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Supplementary Materials: 3-(N,N-Diphenylamino)carbazole Donor Containing Bipolar Derivatives with Very High Glass Transition Temperatures as Potential TADF Emitters for OLEDs

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Instrumentation

NMR spectra were recorded using a Bruker DPX 250 apparatus (Bruker, Billerica, MA, USA). Mass spectra were obtained on a Varian MAT-312-Spectrometer Waters ZQ 200 spectro-chromatograph (Bruker). Fourier transform infrared (FTIR) spectra were measured using a Bio-Rad Digilab FTS-40 spectrometer (Bruker).

Ultraviolet (UV) spectra were measured with a Shimadzu UV-1601PC spectrophotometer (Bruker).

Fluorescence (FL) spectra were recorded with a charge-coupled-device (CCD) Aminco-Bowman Series 2 spectrograph (Bruker).

Differential scanning calorimetry (DSC) measurements were carried out using a TA Instrument DSC-2920 low-temperature scanning calorimeter (TA Instruments, Alzenau, Germany).

Thermogravimetric analysis (TGA) was performed on a TA Instrument 2950 TGA thermal analyzer (TA Instruments). The TGA and DSC measurements were recorded in a nitrogen atmosphere at a heating rate of 10 °C/min.

Citation: Tavgeniene, D.; Beresneviciute, R.; Blazevicius, D.; Krucaite, G.; Jacunskaite, G.; Sudheendran Swayamprabha, S.; Jou, J.-H.; Grigalevicius, S. 3-(N,N-Diphenylamino)carbazole Donor Containing Bipolar Derivatives with very High Glass Transition Temperatures as Potential TADF Emitters for OLEDs. *Coatings* **2022**, *12*, 932. https://doi.org/10.3390/coatings12070932

Academic Editor: Chen Tei-Chen

Received: 6 June 2022
Accepted: 29 June 2022
Published: 1 July 2022

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Table S1. Photophysical, thermal, and electrochemical characteristics of the objective derivatives **6**–**8**.

Material	λ_{abs}[a] (nm)	λ_{PL}[b] (nm)	λ_{PL}[c] (nm)	T_g[d] (°C)	T_d[e] (°C)	HOMO/LUMO[f] (−eV)
6	360	466	472	173	389	5.62/2.91
7	370	421	460	111	351	5.61/2.95
8	345	545	549	159	398	5.58/2.79

[a] Absorbance peaks; [b] Photoluminescence (PL) spectra peak measured at room temperature from toluene solution; [c] Photoluminescence (PL) spectra peak measured at room temperature from thin film; [d] Glass transition temperature; [e] Decomposition temperature; [f] the redox potential obtained using a cyclic voltammetry (CV) technique gives HOMO and LUMO. The potential to semi-oxidation ($E_{1/2}^{ox}$) from $(E_{p1} + E_{p2})/2 - 0.48$ has been computed, where 0.48 is correctly estimated as the value of ferrocenium/ferrocene (Fc^+/Fc) has been included in the internal standard. Then the energy from the HOMO = $-(E_{1/2}^{ox} + 4.8)$ was found. The LUMO energy level was calculated by removing the gap from HOMO, [$E_{LUMO} = -E_{HOMO} + Eg$].

Table S2. Summarized electroluminescent properties of the described OLEDs.

Dopant	Dopant (wt%)	$PE_{100}/CE_{100}/EQE_{100}$ (lm W^{-1}/cd A^{-1}/%)	$PE_{1000}/CE_{1000}/EQE_{1000}$ (lm W^{-1}/cd A^{-1}/%)	CIE_{xy} Coordinates	Max. Lum. (cd m^{-2})
6	5	1.6/2.5/1.5	0.3/0.7/0.4	(0.17, 0.24)	3160
	10	1.7/2.8/1.6	1.0/2.4/1.4	(0.18, 0.25)	2598
	15	2.2/3.2/1.7	1.2/2.5/1.4	(0.18, 0.27)	2632
	20	2.2/3.2/1.6	1.2/2.4/1.3	(0.18, 0.28)	2442
7	5	1.2/1.9/1.3	0.3/0.7/-	(0.17, 0.21)	1005
	10	0.5/1.0/0.6	-/-/-	(0.18, 0.23)	825
	15	1.1/1.9/1.1	-/-/-	(0.18, 0.24)	926

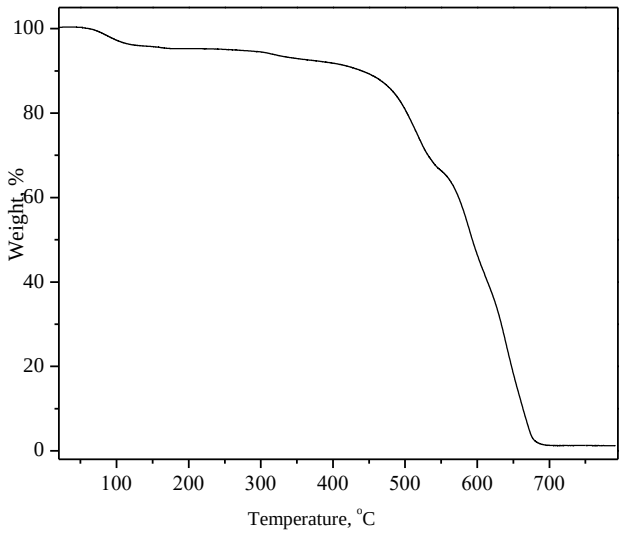

Figure S1. TGA curve of compound **6**. Heating rate: 10 °C min^{-1}.

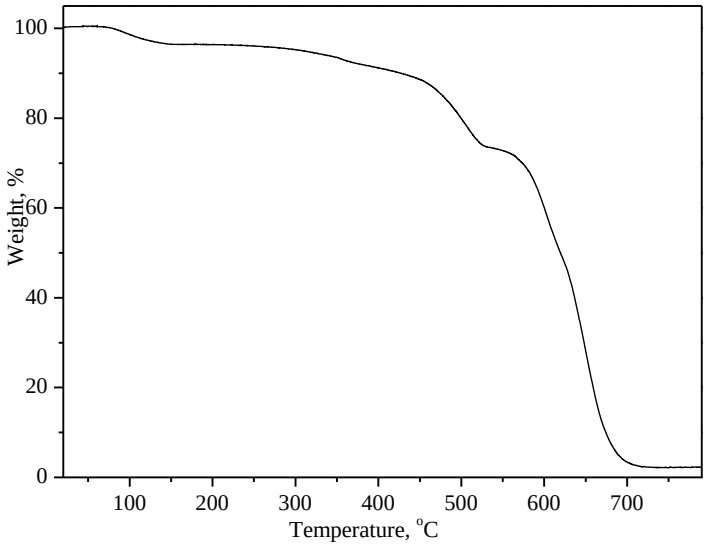

Figure S2. TGA curve of compound **8**. Heating rate: 10 °C min⁻¹.

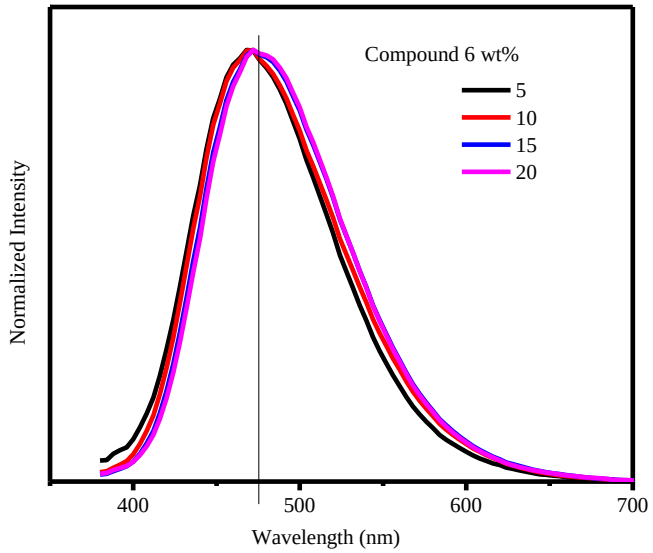

Figure S3. Emission spectra of OLEDs using emitter **6** in CBP host.