Electronic Supplementary Information for

Identification and Isolation of Highly Emissive Cinnamic Derivatives in π-Stacked Polybenzofulvene Derivatives for Optoelectronic Applications

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Table ESI1. Optical properties of cinnamic derivatives **1a-c** compared with those of the corresponding polybenzofulvene derivatives poly-6-DMFL-**BF3k**, poly-6-MCBZ-**BF3k**, and poly-6-TPA-**BF3k**.

	solution[a]			powder	
compound or polymer	λ_{ab} (nm)	λ_{emi} (nm)	QY (%)	λ_{emi} (nm)	QY (%)
1a	334	430	57	407	64 [b]
poly-6-DMFL-**BF3k** [c]	295, 319, 345	465	21	486 [d]	24 [d]
1b	242, 302, 347	480	77	448, 466	69 [e]
poly-6-MCBZ-**BF3k** [c]	290, 350	497	17	535	19
1c	292, 371	540	78	470	80 [f]
poly-6-TPA-**BF3k** [c]	305, 377	495	46	530	35

[a] dichloromethane, [b] λ_{ex} = 350 nm, [c] see ref [1], [d] cast films from dichloromethane solutions, [e] λ_{ex} = 380 nm, [f] λ_{ex} = 420 nm.

Table ESI2.TD-DFT (MPW1K/6-311+G(2d,p) computed absorption maxima (λ_a^{max}, nm), vertical excitation energies (E_{exc}, eV), oscillator strengths (*f*) and composition in terms of molecular orbitals for the lowest singlet-singlet excitation of **1a, 1b, 1c'** and **1c''** in CH_2Cl_2 and for **1c**, **1c'** and **1c''** in gas-phase.

Molecules		Excited states	λ^a_{max}	E_{exc}	f	Transition (%)
1a	CH_2Cl_2	1	336	3.68	1.70	89% H→L
1b	CH_2Cl_2	1	336	3.69	1.64	85% H-1→L
		2	325	3.82	0.06	72% H→L
		3	275	4.51	0.08	31% H→L+1 24% H-2→L
		8	238	5.21	0.31	35% H→L+3 14% H-3→L
		9	232	5.35	0.34	31% H-3→L 8%H-1→L+2
1c	Gas-phase	1	367	3.38	0.09	62% H-2→L+1
		3	358	3.46	0.21	56% H-3→L
		4	349	3.56	2.67	29% H-1→L+3 13% H-2→L+1 9% H-2→L
1c'	CH_2Cl_2	1	364	3.40	1.30	85% H→L
		3	286	4.34	0.31	82% H→L+3
		4	285	4.34	0.21	64% H-1→L 9% H→L+3
1c'	Gas-phase	1	351	3.52	1.17	82% H→L
		3	283	4.37	0.22	88% H→L+3
		4	278	4.46	0.22	64% H-1→L
1c''	CH_2Cl_2	2	366	3.38	2.54	51% H-1→L
		8	287	4.33	0.19	45% H→L+6
		9	287	4.33	0.37	45% H→L+7
		10	284	4.36	0.51	44% H-3→L 9% H-1→L+7
1c''	Gas-phase	2	356	3.48	2.24	53% H-1→L 24% H-2→L+1
		7	286	4.34	0.28	31% H-1→L+6 26% H→L+7
		8	285	4.34	0.14	40% H→L+6 34% H-1→L+7
		10	277	4.47	0.42	40% H-3→L 23% H-2→L+1

References

[1] A. Cappelli, V. Razzano, G. Fabio, M. Paolino, G. Grisci, G. Giuliani, A. Donati, R. Mendichi, W. Mróz, F. Villafiorita-Monteleone, C. Botta, Side chain engineering in π-stacked polybenzofulvene derivatives bearing electron-rich chromophores for OLED applications, RSC Adv. 5 (2015) 101377–101385. doi:10.1039/c5ra21164f.