Supporting Information

Experimental Study on Arsoles; Structural Variation, Optical and Electronic Properties, and Emission Behavior

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Contents:

1. NMR spectra

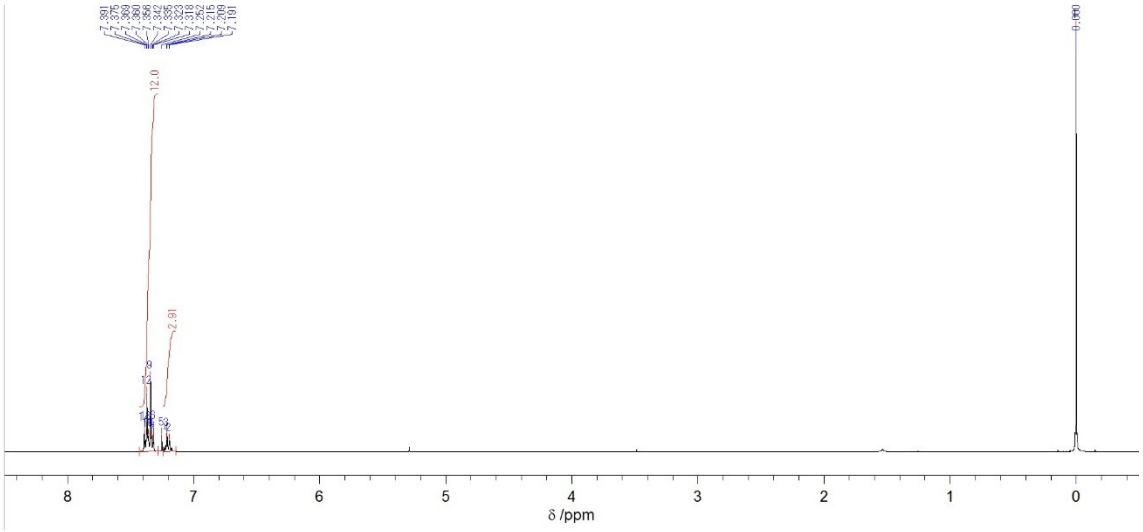


Figure S1. ^{1}H NMR spectrum (400 MHz) of **5b** in $CDCl_3$.

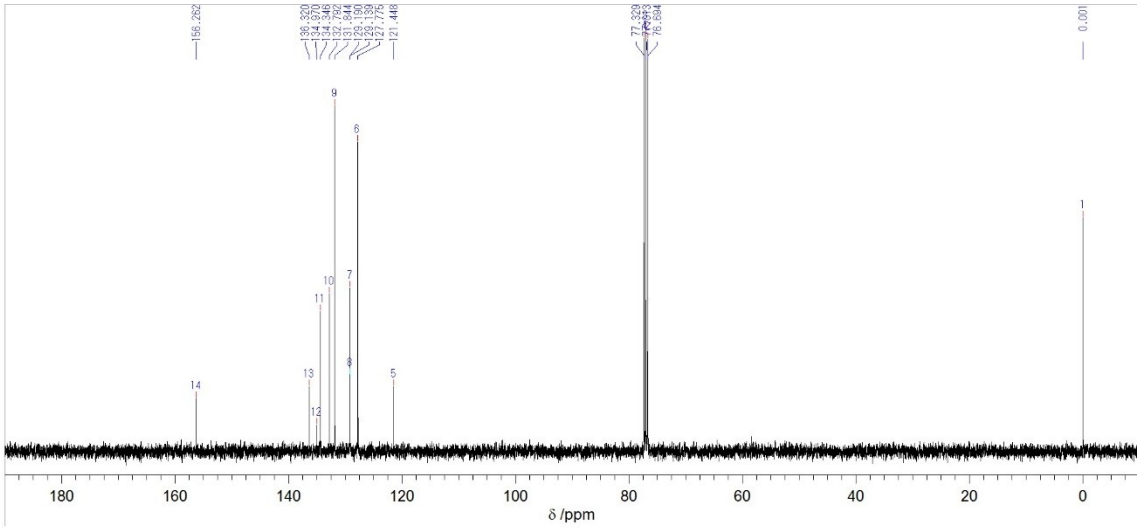


Figure S2. ^{13}C NMR spectrum (100 MHz) of **5b** in $CDCl_3$.

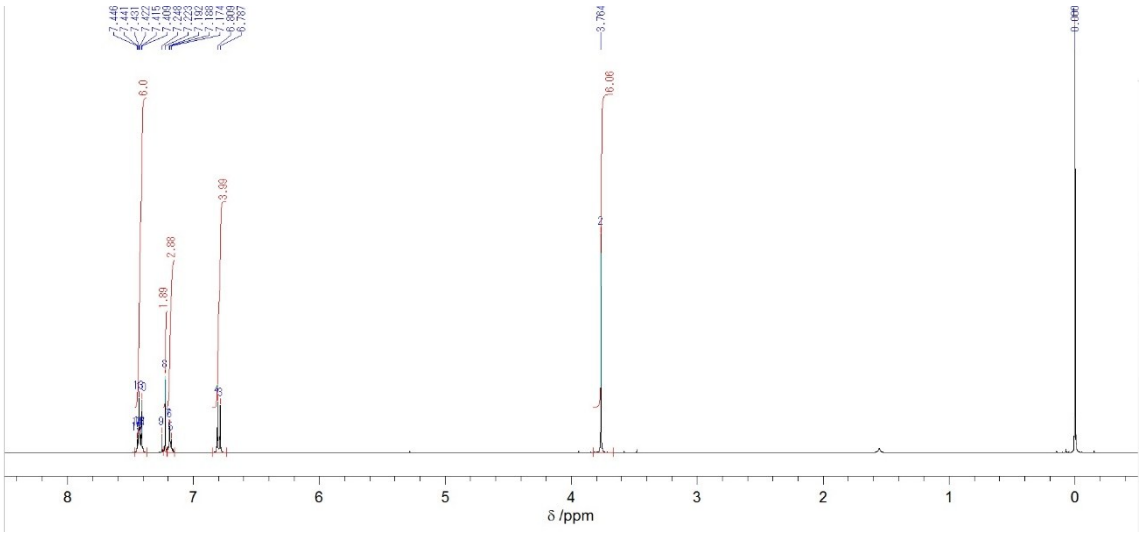


Figure S3. ^{1}H NMR spectrum (400 MHz) of **5d** in $CDCl_3$.

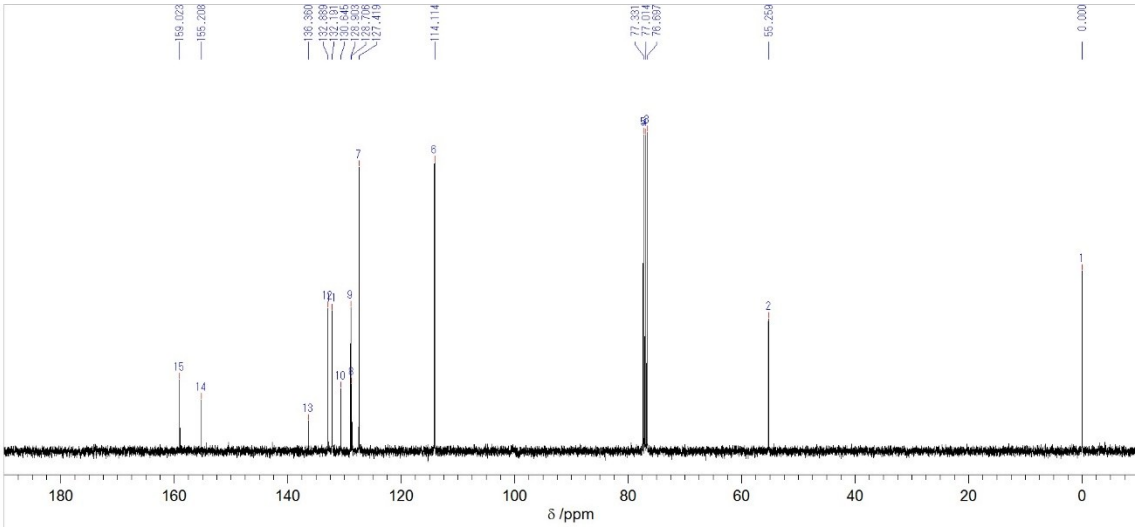


Figure S4. ^{13}C NMR spectrum (100 MHz) of **5d** in $CDCl_3$.

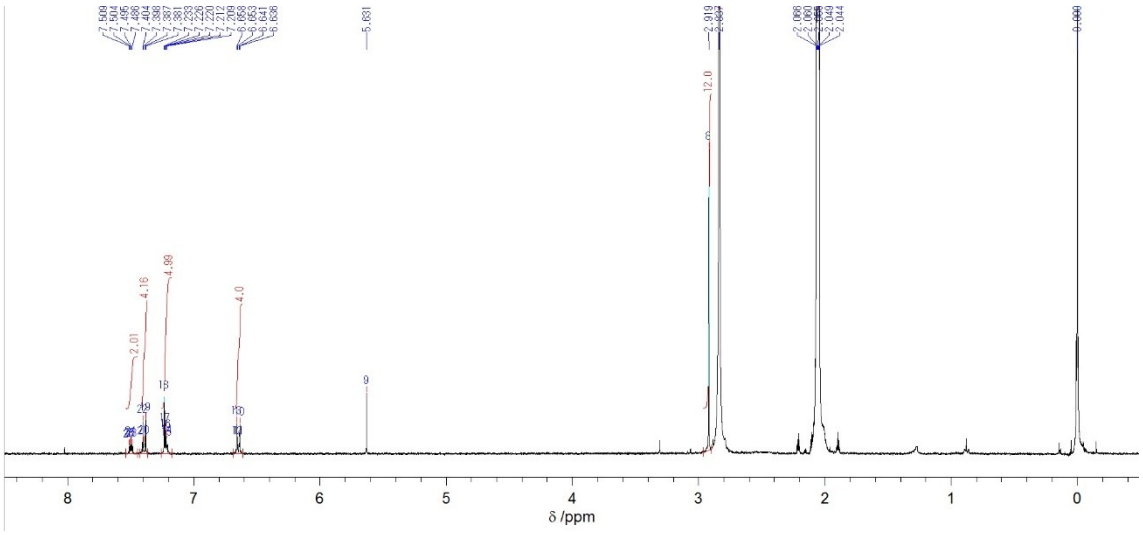


Figure S5. ^{1}H NMR spectrum (400 MHz) of **5e** in acetone-d_6.

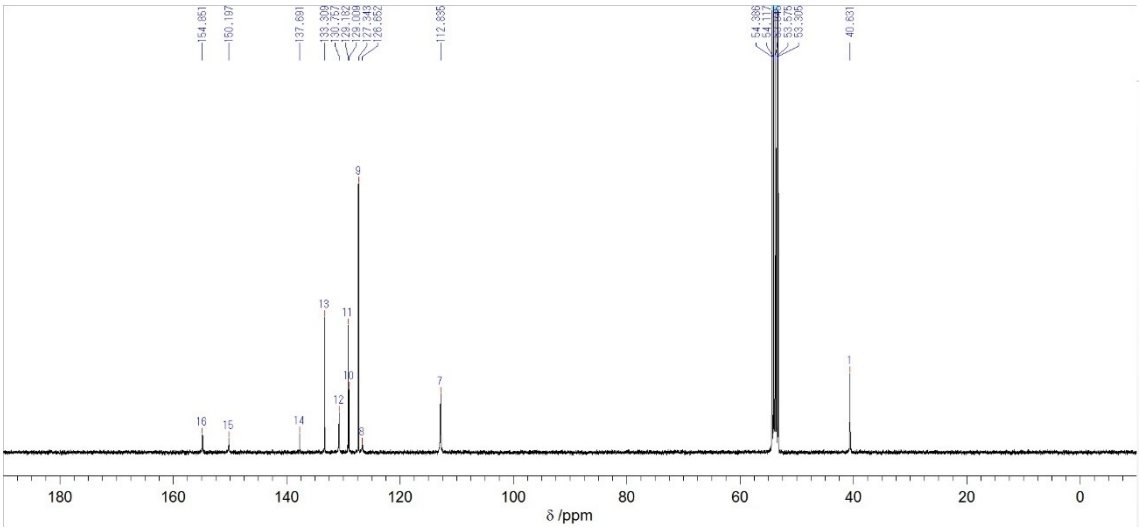


Figure S6. ^{13}C NMR spectrum (100 MHz) of **5e** in CD_2Cl_2.

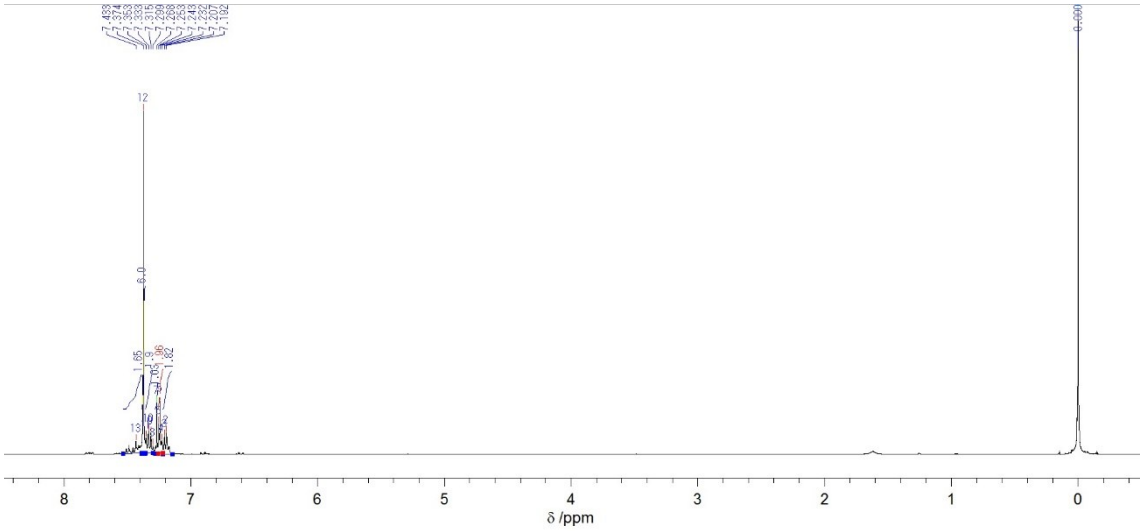


Figure S7. ^{1}H NMR spectrum (400 MHz) of **6b** in $CDCl_3$.

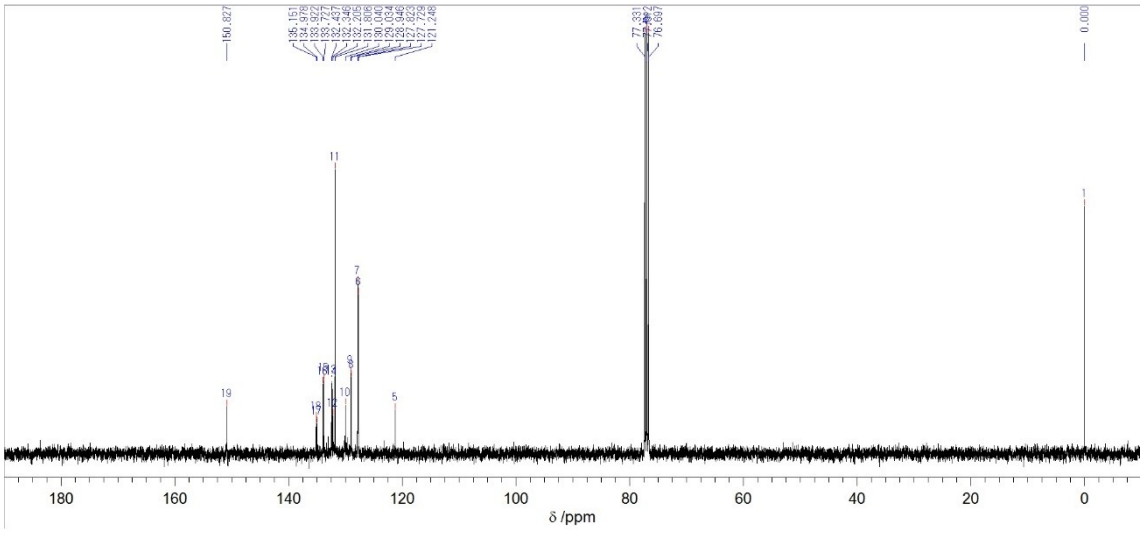


Figure S8. ^{13}C NMR spectrum (100 MHz) of **6b** in $CDCl_3$.

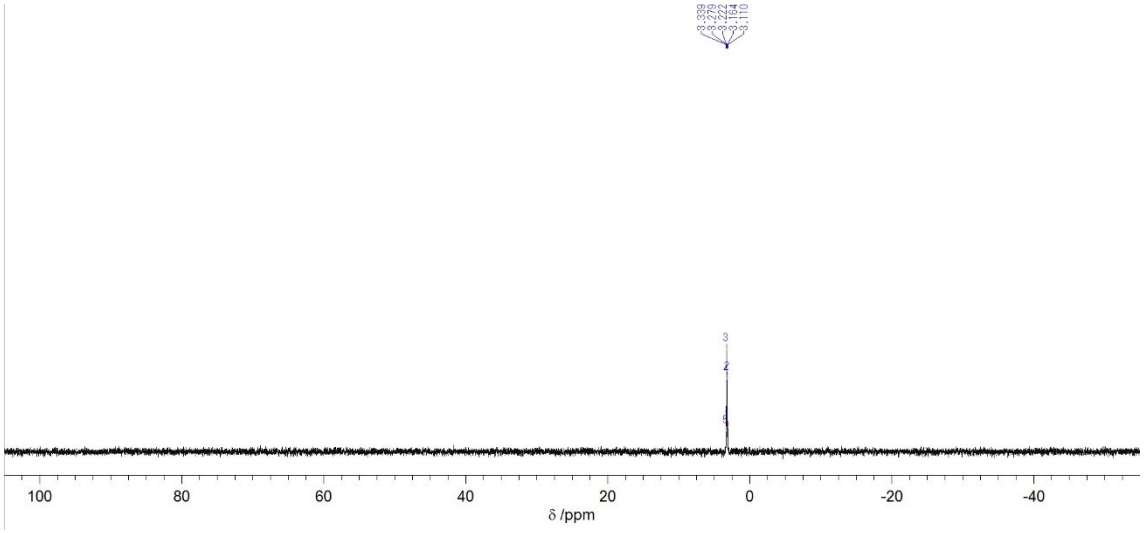


Figure S9. ^{31}P NMR spectrum (161.5 MHz) of **6b** in $CDCl_3$.

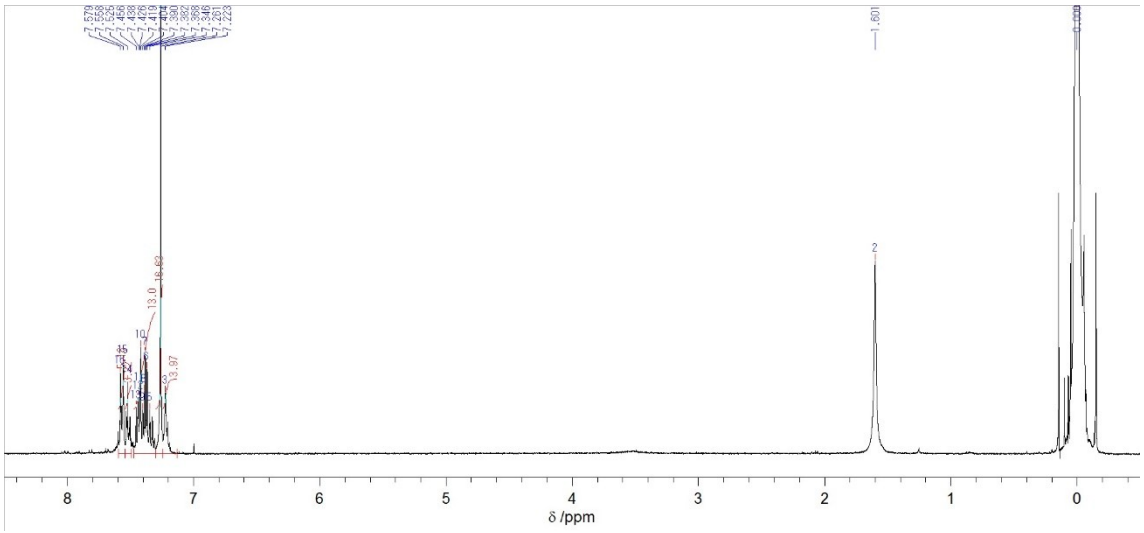


Figure S10. ^{1}H NMR spectrum (400 MHz) of **7a** in $CDCl_3$.

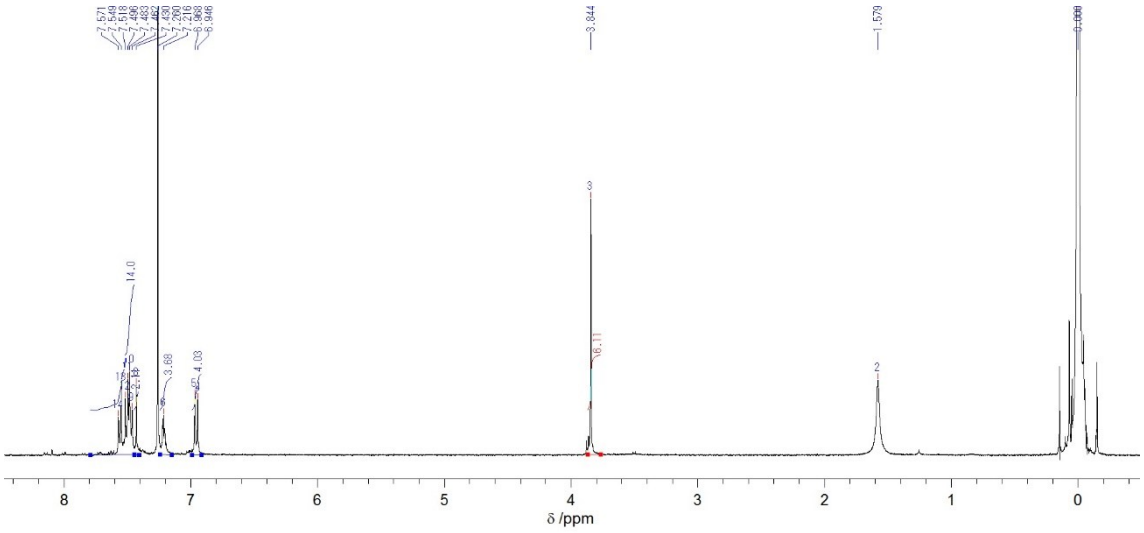


Figure S11. ^{1}H NMR spectrum (400 MHz) of **7b** in $CDCl_3$.

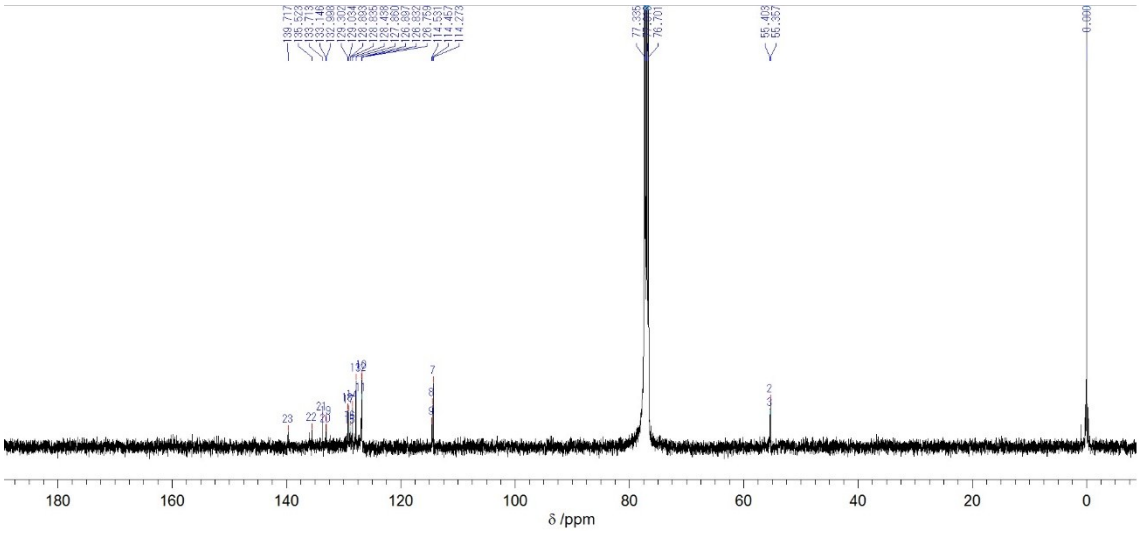


Figure S12. ^{13}C NMR spectrum (100 MHz) of **7b** in $CDCl_3$.

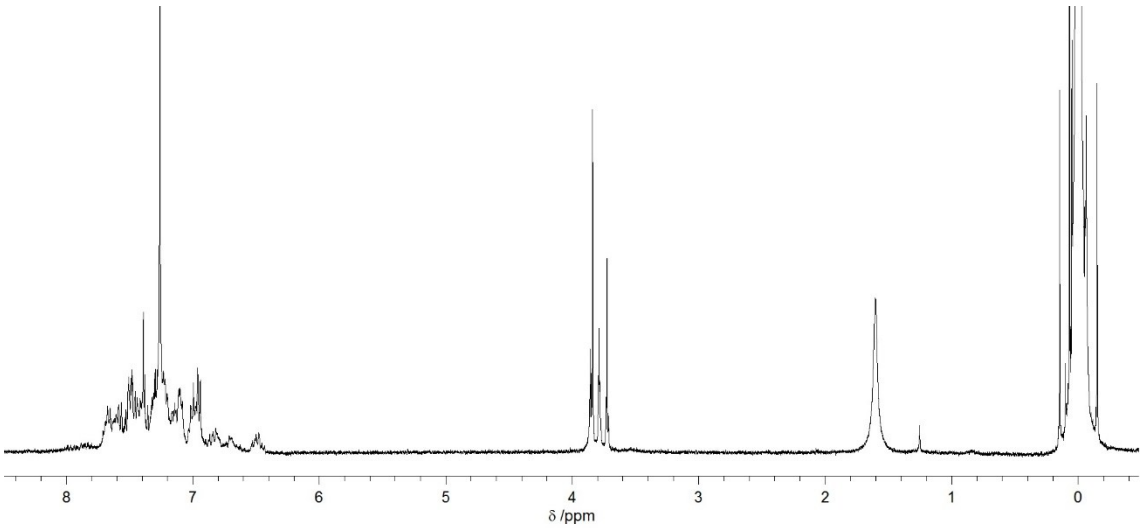


Figure S13. ^{1}H NMR spectrum (400 MHz) in $CDCl_3$ measured after employment of Suzuki-Miyaura coupling reaction with **6b** and 4-methoxyphenylboronic acid.

2. Crystallographic data

Table S1. Crystallographic Data.

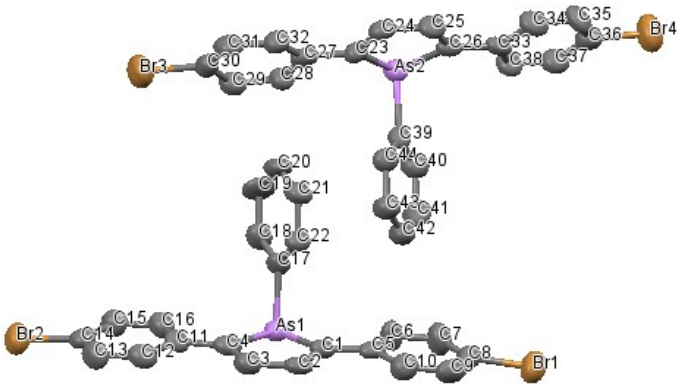
	5b	**5d**	**5e**
Crystal data			
Empirical formula	$C_{22}H_{15}AsBr_2$	$C_{22}H_{15}AsBr_2$	$C_{26}H_{27}AsN_2$
Formula weight	514.09	514.09	442.43
Crystal Dimension [mm^3]	0.143 × 0.130 × 0.040	0.200 × 0.200 × 0.200	0.230 × 0.190 × 0.030
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1/n$
a [Å]	14.854(9)	14.854(9)	16.513(9)
b [Å]	5.972(3)	5.972(3)	6.169(3)
c [Å]	21.848(13)	21.848(13)	22.038(13)
α [°]	-	-	-
β [°]	98.216(7)	98.216(7)	105.993(6)
γ [°]	-	-	-
Volume [$Å^3$]	1918(2)	1918(2)	2158(2)
D_{calcd} [$g \cdot cm^{-3}$]	1.780	1.780	1.362
Z	4	4	4
F(000)	1000.00	1000.00	920.00
Data Collection			
Temperature [°C]	23.0	23.0	23.0
$2\theta_{max}$ [°]	55.1	55.0	55.1
Tmin/Tmax	0.605 / 0.788	0.624 / 0.708	0.833 / 0.953
Refinement			
No. of Observed Data	8824	4562	4948
No. of Parameters	451	244	262
R1[a], wR2[b]	0.0620, 0.0890	0.0440, 0.1158	0.0541, 0.1224
Goodness of Fit Indictor	1.000	1.083	1.065

[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 #1449110 (**5b**), 1449111 (**5d**), and 1449112 (**5e**).

The crystallographic data of **5a**, **5c**, and **6a** have been reported in the previous literature.[1]

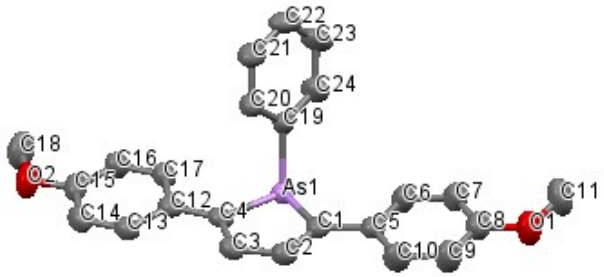
Table S2. ORTEP drawing (ellipsoids at 50% probability), selected angles (deg) and distance (Å) of **5b**.



interplanar angles (°)	As(1)C(1)C(2)C(3)C(4)-C(5)C(6)C(7)C(8)C(9)C(10)	7.03
	As(1)C(1)C(2)C(3)C(4)-C(11)C(12)C(13)C(14)C(15)C(16)	5.38
	As(2)C(23)C(24)C(25)C(26)-C(27)C(28)C(29)C(30)C(31)C(32)	2.75
	As(2)C(23)C(24)C(25)C(26)-C(33)C(34)C(35)C(36)C(37)C(38)	6.98
distance (Å)	As(1)-C(1)	1.95(1)
	As(1)-C(4)	1.95(1)
	As(1)-C(17)	1.944(8)
	C(1)-C(2)	1.36(1)
	C(2)-C(3)	1.44(1)
	C(3)-C(4)	1.35(1)
	C(1)-C(5)	1.46(2)
	C(4)-C(11)	1.47(2)
	As(2)-C(23)	1.94(1)
	As(2)-C(26)	1.96(1)
	As(2)-C(39)	1.96(1)
	C(23)-C(24)	1.34(1)
	C(24)-C(25)	1.44(2)
	C(25)-C(26)	1.37(1)
	C(23)-C(27)	1.47(2)
	C(26)-C(33)	1.49(2)
angle (°)	C(1)-As(1)-C(4)	87.3(4)

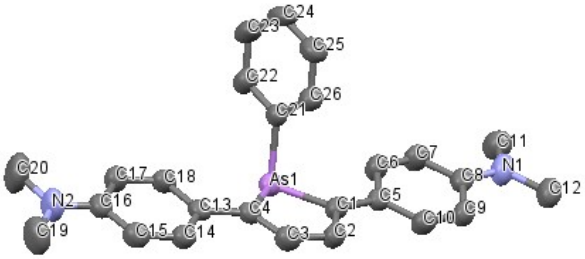
C(1)-As(1)-C(17)	100.6(4)
C(4)-As(1)-C(17)	100.1(4)
As(1)-C(1)-C(2)	108.6(7)
C(1)-C(2)-C(3)	117.6(9)
C(2)-C(3)-C(4)	117.3(9)
As(1)-C(4)-C(3)	108.9(7)
As(1)-C(1)-C(5)	122.3(7)
As(1)-C(4)-C(11)	122.9(8)
C(2)-C(1)-C(5)	128.5(9)
C(3)-C(4)-C(11)	128(1)
C(23)-As(2)-C(26)	87.2(4)
C(23)-As(2)-C(39)	100.4(4)
C(26)-As(2)-C(39)	102.6(4)
As(2)-C(23)-C(24)	109.2(7)
C(23)-C(24)-C(25)	118.8(9)
C(24)-C(25)-C(26)	116.2(9)
As(2)-C(26)-C(25)	108.3(7)
As(2)-C(23)-C(27)	123.7(7)
As(2)-C(26)-C(33)	122.9(7)
C(24)-C(23)-C(27)	127(1)
C(25)-C(26)-C(33)	128.1(9)

Table S3. ORTEP drawing (ellipsoids at 50% probability), selected angles (deg) and distance (Å) of **5d**.



interplanar angles (°)	As(1)C(1)C(2)C(3)C(4)-C(5)C(6)C(7)C(8)C(9)C(10)	3.84
	As(1)C(1)C(2)C(3)C(4)-C(12)C(13)C(14)C(15)C(16)C(17)	2.69
distance (Å)	As(1)-C(1)	1.949(6)
	As(1)-C(4)	1.942(5)
	As(1)-C(19)	1.960(5)
	C(1)-C(2)	1.346(8)
	C(2)-C(3)	1.447(8)
	C(3)-C(4)	1.349(9)
	C(1)-C(5)	1.469(8)
	C(4)-C(12)	1.470(8)
angle (°)	C(1)-As(1)-C(4)	87.2(3)
	C(1)-As(1)-C(19)	102.1(3)
	C(4)-As(1)-C(19)	101.6(3)
	As(1)-C(1)-C(2)	109.0(4)
	C(1)-C(2)-C(3)	117.1(5)
	C(2)-C(3)-C(4)	117.6(5)
	As(1)-C(4)-C(3)	108.8(4)
	As(1)-C(1)-C(5)	123.9(4)
	As(1)-C(4)-C(12)	123.6(4)
	C(2)-C(1)-C(5)	126.7(6)
	C(3)-C(4)-C(12)	127.4(5)

Table S4. ORTEP drawing (ellipsoids at 50% probability), selected angles (deg) and distance (Å) of **5e**.



interplanar angles (°)	As(1)C(1)C(2)C(3)C(4)-C(5)C(6)C(7)C(8)C(9)C(10)	7.36
	As(1)C(1)C(2)C(3)C(4)-C(13)C(14)C(15)C(16)C(17)C(18)	6.19
distance (Å)	As(1)-C(1)	1.948(3)
	As(1)-C(4)	1.950(3)
	As(1)-C(21)	1.949(4)
	C(1)-C(2)	1.341(5)
	C(2)-C(3)	1.446(4)
	C(3)-C(4)	1.347(5)
	C(1)-C(5)	1.460(4)
	C(4)-C(13)	1.460(5)
angle (°)	C(1)-As(1)-C(4)	87.4(1)
	C(1)-As(1)-C(21)	100.8(1)
	C(4)-As(1)-C(21)	100.4(1)
	As(1)-C(1)-C(2)	108.4(3)
	C(1)-C(2)-C(3)	117.8(3)
	C(2)-C(3)-C(4)	117.5(3)
	As(1)-C(4)-C(3)	108.3(3)
	As(1)-C(1)-C(5)	123.4(2)
	As(1)-C(4)-C(13)	123.4(3)
	C(2)-C(1)-C(5)	128.0(3)
	C(3)-C(4)-C(13)	128.0(3)

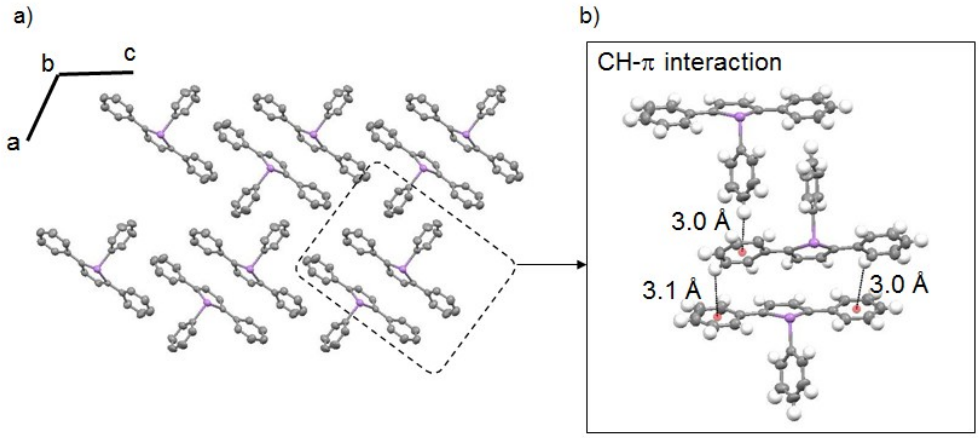


Figure S14 (a) Packing structure of **5a**. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.

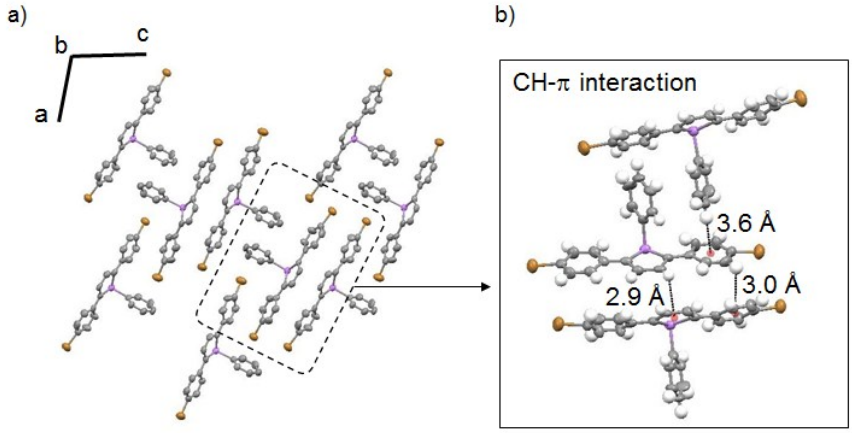


Figure S15 (a) Packing structure of **5b**. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.

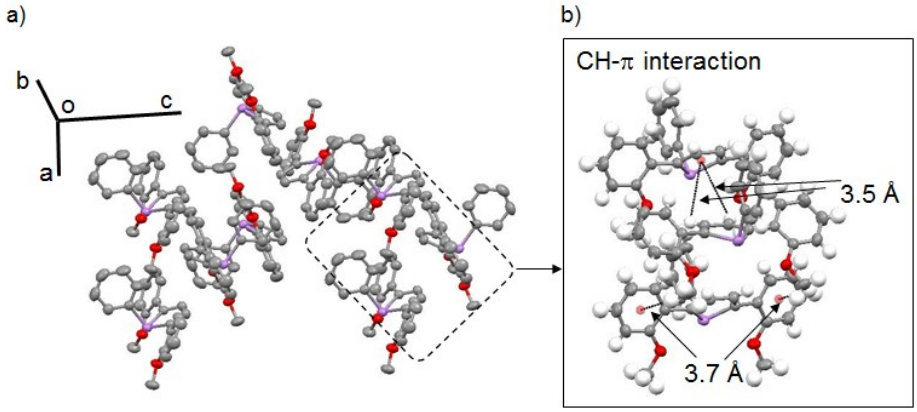


Figure S16 (a) Packing structure of **5c**. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.

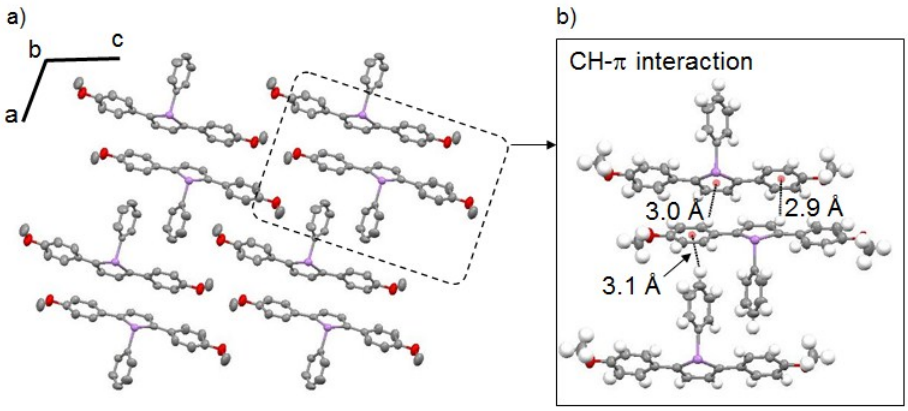


Figure S17 (a) Packing structure of **5d**. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.

3. Optical properties

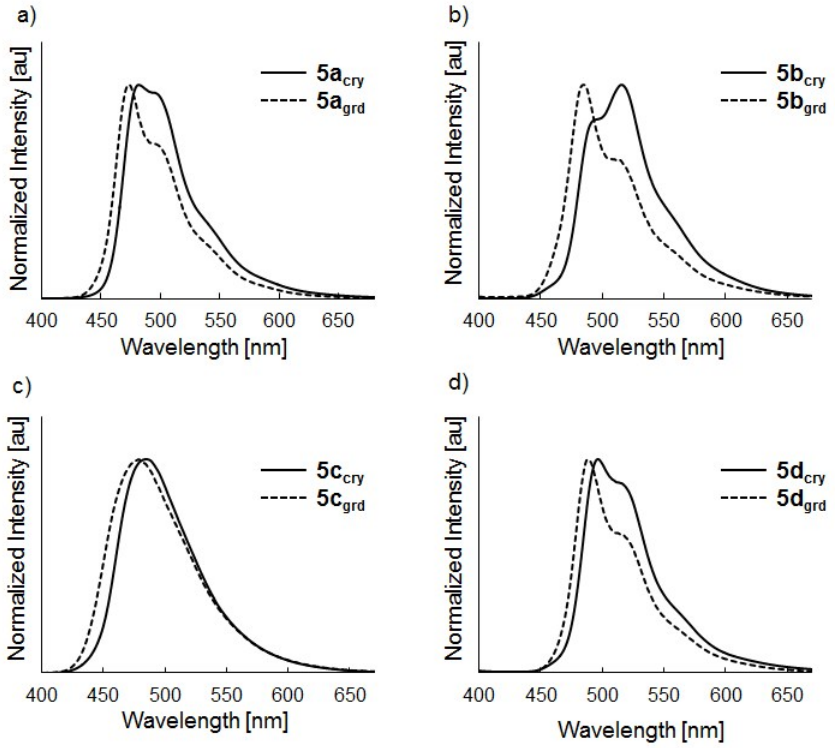


Figure S18. PL spectra of $\mathbf{5}_{\mathbf{cry}}$ and $\mathbf{5}_{\mathbf{grd}}$ (excited at 350 nm).

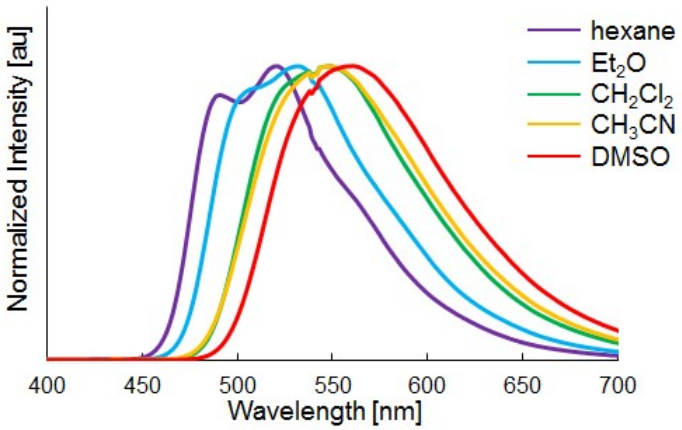


Figure S19. PL spectra of **5e** in various solvents.

4. CV data

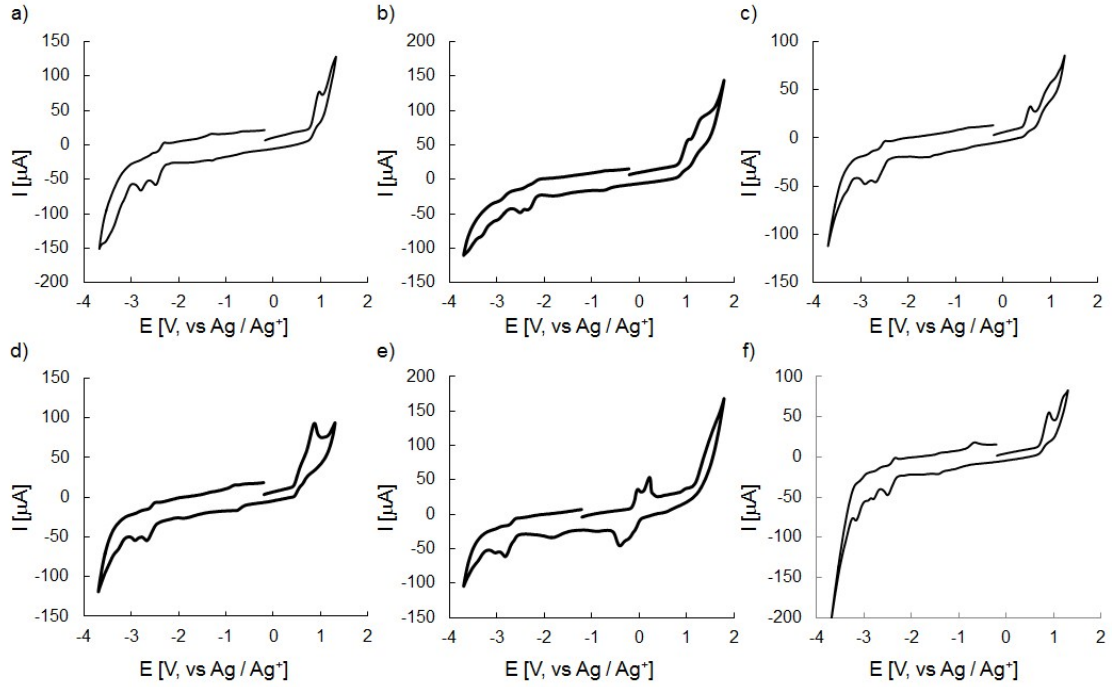


Figure S20. Cyclic voltammograms of (a) **5a** (b) **5b**, (c) **5c**, (d) **5d**, (e) **5e** and (f) **6a** measured in THF solutions (c = 0.1 M) at the scan rate of 100 mV/s under N_2. The working electrode was a glassy carbon, the counter electrode was a platinum wire, and the reference electrode was an Ag^0 / Ag^+.

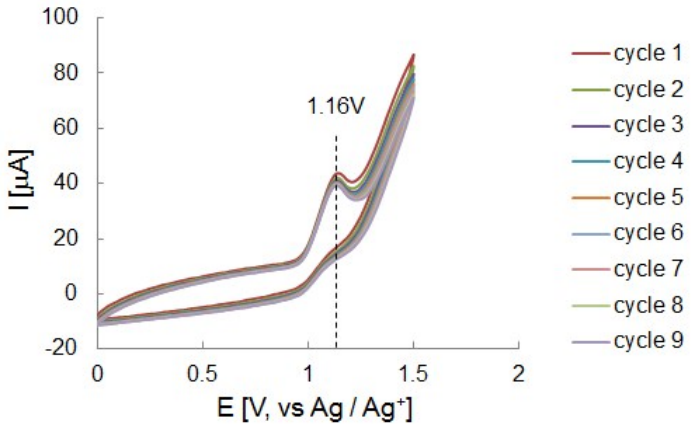


Figure S21. Cyclic voltammograms of **5a** measured in THF solutions (c = 0.1 M) at the scan rate of 100 mV/s under N_2. The working electrode was a glassy carbon, the counter electrode was a platinum wire, and the reference electrode was an Ag^0 / Ag^+.

5. XRD patterns

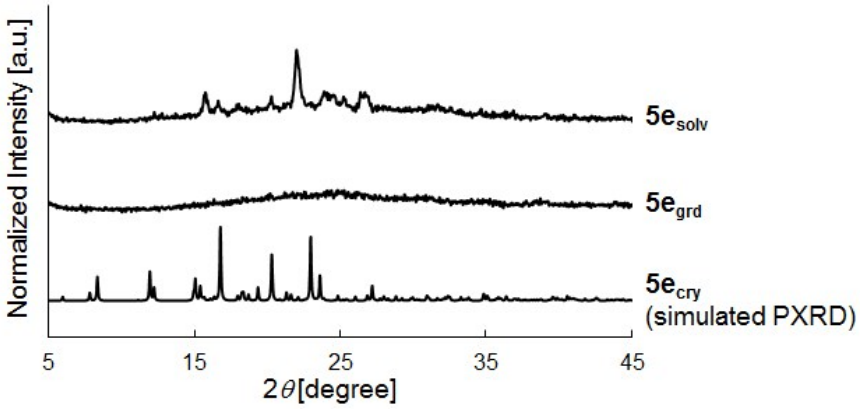


Figure S22. XRD patterns of **5e$_{grd}$** and **5e$_{solv}$**, and simulated PXRD of **5e$_{cry}$**.

6. Theoretical calculations

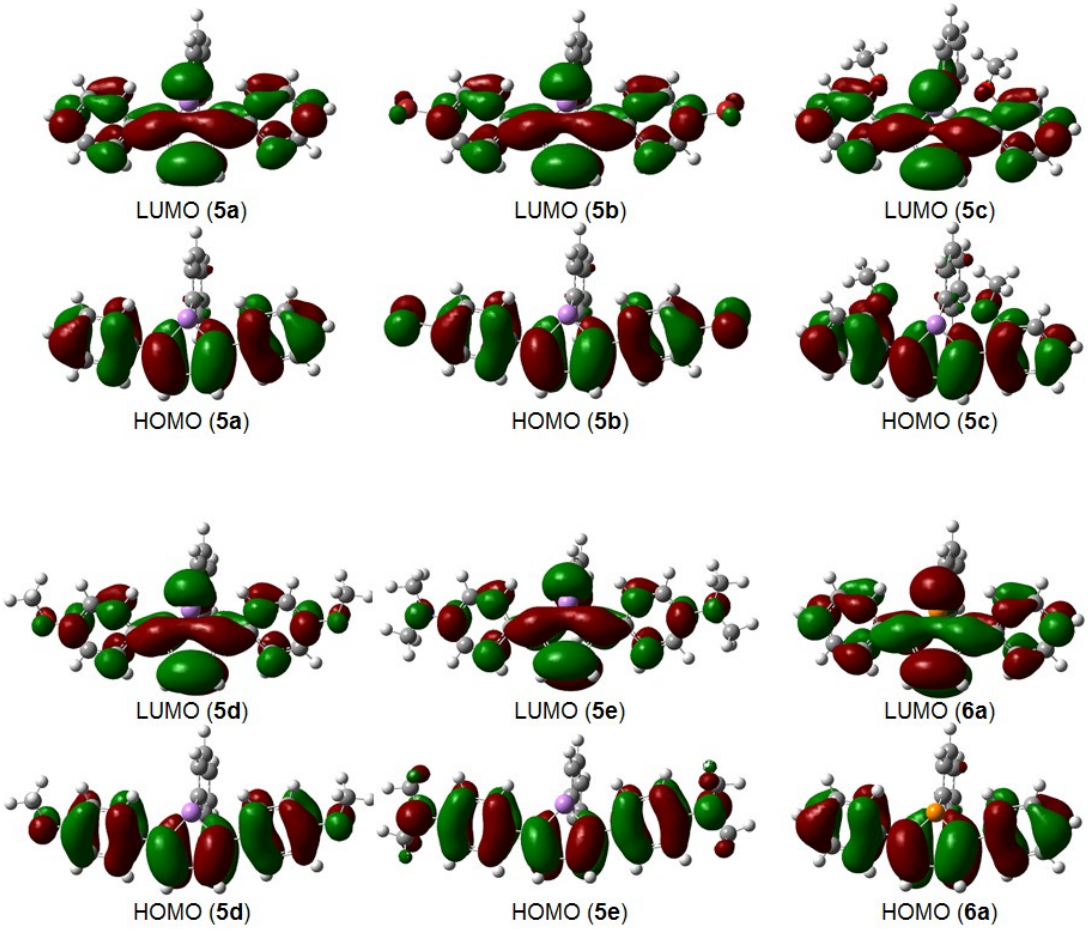


Figure S23. Molecular orbitals of the HOMO and LUMO. The geometries were optimized by DFT calculation at the B3LYP/6-31G+(d) level of theory; calculated with the Gaussian 09 suit program.[2]

Table S5. Calculated energy levels, HOMO-LUMO transition energies, and torsion angles.[a]

	Optimized geometry[b]				Single crystal XRD[c]		
	HOMO [eV][d]	LUMO [eV][d]	E_{ex} [nm][e]	torsion angle [°][f]	HOMO [eV][d]	LUMO [eV][d]	torsion angle [°][f]
5a	-5.51	-2.00	397.5	26.1	-5.49	-1.96	3.6
5b	-5.72	-2.32	410.9	25.2	-5.74, -5.47[g]	-2.34, -2.18[g]	1.9, 3.6[g]
5c	-5.05	-1.78	429.7	18.5	-5.25	-1.39	42.1
5d	-5.09	-1.74	416.7	25.2	-5.09	-1.71	0.4
5e	-4.55	-1.48	454.0	23.7	-4.31	-1.25	2.9
6a	-5.52	-1.92	388.8	30.8	-5.45	-1.96	0.5

[a]All calculation were performed at the B3LYP/6-31G+(d) level of theory with the Gaussian 09 suit program. [b]Structures optimized by DFT calculation [c]Structures obtained by single crystal X-ray diffraction. [d]DFT calculation. [e]TD-DFT calculation. [f]Torsion angles of the cyclopentadiene and aryl groups. [g]**5b** adopt two different conformations in the single crystal.

Table S6. Atom coordinates and absolute energy levels for **5a** optimized in the S_0 state.

5a (S_0 state): E(RB3LYP) = -3082.40024809 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.72572	-2.0601	1.026729
2	6	0	0.724739	-2.06061	1.026328
3	6	0	-1.34727	-1.16683	0.206008
4	6	0	1.346589	-1.1679	0.205249
5	33	0	-0.00031	-0.25437	-0.87536
6	1	0	-1.27258	-2.7738	1.641359
7	1	0	1.271781	-2.77443	1.640687
8	6	0	-2.78854	-0.97638	0.043082
9	6	0	2.787918	-0.97747	0.042504
10	6	0	0.000525	1.523448	-0.04778
11	6	0	0.000974	1.714166	1.339331
12	6	0	0.000645	2.64176	-0.8889
13	6	0	0.001269	3.935141	-0.35448
14	6	0	0.001635	3.001945	1.877172
15	6	0	0.001802	4.116102	1.029793
16	1	0	0.000247	2.507518	-1.96829
17	1	0	0.001274	4.795672	-1.01907
18	1	0	0.00085	0.853189	2.002815
19	1	0	0.001918	3.137995	2.956049
20	1	0	0.00244	5.119192	1.449029
21	6	0	-3.69056	-1.31528	1.073864
22	6	0	-3.32538	-0.43956	-1.14463
23	6	0	-4.70266	-0.28362	-1.31005
24	6	0	-5.06681	-1.16643	0.907471
25	6	0	-5.58125	-0.64126	-0.2835
26	1	0	-2.65432	-0.18157	-1.96033
27	1	0	-5.09072	0.121673	-2.24061
28	1	0	-3.30449	-1.69373	2.01708
29	1	0	-5.74067	-1.44018	1.714966
30	1	0	-6.6545	-0.51655	-0.41048
31	6	0	3.689873	-1.31744	1.073212
32	6	0	3.324652	-0.43957	-1.14438
33	6	0	4.702255	-0.28352	-1.30983
34	6	0	5.06608	-1.1685	0.90709
35	6	0	5.58043	-0.64235	-0.28363
36	1	0	2.654198	-0.18037	-1.9602
37	1	0	5.090221	0.12255	-2.24001
38	1	0	3.303584	-1.69656	2.016058
39	1	0	5.739886	-1.44299	1.714351
40	1	0	6.653803	-0.51771	-0.41033

Table S7. Atom coordinates and absolute energy levels for **5b** optimized in the S_0 state.

5b (S_0 state): E(RB3LYP) = -8224.66074937 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.724727	-1.866741	1.286906
2	6	0	0.724511	-1.866876	1.28687
3	6	0	-1.344423	-1.019255	0.417524
4	6	0	1.344321	-1.019534	0.417434
5	33	0	-0.000003	-0.15225	-0.70113
6	1	0	-1.271239	-2.551886	1.933448
7	1	0	1.270893	-2.552108	1.933429
8	6	0	-2.782729	-0.845744	0.23341
9	6	0	2.782628	-0.846048	0.233331
10	6	0	0.000162	1.659571	0.04728
11	6	0	0.000317	1.911364	1.424748
12	6	0	0.000086	2.738571	-0.843833
13	6	0	0.000161	4.054443	-0.367581
14	6	0	0.000395	3.221751	1.904204
15	6	0	0.000314	4.296551	1.007263
16	1	0	-0.000026	2.557019	-1.916291
17	1	0	0.000104	4.884066	-1.070126
18	1	0	0.000378	1.081084	2.126373
19	1	0	0.000521	3.406371	2.975715
20	1	0	0.000369	5.317389	1.380955
21	6	0	-3.694693	-1.142712	1.267378
22	6	0	-3.309679	-0.37225	-0.984541
23	6	0	-4.681759	-0.227921	-1.178144
24	6	0	-5.06838	-1.013829	1.084289
25	6	0	-5.553643	-0.548823	-0.139187
26	1	0	-2.635541	-0.149283	-1.807038
27	1	0	-5.067362	0.129588	-2.127255
28	1	0	-3.323212	-1.473483	2.233157
29	1	0	-5.754528	-1.251697	1.890668
30	35	0	-7.431098	-0.349487	-0.392664
31	6	0	3.694661	-1.143719	1.267043
32	6	0	3.309534	-0.371747	-0.984323
33	6	0	4.6816	-0.227243	-1.177884
34	6	0	5.068335	-1.014689	1.083994
35	6	0	5.553541	-0.548887	-0.139206
36	1	0	2.635375	-0.148247	-1.806658
37	1	0	5.067153	0.130928	-2.126767
38	1	0	3.323255	-1.47516	2.23262
39	1	0	5.754518	-1.253105	1.890182
40	35	0	7.43099	-0.349503	-0.392678

Table S8. Atom coordinates and absolute energy levels for **5c** optimized in the S_0 state.

5c (S_0 state): E(RB3LYP) = -3311.37744694 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.736145	-2.28687	-1.04546
2	6	0	-0.71287	-2.2995	-1.03695
3	6	0	1.357572	-1.25947	-0.39872
4	6	0	-1.34437	-1.28303	-0.3828
5	33	0	0.002305	-0.17241	0.504085
6	1	0	1.285782	-3.09424	-1.52913
7	1	0	-1.25404	-3.11635	-1.51417
8	6	0	2.800477	-1.04248	-0.29418
9	6	0	-2.7894	-1.09102	-0.26104
10	6	0	-0.01851	1.414849	-0.65072
11	6	0	-0.02625	1.337794	-2.04898
12	6	0	-0.02552	2.674072	-0.03989
13	6	0	-0.03925	3.84155	-0.8125
14	6	0	-0.04084	2.497841	-2.82429
15	6	0	-0.04788	3.754367	-2.20554
16	1	0	-0.01849	2.748429	1.045049
17	1	0	-0.04457	4.813224	-0.32449
18	1	0	-0.02179	0.365616	-2.53493
19	1	0	-0.04674	2.425381	-3.90887
20	1	0	-0.05924	4.658356	-2.80906
21	6	0	3.67609	-1.56872	-1.26978
22	6	0	3.373019	-0.31711	0.771911
23	6	0	4.765585	-0.14712	0.864281
24	6	0	5.04989	-1.41444	-1.17921
25	6	0	5.604518	-0.70011	-0.10951
26	8	0	2.440794	0.198447	1.770084
27	1	0	5.190318	0.402379	1.688761
28	1	0	3.26241	-2.10111	-2.12154
29	1	0	5.711344	-1.82364	-1.93794
30	1	0	6.66735	-0.61416	-0.0993
31	6	0	-3.66805	-1.63377	-1.22512
32	6	0	-3.36067	-0.37441	0.810768
33	6	0	-4.75457	-0.22821	0.921714
34	6	0	-5.04301	-1.50323	-1.117
35	6	0	-5.59622	-0.79702	-0.03992
36	8	0	-2.42409	0.157557	1.796468
37	1	0	-5.17814	0.315764	1.749913
38	1	0	-3.2561	-2.16022	-2.0817
39	1	0	-5.70699	-1.92481	-1.86611
40	1	0	-6.66015	-0.72943	-0.01722
41	6	0	3.131735	0.727448	2.934946
42	6	0	-3.07486	1.067246	2.726037
43	1	0	3.728735	-0.06701	3.401437
44	1	0	3.776753	1.56289	2.635919
45	1	0	2.373847	1.087507	3.643587
46	1	0	-3.50949	1.910806	2.173264
47	1	0	-3.85364	0.534462	3.283517
48	1	0	-2.3135	1.435652	3.427463

Table S9. Atom coordinates and absolute energy levels for **5d** optimized in the S_0 state.

5d (S_0 state): E(RB3LYP) = -3311.39347498 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.734052	-1.995523	1.249384
2	6	0	0.715723	-2.004414	1.24532
3	6	0	-1.351583	-1.116364	0.409775
4	6	0	1.339139	-1.132801	0.402692
5	33	0	-0.003061	-0.221925	-0.683972
6	1	0	-1.283172	-2.697204	1.875466
7	1	0	1.259272	-2.713519	1.868565
8	6	0	-2.789302	-0.928114	0.235235
9	6	0	2.77862	-0.962065	0.221395
10	6	0	0.00973	1.564347	0.123788
11	6	0	0.014711	1.770036	1.508487
12	6	0	0.014221	2.672561	-0.73054
13	6	0	0.023873	3.971308	-0.211169
14	6	0	0.024338	3.063421	2.031607
15	6	0	0.028723	4.167963	1.171018
16	1	0	0.010506	2.526527	-1.809165
17	1	0	0.026703	4.824368	-0.885388
18	1	0	0.011447	0.916815	2.18179
19	1	0	0.028286	3.211961	3.108962
20	1	0	0.035818	5.175713	1.579062
21	6	0	-3.702015	-1.250829	1.258617
22	6	0	-3.319678	-0.413731	-0.961838
23	6	0	-4.692676	-0.252735	-1.150715
24	6	0	-5.073898	-1.105734	1.083011
25	6	0	-5.577441	-0.59979	-0.118908
26	1	0	-2.646653	-0.169342	-1.778771
27	1	0	-5.051451	0.136834	-2.090266
28	1	0	-3.331297	-1.614462	2.213011
29	1	0	-5.756404	-1.36657	1.885816
30	8	0	-7.026483	-0.470834	-0.204777
31	6	0	3.692193	-1.297916	1.239265
32	6	0	3.309601	-0.455411	-0.978528
33	6	0	4.683414	-0.310893	-1.174515
34	6	0	5.0649	-1.170823	1.056659
35	6	0	5.568875	-0.668905	-0.146529
36	1	0	2.635279	-0.202378	-1.792565
37	1	0	5.04227	0.07186	-2.117399
38	1	0	3.322256	-1.658142	2.195205
39	1	0	5.747598	-1.441405	1.856044
40	8	0	7.020836	-0.560869	-0.237913
41	6	0	7.442552	0.102116	-1.459957
42	6	0	-7.450254	-0.045836	-1.527751
43	1	0	-7.020176	0.936301	-1.756815
44	1	0	-7.130681	-0.786219	-2.27344
45	1	0	-8.54594	0.026274	-1.525336
46	1	0	7.29283	-0.571407	-2.314892
47	1	0	6.871665	1.027044	-1.599642
48	1	0	8.509771	0.344876	-1.36247

Table S10. Atom coordinates and absolute energy levels for **5e** optimized in the S_0 state.

5e (S_0 state): E(RB3LYP) = -3350.34343066 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.72819	-1.96804	1.128738
2	6	0	0.720235	-1.97098	1.137393
3	6	0	-1.35085	-1.06895	0.313603
4	6	0	1.355775	-1.07826	0.323905
5	33	0	0.009053	-0.1224	-0.73153
6	1	0	-1.27698	-2.68672	1.73653
7	1	0	1.256426	-2.69631	1.748594
8	6	0	-2.78489	-0.87053	0.141803
9	6	0	2.791921	-0.91676	0.130013
10	6	0	-0.0052	1.616636	0.179862
11	6	0	0.06824	1.750252	1.571291
12	6	0	-0.08009	2.770427	-0.60996
13	6	0	-0.08953	4.039889	-0.02133
14	6	0	0.059395	3.014223	2.163816
15	6	0	-0.01964	4.162896	1.368031
16	1	0	-0.13071	2.681505	-1.6931
17	1	0	-0.15081	4.926853	-0.64754
18	1	0	0.127929	0.862875	2.196145
19	1	0	0.115067	3.104388	3.246277
20	1	0	-0.02488	5.147097	1.830251
21	6	0	-3.71492	-1.24675	1.133336
22	6	0	-3.32315	-0.29114	-1.02351
23	6	0	-4.69104	-0.11257	-1.20225
24	6	0	-5.08337	-1.07463	0.9708
25	6	0	-5.61698	-0.48148	-0.19931
26	1	0	-2.65401	-0.00711	-1.83204
27	1	0	-5.03159	0.318178	-2.13625
28	1	0	-3.35819	-1.67879	2.064823
29	1	0	-5.73707	-1.39039	1.77565
30	7	0	-6.9872	-0.25779	-0.34571
31	6	0	3.740502	-1.45996	1.020584
32	6	0	3.314931	-0.20251	-0.96603
33	6	0	4.680545	-0.0463	-1.17381
34	6	0	5.108861	-1.33058	0.818618
35	6	0	5.625742	-0.62655	-0.29668
36	1	0	2.631949	0.231322	-1.69202
37	1	0	5.004029	0.521862	-2.03804
38	1	0	3.403445	-1.99317	1.90597
39	1	0	5.777055	-1.76822	1.551288
40	7	0	6.996165	-0.52688	-0.52817
41	6	0	-7.49818	0.108521	-1.65905
42	6	0	-7.91453	-0.97897	0.515777
43	6	0	7.476373	0.45805	-1.48743
44	6	0	7.919065	-0.91107	0.529882
45	1	0	-7.02191	1.026482	-2.01739
46	1	0	-7.344	-0.6808	-2.41504
47	1	0	-8.56975	0.305996	-1.5784
48	1	0	-7.89516	-2.06937	0.347129

49	1	0	-7.69467	-0.78892	1.570101
50	1	0	-8.92759	-0.6152	0.326687
51	1	0	7.054493	0.27225	-2.48064
52	1	0	7.230005	1.492842	-1.19494
53	1	0	8.561855	0.370066	-1.57202
54	1	0	7.824499	-0.28061	1.430221
55	1	0	7.760851	-1.95475	0.821676
56	1	0	8.941999	-0.82881	0.15512

Table S11. Atom coordinates and absolute energy levels for **6a** optimized in the S_0 state.

6a (S_0 state): E(RB3LYP) = -1189.93745786 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.72332	-2.08211	0.952526
2	6	0	0.723416	-2.08208	0.95252
3	6	0	-1.32351	-1.18715	0.12253
4	6	0	1.32355	-1.1871	0.122517
5	15	0	0.000008	-0.3205	-0.88597
6	1	0	-1.27984	-2.79209	1.562496
7	1	0	1.27999	-2.79203	1.562486
8	6	0	-2.7583	-0.97307	-0.07001
9	6	0	2.758318	-0.97299	-0.07002
10	6	0	-0.00002	1.38311	-0.09773
11	6	0	-2.3E-05	1.570419	1.290254
12	6	0	-3.6E-05	2.494204	-0.94807
13	6	0	-5.5E-05	3.788478	-0.41509
14	6	0	-4.2E-05	2.861557	1.820685
15	6	0	-5.8E-05	3.973068	0.968961
16	1	0	-3.6E-05	2.35479	-2.02697
17	1	0	-6.8E-05	4.646826	-1.08225
18	1	0	-1.2E-05	0.71026	1.954953
19	1	0	-4.5E-05	3.001488	2.898904
20	1	0	-7.2E-05	4.977505	1.385003
21	6	0	-3.68213	-1.27905	0.952506
22	6	0	-3.26519	-0.44604	-1.27579
23	6	0	-4.63455	-0.25601	-1.46064
24	6	0	-5.05039	-1.09359	0.764699
25	6	0	-5.53612	-0.58027	-0.44313
26	1	0	-2.57742	-0.20923	-2.08339
27	1	0	-4.99793	0.146116	-2.40319
28	1	0	-3.31891	-1.64878	1.907648
29	1	0	-5.73981	-1.33683	1.569596
30	1	0	-6.60306	-0.43093	-0.5866
31	6	0	3.682082	-1.27911	0.952492
32	6	0	3.265195	-0.44587	-1.27574
33	6	0	4.63459	-0.25585	-1.46057
34	6	0	5.050343	-1.09368	0.764647
35	6	0	5.53617	-0.58027	-0.44312
36	1	0	2.577583	-0.20893	-2.08342
37	1	0	4.997955	0.146391	-2.40308
38	1	0	3.319	-1.64862	1.907765
39	1	0	5.73992	-1.33706	1.569383
40	1	0	6.60312	-0.43097	-0.58656

7. References

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