Supporting Information

4-Aryldithieno[3,2-*b*:2',3'-*d*]arsoles: effects of the As-substituent on the structure, photophysical properties, and stability

Chisa Takahara,[a] Suzuka Iwasaki,[a] Hyota Kihara,[a] Yusuke Miyake,[a] Hiroaki Imoto*,[a] and Kensuke Naka*[a,b]

[a] Faculty of Molecular Chemistry and Engineering, Graduate School of Science and Technology, Kyoto Institute of Technology, Goshokaido-cho, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan
[b] Materials Innovation Lab, Kyoto Institute of Technology, Goshokaido-cho, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan.

Contents:

1. NMR Spectra

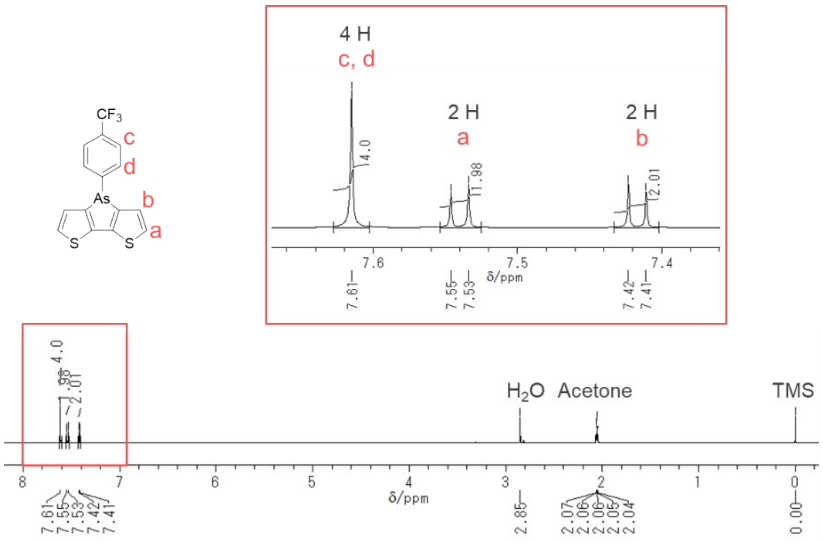


Figure S1. ^{1}H-NMR spectrum (400 MHz) of **3** in Acetone-d_6.

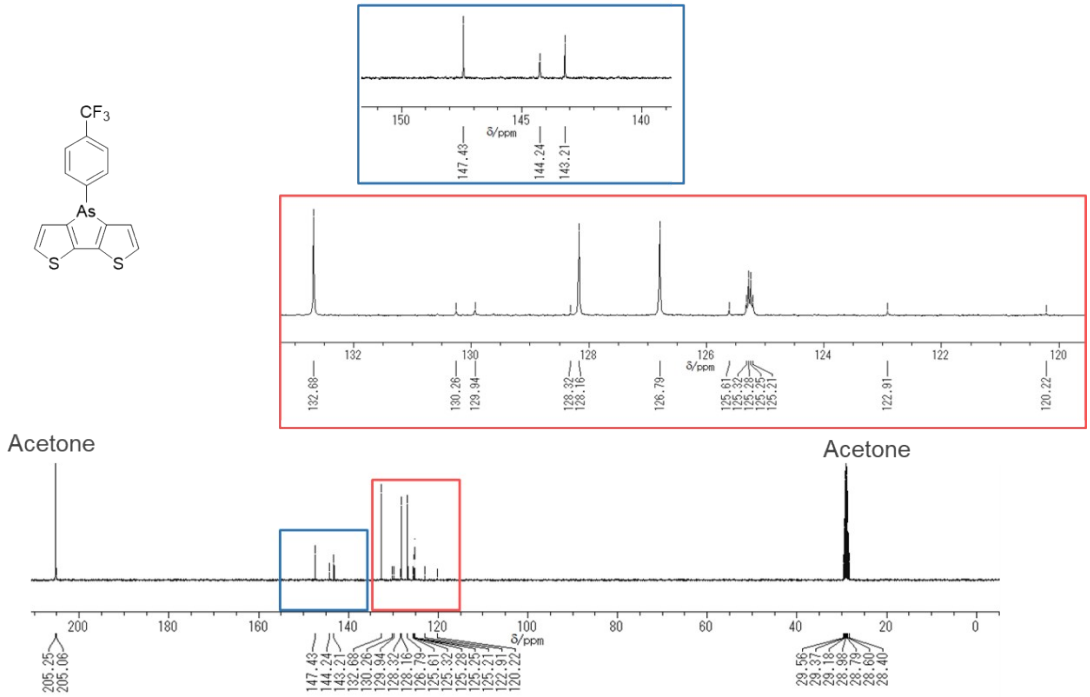


Figure S2. ^{13}C-NMR spectrum (100 MHz) of **3** in Acetone-d_6.

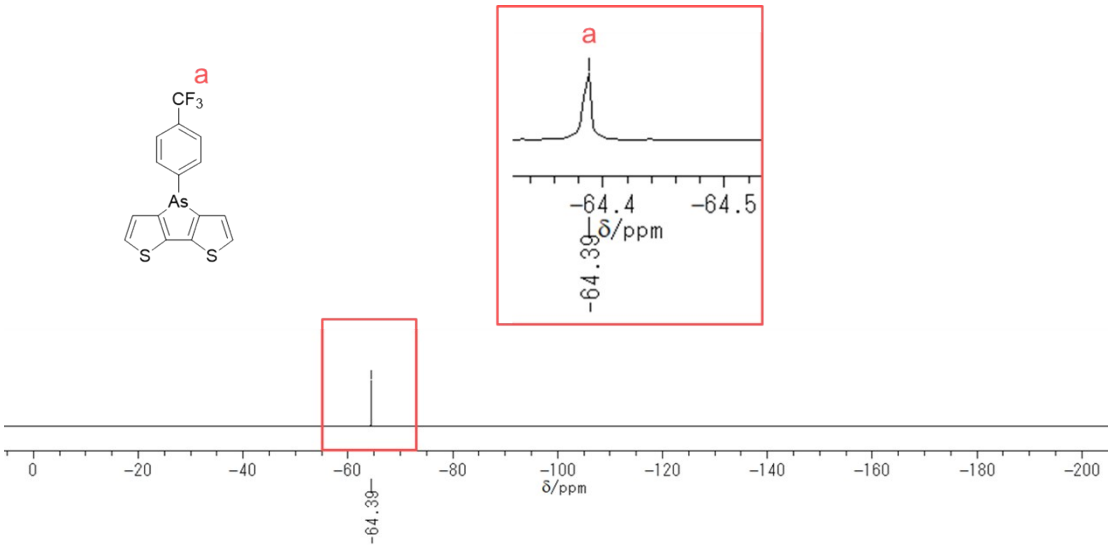


Figure S3. ^{19}F-NMR spectrum (376 MHz) of **3** in Acetone-d_6.

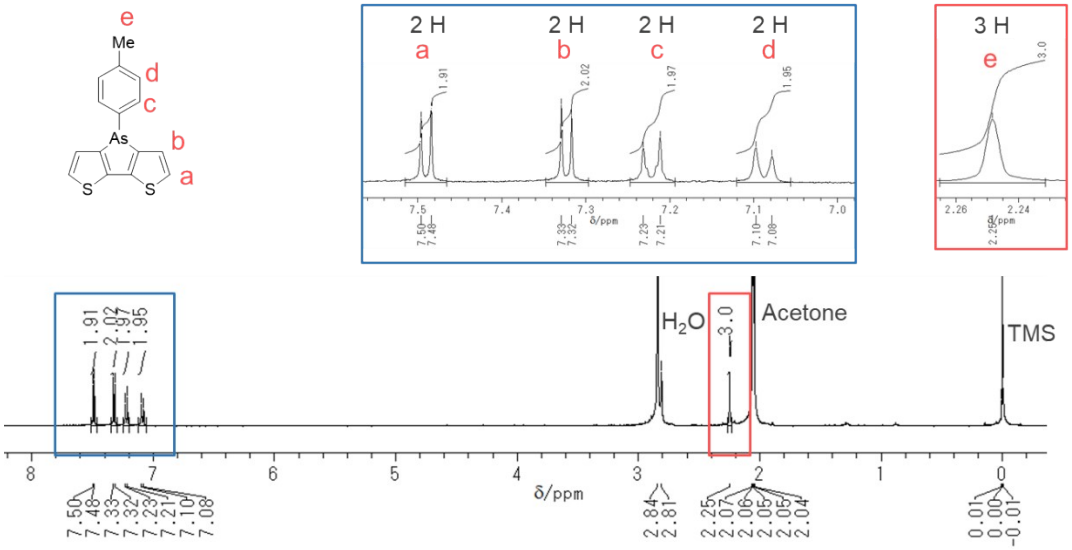


Figure S4. ^{1}H-NMR spectrum (400 MHz) of **4** in Acetone-d_6.

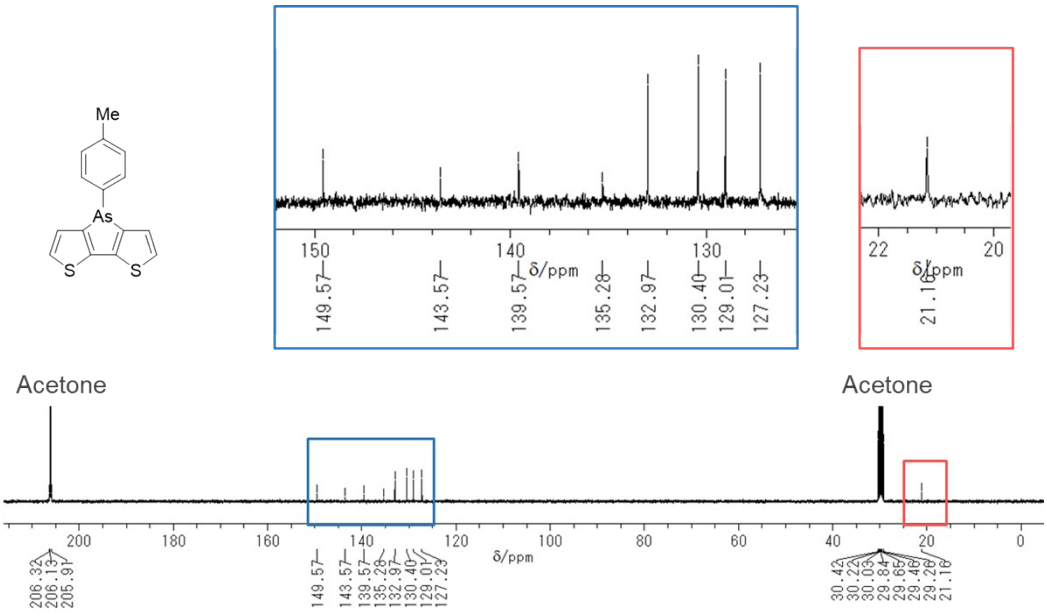


Figure S5. ^{13}C-NMR spectrum (100 MHz) of **4** in Acetone-d_6.

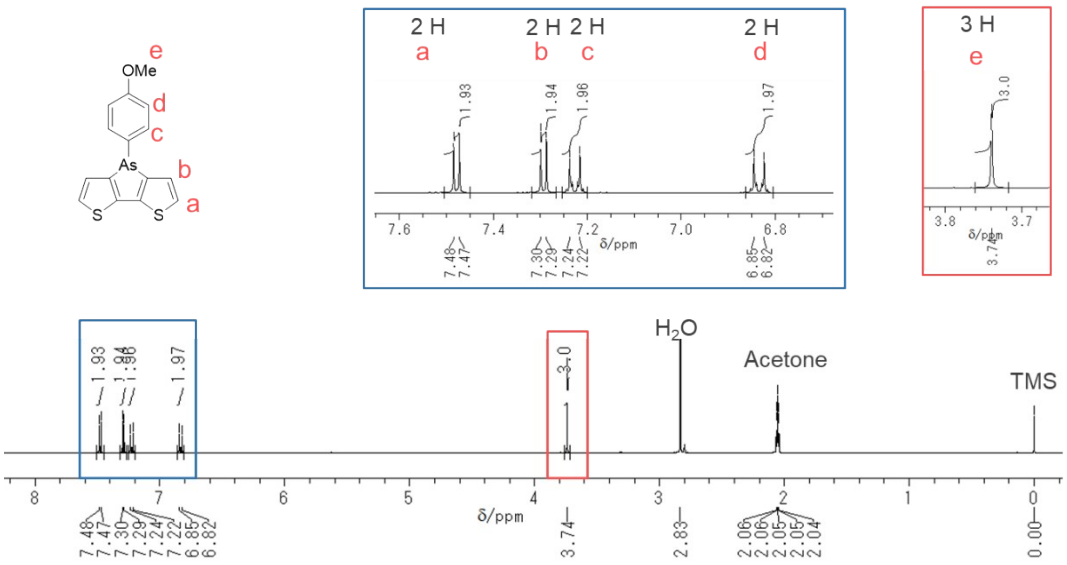


Figure S6. ^{1}H-NMR spectrum (400 MHz) of **5** in Acetone-d_6.

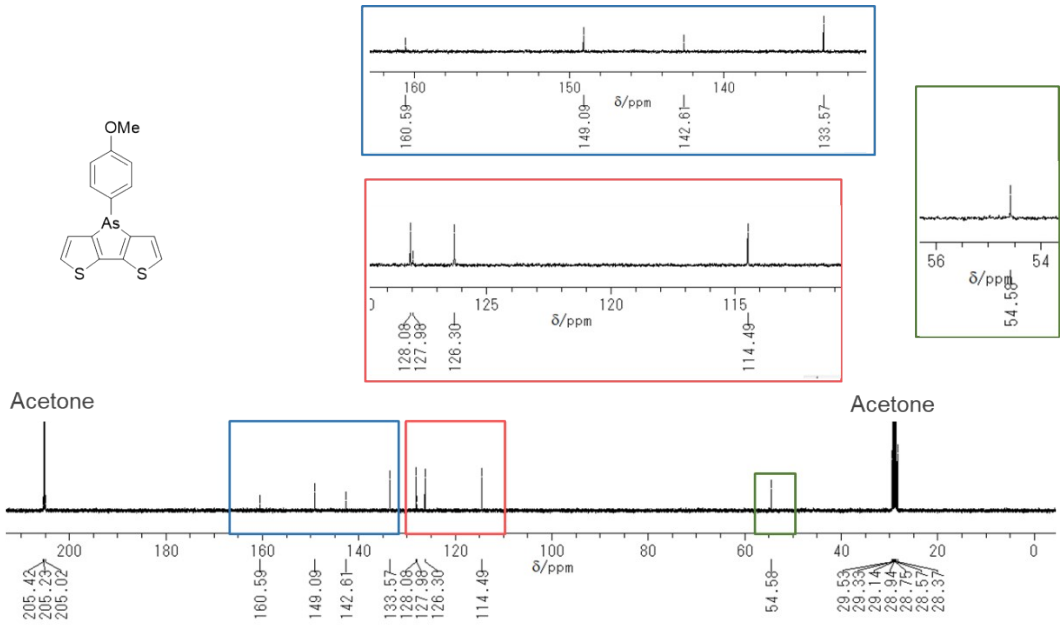


Figure S7. ^{13}C-NMR spectrum (100 MHz) of **5** in Acetone-d_6.

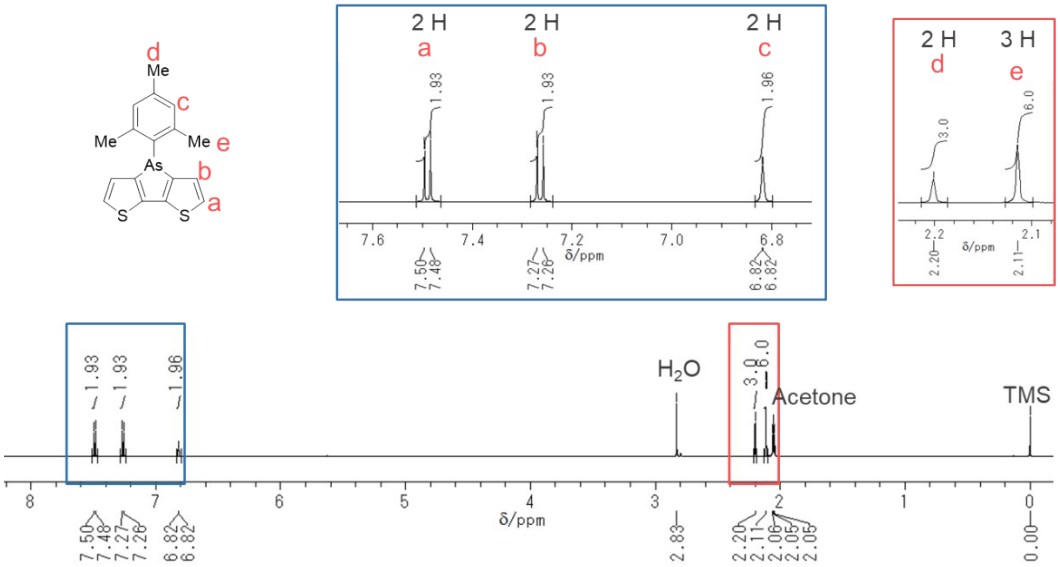


Figure S8. ^{1}H-NMR spectrum (400 MHz) of **6** in Acetone-d_6.

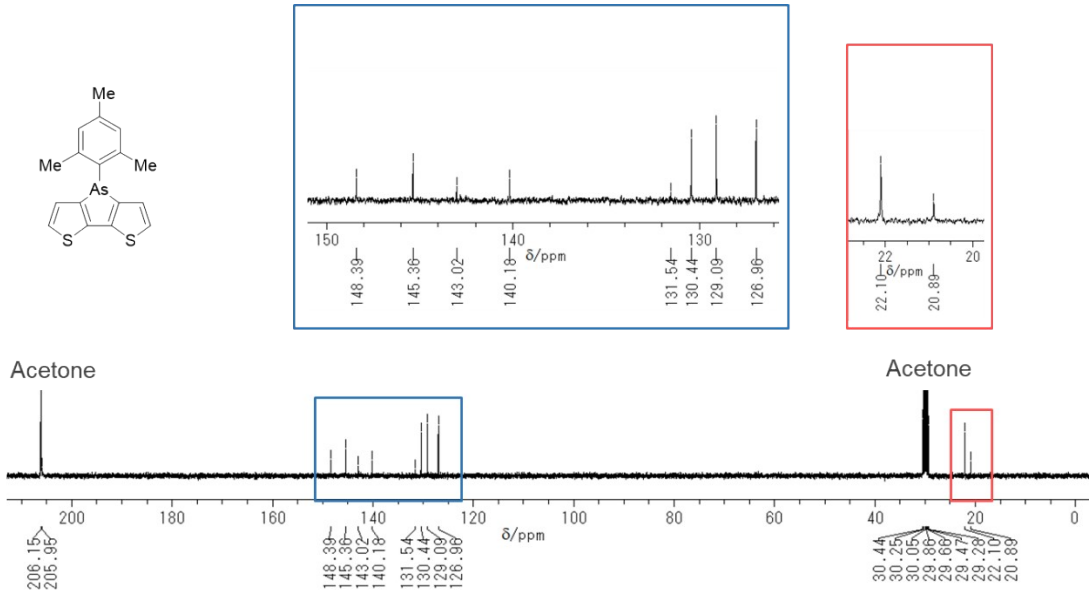


Figure S9. ^{13}C-NMR spectrum (100 MHz) of **6** in Acetone-d_6.

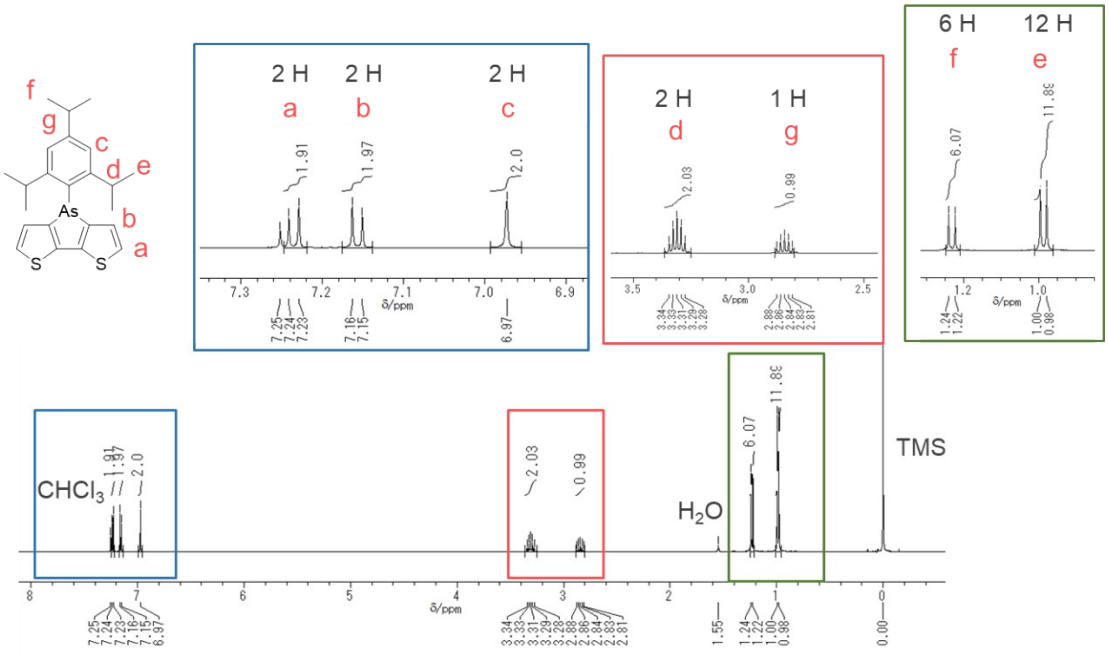


Figure S10. H-NMR spectrum (400 MHz) of **7** in Acetone-d_6.

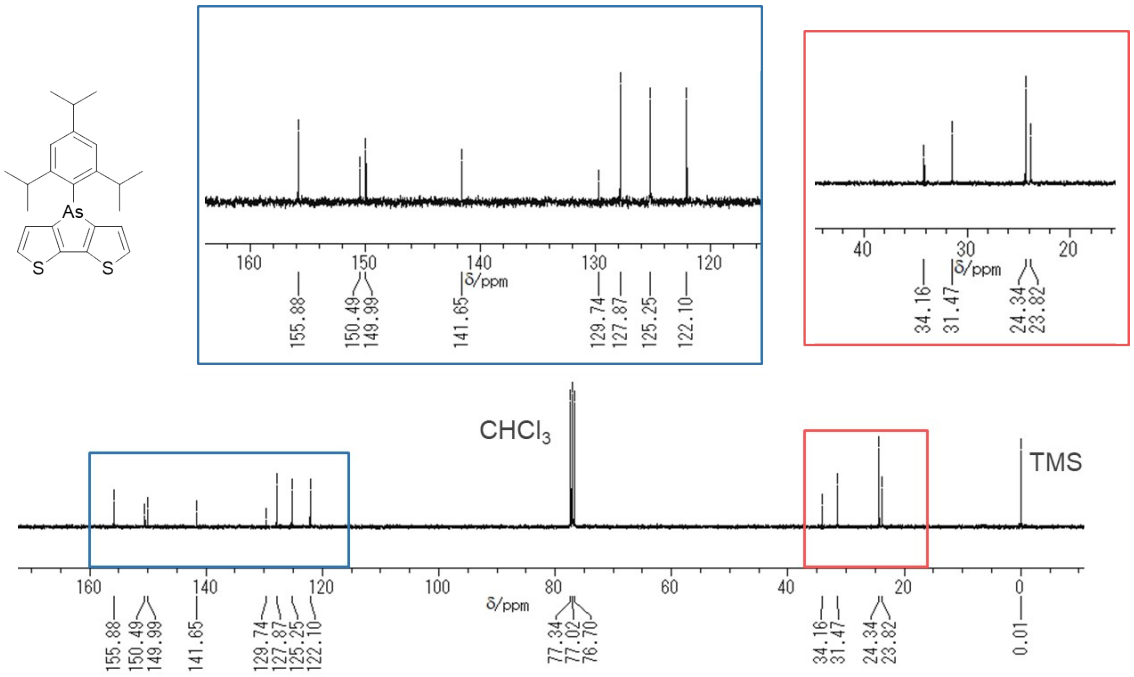


Figure S11. ^{13}C-NMR spectrum (100 MHz) of **7** in Acetone-d_6.

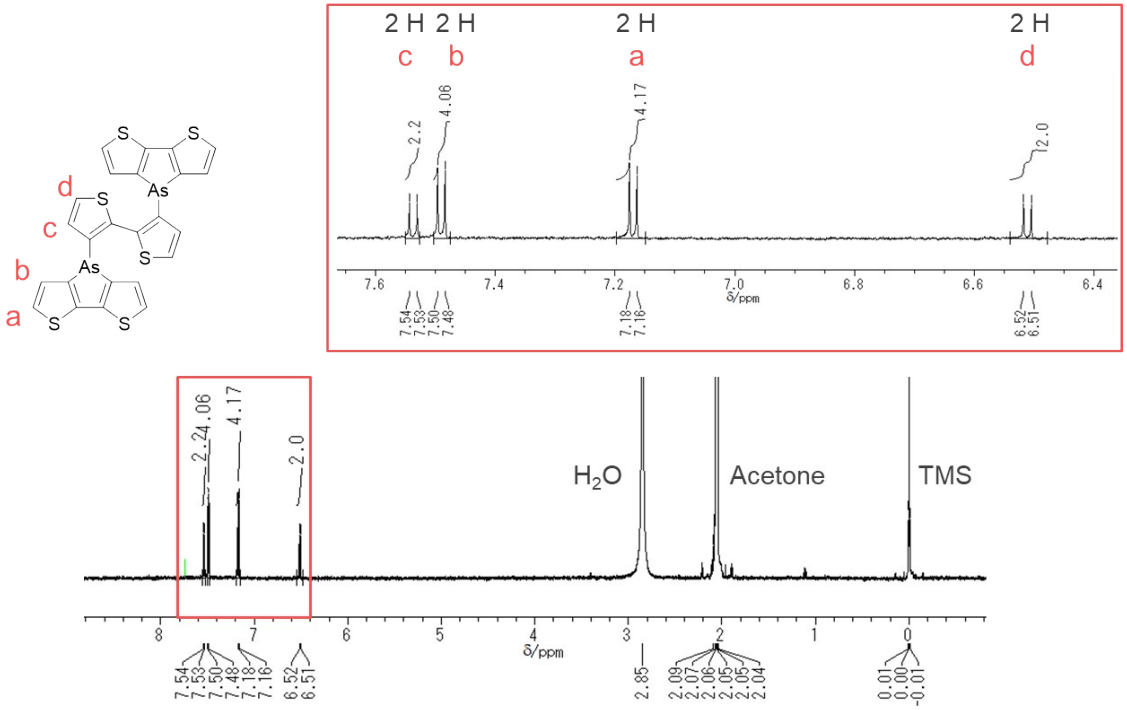


Figure S12. H-NMR spectrum (400 MHz) of **1'** in Acetone-d_6.

2. Generation of DTA bromide 1

*Generation of 4-bromodithieno[3,2-b:2',3'-d]arsole (**1**) and 4-iododithieno[3,2-b:2',3'-d]arsole.*

To an Et_2O solution (40 mL) of 3,3'-dibromo-2,2'-bithiophene (324 mg, 1.0 mmol) was added *n*-BuLi (1.6 M in *n*-hexane, 1.3 mL, 2.1 mmol) at -78 °C under N_2 atmosphere. The reaction solution was warmed to room temperature, and stirred for 30 min at room temperature. The resultant solution was slowly added to an Et_2O solution (7.3 mL) of $AsBr_3$ (316 mg, 1.0 mmol) with a cannula at 0 °C under N_2 atmosphere. The reaction solution was warmed to room temperature, and stirred for 3 h to prepare solution of **1**. Under ambient condition, **1** was gradually decomposed, and thus we failed isolation of **1**. The generation of **1** was confirmed by ^{1}H-NMR spectrum. ^{1}H-NMR (Acetone-d_6, 400 MHz): δ 7.46 (d, J = 4.8 Hz, 2H), 7.34 (d, J = 4.8 Hz, 2H) ppm.

Then, the solvents were removed *in vacuo*, and KI (300 mg, 2.0 mmol) and acetone (40 mL) were added to the residue at room temperature under N_2 atmosphere. The reaction mixture was stirred overnight, and the solvents were removed *in vacuo*. The reside was washed with EtOH and *n*-hexane, extracted with Et_2O, and purified by recrystallization from CH_2Cl_2/MeOH to obtain 4-iododithieno[3,2-*b*:2',3'-*d*]arsole (42 mg, 0.11 mmol, 11%) as dark red solids. ^{1}H-NMR (Acetone-d_6, 400 MHz): δ 7.53 (d, J = 4.8 Hz, 2H), 7.40 (d, J = 4.8 Hz, 2H) ppm.

*Synthesis of DTA dimer **1'** (shown in Scheme 2b of the main text).*

To an Et_2O solution (10 mL) of 3,3'-dibromo-2,2'-bithiophene (324 mg, 1.0 mmol) was added *n*-BuLi (1.6 M in *n*-hexane, 1.3 mL, 2.1 mmol) at -78 °C under N_2 atmosphere. The reaction solution was warmed to room temperature, and stirred for 30 min at room temperature. The reaction solution was cooled to -78 °C again, and an Et_2O solution (3 mL) of $AsBr_3$ (316 mg, 1.0 mmol) was added. The reaction solution was warmed to room temperature, and stirred overnight. The reaction was quenched by addition of distilled water at 0 °C. The volatiles were removed *in vacuo*, and the residue was washed with Et_2O to obtain **1'** (128 mg, 0.20 mmol, 40%) as yellow solids. ^{1}H-NMR (Acetone-d_6, 400 MHz): δ 7.54 (d, J = 5.2 Hz, 2H), 7.49 (d, J = 5.2 Hz, 2H), 7.17 (d, J = 5.2 Hz, 2H), 6.51 (d, J = 5.2 Hz, 2H) ppm. ^{13}C-NMR spectrum was unable to be measured because of the low solubility. HR-FAB-MASS: (m/z): calculated for $C_{24}H_{13}S_6As_2$ $[M+H]^+$: 641.7695, found: 642.7781.

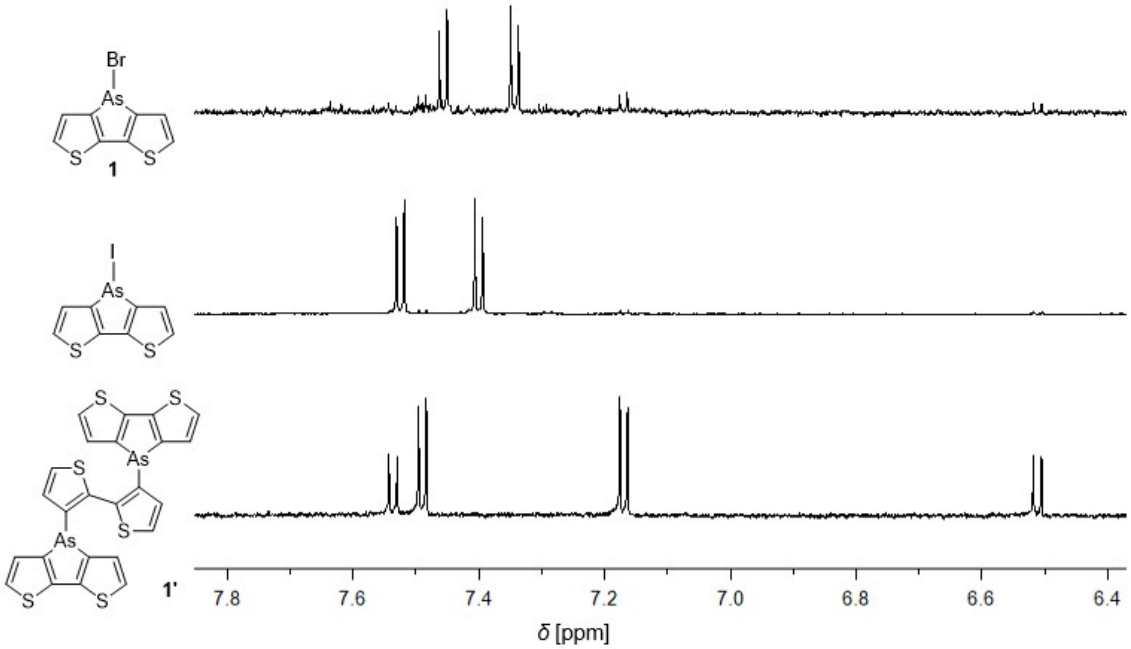


Figure S13. ^{1}H-NMR spectra (400 MHz) of **1** (crude), 4-iododithieno[3,2-*b*:2',3'-*d*]arsole, and **1'** in Acetone-d_6.

3. X-ray crystallographic data for single crystalline products

Table S1. Crystallographic Data of **2-1**, **3** and **4**.

	2-1	**3**	**4**
Crystal data			
Empirical Formula	$C_{14}H_9AsS_2$	$C_{15}H_8AsF_3S_2$	$C_{15}H_{11}AsS_2$
Formula Weight	316.25	384.25	330.28
Crystal Dimension, mm^3	0.42 × 0.17 × 0.04	0.28 × 0.21 × 0.19	0.88 × 0.67 × 0.37
Crystal System	orthorhombic	orthorhombic	orthorhombic
Space Group	*P*na2_1	*P*na2_1	*P*na2_1
a, Å	12.6354(8)	12.886(18)	12.610(12)
b, Å	5.8417(7)	5.795(8)	5.954(6)
c, Å	33.241(3)	38.75(7)	36.39(3)
α, deg	90	90	90
β, deg	90	90	90
γ, deg	90	90	90
Volume, $Å^3$	2453.6(4)	2893(8)	2732(4)
D_{calcd}, g cm^{-3}	1.712	1.764	1.606
Z	8	8	8
F(000)	1264.0	1520.0	1328.0
Data Collection			
Temperature, deg	-180	25	25
2θmax, deg	52.7	52.7	65.2
Tmin/Tmax	0.056 / 0.514	0.211 / 1.000	0.747 / 0.886
Refinement			
No. of Observed Data	4214	5509	6651
No. of Parameters	307	411	303
R1[a], wR2[b]	0.0463, 0.0984	0.0488, 0.1169	0.0600, 0.1841
Goodness of Fit Indictor	1.019	1.026	0.838

[a]$R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma |Fo|$ [b]$wR2 = [\ \Sigma\ w\ ((Fo^2-Fc^2)^2 / \Sigma\ w\ (Fo^2)^2\ ]^{1/2}$ $w = [\ \sigma^2(Fo^2)\ ]^{-1}$

CCDC# 2173950 (**2-1**), 2173953 (**3**), 2173951 (**4**)

Table S2. Crystallographic Data of **5**-**7**.

	5	**6**	**7**
Crystal data			
Empirical Formula	$C_{15}H_{11}AsOS_2$	$C_{17}H_{15}AsS_2$	$C_{23}H_{27}AsS_2$
Formula Weight	346.28	358.33	442.48
Crystal Dimension, mm^3	0.82 × 0.38 × 0.27	0.55 × 0.198 × 0.11	0.74× 0.27× 0.17
Crystal System	monoclinic	triclinic	monoclinic
Space Group	*Cc*	*P*-1	$P2_1/c$
a, Å	10.729(6)	8.343(5)	10.564(15)
b, Å	16.495(10)	14.016(8)	16.002(6)
c, Å	8.178(6)	14.594(8)	18.488(3)
α, deg	90	69.81(5)	90
β, deg	100.39(7)	80.16(5)	135.57(3)
γ, deg	90	79.86(5)	90
Volume, $Å^3$	1423(16)	1565(17)	2188(8)
D_{calcd}, g cm^{-3}	1.616	1.520	1.343
Z	4	4	4
F(000)	696.0	728.0	920.0
Data Collection			
Temperature, deg	-180	-180	-180
2θmax, deg	52.7	52.7	52.7
Tmin/Tmax	0.548 / 1.000	0.789 / 0.952	0.984/0.994
Refinement			
No. of Observed Data	1730	6408	4464
No. of Parameters	173	367	241
R1[a], wR2[b]	0.0253, 0.0672	0.0379, 0.0930	0.0304, 0.1353
Goodness of Fit Indictor	1.050	0.990	0.612

[a]$R1 = \Sigma \, | \, |Fo| - |Fc| \, | \, / \, \Sigma \, |Fo|$ [b]$wR2 = [\, \Sigma \, w \, ((Fo^2-Fc^2)^2 \, / \, \Sigma \, w \, (Fo^2)^2 \,]^{1/2}$ $w = [\, \sigma^2(Fo^2) \,]^{-1}$

CCDC# 2173952 (**5**), 2173949 (**6**), 2173954 (**7**)

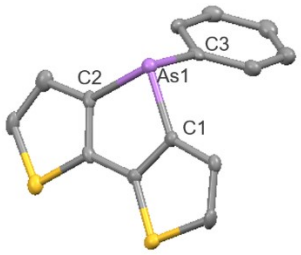
Table S3. Crystallographic Data of **1'** and 4-iododithieno[3,2-*b*:2',3'-*d*]arsole

	1'	4-iododithieno[3,2-*b*:2',3'-*d*]arsole
Crystal data		
Empirical Formula	$C_{24}H_{12}As_2S_6$	$C_8H_4AsIS_2$
Formula Weight	642.54	366.05
Crystal Dimension, mm^3	0.869 × 0.367 × 0.154	0.638 × 0.271 × 0.148
Crystal System	triclinic	monoclinic
Space Group	*P*-1	*I2/a*
a, Å	8.305(6)	14.292(10)
b, Å	10.006(7)	4.979(4)
c, Å	14.215(10)	28.392(17)
α, deg	84.62(6)	90
β, deg	87.42(4)	91.38(6)
γ, deg	88.56(6)	90
Volume, $Å^3$	1175(14)	2020(2)
D_{calcd}, g cm^{-3}	1.817	2.407
Z	2	8
F(000)	636.0	1360.0
Data Collection		
Temperature, deg	-180	25
2θmax, deg	52.7	52.7
Tmin/Tmax	0.388 / 0.799	0.848 / 0.948
Refinement		
No. of Observed Data	4796	2059
No. of Parameters	289	109
R1[a], wR2[b]	0.0514, 0.1372	0.0280, 0.0735
Goodness of Fit Indictor	1.015	1.098

[a] $R1 = \Sigma \, | \, |Fo| - |Fc| \, | \, / \, \Sigma \, |Fo|$ [b] $wR2 = [\, \Sigma \, w \, ((Fo^2-Fc^2)^2 \, / \, \Sigma \, w \, (Fo^2)^2 \,]^{1/2}$ $w = [\, \sigma^2(Fo^2) \,]^{-1}$

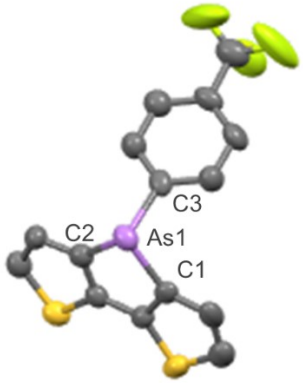
CCDC# 2173955 (**1'**) and 2173948 (4-iododithieno[3,2-*b*:2',3'-*d*]arsole)

Table S4. ORTEP and selected bond lengths and angles of **2-1**.



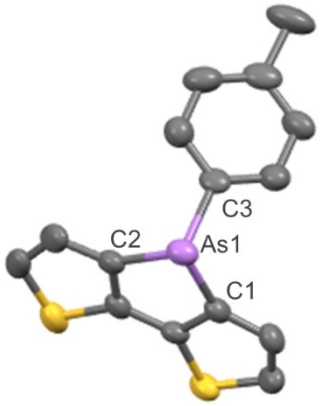
	distance(Å)		angle(°)
As(1)-C(1)	1.94(1)	C(1)-As(1)-C(2)	85.5(4)
As(1)-C(2)	1.95(1)	C(1)-As(1)-C(3)	98.1(4)
As(1)-C(3)	1.96(1)	C(2)-As(1)-C(3)	98.2(4)

Table S5. ORTEP and selected bond lengths and angles of **3**.



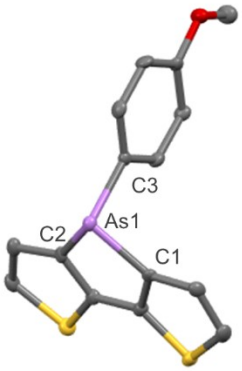
	distance(Å)		angle(°)
As(1)-C(1)	1.95(1)	C(1)-As(1)-C(2)	86.3(4)
As(1)-C(2)	1.92(1)	C(1)-As(1)-C(3)	98.7(3)
As(1)-C(3)	1.96(5)	C(2)-As(1)-C(3)	99.3(3)

Table S6. ORTEP and selected bond lengths and angles of **4**.



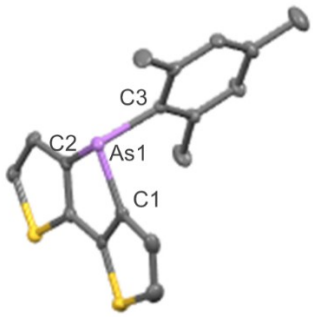
	distance(Å)		angle(°)
As(1)-C(1)	1.95(1)	C(1)-As(1)-C(2)	85.9(4)
As(1)-C(2)	1.94(1)	C(1)-As(1)-C(3)	97.9(3)
As(1)-C(3)	1.98(5)	C(2)-As(1)-C(3)	99.6(3)

Table S7. ORTEP and selected bond lengths and angles of **5**.



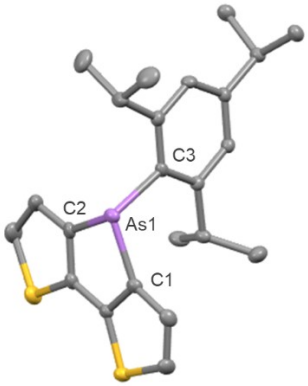
	distance(Å)		angle(°)
As(1)-C(1)	1.96(4)	C(1)-As(1)-C(2)	85.2(2)
As(1)-C(2)	1.95(4)	C(1)-As(1)-C(3)	99.5(2)
As(1)-C(3)	1.96(4)	C(2)-As(1)-C(3)	100.1(2)

Table S8. ORTEP and selected bond lengths and angles of **6**.



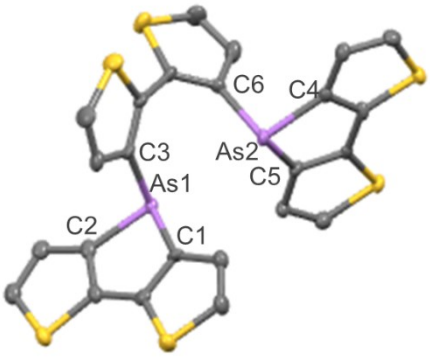
	distance(Å)		angle(°)
As(1)-C(1)	1.96(4)	C(1)-As(1)-C(2)	85.2(2)
As(1)-C(2)	1.95(4)	C(1)-As(1)-C(3)	99.5(2)
As(1)-C(3)	1.96(4)	C(2)-As(1)-C(3)	100.1(2)

Table S9. ORTEP and selected bond lengths and angles of **7**.



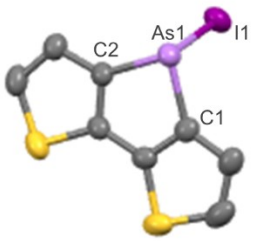
	distance(Å)		angle(°)
As(1)-C(1)	1.96(2)	C(1)-As(1)-C(2)	85.8(1)
As(1)-C(2)	1.95(3)	C(1)-As(1)-C(3)	110.5(1)
As(1)-C(3)	2.00(2)	C(2)-As(1)-C(3)	99.3(1)

Table S10. ORTEP and selected bond lengths and angles of **1'**.



	distance(Å)		angle(°)
As(1)-C(1)	1.96(5)	C(1)-As(1)-C(2)	84.9(2)
As(1)-C(2)	1.97(5)	C(1)-As(1)-C(3)	97.7(2)
As(1)-C(3)	1.95(6)	C(2)-As(1)-C(3)	100.7(2)
As(2)-C(4)	1.94(5)	C(4)-As(2)-C(5)	85.2(2)
As(2)-C(5)	1.96(6)	C(4)-As(2)-C(6)	97.4(2)
As(2)-C(6)	1.95(6)	C(5)-As(2)-C(6)	101.3(2)

Table S11. ORTEP and selected bond lengths and angles of 4-iododithieno[3,2-*b*:2',3'-*d*]arsole.



	distance(Å)		angle(°)
As(1)-C(1)	1.96(5)	C(1)-As(1)-C(2)	97.6(1)
As(1)-C(2)	1.96(5)	C(1)-As(1)-I(1)	84.9(1)
As(1)-I(1)	2.60(6)	C(2)-As(1)-I(1)	98.1(1)

Table S12. Wiberg bond indices (WBI) of the As–C, C=C, and C–C bonds in the arsole rings for the crystal structures.[a]

	As–C	C=C	C–C
2-1	0.91, 0.90	1.51, 1.49	1.11
3	0.90, 0.90	1.51, 1.48	1.12
4	0.90, 0.90	1.47, 1.47	1.14
5	0.89, 0.89	1.49, 1.49	1.12
6	0.90, 0.89	1.49, 1.48	1.12
7	0.90, 0.89	1.49, 1.48	1.13

[a] Estimated by DFT calculations (B3LYP/def2tzvp)

4. Photophysical data

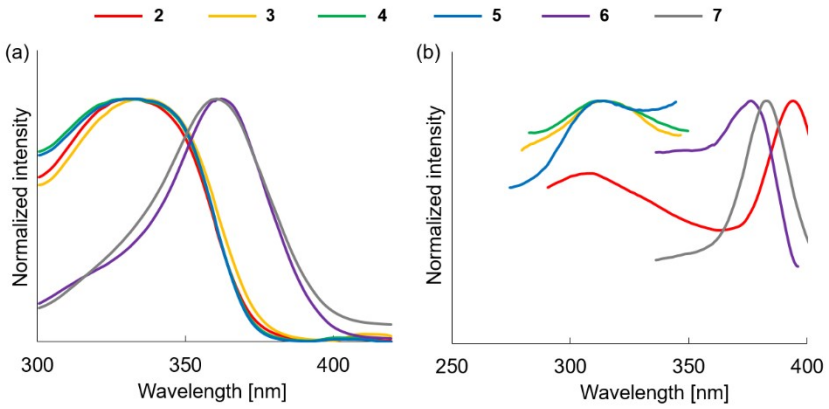


Figure S14. Excitation spectra (monitored at emission maxima) of **2**-**7** measured in (a) solutions (1.0×10^{-4} mol/L in THF) and (b) the solid states at 298 K.

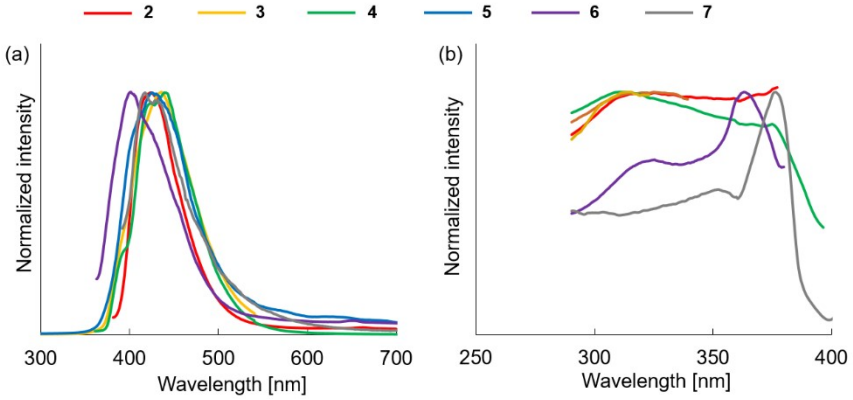


Figure S15. (a) Emission (excited at excitation maxima) and (b) excitation (monitored at emission maxima) spectra of **2**-**7** measured in the solid states at 77 K.

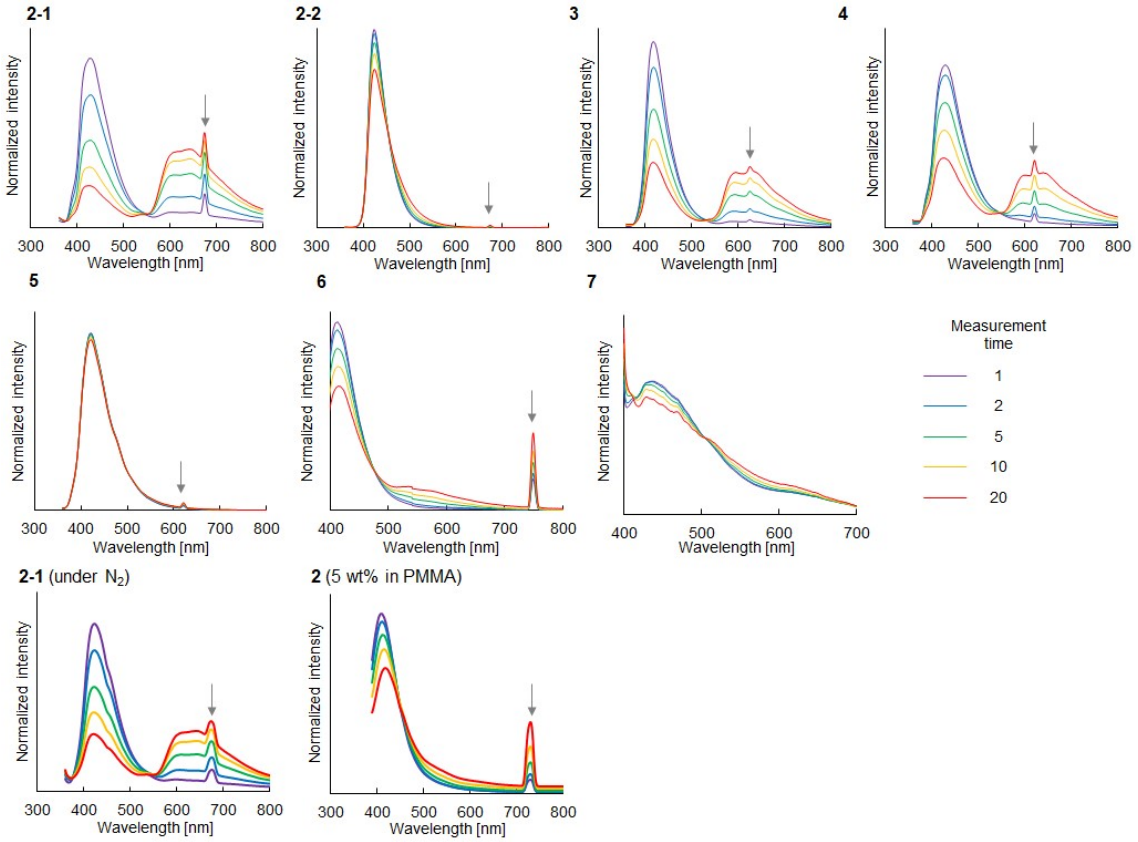


Figure S16. PL spectra of **2-1**, **2-2**, **3**-**7**, **2-1** (under N_2), and **2** (5 wt% in PMMA) measured 20 times. Arrows indicate light scattering.

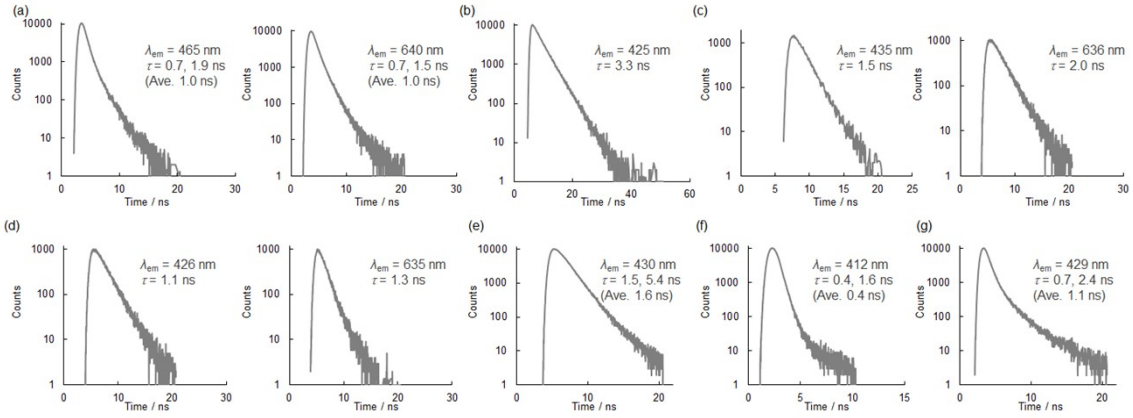


Figure S17. The emission decay kinetics of (a) **2-1**, (b) **2-2**, (c) **3**, (d) **4**, (e) **5**, (f) **6**, and (g) **7** at 298 K in the solid states (excited at 340 nm (**3**-**5**) or 365 nm (**2-1**, **2-2**, **6**, and **7**)). For **2-1**, **3** and **4**, the decay kinetics of the longer-wavelength emissions (monitored at 640 nm (**2-1**), 636 nm (**3**), 635 nm (**4**)) were also measured after UV-irradiation to partially decompose the solid samples.

5. XRD data for crystal polymorphs of 2

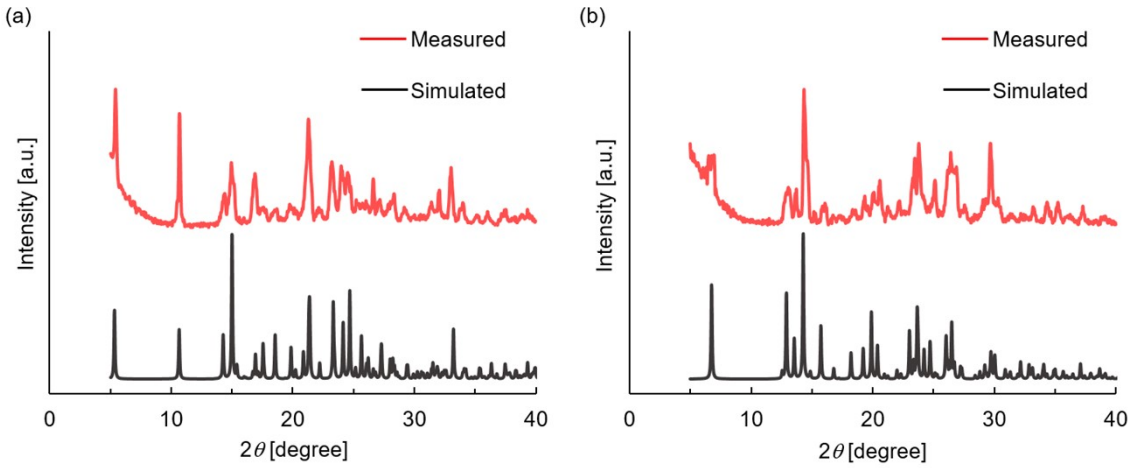


Figure S18. PXRD patterns of (a) **2-1** and (b) **2-2**: measured and simulated by the single crystal XRD data.

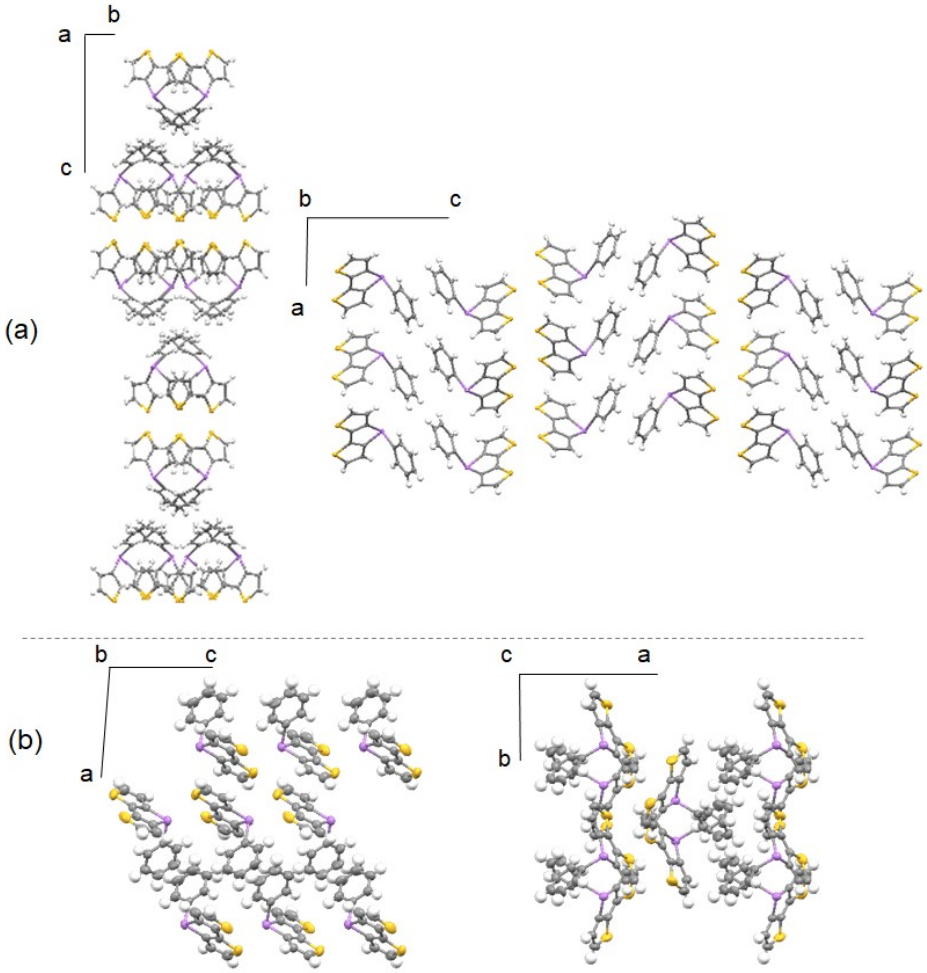


Figure S19. Crystal packing of (a) **2-1** and (b) **2-2**.

6. ESR data

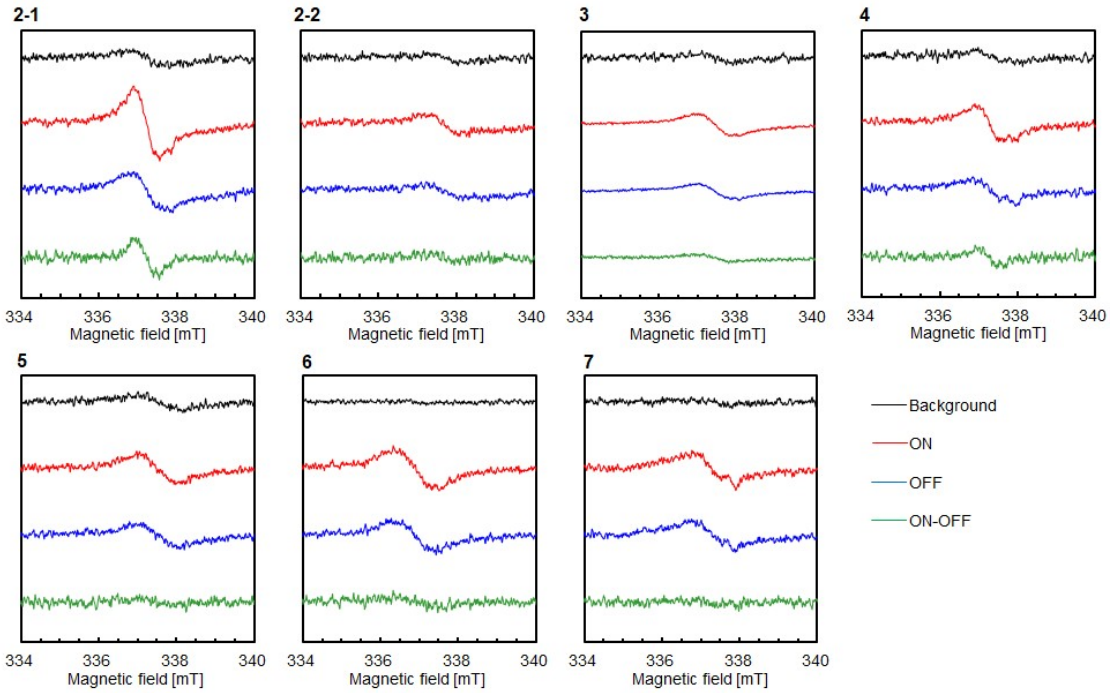


Figure S20. ESR spectra of (c) **2-1** and (d) **2-2** before (black), during (red), and after (blue) UV-irradiation. Difference in the spectra during and after UV-irradiation is also shown (green).

7. DFT calculations

Cartesian coordinates in the structures optimized by DFT calculations

2 (S_0): *E*(B3LYP/def2svp) = -3570.296517 hartree

Number	Atom	X	Y	Z
1	As	0.540255	-2.1E-05	-1.38286
2	S	-2.79466	-1.89045	0.783042
3	S	-2.79457	1.890537	0.783073
4	C	-0.62404	-1.33276	-0.52279
5	C	-1.69345	-0.7234	0.121026
6	C	-1.69343	0.723442	0.121025
7	C	-0.62399	1.332762	-0.5228
8	C	-0.70131	-2.75435	-0.48567
9	C	-1.81229	-3.19918	0.191674
10	C	-1.81218	3.19923	0.191669
11	C	-0.70121	2.754358	-0.48567
12	C	2.076826	-3E-05	-0.13335
13	C	1.933971	-8.2E-05	1.262892
14	C	3.062962	-8.2E-05	2.084975
15	C	4.345275	-3E-05	1.521808
16	C	4.494572	2.05E-05	0.133457
17	C	3.362817	1.96E-05	-0.69162
18	H	0.030952	-3.42892	-0.93241
19	H	-2.11813	-4.22726	0.381489
20	H	-2.11798	4.227323	0.38147
21	H	0.031073	3.4289	-0.93242
22	H	0.936578	-0.00012	1.709741
23	H	2.942949	-0.00012	3.171731
24	H	5.226902	-3E-05	2.168124
25	H	5.492874	6.02E-05	-0.31225
26	H	3.487015	5.69E-05	-1.77863

2 (S_0): *E*(B3LYP/6-31G+(d,p)) = -3569.101740 hartree

Number	Atom	X	Y	Z

1	As	0.533399	-7.7E-06	-1.34334
2	S	-2.81682	-1.89274	0.758685
3	S	-2.81681	1.892756	0.758683
4	C	-0.61293	-1.32915	-0.48739
5	C	-1.69238	-0.72257	0.135222
6	C	-1.69238	0.722581	0.135216
7	C	-0.61293	1.329146	-0.4874
8	C	-0.69772	-2.74914	-0.47439
9	C	-1.82072	-3.20096	0.172234
10	C	-1.8207	3.200967	0.172223
11	C	-0.6977	2.749139	-0.4744
12	C	2.083583	-4.3E-06	-0.13705
13	C	1.968268	5E-07	1.258456
14	C	3.107039	2.3E-06	2.064235
15	C	4.379154	-1.1E-06	1.479709
16	C	4.50421	-6E-06	0.089426
17	C	3.358388	-7.8E-06	-0.71445
18	H	0.037522	-3.41404	-0.91325
19	H	-2.13217	-4.22263	0.342367
20	H	-2.13214	4.222644	0.342354
21	H	0.037544	3.414026	-0.91327
22	H	0.984989	2.9E-06	1.719917
23	H	3.00462	6.1E-06	3.145878
24	H	5.266367	1E-07	2.106533
25	H	5.488115	-8.9E-06	-0.37121
26	H	3.461916	-1.2E-05	-1.79673

2 (S_1): *E*(B3LYP/6-31G+(d,p)) = -3568.980284 hartree

Number	Atom	X	Y	Z
1	As	0.553409	0.000156	-1.40472
2	S	-2.78197	-1.88905	0.877292
3	S	-2.7819	1.888976	0.877725
4	C	-0.61278	-1.30423	-0.56541
5	C	-1.66331	-0.69131	0.226945

6	C	-1.6633	0.691342	0.227081
7	C	-0.6128	1.304389	-0.56521
8	C	-0.78654	-2.69291	-0.65096
9	C	-1.87327	-3.15964	0.071031
10	C	-1.87322	3.159705	0.071654
11	C	-0.78653	2.693084	-0.65048
12	C	2.108811	-5.5E-05	-0.11351
13	C	1.955169	-0.00077	1.277553
14	C	3.071958	-0.00087	2.116567
15	C	4.358594	-0.00025	1.565531
16	C	4.521879	0.000445	0.177453
17	C	3.39755	0.000541	-0.65554
18	H	-0.13721	-3.36036	-1.20687
19	H	-2.19936	-4.18626	0.177947
20	H	-2.19928	4.186302	0.178767
21	H	-0.13721	3.360624	-1.20629
22	H	0.960159	-0.00127	1.715027
23	H	2.942412	-0.00142	3.195772
24	H	5.229052	-0.00033	2.215675
25	H	5.519461	0.000901	-0.25431
26	H	3.528005	0.00108	-1.7366

3 (S_0): *E*(B3LYP/def2svp) = -3907.084005 hartree

Number	Atom	X	Y	Z
1	As	-0.93003	-0.02607	1.665337
2	S	-3.53033	1.921995	-1.30313
3	S	-3.55552	-1.85913	-1.35414
4	C	-1.80524	1.328112	0.539149
5	C	-2.66077	0.736405	-0.38171
6	C	-2.67051	-0.71048	-0.40116
7	C	-1.82327	-1.33811	0.50337
8	C	-1.85975	2.7507	0.502846
9	C	-2.73979	3.213785	-0.44684
10	C	-2.78255	-3.18389	-0.53299

11	C	-1.89675	-2.75831	0.428839
12	C	0.883052	-0.02793	0.858003
13	C	1.108189	0.00616	-0.52703
14	C	2.40781	0.001411	-1.03101
15	C	3.501029	-0.0361	-0.1531
16	C	3.28715	-0.07327	1.226888
17	C	1.980652	-0.06873	1.727476
18	H	-1.27467	3.413009	1.142991
19	H	-2.97597	4.246916	-0.69863
20	H	-3.03241	-4.20663	-0.81246
21	H	-1.32083	-3.44537	1.050953
22	H	0.262577	0.033533	-1.21832
23	H	2.57734	0.019869	-2.10971
24	H	4.137853	-0.11135	1.909691
25	H	1.822665	-0.09976	2.809236
26	C	4.903451	0.011368	-0.70772
27	F	5.009334	-0.68567	-1.85345
28	F	5.28297	1.274435	-0.98437
29	F	5.804569	-0.48903	0.155179

4 (S_0): *E*(B3LYP/def2svp) = -3609.585632 hartree

Number	Atom	X	Y	Z
1	As	0.073905	-1.4E-05	1.526014
2	S	-2.96888	1.890554	-1.03546
3	S	-2.96917	-1.89036	-1.03524
4	C	-0.97574	1.332638	0.528359
5	C	-1.95763	0.723455	-0.24239
6	C	-1.95771	-0.72333	-0.24235
7	C	-0.97588	-1.33258	0.528425
8	C	-1.04756	2.754257	0.481308
9	C	-2.06657	3.199333	-0.32765
10	C	-2.06701	-3.19921	-0.32735
11	C	-1.0479	-2.75419	0.481518
12	C	1.752723	-5.9E-05	0.481765

13	C	1.793478	-0.00047	-0.92192
14	C	3.015565	-0.00045	-1.59183
15	C	4.235167	-6.4E-05	-0.88863
16	C	4.185255	0.000422	0.511029
17	C	2.960206	0.000401	1.189968
18	H	-0.37574	3.428738	1.014848
19	H	-2.34657	4.227454	-0.55379
20	H	-2.34716	-4.22731	-0.55339
21	H	-0.37615	-3.42872	1.015087
22	H	0.86306	-0.00078	-1.49555
23	H	3.027034	-0.00074	-2.68627
24	H	5.117252	0.00083	1.083903
25	H	2.954059	0.000756	2.284128
26	C	5.548577	-0.00036	-1.63174
27	H	5.639519	0.885075	-2.28312
28	H	6.405316	-0.0002	-0.94193
29	H	5.639432	-0.88641	-2.28236

5 (S_0): *E*(B3LYP/def2svp) = -3684.735152 hartree

Number	Atom	X	Y	Z
1	As	-0.27021	-1.4E-05	1.546616
2	S	-3.24533	1.890428	-1.09449
3	S	-3.24558	-1.89021	-1.09437
4	C	-1.2935	1.332595	0.520953
5	C	-2.25516	0.723486	-0.27484
6	C	-2.25525	-0.72335	-0.2748
7	C	-1.29366	-1.33253	0.521018
8	C	-1.36401	2.754215	0.471422
9	C	-2.36157	3.199319	-0.36386
10	C	-2.36198	-3.19917	-0.36366
11	C	-1.36435	-2.75415	0.471576
12	C	1.436445	-9.5E-05	0.558687
13	C	1.525519	-0.00047	-0.84613
14	C	2.76141	-0.0005	-1.47977

15	C	3.950386	-0.00016	-0.72345
16	C	3.876145	0.00024	0.676442
17	C	2.62121	0.000257	1.301476
18	H	-0.70593	3.428783	1.021741
19	H	-2.63507	4.227409	-0.59794
20	H	-2.63563	-4.22724	-0.59767
21	H	-0.70635	-3.42876	1.021934
22	H	0.615078	-0.00074	-1.45087
23	H	2.842155	-0.00078	-2.56893
24	H	4.777722	0.000573	1.289454
25	H	2.580414	0.000546	2.394946
26	O	5.105419	-0.00025	-1.43271
27	C	6.338036	0.000093	-0.74838
28	H	6.457556	-0.89766	-0.11517
29	H	7.122787	-0.00017	-1.51677
30	H	6.4574	0.898374	-0.11591

6 (S_0): *E*(B3LYP/def2svp) = -3688.153685 hartree

Number	Atom	X	Y	Z
1	As	0.025059	-0.00282	1.281527
2	S	-3.40622	1.89283	-0.69575
3	S	-3.40953	-1.88584	-0.70207
4	C	-1.13734	1.332157	0.433993
5	C	-2.26082	0.723453	-0.11492
6	C	-2.26209	-0.72043	-0.11732
7	C	-1.1397	-1.33294	0.429582
8	C	-1.21328	2.754329	0.395494
9	C	-2.3722	3.200225	-0.19497
10	C	-2.37783	-3.19672	-0.20563
11	C	-1.21814	-2.75483	0.386345
12	C	1.721265	-0.00212	0.236369
13	C	1.819207	-0.0002	-1.17664
14	C	3.09412	-0.00034	-1.76674
15	C	4.270671	-0.00156	-1.01364

16	C	4.1505	-0.005	0.380782
17	C	2.904784	-0.00491	1.021918
18	H	-0.4448	3.428373	0.777677
19	H	-2.68669	4.228757	-0.36771
20	H	-2.69412	-4.22411	-0.38181
21	H	-0.45086	-3.4315	0.766287
22	H	3.162157	-5.5E-05	-2.85878
23	H	5.05697	-0.00845	0.994097
24	C	0.619687	0.000721	-2.09082
25	H	-0.01556	-0.8826	-1.92605
26	H	-0.01663	0.882619	-1.92273
27	H	0.93395	0.002905	-3.14441
28	C	2.892894	-0.00912	2.538407
29	H	2.379162	0.872764	2.95332
30	H	2.377844	-0.89249	2.948537
31	H	3.920738	-0.01094	2.929517
32	C	5.628802	0.011082	-1.67113
33	H	6.15699	0.95982	-1.47444
34	H	6.269728	-0.79779	-1.28349
35	H	5.553005	-0.10889	-2.76189

6 (S_0): *E*(B3LYP/6-31G+(d,p)) = -3687.058323 hartree

Number	Atom	X	Y	Z
1	As	0.02894	-0.00036	1.253596
2	S	-3.41053	1.89016	-0.68283
3	S	-3.41089	-1.88958	-0.68347
4	C	-1.12522	1.330346	0.4149
5	C	-2.25027	0.721122	-0.12238
6	C	-2.25037	-0.72094	-0.1227
7	C	-1.12538	-1.33055	0.414271
8	C	-1.20596	2.751016	0.389567
9	C	-2.36881	3.19993	-0.18472
10	C	-2.36928	-3.19971	-0.18606
11	C	-1.20636	-2.7512	0.388404

12	C	1.711507	-0.00019	0.230999
13	C	1.820948	0.000314	-1.17735
14	C	3.098029	0.000514	-1.75821
15	C	4.26522	0.00025	-0.99274
16	C	4.135363	-0.00029	0.399174
17	C	2.884015	-0.00047	1.025681
18	H	-0.43794	3.417238	0.765999
19	H	-2.68594	4.221208	-0.34698
20	H	-2.68653	-4.22087	-0.34879
21	H	-0.4384	-3.41769	0.764501
22	H	3.177119	0.000861	-2.84298
23	H	5.031562	-0.00057	1.016047
24	C	0.627326	0.000661	-2.10147
25	H	-0.00601	-0.87713	-1.94376
26	H	-0.00547	0.878855	-1.94374
27	H	0.953439	0.000573	-3.14502
28	C	2.856613	-0.00097	2.543669
29	H	2.342831	0.877652	2.947532
30	H	2.34123	-0.87885	2.947027
31	H	3.876469	-0.00199	2.938221
32	C	5.628643	0.000448	-1.64248
33	H	6.208797	0.88256	-1.34694
34	H	6.209173	-0.88134	-1.34673
35	H	5.551282	0.000307	-2.73339

6 (S_1): *E*(B3LYP/6-31G+(d,p)) = -3686.934836 hartree

Number	Atom	X	Y	Z
1	As	-0.03665	0.003602	1.329263
2	S	3.484625	-1.81969	-0.72616
3	S	3.312118	1.957516	-0.88225
4	C	1.212187	-1.27835	0.570708
5	C	2.287836	-0.64659	-0.16968
6	C	2.228671	0.732009	-0.22065
7	C	1.0774	1.323111	0.436805

8	C	1.418463	-2.65966	0.687455
9	C	2.564386	-3.10337	0.04386
10	C	2.236218	3.213714	-0.28599
11	C	1.131758	2.723705	0.393096
12	C	-1.74651	-0.02	0.226056
13	C	-1.82484	-0.18059	-1.17279
14	C	-3.08655	-0.22276	-1.78502
15	C	-4.27099	-0.11036	-1.05294
16	C	-4.17205	0.051163	0.332237
17	C	-2.93396	0.09511	0.985586
18	H	0.754958	-3.33836	1.21233
19	H	2.934577	-4.1193	-0.00945
20	H	2.487825	4.250442	-0.46962
21	H	0.384383	3.380711	0.824611
22	H	-3.14178	-0.34545	-2.86511
23	H	-5.08228	0.147791	0.921687
24	C	-0.60548	-0.30961	-2.05744
25	H	0.053752	0.559516	-1.97338
26	H	-0.00575	-1.18656	-1.79348
27	H	-0.90272	-0.40763	-3.10541
28	C	-2.93937	0.274136	2.494201
29	H	-2.46134	-0.56507	3.010125
30	H	-2.40563	1.178105	2.806192
31	H	-3.96725	0.352307	2.860159
32	C	-5.61973	-0.16391	-1.73103
33	H	-6.18975	-1.04497	-1.412
34	H	-6.22409	0.717009	-1.48539
35	H	-5.51805	-0.20914	-2.81921

7 (S_0): *E*(B3LYP/def2svp) = -3923.856060 hartree

Number	Atom	X	Y	Z
1	As	-0.76172	1.375269	0.000219
2	S	-4.14632	-0.67527	-1.88983
3	S	-4.14602	-0.67617	1.889858

4	C	-1.88974	0.482941	-1.33308
5	C	-3.00694	-0.07883	-0.72184
6	C	-3.00683	-0.07914	0.721968
7	C	-1.88956	0.48238	1.333291
8	C	-1.96913	0.444768	-2.75535
9	C	-3.1212	-0.16059	-3.19856
10	C	-3.12065	-0.16213	3.198663
11	C	-1.96868	0.44347	2.75555
12	C	1.012903	0.450679	1.25E-05
13	C	1.203037	-0.9588	-0.00024
14	C	2.508993	-1.46625	-0.00027
15	C	3.640493	-0.64298	-4.9E-05
16	C	3.430471	0.735951	0.000207
17	C	2.147241	1.308097	0.000243
18	H	-1.20779	0.838499	-3.43084
19	H	-3.43423	-0.33938	-4.22652
20	H	-3.4335	-0.34146	4.226586
21	H	-1.20724	0.836883	3.431111
22	H	2.64339	-2.55098	-0.00047
23	H	4.302766	1.395519	0.000375
24	C	0.062405	-1.97405	-0.00053
25	H	-0.87981	-1.42098	-0.00061
26	C	2.079903	2.839703	0.000491
27	H	1.021996	3.135785	0.000638
28	C	5.04991	-1.22071	-0.0001
29	H	5.744537	-0.36262	0.000353
30	C	2.703913	3.44179	-1.27089
31	H	2.582711	4.537521	-1.27838
32	H	3.782807	3.227379	-1.34142
33	H	2.225613	3.042136	-2.17914
34	C	2.704162	3.441418	1.271923
35	H	2.226098	3.041438	2.180151
36	H	3.783089	3.227071	1.34215
37	H	2.582871	4.537138	1.279795
38	C	5.335217	-2.04132	1.269693

39	H	6.380152	-2.39245	1.280679
40	H	5.166724	-1.44371	2.179206
41	H	4.685927	-2.93024	1.328976
42	C	5.335504	-2.04021	-1.27056
43	H	4.686175	-2.92904	-1.33077
44	H	5.167256	-1.44179	-2.17958
45	H	6.380426	-2.39138	-1.2816
46	C	0.066874	-2.84176	-1.27164
47	H	0.02455	-2.21972	-2.17902
48	H	0.967838	-3.47391	-1.33662
49	H	-0.80915	-3.51077	-1.2813
50	C	0.066541	-2.8421	1.270354
51	H	0.023985	-2.22029	2.177881
52	H	-0.80949	-3.51111	1.279618
53	H	0.967501	-3.47425	1.335366