

Supporting Information

The development of anthracene derivatives for organic light-emitting diodes

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Table 1. The photophysical and thermal property data for compounds referred in the Feature article.

compounds	λ (nm) ^a	T _d (°C) [§]	T _m (°C)	T _g (°C)	HOMO(eV)	LUMO (eV)	E _g (eV)	Ref.
8	414 ^b	---	---	---	5.84	2.89	2.95	9
9	421 ^b	---	---	---	5.78	2.82	2.96	9
10	420 ^b	---	---	---	5.96	2.99	2.97	9
11	427 ^b	---	---	---	6.67	2.70	2.97	9
12	410	300	---	---	5.96	2.84	3.12	10
13	430 ^b	---	---	---	5.88	2.87	3.01	9
14	454 ^c	---	---	---	5.8	2.8	3.0	11b
16	431	397	255	120	5.5	2.5	3.0	13
19	416, 434	510	---	---	5.57	2.59	2.98	14
20	430	535	---	---	5.55	2.58	2.97	14
21	414, 432	542	---	---	5.61	2.61	3.00	14
22	422, 440	539	---	---	5.59	2.60	2.99	14
23	421	---	288	116	5.50	2.48	3.02	15
24	416	---	294	125	5.50	2.48	3.02	15
25	417	---	164	84	5.49	2.46	3.03	15
26	420	---	219	123	5.49	2.48	3.01	15
27	421	---	242	126	5.50	2.50	3.00	15
28	425	---	292	153	5.48	2.48	3.00	15
30	440	419	294	133	5.83	2.95	2.88	16b
31	435	324	---	---	5.83	2.87	---	16c
32	419, 437	392	---	---	5.85	2.91	---	16c

33	433 ^d	410	366	2.96	5.55	2.59	2.96	17a
34	433 ^d	464	310	2.95	5.53	2.58	2.95	17a
35	436 ^d	470	340	2.94	5.54	2.60	2.94	17a
36	416, 436	410	---	206	6.03	2.92	2.96	17c
37	415, 436	410 ^h	391	207	5.91	2.89	---	17d
38	421, 433	441	298	138	5.58	2.53	3.05	18
39	425	400	262	132	5.55	2.51	3.04	18
40	432	401.8	236.5	132.5	5.58	2.60	2.98	13
41	431	412.1	265.2	133.8	5.58	2.60	2.98	13
42	437	458	---	---	5.55	2.57	2.98	20
43	435	480	---	---	5.55	2.57	2.98	20
44	435	504	---	---	5.58	2.61	2.97	20
45	435	525	---	---	5.57	2.61	2.96	20
46	414, 425	358	320	---	5.22	2.10	---	21
47	415	367	333	---	5.21	2.18	---	21
48	403, 422	323	275	---	5.23	2.11	---	21
49	409, 425	397	283	---	5.25	2.15	---	21
50	426	429	350	---	5.28	2.28	---	21
51	439	449	389	---	5.26	2.28	---	21
52	438	410	---	---	5.91	3.05	2.96	23
53	448 ^e	445	298	155	5.7	2.9		24
54	482	381.5	290.0	135.6	5.63	2.61	3.02	25a
55	495	356.3	345.0	155.3	5.65	2.62	3.03	25a
56	451	401.7	337.0	---	5.62	2.67	2.95	25a
57	462	408.4	398.0	---	5.59	2.64	2.95	25a
58	441	---	406	---	5.69	2.76	2.93	26
59	442	353	283	---	5.79	2.92	2.87	16b
60	442	429	388	165	5.82	2.88	2.94	16b
61	438	358	---	131	5.6	2.7	2.9	28
62	438	---	---	---	5.54	2.68	---	30
63	402, 423	441	417	159	5.59	2.59	3.03	31
64	416, 431	488	438	241	5.55	2.54	3.02	31
65	414, 433	495	475	257	5.55	2.55	3.02	31
66	446	510	391	227	5.85	3.92	---	16a
67	---	---	---	---	---	---	---	
69	425 ^f	450	397	223	5.47	2.45	3.02	35
72	425 ^e	---	220	174.1	5.83	2.79	3.04	37b

73	432 ^e	---	350	282.4	5.80	2.78	3.02	37a
74	428 ^d	393	351	252	5.87	2.91	---	37c
75	426 ^d	413	339	261	5.89	2.93	---	37c
76	432 ^d	435	381	250	5.84	2.89	---	37c
78	450 ^e	389	304	204	5.94	3.09	---	40
79	453 ^e	439	350	237	5.87	3.03	---	40
80	457	320	---	---	5.65	2.87	2.78	41
81	470	>400	---	162	5.8	2.91	2.89	41
82	520	>400	---	---	5.22	2.9	2.32	41
83	431 ^d	382	292	---	5.58	2.60	2.98	38
84	435 ^d	386	---	132	5.59	2.68	2.91	38
85	441, 463	340	---	251	5.61	2.73	2.88	42
86	441, 463	358	---	248	5.63	2.77	2.86	42
87	453, 475	300	---	194	5.70	2.89	2.81	42
98	442 ^d	430	---	168	6.17	3.09	3.04	23
99	400, 422 ^f	401	216	102	5.85	2.75	---	46
100	413 ^f	442	252	148	5.91	2.89	---	46
101	421 ^f	486	282	177	5.90	2.90	---	46
102	426	368	---	140	5.86	2.84	3.02	43
103	438	490	---	94	5.83	2.89	2.94	43
104	430	440	---	141	5.65	2.77	2.88	43
105	420	358	---	89	5.90	2.95	2.95	43
106	472	410	255	142	5.25	2.38	---	48
107	466	405	353	170	5.18	2.33	---	48
108	470	415	393	201	5.16	2.33	---	48
109	467	400		140	5.57	2.60	---	48
110	450	410	264	157	5.31	2.38	---	48
111	467	405	375	138	5.21	2.34	---	48
113	498	---	---	---	5.50	2.67	2.83	49
114	489	---	---	---	5.46	2.60	2.86	49
115	492	---	---	---	5.54	2.58	2.96	49
116	454 ^f	420	351	---	5.22	2.33	2.89	50
117	438	---	---	104	5.70	2.94	---	52a
118	439	---	---	129	5.66	2.91	---	52a
119	444	---	---	162	5.63	2.93	---	52a
120	474 ^d	427	305	130	5.35	2.48	2.87	17b
121	476	479	272	139	5.37	2.50	2.87	17b

124	431 ^d	388	274	135	5.58	2.66	2.88	51
125	524	---	373	227	5.54	3.11	---	53a
126	536	---	332	223	5.54	3.11	---	53a
127	526	---	248	169	5.51	3.05	---	53a
128	524	---	---	---	5.57	3.11	2.46	53b
129	530	---	---	---	5.49	3.05	2.44	53b
130	546	---	---	---	5.45	3.06	2.39	53b
131	553	---	---	---	5.37	3.01	2.36	53b
132	560,579	---	---	---	5.2	2.8	---	54
133	443	300	---	---	5.4	2.36	3.04	55
134	441	395	---	---	5.41	2.37	3.04	55
135	431	419	---	---	5.50	2.45	3.05	55
136	435	326	196	89	5.47	2.42	3.05	55
137	427	---	---	214	5.54	2.54	---	56
138	428	---	---	187	5.56	2.57	---	56
139	418, 436	411	---	177	5.50	2.55	---	57
140	410, 430	437	---	115	5.67	2.64	---	57
141	414, 434	454	---	149	5.61	2.61	---	57
143	438	502	355	192	6.02	3.07	---	16a
144	512 ^d	461	276	97	5.92	3.19	---	59
145	514 ^d	400	288	106	6.02	3.11	---	59
146	512 ^d	445	228	83	6.00	3.16	---	59
147	518 ^d	430	262	108	6.04	3.10	---	59
148	518 ^d	457	296	131	6.03	3.13	---	59
149	517 ^d	458	180	52	5.97	3.15	---	59
150	456 ^d	460	---	---	6.67	3.71	2.96	60
151	447 ^d	418	---	---	6.72	3.7	3.00	60
152	447 ^d	420	---	---	6.66	3.68	2.98	60
153	430 ^d	430	---	---	6.75	3.7	3.05	60
154	421 ^d	410	---	92	6.83	3.71	3.12	60
157	435	460	---	146	5.60	2.50	---	62
158	456	---	---	---	5.65	2.65	---	63
159	503	---	---	---	5.71	2.76	---	63
160	---	442	268	97	5.9	2.8	3.1	64
161	415, 431 ^f	471	---	226	5.51	2.47	---	66a
162	433 ^f	475	---	154	5.38	2.48	---	66a
163	430 ^f	466	---	173	5.32	2.24	---	66a

164	433 ^f	474	---	180	5.27	2.36	---	66a
165	438 ^f	---	378	165	5.30	2.40	---	66b
166	434 ^f	---	376	229	5.46	2.45	---	66b
167	442 ^f	---	---	189	5.45	2.46	---	66b
168	441 ^f	---	---	---	5.48	2.53	---	66b
169	496	460.4	310.6	144.1	5.33	2.40	2.93	7
170	496	481.0	349.8	152.7	5.29	2.32	2.97	7
171	493	486.0	276.1	161.5	5.33	2.41	2.92	7
172	498	519.7	398.8	---	5.28	2.32	2.96	7
175	474 ^f	---	---	223	5.00	2.41	---	68
176	436	484	---	166	5.57	2.65	2.92	69
177	436	504	---	189	5.54	2.59	2.95	69
178	436	497	---	260	5.52	2.58	2.94	69
179	437	427	---	231	5.50	2.57	2.93	69

^a Obtained in CH₂Cl₂ solution. ^b Obtained in 1,2-dichloroethane solution. ^c Obtained in the film. ^d Obtained in the chloroform. ^e Obtained in the THF. ^f Obtained in the toluene. ^g 5% weight loss. ^h 3% weight loss.

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