

Blue emitting C₂-symmetrical dibenzothiazolyl-substituted pyrrole, furan and thiophene

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Electronic Supplementary Information

Bond Lengths [Å] and Angles [°] for 2

C12A–N2A	1.338(12)
C12A–C11	1.470(9)
C12A–S2A	1.752(10)
S2A–C13A	1.737(7)
C13A–C14A	1.3900
C13A–C19A	1.3900
C14A–C15A	1.3900
C15A–C16A	1.3900
C16A–C18A	1.3900
C18A–C19A	1.3900
C19A–N2A	1.387(9)
C12B–N2B	1.298(12)
C12B–C11	1.472(9)
C12B–S2B	1.767(10)
S2B–C13B	1.703(7)
C13B–C14B	1.3900
C13B–C19B	1.3900
C14B–C15B	1.3900
C15B–C16B	1.3900
C16B–C18B	1.3900
C18B–C19B	1.3900
C19B–N2B	1.399(9)
S1–C6	1.737(3)
S1–C7	1.751(6)
O1–C11	1.369(6)
O1–C8	1.379(7)
N1–C7	1.291(7)
N1–C1	1.384(5)
C1–C2	1.3900
C1–C6	1.3900
C2–C3	1.3900
C3–C4	1.3900
C4–C5	1.3900
C5–C6	1.3900
C7–C8	1.450(7)
C8–C9	1.351(8)
C9–C10	1.425(7)
C9–C20	1.473(8)
C10–C11	1.364(8)
C10–C26B	1.474(7)
C10–C26A	1.488(7)
C20–C25	1.382(7)
C20–C21	1.393(9)
C21–C22	1.368(7)
C22–C23	1.3900
C23–C24	1.3900
C24–C25	1.3900
C26A–C27A	1.3900
C26A–C31A	1.3900
C27A–C28A	1.3900
C28A–C29A	1.3900
C29A–C30A	1.3900
C30A–C31A	1.3900
C26B–C27B	1.3900
C26B–C31B	1.3900

C27B–C28B	1.3900
C28B–C29B	1.3900
C29B–C30B	1.3900
C30B–C31B	1.3900
N2A–C12A–C11	122.6(8)
N2A–C12A–S2A	118.8(6)
C11–C12A–S2A	118.2(7)
C13A–S2A–C12A	87.3(4)
C14A–C13A–C19A	120.0
C14A–C13A–S2A	130.0(4)
C19A–C13A–S2A	109.7(4)
C15A–C14A–C13A	120.0
C14A–C15A–C16A	120.0
C18A–C16A–C15A	120.0
C16A–C18A–C19A	120.0
N2A–C19A–C18A	121.7(6)
N2A–C19A–C13A	118.3(6)
C18A–C19A–C13A	120.0
C12A–N2A–C19A	105.7(7)
N2B–C12B–C11	122.4(8)
N2B–C12B–S2B	116.7(6)
C11–C12B–S2B	121.0(7)
C13B–S2B–C12B	87.9(4)
C14B–C13B–C19B	120.0
C14B–C13B–S2B	128.6(3)
C19B–C13B–S2B	111.2(4)
C13B–C14B–C15B	120.0
C14B–C15B–C16B	120.0
C18B–C16B–C15B	120.0
C16B–C18B–C19B	120.0
C18B–C19B–C13B	120.0
C18B–C19B–N2B	124.9(5)
C13B–C19B–N2B	115.1(5)
C12B–N2B–C19B	108.8(7)
C6–S1–C7	87.9(2)
C11–O1–C8	105.7(4)
C7–N1–C1	111.1(5)
N1–C1–C2	125.8(2)
N1–C1–C6	114.2(2)
C2–C1–C6	120.0
C1–C2–C3	120.0
C4–C3–C2	120.0
C5–C4–C3	120.0
C4–C5–C6	120.0
C5–C6–C1	120.0
C5–C6–S1	129.45(10)
C1–C6–S1	110.55(10)
N1–C7–C8	123.3(5)
N1–C7–S1	116.2(4)
C8–C7–S1	120.5(4)
C9–C8–O1	111.0(4)
C9–C8–C7	135.0(5)
O1–C8–C7	113.8(5)
C8–C9–C10	106.3(5)
C8–C9–C20	128.9(5)
C10–C9–C20	124.8(5)
C11–C10–C9	106.4(5)

C11–C10–C26B	125.6(5)
C9–C10–C26B	128.0(6)
C11–C10–C26A	127.5(5)
C9–C10–C26A	125.9(6)
C26B–C10–C26A	5.9(5)
C10–C11–O1	110.6(4)
C10–C11–C12A	136.5(6)
O1–C11–C12A	112.7(6)
C10–C11–C12B	132.0(6)
O1–C11–C12B	117.2(6)
C12A–C11–C12B	4.6(7)
C25–C20–C21	117.8(5)
C25–C20–C9	121.2(5)
C21–C20–C9	120.9(5)
C22–C21–C20	122.8(6)
C21–C22–C23	118.7(3)
C24–C23–C22	120.0
C23–C24–C25	120.0

Bond Lengths [Å] and Angles [°] for 3

S1–C6	1.738(4)
S1–C7	1.746(4)
S2–C8	1.728(4)
S2–C11	1.729(4)
S3–C13	1.739(4)
S3–C12	1.754(4)
N1–C7	1.300(5)
N1–C1	1.394(5)
N2–C12	1.296(5)
N2–C18	1.389(5)
C1–C2	1.385(6)
C1–C6	1.399(6)
C2–C3	1.388(6)
C3–C4	1.395(6)
C4–C5	1.375(6)
C5–C6	1.395(6)
C7–C8	1.446(5)
C8–C9	1.368(6)
C9–C10	1.407(6)
C10–C11	1.370(6)
C11–C12	1.453(5)
C13–C14	1.395(6)
C13–C18	1.404(6)
C14–C15	1.378(6)
C15–C16	1.391(6)
C16–C17	1.383(6)
C17–C18	1.392(6)
C6–S1–C7	88.94(19)
C8–S2–C11	91.1(2)
C13–S3–C12	88.58(19)
C7–N1–C1	110.4(3)
C12–N2–C18	110.4(3)
C2–C1–N1	124.8(4)
C2–C1–C6	120.1(4)
N1–C1–C6	115.1(4)
C1–C2–C3	118.7(4)
C2–C3–C4	120.7(4)
C5–C4–C3	121.3(4)
C4–C5–C6	117.9(4)
C5–C6–C1	121.3(4)
C5–C6–S1	129.2(3)
C1–C6–S1	109.4(3)
N1–C7–C8	123.3(4)
N1–C7–S1	116.1(3)
C8–C7–S1	120.4(3)
C9–C8–C7	129.8(4)
C9–C8–S2	111.5(3)
C7–C8–S2	118.7(3)
C8–C9–C10	113.3(4)
C11–C10–C9	112.3(4)
C10–C11–C12	128.7(4)
C10–C11–S2	111.9(3)
C12–C11–S2	119.4(3)
N2–C12–C11	124.0(4)
N2–C12–S3	116.3(3)

C11–C12–S3	119.7(3)
C14–C13–C18	121.5(4)
C14–C13–S3	129.0(3)
C18–C13–S3	109.5(3)
C15–C14–C13	118.0(4)
C14–C15–C16	121.0(4)
C17–C16–C15	121.2(4)
C16–C17–C18	118.8(4)
N2–C18–C17	125.4(4)
N2–C18–C13	115.2(4)
C17–C18–C13	119.4(4)

Simulated Absorption Spectra

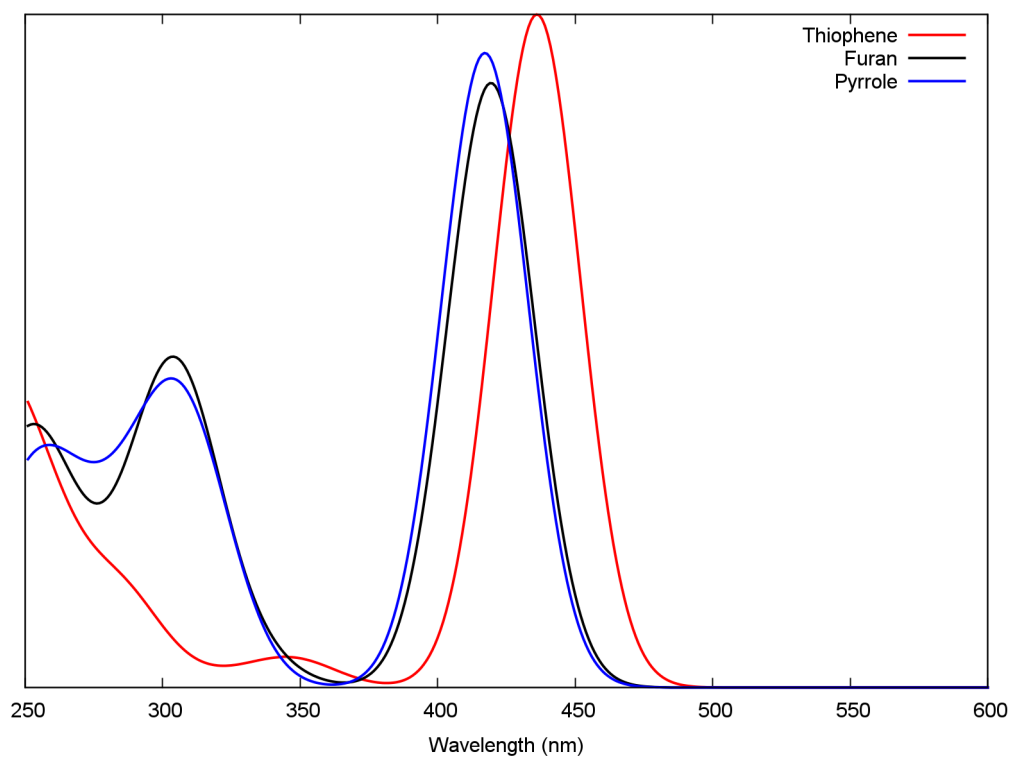


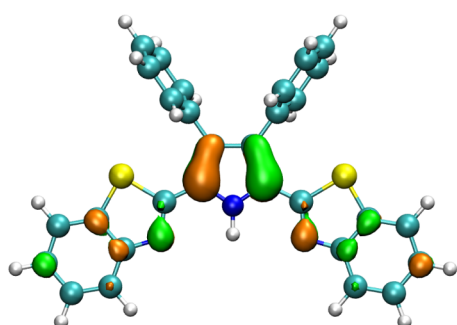
Figure S1. Simulated absorption spectra for **1**, **2**, and **3**.

Calculated Transitions for 1

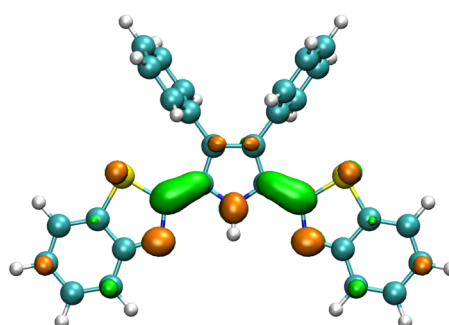
Wavelength	Intensity	Levels	Character
417.16 nm	1.3965	HOMO -> LUMO	99.2 %
317.78 nm	0.0560	HOMO-3 -> LUMO HOMO-1 -> LUMO	3.2 % 90.6 %
316.36 nm	0.0027	HOMO-2 -> LUMO	94.6 %
313.77 nm	0.1787	HOMO-3 -> LUMO HOMO-1 -> LUMO HOMO -> LUMO+1	6.4 % 2.5 % 87.4 %
303.39 nm	0.3706	HOMO-4 -> LUMO HOMO-3 -> LUMO HOMO -> LUMO+1	9.8 % 79.3 % 7.6 %
293.03 nm	0.0781	HOMO-4 -> LUMO HOMO-3 -> LUMO	85.5 % 8.9 %
288.71 nm	0.0242	HOMO-6 -> LUMO HOMO-5 -> LUMO	10.5 % 87.2 %
284.93 nm	0.0213	HOMO -> LUMO+2 HOMO -> LUMO+4	89.7 % 6.9 %
282.39 nm	0.0014	HOMO-6 -> LUMO HOMO-5 -> LUMO	86.2 % 9.4 %
279.29 nm	0.0553	HOMO -> LUMO+3 HOMO -> LUMO+5	79.6 % 11.8 %
277.33 nm	0.0020	HOMO -> LUMO+2 HOMO -> LUMO+4 HOMO -> LUMO+6	6.2 % 83.5 % 2.7 %
277.20 nm	0.0002	HOMO-7 -> LUMO HOMO -> LUMO+5	81.9 % 14.2 %
273.01 nm	0.0566	HOMO-7 -> LUMO HOMO-2 -> LUMO+1 HOMO -> LUMO+3 HOMO -> LUMO+5	13.9 % 3.0 % 11.8 % 64.8 %
267.70 nm	0.0859	HOMO-8 -> LUMO	94.6 %
267.26 nm	0.0127	HOMO-1 -> LUMO+1 HOMO -> LUMO+6	7.1 % 84.7 %
259.90 nm	0.0222	HOMO-2 -> LUMO+1 HOMO -> LUMO+7	5.9 % 87.6 %

258.10 nm	0.0009	HOMO-11 -> LUMO+1	5.9 %
		HOMO-10 -> LUMO	92.4 %
257.72 nm	0.0014	HOMO-11 -> LUMO	91.8 %
		HOMO-10 -> LUMO+1	6.0 %
253.00 nm	0.0697	HOMO-9 -> LUMO	7.0 %
		HOMO-3 -> LUMO+1	2.1 %
		HOMO-1 -> LUMO+1	73.3 %
		HOMO -> LUMO+4	2.7 %
		HOMO -> LUMO+6	7.2 %
		HOMO -> LUMO+11	2.6 %
251.08 nm	0.2594	HOMO-2 -> LUMO+1	76.4 %
		HOMO -> LUMO+5	4.4 %
		HOMO -> LUMO+7	4.7 %
		HOMO -> LUMO+8	6.5 %
249.57 nm	0.0075	HOMO-2 -> LUMO+1	5.5 %
		HOMO -> LUMO+8	80.5 %
		HOMO -> LUMO+10	6.0 %
248.32 nm	0.0004	HOMO-9 -> LUMO	66.5 %
		HOMO-4 -> LUMO+1	6.4 %
		HOMO-3 -> LUMO+1	8.0 %
		HOMO-1 -> LUMO+1	6.6 %
		HOMO -> LUMO+11	6.5 %
246.72 nm	0.0133	HOMO-4 -> LUMO+1	2.7 %
		HOMO-3 -> LUMO+1	2.5 %
		HOMO -> LUMO+9	81.6 %
		HOMO -> LUMO+17	4.9 %
245.03 nm	0.0372	HOMO-9 -> LUMO	8.6 %
		HOMO-5 -> LUMO+2	2.6 %
		HOMO-4 -> LUMO+1	25.1 %
		HOMO-3 -> LUMO+1	42.6 %
		HOMO-1 -> LUMO+1	3.8 %
		HOMO -> LUMO+9	4.9 %
243.67 nm	0.0001	HOMO -> LUMO+8	5.5 %
		HOMO -> LUMO+10	70.4 %
		HOMO -> LUMO+13	18.1 %

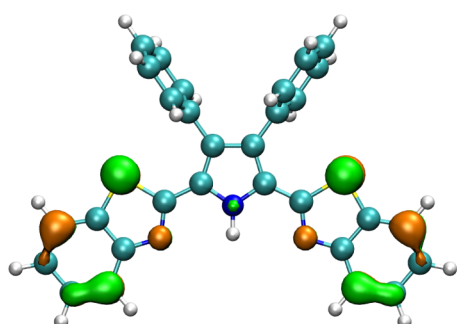
Selected Orbital Representations for 1



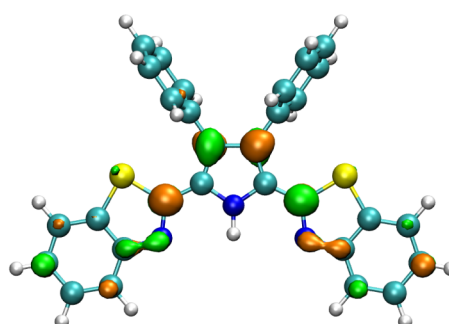
HOMO



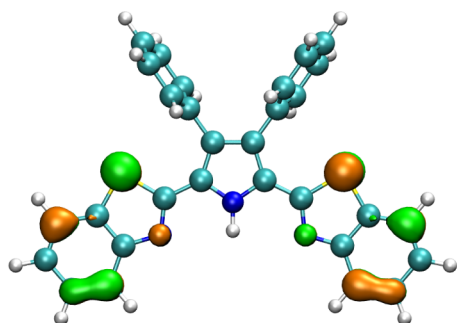
LUMO



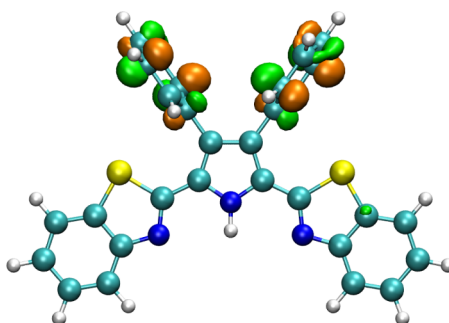
HOMO-1



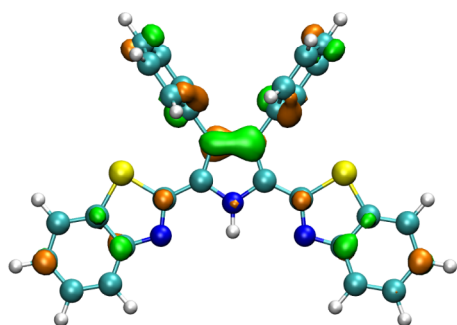
LUMO+1



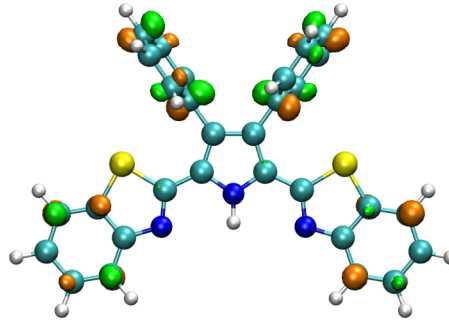
HOMO-2



LUMO+2



HOMO-3



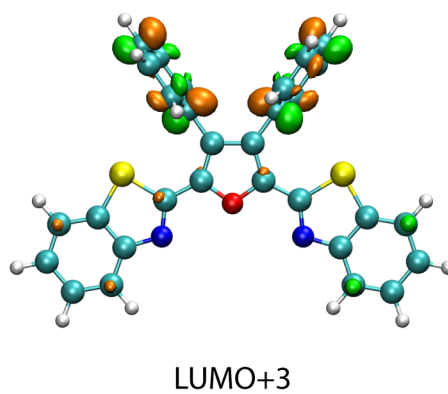
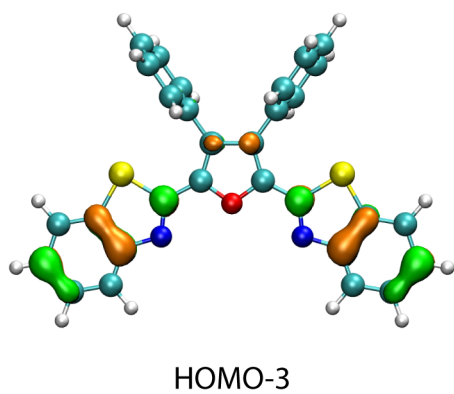
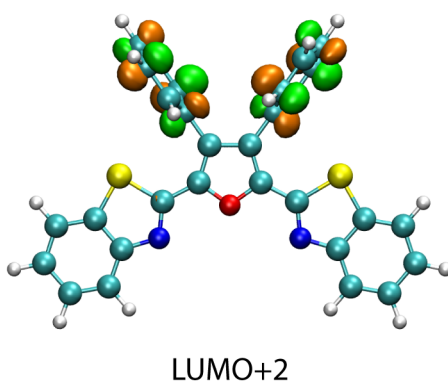
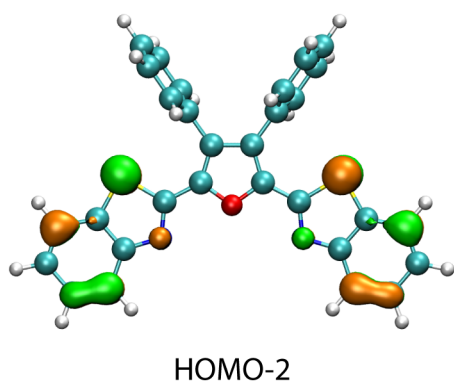
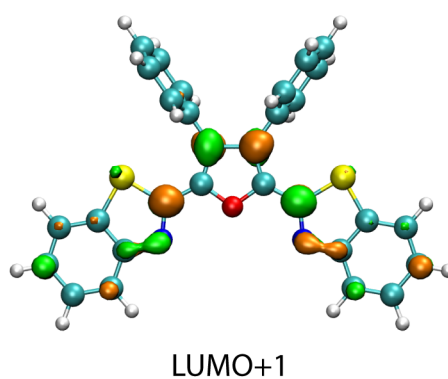
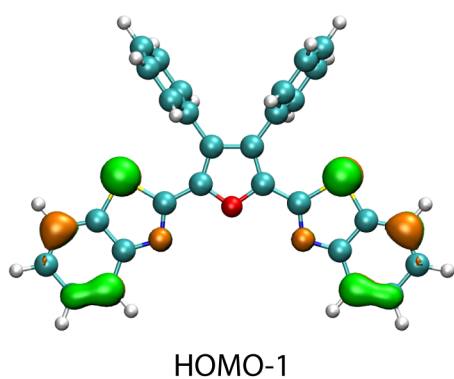
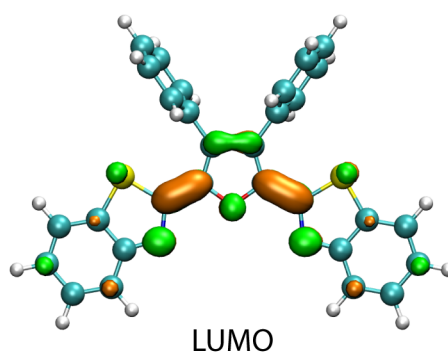
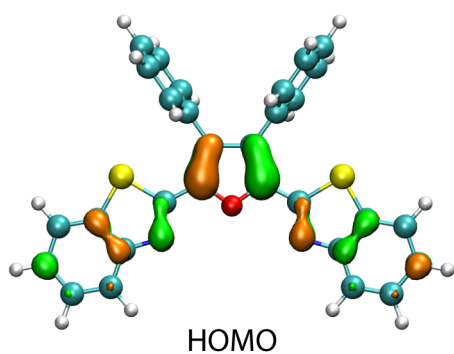
LUMO+3

Calculated Transitions for 2

Wavelength	Intensity	Levels	Character
419.38 nm	1.3305	HOMO -> LUMO	99.2 %
333.09 nm	0.0508	HOMO-1 -> LUMO	96.2 %
332.98 nm	0.0009	HOMO-2 -> LUMO	97.0 %
313.87 nm	0.0756	HOMO-4 -> LUMO	3.2 %
		HOMO-3 -> LUMO	81.1 %
		HOMO -> LUMO+1	13.4 %
304.39 nm	0.5001	HOMO-4 -> LUMO	14.6 %
		HOMO-3 -> LUMO	7.1 %
		HOMO -> LUMO+1	74.8 %
300.44 nm	0.0275	HOMO-6 -> LUMO	17.9 %
		HOMO-5 -> LUMO	80.8 %
298.27 nm	0.1199	HOMO-4 -> LUMO	80.7 %
		HOMO-3 -> LUMO	8.2 %
		HOMO -> LUMO+1	8.4 %
293.87 nm	0.0026	HOMO-6 -> LUMO	80.8 %
		HOMO-5 -> LUMO	18.0 %
286.03 nm	0.0041	HOMO-7 -> LUMO	97.3 %
277.98 nm	0.0220	HOMO -> LUMO+2	93.7 %
		HOMO -> LUMO+4	4.0 %
273.07 nm	0.0000	HOMO-10 -> LUMO+1	4.9 %
		HOMO-9 -> LUMO	93.6 %
272.45 nm	0.0009	HOMO-10 -> LUMO	92.2 %
		HOMO-9 -> LUMO+1	5.1 %
271.20 nm	0.0310	HOMO -> LUMO+3	91.8 %
270.20 nm	0.0003	HOMO-1 -> LUMO+1	7.1 %
		HOMO -> LUMO+2	3.3 %
		HOMO -> LUMO+4	84.6 %
266.33 nm	0.0004	HOMO-2 -> LUMO+1	22.5 %
		HOMO -> LUMO+5	69.6 %
262.56 nm	0.0172	HOMO-1 -> LUMO+1	35.5 %
		HOMO -> LUMO+4	5.3 %
		HOMO -> LUMO+6	49.9 %
255.36 nm	0.2989	HOMO-2 -> LUMO+1	49.3 %
		HOMO -> LUMO+3	3.6 %

		HOMO -> LUMO+5	18.3 %
		HOMO -> LUMO+7	25.0 %
252.67 nm	0.0245	HOMO-8 -> LUMO	21.9 %
		HOMO-1 -> LUMO+1	34.4 %
		HOMO -> LUMO+4	3.2 %
		HOMO -> LUMO+6	34.9 %
		HOMO -> LUMO+11	2.5 %
250.25 nm	0.0148	HOMO-8 -> LUMO	66.1 %
		HOMO-1 -> LUMO+1	16.8 %
		HOMO -> LUMO+6	7.4 %
249.73 nm	0.1009	HOMO-2 -> LUMO+1	20.2 %
		HOMO -> LUMO+5	5.3 %
		HOMO -> LUMO+7	65.3 %
243.52 nm	0.0032	HOMO-4 -> LUMO+1	11.5 %
		HOMO-3 -> LUMO+1	73.8 %
		HOMO-2 -> LUMO+2	3.2 %
		HOMO-1 -> LUMO+5	2.7 %
242.55 nm	0.1041	HOMO-11 -> LUMO	88.4 %
		HOMO -> LUMO+8	2.9 %
241.63 nm	0.0107	HOMO-11 -> LUMO	3.1 %
		HOMO -> LUMO+8	68.2 %
		HOMO -> LUMO+10	15.8 %
240.64 nm	0.0008	HOMO-6 -> LUMO+4	3.0 %
		HOMO-5 -> LUMO+2	6.5 %
		HOMO-4 -> LUMO+1	9.9 %
		HOMO-3 -> LUMO+1	9.7 %
		HOMO-2 -> LUMO+2	17.1 %
		HOMO-2 -> LUMO+4	6.7 %
		HOMO-1 -> LUMO+3	13.1 %
		HOMO -> LUMO+9	14.2 %
240.22 nm	0.0117	HOMO-7 -> LUMO+2	4.0 %
		HOMO-6 -> LUMO+1	14.3 %
		HOMO-6 -> LUMO+3	2.9 %
		HOMO-4 -> LUMO+2	2.7 %
		HOMO-4 -> LUMO+4	4.7 %
		HOMO-3 -> LUMO+2	3.4 %
		HOMO-2 -> LUMO+3	15.1 %
		HOMO-2 -> LUMO+5	2.4 %
		HOMO-1 -> LUMO+2	24.2 %
		HOMO-1 -> LUMO+4	3.5 %
		HOMO -> LUMO+7	4.6 %

Selected Orbital Representations for 2

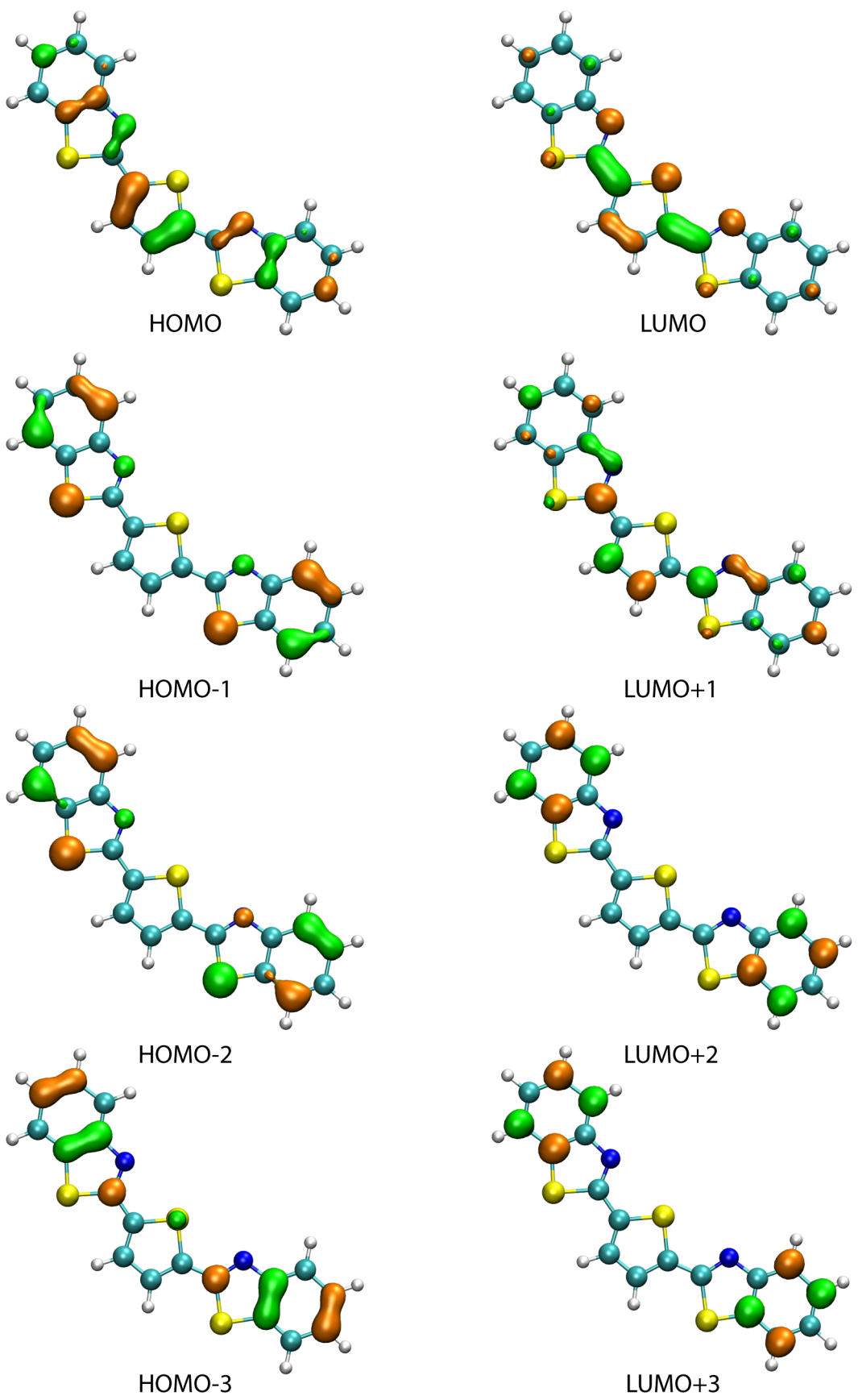


Calculated Transitions for 3

Wavelength	Intensity	Levels	Character
436.10 nm	1.4813	HOMO -> LUMO	99.2 %
347.57 nm	0.0585	HOMO-1 -> LUMO	97.3 %
345.62 nm	0.0022	HOMO-2 -> LUMO	97.8 %
322.61 nm	0.0197	HOMO-3 -> LUMO	96.6 %
302.05 nm	0.0002	HOMO-4 -> LUMO HOMO -> LUMO+1	40.9 % 56.4 %
284.01 nm	0.2064	HOMO-4 -> LUMO HOMO -> LUMO+1	57.2 % 40.5 %
281.51 nm	0.0005	HOMO-7 -> LUMO+1 HOMO-6 -> LUMO	3.4 % 96.0 %
274.41 nm	0.0000	HOMO-7 -> LUMO HOMO-6 -> LUMO+1	94.6 % 4.6 %
263.87 nm	0.0034	HOMO-5 -> LUMO HOMO-3 -> LUMO+3 HOMO-2 -> LUMO+6 HOMO-1 -> LUMO+1 HOMO -> LUMO+2	2.4 % 3.1 % 3.2 % 31.8 % 54.2 %
263.29 nm	0.0026	HOMO-3 -> LUMO+2 HOMO-2 -> LUMO+1 HOMO-1 -> LUMO+6 HOMO -> LUMO+3	3.4 % 29.4 % 2.8 % 60.4 %
257.58 nm	0.0456	HOMO-5 -> LUMO HOMO -> LUMO+2 HOMO -> LUMO+6	86.1 % 5.7 % 5.9 %
249.92 nm	0.0000	HOMO-3 -> LUMO+5 HOMO -> LUMO+4 HOMO -> LUMO+7	3.8 % 89.0 % 2.8 %
249.04 nm	0.1144	HOMO-5 -> LUMO HOMO-1 -> LUMO+1 HOMO -> LUMO+2	3.2 % 62.2 % 30.4 %
247.70 nm	0.3157	HOMO-2 -> LUMO+1 HOMO -> LUMO+3	64.5 % 31.9 %
246.75 nm	0.0016	HOMO-3 -> LUMO+4 HOMO -> LUMO+5 HOMO -> LUMO+8	4.9 % 88.3 % 4.1 %

240.47 nm	0.0029	HOMO-8 -> LUMO	3.5 %
		HOMO-4 -> LUMO+1	2.4 %
		HOMO-3 -> LUMO+1	73.8 %
		HOMO-2 -> LUMO+2	5.6 %
		HOMO-1 -> LUMO+3	6.8 %
		HOMO -> LUMO+2	3.3 %
236.69 nm	0.0448	HOMO-8 -> LUMO	16.2 %
		HOMO-3 -> LUMO+1	12.6 %
		HOMO-2 -> LUMO+2	5.5 %
		HOMO-1 -> LUMO+3	6.5 %
		HOMO -> LUMO+6	53.8 %
233.29 nm	0.0000	HOMO-9 -> LUMO	64.0 %
		HOMO-2 -> LUMO+3	11.2 %
		HOMO-1 -> LUMO+2	13.5 %
		HOMO -> LUMO+3	2.1 %
		HOMO -> LUMO+10	4.8 %
232.43 nm	0.0000	HOMO -> LUMO+4	3.4 %
		HOMO -> LUMO+7	90.8 %
229.29 nm	0.0060	HOMO-8 -> LUMO	73.4 %
		HOMO -> LUMO+6	20.4 %
229.20 nm	0.0000	HOMO-2 -> LUMO+5	38.9 %
		HOMO-1 -> LUMO+4	48.8 %
		HOMO -> LUMO+5	2.1 %
		HOMO -> LUMO+11	2.9 %
228.90 nm	0.0000	HOMO-2 -> LUMO+4	47.0 %
		HOMO-1 -> LUMO+5	41.5 %
		HOMO -> LUMO+7	3.5 %
225.82 nm	0.0005	HOMO -> LUMO+8	8.6 %
		HOMO -> LUMO+11	77.8 %
		HOMO -> LUMO+14	6.0 %
225.29 nm	0.0428	HOMO-9 -> LUMO	30.9 %
		HOMO-2 -> LUMO+3	26.7 %
		HOMO-1 -> LUMO+2	35.2 %
224.24 nm	0.3715	HOMO-4 -> LUMO+1	62.2 %
		HOMO-2 -> LUMO+2	12.5 %
		HOMO-1 -> LUMO+3	14.6 %
		HOMO -> LUMO+6	4.8 %

Orbital Representation for 3



Photophysics of 1 in Polystyrene

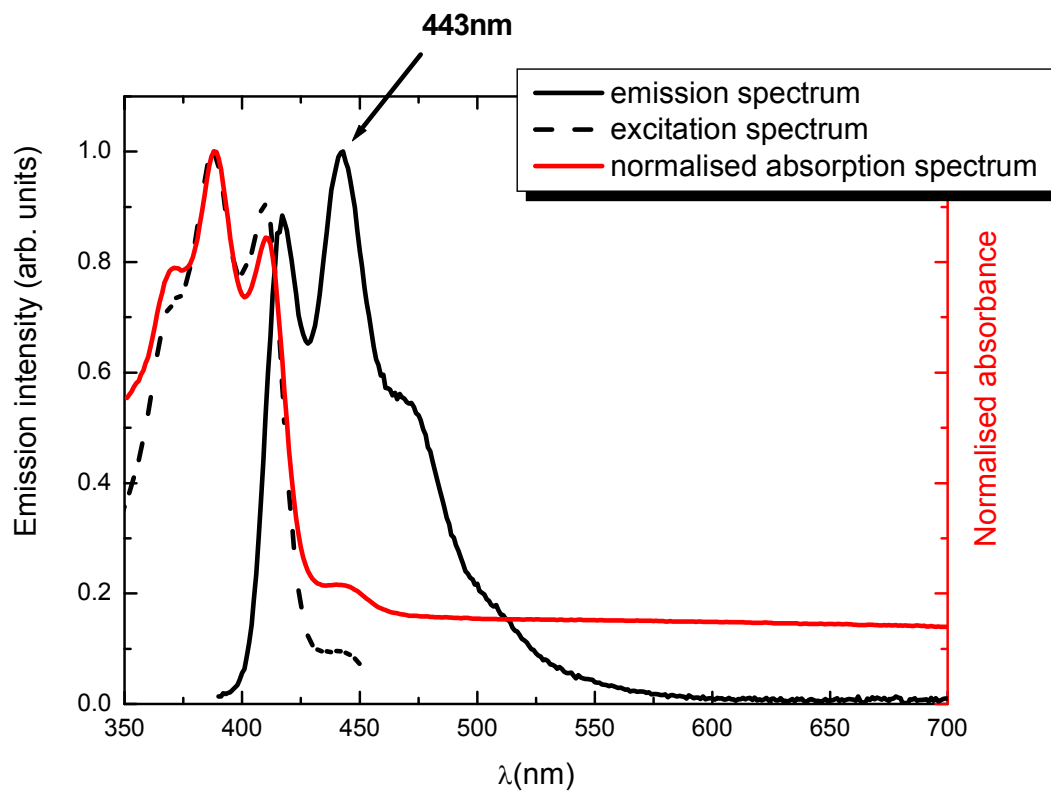


Figure S2. Absorption, excitation and emission profiles of a polystyrene matrix doped with 0.1% of **1**. The emission profiles was measured at $\lambda_{\text{ex}}=360$ nm.