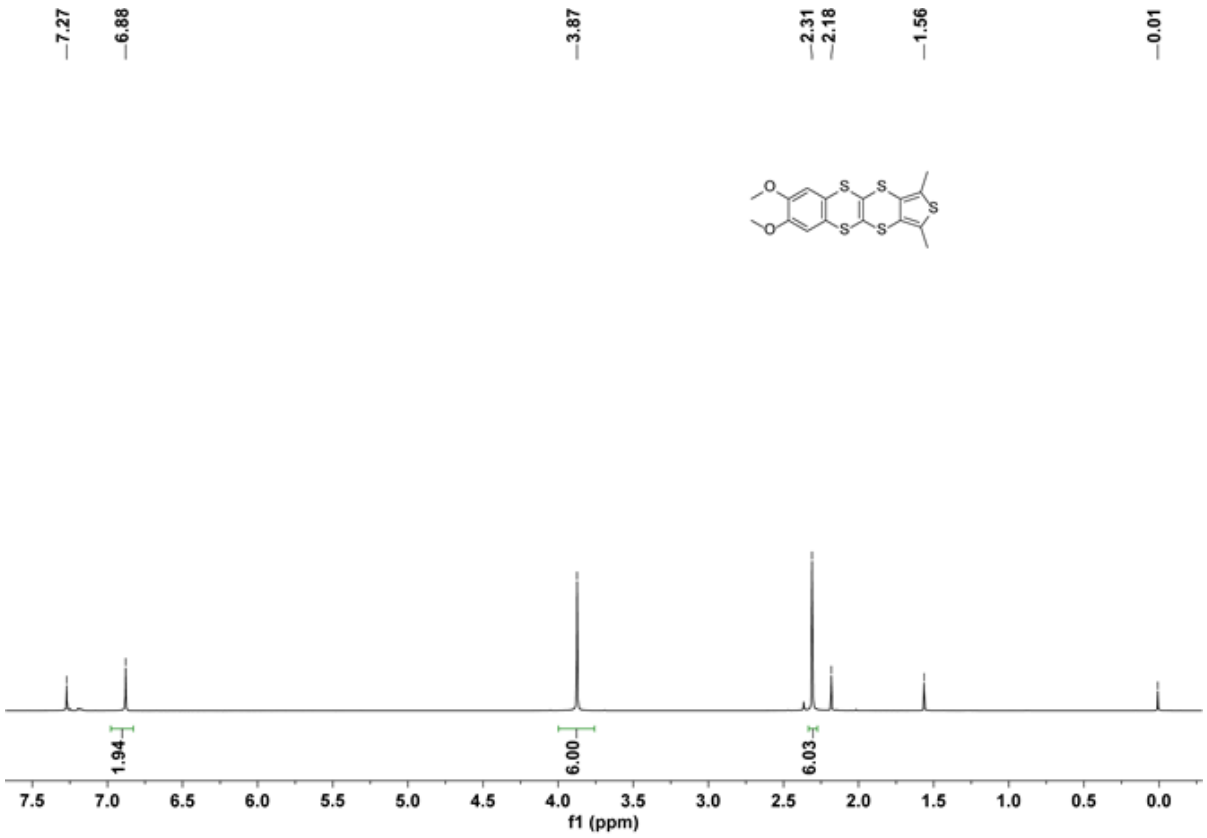
f1 (ppm)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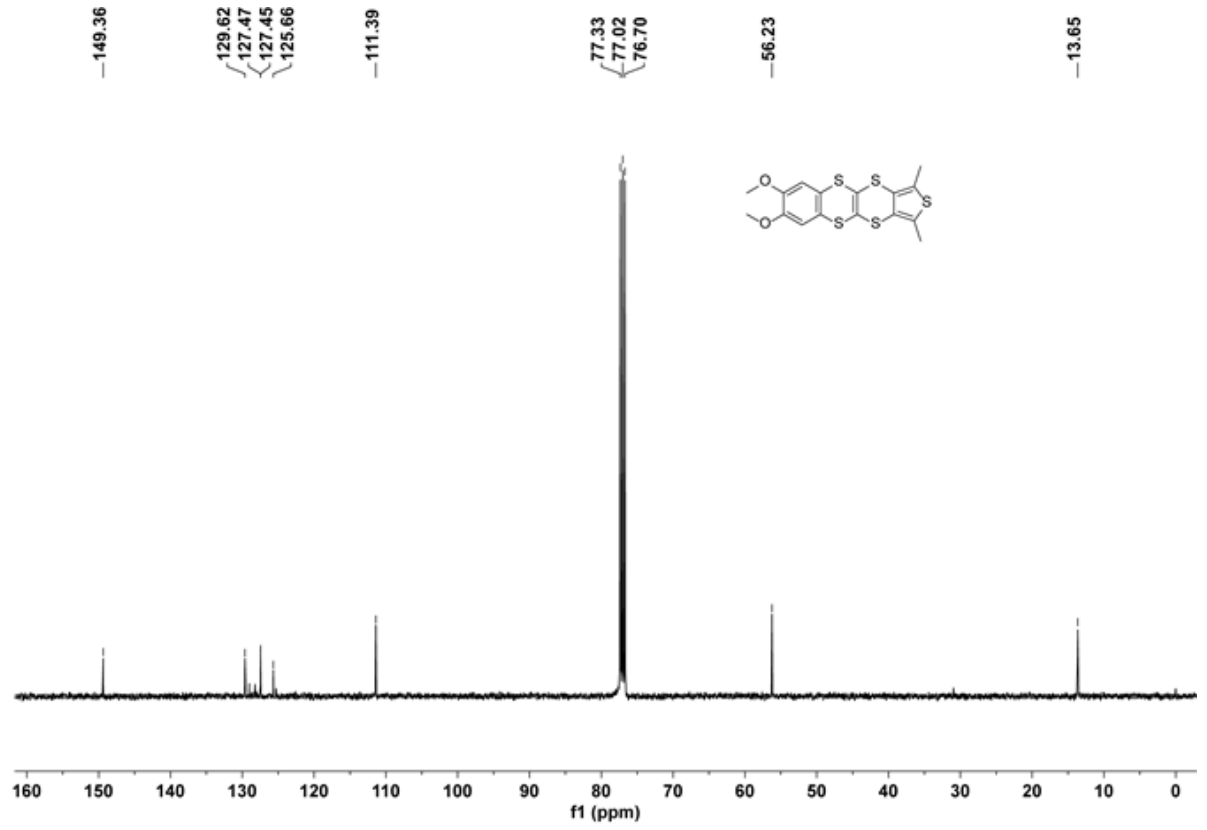
6.03
f1 (ppm)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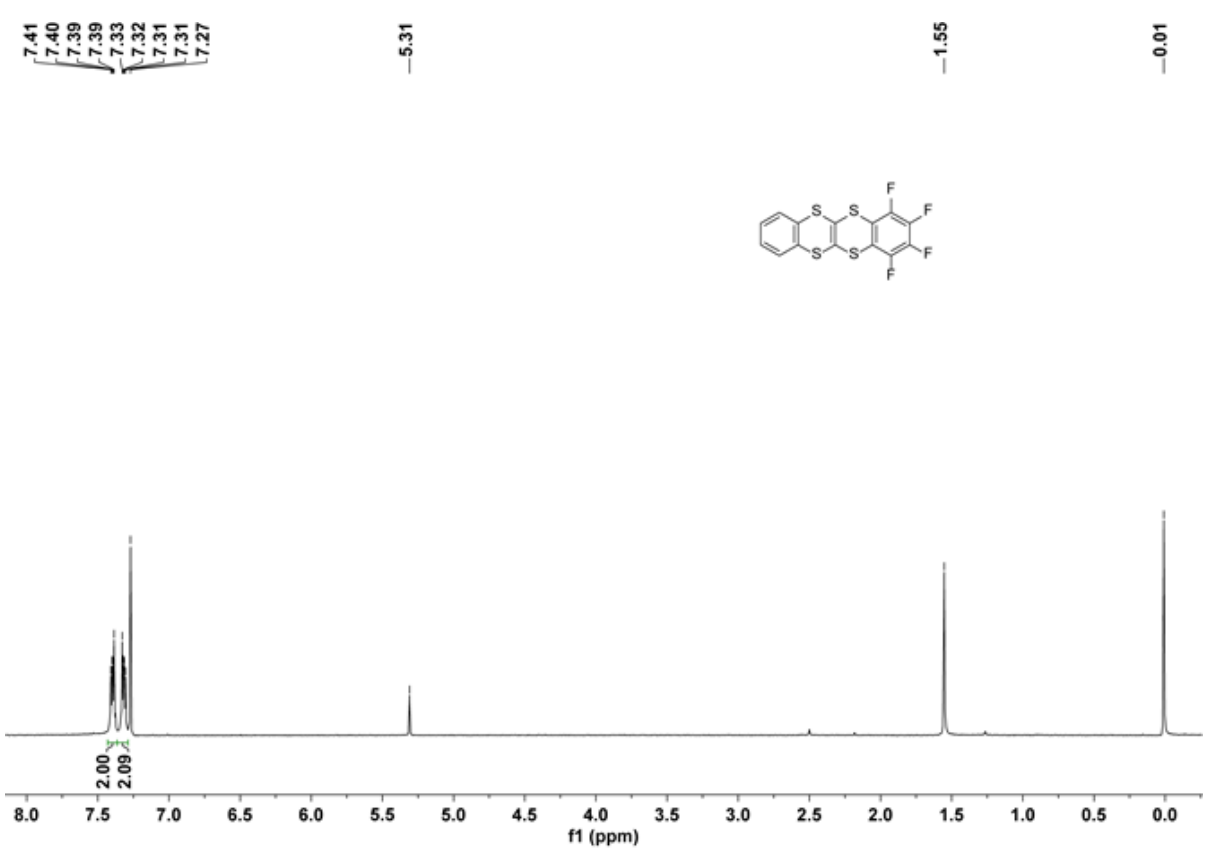
13.65
f1 (ppm)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7.33
7.32
7.31
7.31
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5.31
1.55
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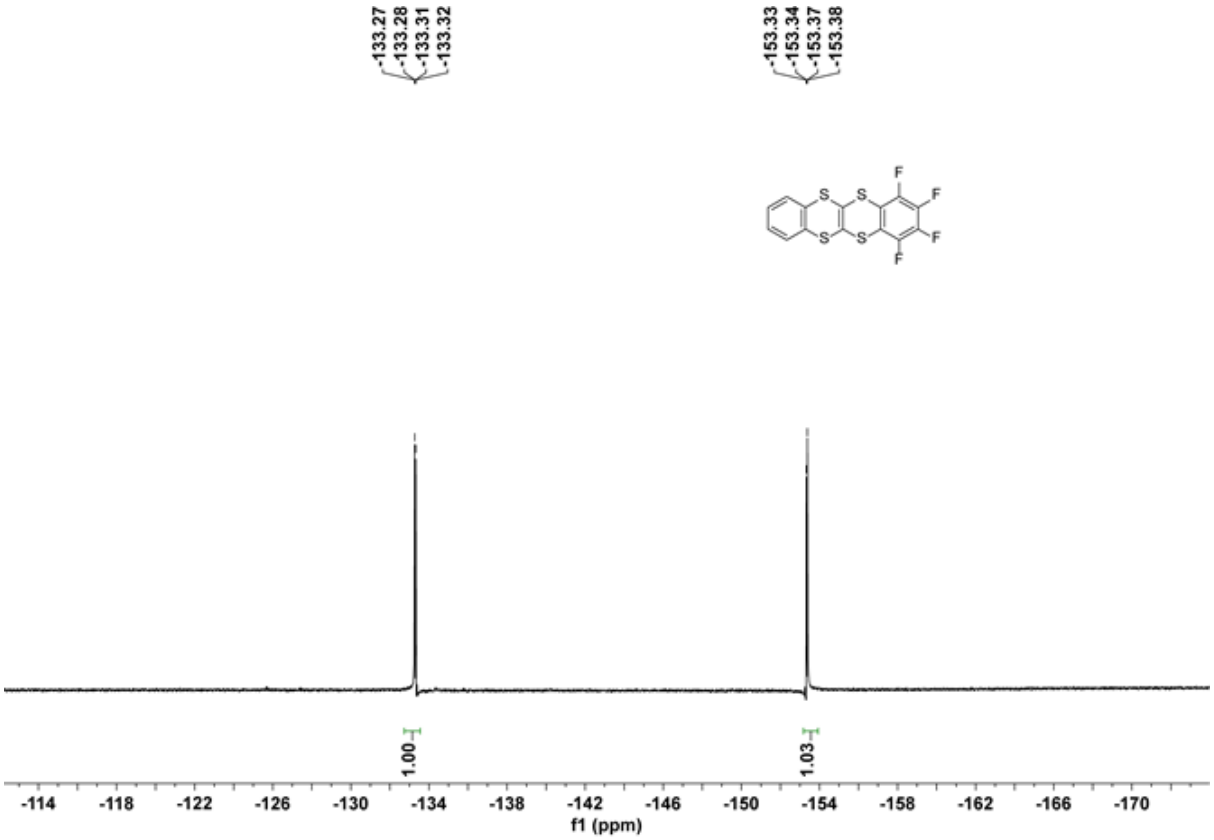
F
S
S
S
S
F
F
F
2.00
2.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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-133.28
-133.31
-133.32
-153.33
-153.34
-153.37
-153.38
F
S
S
S
S
F
F
F
1.00
1.03
-114
-118
-122
-126
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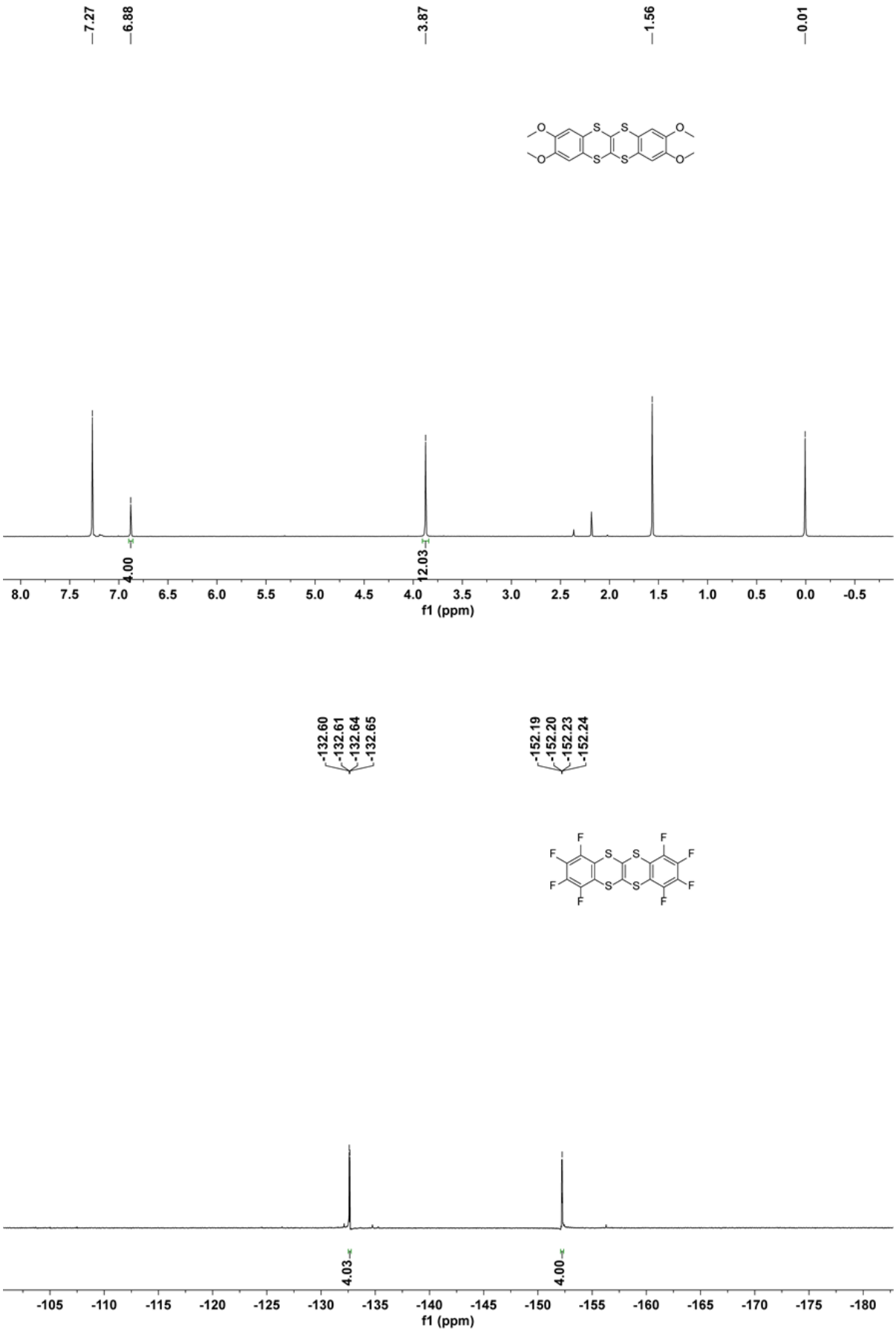
-134
-138
-142
-146
-150
-154
-158
-162
-166
-170
f1 (ppm)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4.00
12.03
f1 (ppm)
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-132.61
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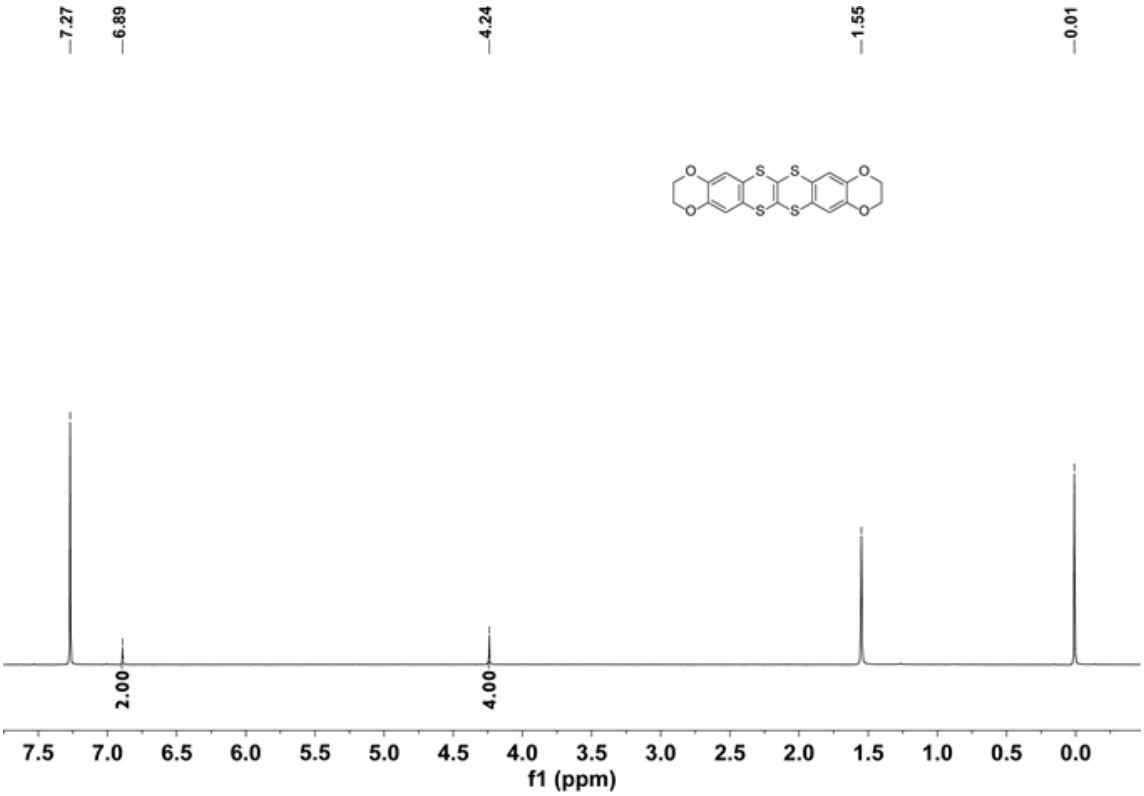
-152.20
-152.23
-152.24
4.03
4.00
f1 (ppm)

Figure S39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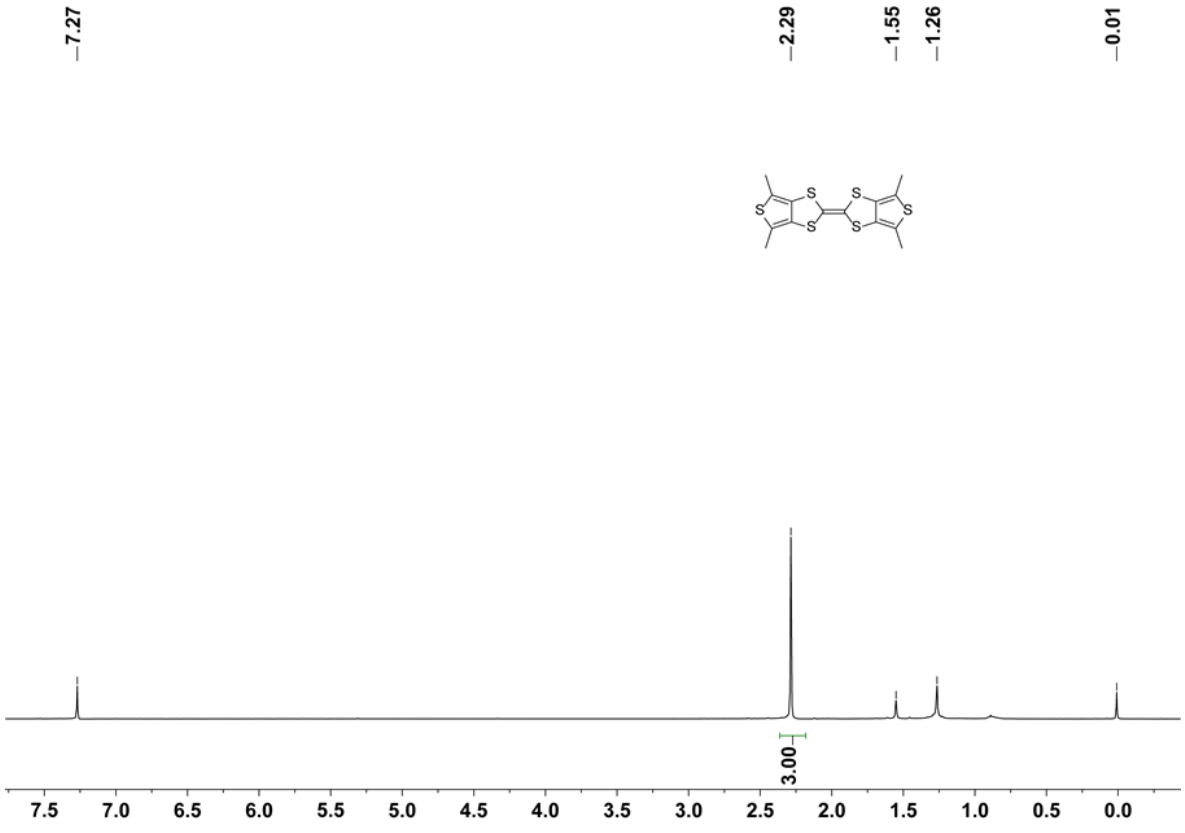
2.00
4.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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1.26
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3.00
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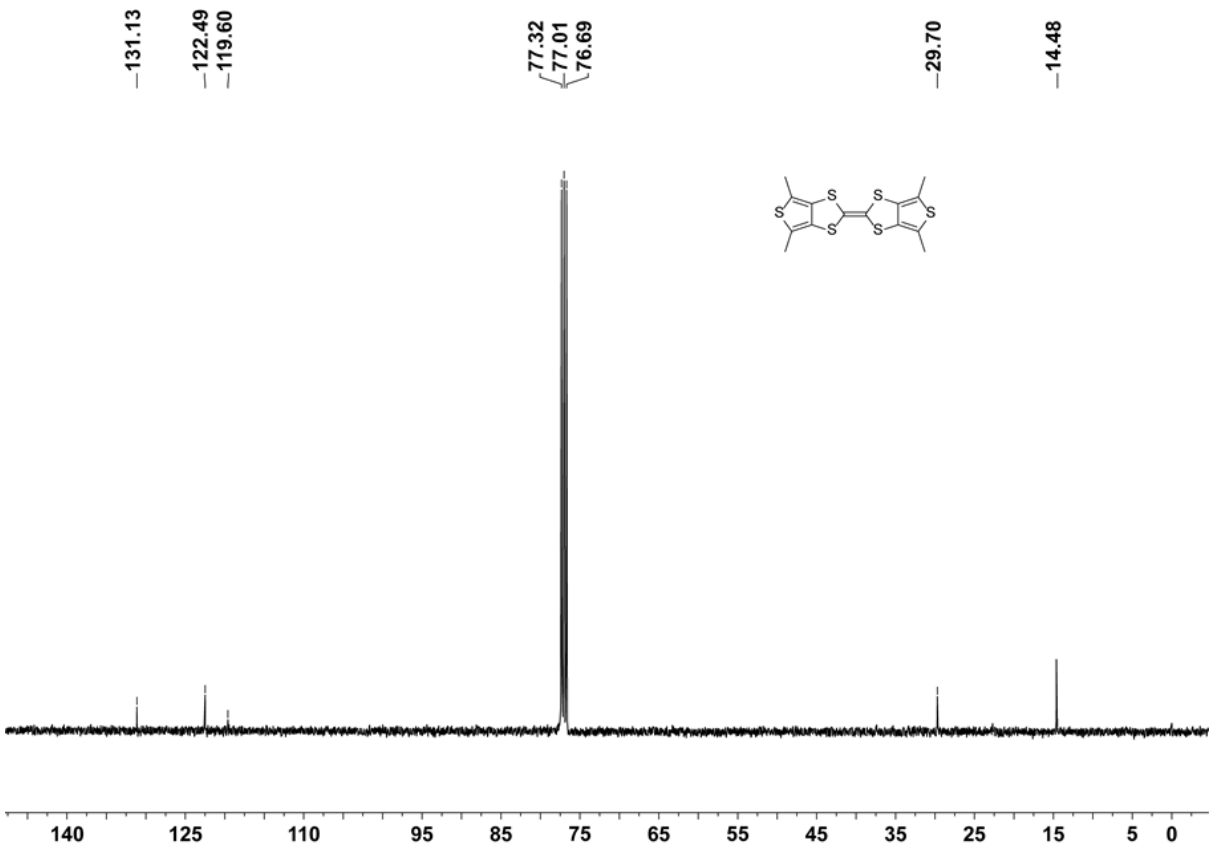
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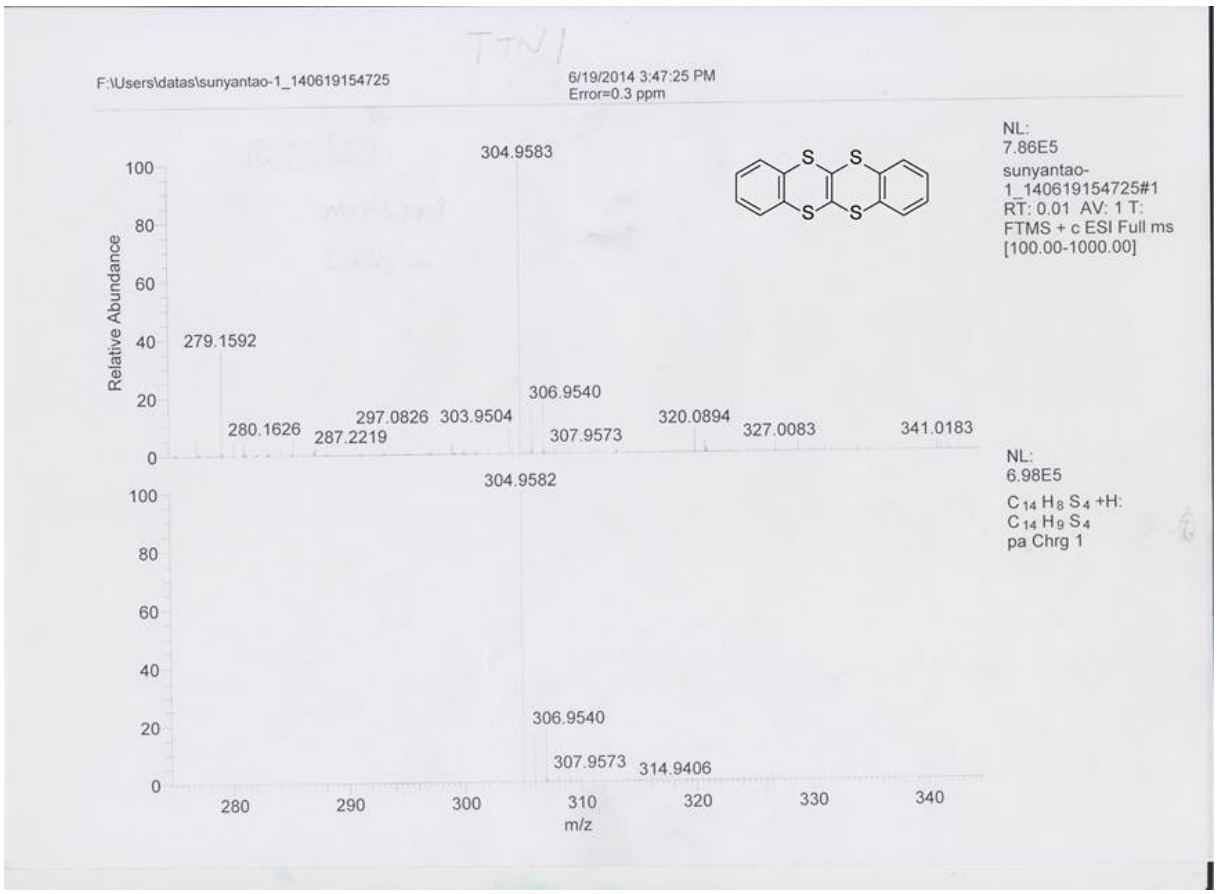
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RT: 0.01 AV: 1 T:
FTMS + c ESI Full ms
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279.1592
306.9540
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303.9504
280.1626
287.2219
307.9573
320.0894
327.0083
341.0183
Relative Abundance
NL:
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C14 H9 S4
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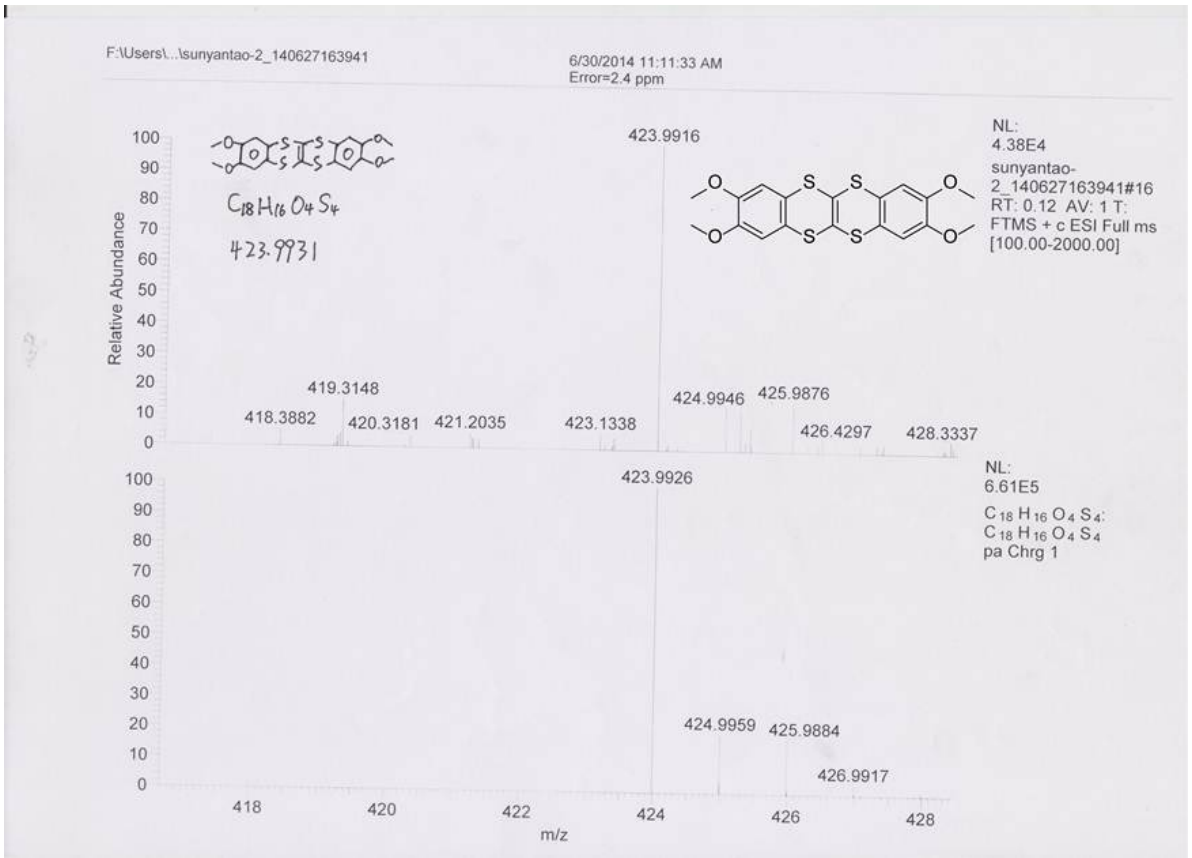
306.9540
307.9573
314.9406
m/z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FTMS + c ESI Full ms
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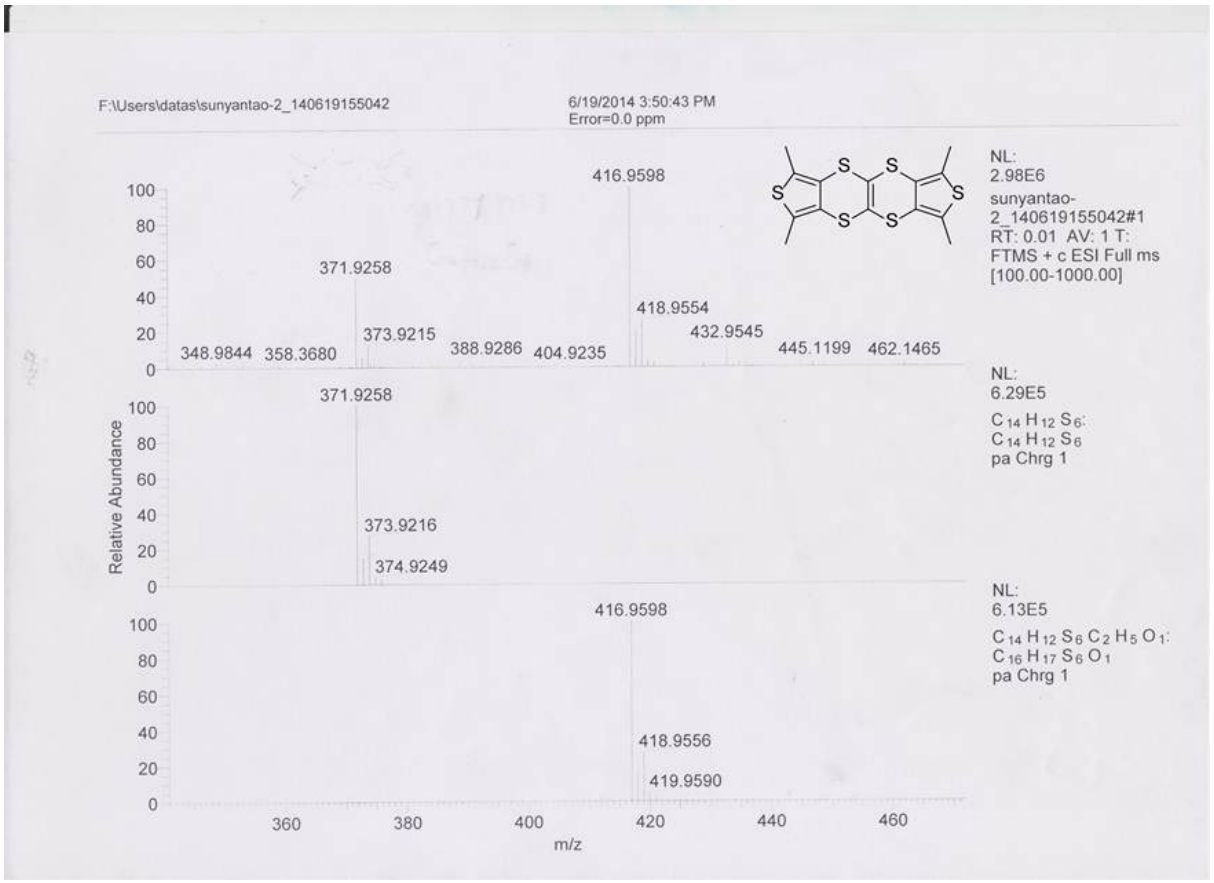
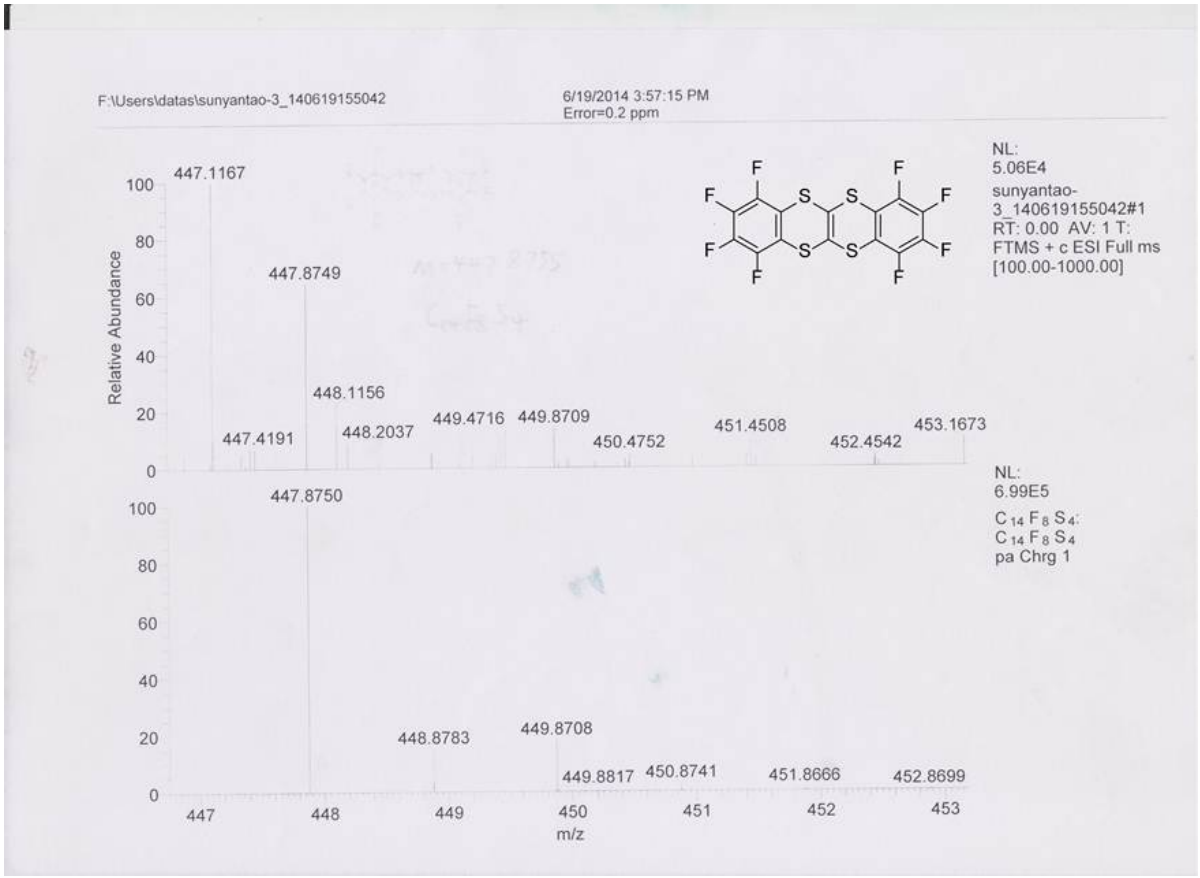
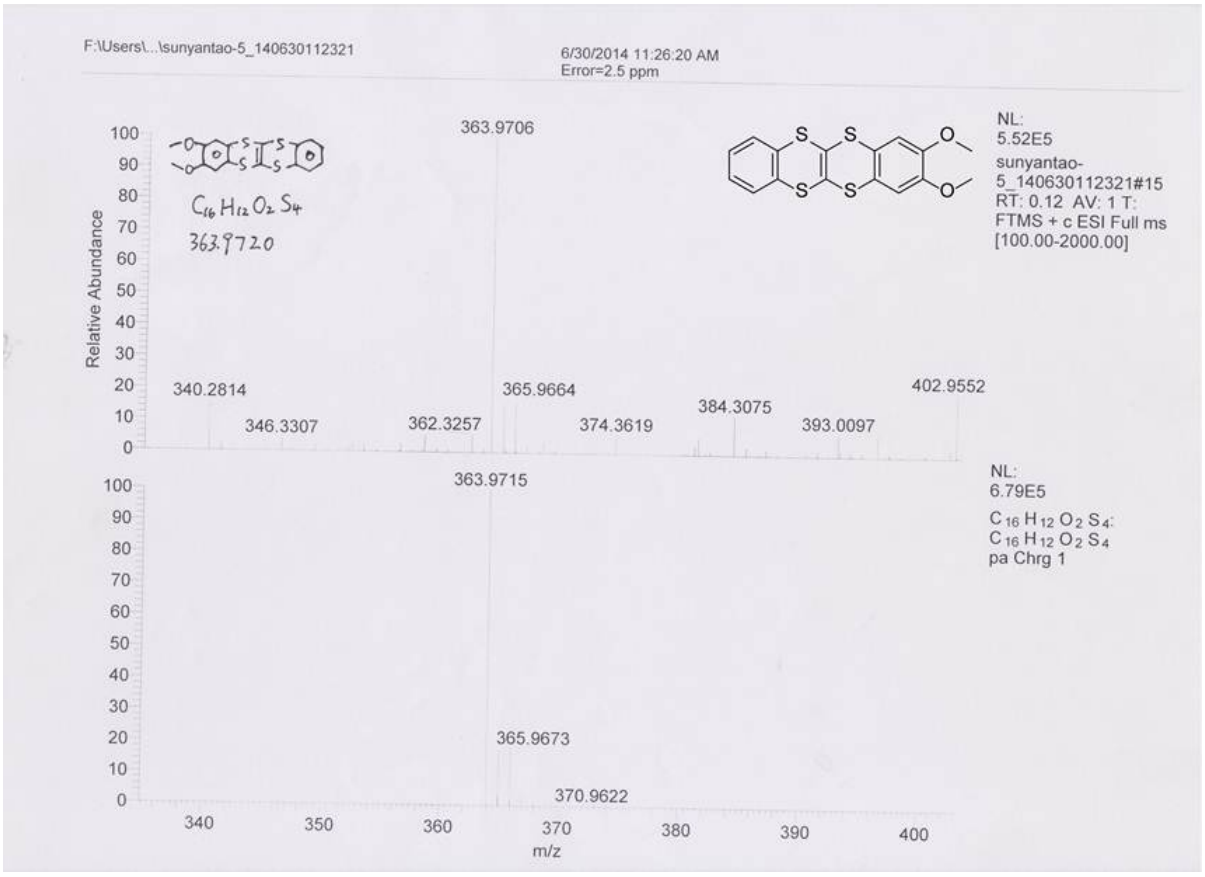
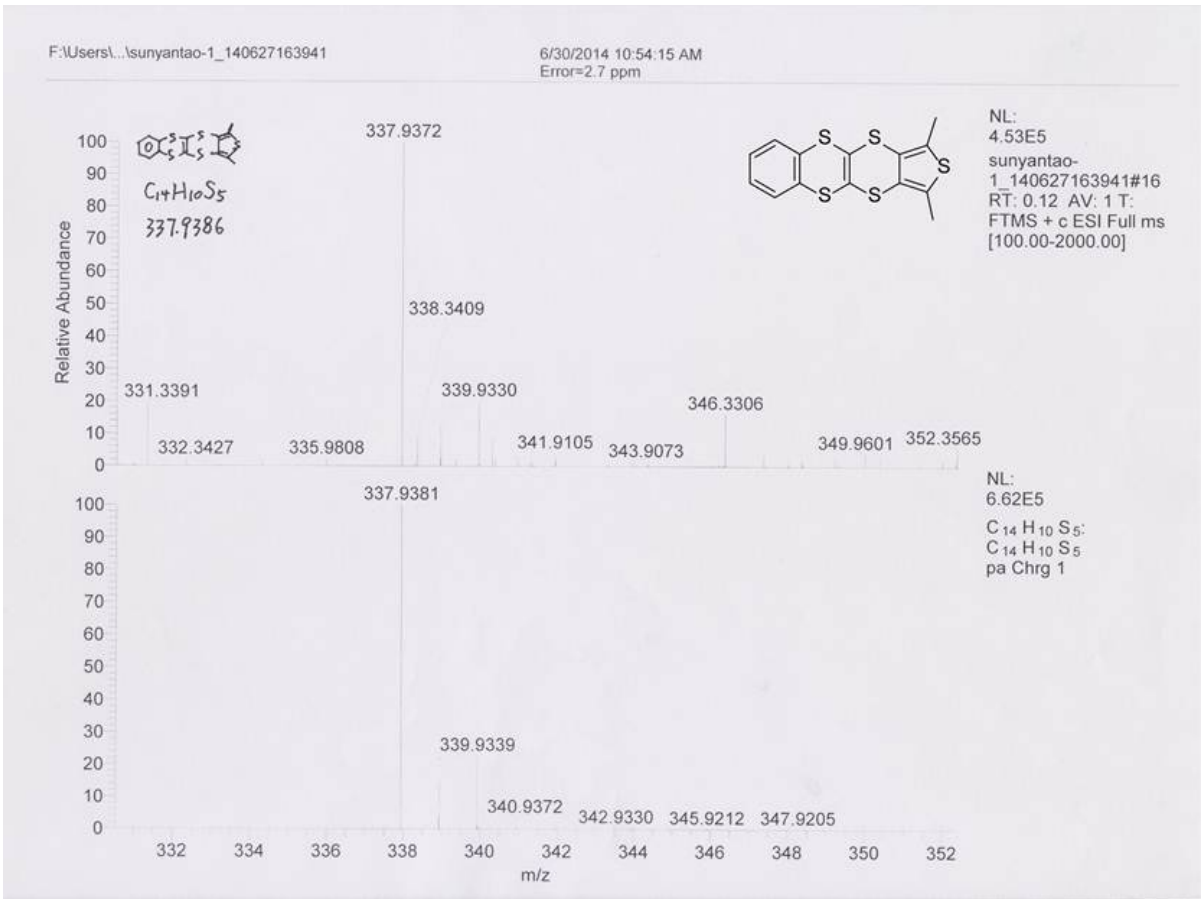
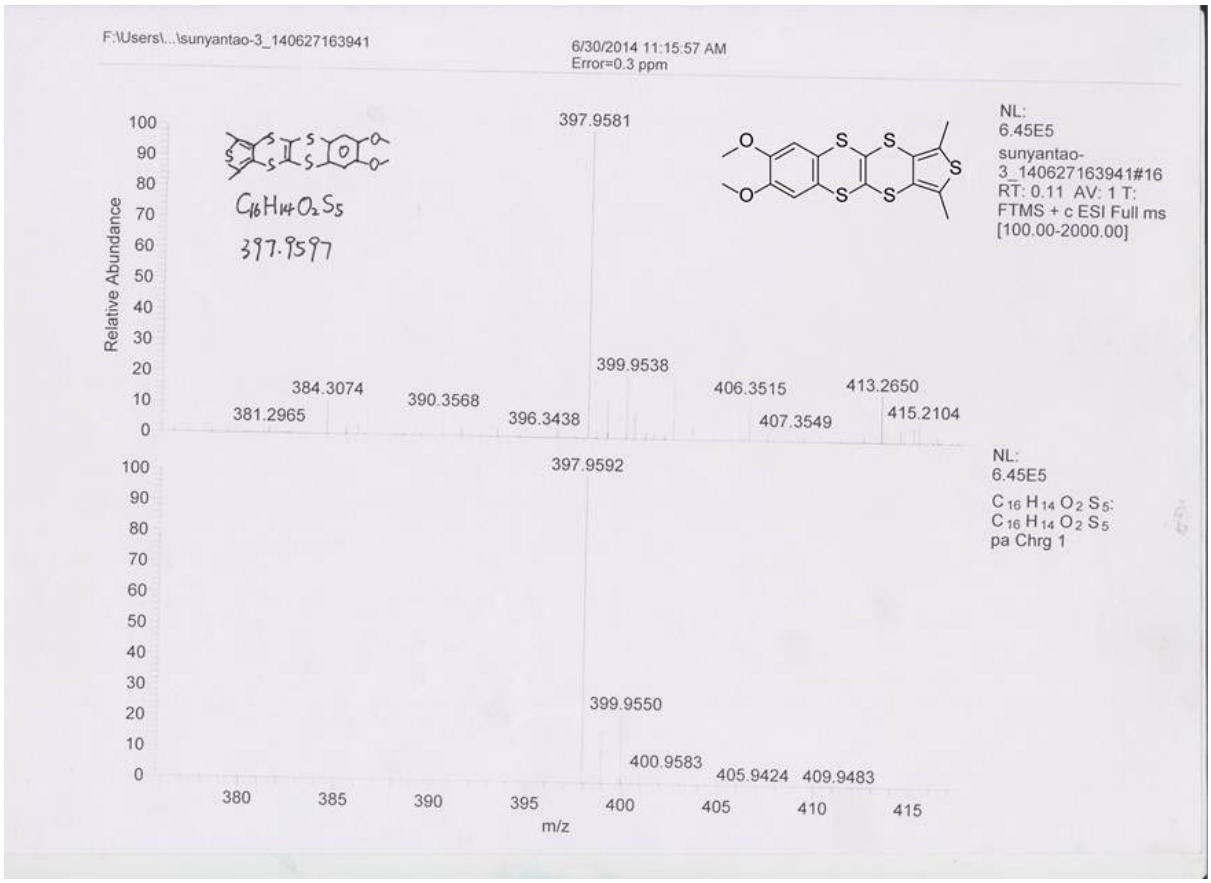
421.2035
423.1338
424.9946
425.9876
426.4297
428.3337
Relative Abundance
NL:
6.61E5
C18 H16 O4 S4:
C18 H16 O4 S4
pa Chrg 1
423.9926
424.9959
425.9884
426.9917
m/z

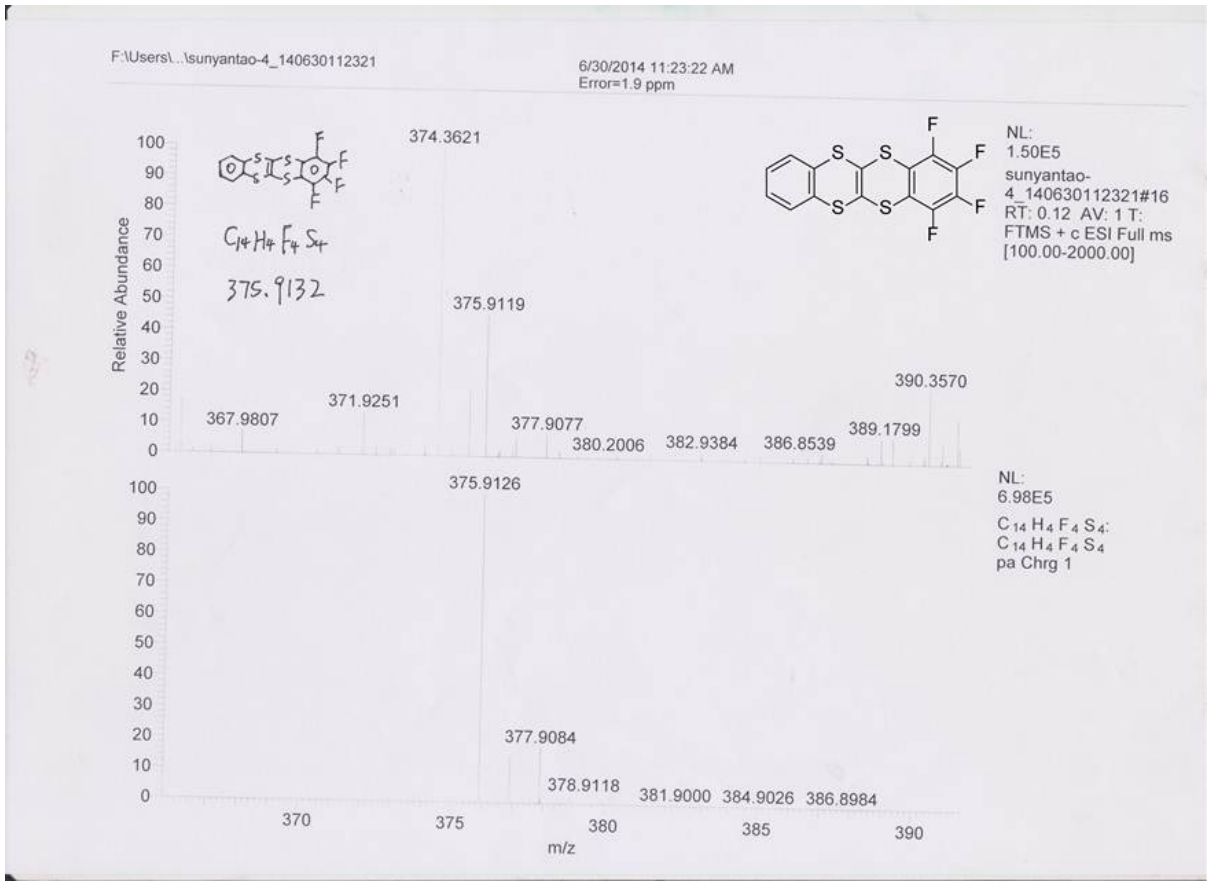

F:\Users\datas\sunyantao-2_140619155042
6/19/2014 3:50:43 PM
Error=0.0 ppm
NL:
2.98E6
sunyantao-2_140619155042#1
RT: 0.01 AV: 1 T:
FTMS + c ESI Full ms
[100.00-1000.00]
NL:
6.29E5
C14 H12 S6:
C14 H12 S6
pa Chrg 1
NL:
6.13E5
C14 H12 S6 C2 H5 O1:
C16 H17 S6 O1
pa Chrg 1
Relative Abundance
m/z

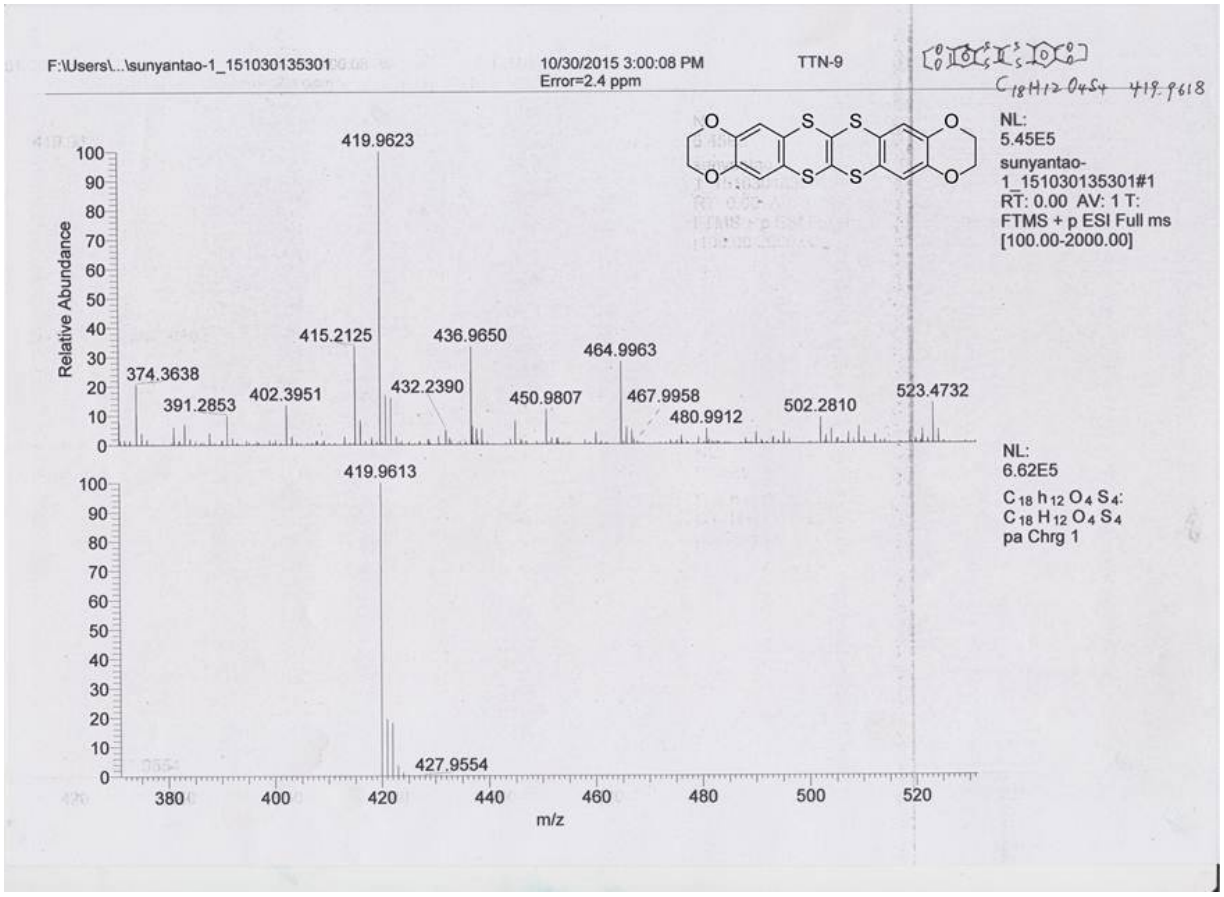

F:\Users\datas\sunyantao-3_140619155042
6/19/2014 3:57:15 PM
Error=0.2 ppm
NL:
5.06E4
sunyantao-3_140619155042#1
RT: 0.00 AV: 1 T:
FTMS + c ESI Full ms
[100.00-1000.00]
NL:
6.99E5
C14 F8 S4:
C14 F8 S4
pa Chrg 1
Relative Abundance
m/z

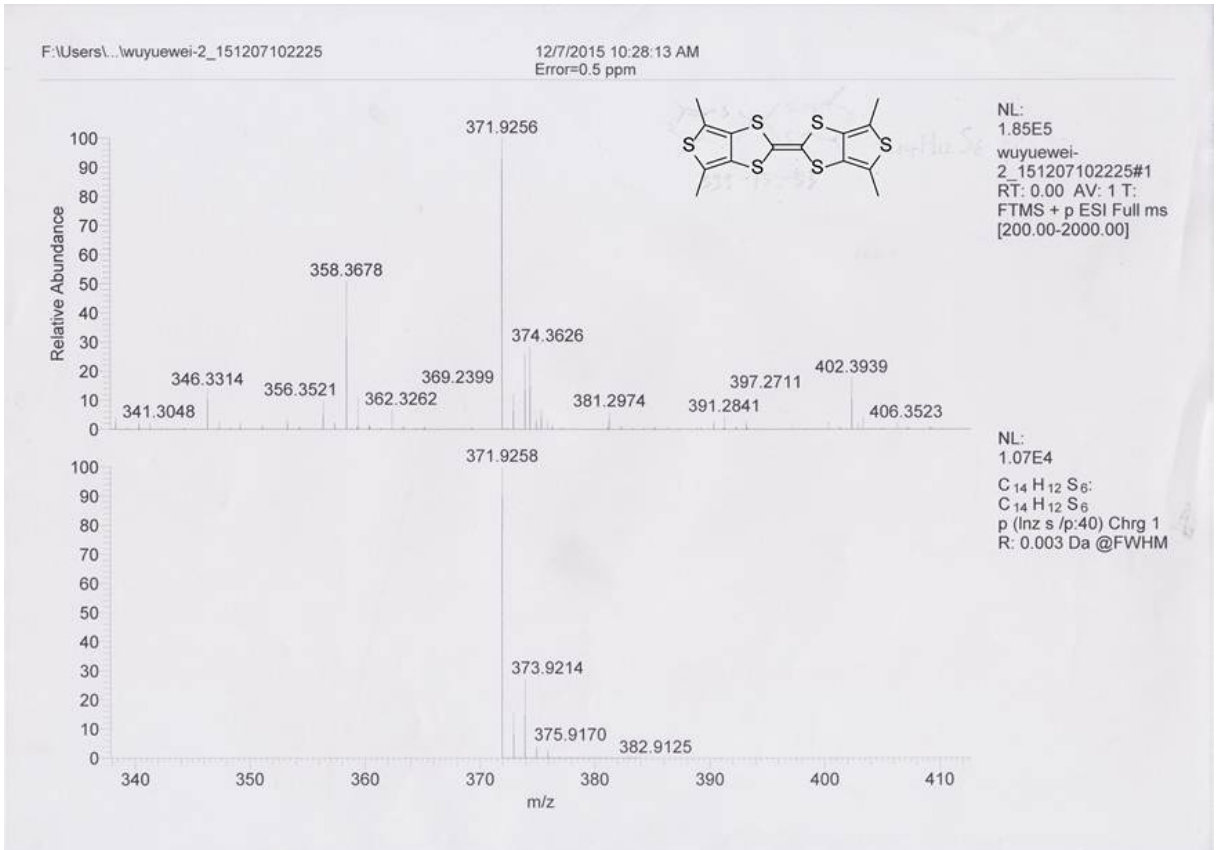

F:\Users\...\sunyantao-5_140630112321
6/30/2014 11:26:20 AM
Error=2.5 ppm
C16 H12 O2 S4
363.9720
363.9706
NL:
5.52E5
sunyantao-5_140630112321#15
RT: 0.12 AV: 1 T:
FTMS + c ESI Full ms
[100.00-2000.00]
340.2814
346.3307
362.3257
365.9664
374.3619
384.3075
393.0097
402.9552
Relative Abundance
NL:
6.79E5
C16 H12 O2 S4:
C16 H12 O2 S4
pa Chrg 1
363.9715
365.9673
370.9622
m/z


F:\Users\...\sunyantao-1_140627163941
6/30/2014 10:54:15 AM
Error=2.7 ppm
C14H10S5
337.9386
337.9372
NL:
4.53E5
sunyantao-1_140627163941#16
RT: 0.12 AV: 1 T:
FTMS + c ESI Full ms
[100.00-2000.00]
331.3391
332.3427
335.9808
338.3409
339.9330
341.9105
343.9073
346.3306
349.9601
352.3565
Relative Abundance
NL:
6.62E5
C14 H10 S5:
C14 H10 S5
pa Chrg 1
337.9381
339.9339
340.9372
342.9330
345.9212
347.9205
m/z


F:\Users\...\sunyantao-3_140627163941
6/30/2014 11:15:57 AM
Error=0.3 ppm
C16H14O2S5
397.9597
397.9581
399.9538
384.3074
390.3568
381.2965
396.3438
406.3515
413.2650
407.3549
415.2104
NL:
6.45E5
sunyantao-3_140627163941#16
RT: 0.11 AV: 1 T:
FTMS + c ESI Full ms
[100.00-2000.00]
Relative Abundance
397.9592
399.9550
400.9583
405.9424
409.9483
NL:
6.45E5
C16 H14 O2 S5:
C16 H14 O2 S5
pa Chrg 1
m/z


F:\Users\...\sunyantao-4_140630112321
6/30/2014 11:23:22 AM
Error=1.9 ppm
C14H4F4S4
375.9132
374.3621
375.9119
371.9251
367.9807
377.9077
380.2006
382.9384
386.8539
389.1799
390.3570
NL:
1.50E5
sunyantao-4_140630112321#16
RT: 0.12 AV: 1 T:
FTMS + c ESI Full ms
[100.00-2000.00]
Relative Abundance
375.9126
377.9084
378.9118
381.9000
384.9026
386.8984
NL:
6.98E5
C14 H4 F4 S4:
C14 H4 F4 S4
pa Chrg 1
m/z


F:\Users\...\sunyantao-1_151030135301
10/30/2015 3:00:08 PM
Error=2.4 ppm
TTN-9
C18H12O4S4 419.9618
NL:
5.45E5
sunyantao-1_151030135301#1
RT: 0.00 AV: 1 T:
FTMS + p ESI Full ms
[100.00-2000.00]
419.9623
415.2125
436.9650
464.9963
374.3638
391.2853
402.3951
432.2390
450.9807
467.9958
480.9912
502.2810
523.4732
NL:
6.62E5
C18 h12 O4 S4:
C18 H12 O4 S4
pa Chrg 1
419.9613
427.9554
Relative Abundance
m/z


F:\Users\...\wuyuewei-2_151207102225
12/7/2015 10:28:13 AM
Error=0.5 ppm
NL:
1.85E5
wuyuewei-2_151207102225#1
RT: 0.00 AV: 1 T:
FTMS + p ESI Full ms
[200.00-2000.00]
371.9256
358.3678
374.3626
346.3314
356.3521
362.3262
369.2399
381.2974
391.2841
397.2711
402.3939
406.3523
341.3048
NL:
1.07E4
C14 H12 S6:
C14 H12 S6
p (lnz s /p:40) Chrg 1
R: 0.003 Da @FWHM
371.9258
373.9214
375.9170
382.9125
Relative Abundance
m/z