Solvent impact on the singlet and triplet states of selected fluorine corroles – absorption, fluorescence, and optoacoustic studies

Electronic Supplementary Information (ESI)

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Table S1 TD-DFT calculated transitions of corrole **1**. The table is limited to the transitions with oscillator strength > 0.1 and wavelength > 200 nm. Additionally, the first transition for the isolated species is also included.

Wavelength (nm)	Osc. Strength	Major contribution
Isolated[21]		
575	0.0568	H-1→→LUMO (17%), HOMO→LUMO (22%), HOMO→L+1 (53%)
560	0.1808	H-1→LUMO (19%), H-1→L+2 (10%), HOMO→LUMO (46%)
515	0.1576	H-1→LUMO (22%), H-1→L+1 (14%), HOMO→L+1 (24%), HOMO→L+2 (33%)
495	0.1214	H-1→LUMO (13%), H-1→L+1 (60%), H-1→L+2 (11%)
391	0.6029	H-1→LUMO (12%), HOMO→L+2 (38%)
382	0.4419	H-2→LUMO (32%), H-2→L+1 (11%), H-1→L+2 (29%)
369	0.505	H-2→LUMO (55%), H-1→L+2 (22%)
361	0.1345	H-2→L+1 (76%)
342	0.156	HOMO→L+3 (77%)
312	0.3245	H-2→L+2 (25%), H-1→L+4 (47%)
In TL		
626	0.1608	HOMO→LUMO (89%)
580	0.1241	H-1→LUMO (55%), HOMO→L+1 (32%)
535	0.3312	H-1→LUMO (40%), H-1→L+2 (12%), HOMO→L+1 (35%)
530	0.115	H-1→L+1 (59%), HOMO→L+2 (33%)
407	0.8755	H-1→L+1 (17%), HOMO→L+2 (48%)
392	1.0567	H-1→L+2 (61%)
370	0.215	H-2→L+1 (82%)
347	0.1327	HOMO→L+3 (87%)
319	0.1329	H-17→LUMO (19%), H-1→L+4 (65%)
317	0.2496	H-2→L+2 (56%)
206	0.1014	H-9→L+3 (10%), H-2→L+11 (35%), HOMO→L+13 (23%)
In CL		
657	0.1639	HOMO→LUMO (93%)
546	0.331	H-1→LUMO (17%), H-1→L+2 (15%), HOMO→L+1 (48%)
531	0.1437	H-1→L+1 (53%), HOMO→L+2 (32%)
407	0.8748	H-1→L+1 (18%), HOMO→L+2 (46%)
392	1.0881	H-1→L+2 (61%)
368	0.1843	H-2→L+1 (84%)
346	0.1269	HOMO→L+3 (88%)
319	0.1113	H-2→L+2 (14%), H-1→L+4 (67%)

316	0.2137	H-2→L+2 (50%)
206	0.1326	H-2→L+11 (48%), HOMO→L+13 (27%)
In DMSO		
691	0.1715	HOMO→LUMO (94%)
551	0.3523	H-1→L+2 (16%), HOMO→L+1 (58%)
531	0.1326	H-1→L+1 (54%), HOMO→L+2 (32%)
408	0.8858	H-1→L+1 (18%), HOMO→L+2 (44%)
392	1.1479	H-1→L+2 (62%)
365	0.1506	H-2→L+1 (86%)
344	0.1138	HOMO→L+3 (89%)
319	0.2547	H-6→LUMO (11%), H-4→LUMO (21%), H-1→L+4 (57%)
316	0.1005	H-4→LUMO (13%), H-2→L+2 (55%)

Table S2 TD-DFT calculated transitions of corrole **2**. The table is limited to the transitions with oscillator strength > 0.1 and wavelength > 200 nm. Additionally, the first transition for the isolated species is also included. H – HOMO, L – LUMO.

Wavelength (nm)	Osc. Strength	Major contribution
Isolated[21]		
547	0.0875	H-1→LUMO (36%), H-1→L+1 (10%), HOMO→LUMO (25%), HOMO→L+1 (27%)
534	0.1511	H-1→LUMO (21%), H-1→L+1 (16%), HOMO→LUMO (40%), HOMO→L+1 (15%)
396	0.7181	H-1→LUMO (18%), HOMO→L+1 (33%)
387	0.7593	H-2→LUMO (16%), H-1→L+1 (37%)
370	0.3045	H-2→LUMO (74%), H-1→L+1 (10%)
322	0.133	H-1→L+2 (39%), H-1→L+3 (11%), HOMO→L+3 (11%)
313	0.1133	H-1→L+3 (48%), HOMO→L+7 (18%)
310	0.1859	H-1→L+4 (79%)
306	0.1107	H-11→LUMO (15%), H-10→LUMO (14%), H-9→LUMO (19%), H-7→LUMO (14%)
In TL		
553	0.2165	H-1→LUMO (22%), H-1→L+1 (14%), HOMO→LUMO (45%), HOMO→L+1 (15%)
541	0.1491	H-1→LUMO (39%), HOMO→LUMO (25%), HOMO→L+1 (25%)
412	0.9916	H-1→LUMO (20%), HOMO→L+1 (42%)
401	1.1947	H-1→L+1 (57%)
369	0.1186	H-2→LUMO (87%)
326	0.1065	H-2→L+1 (12%), H-1→L+2 (44%), H-1→L+3 (10%)
317	0.1415	H-1→L+3 (54%), HOMO→L+7 (16%)
315	0.2002	H-1→L+4 (84%)

251	0.1033	H-2→L+2 (10%), H-2→L+3 (31%), H-2→L+4 (16%), H-1→L+11 (20%)
In CL		
552	0.2075	H-1→LUMO (21%), H-1→L+1 (15%), HOMO→LUMO (46%), HOMO→L+1 (14%)
539	0.1366	H-1→LUMO (39%), HOMO→LUMO (24%), HOMO→L+1 (25%)
411	0.9813	H-1→LUMO (20%), HOMO→L+1 (42%)
400	1.2065	H-1→L+1 (57%)
366	0.1051	H-2→LUMO (87%)
317	0.1414	H-1→L+3 (56%), HOMO→L+7 (11%)
314	0.2202	H-1→L+4 (81%)
251	0.1193	H-2→L+3 (29%), H-2→L+4 (10%), H-1→L+11 (27%)
In DMSO		
551	0.2192	H-1→LUMO (18%), H-1→L+1 (16%), HOMO→LUMO (50%), HOMO→L+1 (12%)
538	0.1192	H-1→LUMO (42%), HOMO→LUMO (20%), HOMO→L+1 (28%)
410	1.0153	H-1→LUMO (20%), HOMO→L+1 (42%)
400	1.2621	H-1→L+1 (57%)
316	0.1256	H-1→L+3 (58%)
313	0.2129	H-1→L+4 (82%)
303	0.11	H-5→LUMO (48%), H-1→L+6 (20%)
249	0.133	H-2→L+3 (31%), H-1→L+11 (32%)