Electronic Supplementary Material (ESI) for Chemical Communications.

Thiophene-fused boracycles as photoactive analogues of diboraanthracenes

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Experimental Section

General Information

All reagents and starting materials were purchased from Sigma-Aldrich, Alfa-Aesar and Spectrochem chemical companies and used as received unless otherwise noted. Chlorinated solvents, acetonitrile, and DMF were distilled from CaH_2. THF and toluene were distilled from Na/benzophenone prior to use. All 400 MHz ^{1}H, 100 MHz ^{13}C, NMR spectra were recorded on a Bruker ARX 400 spectrometer operating at 400 MHz. All ^{1}H and ^{13}C NMR spectra were referenced internally to solvent signals. All NMR spectra were recorded at ambient temperature. ESI mass spectra were recorded on Bruker, micrOTOF-QII mass spectrometer. The absorbance spectra were recorded on a JASCO V-730 UV-Visible spectrometer. The fluorescence spectra were recorded using Edinburgh FS5 spectrofluorometer. Absolute fluorescence quantum yields of compounds **3-5** were measured by integrating sphere method using Edinburgh FS5 spectrofluorometer. The fluorescence spectra are corrected for the instrumental response. Cyclic voltammetry measurements were performed with a conventional three electrode cell using an electrochemical workstation (CH Instrument, Model: 1100A) The three-electrode system consisted of a Glassy carbon working electrode, a Pt wire as the secondary electrode, and a Ag wire as the reference electrode. The voltammograms were recorded with ca. 1.0 x10^{-3} M solution in THF containing Bu_4NPF_6 (0.1 M) as the supporting electrolyte. The scans were referenced after the addition of a small amount of ferrocene as the internal standard. Single-crystal X-ray diffraction data for compound **3** were collected on a Rigaku SuperNova fine-focused dual diffractometer, with Cu Kα radiation (λ = 1.54178 Å) equipped with a PILATUS200K detector and for compound **4** were collected on a Bruker APEX-II diffractometer using Mo-Kα radiation (0.71073 Å). Using Olex2, the structures were solved with the ShelXS structure solution program using Direct Methods and refined with the ShelXL refinement package using Least Squares minimization. All non-hydrogen atoms were refined with anisotropic displacement coefficients. The H atoms were placed at calculated positions and were refined as riding atoms. Crystallographic data for compounds **3** & **4** have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC- 2091448-2091449. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk). DFT calculations were performed with the Gaussian09 program.[1] The structures were optimized using 6-31G(d,p) (B3LYP) as the basis set. Frequency calculations confirmed the optimized structures to be local minimum structures. Excitation data were determined using TD-DFT (B3LYP/631g(d,p))–calculations.

References:

Gaussian 09 (Rev. C.02), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, _. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Synthesis of compound 2: To a suspension of 3,4-bis(chloromercurio)2,5-dimethylthiophene (**1**) (2.00 g, 3.42 mmol) in toluene (50 mL) in a seal tube was added BCl_3 (4 mL in CH_2Cl_2) inside a glovebox. The tube was closed and heated at 100 ºC in an oil bath for 12h. After cooling to room temp, the resulting mixture was filtered inside the glovebox and kept for crystallization. Fluffy white needles formed were filtered to give compound **2**. Yield: 0.322 g (30%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.82 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ=155.27, 128.38, 17.35. ^{11}B NMR (128 MHz, $CDCl_3$) δ =49.96.

General procedure for the synthesis of compounds 3-5: A solution of arylmagnesium bromide (6 mL, 1M in THF) was added to a solution of compound **2** (0.50 g) in toluene (20 mL) in a sealed tube. The resulting mixture was then refluxed for 12h. After 12h, the compound was extracted with water and dichloromethane (3 x 50 mL). The organic phase was collected and dried over anhydrous sodium sulphate. The solvent was concentrated and the product was purified using silica gel column chromatography (EtOAc/ *n*-hexane (5:95)).

Synthesis of compound 3: The quantities involved are as follows, xylylmagnesium bromide (6 mL, 1M in THF), compound **2** (0.50 g), and toluene (20 mL). Yield: 0.298 g (41%). Mp: 248 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ= 7.18 - 7.14 (m, 2H), 7.01 (d, *J* = 4.0 Hz, 4H), 2.17 (s, 12H), 1.96 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ=156.29, 145.14, 136.17, 126.83, 126.58, 21.97, 14.97. ^{11}B NMR (128 MHz, $CDCl_3$) δ=56.71. HR-MS (ESI): calcd for $C_{28}H_{30}B_2S_2[M+H]^+$: 453.2058, Found: 453.2042. IR (KBr): ν(cm^{-1}) =2959(m), 2912(m), 1607(m), 1463(m), 1259(m), 1104(m), 761(m), 699(m).

Synthesis of compound 4: The quantities involved are as follows, mesitylmagnesium bromide (6 mL, 1M in THF), compound **2** (0.50 g), and toluene (20 mL). Yield: 0.312 g (40%). Mp: 253 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.84 (s, 4H), 2.33 (s, 6H), 2.12 (s, 12H), 1.97 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 156.26, 145.49, 144.24, 136.26, 136.16, 127.57, 21.98, 21.37, 15.10. ^{11}B NMR (128 MHz, $CDCl_3$) δ = 56.36. HR-MS (ESI): calcd for $C_{30}H_{34}B_2S_2[M+H]^+$: 481.2371, Found: 481.2348. Anal. Calcd for $C_{30}H_{34}B_2S_2$: C 75.02; H 7.13; S 13.35. Found: C

74.89; H 7.037; S 13.525. IR (KBr): ν(cm^{-1}) = 2959(m), 2910(m), 1605(m), 1465(m), 1302(m), 1255(m), 1104(m), 851(m), 794(m), 681(m).

Synthesis of compound 5: The quantities involved are as follows, 2,4,6-triisopropylphenylmagnesium bromide (6 mL, 1M in THF), compound **2** (0.50 g), and toluene (20 mL). Yield: 0.328 g (32%). Mp: 255 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.00 (s, 4H), 2.92 (h, *J* = 8 Hz, 2H), 2.61 (h, *J* = 8 Hz, 4H), 1.98 (s, 12H), 1.29 (d, *J* = 8 Hz, 2H), 1.11 (d, *J* = 8 Hz, 24H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 156.12, 148.40, 146.96, 120.44, 34.94, 34.34, 24.41, 24.33, 15.87. ^{11}B NMR (128 MHz, $CDCl_3$) δ = 57.79. HR-MS (ESI): calcd for $C_{42}H_{58}B_2S_2[M+Na]^+$: 671.4072, Found: 671.4033. IR (KBr): ν(cm^{-1}) = 2959(m), 2925(m), 1602(m), 1455(m), 1247(m), 1090(m), 876(m), 790(m), 689(m).

Table S1: Photophysical data of compound **3-5**

Compound	**Solvent**	**λ_{absmax}(nm)(log ε)**	**λ_{em}(nm)**	**Φ_F**
3	CH_2Cl_2	275(4.874), 351(4.098), 365(4.225)	378, 395	5.89
	THF	275(4.838), 351(4.021), 367(4.166)	377, 394	4.73
	Cyclohexane	277(4.952), 351(3.963), 367(4.130)	372, 390	5.22
4	CH_2Cl_2	275(4.725), 351(3.959), 365(4.077)	378, 395	5.37
	THF	275(4.966), 351(4.149), 367(4.287)	376, 394	5.23
	Cyclohexane	276(4.769), 351(4.148), 367(4.315)	373, 390	4.69
5	CH_2Cl_2	275(4.760), 348(3.894), 363(4.007)	376, 393	7.06
	THF	275(4.777), 349(3.859), 363(3.954)	375, 392	6.24
	Cyclohexane	277(4.784), 348(3.947), 363(4.080)	371, 388	4.35

Table S2: Crystal data and structure refinement parameters for compounds **3** and **4.**

Compound	**3**	**4**
Empirical formula	$C_{28}H_{30}B_2S_2$	$C_{30}H_{34}B_2S_2$
Formula weight	452.26	480.31
Temperature/K	297.6(8)	296.15
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	10.54815(16)	7.3621(3)
b/Å	14.5492(2)	16.4766(7)
c/Å	8.34333(15)	11.3205(5)
α/°	90	90
β/°	97.4946(16)	93.878(2)
γ/°	90	90
Volume/$Å^3$	1269.49(4)	1370.06(10)
Z	2	2
ρcalcg/cm3	1.183	1.164
μ/mm-1	1.979	0.211
F(000)	480.0	512.0
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)
2 θ range for data collection/°	8.454 to 150.788	4.372 to 56.714
Index ranges	$-13 \leq h \leq 12$, $-17 \leq k \leq 9$, $-9 \leq l \leq 10$	$-9 \leq h \leq 9$, $-21 \leq k \leq 21$, $-15 \leq l \leq 15$
Reflections collected	9588	22133
Independent reflections	2563[R_{int} = 0.0963, R_{sigma} = 0.0555]	3394[R_{int} = 0.0345, R_{sigma} = 0.0218]
Data/restraints/parameters	2563/0/150	3394/0/159
Goodness-of-fit on F2	1.112	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0680, wR_2 = 0.1955	R_1 = 0.0467, wR_2 = 0.1309
Final R indexes [all data]	R_1 = 0.0749, wR_2 = 0.2030	R_1 = 0.0610, wR_2 = 0.1429
Largest diff. peak/hole / e $Å^{-3}$	0.31 and -0.32	0.31 and -0.23

Table S3: Frontier orbital energies derived from UV/Vis onset absorption and electrochemical data

Compound	HOMO-LUMO gap[a]	LUMO[b]	HOMO[c]
3	3.28	-2.01	-5.29
4	3.28	-2.03	-5.31
5	3.30	-1.98	-5.28

[a] Estimated from the absorption onset of the longest-wavelength UV band. [b] Calculated from E_{pc} of the first reduction wave referenced to Fc/Fc+. [c] Calculated from the HOMO–LUMO gap and the LUMO.

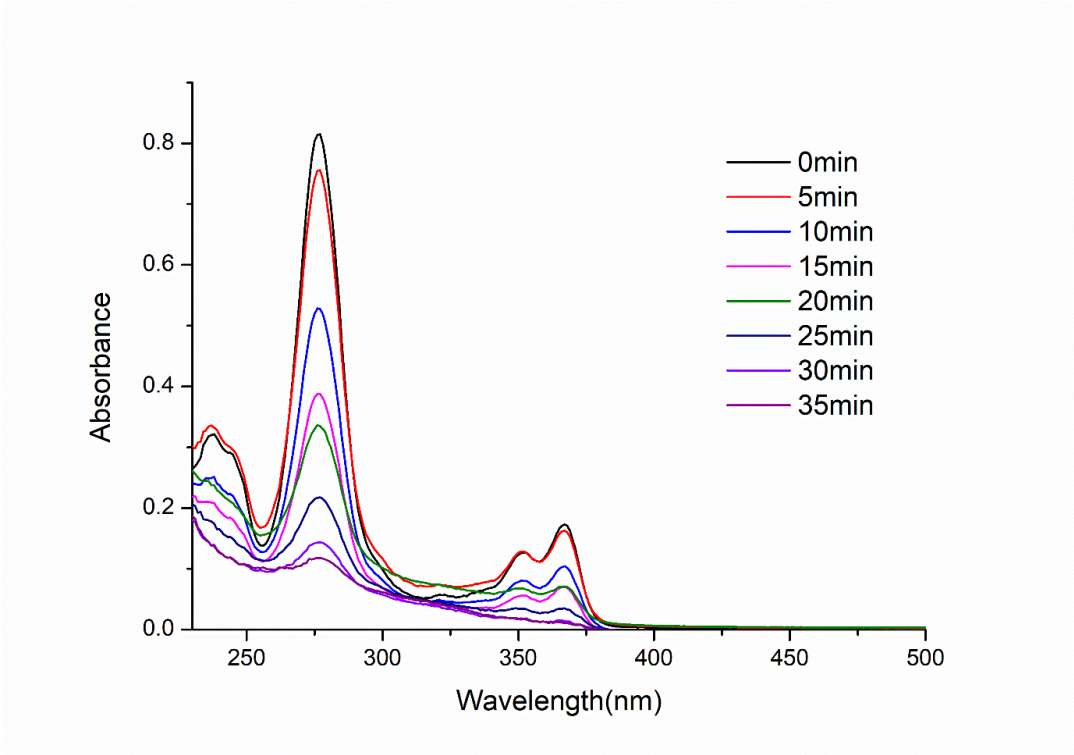


Figure S1: UV Spectra of compound **3** in THF(10^{-5}M) after passing of UV light (365nm).

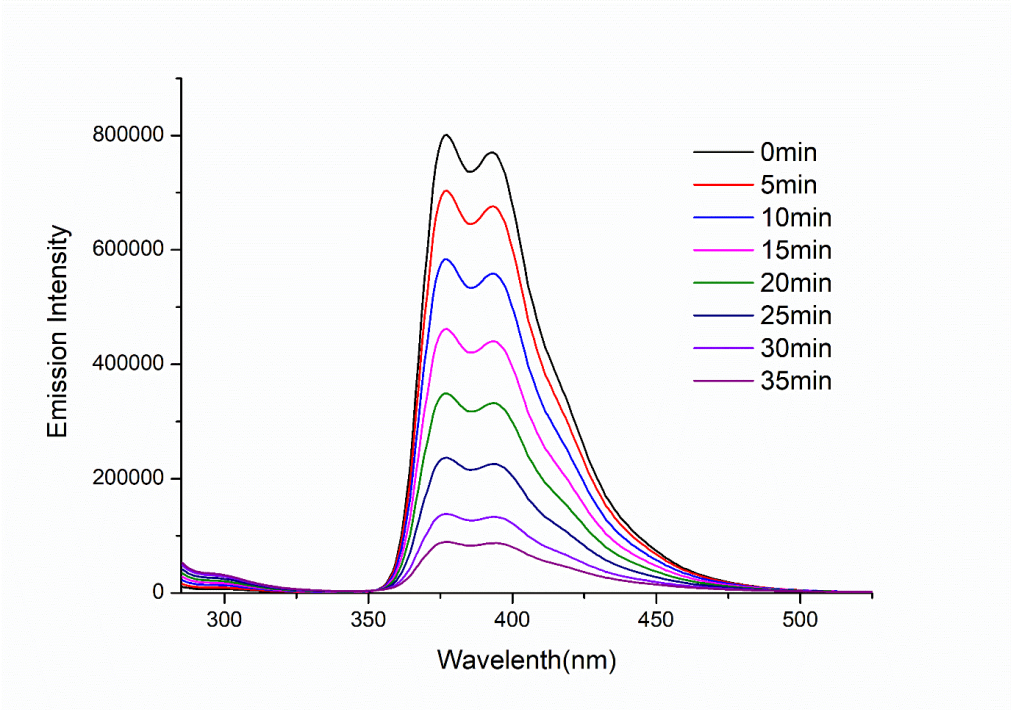


Figure S2: Emission spectra of compound **3** in THF(10^{-5}M) after passing of UV light (365nm).

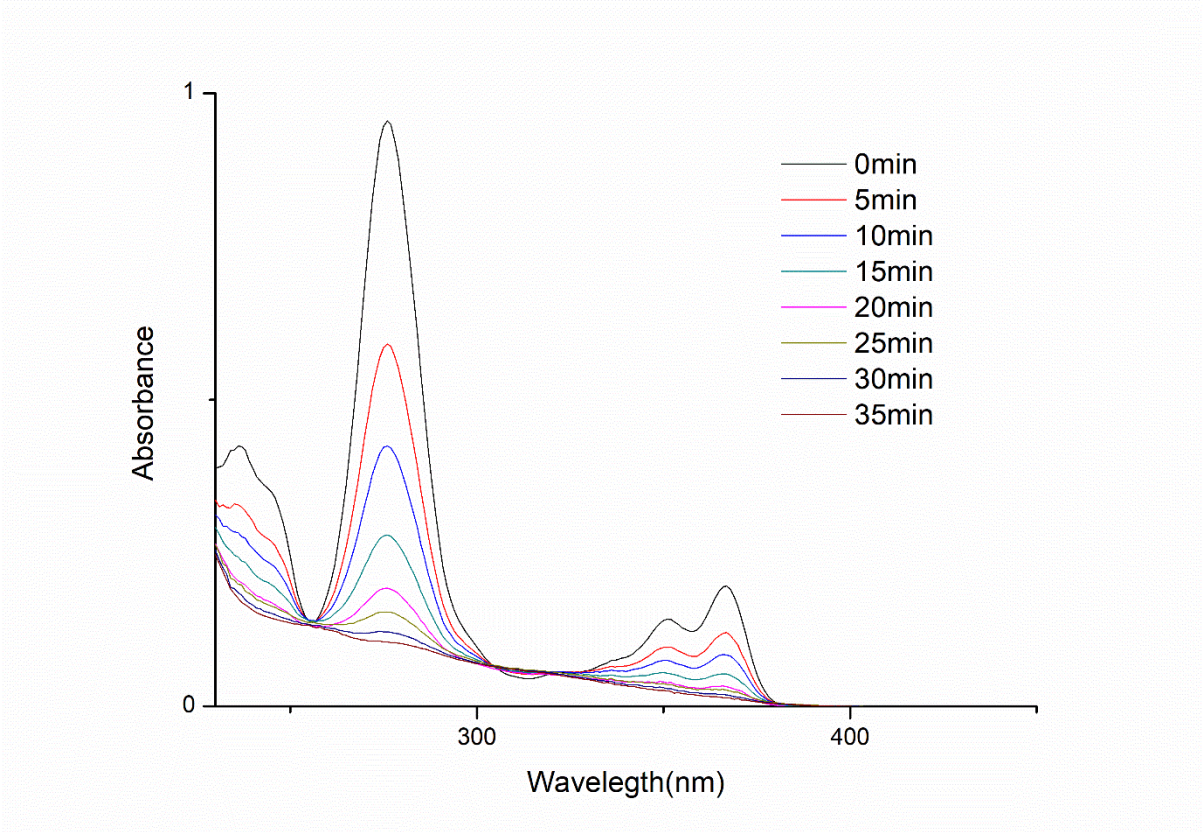


Figure S3: UV spectra of compound **4** in THF(10^{-5}M) after passing of UV light (365nm).

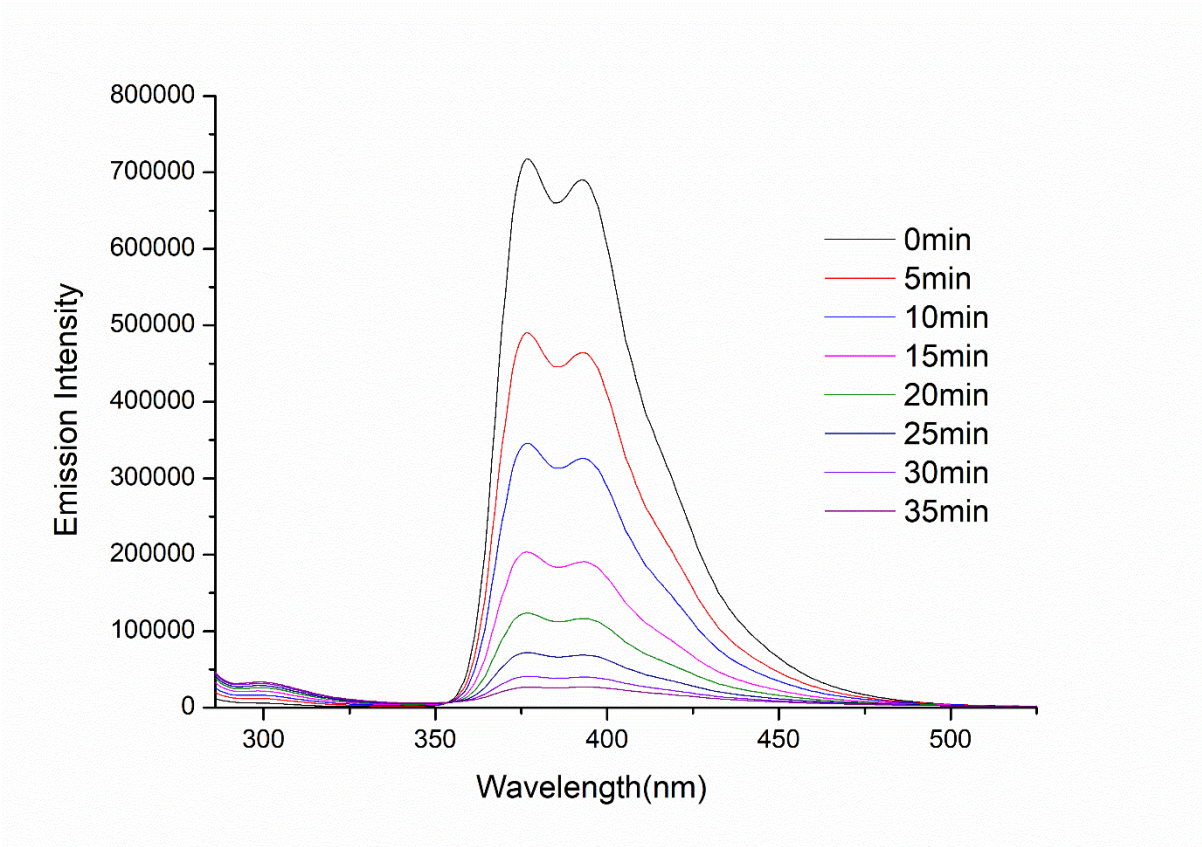


Figure S4: Emission spectra of compound **4** in THF(10^{-5}M) after passing of UV light (365nm).

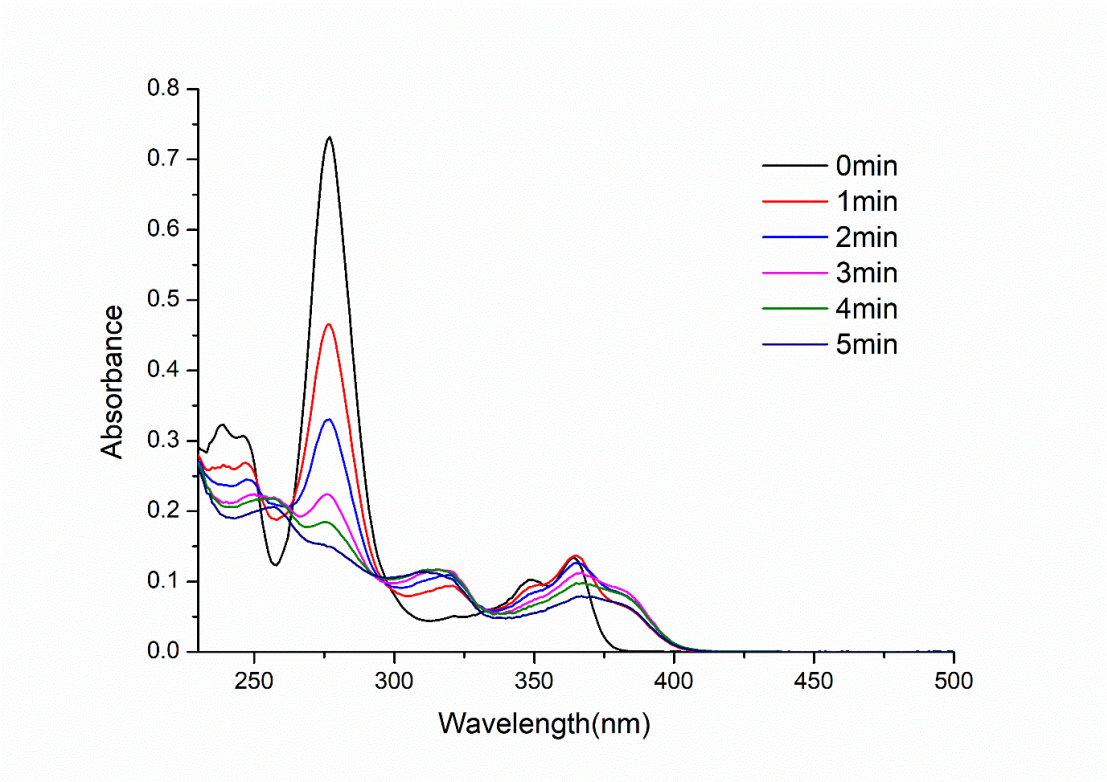


Figure S5: UV Spectra of compound **5** in THF(10^{-5}M) after passing of UV light (365nm).

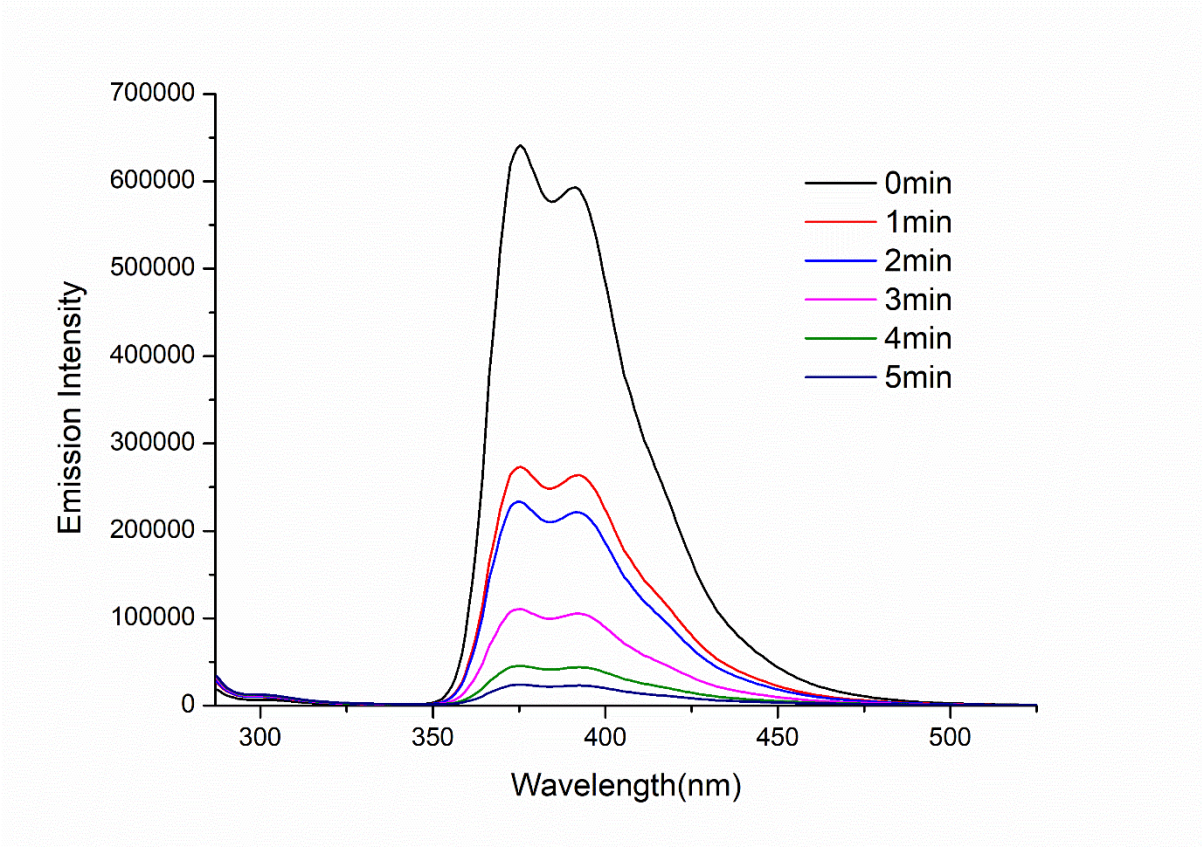


Figure S6: Emission spectra of compound **5** in THF(10^{-5}M) after passing of UV light (365nm).

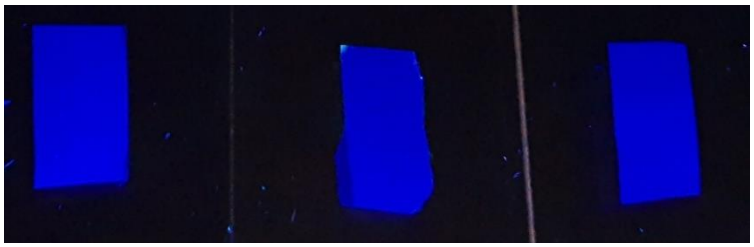


Figure S7: Photograph of compounds **3-5** (from left to right) in PMMA film (4wt%).

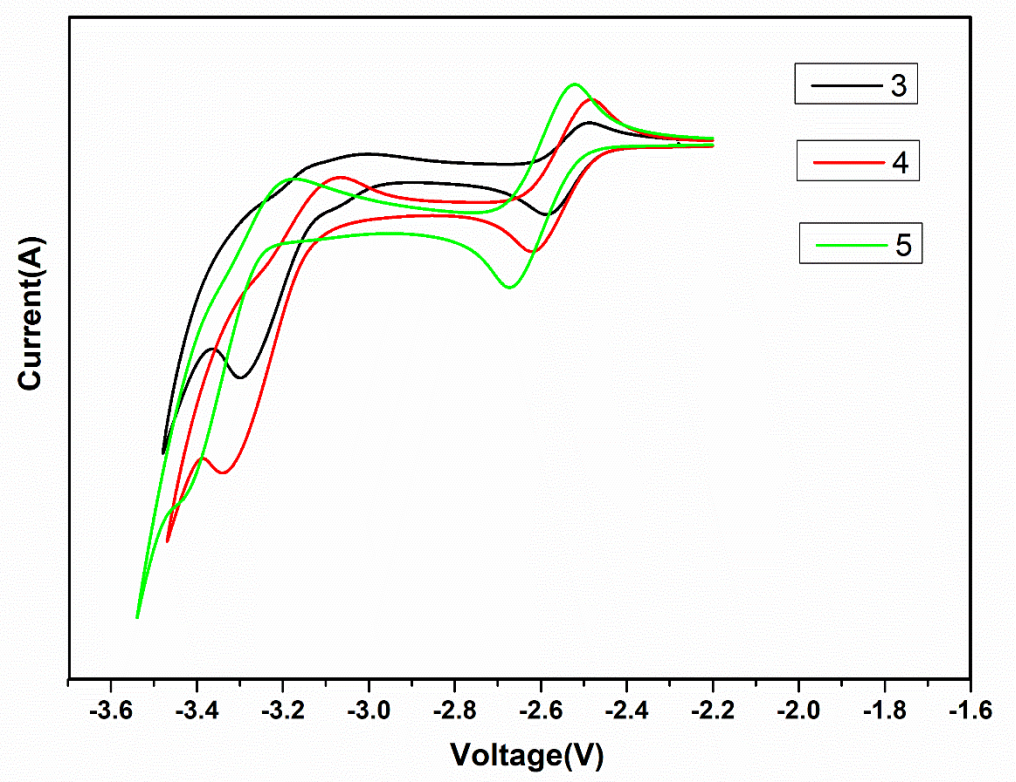
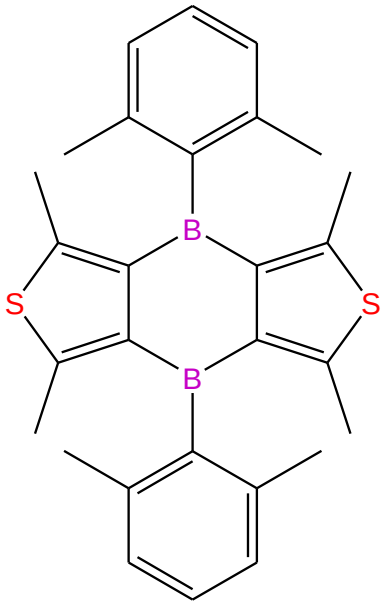
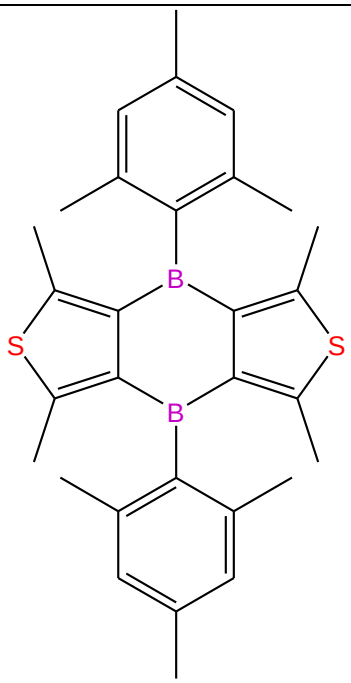
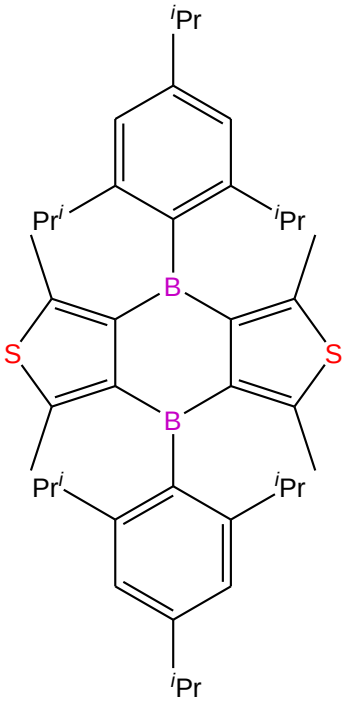
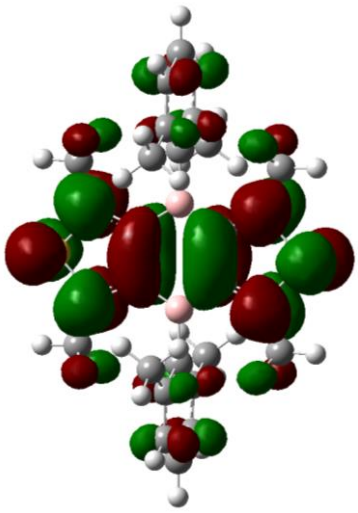
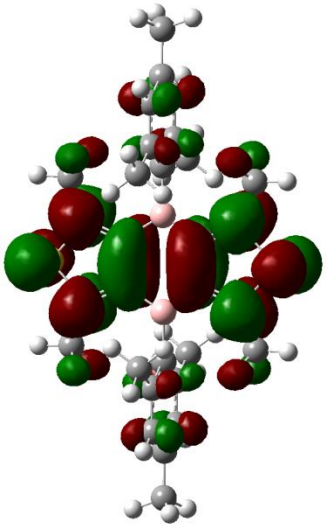
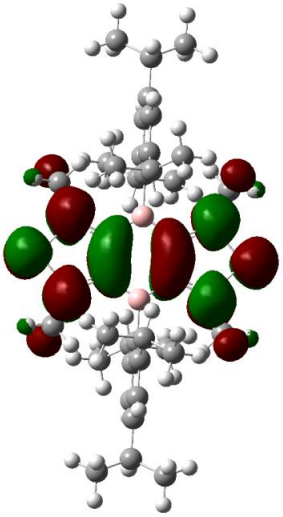


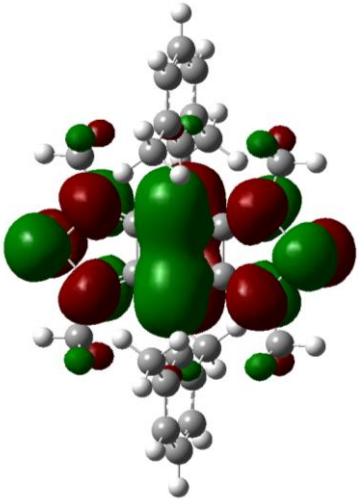
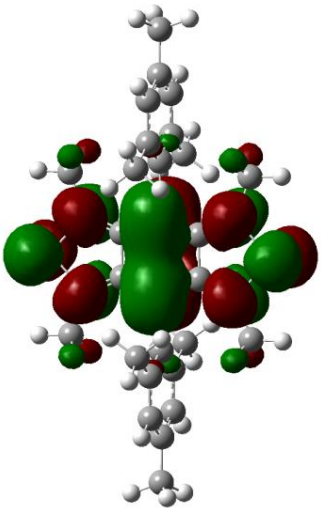
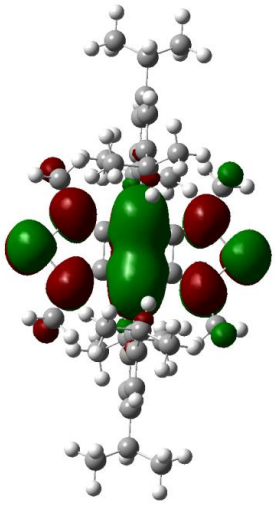
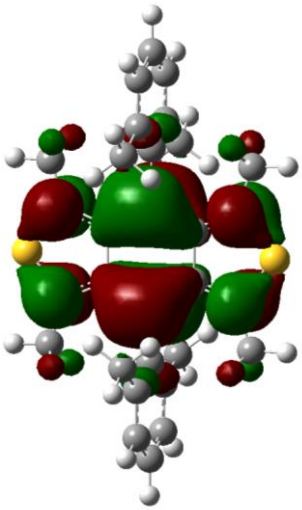
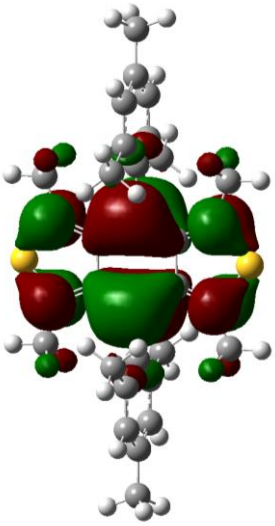
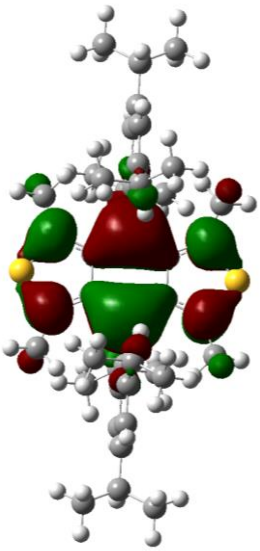
Figure S8: Cyclic Voltammogram of compounds **3-5** (vs. Ferrocene/Ferrocenium) with 0.1 M Bu_4NPF_6 as the supporting electrolyte (scan rate 50 mV/s) in DME.

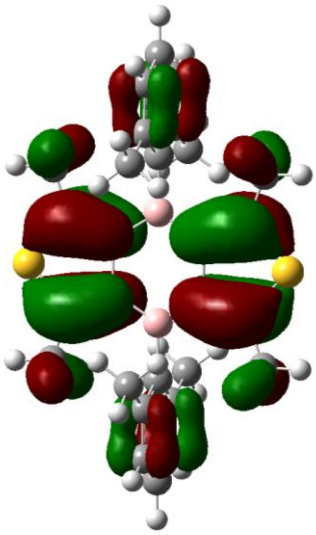
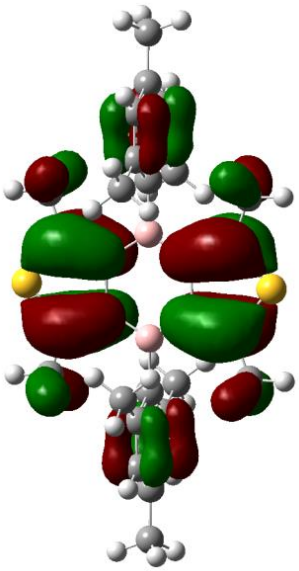
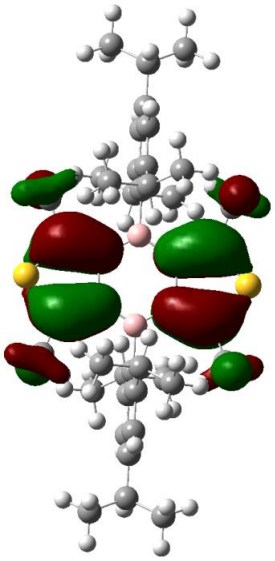
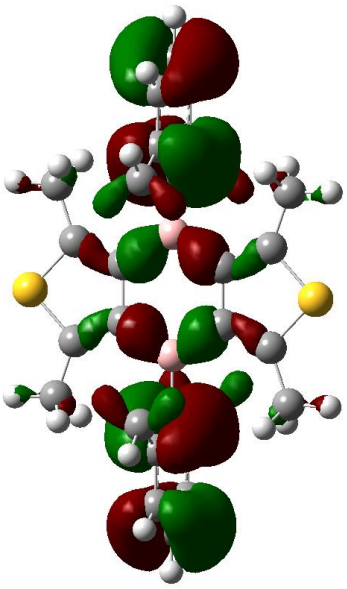
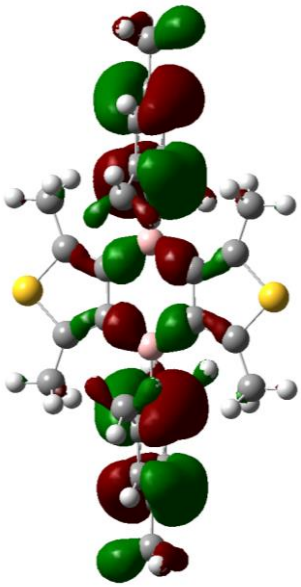
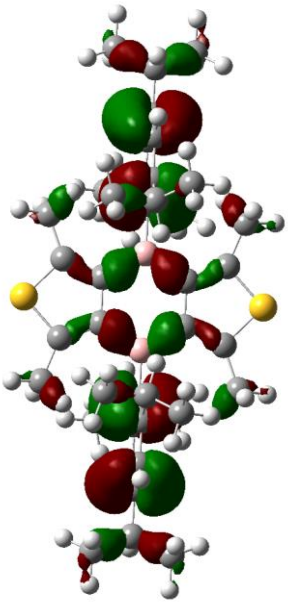
Table S4. Calculated electronic transitions for compound **3-5** from TD-DFT ((B3LYP/631g(d,p))– PCM solvation (THF))) calculations

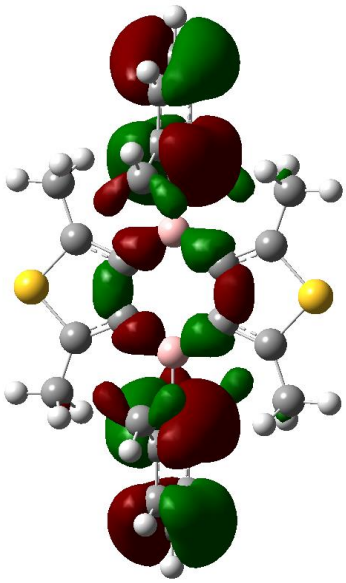
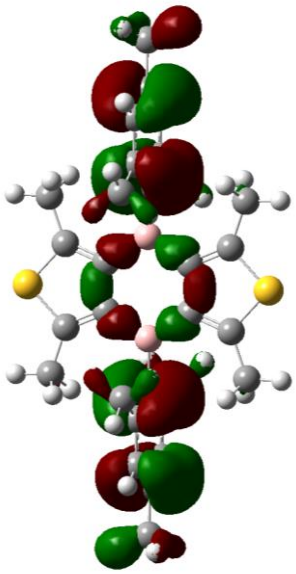
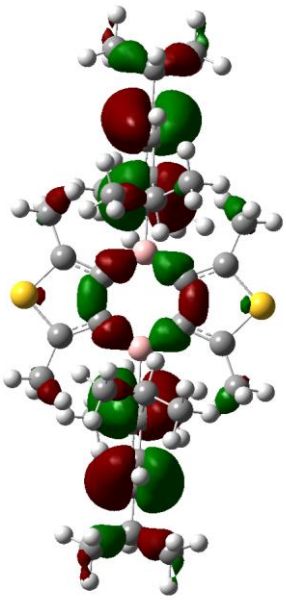
Compound	Transition	MO contributions	Energy gap eV (nm)	Oscillator strength/f
3	$S_0 \rightarrow S_1$	HOMO-6→LUMO+1 (17%)	3.48 (355)	0.1655
	$S_0 \rightarrow S_2$	HOMO→LUMO (66%) HOMO-2→LUMO+1(22%)	3.52 (351)	0.0000
	$S_0 \rightarrow S_3$	HOMO-1→LUMO(67%) HOMO-2→LUMO(66%)	3.56 (348)	0.0000
	$S_0 \rightarrow S_4$	HOMO-1→LUMO+1(25%) HOMO-6→LUMO(41%) HOMO-3→LUMO(44%)	3.74 (331)	0.0000
	$S_0 \rightarrow S_5$	HOMO→LUMO+1(35%) HOMO-6→LUMO(52%) HOMO-4→LUMO+1(16%) HOMO-3→LUMO(45%)	3.86 (321)	0.0000
4	$S_0 \rightarrow S_1$	HOMO-2→LUMO+1 (22%)	3.37 (368)	0.0000
	$S_0 \rightarrow S_2$	HOMO-1→LUMO (67%) HOMO-2→LUMO(66%)	3.39 (365)	0.0000
	$S_0 \rightarrow S_3$	HOMO-1→LUMO+1(25%) HOMO-6→LUMO+1(17%)	3.48 (355)	0.1599
	$S_0 \rightarrow S_4$	HOMO→LUMO(66%)	3.73 (332)	0.0000

	$S_0 \rightarrow S_5$	HOMO-6→LUMO(35%) HOMO-3→LUMO(48%) HOMO→LUMO+1(35%) HOMO-6→LUMO(54%) HOMO-4→LUMO+1(15%) HOMO-3→LUMO(42%)	3.85 (321)	0.0000
5	$S_0 \rightarrow S_1$	HOMO-2→LUMO+1 (25%)	3.44 (360)	0.0000
	$S_0 \rightarrow S_2$	HOMO-1→LUMO (66%) HOMO-2→LUMO(63%)	3.46 (357)	0.0184
	$S_0 \rightarrow S_3$	HOMO-1→LUMO+1(30%) HOMO-6→LUMO+1(21%)	3.60 (343)	0.1567
	$S_0 \rightarrow S_4$	HOMO→LUMO(65%) HOMO-6→LUMO(40%) HOMO-4→LUMO+1(16%) HOMO-3→LUMO(49%)	3.80 (325)	0.0000
	$S_0 \rightarrow S_5$	HOMO→LUMO+1(25%) HOMO-6→LUMO(33%) HOMO-4→LUMO(10%) HOMO-4→LUMO+1(18%) HOMO-3→LUMO(43%) HOMO→LUMO+1(38%)	3.82 (324)	0.0002

Compound	 **3**	 **4**	 **5**
LUMO+2	 -0.0544 eV	 -0.0816 eV	 -0.0272 eV

LUMO+1	 -1.387 eV	 -1.360 eV	 -1.4144 eV
LUMO	 -1.741 eV	 -1.714 eV	 -1.632 eV

HOMO	 -5.766 eV	 -5.739 eV	 -5.7936 eV
HOMO-1	 -6.066 eV	 -5.848 eV	 -5.8752 eV

HOMO-2	 -6.120 eV	 -5.875 eV	 -5.9024 eV

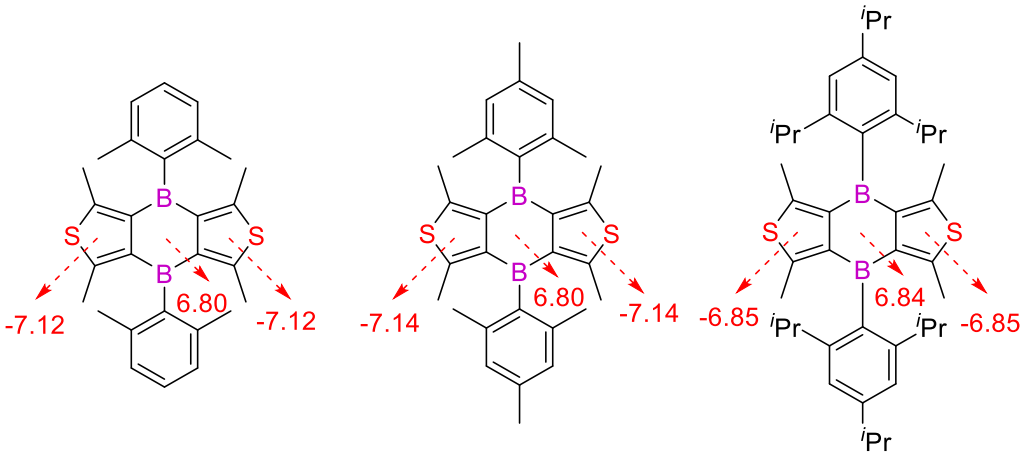


Figure S9: NICS values of thiophene and B_2C_4 ring of compounds **3-5**.

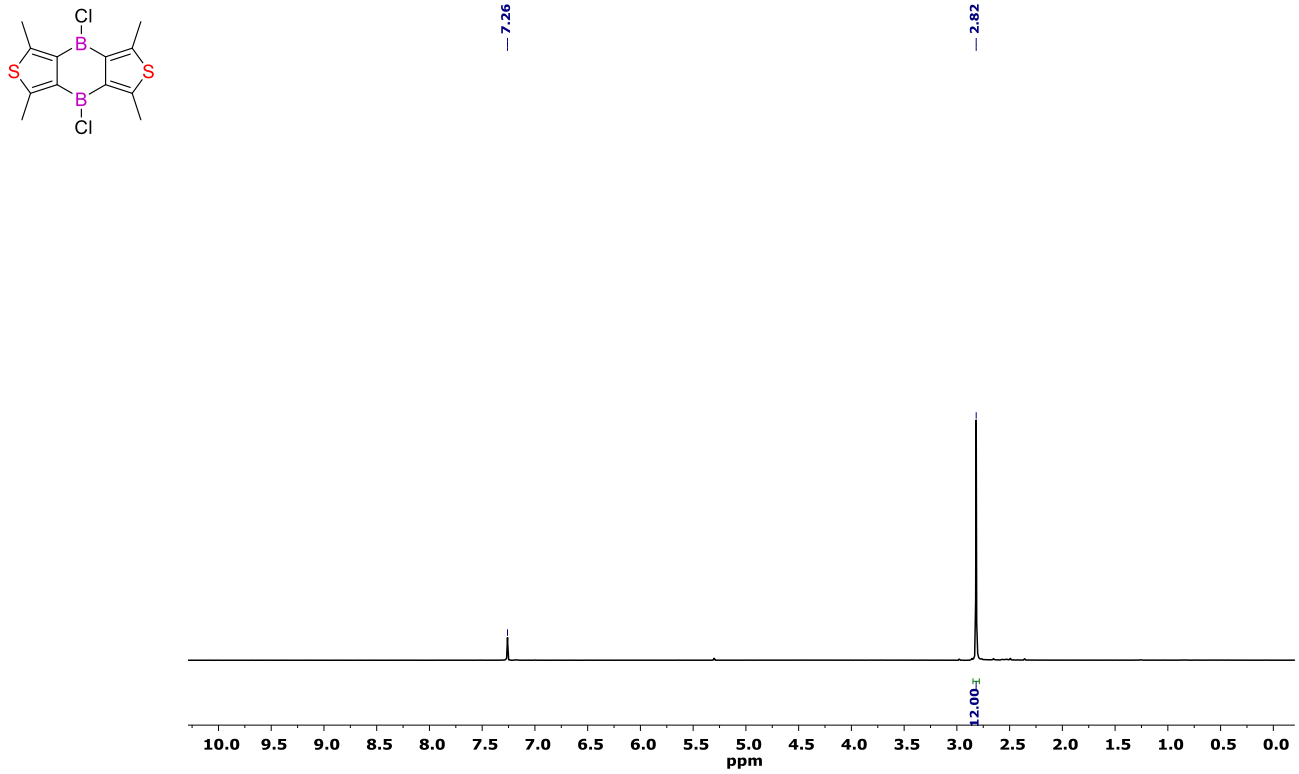


Figure **S10**:[1]H NMR spectrum of compound **2** in $CDCl_3$.

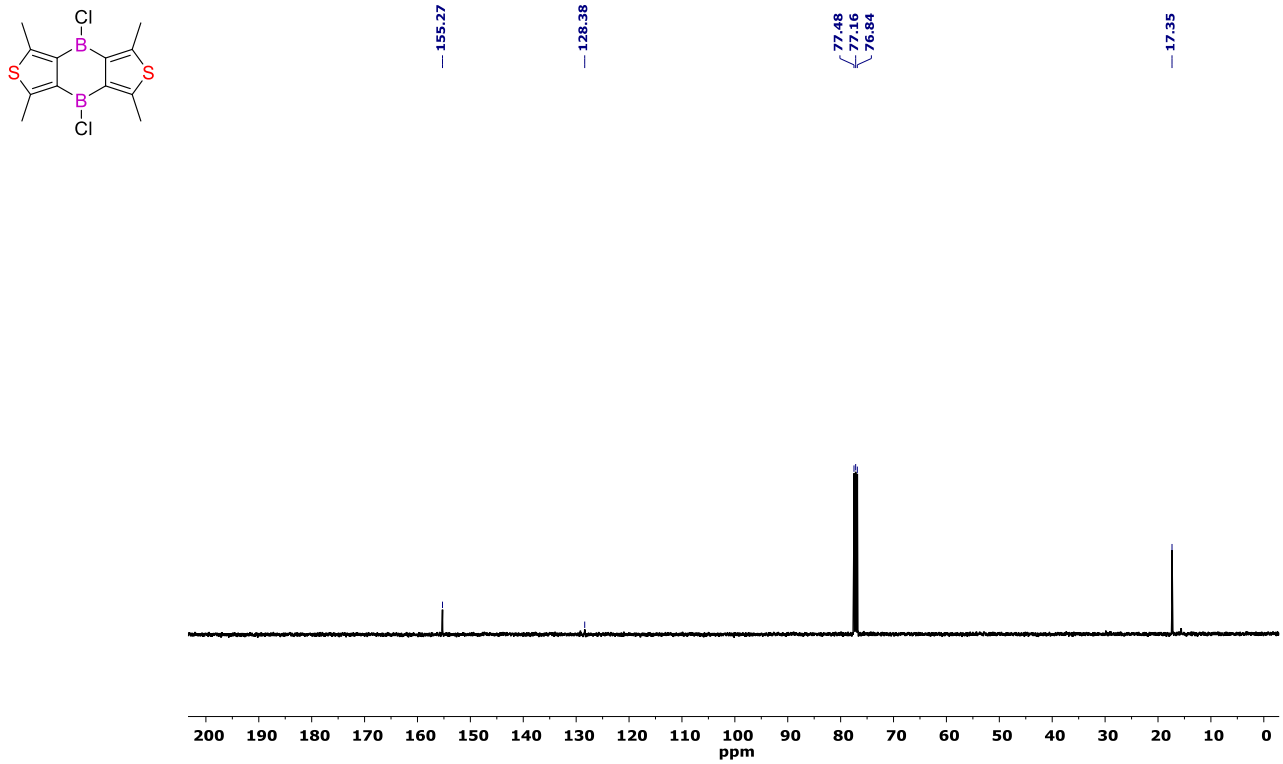


Figure **S11**:[13]C NMR spectrum of compound **2** in $CDCl_3$.

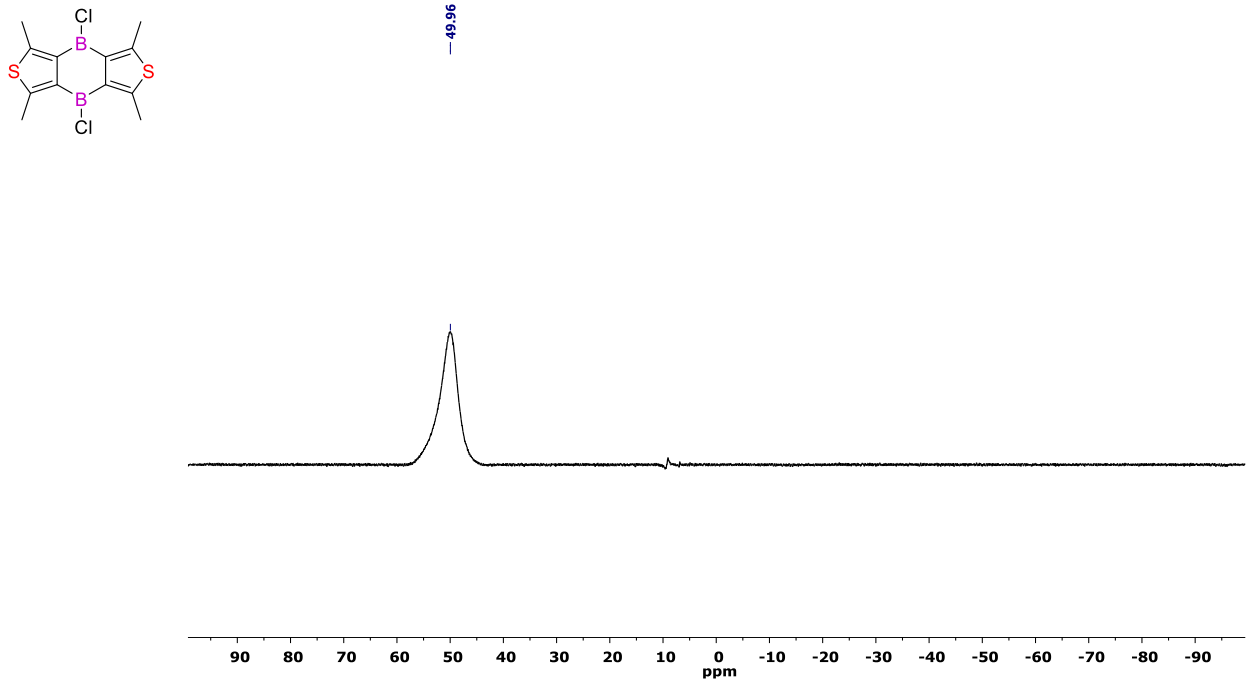


Figure **S12**:^{11}B NMR spectrum of compound **2** in $CDCl_3$.

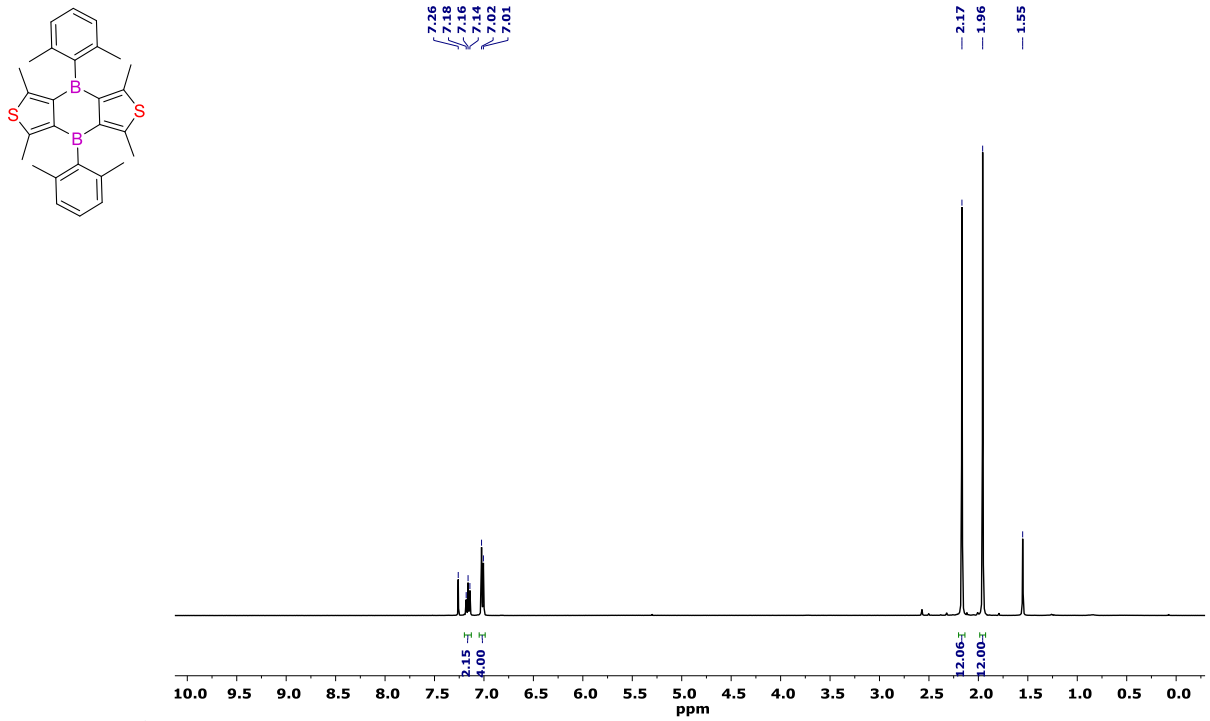


Figure **S13**:^{1}H NMR spectrum of compound **3** in $CDCl_3$.

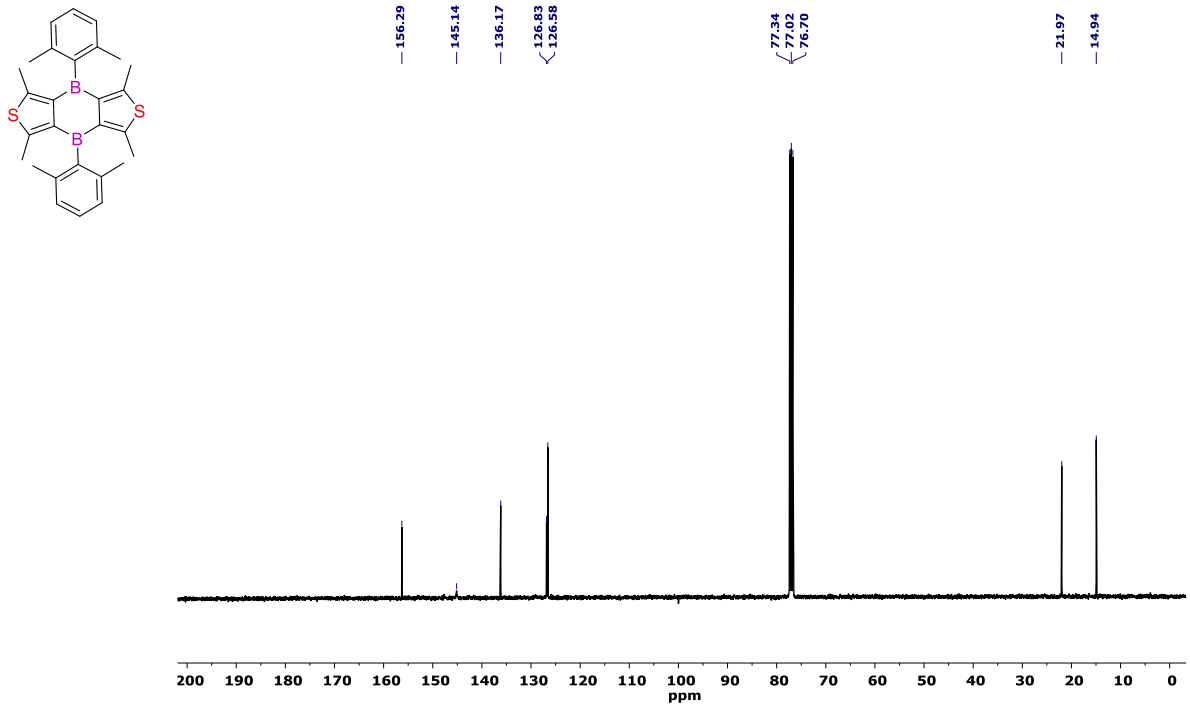


Figure **S14**:^{13}C NMR spectrum of compound **3** in $CDCl_3$.

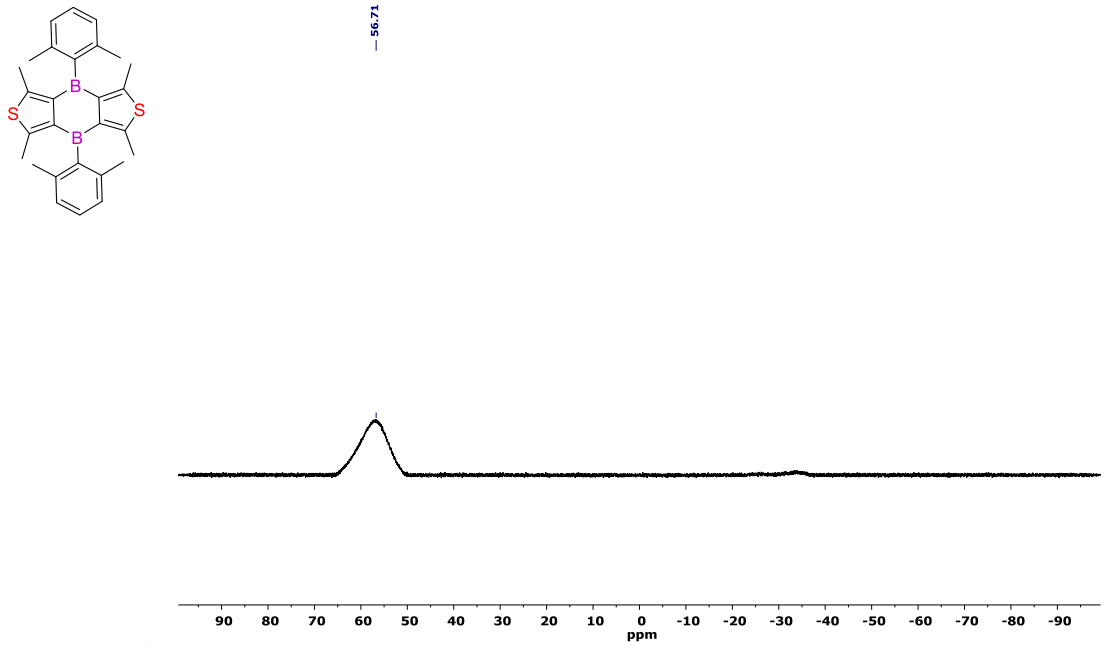


Figure **S15**:^{11}B NMR spectrum of compound **3** in $CDCl_3$.

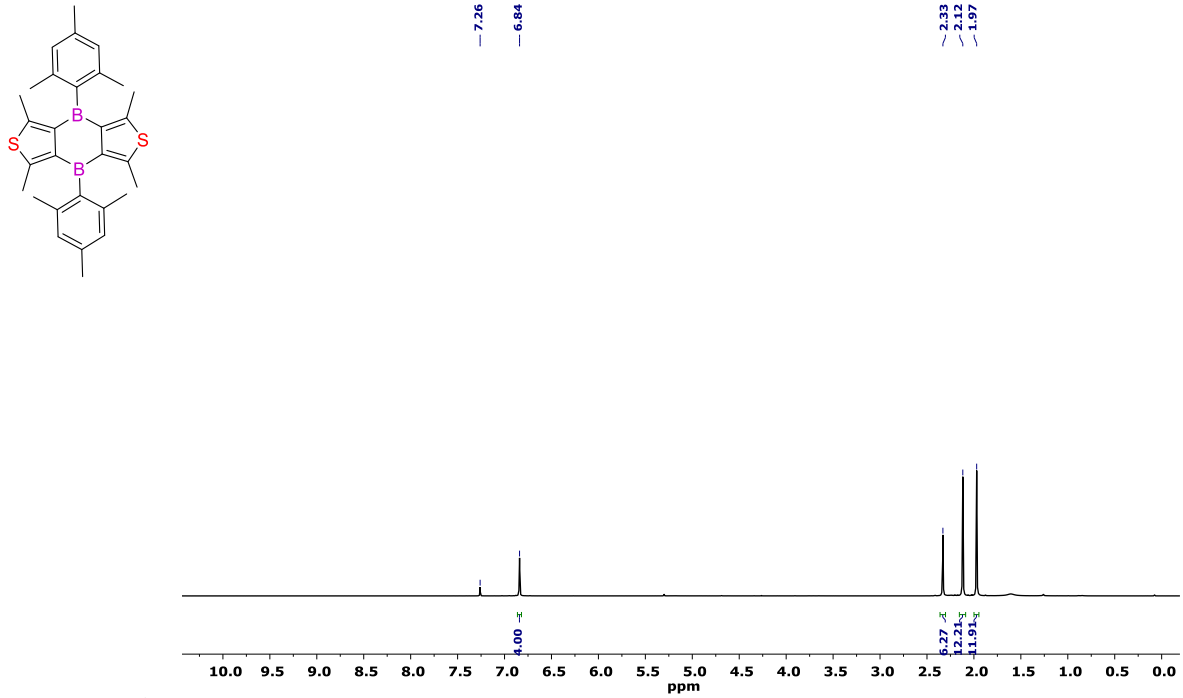


Figure **S16**:[1]H NMR spectrum of compound **4** in $CDCl_3$.

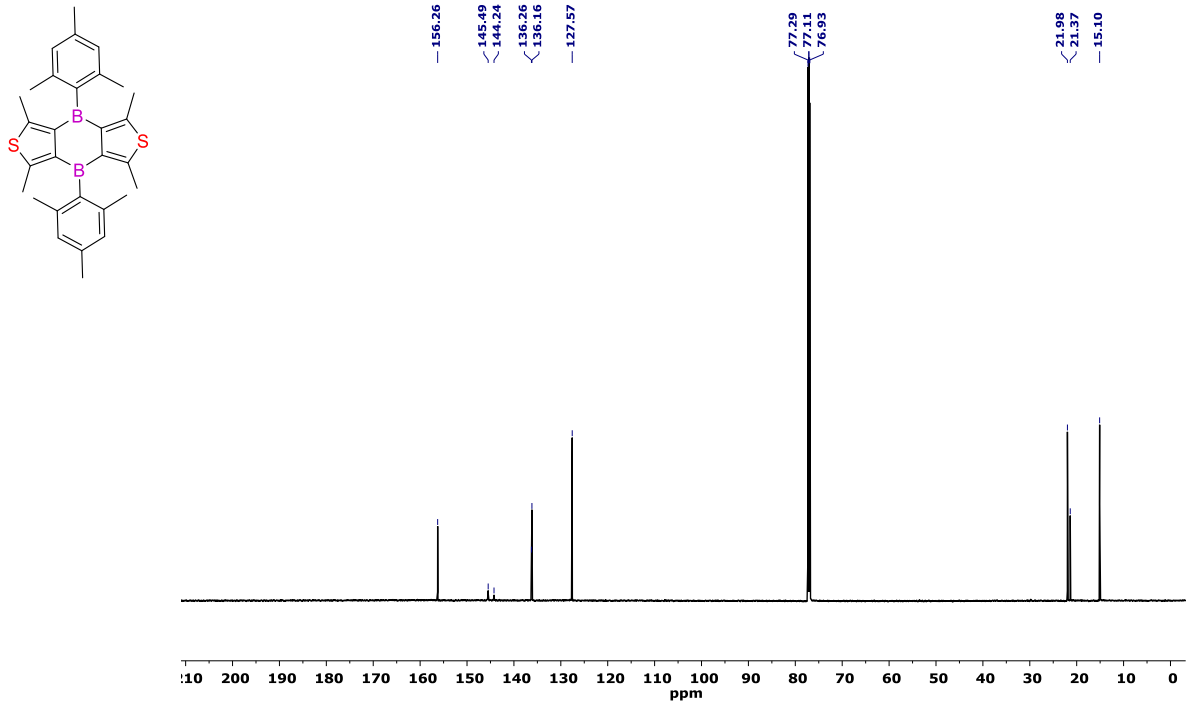


Figure **S17**:[13]C NMR spectrum of compound **4** in $CDCl_3$.

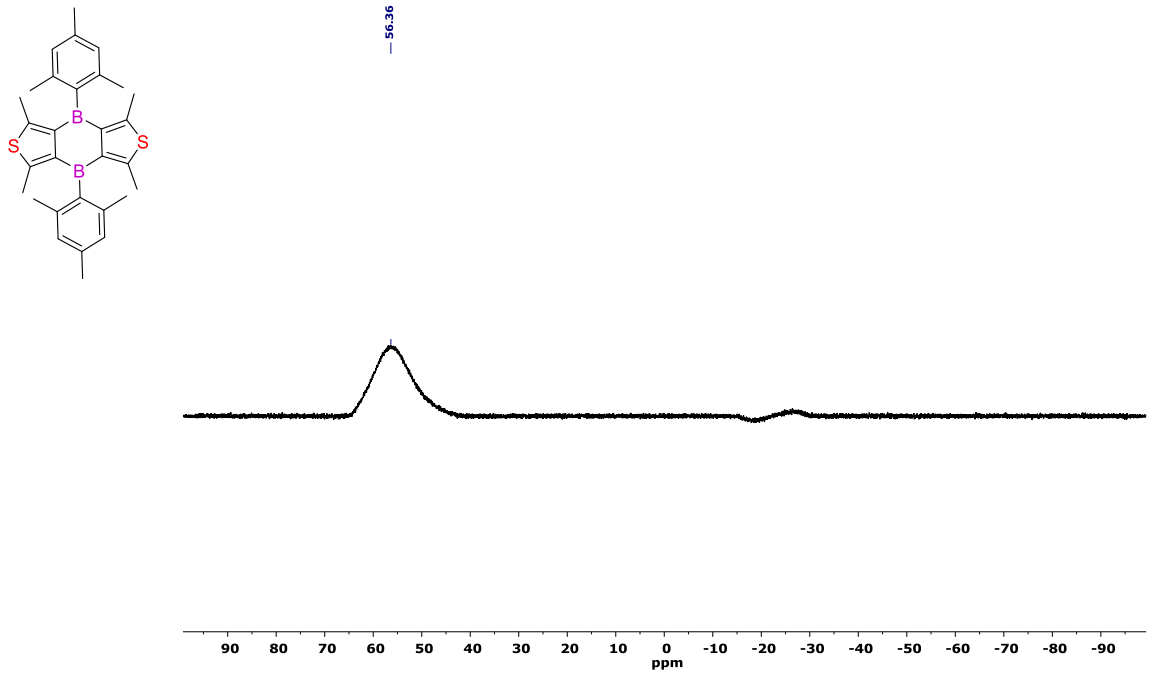


Figure **S18**:[11]B NMR spectrum of compound **4** in $CDCl_3$.

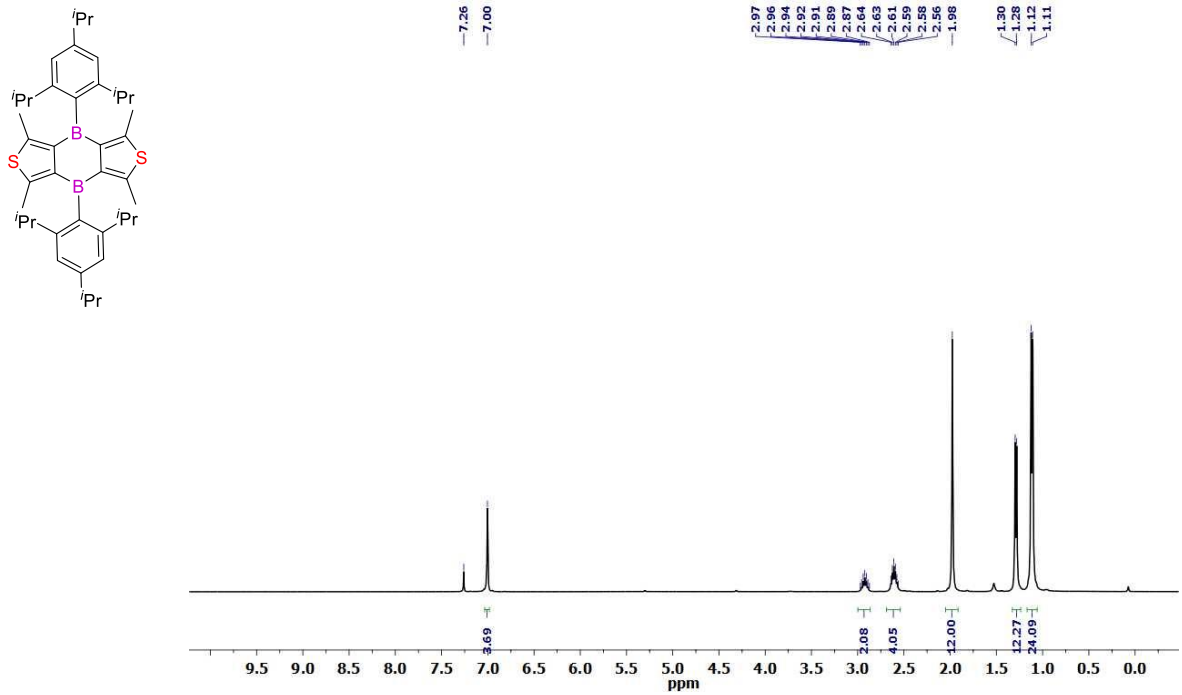


Figure **S19**:[1]H NMR spectrum of compound **5** in $CDCl_3$.

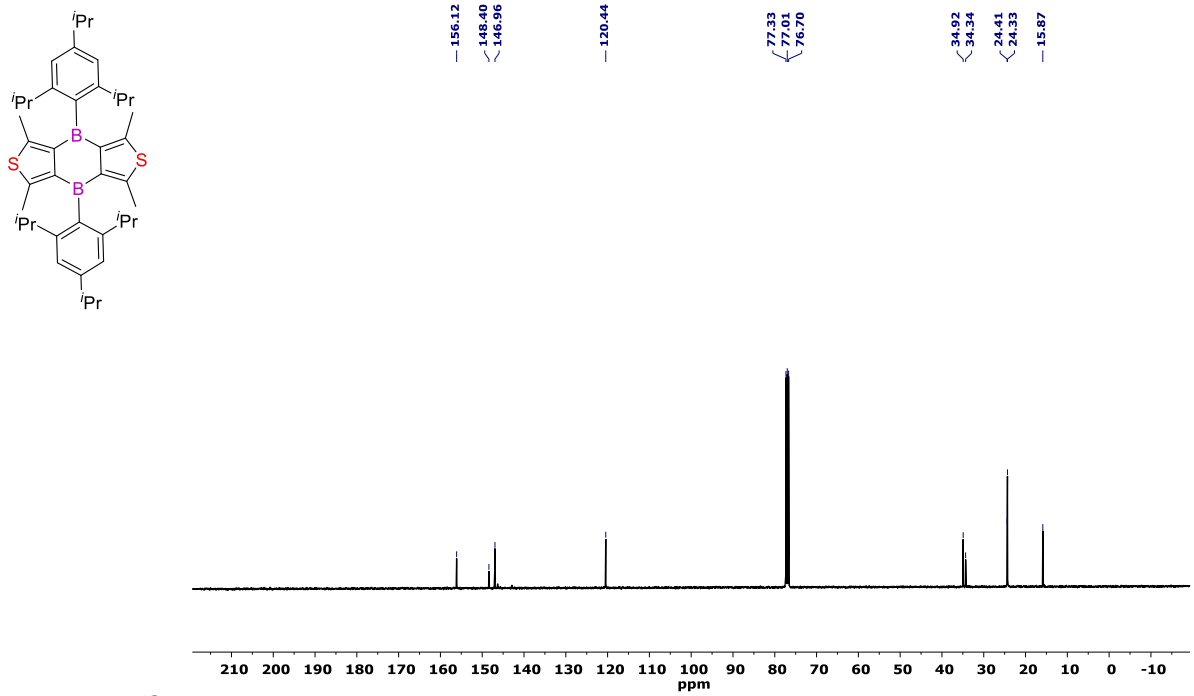


Figure **S20**:[13]C NMR spectrum of compound **5** in $CDCl_3$.

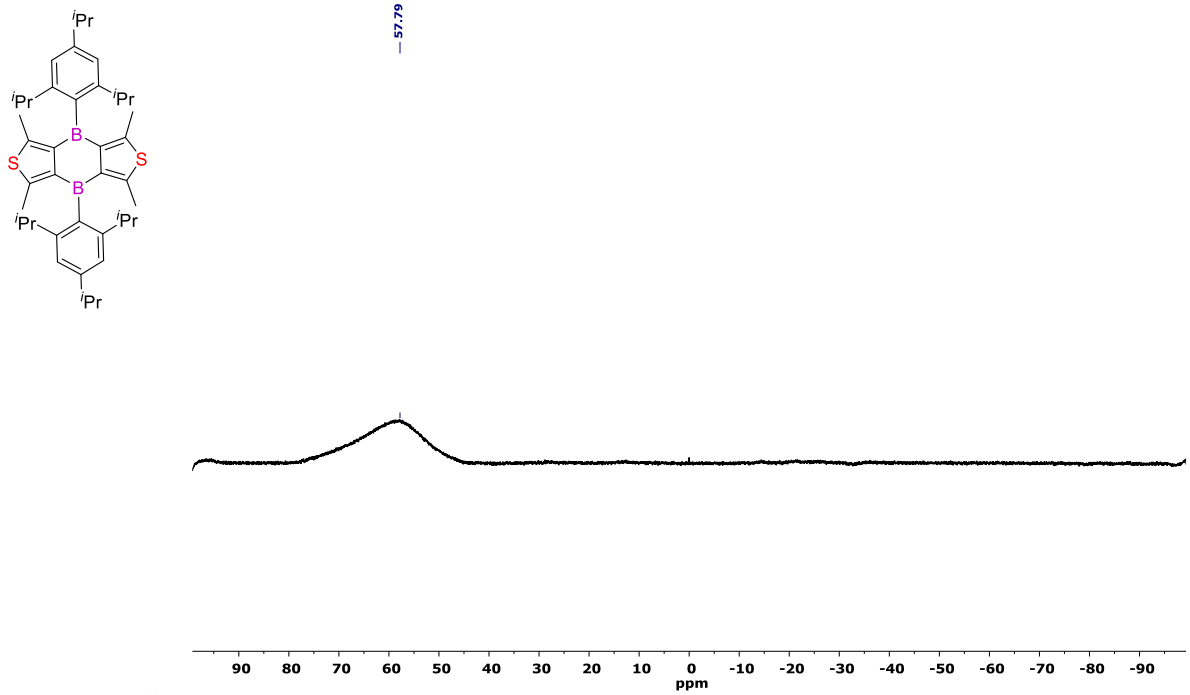
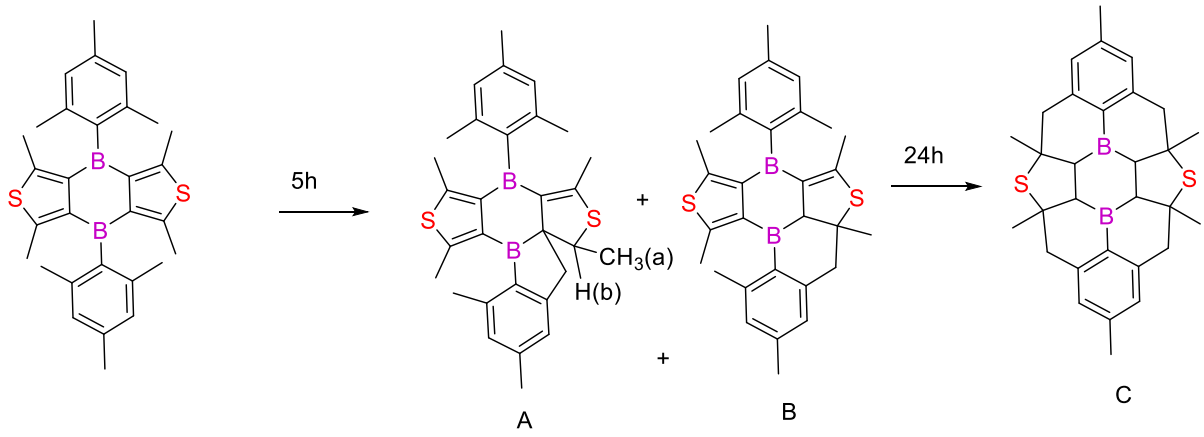


Figure **S21**:[11]B NMR spectrum of compound **5** in $CDCl_3$.

Photoirradiation studies of compounds 3-5.

Compound **4** was subjected to photolysis. The ^{1}H (^{1H}-^{1}H COSY),^{13}C (^{13}C-DEPT-135) & ^{11}B NMR of compound **4** was recorded after 5h and 24h. After 5h, the ^{1}H, ^{1}H-COSY, ^{13}C and ^{13}C DEPT-135 reveal the presence of species A & B as major products. Formation of a doublet (Figure S23-S25, CH_3 (a)) at 1.26 ppm and quartet at 3.38 ppm (H(b)) was observed which corresponds to species A. In addition to that presence of two carbons (–CH_2-) with different environment was also observed using ^{13}C DEPT-135 experiment (Figure S27), which suggest that more than one species is formed during the photolysis. The second species is assigned as B. However, after 24h photolysis, presence of a symmetrical product C was observed. A similar phenomenon was observed for compound **3** and **5**. Further studies needed to reveal the pathways involved in this process and also other species involved in the processes.



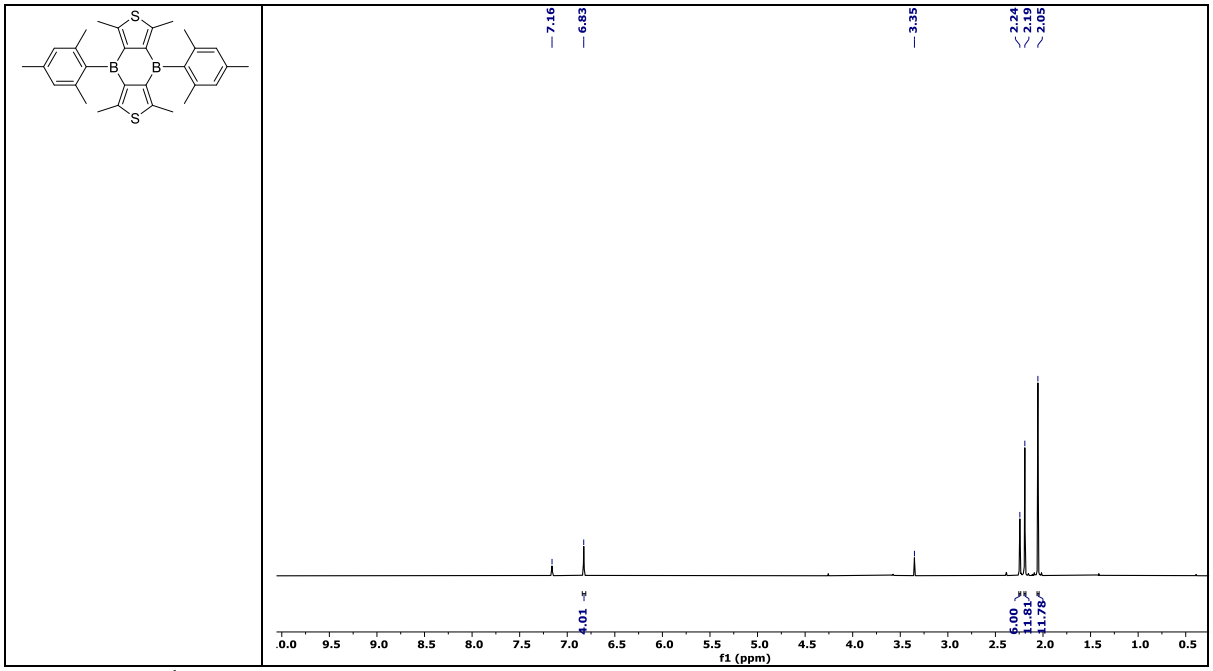


Figure S22: ^{1}H NMR spectrum of compound **4** in C_6D_6.

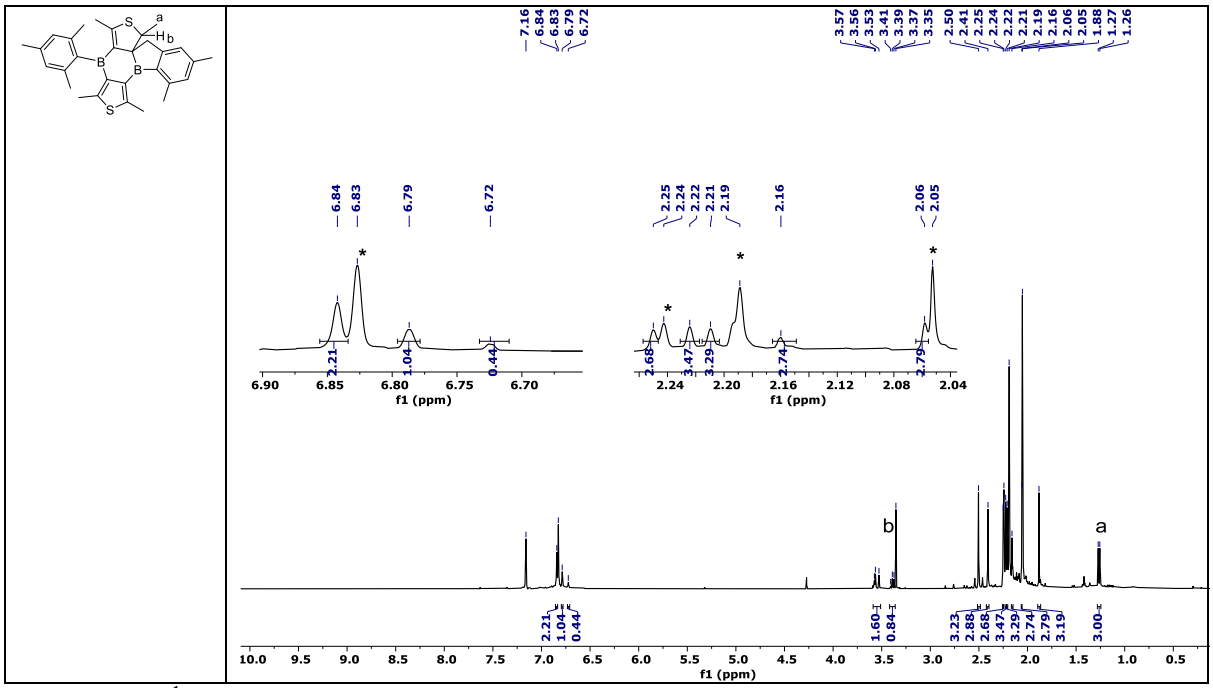


Figure S23: ^{1}H NMR spectrum of compound **4** in C_6D_6 after irradiation of UV light for 5h. Starting material peaks are marked with asterisk (*).

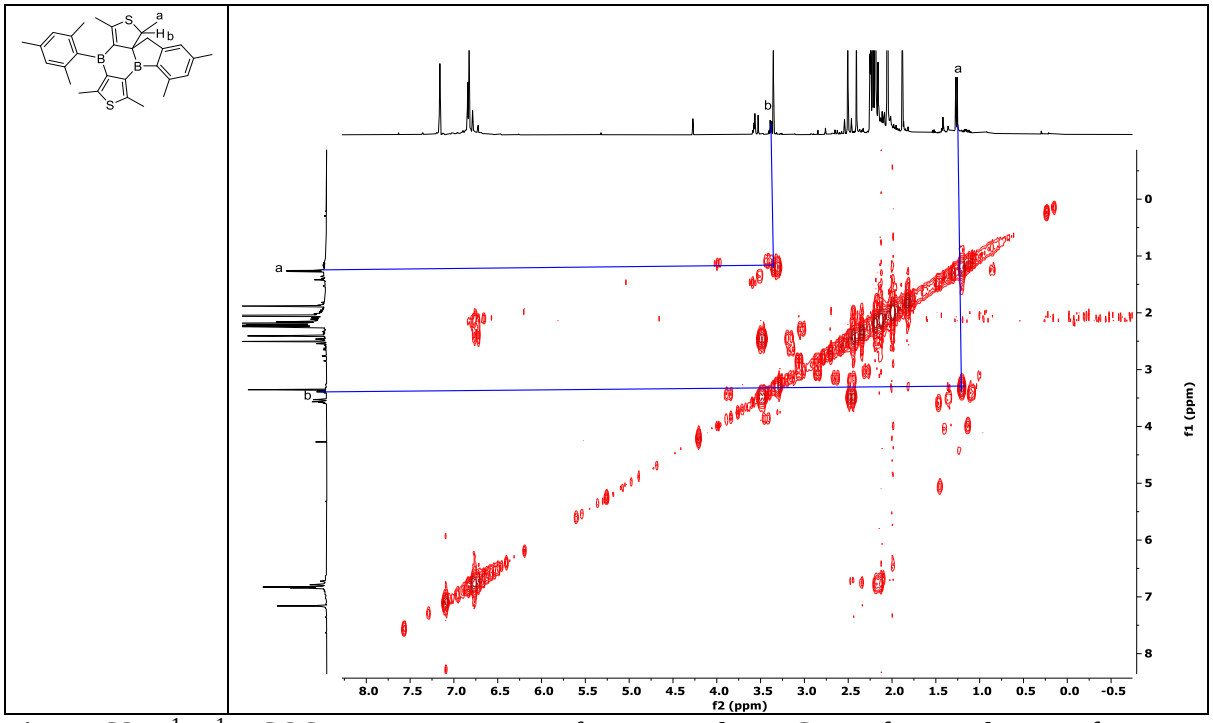


Figure S24: ^{1}H-^{1}H COSY NMR spectrum of compound **4** in C_6D_6 after irradiation of UV light for 5h.

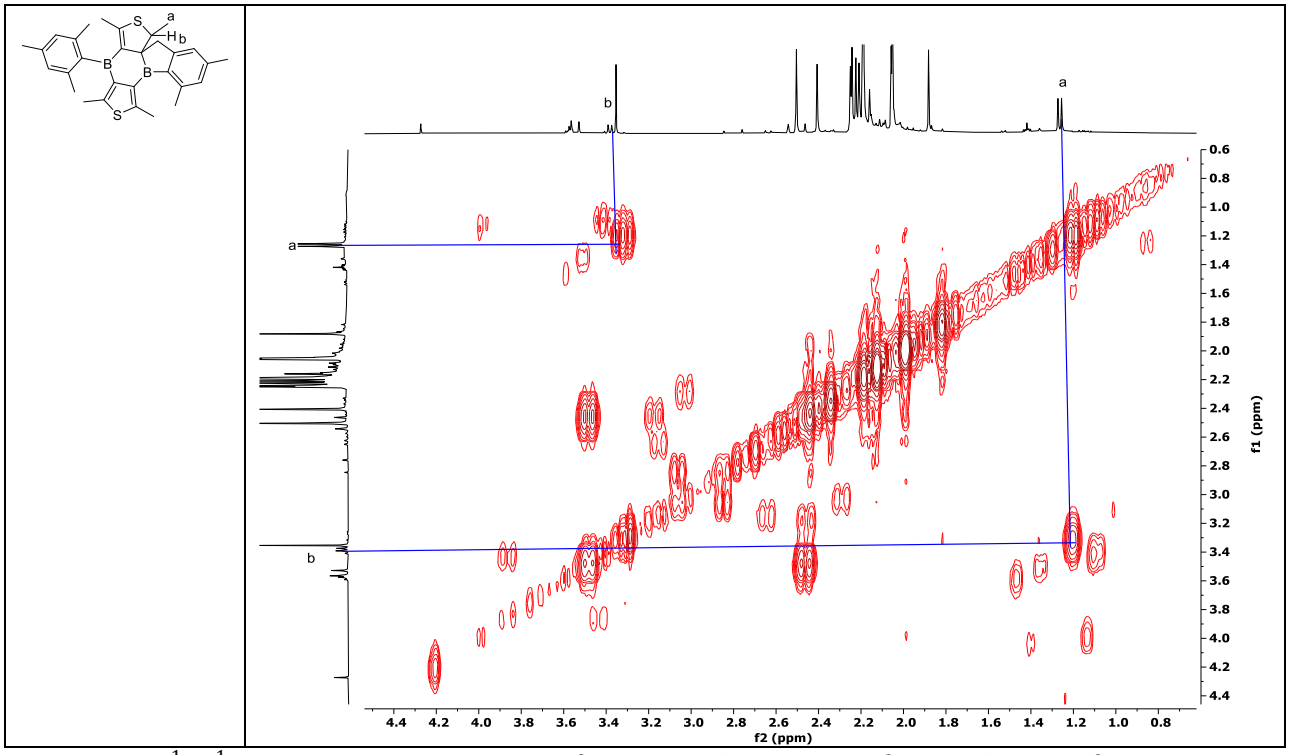


Figure S25: ^{1}H-^{1}H COSY NMR spectrum of compound **4** in C_6D_6 after irradiation of UV light for 5h.

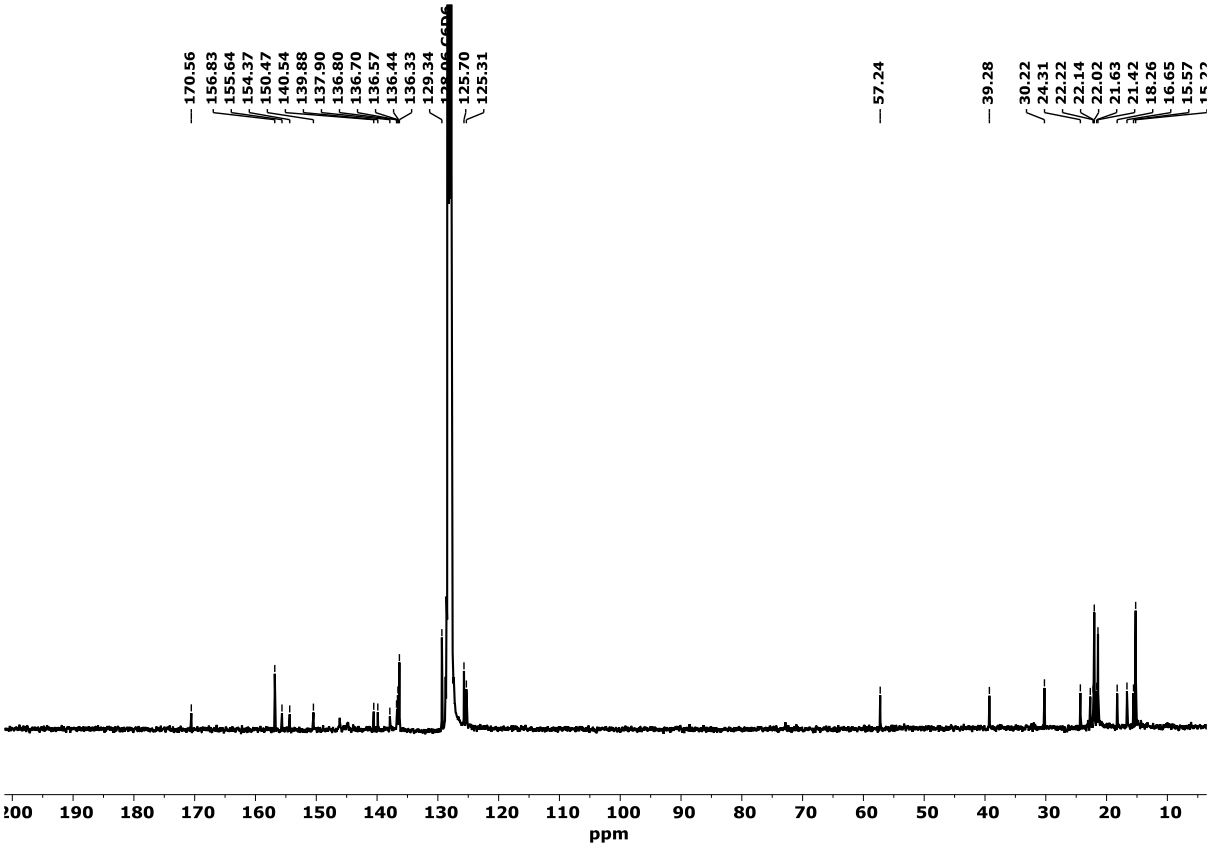


Figure S26: ^{13}C NMR of compound **4** in C_6D_6 after irradiation of UV light for 5h.

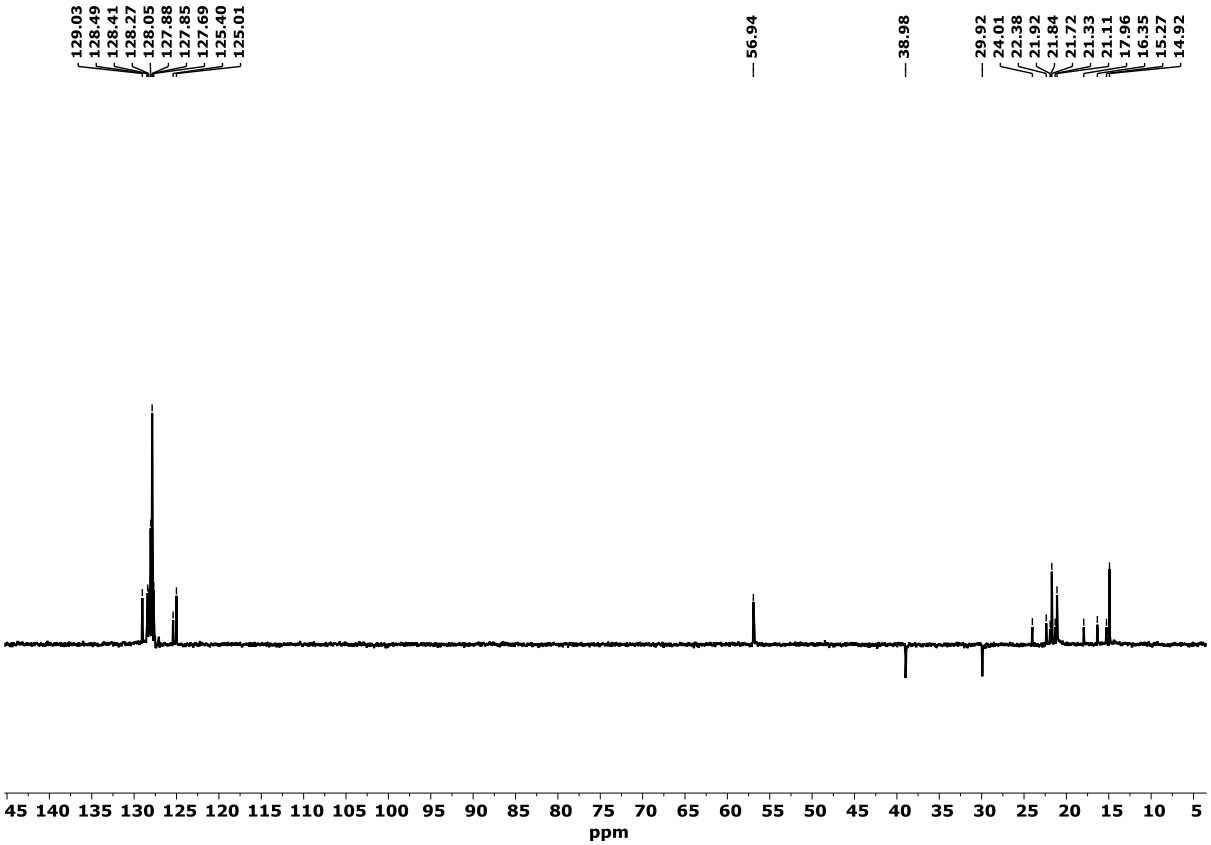


Figure S27: ^{13}C DEPT-135 NMR of compound **4** in C_6D_6 after irradiation of UV light for 5h.

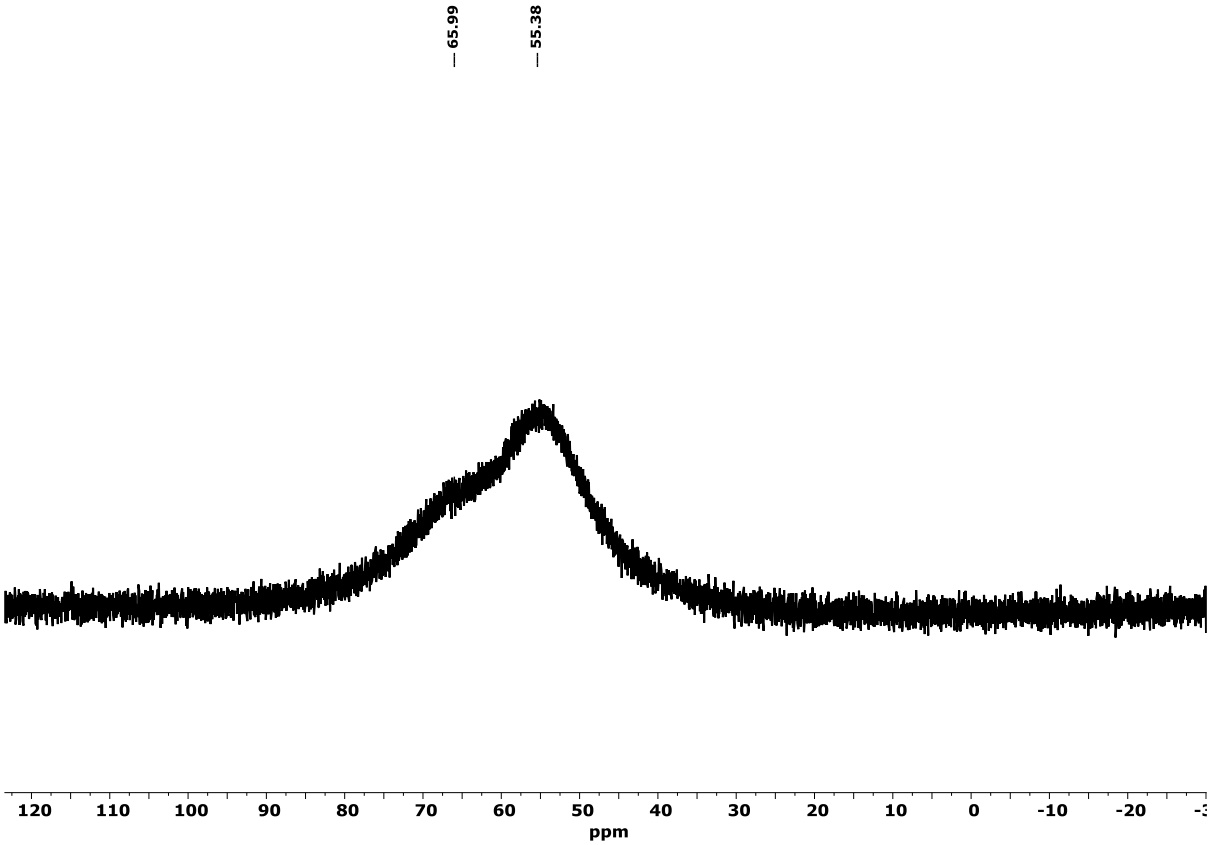


Figure S28: ^{11}B of compound **4** in C_6D_6 after irradiation of UV light for 5h.

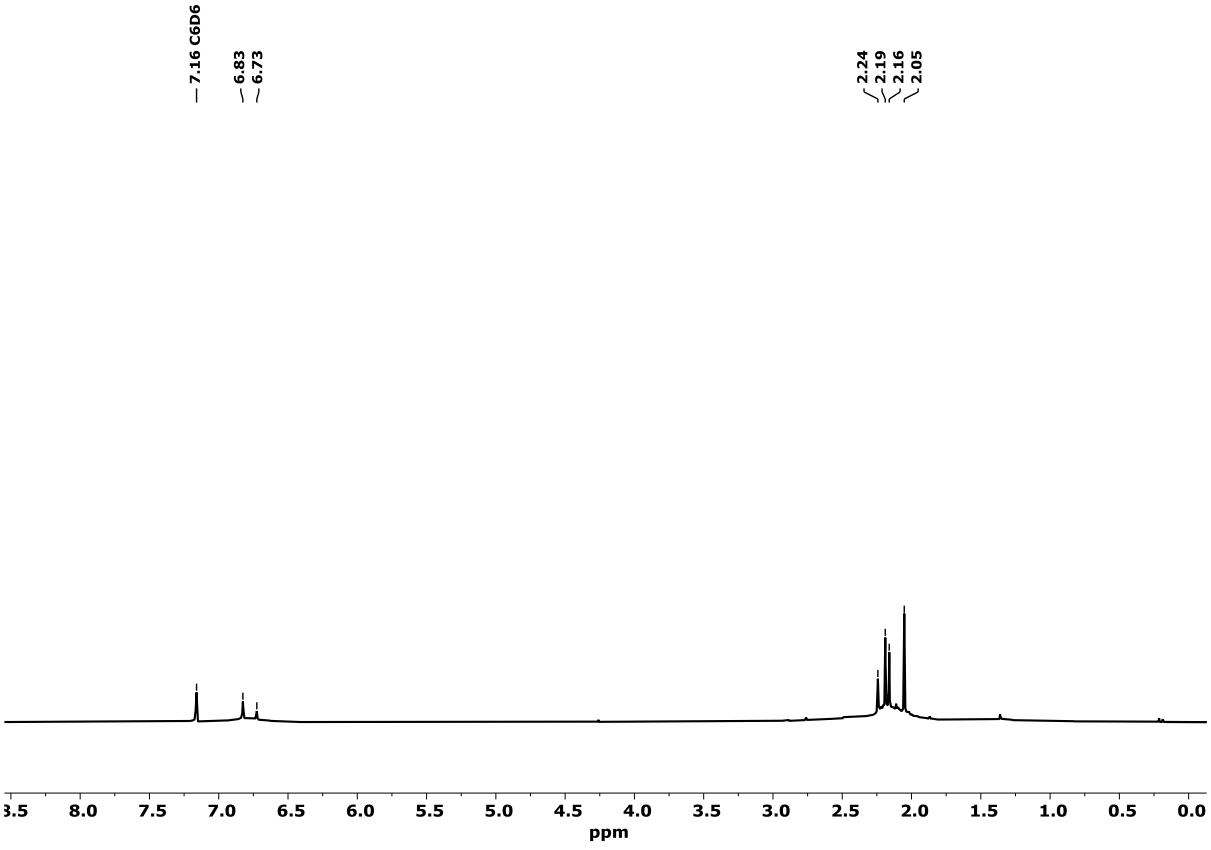


Figure S29: ^{1}H NMR of compound **4** in C_6D_6 after irradiation of UV light for 24h.

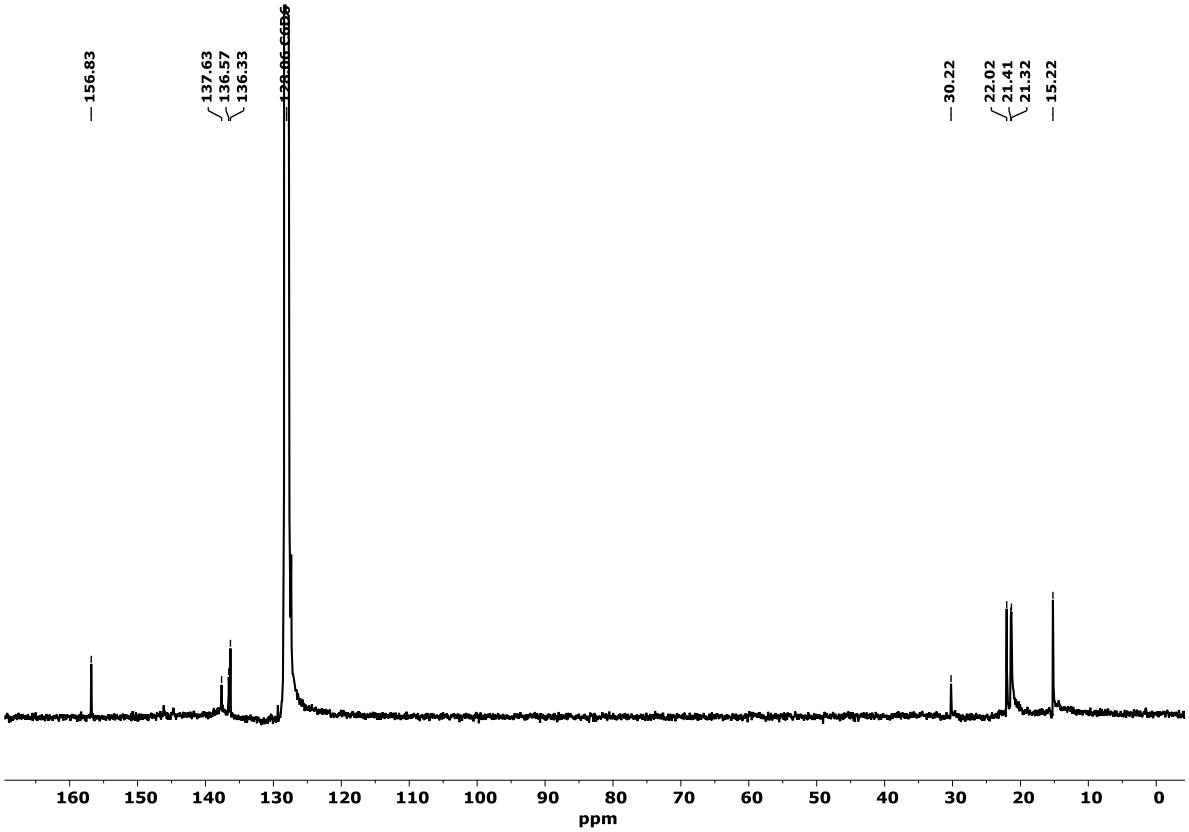


Figure S30: ^{13}C NMR of compound **4** in C_6D_6 after irradiation of UV light for 24h.

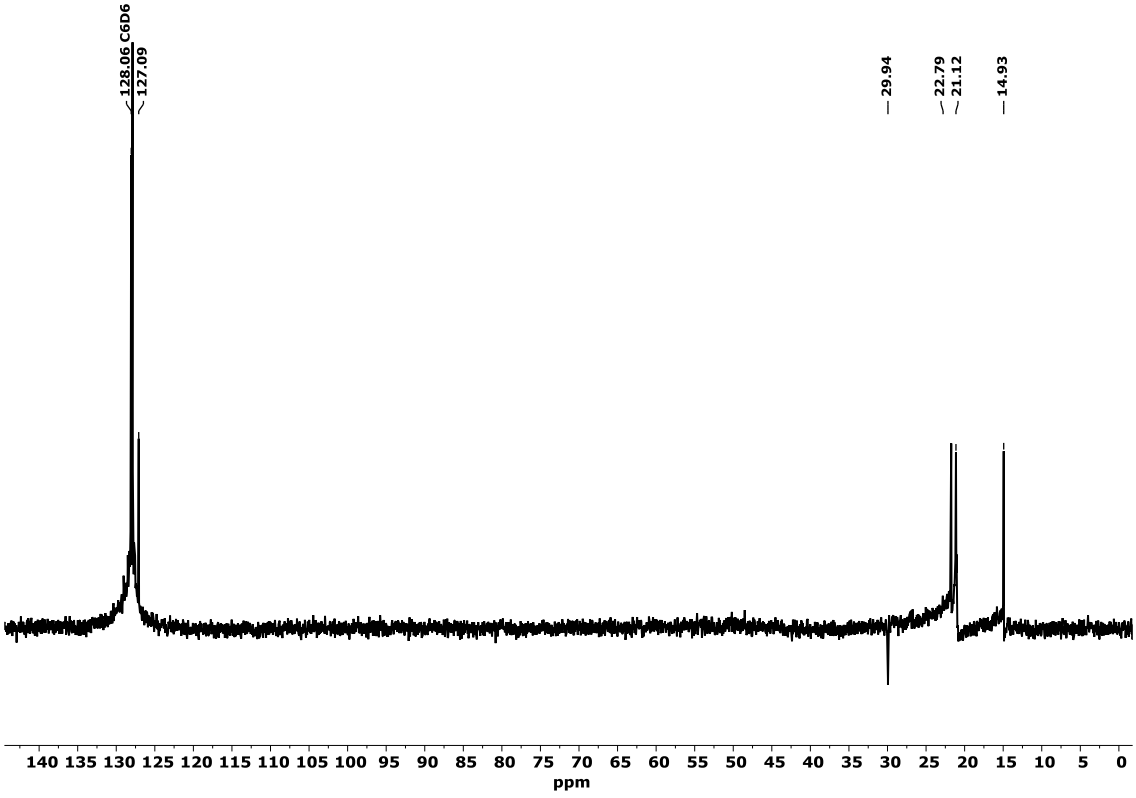


Figure S31: ^{13}C DEPT-135 NMR of compound **4** in C_6D_6 after irradiation of UV light for 24h.

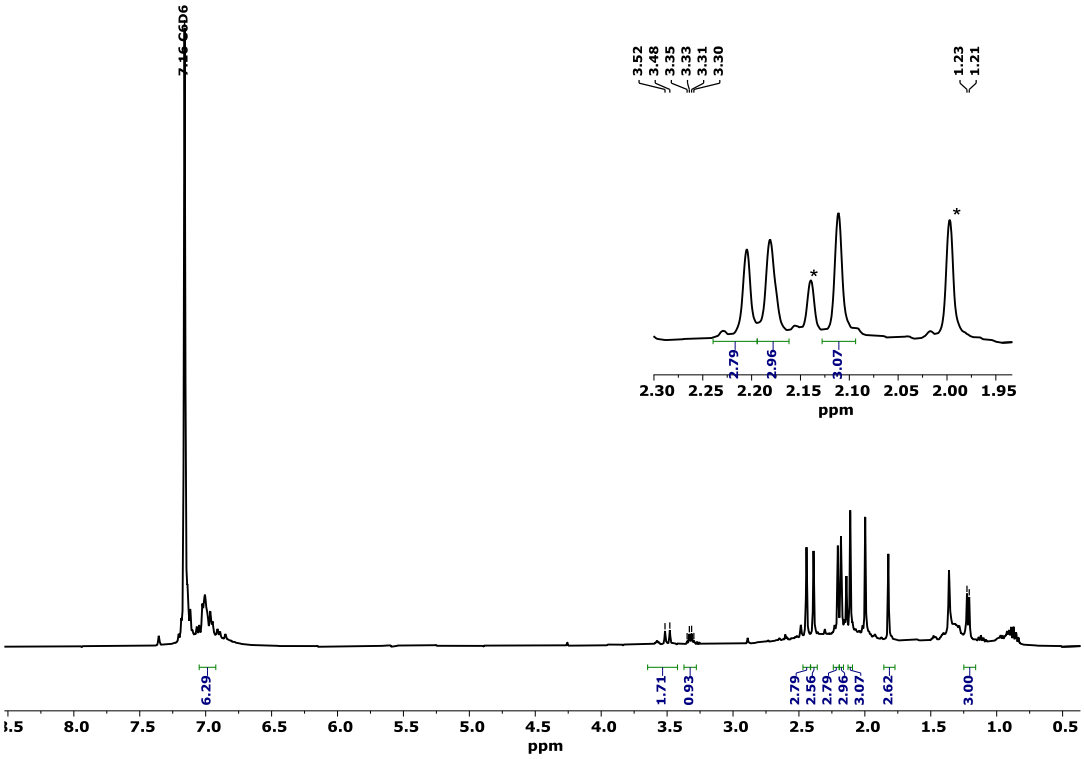


Figure S32: ^{1}H NMR of compound **3** in C_6D_6 after irradiation of UV light for 5h.

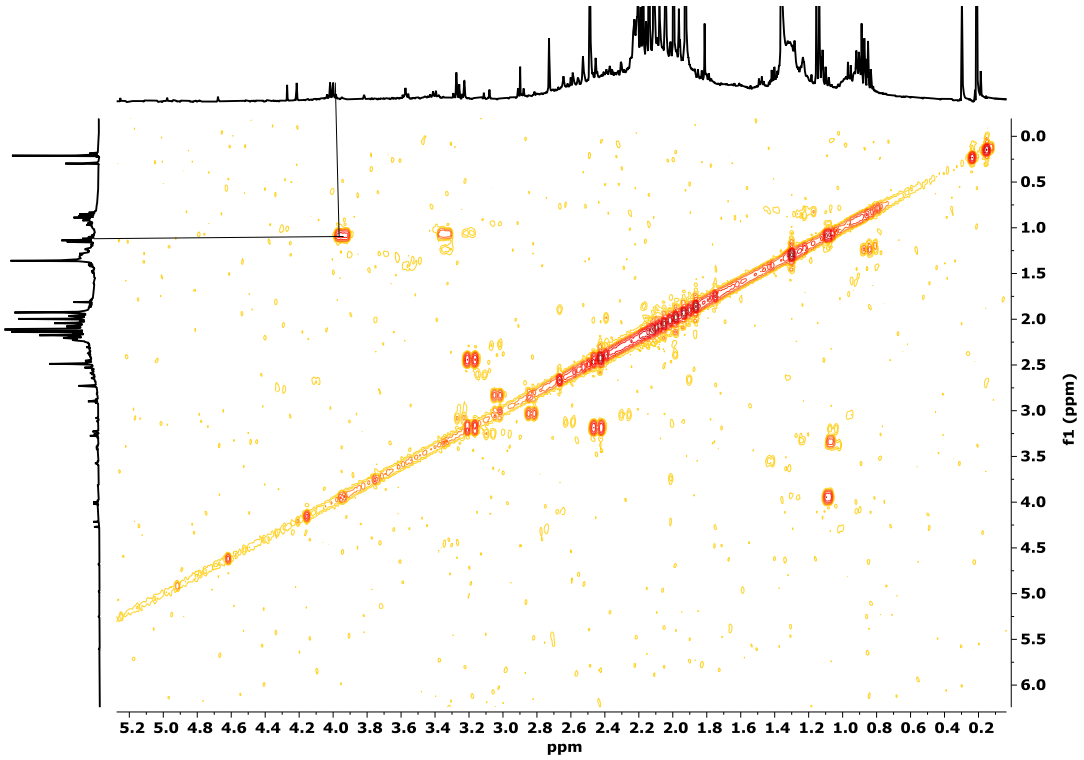


Figure S33: ^{1}H-^{1}H COSY of compound **3** in C_6D_6 after irradiation of UV light for 5h.

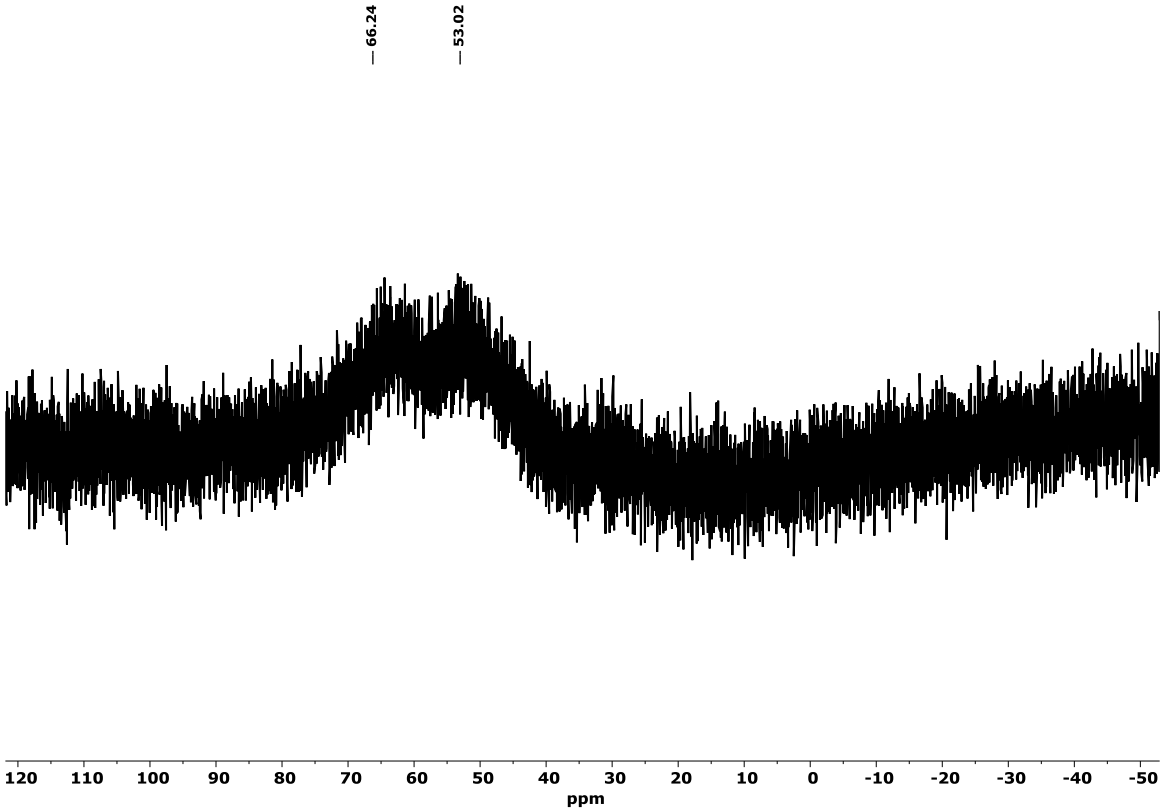


Figure S34: ^{11}B NMR of compound **3** in C_6D_6 after irradiation of UV light for 5h.

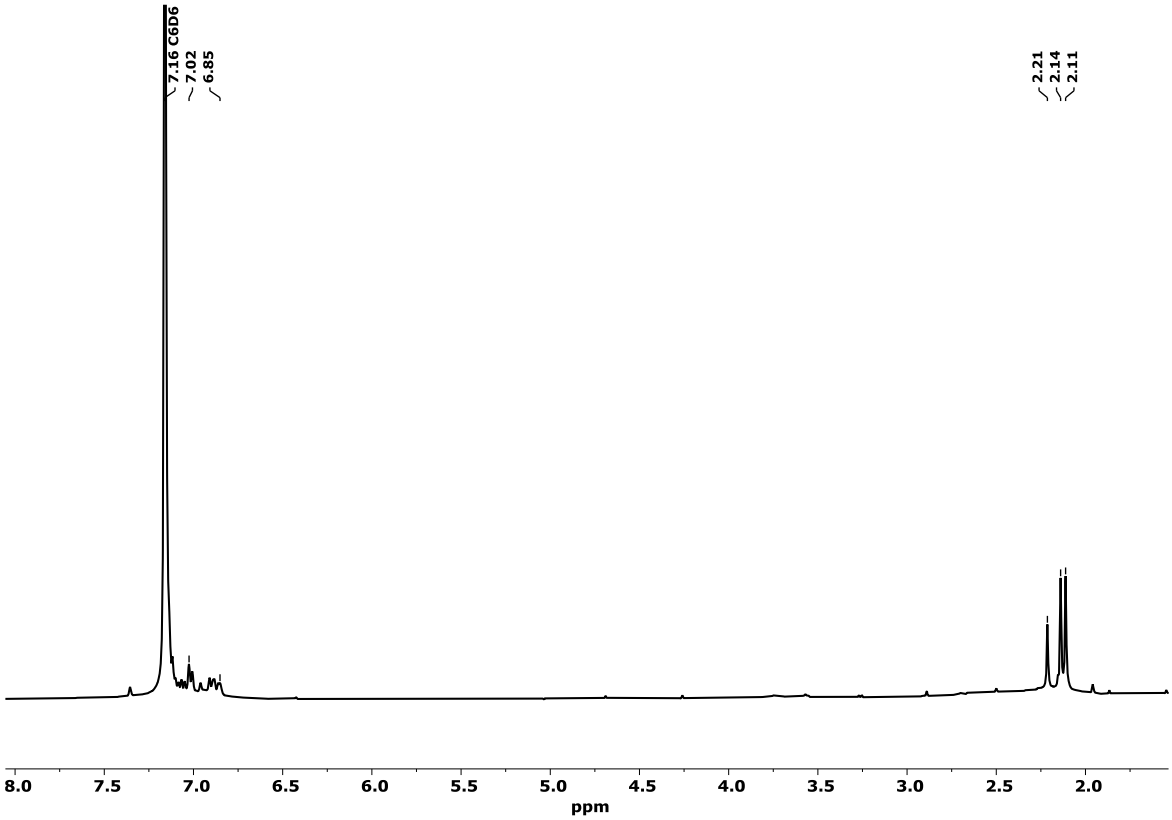


Figure S35: ^{1}H NMR of compound **3** in C_6D_6 after irradiation of UV light for 24h.

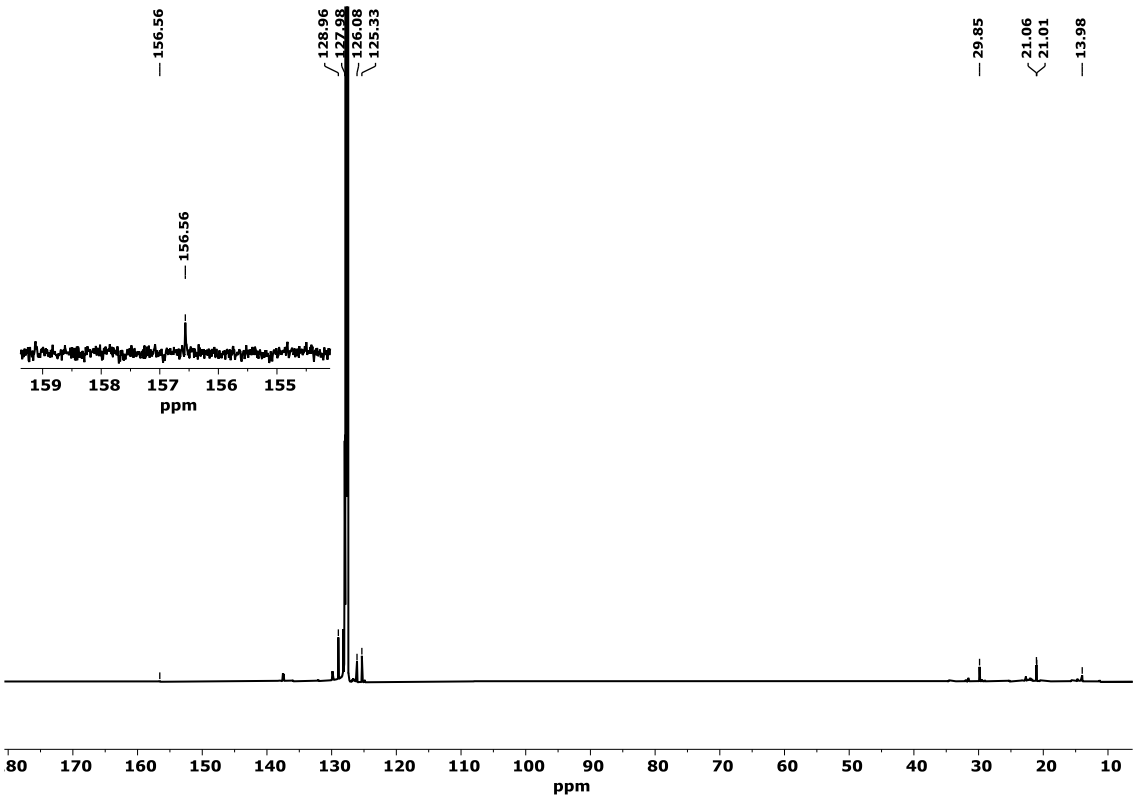


Figure S36: ^{13}C NMR of compound **3** in C_6D_6 after irradiation of UV light for 24h.

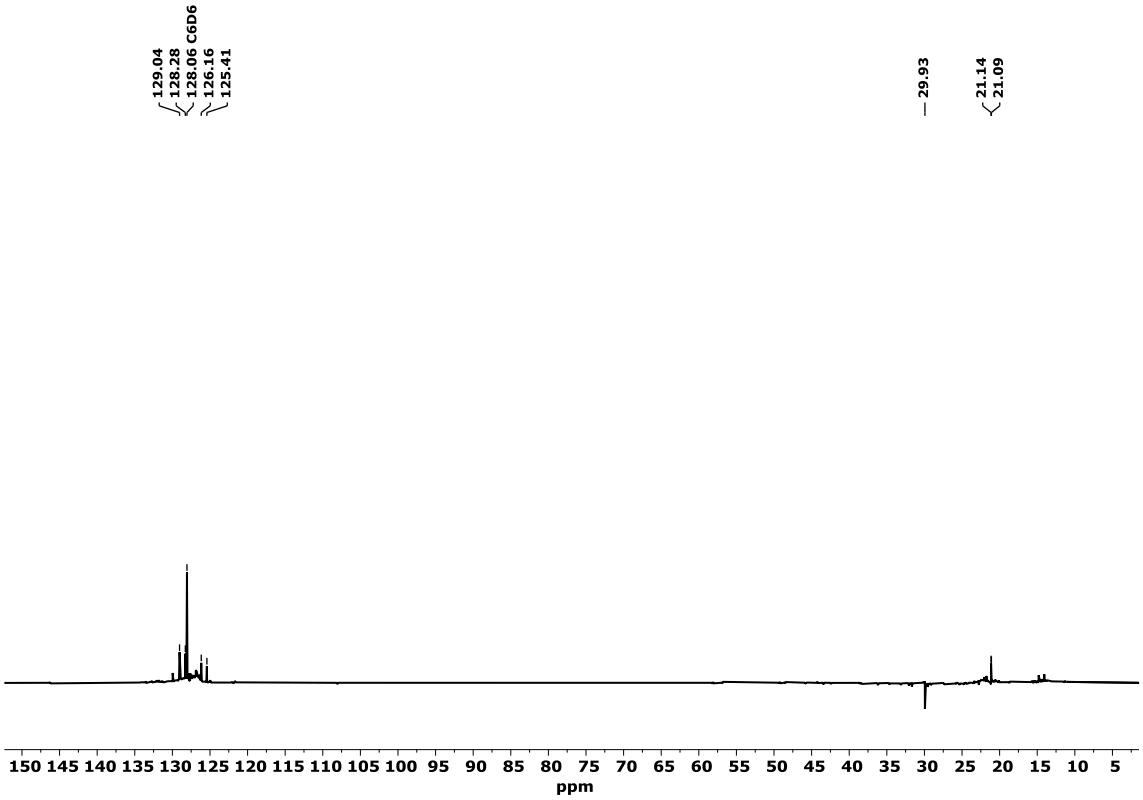


Figure S37: ^{13}C DEPT-135 NMR of compound **3** in C_6D_6 after irradiation of UV light for 24h.

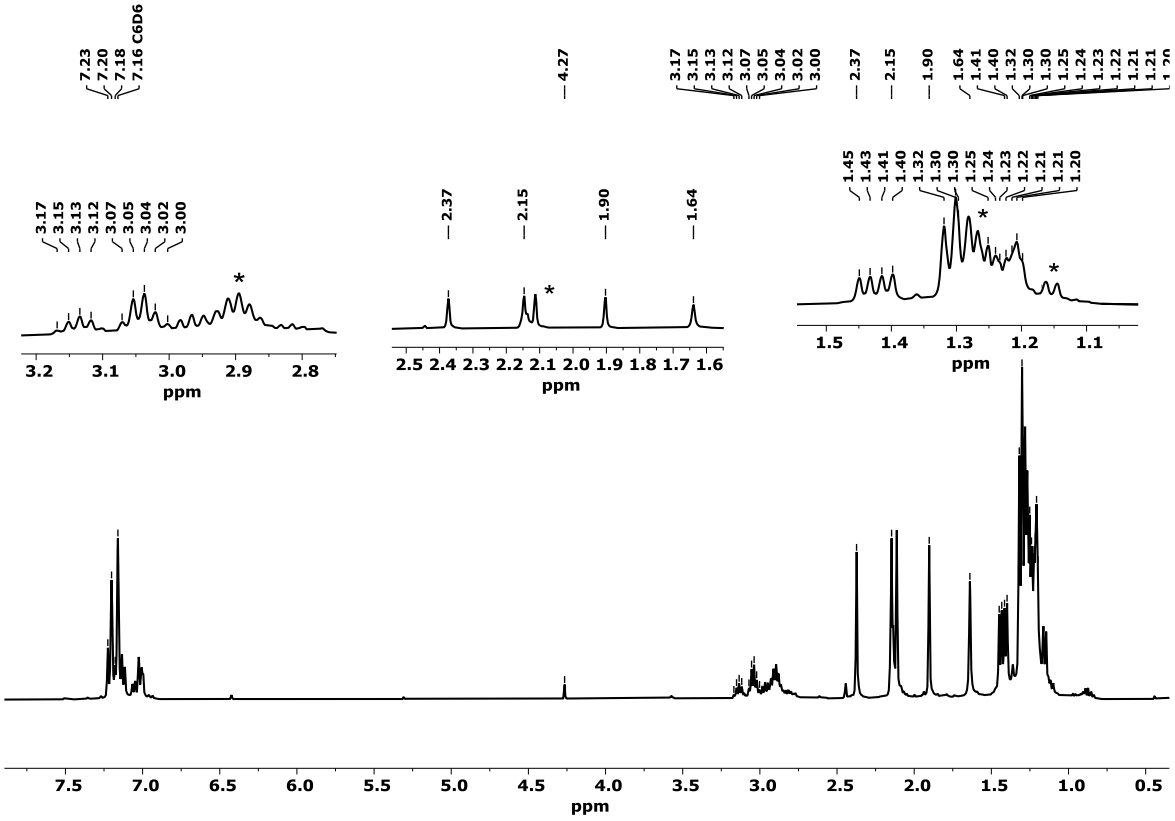


Figure S38: ^{1}H NMR of compound **5** in C_6D_6 after irradiation of UV light for 5h.

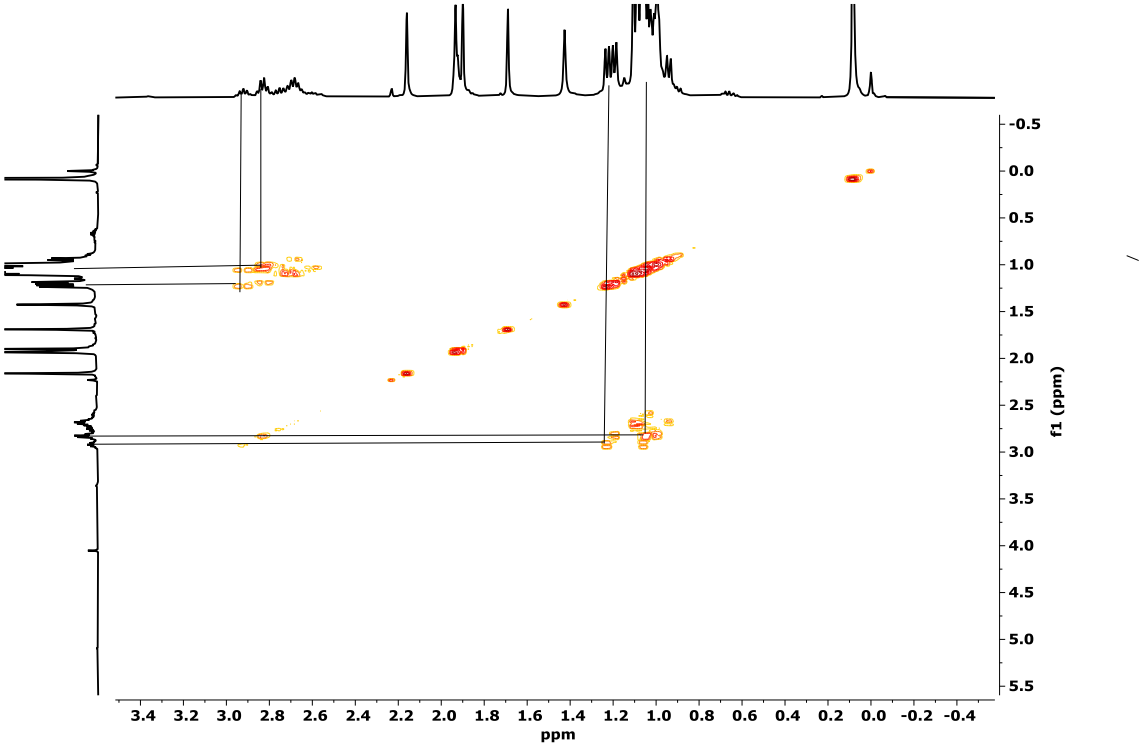


Figure S39: ^{1}H-^{1}H COSY of compound **5** in C_6D_6 after irradiation of UV light for 5h.

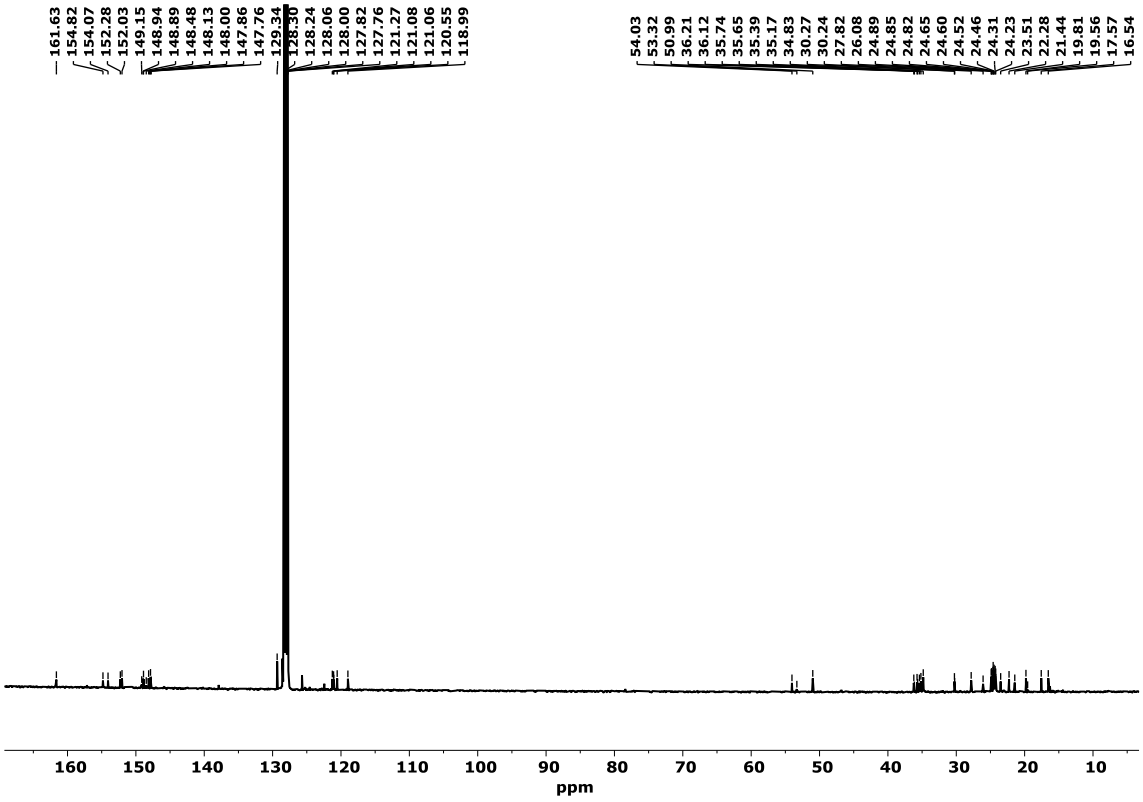


Figure S40: ^{13}C NMR of compound **5** in C_6D_6 after irradiation of UV light for 5h.

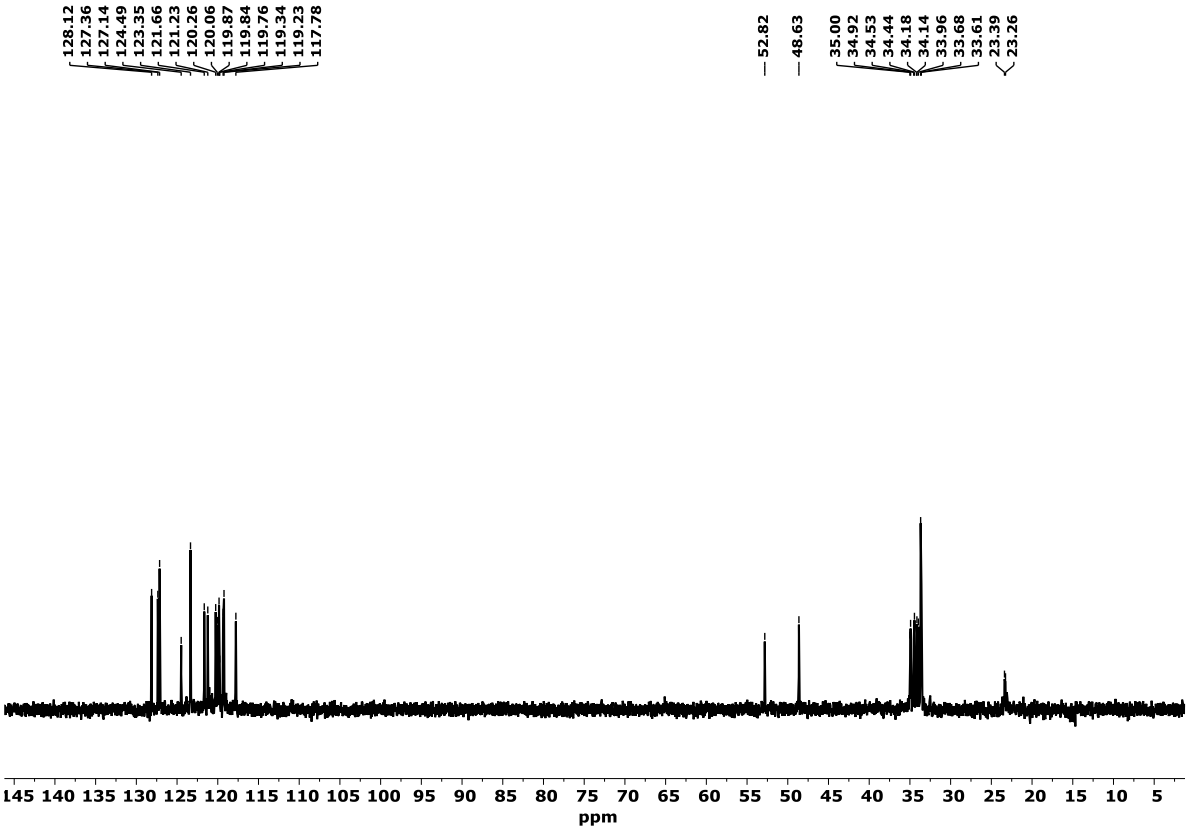


Figure S41: ^{13}C DEPT-135 NMR of compound **5** in C_6D_6 after irradiation of UV light for 5h.

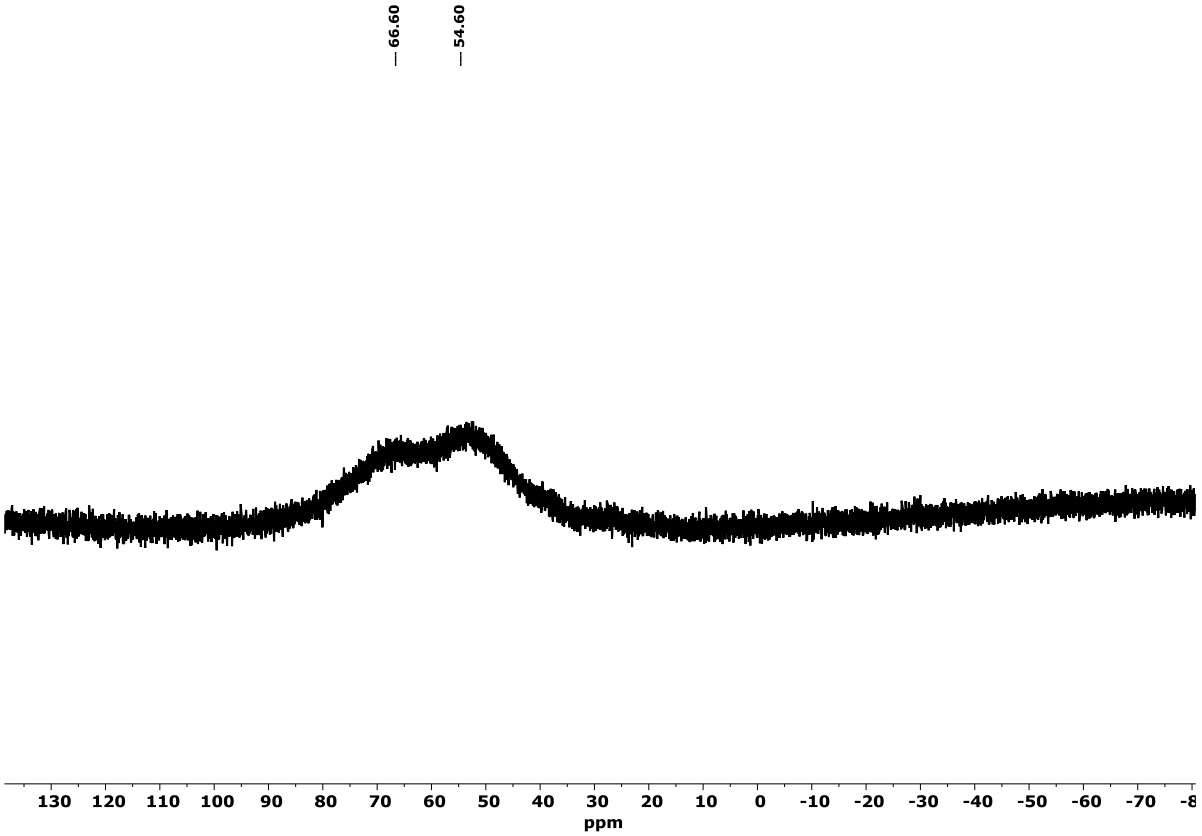


Figure S42: ^{11}B of compound **5** in C_6D_6 after irradiation of UV light for 5h.

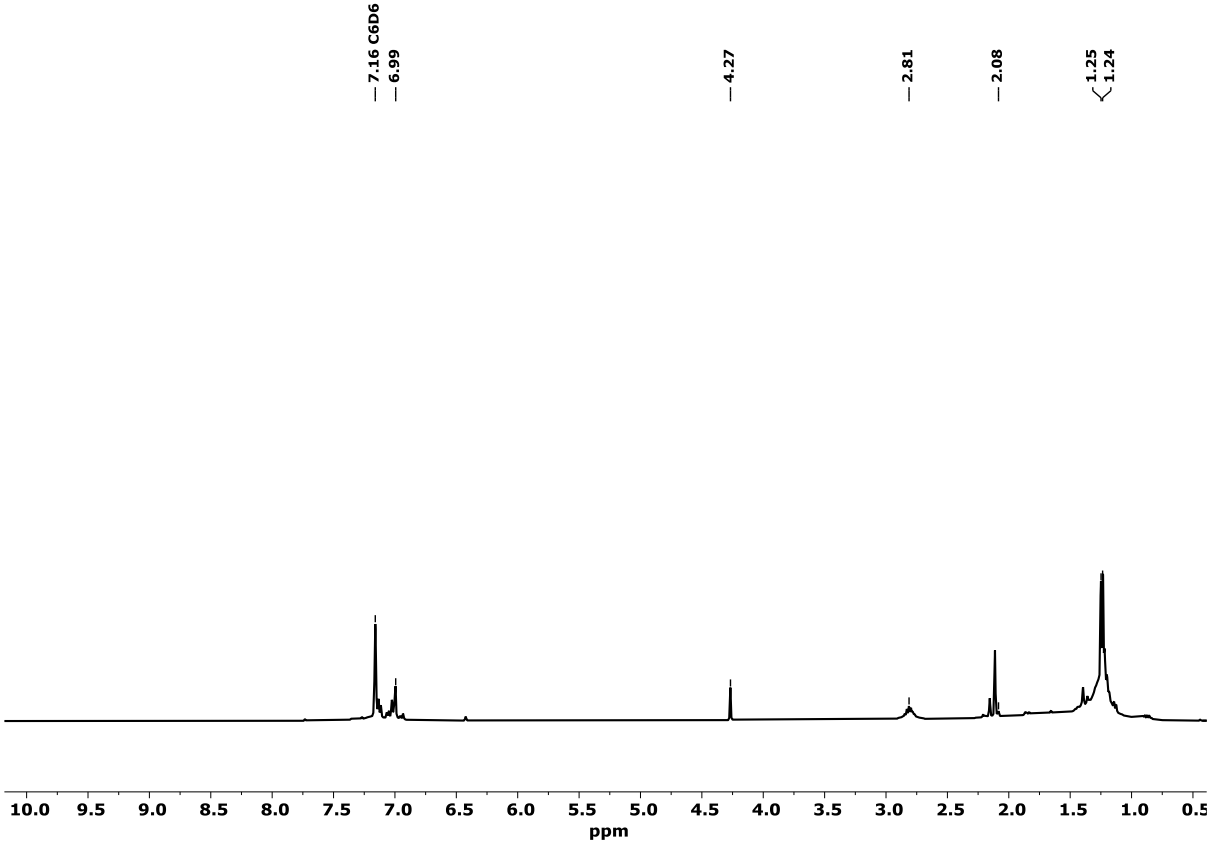


Figure S43: ^{1}H NMR of compound **5** in C_6D_6 after irradiation of UV light for 24h.

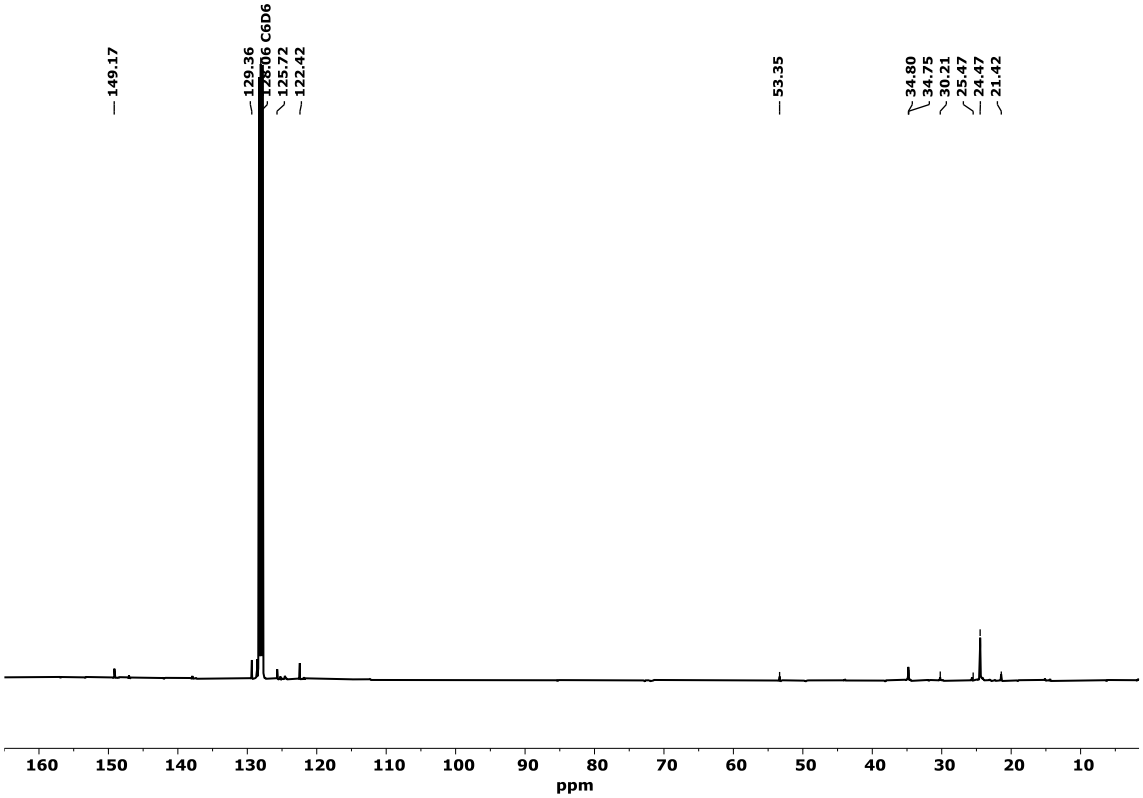


Figure S44: ^{13}C NMR of compound **5** in C_6D_6 after irradiation of UV light for 24h.

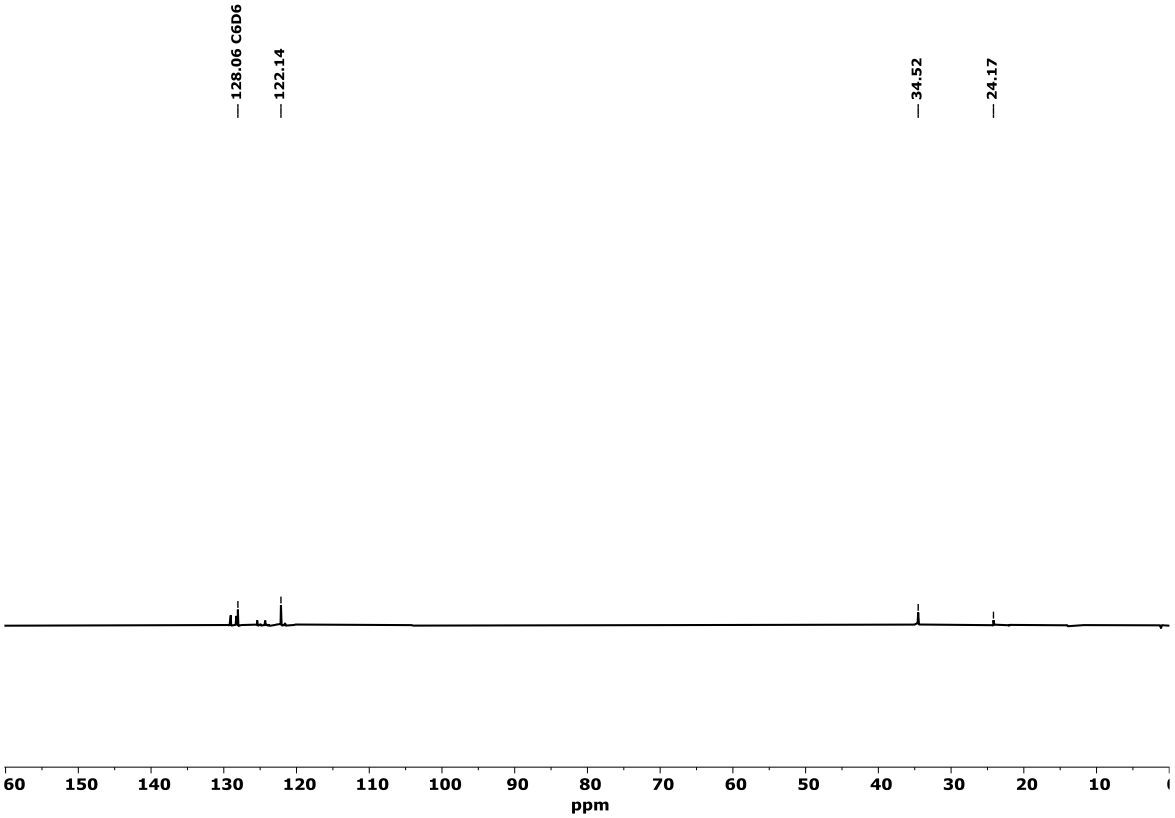


Figure S45: ^{13}C DEPT-135 NMR of compound **5** in C_6D_6 after irradiation of UV light for 24h.

Optimized x,y,z coordinates for compounds **3-5** calculated on Gaussian 03 at the B3LYP//6-31g(d,p) level

Compound **3**

Center Type	Atomic	Atomic Coordinates (Angstroms) X	Y	Z
S		0.000025	-3.805492	-0.000013
C		-5.948332	-0.000006	0.000009
C		-5.247460	-0.000011	1.204276
H		-5.790086	-0.000012	2.146704
C		-3.847330	-0.000017	1.218217
C		-3.129969	-0.000017	0.000007
C		-0.732906	1.326730	0.000002
C		-0.732884	-1.326738	0.000001
C		-3.847332	-0.000011	-1.218202
C		-5.247461	-0.000006	-1.204259
H		-5.790090	-0.000003	-2.146685
C		-3.108449	-0.000019	2.540728
H		-3.802559	-0.000034	3.385869
H		-2.460163	0.878810	2.640393
H		-2.460141	-0.878833	2.640378
C		-1.265108	2.606545	-0.000006
C		-1.265072	-2.606560	-0.000006
C		-2.686976	-3.100899	-0.000010
H		-3.233986	-2.745547	0.877256
H		-2.721707	-4.193796	-0.000022
H		-3.233988	-2.745526	-0.877266
C		-2.687016	3.100872	-0.000009
H		-3.234035	2.745480	0.877234
H		-3.234014	2.745530	-0.877287
H		-2.721757	4.193769	0.000021
C		-3.108453	-0.000007	-2.540715
H		-3.802565	-0.000035	-3.385854
H		-2.460132	-0.878812	-2.640362
H		-2.460180	0.878832	-2.640383
B		-1.546332	-0.000013	0.000004
S		-0.000025	3.805493	-0.000015
C		5.948332	0.000004	0.000008
C		5.247461	-0.000004	-1.204259
H		5.790088	-0.000014	-2.146686
C		3.847331	0.000002	-1.218201
C		3.129969	0.000017	0.000008
C		0.732906	-1.326729	0.000007
C		0.732884	1.326739	-0.000001
C		3.847331	0.000025	1.218218
C		5.247460	0.000019	1.204276

H	5.790088	0.000026	2.146703
C	3.108452	-0.000016	-2.540713
H	3.802564	0.000037	-3.385853
H	2.460205	-0.878874	-2.640388
H	2.460104	0.878769	-2.640356
C	1.265108	-2.606544	0.000006
C	1.265072	2.606561	-0.000014
C	2.686976	3.100900	-0.000030
H	3.233966	2.745567	-0.877317
H	2.721707	4.193797	0.000005
H	3.234008	2.745508	0.877205
C	2.687016	-3.100871	0.000004
H	3.233996	-2.745577	-0.877306
H	3.234053	-2.745430	0.877215
H	2.721757	-4.193768	0.000092
C	3.108450	0.000041	2.540729
H	3.802560	0.000032	3.385870
H	2.460168	0.878874	2.640384
H	2.460138	-0.878770	2.640389
B	1.546332	0.000013	0.000007
H	-7.034740	-0.000004	0.000010
H	7.034740	0.000002	0.000009

Compound **4**

Center Type	Atomic X	Atomic Y	Coordinates (Angstroms) Z
S	-0.002955	-3.805415	-0.000041
C	-5.973237	0.009170	0.000010
C	-5.251670	0.009834	1.197365
H	-5.791623	0.015825	2.142593
C	-3.852546	0.004997	1.214162
C	-3.130250	0.002070	-0.000039
C	-0.731886	1.327142	-0.000044
C	-0.733886	-1.325981	-0.000042
C	-3.852567	0.005002	-1.214184
C	-5.251723	0.009845	-1.197337
H	-5.791703	0.015841	-2.142545
C	-3.119395	0.007636	2.539958
H	-3.816595	0.007806	3.382561
H	-2.472260	0.887204	2.640937
H	-2.470492	-0.870389	2.642834
C	-1.263111	2.607278	-0.000009
C	-1.267108	-2.605279	-0.000038
C	-2.689505	-3.098260	-0.000032
H	-3.236039	-2.742067	0.877196
H	-2.725206	-4.191183	-0.000029
H	-3.236045	-2.742068	-0.877257

C	-2.684702	3.102578	-0.000003
H	-3.231897	2.747480	0.877254
H	-3.231984	2.747247	-0.877106
H	-2.718618	4.195550	-0.000141
C	-3.119484	0.007628	-2.540020
H	-3.816728	0.007897	-3.382586
H	-2.470672	-0.870457	-2.642968
H	-2.472270	0.887138	-2.640998
C	-7.483748	-0.019065	0.000108
H	-7.893858	0.473504	-0.886904
H	-7.893876	0.479160	0.883970
H	-7.863799	-1.048658	0.003453
B	-1.547248	0.001186	-0.000048
S	0.002962	3.805424	0.000045
C	5.973234	-0.009188	0.000080
C	5.251711	-0.009771	-1.197313
H	5.791701	-0.015709	-2.142521
C	3.852597	-0.004922	-1.214163
C	3.130247	-0.002069	0.000018
C	0.731884	-1.327132	-0.000063
C	0.733885	1.325988	-0.000015
C	3.852510	-0.005090	1.214183
C	5.251675	-0.009938	1.197389
H	5.791619	-0.015998	2.142616
C	3.119488	-0.007475	-2.539983
H	3.816715	-0.007683	-3.382564
H	2.472286	-0.886988	-2.640999
H	2.470661	0.870606	-2.642860
C	1.263114	-2.607265	-0.000060
C	1.267110	2.605284	0.000024
C	2.689509	3.098261	0.000059
H	3.236076	2.742044	-0.877138
H	2.725214	4.191184	0.000033
H	3.236013	2.742088	0.877314
C	2.684709	-3.102555	-0.000023
H	3.232114	-2.746932	-0.876925
H	3.231774	-2.747741	0.877433
H	2.718634	-4.195527	-0.000508
C	3.119384	-0.007779	2.539995
H	3.816600	-0.008167	3.382584
H	2.470632	0.870345	2.642999
H	2.472102	-0.887250	2.640878
C	7.483745	0.019033	0.000009
H	7.893797	-0.472047	0.887867
H	7.893922	-0.480682	-0.882995
H	7.863806	1.048615	-0.005079
B	1.547246	-0.001179	-0.000033

Compound **5**

Center Type	Atomic	Atomic Coordinates (Angstroms) X	Y	Z
S		0.011611	-3.571675	1.337168
C		-5.979439	0.076326	0.199282
C		-5.215276	0.549636	1.268206
H		-5.731675	0.933694	2.144929
C		-3.814879	0.548747	1.239293
C		-3.137719	0.033900	0.108344
C		-0.739005	1.256134	-0.436214
C		-0.731359	-1.241779	0.486138
C		-3.903118	-0.461979	-0.976974
C		-5.300083	-0.420910	-0.918449
H		-5.876347	-0.789983	-1.762896
C		-3.035820	1.071268	2.450145
H		-1.993068	1.208308	2.135583
C		-1.271819	2.461089	-0.869559
C		-1.256318	-2.437415	0.953525
C		-2.663687	-2.931958	1.146857
H		-3.359781	-2.114751	1.321308
H		-2.719764	-3.625083	1.992406
H		-3.010876	-3.476678	0.260998
C		-2.679313	2.982025	-0.973425
H		-2.964701	3.520213	-0.061924
H		-3.399624	2.179969	-1.117703
H		-2.771816	3.687393	-1.805482
C		-3.216136	-1.011762	-2.230876
H		-2.163430	-1.189324	-1.975807
C		-7.501580	0.111235	0.255041
H		-7.777083	0.506591	1.241768
B		-1.550276	0.015296	0.053628
S		-0.011282	3.572035	-1.337416
C		5.979358	-0.077029	-0.199917
C		5.214515	-0.549213	-1.268869
H		5.730397	-0.932906	-2.146054
C		3.814153	-0.547713	-1.239387
C		3.137694	-0.033397	-0.107734
C		0.738969	-1.255587	0.436406
C		0.731397	1.242839	-0.484309
C		3.903796	0.461396	0.977566
C		5.300728	0.419757	0.918435
H		5.877504	0.787971	1.762901
C		3.034432	-1.069254	-2.450193
H		1.992145	-1.207836	-2.134705
C		1.271963	-2.460783	0.868757
C		1.256558	2.438305	-0.951717
C		2.664027	2.932925	-1.143950
H		3.360705	2.115545	-1.315281

H	2.721278	3.623973	-1.991131
H	3.009323	3.480060	-0.258808
C	2.679441	-2.982254	0.970036
H	2.963723	-3.518470	0.057022
H	3.400073	-2.180640	1.115320
H	2.772708	-3.689452	1.800445
C	3.217501	1.010751	2.232030
H	2.165537	1.191988	1.976409
C	7.501475	-0.112560	-0.256411
H	7.776284	-0.508086	-1.243265
B	1.550268	-0.014412	-0.052358
C	-3.794092	-2.360289	-2.698595
H	-4.816860	-2.255224	-3.075952
H	-3.188396	-2.770070	-3.513882
H	-3.812696	-3.095356	-1.888594
C	-3.239645	0.006863	-3.387792
H	-4.269520	0.257554	-3.666109
H	-2.727360	0.933247	-3.115072
H	-2.742336	-0.402527	-4.274304
C	-8.089763	1.063765	-0.803155
H	-7.857418	0.720487	-1.817240
H	-9.180225	1.120092	-0.712671
H	-7.685721	2.074909	-0.693591
C	-8.119076	-1.294399	0.134204
H	-7.730076	-1.965546	0.906176
H	-9.208703	-1.249002	0.239013
H	-7.898685	-1.744094	-0.840095
C	-3.534799	2.440036	2.948556
H	-3.562501	3.178862	2.142254
H	-4.541546	2.375075	3.374814
H	-2.873868	2.821526	3.734191
C	-3.032111	0.052368	3.607097
H	-4.052840	-0.158765	3.945326
H	-2.573420	-0.892871	3.305116
H	-2.468303	0.440551	4.462804
C	3.534306	-2.436721	-2.951263
H	4.539930	-2.369777	-3.379878
H	3.565065	-3.176403	-2.145852
H	2.872105	-2.818311	-3.735775
C	3.028528	-0.048563	-3.605541
H	2.569460	0.895824	-3.301463
H	4.048708	0.163841	-3.944605
H	2.464021	-0.435848	-4.461199
C	3.799176	2.356551	2.702941
H	4.821098	2.247526	3.081479
H	3.821197	3.092940	1.894241
H	3.193747	2.766781	3.518194
C	3.237071	-0.010274	3.386888
H	2.722788	-0.934796	3.111623
H	4.265994	-0.264099	3.665882

H	2.739745	0.398536	4.273663
C	8.119525	1.292877	-0.136018
H	9.209116	1.247072	-0.241025
H	7.730613	1.963985	-0.908067
H	7.899452	1.742855	0.838219
C	8.089880	-1.065226	0.801525
H	9.180271	-1.121949	0.710434
H	7.858249	-0.721830	1.815733
H	7.685429	-2.076238	0.692236
