

Supporting Information

A Phosphorescent OLED with Efficiency Roll-Off Lower than 1% at 10,000 cd/m² Achieved by Reducing the Carrier Mobility of the Donors in Exciplex Co-host System

Chun-Hao Chiu^a, Nurul Ridho Al Amin^{b,c,d}, Jia-Xun Xie^a, Chih-Chien Lee^d, Dian Luo^c, Sajal Biring^{b,c}, Kevin Sutanto^{b,c}, Shun-Wei Liu^{b,c,*}, Chih-Hsin Chen^{a,*}

^aDepartment of Chemistry, Tamkang University, New Taipei City 251, Taiwan

^bOrganic Electronics Research Center, Ming Chi University of Technology, New Taipei City 24301, Taiwan

^cDepartment of Electronic Engineering, Ming Chi University of Technology, New Taipei City 24301, Taiwan

^dDepartment of Electronic Engineering, National Taiwan University of Science and Technology, Taipei 10617, Taiwan

*Corresponding authors: chc@mail.tku.edu.tw (Chih-Hsin Chen)

swliu@mail.mcut.edu.tw (Shun-Wei Liu)

Table S1. The decay lifetime of BCzPh-pimi, BCzPh-mimi and their blended films with B3PyMPM.

sample	TRPL decay curve	
	T ₁ (ns)	T ₂ (ns)
BCzPh-pimi	5.39	---
BCzPh-mimi	9.46	---
BCzPh-pimi/B3PyMPM	63.73	274.79
BCzPh-mimi/B3PyMPM	54.16	263.21

Table S2. The hole mobility of hole only device (HOD) and electron mobility of electron only device (EOD) by SCLC methods.

sample	hole mobility (cm ² V ⁻¹ s ⁻¹)	electric field (V cm ⁻¹) ^{1/2}
BCzPh-pimi	2.80 x 10 ⁻⁶	850 - 950
BCzPh-mimi	1.13 x 10 ⁻⁶	850 - 950
BCzPh	1.13 x 10 ⁻⁵	700 - 800
sample	electron mobility (cm ² V ⁻¹ s ⁻¹)	electric field (V cm ⁻¹) ^{1/2}
BCzPh-pimi	1.39 x 10 ⁻⁹	850 - 950
BCzPh-mimi	5.98 x 10 ⁻⁹	800 - 900
B3PyMPM	7.79 x 10 ⁻⁶	800 - 900

Table S3. Summary of the UV and PL spectra data of BCzPh-pimi and BCzPh-mimi.

compound	solvent	toluene	DPE	diethyl ether	DCM	DMF	ACN
	polarity	0.01	0.08	0.16	0.22	0.27	0.31
BCzPh-pimi	UV (nm)	338	340	335	334	325	327
	PL (nm)	403	412	403	452	464	476
	$\nu_a-\nu_f$ (cm ⁻¹)	4894	5139	5036	7816	9217	9572
BCzPh-mimi	UV (nm)	304	305	302	303	302	301
	PL (nm)	404	409	403	458	475	498
	$\nu_a-\nu_f$ (cm ⁻¹)	8203	8337	8298	11169	12059	13142

DPE: diphenyl ether; DCM: dichloromethane; DMF: dimethylformamide; ACN: acetonitrile.

Table S4. The calculated excited-state dipole moments of BCzPh-pimi and BCzPh-mimi.

compound	μ_g^a (Debye)	excited-state dipole (Debye)	
		LE ^b	CT ^c
BCzPh-pimi	3.46	8.15	32.68
BCzPh-mimi	4.22	8.10	33.73

^a μ_g is calculated by using the DFT method at the B3LYP/6-31G(d) levels. ^bCalculated from the slope of the fitted line in the low-polarity solvents. ^cCalculated from the slope of the fitted line in the high-polarity solvents. The excited-state dipole moment can be calculated from the slope of Lippert–Mataga plot, Stokes shift ($\nu_a-\nu_f$) against the solvent polarizability, f , according to the Lippert–Mataga equation.²⁴

Table S5. The hole only device (HOD) hole mobility and electron only device (EOD) electron mobility by SCLC methods.

sample	hole mobility ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	electric field (V cm^{-1}) ^{1/2}
BCzPh-pimi	2.80×10^{-6}	850 – 950
BCzPh-mimi	1.13×10^{-6}	850 – 950
BCzPh	1.13×10^{-5}	700 – 800
BCzPh-pimi:B3PyMPM	2.79×10^{-9}	900 – 1000
BCzPh-mimi:B3PyMPM	7.48×10^{-10}	950 – 1050
sample	electron mobility ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	electric field (V cm^{-1}) ^{1/2}
BCzPh-pimi	1.39×10^{-9}	850 – 950
BCzPh-mimi	5.98×10^{-9}	800 – 900
B3PyMPM	7.79×10^{-6}	800 – 900
BCzPh-pimi:B3PyMPM	7.45×10^{-8}	900 – 1000
BCzPh-mimi:B3PyMPM	2.67×10^{-10}	950 – 1050

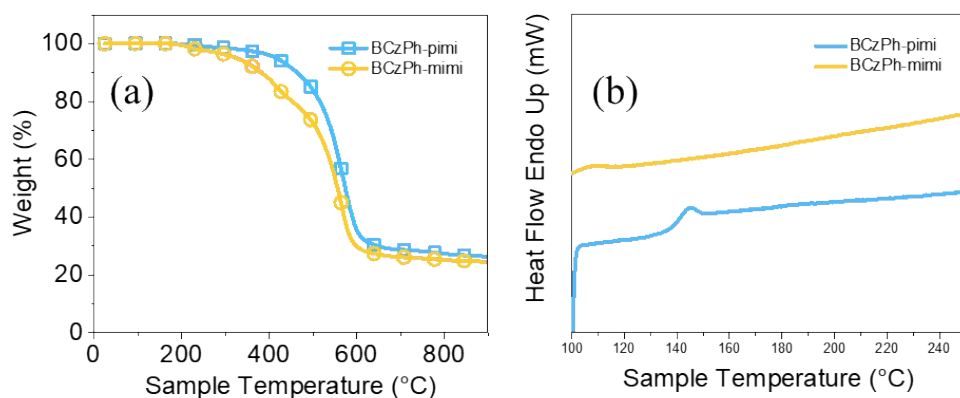


Figure S1. (a) TGA and (b) DSC curves of BCzPh-pimi and BCzPh-mimi.

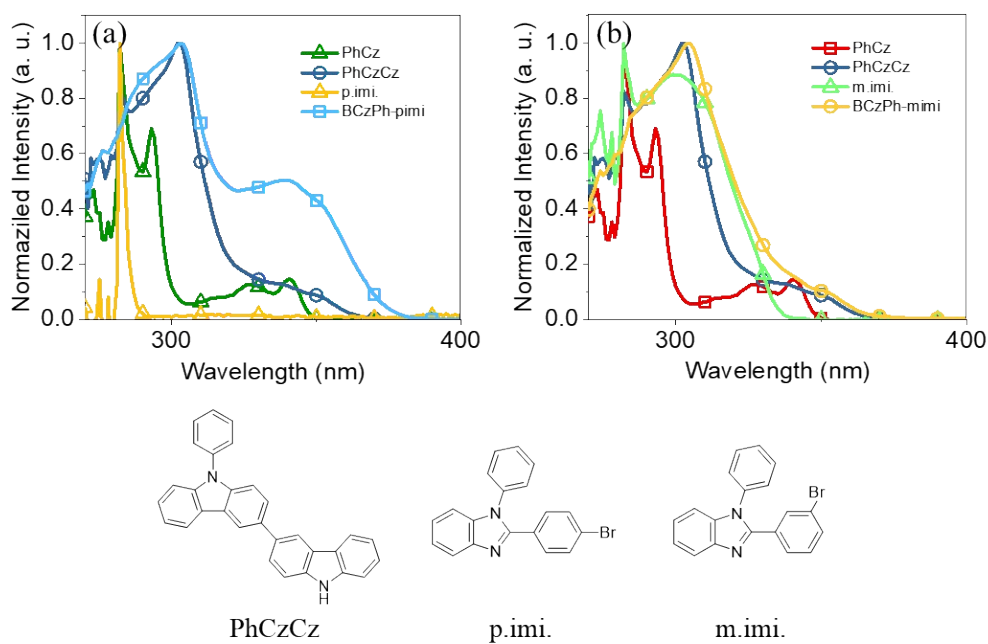


Figure S2. UV-Vis spectra and molecular structure of each moiety of (a) BCzPh-pimi and (c) BCzPh-mimi in toluene.

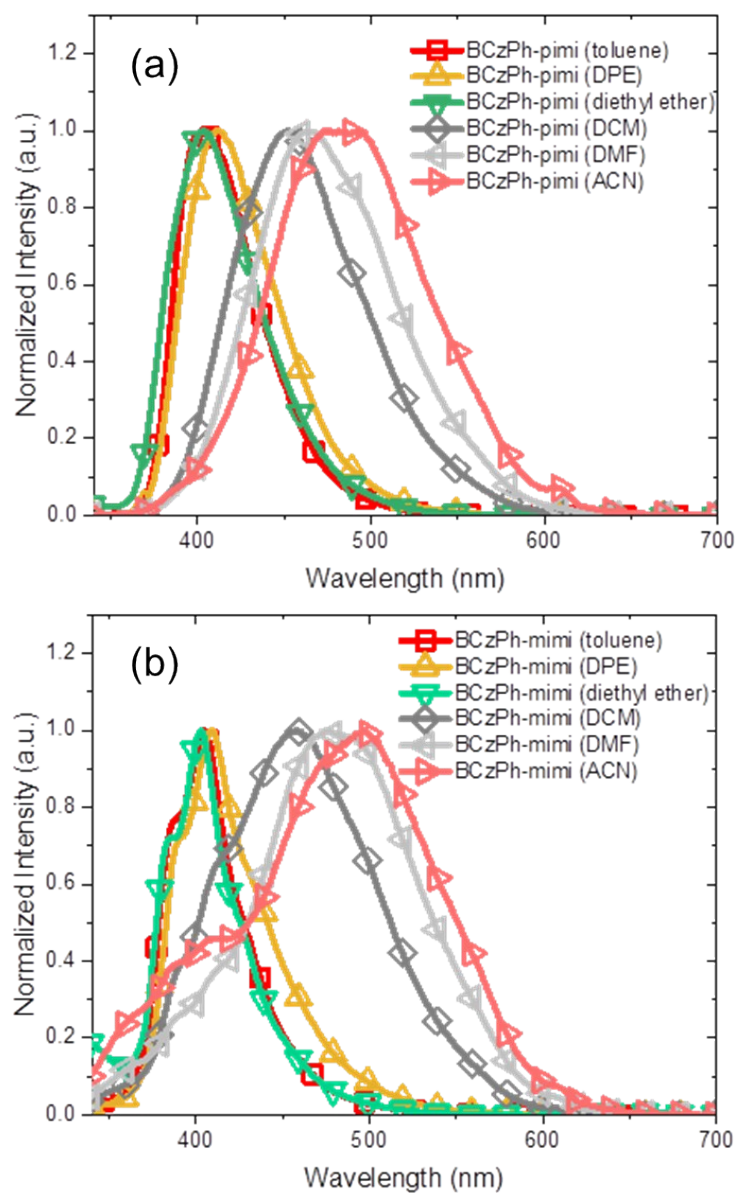


Figure S3. Fluorescence spectra of BCzPh-pimi, BCzPh-mimi in toluene and dichloromethane (DCM) at 1×10^{-5} M.

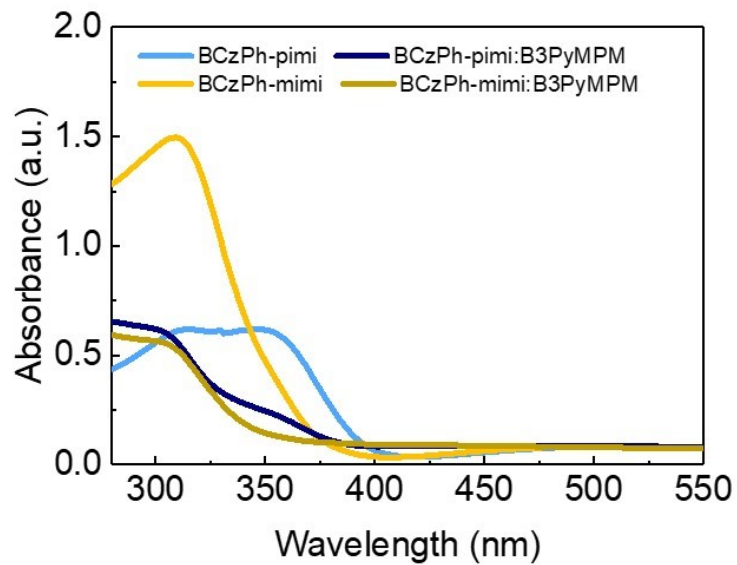


Figure S4. UV-Vis spectra of the bare films of BCzPh-pimi, BCzPh-mimi and their blended films with B3PyMPM measured in room temperature.

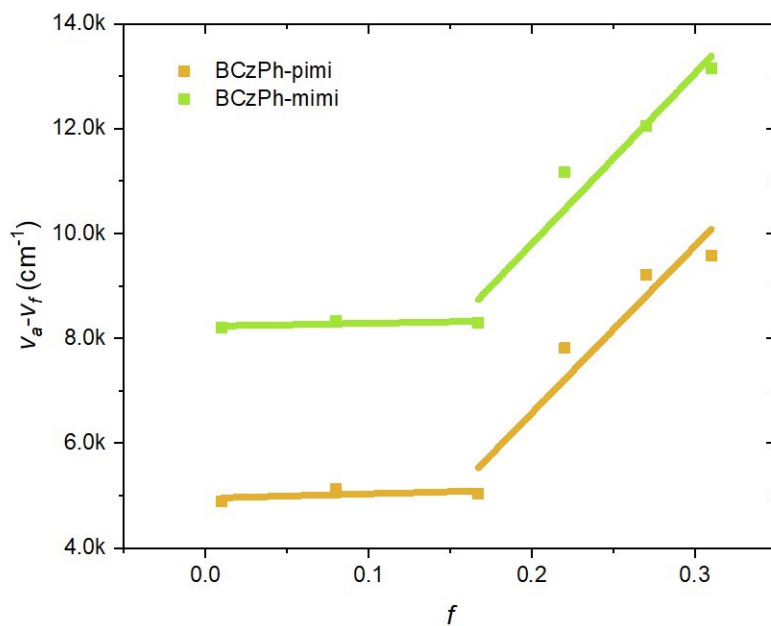


Figure S5. The fitted linear correlation of the Stokes shift against the different solvent polarizability for BCzPh-pimi and BCzPh-mimi.

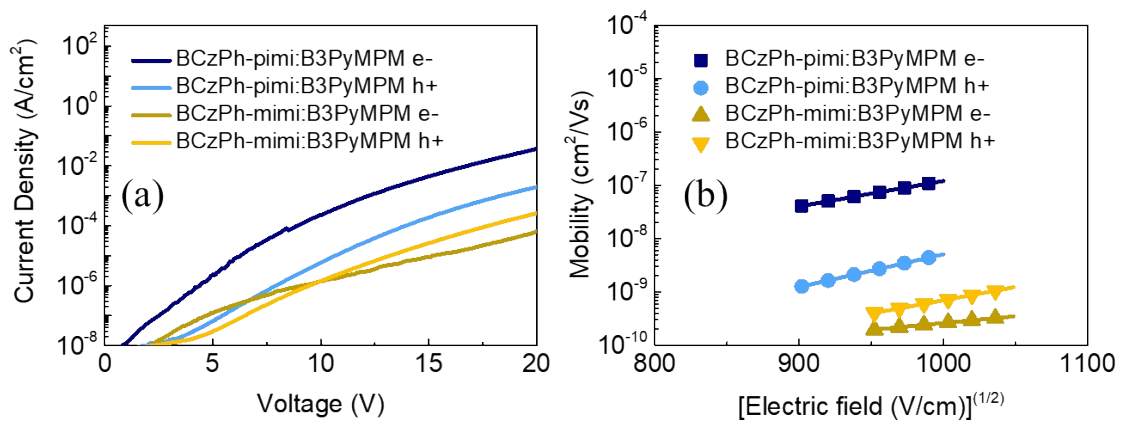


Figure S6. The mobility measurement for the blended films of BCzPh-pimi:B3PyMPM and BCzPh-mimi:B3PyMPM. (a) Current density of hole and electron only device. (b) Hole and electron only device mobility.

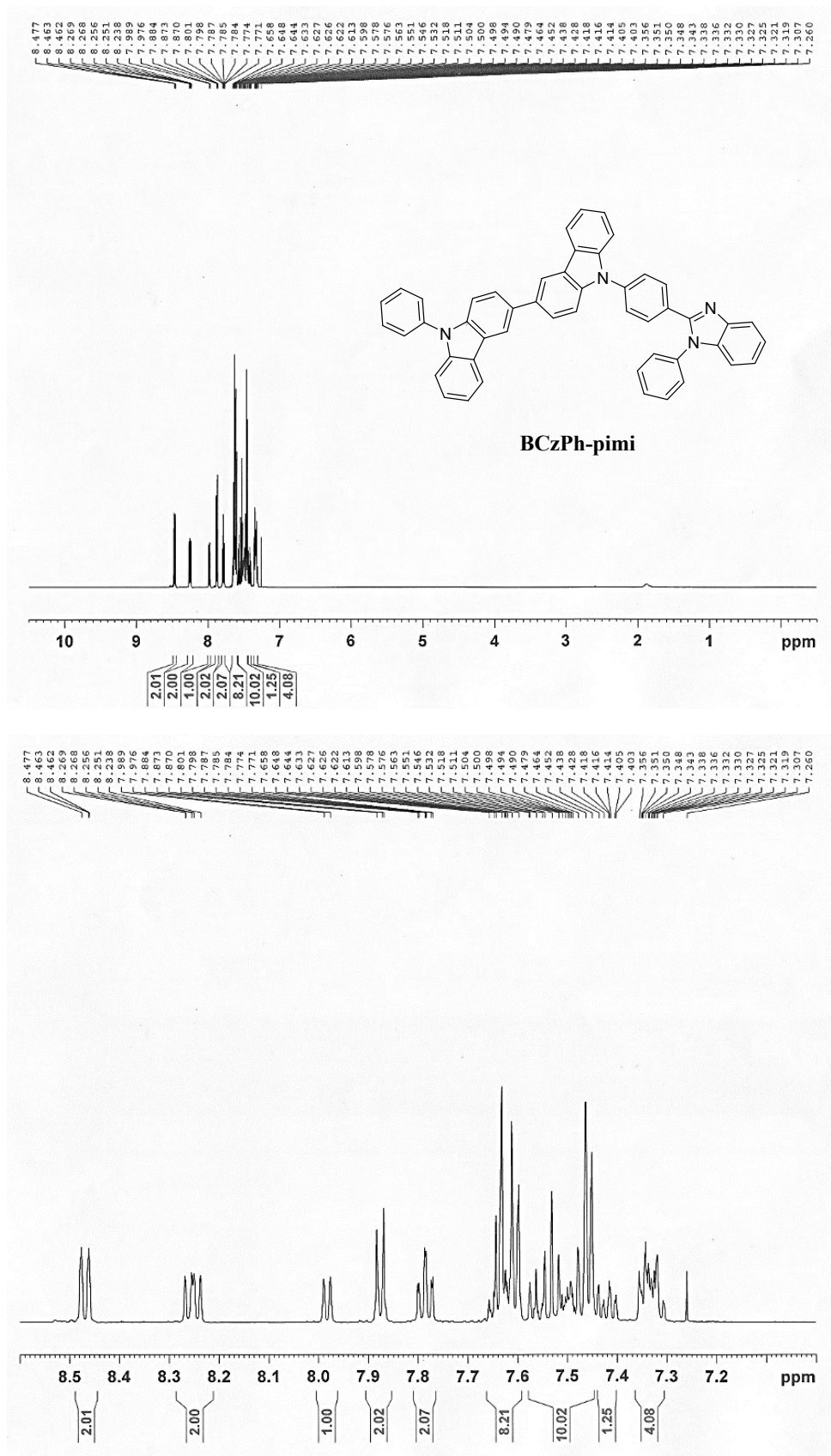


Figure S7. ^1H NMR spectrum of BCzPh-pimi in CDCl_3 .

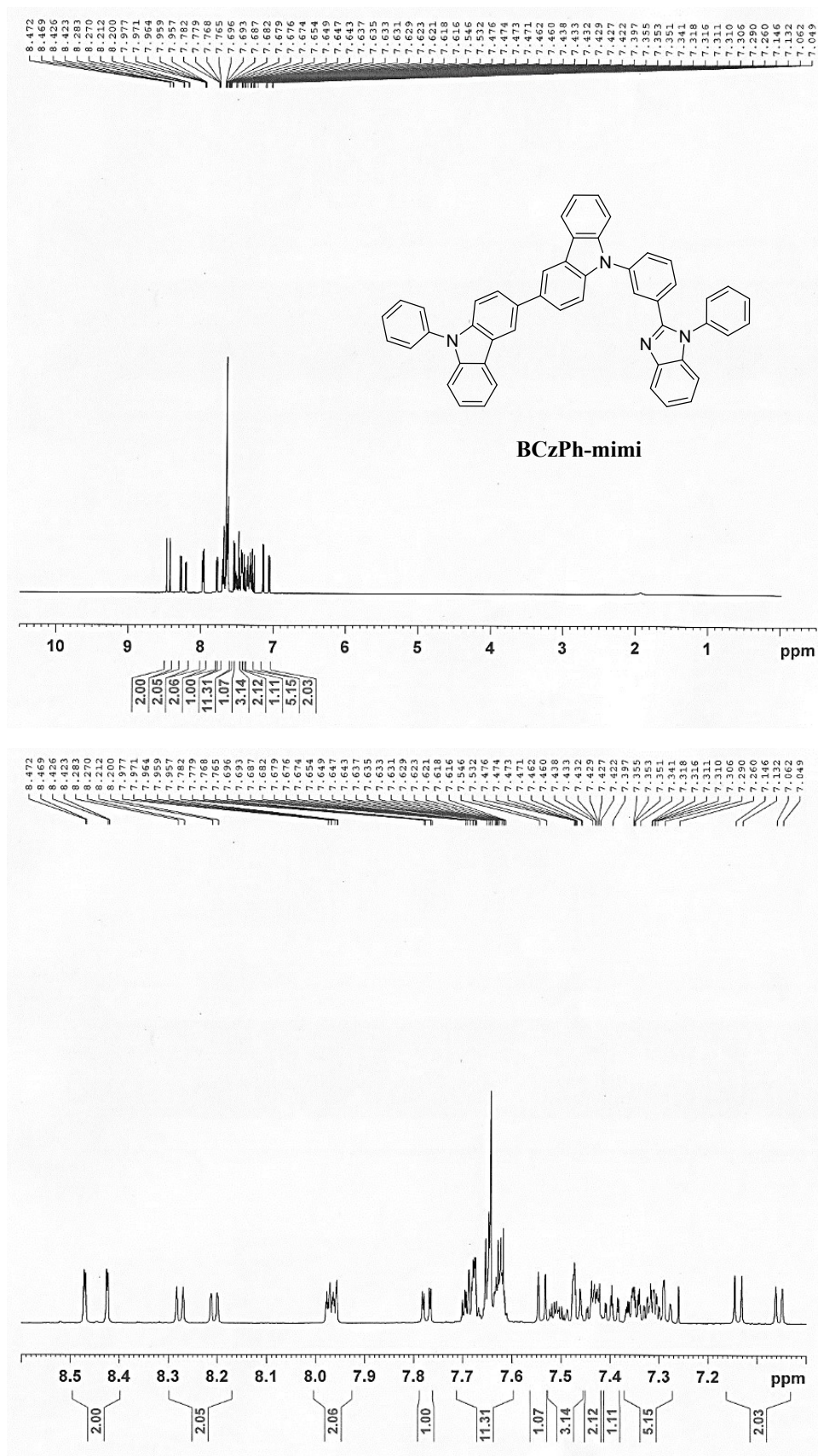


Figure S8. ^1H NMR spectrum of BCzPh-mimi in CDCl_3 .

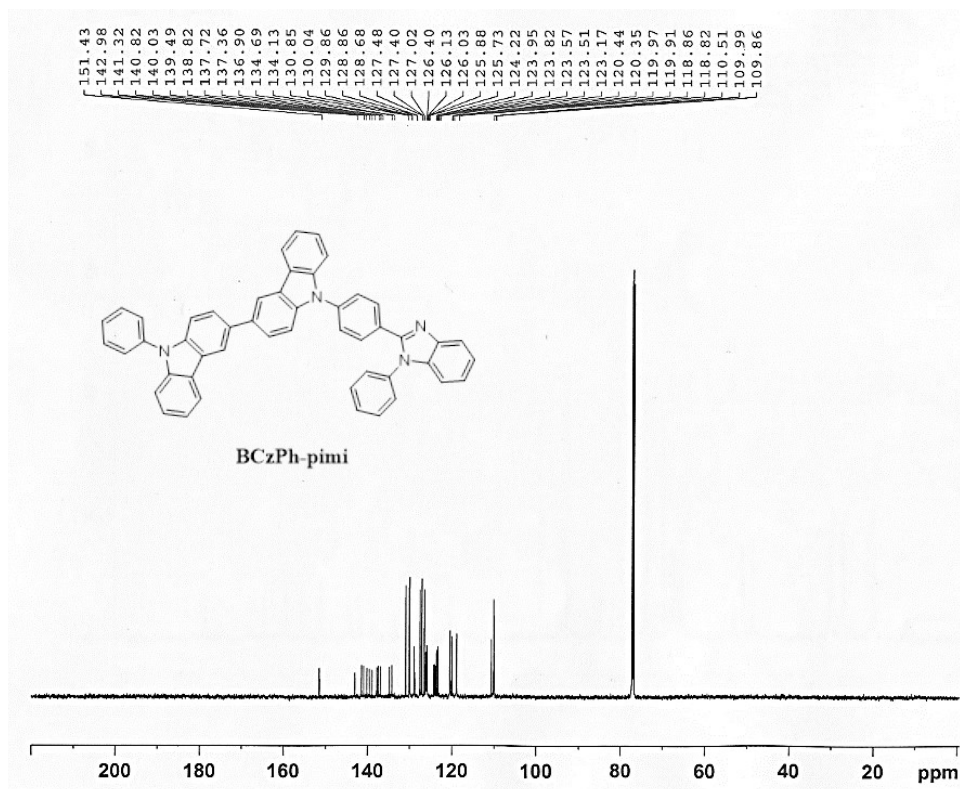


Figure S9. ¹³C NMR spectrum of BCzPh-pimi in CDCl₃.

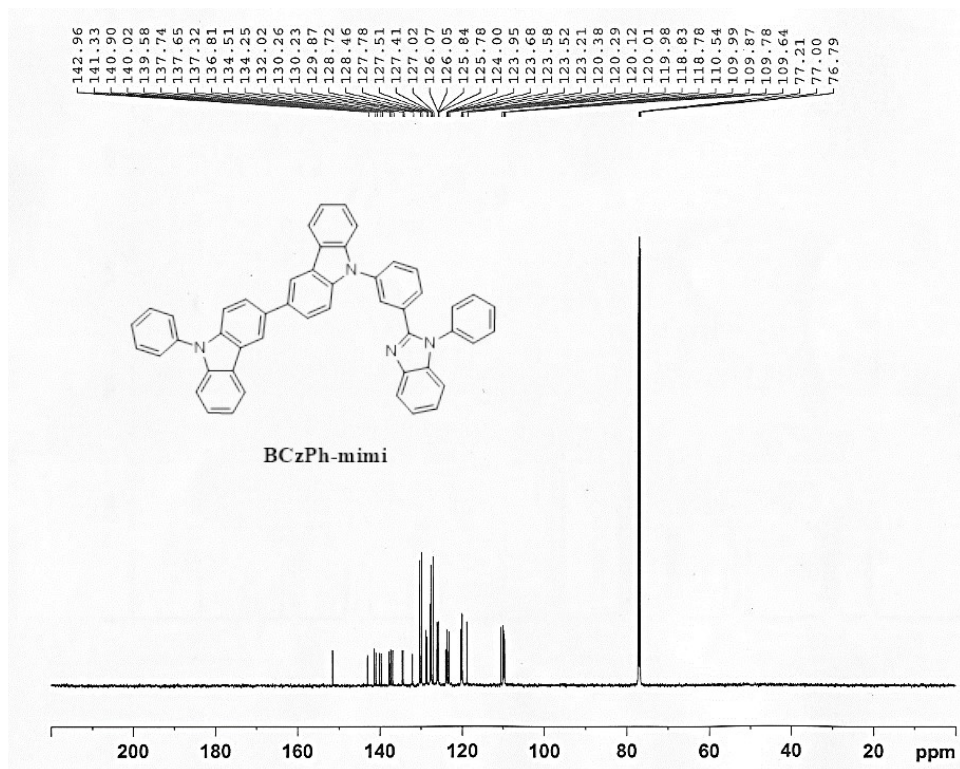


Figure S10. ¹³C NMR spectrum of isolated compound BCzPh-mimi in CDCl₃.

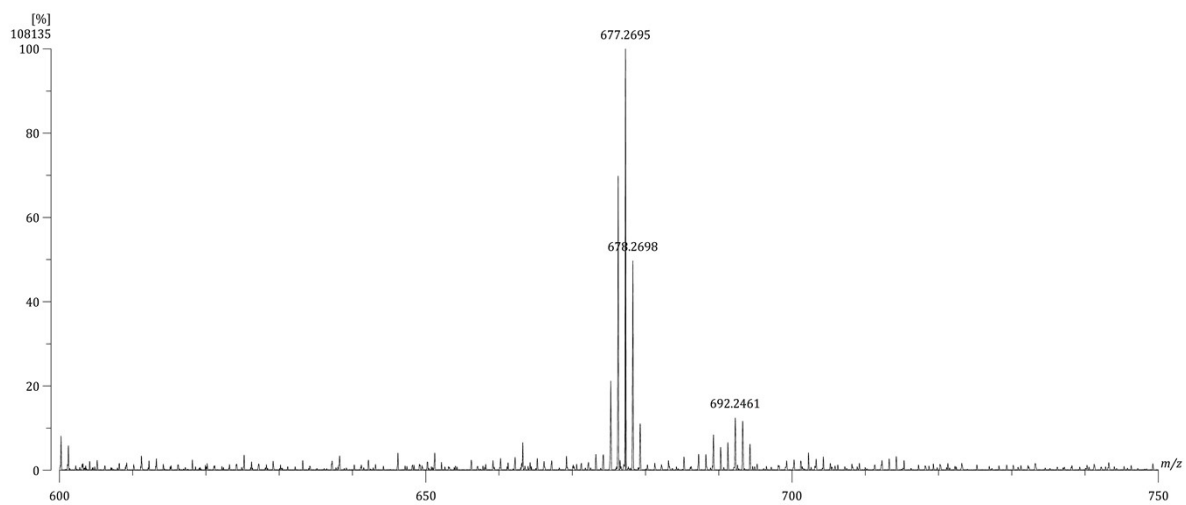


Figure S11. Mass spectrum of BCzPh-pimi.

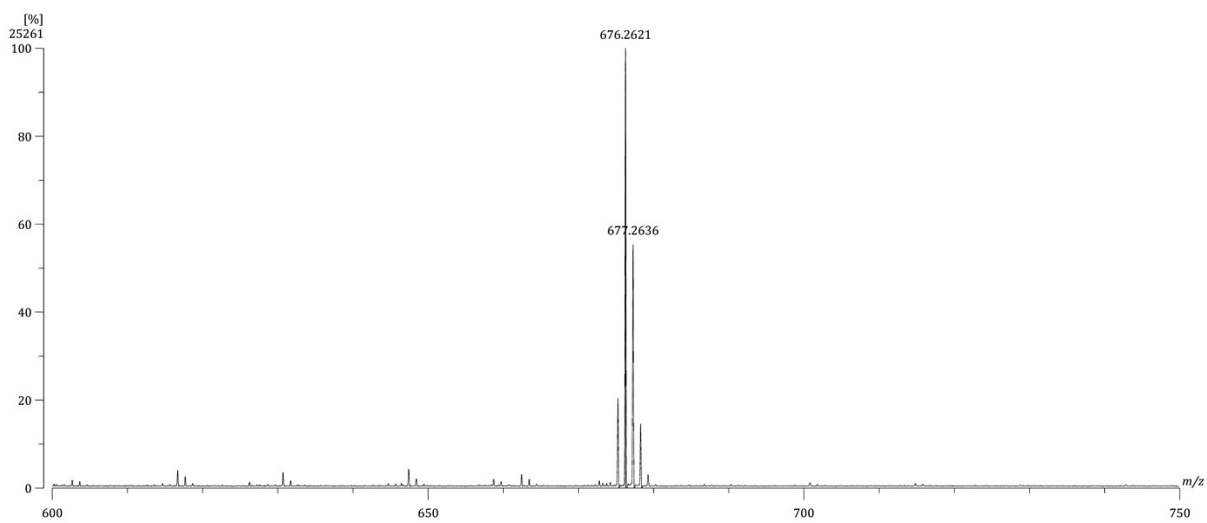


Figure S12. Mass spectrum of BCzPh-mimi.