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Electronic Supplementary Information

Sulfur-bridged tetraphenylethylene AIEgens for deep-blue organic light-emitting diodes

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Table of Contents

1. HRMS and NMR spectra

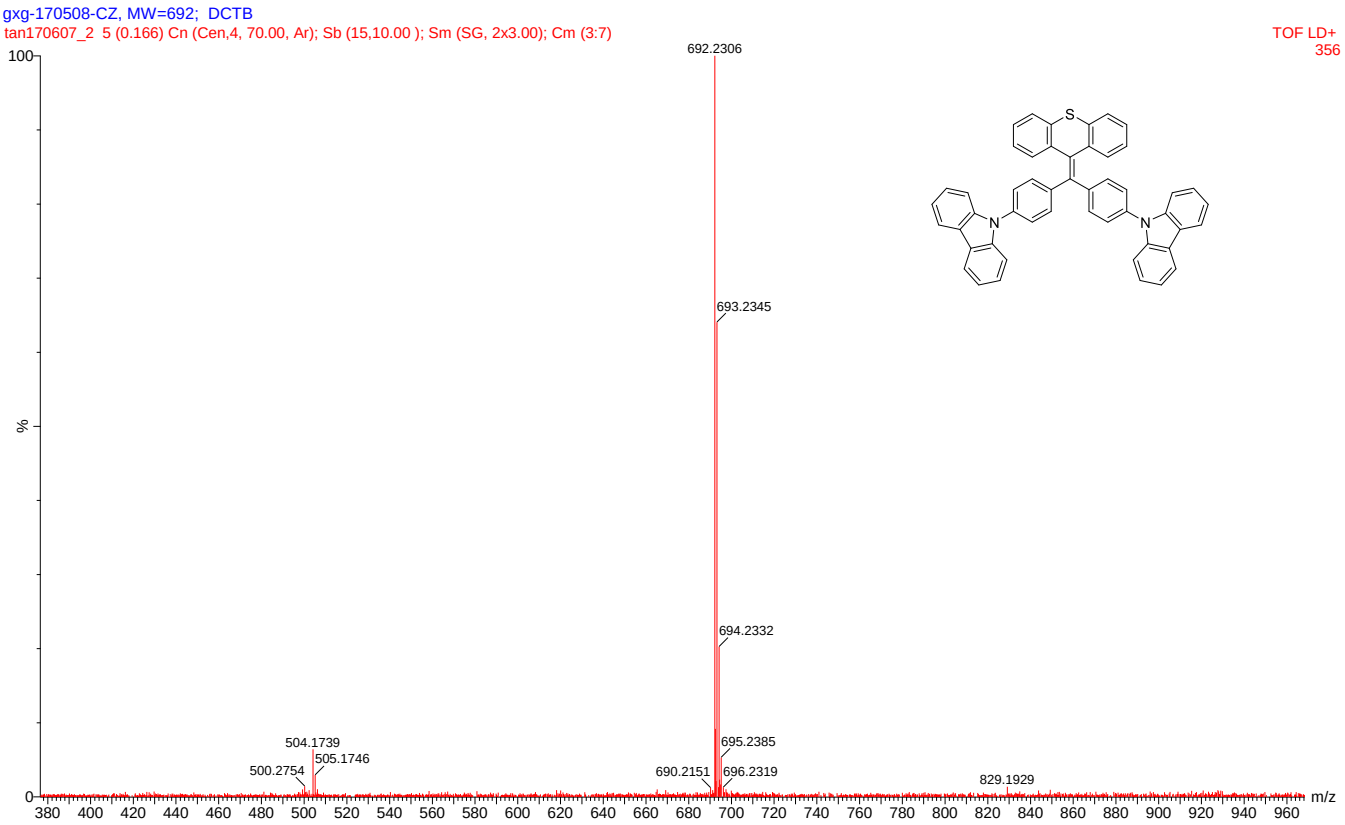
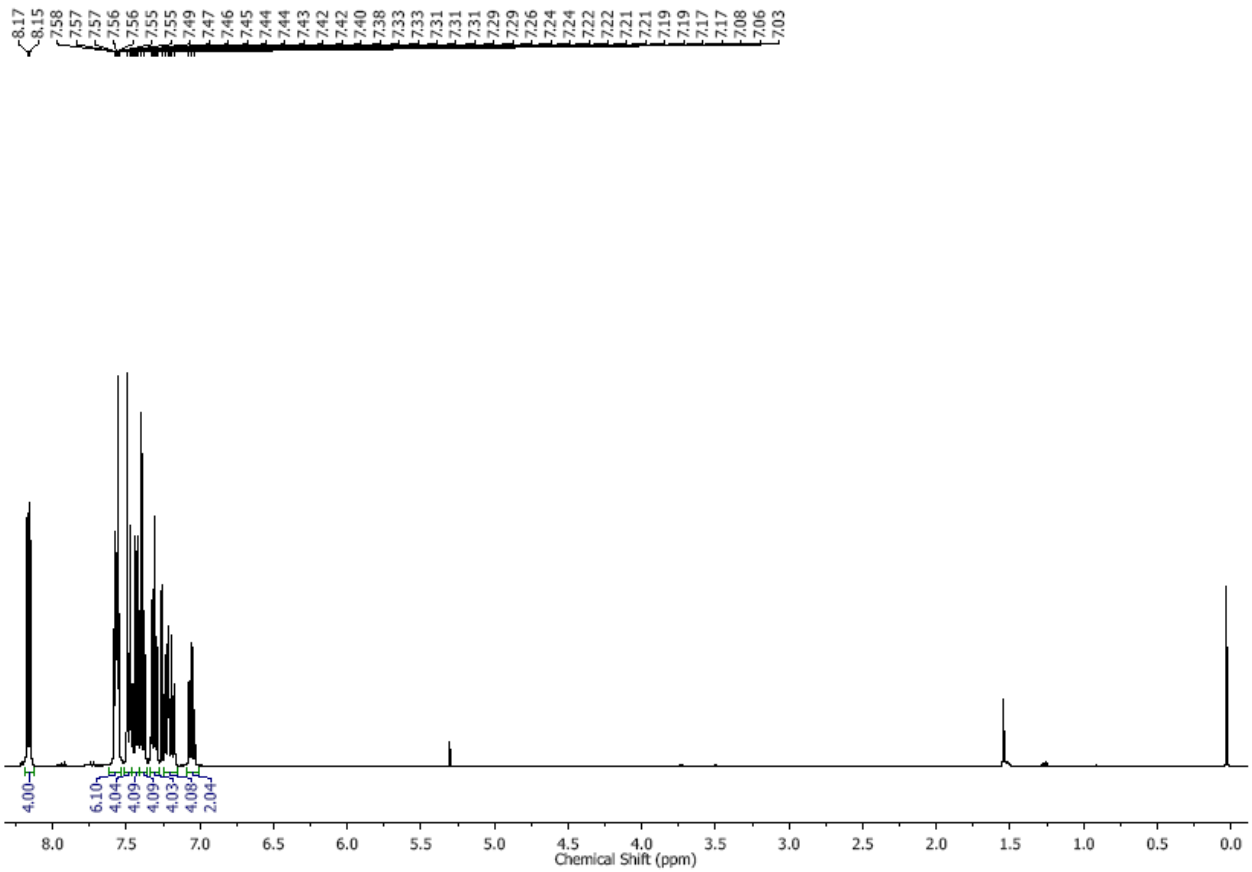


Figure S1. HRMS of compound **1**.



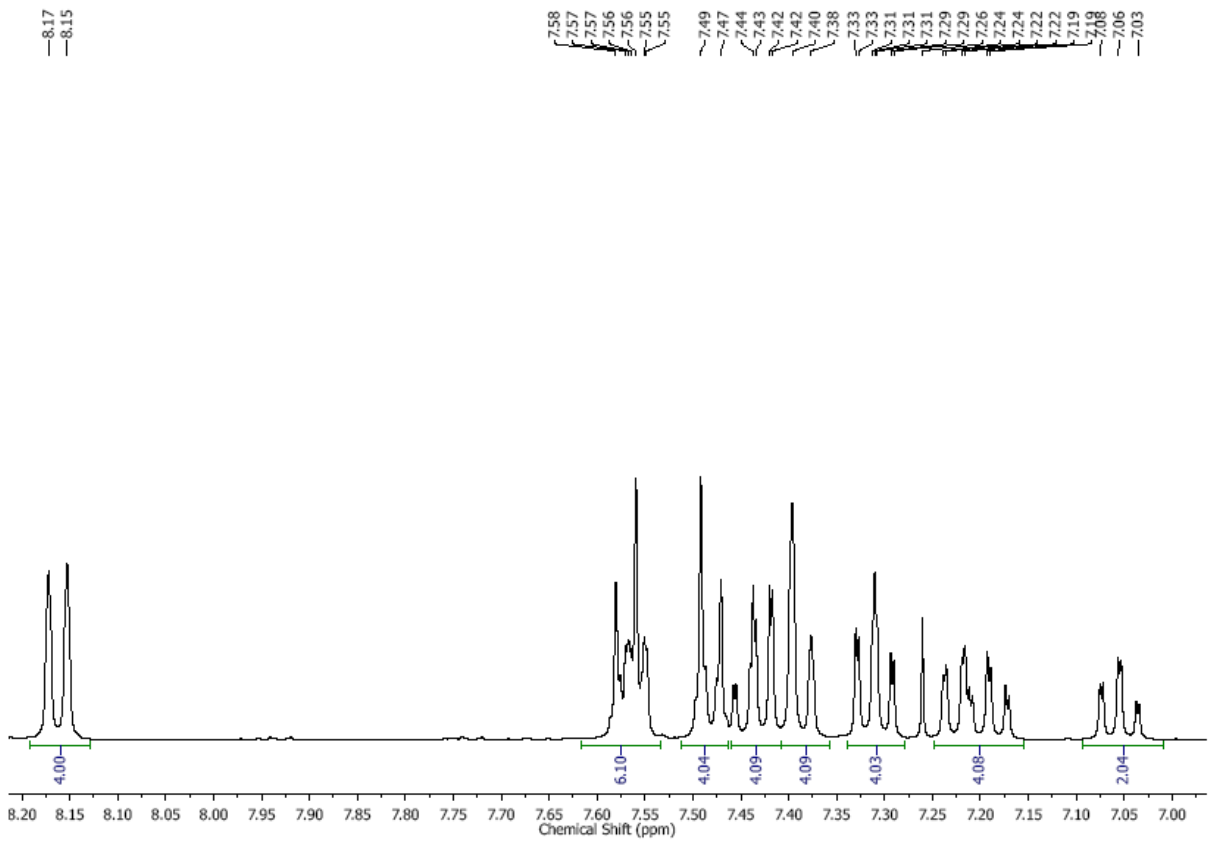


Figure S2. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

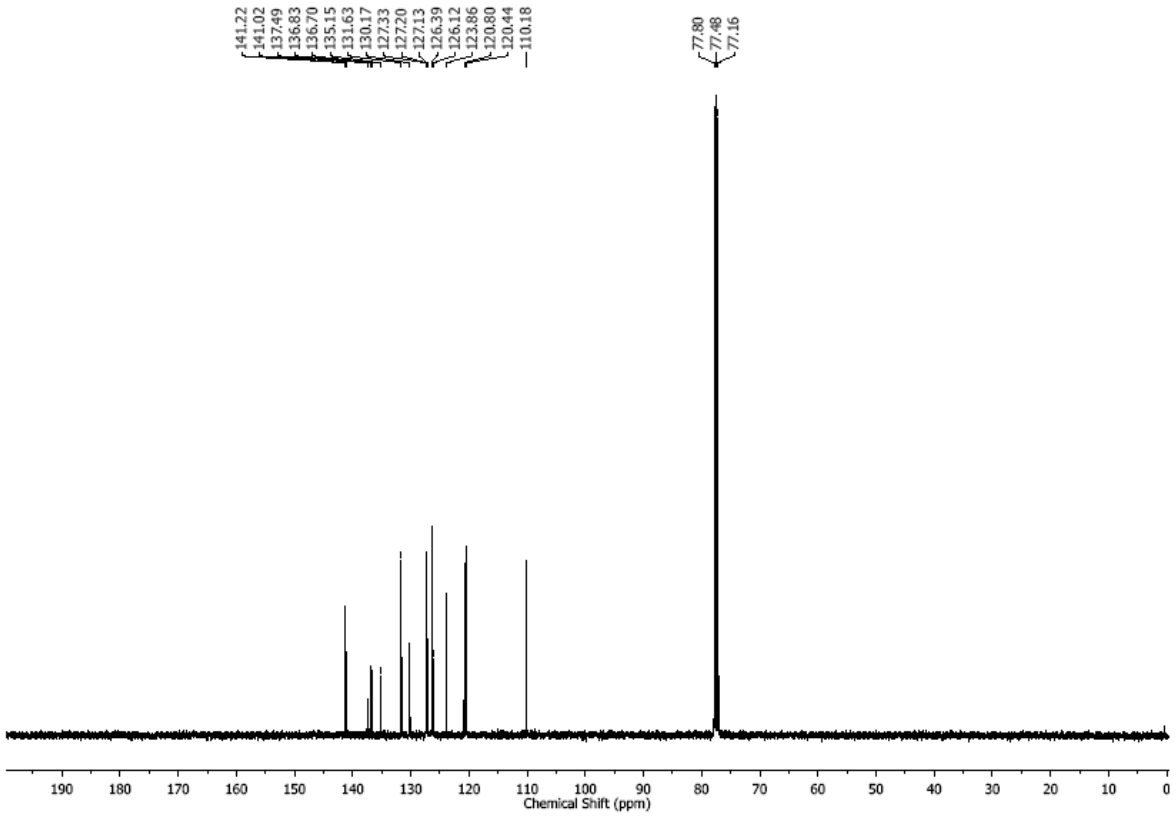


Figure S3. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

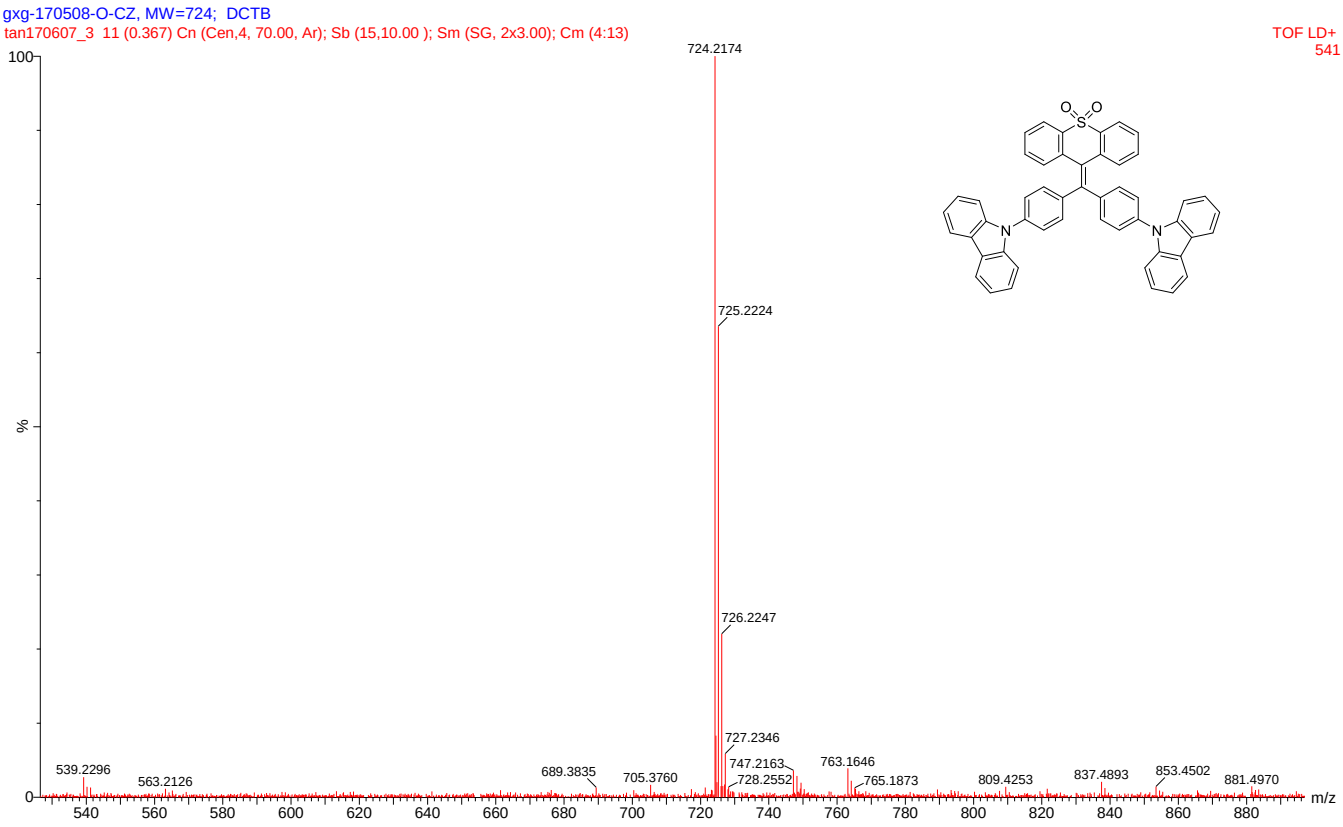
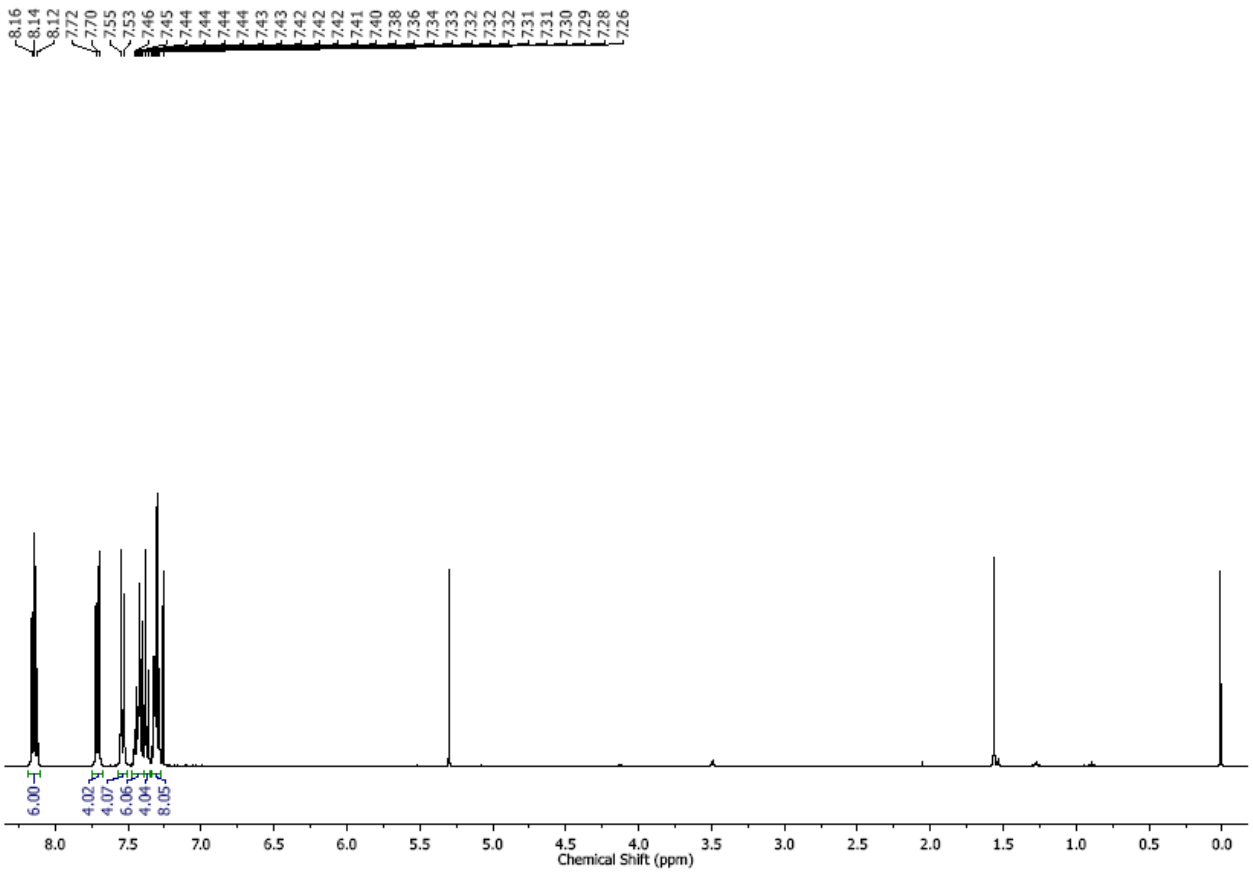


Figure S4. HRMS spectrum of compound **2**.



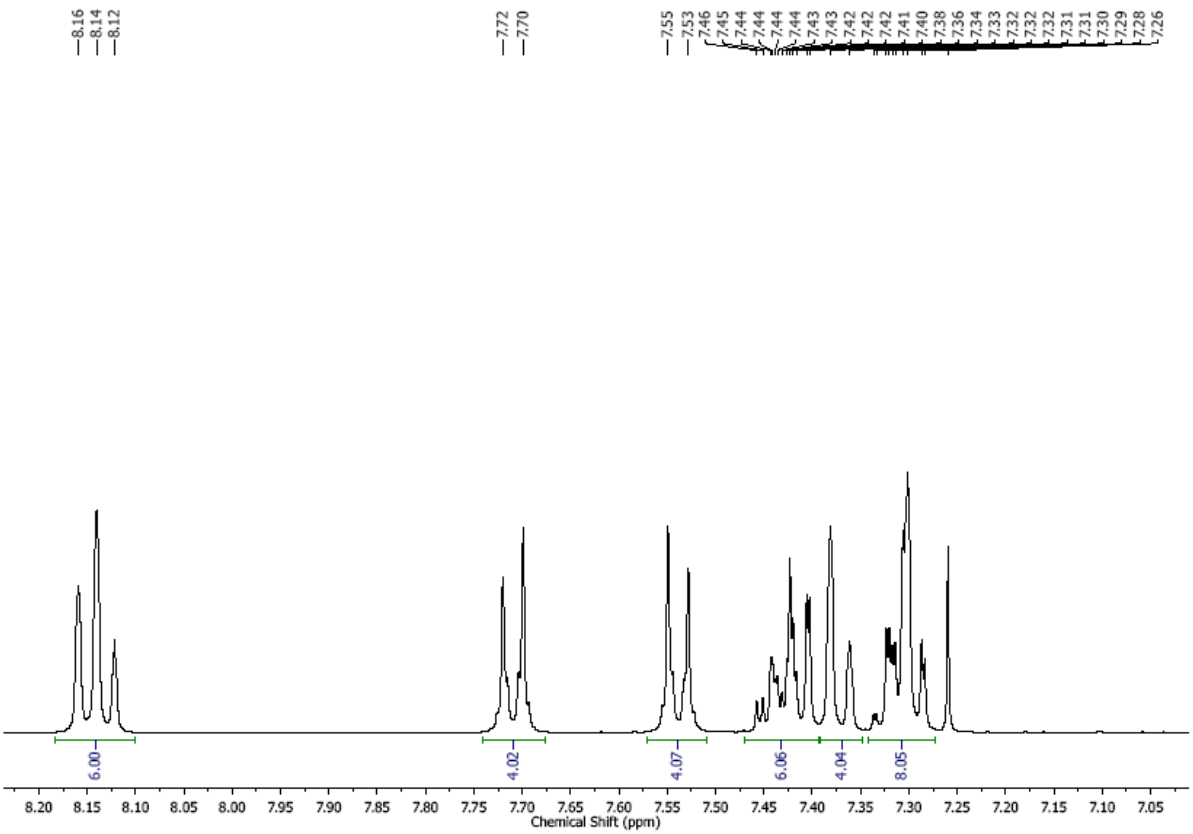


Figure S5. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

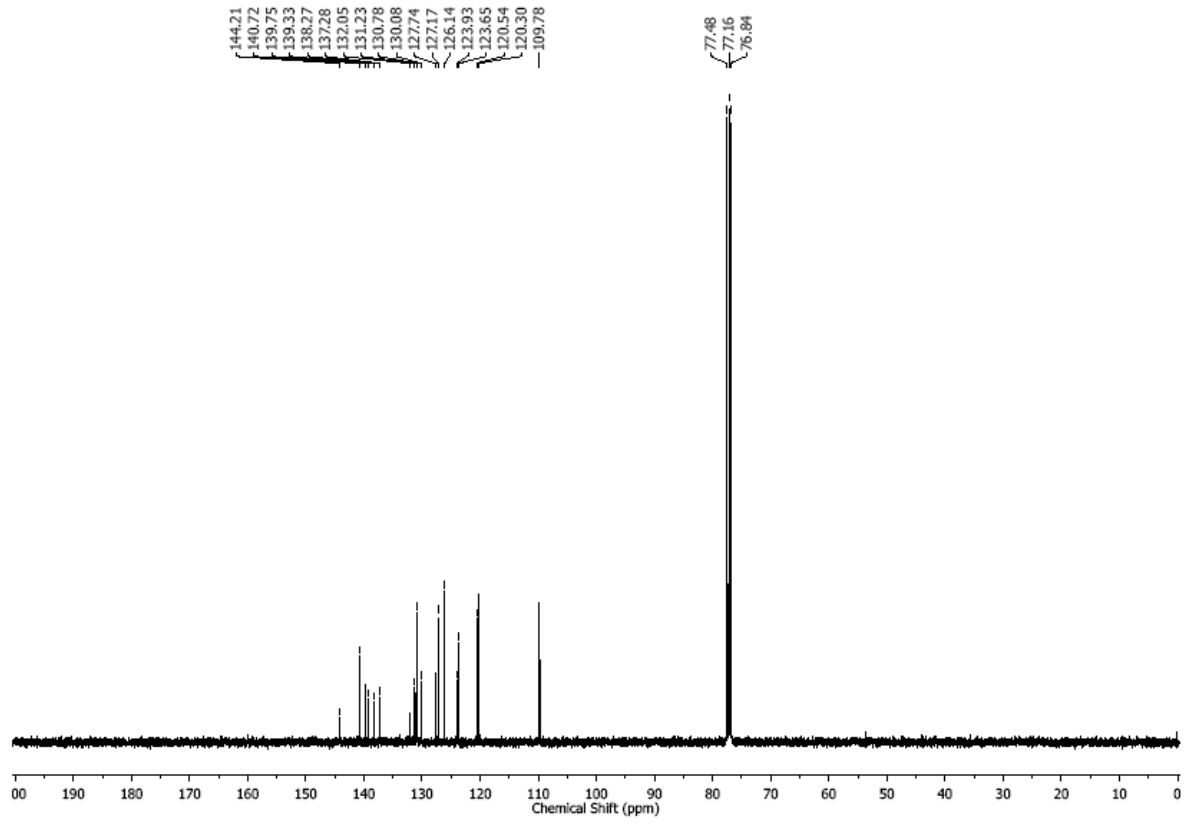


Figure S6. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

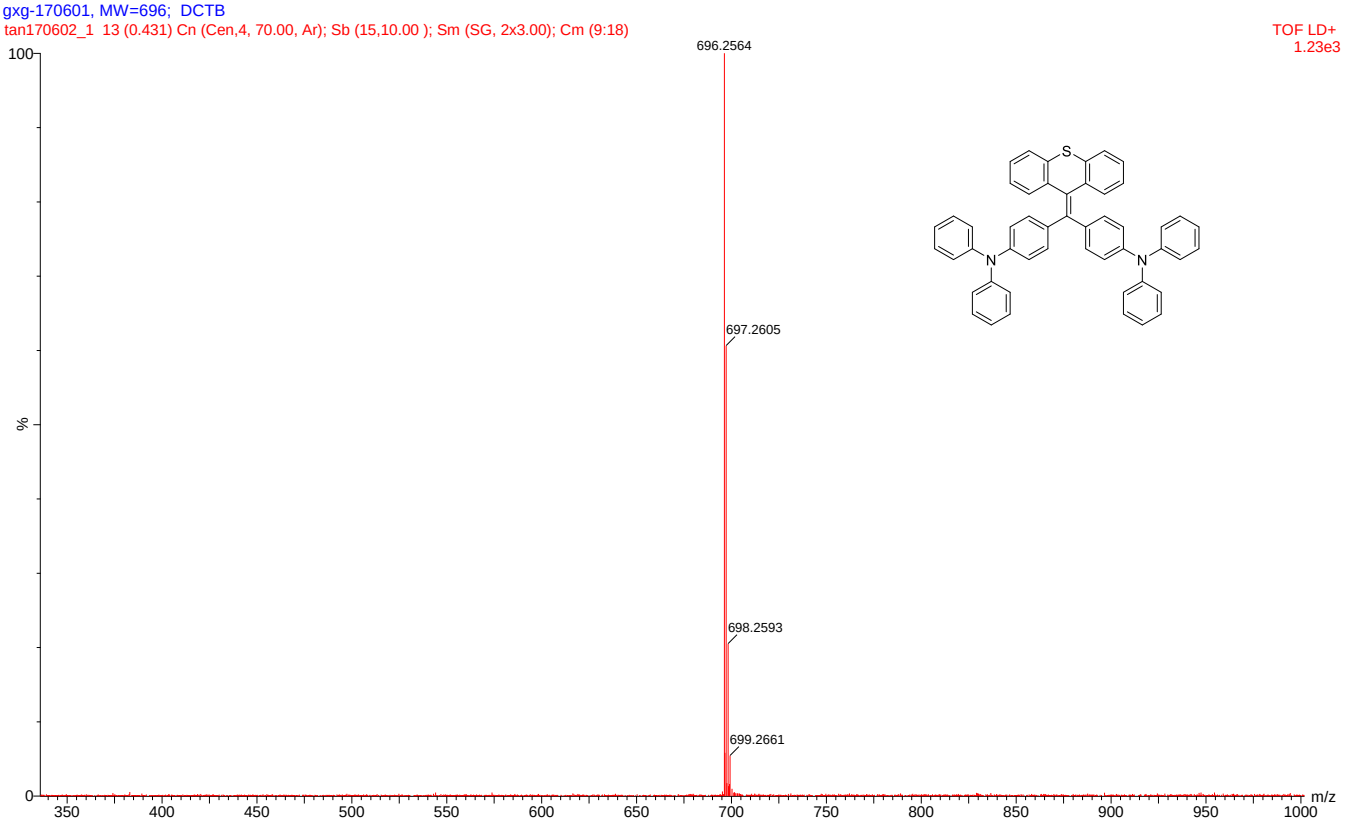
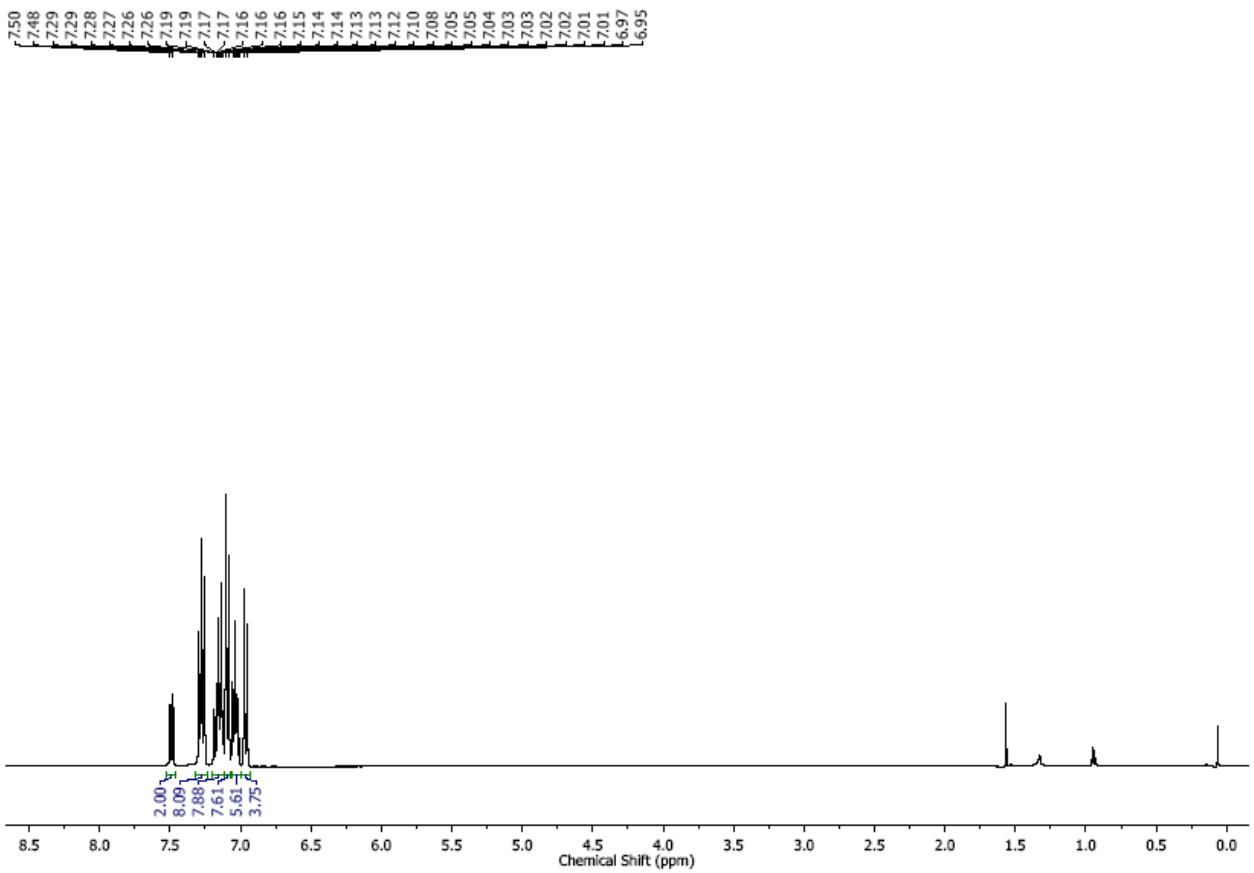


Figure S7. HRMS spectrum of compound **3**.



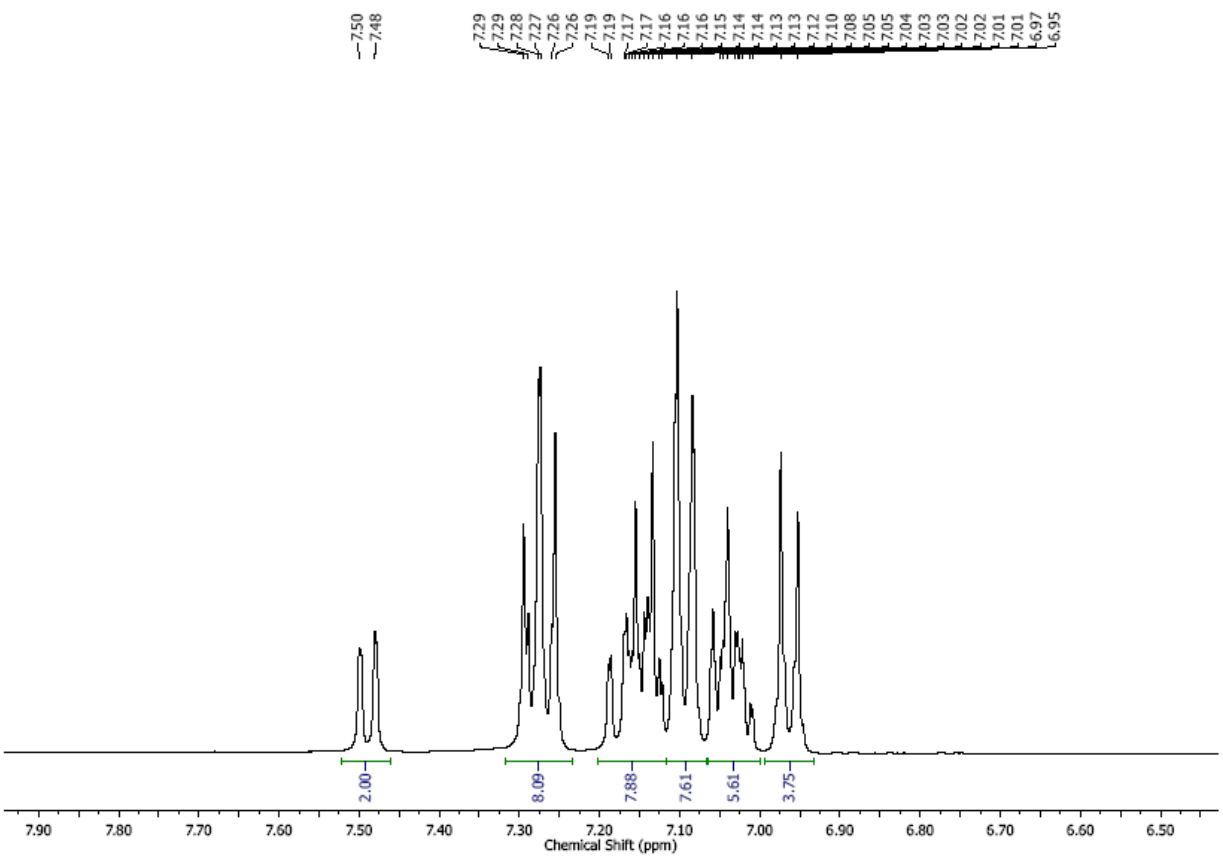


Figure S8. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

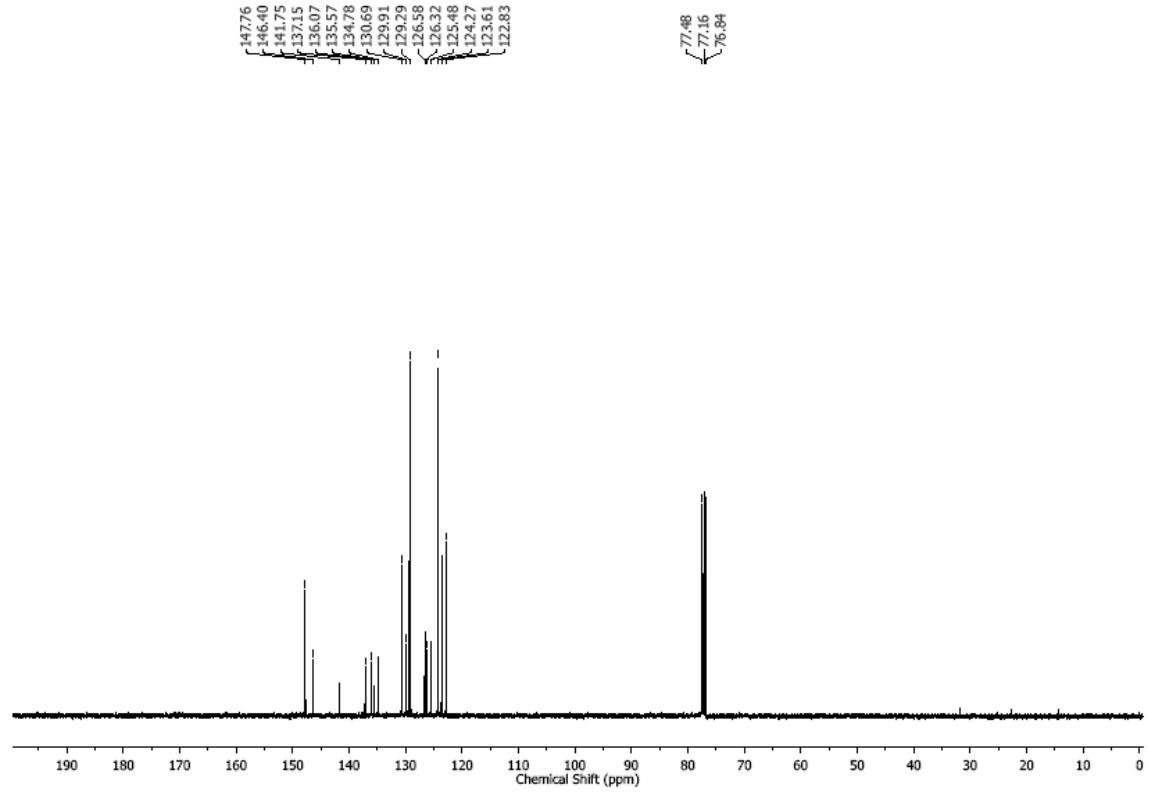


Figure S9. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

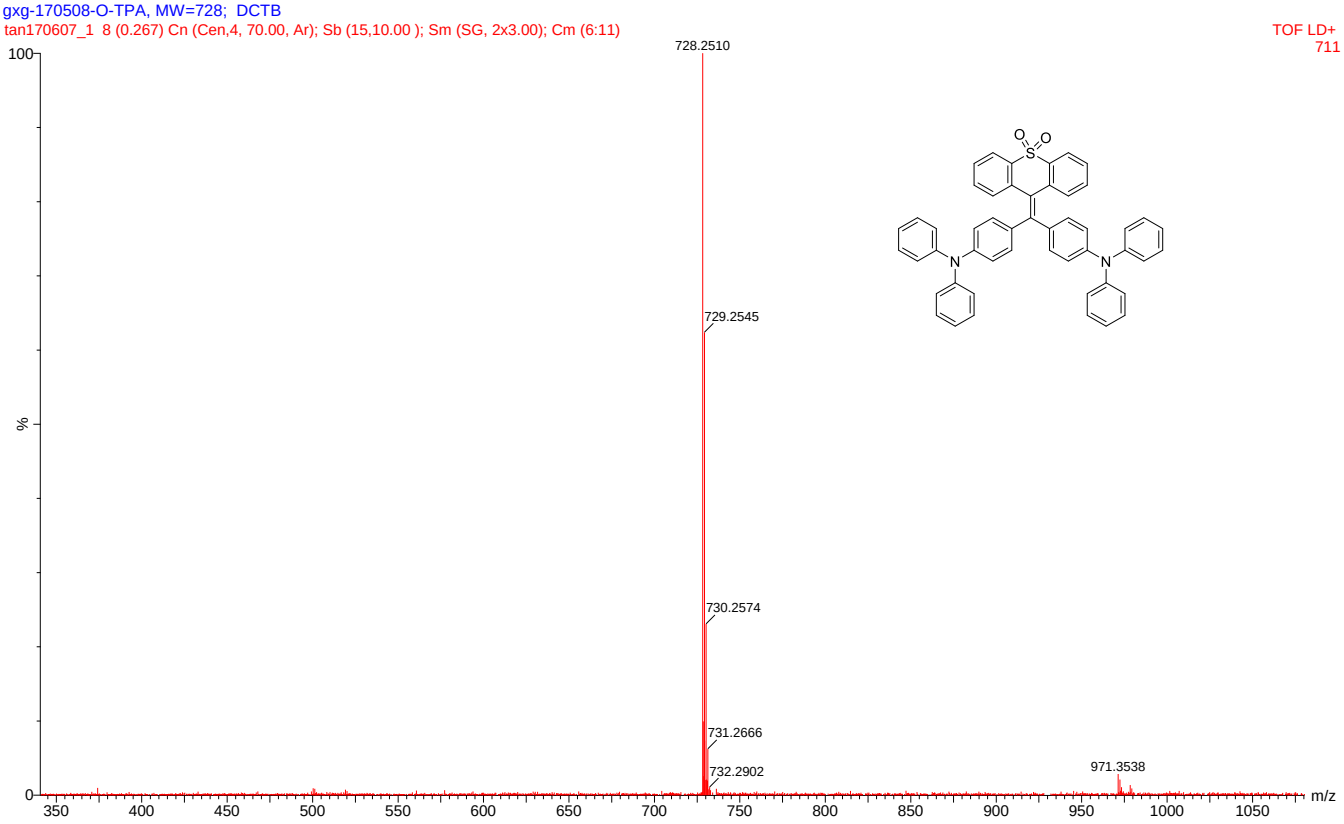
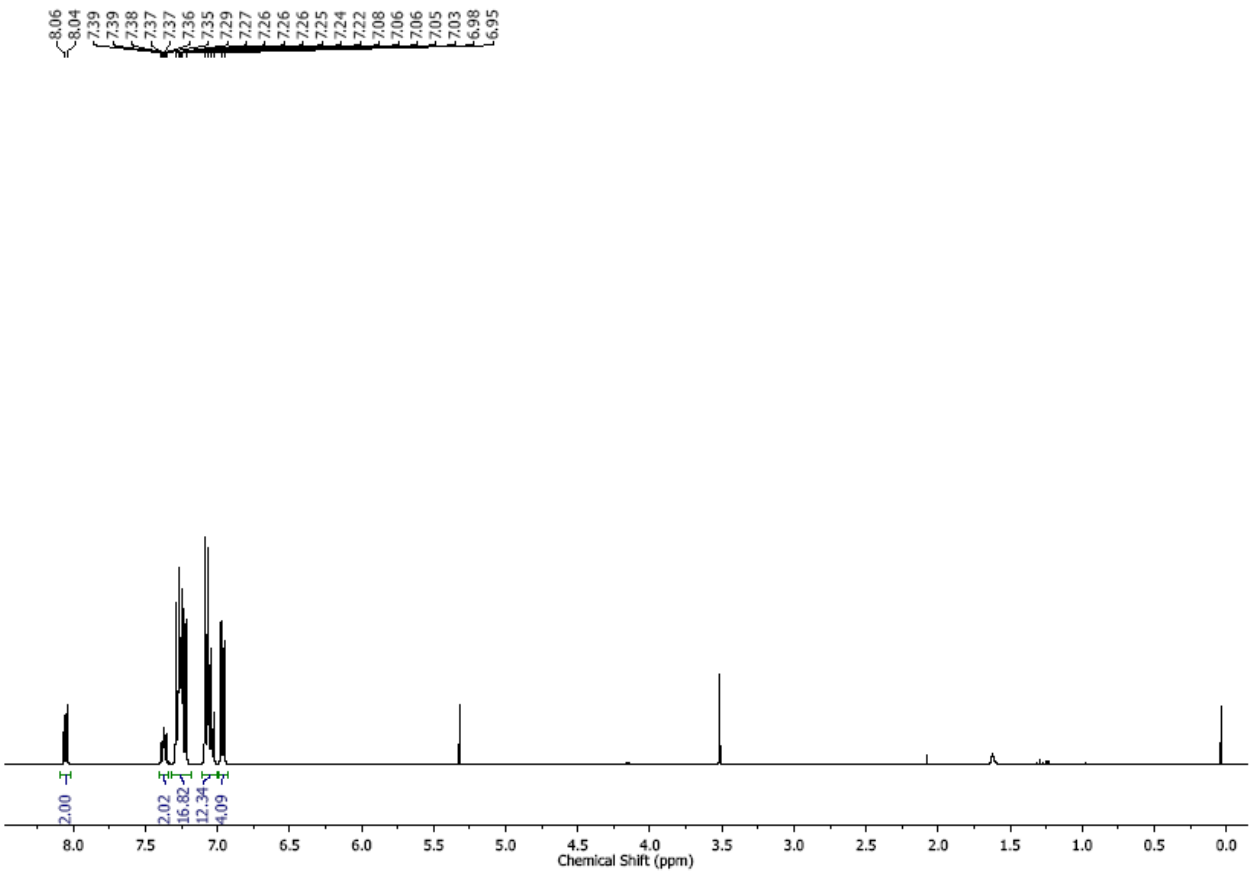


Figure S10. HRMS spectrum of compound **4**.



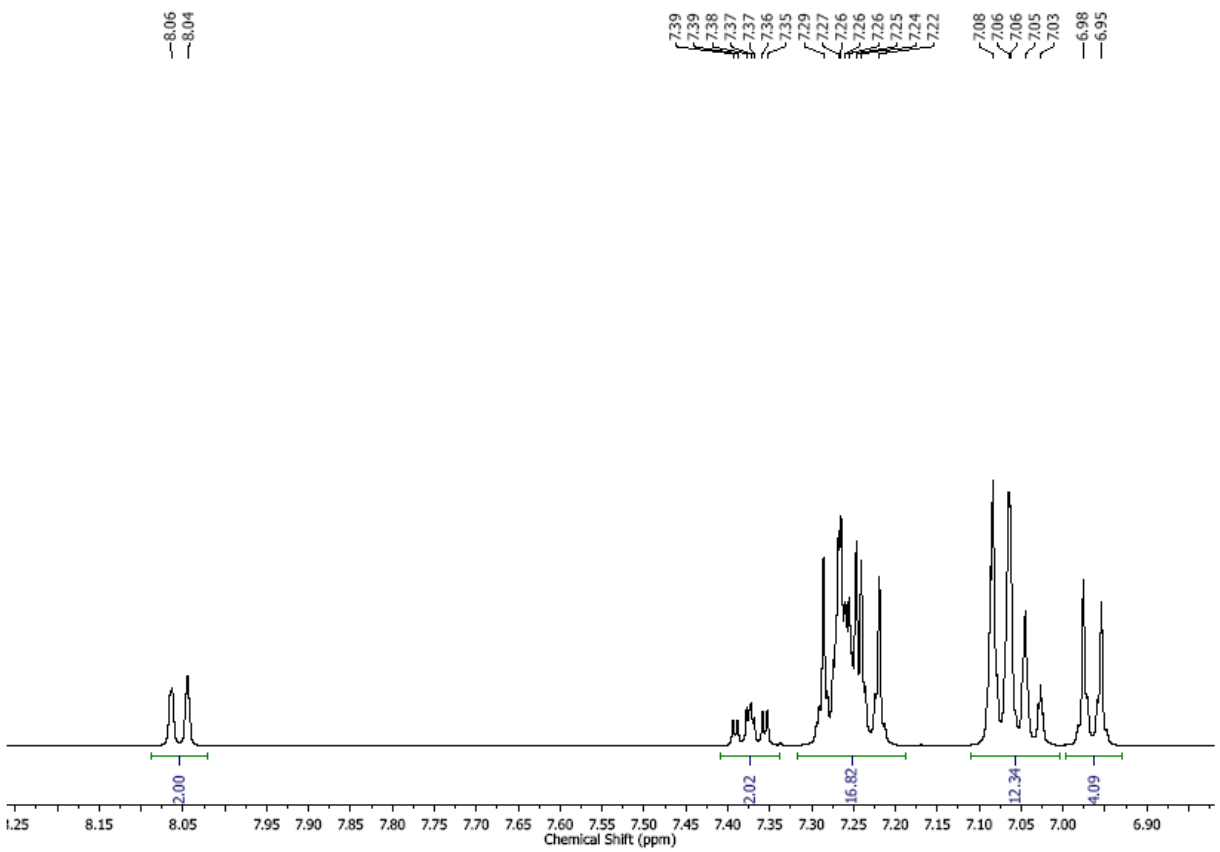


Figure S11. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

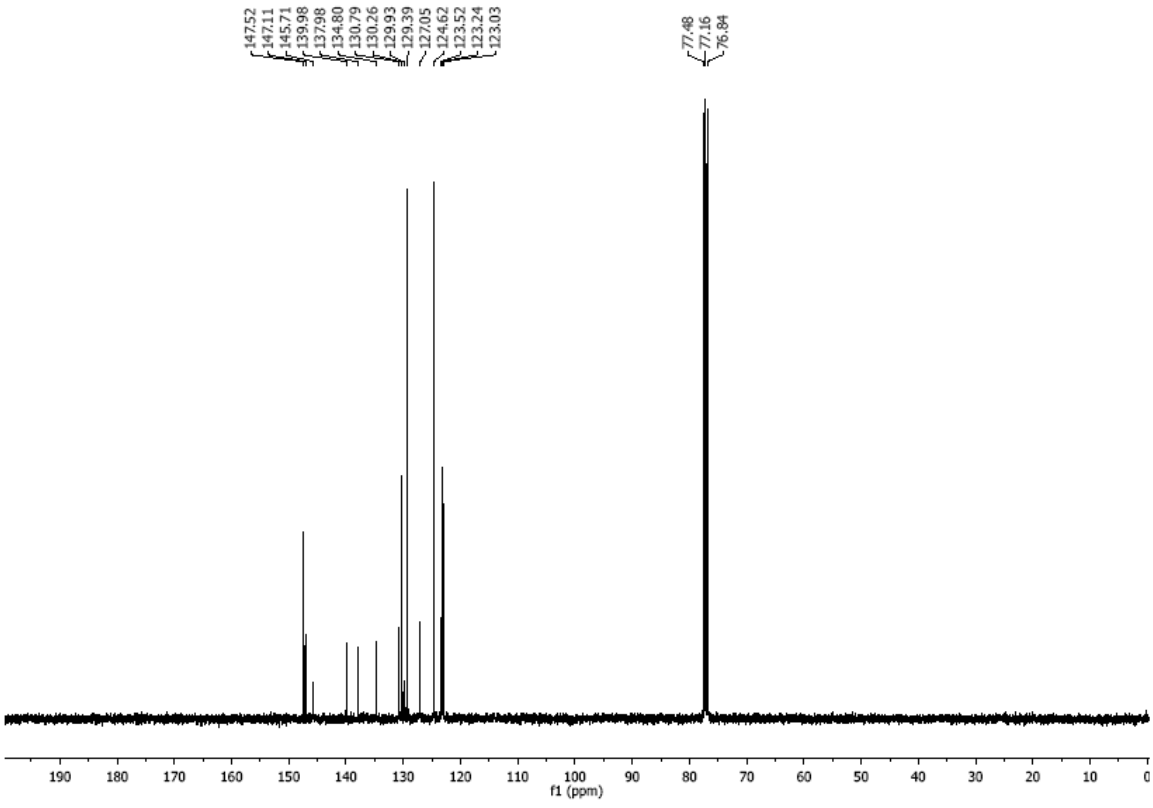


Figure S12. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

2. Single Crystal X-ray Crystallography

Suitable single crystals of sulfur-bridged TPE derivatives were selected under oil under ambient conditions. Single crystal X-ray diffraction intensity data were collected in a stream of cold nitrogen at 100K on a SuperNova, dual Cu/Mo Atlas diffractometer or at 90K on a Bruker APEX DUO diffractometer. Using Olex2, [1] the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL[3] refinement package using Least Squares minimization. The details concerning x-ray crystallographic structure solutions and refinement for TPE derivatives are tabulated in **Table S1**.

Table S1. The crystallographic details of sulfur-bridged TPE derivatives.

	1	**3**	**4**
CCDC No.	1826997	1826670	1826998
empirical formula	$C_{50}H_{32}N_2S$	$C_{50}H_{36}N_2S$	$C_{50}H_{36}N_2O_2S \cdot CHCl_3$
formula weight	692.83	696.91	848.23
crystal dimensions, mm	0.4 × 0.04 × 0.03	0.3 × 0.1 × 0.1	0.4 × 0.05 × 0.03
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1$	$P2_1/n$	$P2_1/c$
a/Å	10.2848(6)	13.4729(6)	15.9689(4)
b/Å	9.0120(5)	11.6041(5)	28.4291(4)
c/Å	19.3052(11)	24.7449(10)	9.49878(19)
α/°	90	90	90
β/°	91.856(5)	97.034(2)	106.722(2)
γ/°	90	90	90
Volume/Å^3	1788.41(17)	3839.5(3)	4129.93(15)
Z	2	4	4
ρ_{calc}, mg/mm^3	1.287	1.206	1.364
F(000)	724.0	1464.0	1760.0
λ/ Å	Cu Kα, λ = 1.54184	Mo Kα, λ = 0.71073	Cu Kα , 1.54184
μ/mm $^{-1}$	1.100	0.122	2.833
temperature/K	100.00(10)	90.00(2)	99.98(10)
2θ range for data collection	8.602° to 134.988°	3.3° to 61.2°	6.562° to 135°
reflections collected	5324	87810	12935
independent reflections. (R_{int})	4010 (0.0412)	11714 (0.0545)	7349 (0.0291)
data/restraints/parameters	4010/1/478	11714/0/478	7349/0/532
goodness-of-fit on F^2	1.001	1.027	1.022
R_1,wR_2 [I>=2σ (I)]	0.0543, 0.1306	0.0430, 0.1038	0.0478, 0.1297
R_1,wR_2 [all data]	0.0683, 0.1409	0.0599, 0.1141	0.0606, 0.1399
largest diff. peak/hole / e Å^{-3}	0.27/-0.37	0.36/-0.36	0.38/-0.58

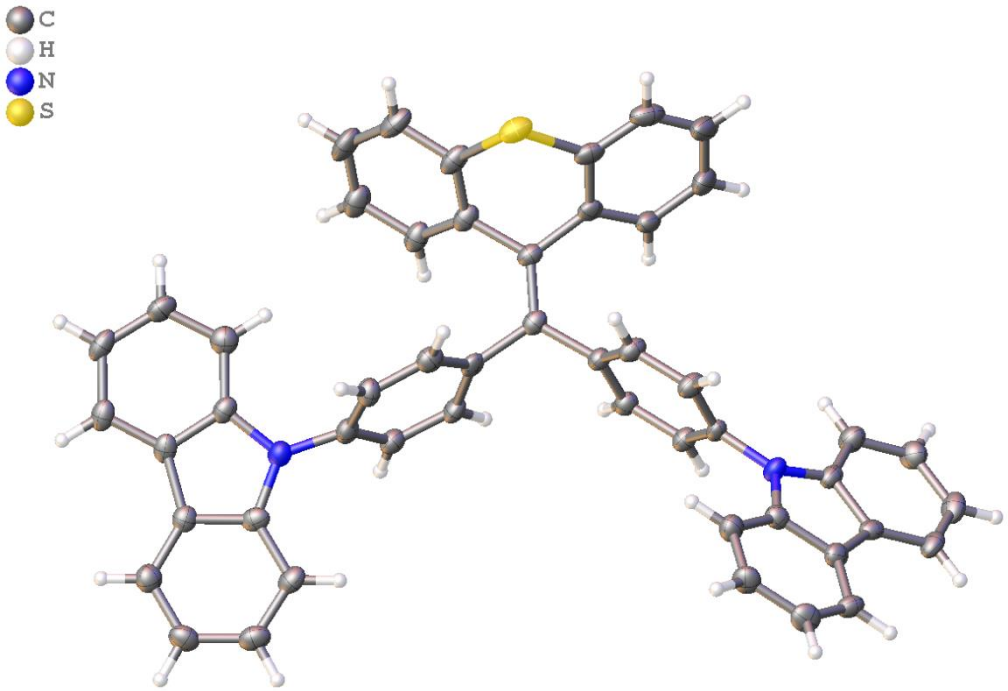


Figure S13. Thermal ellipsoids drawing of sulfur-bridged TPE derivative **1**.

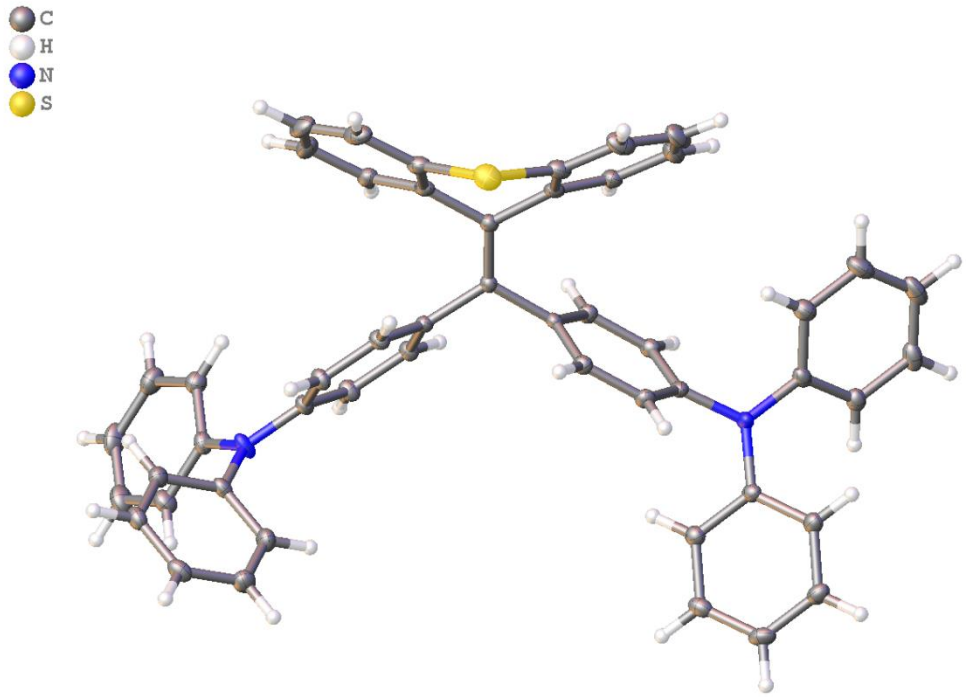


Figure S14. Thermal ellipsoids drawing of sulfur-bridged TPE derivative **3**.

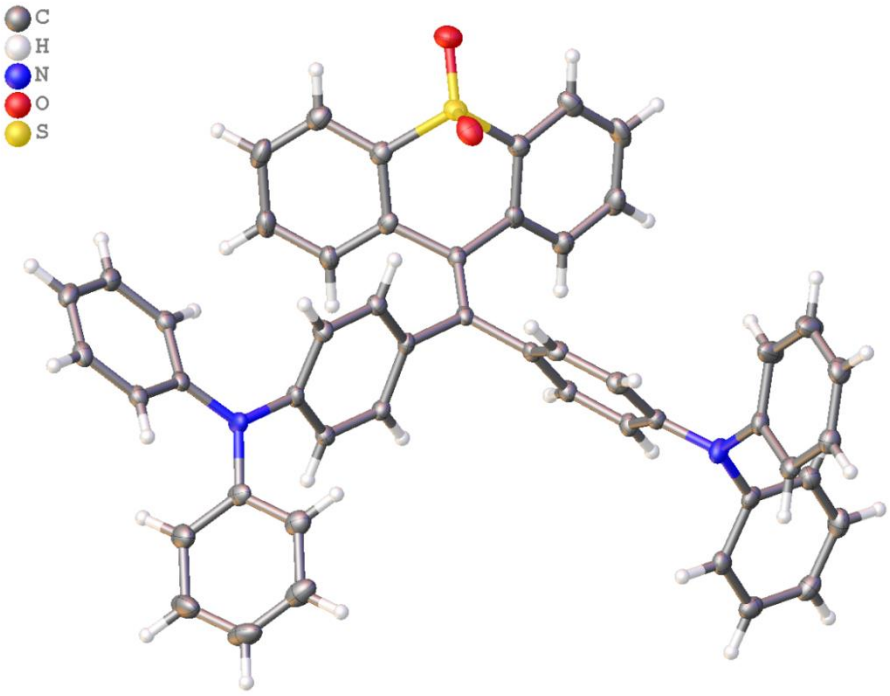


Figure S15. Thermal ellipsoids drawing of sulfur-bridged TPE derivative **4**.

3. AIE properties

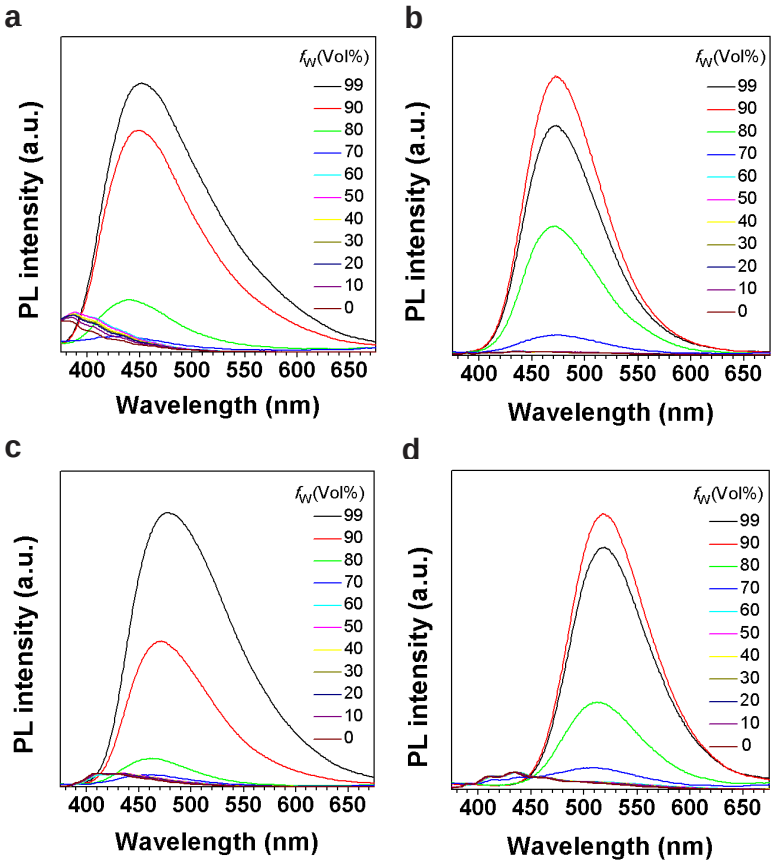


Figure S16. (a) **1**, (b) **2**, (c) **3**, (d) **4** AIE curves of sulfur-bridged tetraphenylethylene derivatives **1-4 in** THF/H_2O mixtures (10^{-5} M) with different water fractions (f_w).

4. OLEDs performances

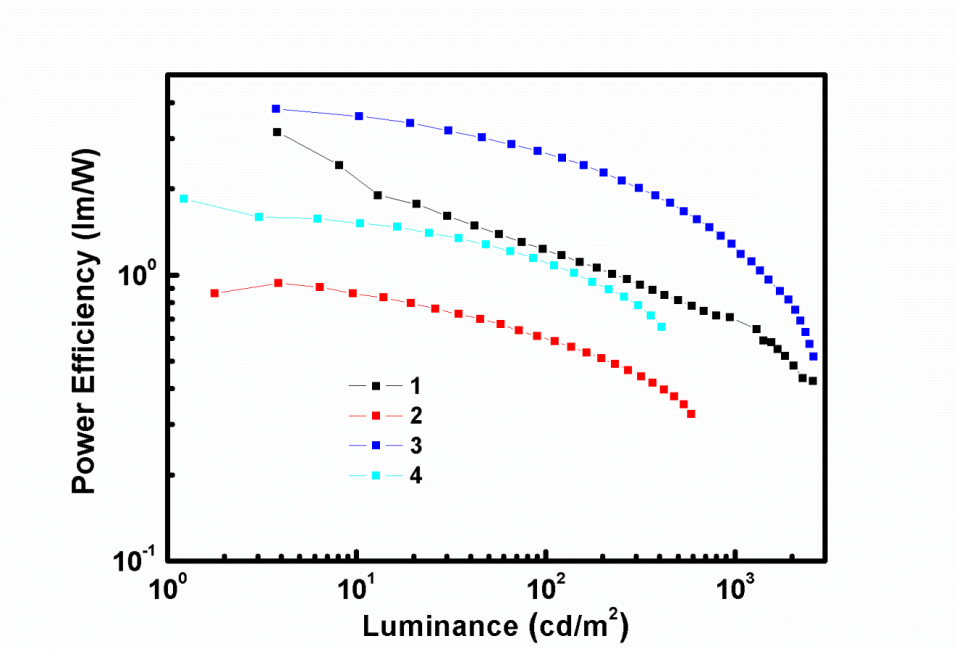


Figure S17. Power efficiency *versus* luminance curves of the non-doped OLEDs based on sulfur-bridged tetraphenylethylene derivatives **1**-**4** as emitters, device configuration: ITO/MoO_3 (10nm)/NPB (40nm)/TCTA (10nm)/EML (10nm)/BmPyPB (40nm)/LiF (1nm)/Al.

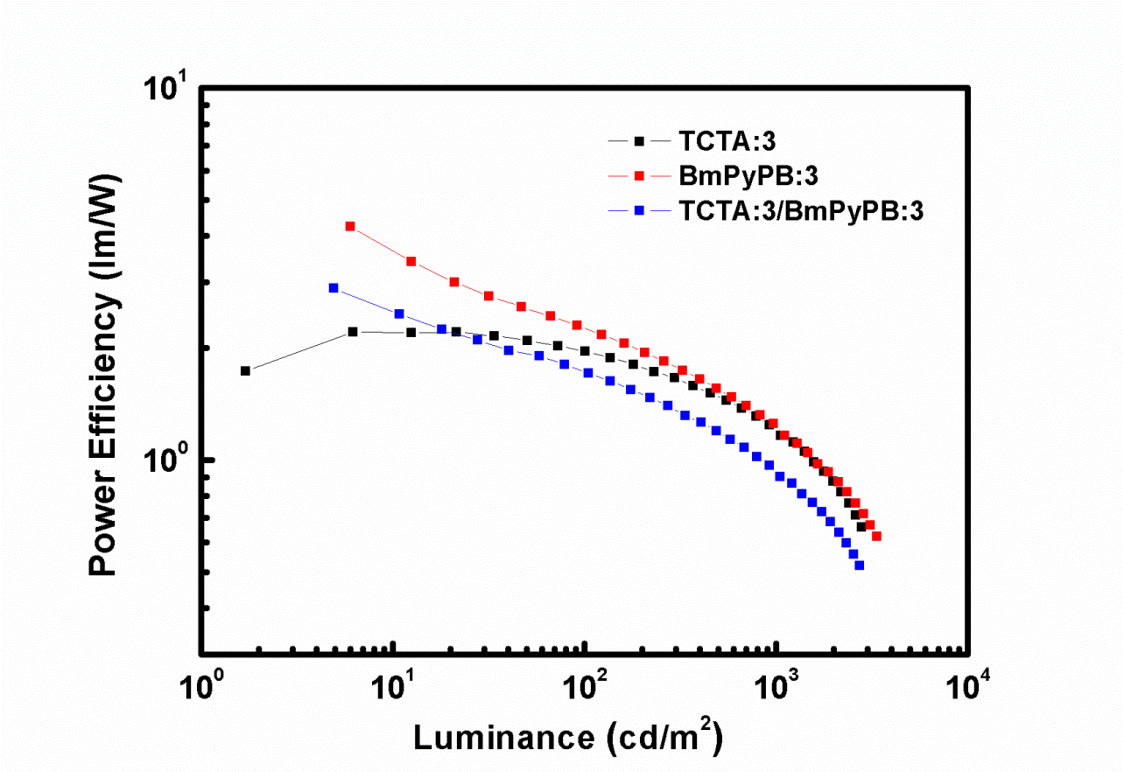


Figure S18. Power efficiency *versus* luminance curves of the doped OLEDs based on sulfur-bridged tetraphenylethylene derivative **3** as dopant, device configuration: ITO/MoO_3 (10nm)/NPB (40nm)/TCTA (10nm)/EML (10nm)/BmPyPB (40nm)/LiF (1nm)/Al.

5. Theoretical calculation

All density functional theory (DFT) calculations were performed using Gaussian 09 (Revision D.01) [4] employing Becke, Lee, Yang and Parr (B3LYP) functional [5] in combination with the 6-311G(d) basis set as implemented in Gaussian 09 (Revision D.01). All geometry optimizations were performed without imposing any symmetry constraints using tightened cutoffs (keyword *Tight*) on forces and step size to ensure adequate convergence and reliability of frequencies computed in a subsequent job step. Ultrafine (pruned (99,590)) integration grid (keyword *Ultrafine*) as implemented in Gaussian 09 (Revision D.01) was used for all calculations. Frequency calculations were used to confirm the identity of all obtained minima (no negative eigenvalues of the Hessian matrix).

Table S2. The optimized geometric structure of **1** in gas phase at the ground state (S_0) performed at B3LYP/6-311G(d) using the Gaussian 09 package.

Atom	x	y	z
N	4.937600	-1.500100	-0.043100
C	3.704900	-0.803900	-0.105500
C	3.119600	-0.298400	1.061500
C	1.911300	0.389500	0.993400
C	1.278000	0.613200	-0.236500
C	-0.014900	1.367100	-0.280200
C	-0.058900	2.724600	-0.237200
C	-1.338200	3.484600	-0.280500
C	-1.582500	4.487100	0.675900
S	-0.349100	4.857300	1.911300
C	1.121900	4.581200	0.934600
C	1.149100	3.576800	-0.054700
C	2.314300	3.442300	-0.825000
H	2.337200	2.706900	-1.620000
C	3.438800	4.224200	-0.574500
H	4.332600	4.090400	-1.177300
C	3.413700	5.177500	0.445700
H	4.287800	5.790600	0.646500
C	2.251100	5.367300	1.189200
H	2.208900	6.135800	1.955800
C	-2.800200	5.177200	0.692900
H	-2.971800	5.948000	1.438900
C	-3.776400	4.885400	-0.257100
H	-4.720000	5.423700	-0.241400
C	-3.528200	3.926300	-1.243900
H	-4.276700	3.714200	-2.002100
C	-2.316000	3.242900	-1.257700
H	-2.123600	2.487200	-2.012400
C	-1.243700	0.520400	-0.234100
C	-1.449000	-0.534100	-1.136800
H	-0.700300	-0.751300	-1.891700
C	-2.619300	-1.288500	-1.107900
H	-2.790600	-2.068100	-1.843300
C	-3.596100	-1.029600	-0.139900
N	-4.804000	-1.768100	-0.120400
C	-4.920800	-3.162100	-0.109500
C	-3.920000	-4.136000	-0.065600
H	-2.870700	-3.861500	-0.044000
C	-4.318100	-5.471300	-0.040900
H	-3.559100	-6.248300	-0.008100

C	-5.677200	-5.831900	-0.053500
H	-5.953200	-6.882400	-0.035500
C	-6.669100	-4.855400	-0.082900
H	-7.720100	-5.132400	-0.081900
C	-6.296400	-3.507200	-0.108200
C	-7.041300	-2.266300	-0.123500
C	-8.406600	-1.961200	-0.145500
H	-9.145300	-2.758300	-0.138700
C	-8.801600	-0.626700	-0.182700
H	-9.858500	-0.376200	-0.198100
C	-7.843800	0.402600	-0.206900
H	-8.172700	1.437600	-0.245900
C	-6.478000	0.126700	-0.184700
H	-5.742900	0.924400	-0.214800
C	-6.089800	-1.214900	-0.131200
C	-3.375400	-0.022700	0.808500
H	-4.115300	0.150400	1.583300
C	-2.218500	0.744100	0.753500
H	-2.061600	1.531000	1.483900
C	1.873400	0.102300	-1.398100
C	3.069800	-0.608900	-1.337300
H	3.520400	-1.012200	-2.238500
H	1.403600	0.276200	-2.362600
H	1.463800	0.788100	1.899100
H	3.624200	-0.436600	2.012500
C	6.086800	-1.190400	-0.778500
C	6.305600	-0.151700	-1.687000
H	5.522200	0.561000	-1.922500
C	7.567600	-0.058200	-2.270700
H	7.763200	0.739900	-2.981900
C	8.590400	-0.970400	-1.956300
H	9.562300	-0.870800	-2.431300
C	8.369600	-1.993900	-1.038600
H	9.162700	-2.692700	-0.785900
C	7.111600	-2.109500	-0.437400
C	6.555300	-3.012400	0.547400
C	7.064300	-4.116100	1.240500
H	8.090200	-4.437000	1.080200
C	6.237900	-4.796600	2.130600
H	6.621200	-5.653900	2.676300
C	4.906900	-4.387500	2.327100
H	4.275400	-4.937200	3.019800
C	4.375500	-3.291700	1.649700
H	3.345300	-2.985100	1.796600
C	5.214800	-2.605900	0.768200

Table S3. The optimized geometric structure of **2** in gas phase at the ground state (S_0) performed at B3LYP/6-311G(d) using the Gaussian 09 package.

Atom	**x**	**y**	**z**
S	-0.231500	4.388400	1.505500
C	-1.554300	4.154500	0.322700
C	-1.371700	3.141100	-0.632800
C	-0.073200	2.404300	-0.667300
C	-0.002800	1.052000	-0.649500
C	1.302800	0.339200	-0.507600
C	2.018000	0.480600	0.691900
C	3.239100	-0.161800	0.870600

C	3.759100	-0.976000	-0.143500
N	5.004100	-1.628200	0.032200
C	6.094200	-1.556800	-0.842700
C	6.232800	-0.837500	-2.032500
H	5.423100	-0.225100	-2.415000
C	7.450000	-0.927100	-2.705400
H	7.582200	-0.378600	-3.634100
C	8.507700	-1.707600	-2.206600
H	9.442900	-1.758100	-2.757000
C	8.367800	-2.409700	-1.012400
H	9.188300	-3.004300	-0.619400
C	7.156200	-2.335900	-0.317100
C	6.685600	-2.902400	0.928800
C	7.261700	-3.752100	1.879300
H	8.279700	-4.109300	1.748100
C	6.511500	-4.135100	2.987700
H	6.947300	-4.792700	3.734300
C	5.189900	-3.682500	3.148300
H	4.617700	-3.999900	4.015700
C	4.592900	-2.835600	2.216400
H	3.569500	-2.497600	2.339800
C	5.356800	-2.443900	1.114200
C	3.043000	-1.138100	-1.335600
C	1.827800	-0.480600	-1.514400
H	1.291900	-0.601700	-2.451200
H	3.442400	-1.781500	-2.113000
H	3.803200	-0.026600	1.787800
H	1.617300	1.121000	1.473100
C	-1.233700	0.215200	-0.529000
C	-1.605900	-0.724600	-1.498900
H	-0.991200	-0.866300	-2.382500
C	-2.790800	-1.446100	-1.373100
H	-3.102000	-2.136700	-2.150300
C	-3.606200	-1.263000	-0.249800
N	-4.829300	-1.966200	-0.132000
C	-5.000300	-3.350300	-0.244600
C	-4.042900	-4.349900	-0.433900
H	-2.989400	-4.107600	-0.526500
C	-4.488200	-5.669300	-0.488700
H	-3.763700	-6.465700	-0.636000
C	-5.850500	-5.989700	-0.353000
H	-6.164300	-7.028500	-0.402000
C	-6.797200	-4.989100	-0.150200
H	-7.849200	-5.236300	-0.034200
C	-6.376500	-3.656200	-0.091500
C	-7.065900	-2.400600	0.117200
C	-8.408600	-2.058200	0.309800
H	-9.171700	-2.831600	0.337600
C	-8.750800	-0.716800	0.458300
H	-9.789500	-0.437800	0.611100
C	-7.763900	0.283300	0.406900
H	-8.052700	1.325200	0.516000
C	-6.419300	-0.030300	0.217200
H	-5.662800	0.746100	0.167400
C	-6.082000	-1.380100	0.085500
C	-3.214700	-0.364800	0.750900
H	-3.833700	-0.249100	1.634700
C	-2.045500	0.373500	0.606000
H	-1.748800	1.083200	1.373500
C	1.135600	3.275200	-0.576600

C	1.161900	4.299800	0.385000
C	2.228500	5.182400	0.519300
C	3.324600	5.040000	-0.332200
C	3.325000	4.032000	-1.300000
C	2.240600	3.162800	-1.428200
H	2.246800	2.389400	-2.188600
H	4.174200	3.926000	-1.969200
H	4.170400	5.715400	-0.245100
H	2.186200	5.960900	1.274400
C	-2.418900	2.907100	-1.532000
C	-3.599800	3.646400	-1.452100
C	-3.754900	4.645800	-0.487000
C	-2.718800	4.910600	0.409100
H	-2.797000	5.687400	1.163100
H	-4.674700	5.221000	-0.437800
H	-4.401700	3.446400	-2.157200
H	-2.305800	2.137400	-2.288000
O	-0.316900	5.734800	2.092800
O	-0.190500	3.200000	2.384700

Table S4. The optimized geometric structure of **3** in gas phase at the ground state (S_0) performed at B3LYP/6-311G(d) using the Gaussian 09 package.

Atom	**x**	**y**	**z**
C	1.315100	-4.423300	-0.031900
S	0.037700	-4.891400	1.124300
C	-1.391900	-4.320200	0.216600
C	-1.314400	-3.164800	-0.587200
C	-0.034700	-2.399500	-0.617600
C	1.174800	-3.248400	-0.792900
C	2.184700	-2.927000	-1.713100
C	3.328700	-3.711100	-1.825800
C	3.475000	-4.850700	-1.028900
C	2.463600	-5.215800	-0.143300
H	2.553800	-6.119800	0.452300
H	4.365300	-5.467900	-1.113000
H	4.104200	-3.436500	-2.535400
H	2.072100	-2.033000	-2.318000
C	0.030800	-1.054300	-0.424000
C	1.317800	-0.327900	-0.232900
C	2.269200	-0.798700	0.689500
H	2.048800	-1.689900	1.268200
C	3.478500	-0.145400	0.879200
H	4.195100	-0.525400	1.599900
C	3.793300	1.001900	0.132200
N	5.051300	1.635500	0.283900
C	6.227400	0.850700	0.416900
C	6.383700	-0.333500	-0.322200
H	5.595000	-0.649200	-0.997600
C	7.535800	-1.103300	-0.178000
H	7.638400	-2.018600	-0.755200
C	8.558000	-0.700400	0.684500
H	9.457800	-1.300000	0.788600
C	8.408300	0.481800	1.413000
H	9.190900	0.805300	2.094400
C	7.251300	1.248500	1.291500
H	7.132800	2.159900	1.868600
C	5.140400	3.053000	0.257300

C	6.168000	3.690800	-0.455000
H	6.896300	3.089400	-0.989600
C	6.252500	5.081600	-0.469100
H	7.054900	5.560300	-1.024500
C	5.307900	5.857900	0.206400
H	5.372900	6.942000	0.186900
C	4.278800	5.224600	0.907500
H	3.540500	5.815100	1.443700
C	4.197500	3.834200	0.943800
H	3.404200	3.342800	1.498100
C	2.837700	1.500800	-0.766200
H	3.060100	2.394000	-1.340900
C	1.615100	0.855900	-0.925600
H	0.894500	1.267200	-1.625100
C	-1.217800	-0.248200	-0.252200
C	-1.748100	0.535900	-1.285600
H	-1.231700	0.587600	-2.240500
C	-2.974400	1.180400	-1.142600
H	-3.394400	1.748400	-1.966600
C	-3.694700	1.068400	0.055000
N	-4.984600	1.647200	0.186000
C	-5.227700	2.947100	-0.327500
C	-4.275300	3.963000	-0.145300
H	-3.363000	3.742800	0.400100
C	-4.499000	5.236900	-0.662600
H	-3.750700	6.010800	-0.512600
C	-5.679100	5.527200	-1.351600
H	-5.854100	6.523800	-1.746400
C	-6.631300	4.520400	-1.526600
H	-7.551100	4.728200	-2.067200
C	-6.408300	3.237600	-1.030100
H	-7.145100	2.455200	-1.179700
C	-6.042600	0.863500	0.717600
C	-6.109300	-0.516300	0.459700
H	-5.345100	-0.987000	-0.150500
C	-7.140200	-1.281500	1.000600
H	-7.170800	-2.348500	0.794900
C	-8.131100	-0.689200	1.786500
H	-8.936600	-1.288700	2.200900
C	-8.071100	0.683900	2.036400
H	-8.829100	1.159400	2.653400
C	-7.033100	1.455300	1.518200
H	-6.982600	2.519200	1.726500
C	-3.139400	0.337200	1.115600
H	-3.687500	0.257400	2.048900
C	-1.923000	-0.316100	0.957300
H	-1.520300	-0.912300	1.771000
C	-2.453600	-2.798400	-1.321500
H	-2.401500	-1.939300	-1.979100
C	-3.649400	-3.501300	-1.198900
H	-4.518600	-3.187700	-1.770700
C	-3.725500	-4.608500	-0.350000
H	-4.655400	-5.161300	-0.248800
C	-2.592500	-5.028800	0.342500
H	-2.629500	-5.915300	0.969400

Table S5. **.** The optimized geometric structure of **4** in gas phase at the ground state (S_0) performed at B3LYP/6-311G(d) using the Gaussian 09 package.

Atom	x	y	z
S	0.066100	-4.477300	0.924600
O	0.066500	-5.910000	1.263300
O	0.139900	-3.466300	2.000300
C	1.368400	-4.131600	-0.252200
C	2.475600	-4.969700	-0.344000
H	2.515700	-5.869600	0.261500
C	3.503100	-4.625100	-1.221700
H	4.378300	-5.262000	-1.309400
C	3.395900	-3.463800	-1.993300
H	4.190000	-3.200500	-2.686800
C	2.272600	-2.642600	-1.897100
H	2.195100	-1.746100	-2.503000
C	1.234500	-2.957000	-1.010300
C	-0.009400	-2.141500	-0.884600
C	-1.274000	-2.936700	-0.891700
C	-2.393900	-2.617600	-1.670800
H	-2.367300	-1.736200	-2.301300
C	-3.536800	-3.417100	-1.633900
H	-4.393300	-3.148300	-2.246400
C	-3.584900	-4.563000	-0.834800
H	-4.476400	-5.182900	-0.817900
C	-2.475500	-4.916100	-0.067000
H	-2.467100	-5.807700	0.551900
C	-1.348900	-4.100000	-0.106100
C	0.012200	-0.802900	-0.664300
C	1.288200	-0.071900	-0.428100
C	2.140600	-0.500100	0.604400
H	1.838500	-1.338800	1.225500
C	3.347600	0.141200	0.847400
H	3.991000	-0.198800	1.652200
C	3.755300	1.221000	0.046400
N	5.013700	1.835300	0.255400
C	6.149800	1.038000	0.559100
C	6.341500	-0.202000	-0.071800
H	5.610600	-0.552100	-0.793800
C	7.453200	-0.982100	0.238600
H	7.584200	-1.941300	-0.255600
C	8.400700	-0.534800	1.162300
H	9.269400	-1.143200	1.396800
C	8.216500	0.702800	1.783100
H	8.940400	1.061100	2.510300
C	7.097500	1.481300	1.494800
H	6.950300	2.436600	1.988300
C	5.150000	3.243000	0.119600
C	6.254900	3.791400	-0.549900
H	7.006300	3.128300	-0.966700
C	6.385900	5.173400	-0.671100
H	7.248000	5.582700	-1.191200
C	5.412900	6.027800	-0.147200
H	5.515000	7.104400	-0.249900
C	4.307800	5.483000	0.511200
H	3.546700	6.135500	0.930800
C	4.178300	4.103200	0.654700
H	3.325800	3.681100	1.177400
C	2.894500	1.671800	-0.967500
H	3.193200	2.510600	-1.587500
C	1.671100	1.045300	-1.183200
H	1.026700	1.409700	-1.977400

C	-1.256000	-0.048100	-0.436300
C	-1.766500	0.872600	-1.359700
H	-1.229300	1.069000	-2.283500
C	-2.996700	1.489900	-1.148400
H	-3.400300	2.171500	-1.890100
C	-3.735600	1.218700	0.013300
N	-5.011900	1.802500	0.213600
C	-5.235000	3.157100	-0.148700
C	-4.271600	4.134300	0.148300
H	-3.362100	3.843100	0.664200
C	-4.481700	5.461500	-0.219500
H	-3.725500	6.205400	0.017600
C	-5.658800	5.841000	-0.869100
H	-5.823100	6.878200	-1.146800
C	-6.622500	4.871700	-1.156700
H	-7.540500	5.150400	-1.667600
C	-6.412900	3.538200	-0.810700
H	-7.158300	2.785300	-1.045600
C	-6.080200	1.003100	0.700600
C	-6.211900	-0.336100	0.297600
H	-5.487800	-0.761800	-0.389800
C	-7.254800	-1.117400	0.790500
H	-7.338000	-2.153400	0.472400
C	-8.193700	-0.577500	1.672400
H	-9.008700	-1.188400	2.049500
C	-8.069600	0.756800	2.066500
H	-8.786700	1.189700	2.759000
C	-7.018500	1.541000	1.595900
H	-6.917400	2.573400	1.914900
C	-3.201700	0.336100	0.966000
H	-3.760900	0.130100	1.872800
C	-1.985900	-0.295300	0.736600
H	-1.594200	-1.003500	1.461900

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