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Electronic Supplementary Information for

Selective dispersion and separation of single-walled carbon nanotubes using conformationally switchable TTFV-phenylacetylene polymers

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1. NMR Spectra for New Compounds

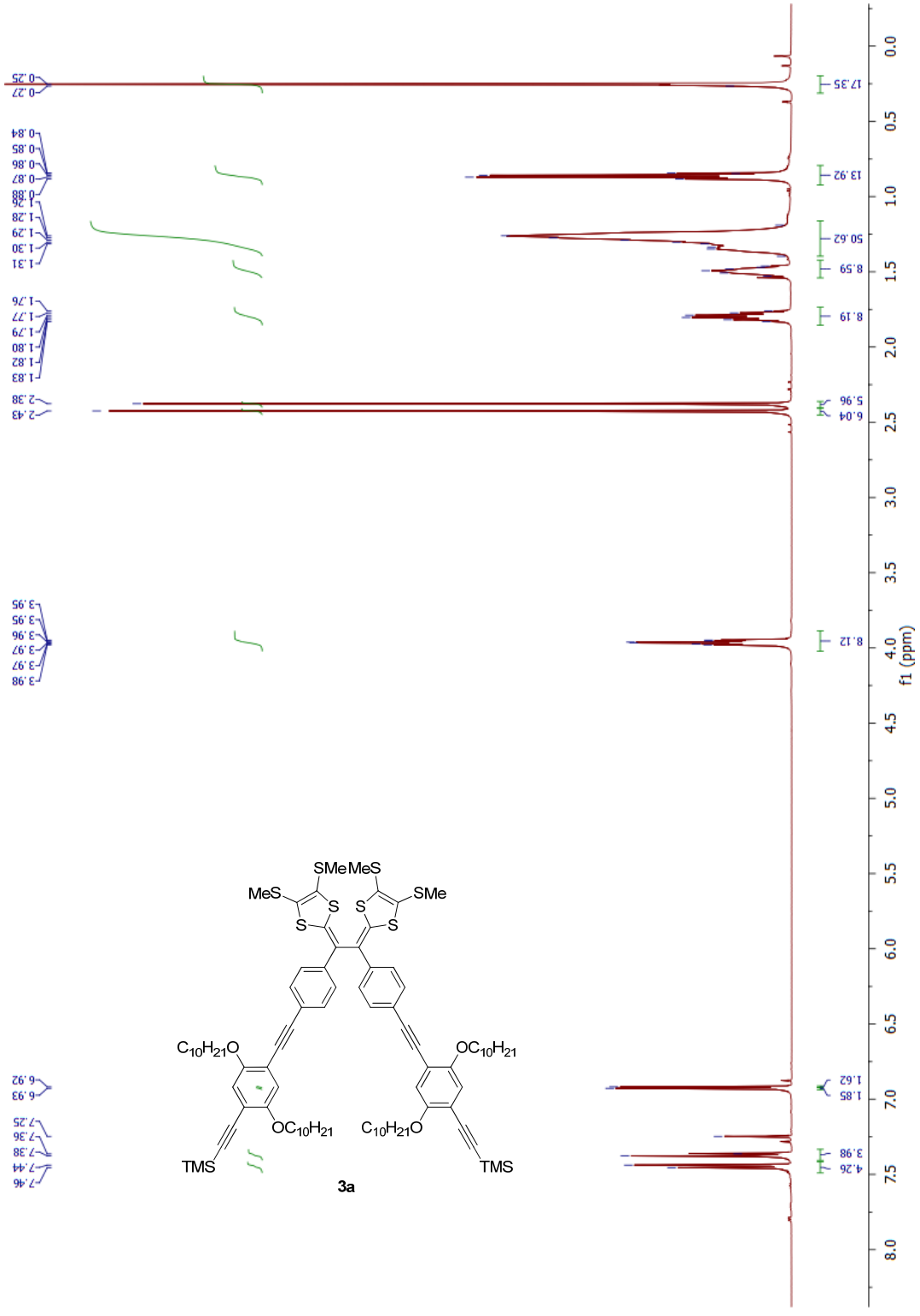

Figure S1: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **3a**.

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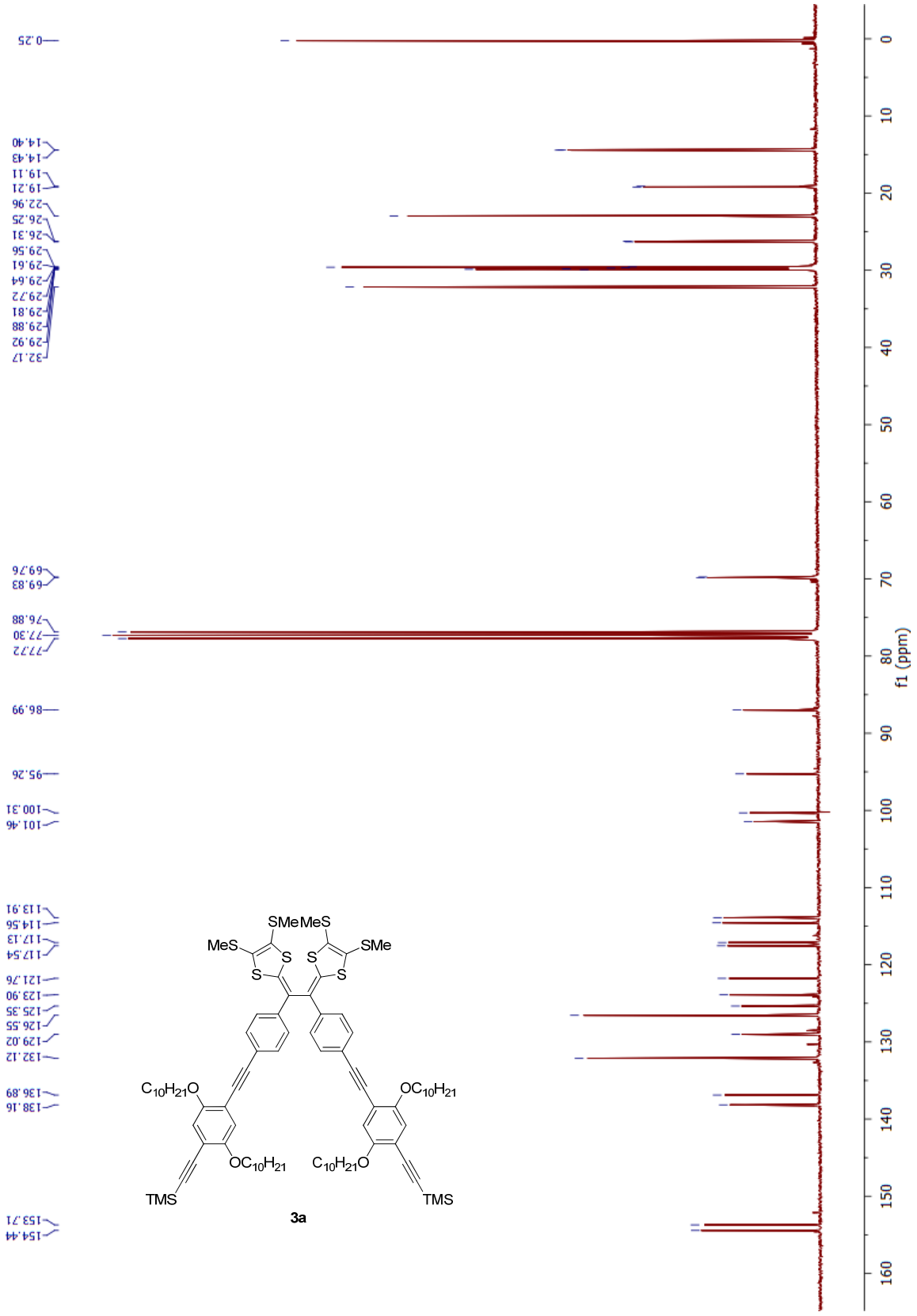

Figure S2: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3a**.

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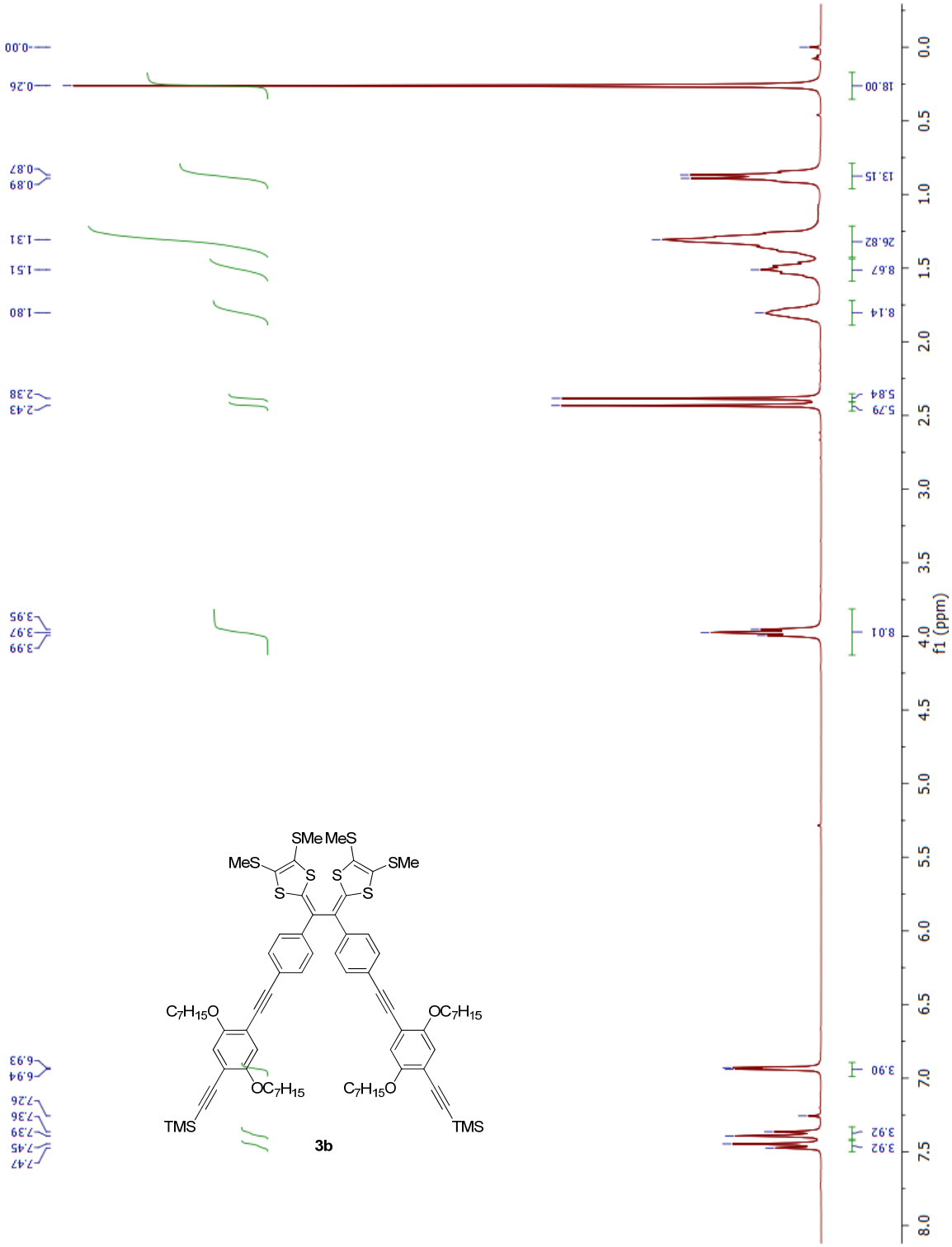

Figure S3: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **3b**.

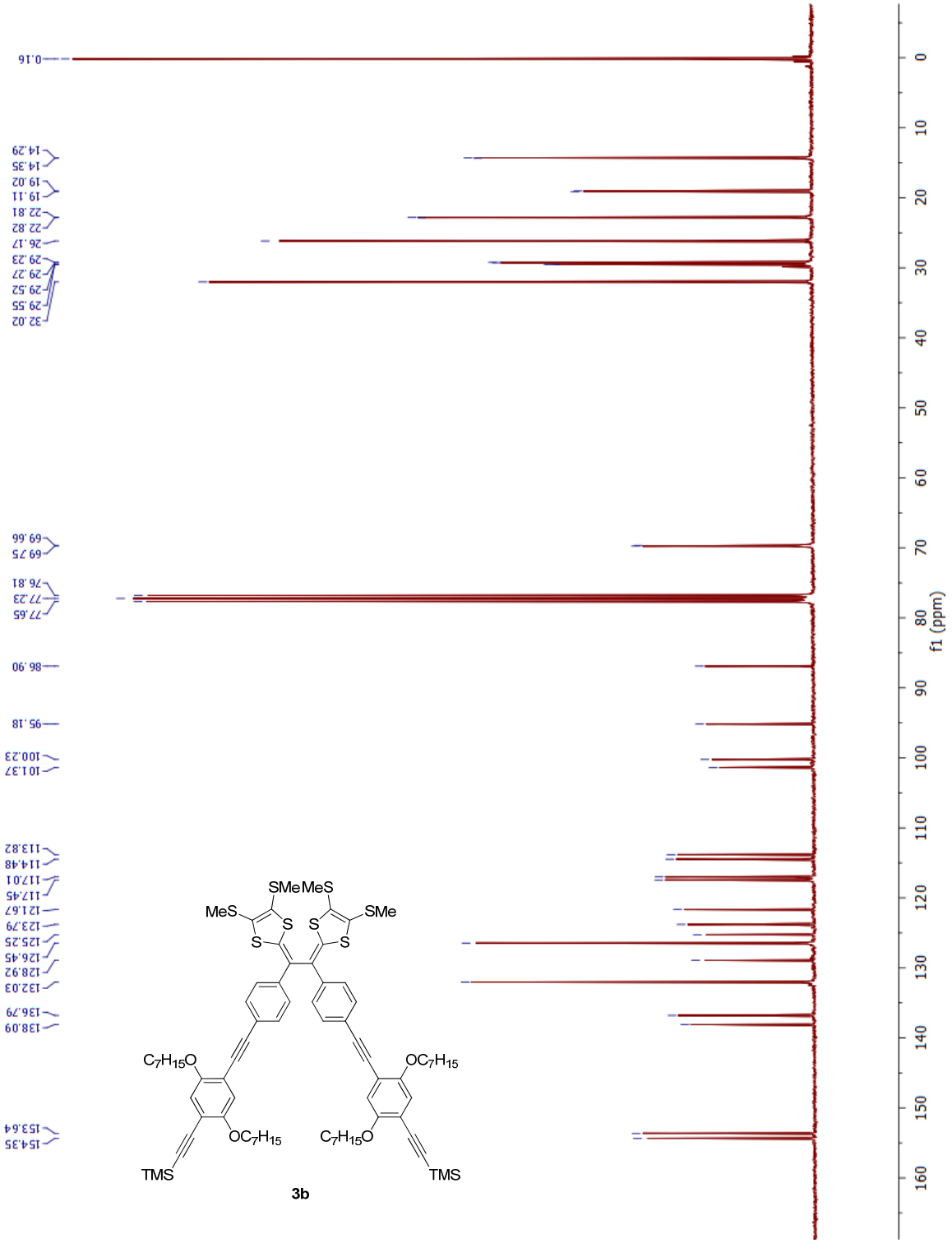

Figure S4: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3b**.

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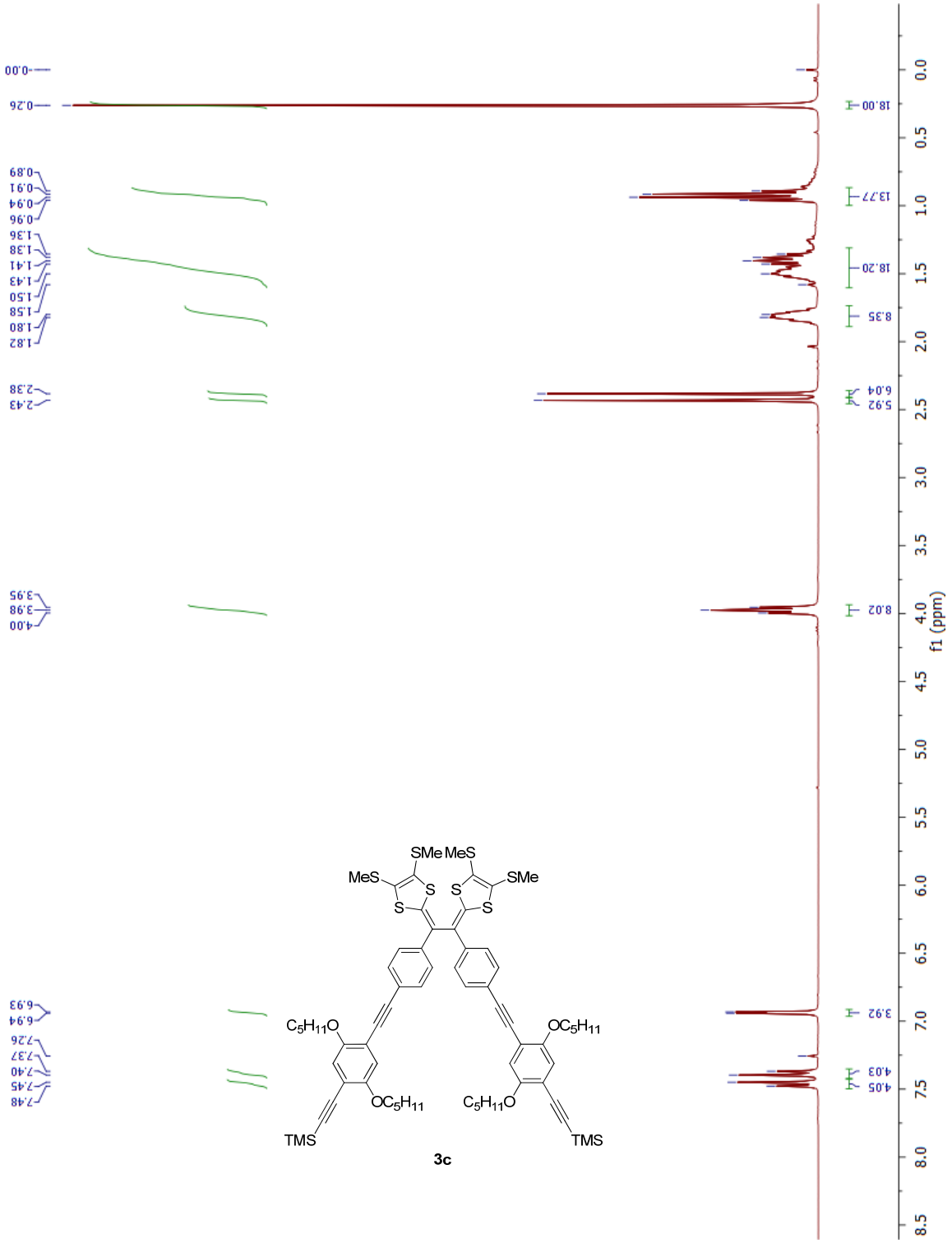

Figure S5: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **3c**.

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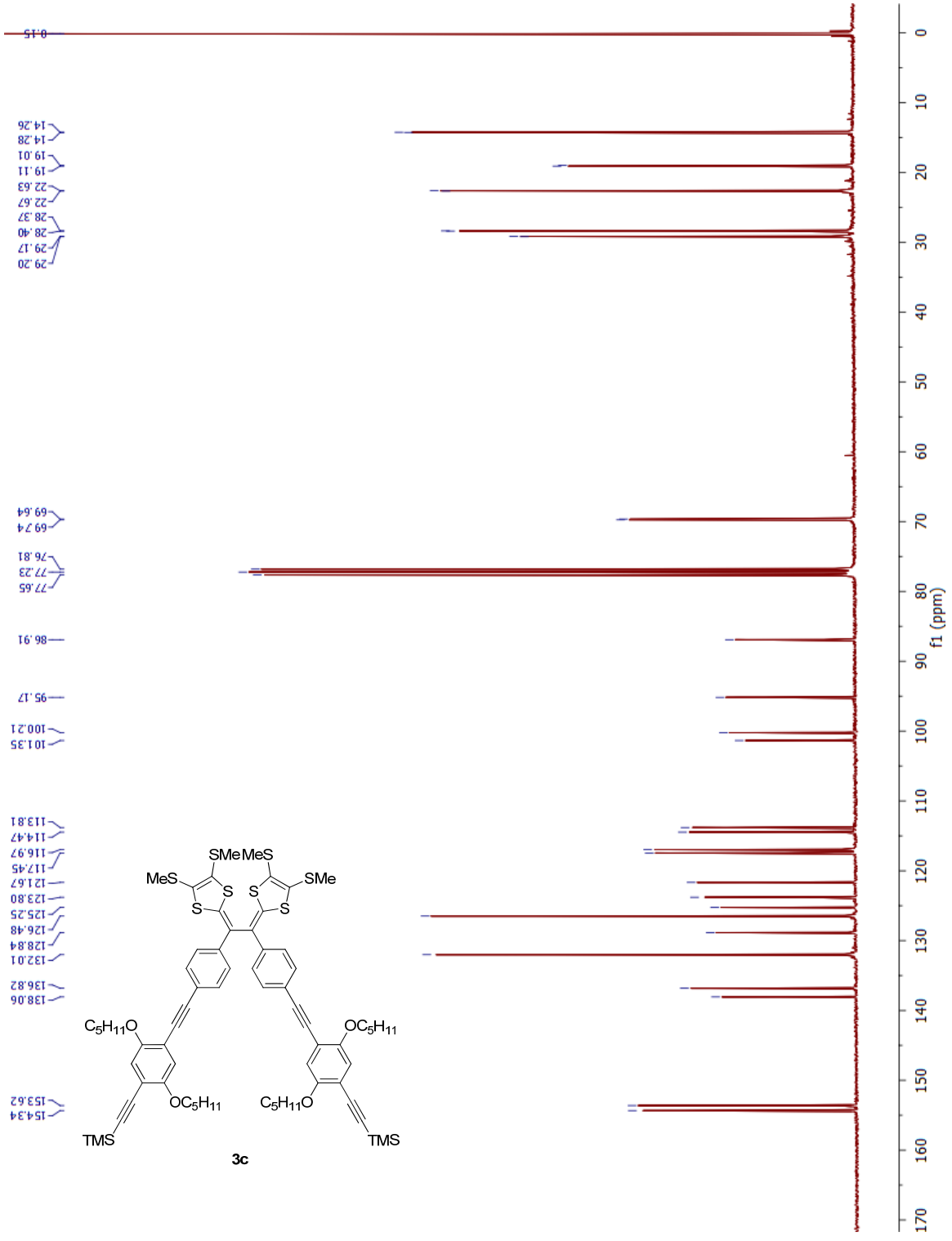

Figure S6: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3c**.

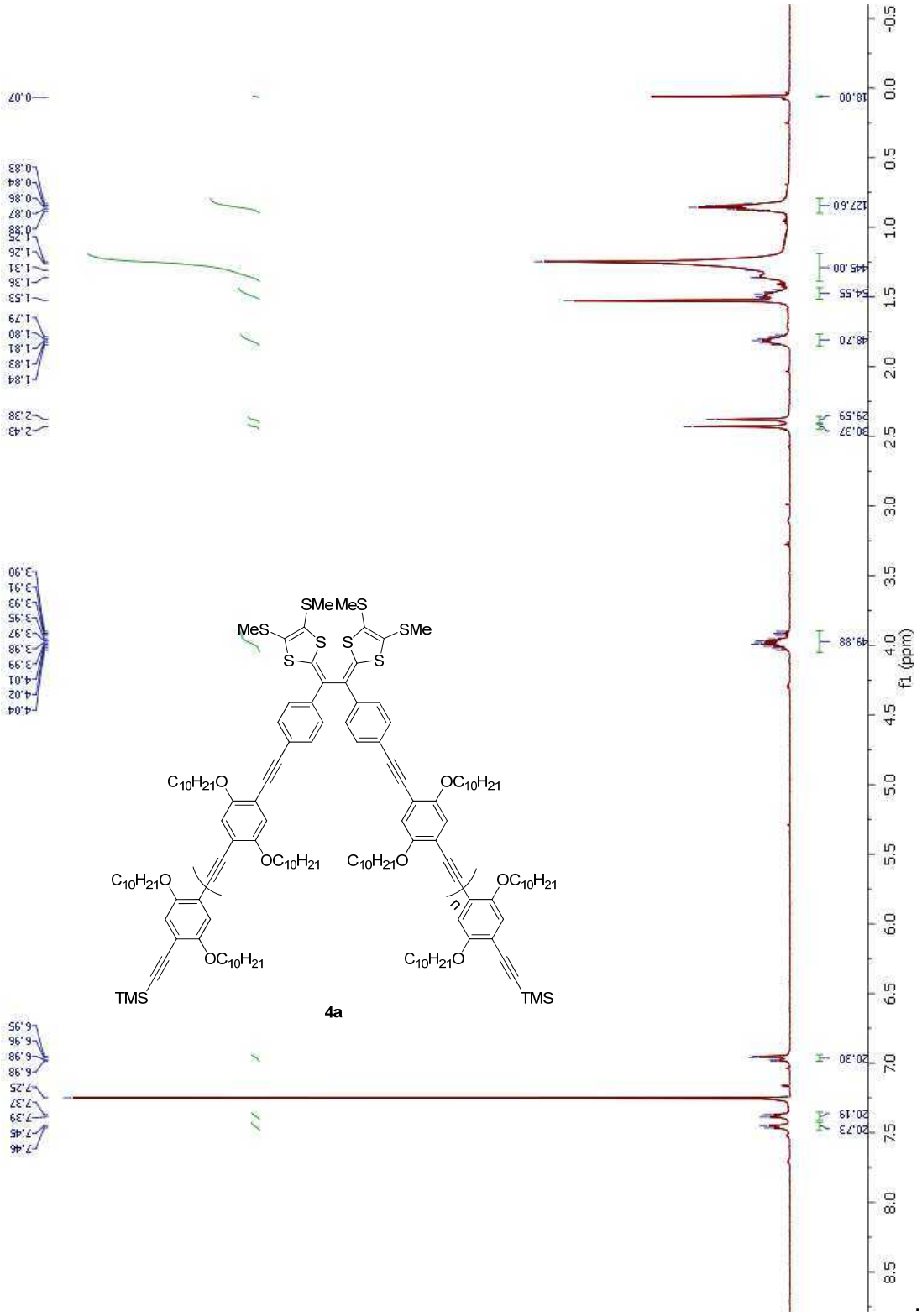

Figure S7: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **4a**.

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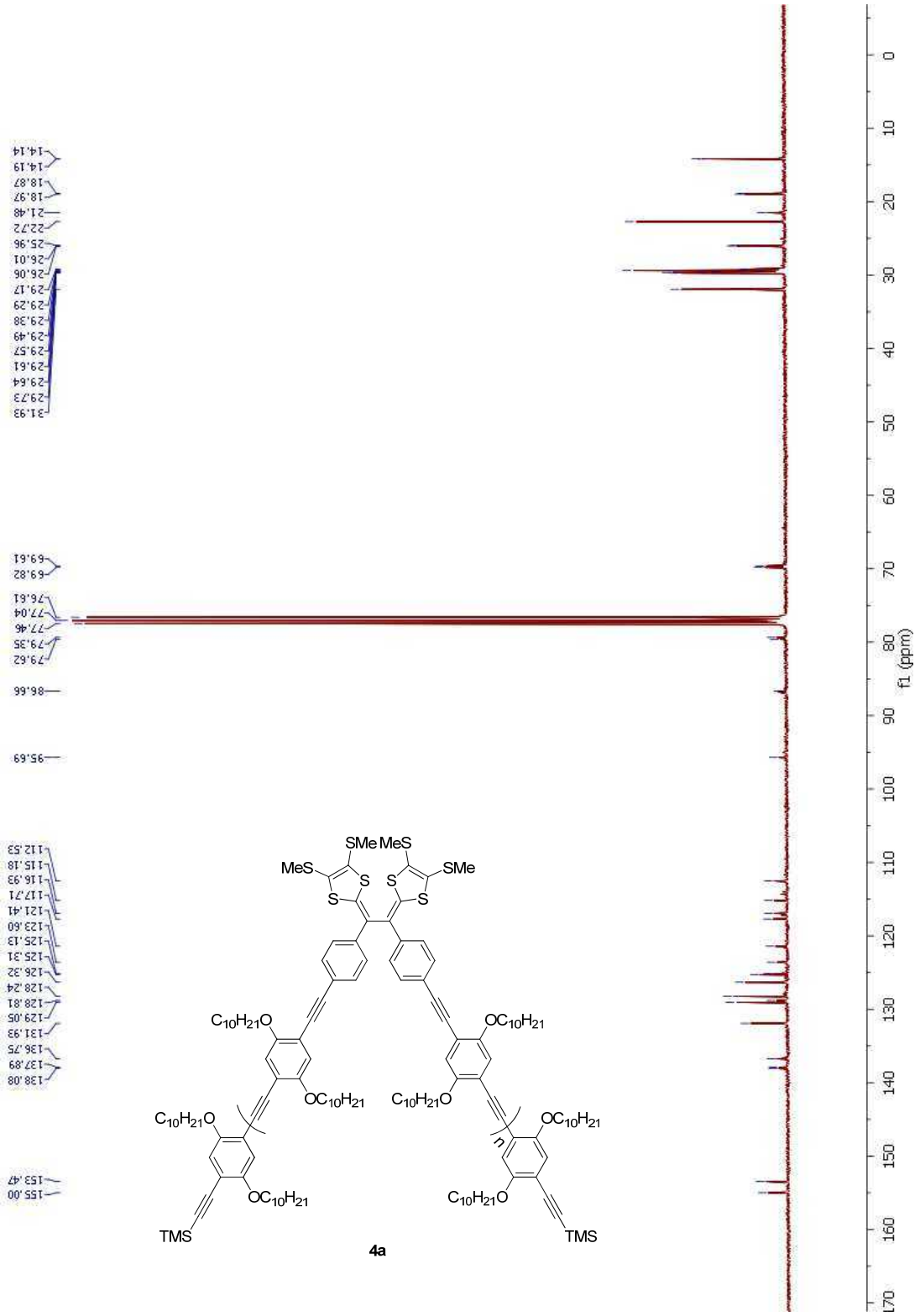

Figure S8: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **4a**.

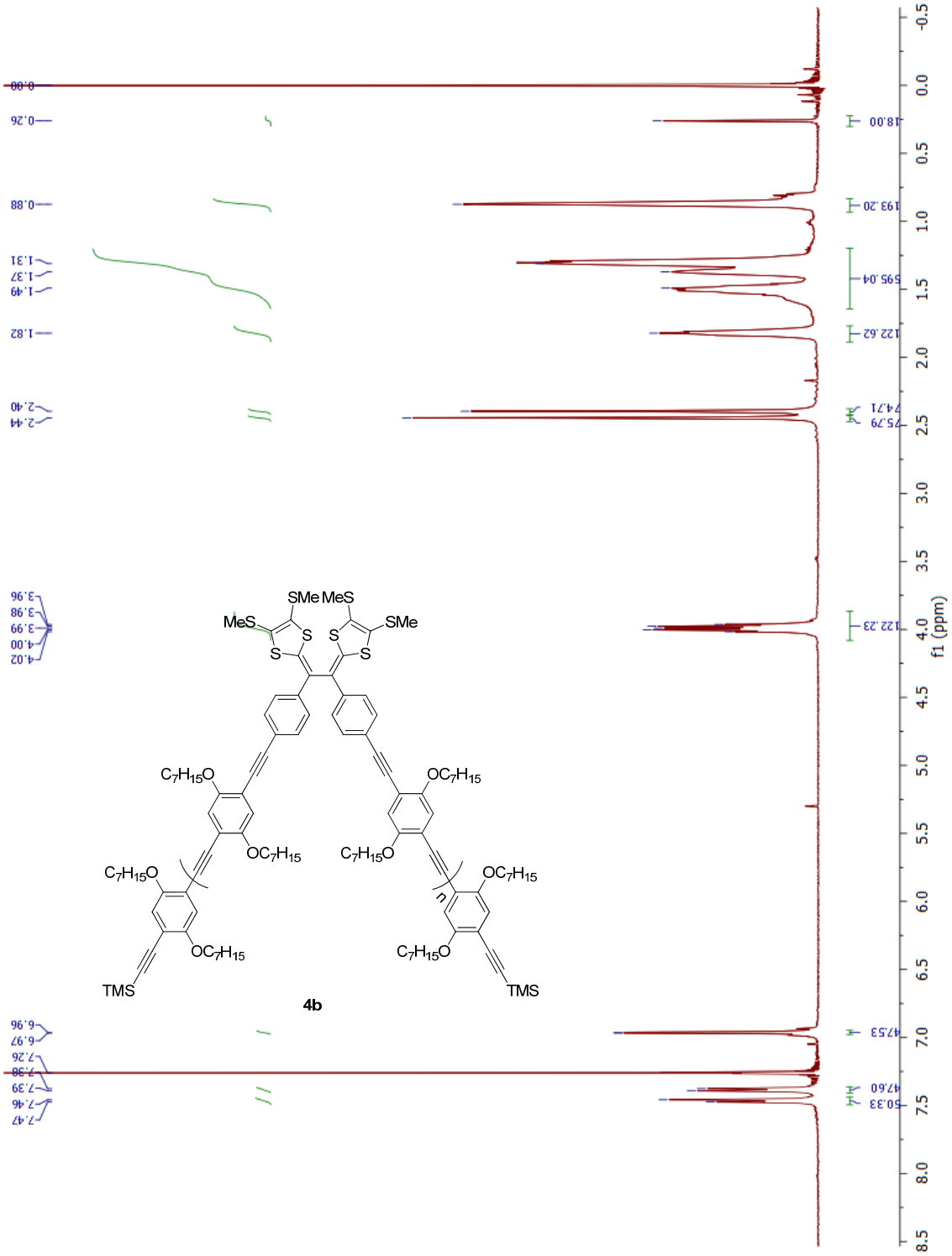

Figure S9: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **4b**.

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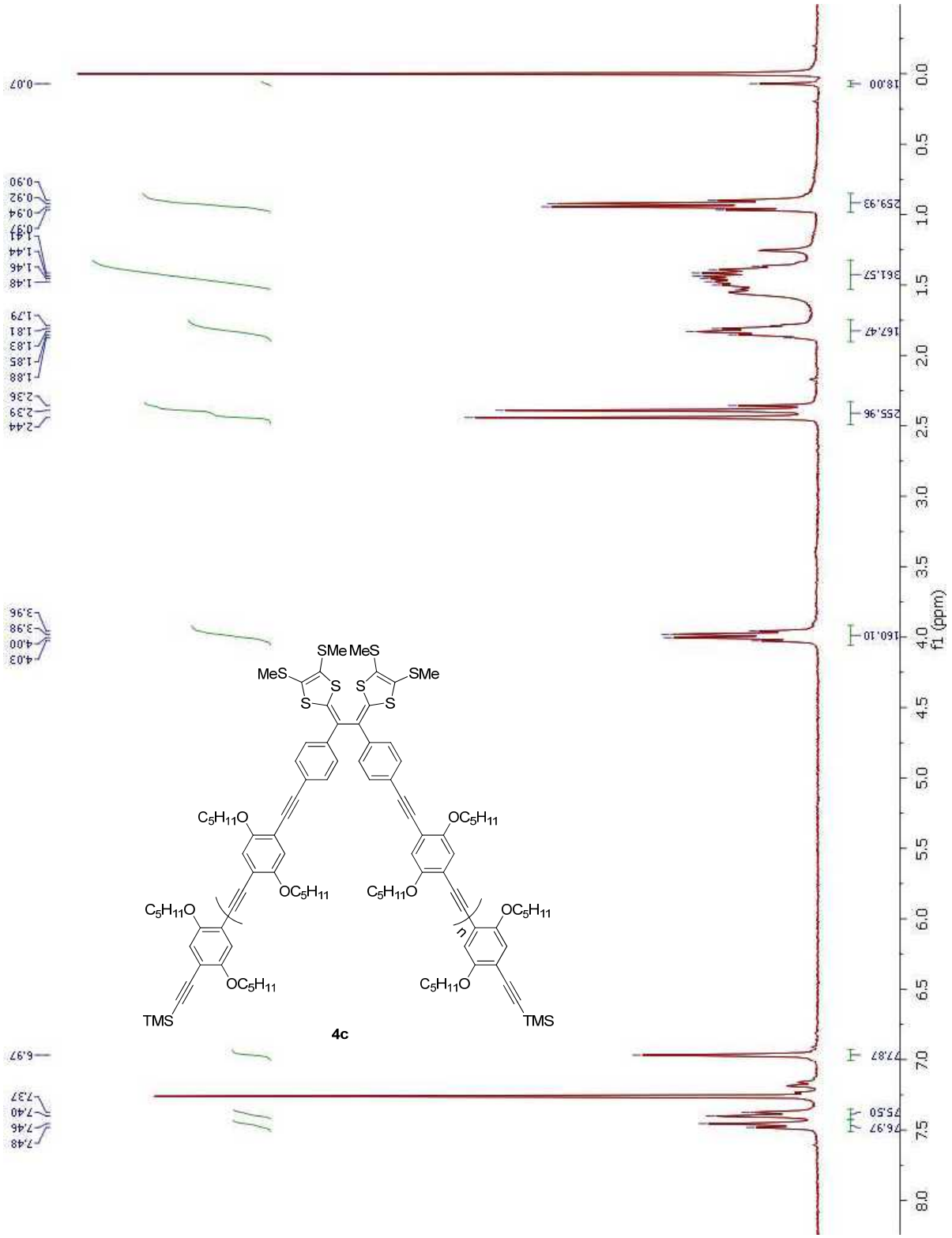

Figure S10: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **4c**.

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2. Procedures for Multi-Cycle Dispersion and Release of SWNTs

2.1 Multi-cycle dispersion-releasing of CoMoCAT SWNTs

Cycle 1

To a toluene solution of polymer **4a** (8.0 mL, 4.5 mg/mL) was added CoMoCAT SWNTs (40 mg). The mixture was ultrasonicated for 30 min, left still for 2 h, and then filtered through a tightly packed cotton plug to remove insoluble components. A clear black SWNT solution was obtained which was characterized by UV-Vis spectral analysis.

To the solution was added an excess amount of trifluoroacetic acid (TFA, 2.0 mL). Precipitation of SWNTs was observed. The mixture was subjected to centrifugation for 15 min to afford a clear yellow solution and SWNT precipitates on the bottom. The top organic layer was carefully transferred to an Erlenmeyer flask by a pipette, washed with aq. Na_2CO_3 solution, and dried over $MgSO_4$ to afford the recovered polymer solution. UV-Vis and ^1H NMR analyses on the recovered polymer showed that the recovered polymer does not undergo any changes in molecular structure. The bottom precipitates was collected and washed sequentially with toluene (20 mL) and acetonitrile (20 mL), and air-dried overnight in the fumehood to afford the released SWNTs (16 mg).

Cycle 2

To the released SWNTs (16 mg) was added a toluene solution of polymer **4a** (3.2 mL, 4.5 mg/mL). The mixture was treated with the same procedure in cycle 1 to afford a SWNT solution, which was characterized by UV-Vis analysis.

To the solution was added an excess amount of TFA (1.0 mL). The mixture was treated with the same procedure in cycle 1 to afford the released SWNTs (3 mg) and the recovered polymer solution.

Cycle 3

To the released SWNTs (3 mg) was added a toluene solution of polymer **4a** (0.6 mL). The mixture was treated with the same procedure in cycle 1 to afford a SWNT solution, which was characterized by UV-Vis analysis.

Then to the solution was added an excess amount of TFA (0.1 mL). The mixture was treated with the same procedure in cycle 1 to give recovered polymer solution and the released SWNTs, the weight of which was not determined due to the small amount.

Table S1. Quantities of starting and recovered CoMoCAT SWNTs, polymer solution, and TFA used in the multi-cycle dispersion-releasing of SWNTs.

	Cycle 1	Cycle 2	Cycle 3
Starting CoMoCAT NTs	40 mg	16 mg	3 mg
Polymer (4.5 mg/mL)	8.0 mL	3.2 mL	0.6 mL
TFA	2.0 mL	1.0 mL	0.1 mL

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Recovered CoMoCAT NTs	16 mg	3 mg*	-

*Low recovery is due to partially protonation of SWNTs and significant mechanical loss during small-quantity sample handling.

2.2 Multi-cycle dispersion-releasing of HiPCO SWNTs

Cycle 1

To a toluene solution of polymer **4a** (32.0 mL, 2.3 mg/mL) was added HiPCO SWNTs (48 mg). The mixture was ultrasonicated for 30 min, left to stand still for 2 h, and filtered through a tightly packed cotton plug to remove insoluble components. A clear black SWNT solution was obtained, which was characterized by UV-Vis spectral analysis.

To the solution was added an excess amount of TFA (3.0 mL), which led to the release of SWNTs as precipitates. The mixture was subjected to centrifugation for 15 min to afford a clear yellow solution and SWNT precipitates on the bottom. The top organic layer was carefully transferred to an Erlenmeyer flask by a pipette, washed with aq. Na_2CO_3 solution, and dried over $MgSO_4$ to afford the recovered polymer solution. The bottom precipitates was washed sequentially with toluene (20 mL) and acetonitrile (20 mL), and air-dried overnight in the fumehood to afford the released SWNTs (10 mg).

Cycle 2

To the released SWNTs (10 mg) was added a toluene solution of polymer **4a** (6.0 ml, 2.3 mg/mL). The mixture was treated with the same procedure in cycle 1 to afford a SWNT solution, which was characterized by UV-Vis analysis.

To the solution was added an excess amount of TFA (0.6 mL). The mixture was treated with the same procedure in cycle 1 to afford the released SWNTs (0.5 mg) and the recovered polymer solution.

Cycle 3

To the released SWNTs (0.5 mg) was added a toluene solution of polymer **4a** (0.3 mL, 2.3 mg/mL). The mixture was treated with the same procedure in cycle 1 to afford a SWNT solution, which was characterized by UV-Vis analysis.

To the solution was added an excess amount of TFA (0.03 mL). The mixture was treated with the same procedure in cycle 1 to give recovered polymer solution and the released SWNTs (trace).

Table S2. Quantities of starting and recovered HiPCO SWNTs, polymer solution, and TFA used in the multi-cycle dispersion-releasing of SWNTs.

	Cycle 1	Cycle 2	Cycle 3
Starting HiPCO NTs	48 mg	10 mg	0.5 mg
Polymer (2.3 mg/mL)	32 mL	6.0 mL	0.3 mL
TFA	3.0 mL	0.6 mL	0.03 mL
Recovered CoMoCAT NTs	10 mg	0.5 mg*	-

*Low recovery is due to partially protonation of SWNTs and significant mechanical loss during small-quantity sample handling.

3. Cross-section Analysis of AFM imaging for 4a and SWNTs

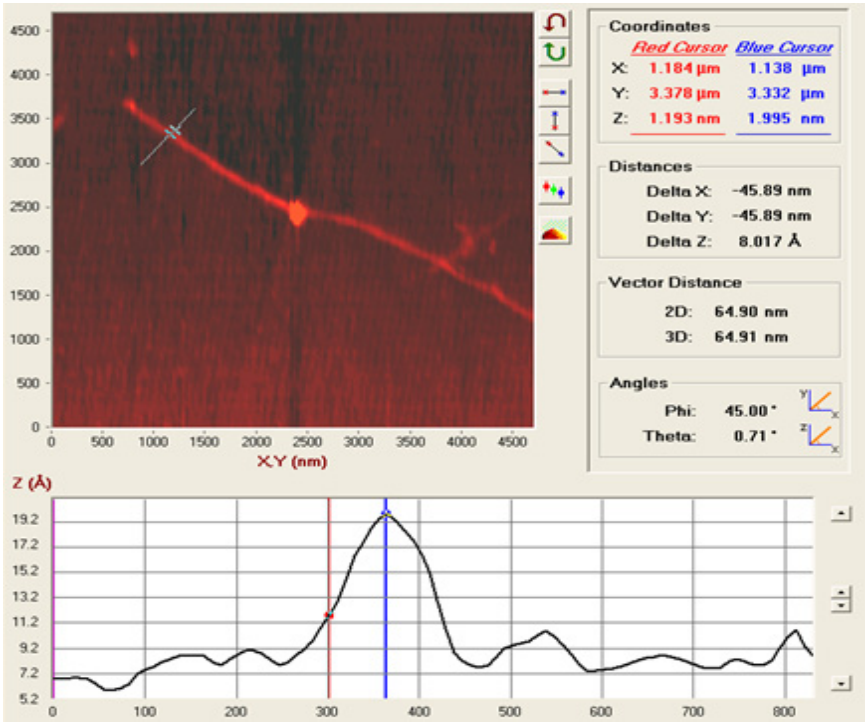

Figure S11: Cross-section analysis showing the feature of a bare single-walled carbon nanotube (height = 0.8 nm).

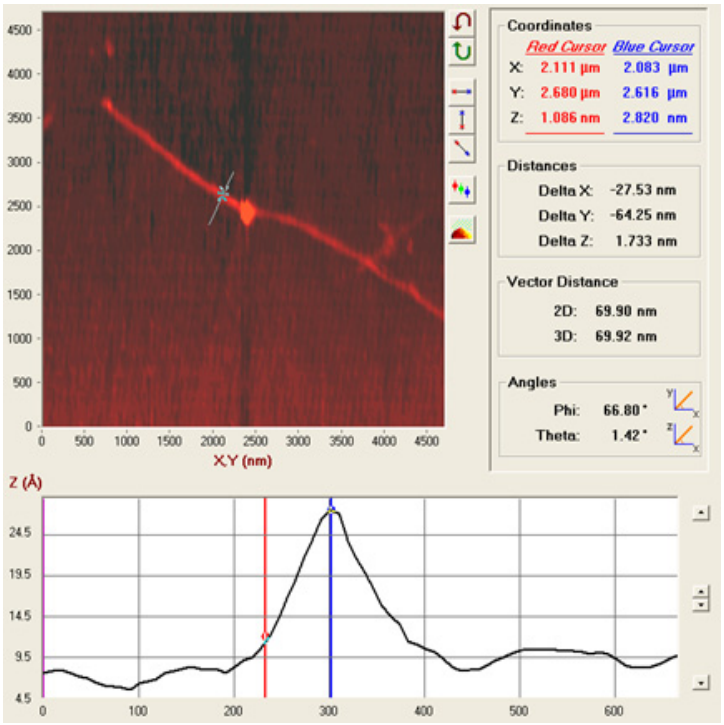

Figure S12: Cross-section analysis showing the feature of a single-walled carbon nanotube wrapped with polymer **4a** (height = 1.7 nm).

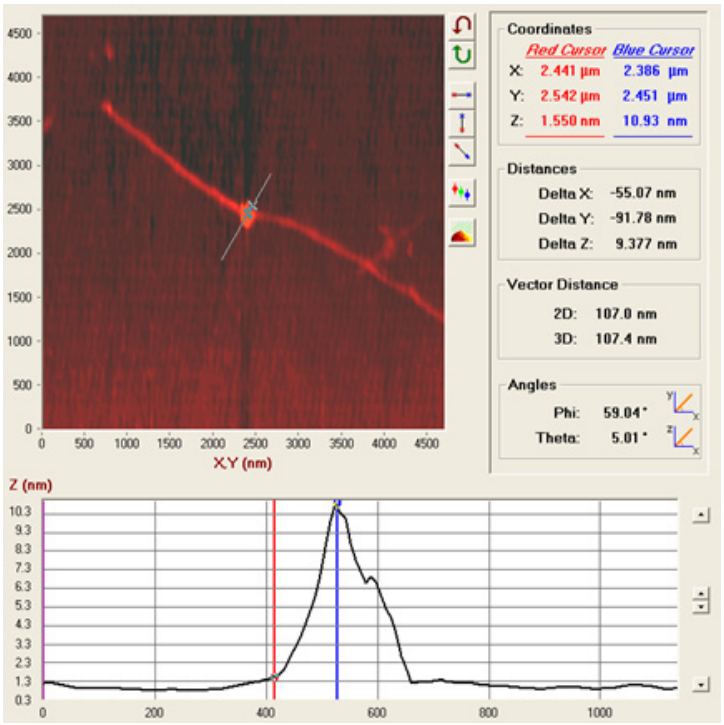

Figure S13: Cross-section analysis showing the feature of a globular aggregate of polymer **4a** on a single-walled carbon nanotube (height = 9.4 nm).

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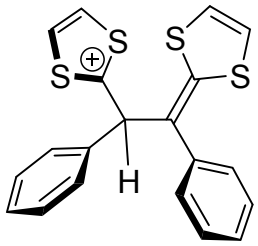
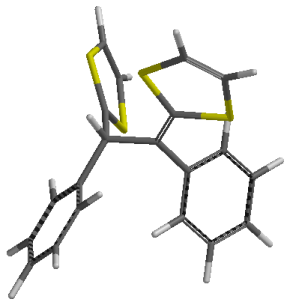
4. Density Functional Theory (DFT) Calculations of Protonated TTFVs

4.1 Geometry Optimization





Optimized at B3LYP/6-311G*, E = -2364.15708 au

C	4.206970	0.412332	1.898412
H	5.202589	0.822290	2.009053
C	3.705887	-0.587441	2.626630
H	4.219274	-1.113866	3.420101
S	2.063773	-1.091498	2.263732
S	3.186990	1.121395	0.662875
C	1.804491	0.044393	0.925810
C	0.685610	0.071570	0.140189
C	0.471343	1.168673	-0.841009
C	0.057996	3.298109	-2.634204
C	0.453970	2.503787	-0.392326
C	0.270448	0.926300	-2.210426
C	0.067164	1.982737	-3.094109
C	0.253434	3.556787	-1.279072
H	0.597007	2.714375	0.662707
H	0.293255	-0.086126	-2.590722
H	-0.074650	1.775865	-4.149366
H	0.249644	4.577496	-0.911616
H	-0.095612	4.116983	-3.328650
C	-0.411949	-0.986536	0.356009
H	-0.020395	-1.727193	1.060772
C	-1.473711	-0.234094	1.111100
S	-2.468422	0.988016	0.441766
S	-1.661911	-0.466373	2.794793
C	-3.204669	1.469731	1.940396
H	-3.927945	2.274186	1.911517
C	-2.822821	0.799279	3.042715
H	-3.186141	0.972655	4.046823

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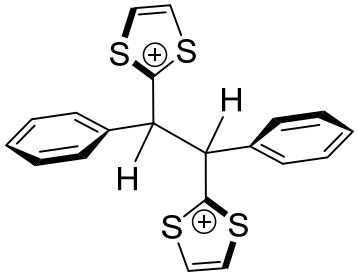
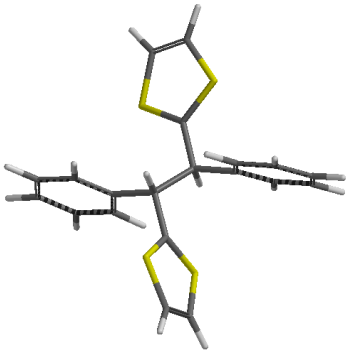
C	-0.832486	-1.794695	-0.873194
C	-1.442219	-3.410862	-3.081865
C	-2.146942	-1.911058	-1.322723
C	0.173919	-2.517697	-1.527883
C	-0.127284	-3.317277	-2.623634
C	-2.448363	-2.711545	-2.426341
H	-2.959715	-1.400689	-0.820139
H	1.200241	-2.449319	-1.179567
H	0.662926	-3.871442	-3.118521
H	-3.475429	-2.788348	-2.765845
H	-1.678144	-4.033093	-3.938021





Optimized at B3LYP/6-311G*, E = -2363.87811 au

C	-4.222242	-1.224330	-0.607477
H	-5.136450	-1.491094	-1.123400
C	-4.112679	-0.930434	0.704676
H	-4.921893	-0.920368	1.424277
S	-2.524796	-0.523334	1.257589
S	-2.758217	-1.142569	-1.521874
C	-1.740837	-0.698800	-0.237144
C	-0.239134	-0.584857	-0.452617
C	0.404743	-1.943640	-0.159888
C	1.590911	-4.434719	0.309392
C	0.490560	-2.452408	1.142991
C	0.904782	-2.702394	-1.224878
C	1.498605	-3.940886	-0.990546
C	1.086786	-3.688792	1.375403
H	0.095570	-1.899136	1.990652
H	0.836856	-2.327774	-2.242406
H	1.883334	-4.519455	-1.822690

H	1.149388	-4.074946	2.386535
H	2.046616	-5.401193	0.492494
C	0.386988	0.628513	0.335579
H	0.354123	0.378927	1.402217
C	1.869714	0.801557	0.010450
S	2.465332	2.290147	-0.553475
S	3.055410	-0.394306	0.260353
C	4.125842	1.826923	-0.620340
H	4.847317	2.560472	-0.958856
C	4.407197	0.565256	-0.228146
H	5.390609	0.111408	-0.204270
C	-0.374094	1.937950	0.143346
C	-1.734982	4.368106	-0.154121
C	-0.771298	2.378852	-1.126905
C	-0.663165	2.730488	1.260277
C	-1.340581	3.938785	1.111979
C	-1.448849	3.587567	-1.272966
H	-0.549219	1.796038	-2.016514
H	-0.355901	2.410122	2.252240
H	-1.557601	4.544841	1.984267
H	-1.748325	3.921057	-2.260291
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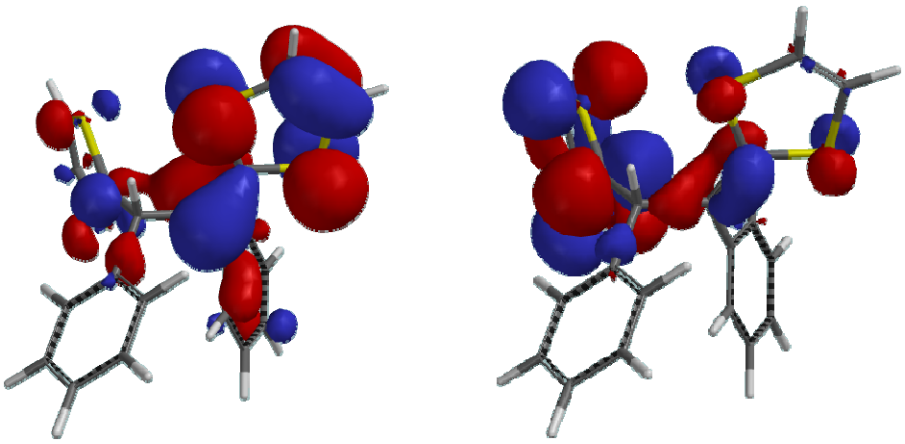
H	-0.101797	-0.383049	-1.517909

4.2 Molecular orbital and electron density properties



(A) (B)

Figure S14: Plots of frontier molecular orbitals of mono-protonated TTFV. (A) HOMO (E = -8.47 eV), (B) LUMO (E = -6.28 eV).

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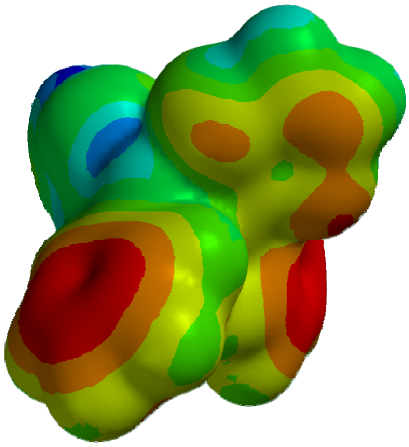

Figure S15: Plots of electrostatic potential map of mono-protonated TTFV.

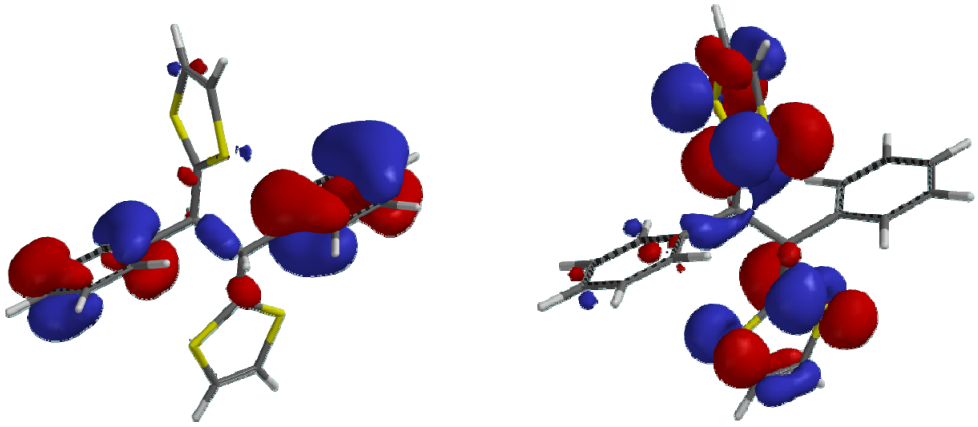

Figure S16: Plots of frontier molecular orbitals of di-protonated TTFV. (A) HOMO (E = -12.82 eV), (B) LUMO (E = -9.59 eV).

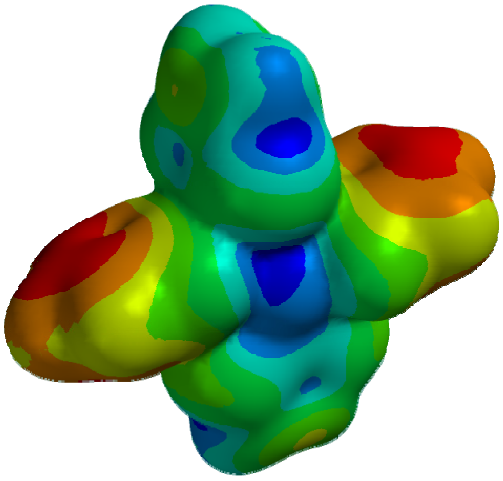

Figure S17: Plots of electrostatic potential map of di-protonated TTFV.