

Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

A Universal Bipolar Host Based on Isonicotinonitrile and Carbazole for Efficient Red, Green and Blue PhOLEDs

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Experimental section

General information

Chemicals and solvents used in the process were reagent grades and purchased from commercial companies without further purification. The ^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were measured using a Bruker AM400 spectrometer. Mass spectra (MS) were obtained on a Waters LCT Premier XE spectrometer. Purity was measured by a SHIMADZU LC-20A liquid chromatograph. The melting point was measured by an INESA WRR melting point apparatus. The ultraviolet-visible (UV-Vis) absorption spectra of the samples were characterized using a Agilent spectrophotometer. Photoluminescence (PL) measurements were conducted by a Agilent fluorescence spectrophotometer at room temperature. The photoluminescence quantum yield (PLQY) was measured by a HAMAMATSU Quantaurus-QY C11347-11 fluorescence spectrophotometer. The cyclic voltammetry (CV) experiments were performed by a Versastat II electrochemical workstation (Princeton applied research). The differential scanning calorimetry (DSC) analysis was performed under a nitrogen atmosphere using a SHIMADZU DSC-60 Plus instrument with a heating scan rate of $10\text{ }^\circ\text{C}/\text{min}$. Thermogravimetric analysis (TGA) was carried out using a SHIMADZU TGA-50/50H instrument under a nitrogen atmosphere with a heating scan rate of $10\text{ }^\circ\text{C}/\text{min}$.

All OLEDs were fabricated on the pre-patterned indium tin oxide (ITO) glass substrate with sheet resistance of $10\ \Omega/\square$. OLEDs have an active area of $3.0\times 3.0\ \text{mm}^2$, defined by the overlap between the ITO anode and Al cathode. The ITO substrates were cleaned first with acetone, deionized water and acetone, and then dried in drying cabinet,

and treated with ultraviolet-ozone for 15 min. After these processes, the cleaned ITO glass substrates were loaded in a vacuum chamber, a base pressure of $\leq 5 \times 10^{-4}$ Pa, for film deposition using thermal evaporation technology. The deposition rate and film thickness were monitored controlled by the calibrated crystal quartz sensors, e.g., the deposition rates of organic materials, MoO₃, LiF, and cathode Al were controlled at about 1 Å/s, 0.3 Å/s, 0.1 Å/s, and 3–6 Å/s, respectively.

The EL spectra and CIE coordinates of all OLEDs were measured by a computer controlled PR-655 spectra scan spectrometer. The current density-voltage-luminance characteristics, current efficiency, and power efficiency were recorded by a computer-controlled Keithley 2400 source integrated with a BM-70A luminance meter. The EQE was calculated from the current density-voltage-luminance curve and spectra data. All samples were immediately characterized after thin films deposition without encapsulation in ambient atmosphere at room temperature.

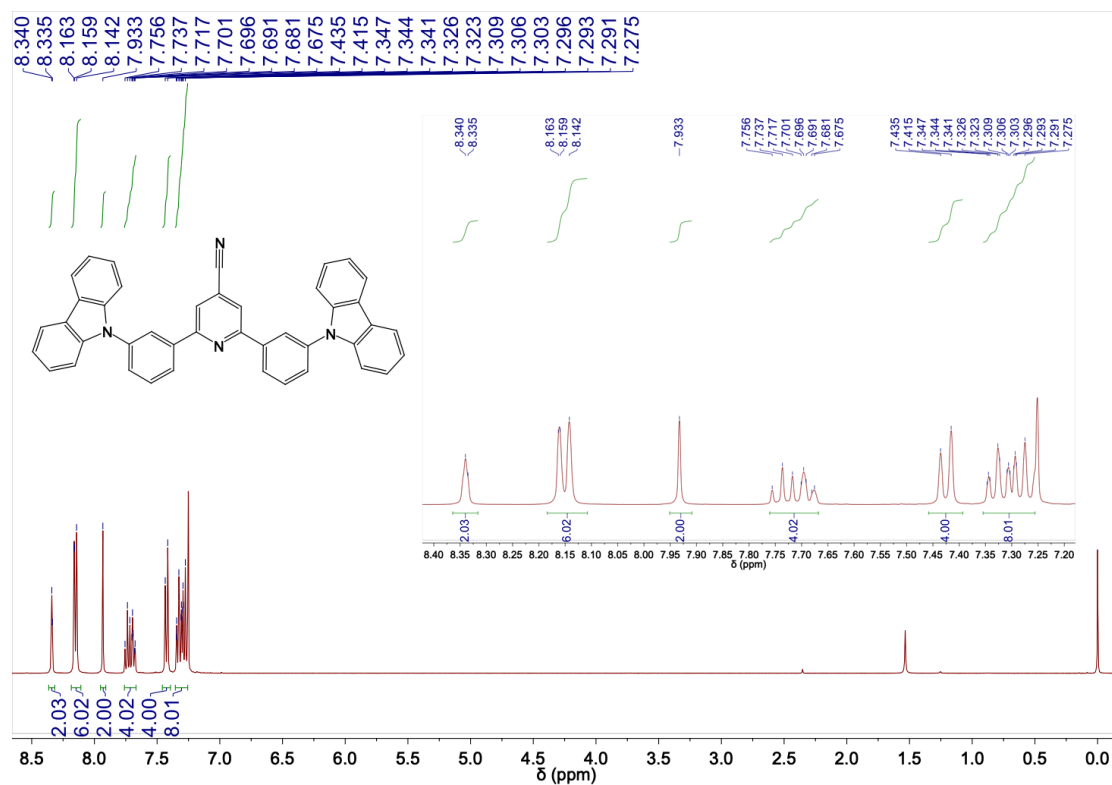


Fig. S1 The ¹H NMR spectra of BCz3PhCN.

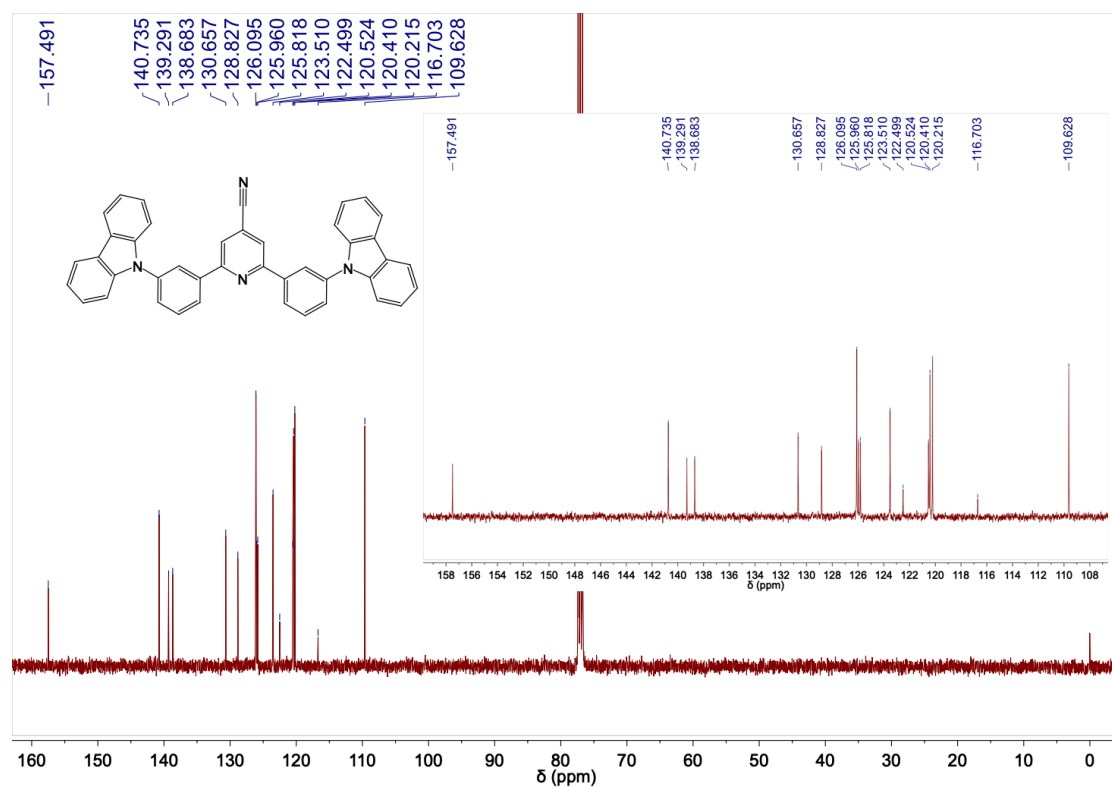


Fig. S2 The ¹³C NMR spectra of BCz3PhCN.

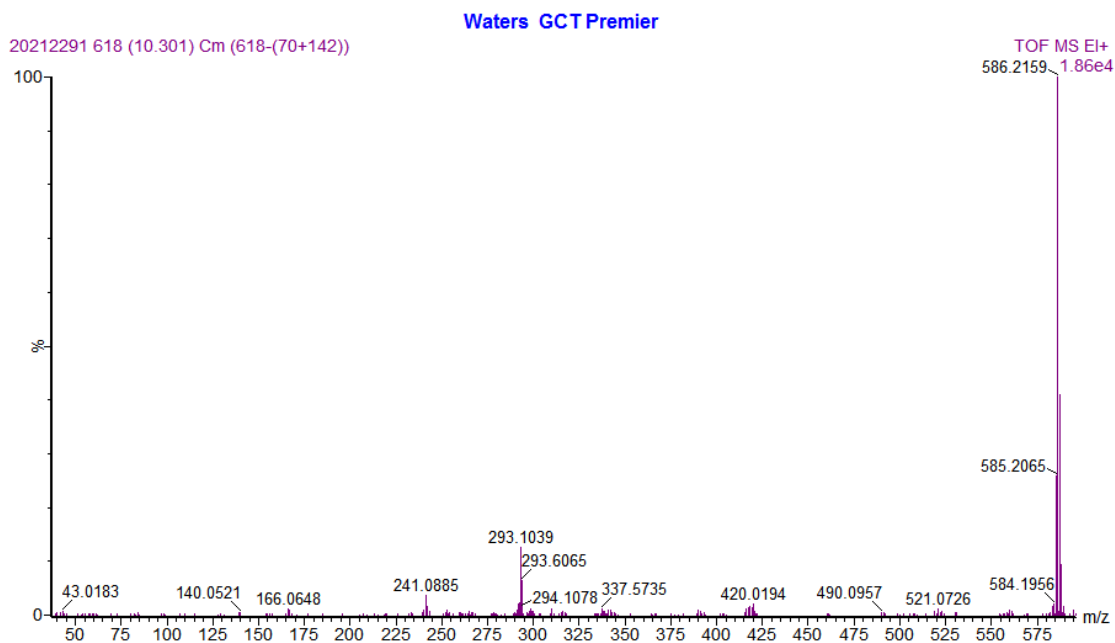


Fig. S3 The MS spectra of **BCz3PhCN**.

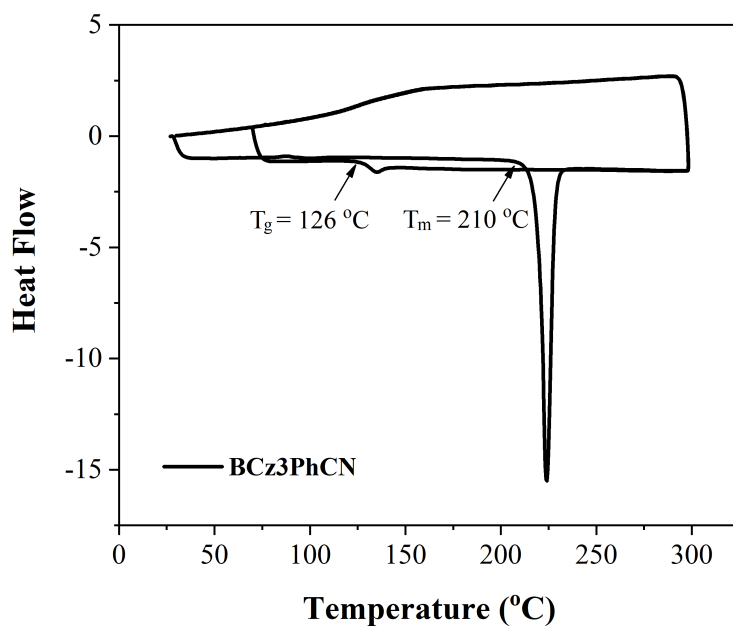


Fig. S4 The whole DSC curve of **BCz3PhCN**.

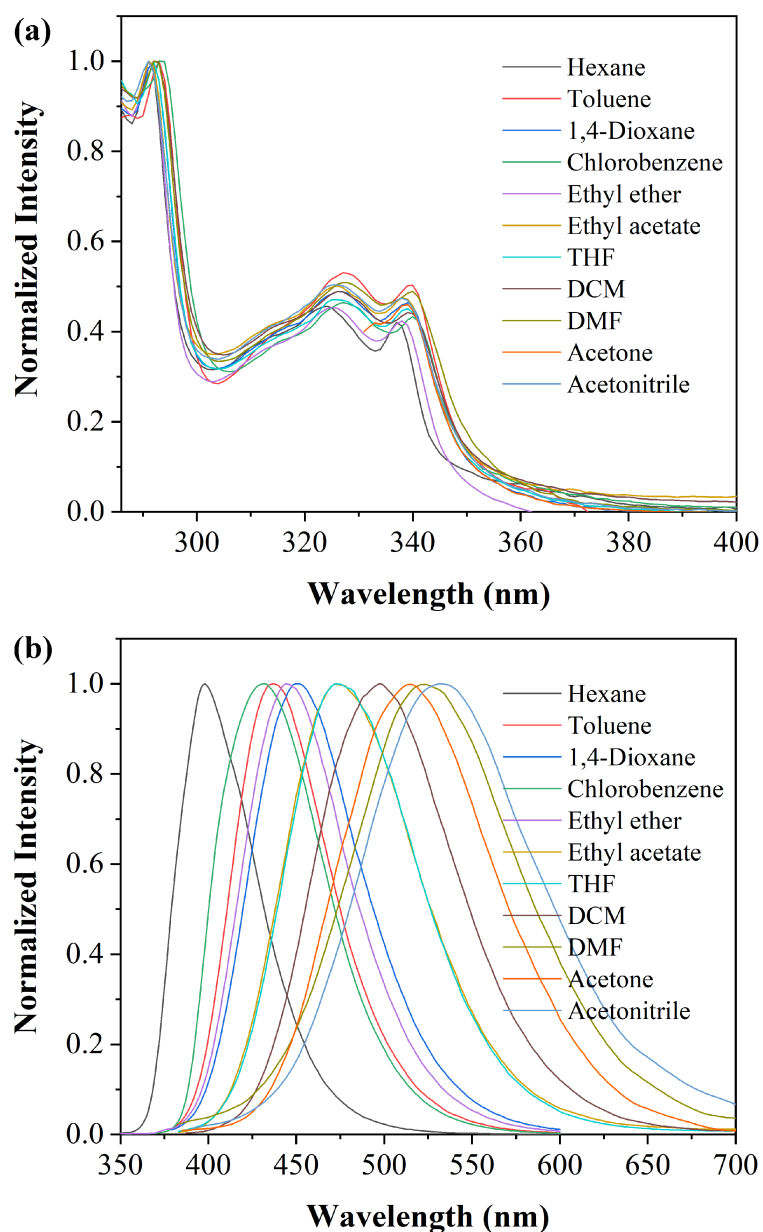


Fig. S5 Normalized absorption (a) and emission (b) spectra of **BCz3PhCN** in various polarity solvents (Concentration: 10^{-5} M).

Table S1 Detailed photophysical data of **BCz3PhCN** in different solvents.

Solvent	ϵ	n	$f(\epsilon, n)$	λ_{abs} (nm)	λ_{pl} (nm)	ν_{a} (cm^{-1})	ν_{f} (cm^{-1})	$\nu_{\text{a}} - \nu_{\text{f}}$ (cm^{-1})
Hexane	1.9	1.3749	0.00126	337	398	29673.59	25125.63	4547.96
Toluene	2.38	1.497	0.01321	340	437	29411.77	22883.30	6528.47
1,4-Dioxane	2.25	1.422	0.02465	339	451	29498.53	22172.95	7325.58
Chlorobenzene	5.62	1.5248	0.14294	340	431	29411.77	23201.86	6209.91
Ethyl ether	4.33	1.3524	0.16675	338	445	29585.80	22471.91	7113.89

Ethyl acetate	6.02	1.3724	0.19964	338	474	29585.80	21097.05	8488.75
THF	7.58	1.4072	0.20957	339	474	29498.53	21097.05	8401.48
DCM	8.93	1.424	0.21717	340	497	29411.77	20120.72	9291.04
DMF	36.7	1.4305	0.27438	340	523	29411.77	19120.46	10291.30
Acetone	20.7	1.3587	0.28431	339	514	29498.53	19455.25	10043.27
Acetonitrile	37.5	1.3441	0.30542	338	532	29585.80	18796.99	10788.81

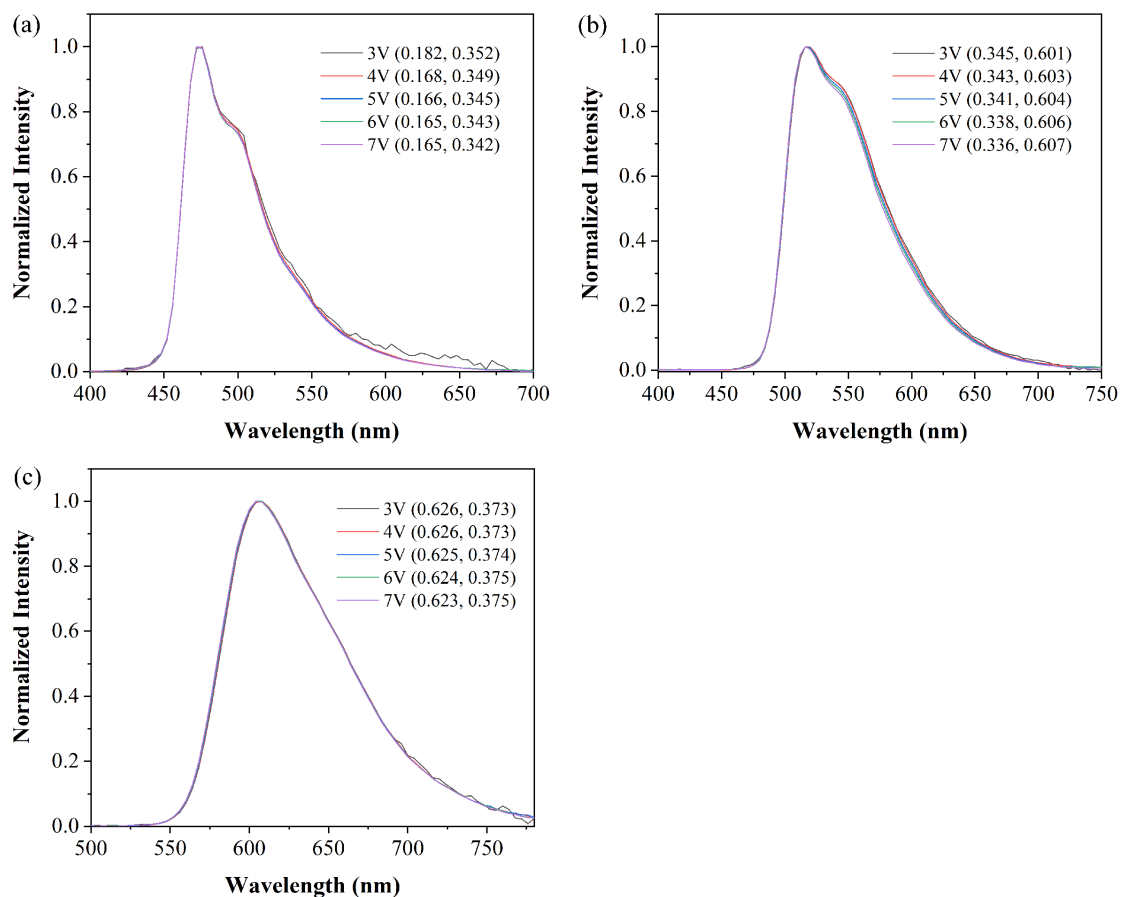


Fig. S6 (a) The EL spectra of device B1 at 3-7 V. (b) The EL spectra of device G1 at 3-7 V. (c) The EL spectra of device R1 at 3-7 V.

Table S2 Comparison of EQE_{\max} between **BCz3PhCN** and other reported red phosphorescent hosts.

Host	Emitter	EQE_{\max} (%)	Reference
BCz3PhCN	Ir(pq)₂acac	26.84	This work
CNTPA-PTZ	Ir(MDQ) ₂ acac	23.4	<i>Dyes and Pigments</i> 162 (2019) 632-639.

BCTrz1	Ir(mphmq) ₂ tmd	24.8	<i>Dyes and Pigments</i> 170 (2019) 107551.
PPI-F-Cz	Ir(MDQ) ₂ acac	20.98	<i>Organic Electronics</i> 69 (2019) 85-91.
D-PY	Ir(MDQ) ₂ acac	26.3	<i>J. Mater. Chem. C</i> , 2021, 9, 2969-2976.
SF	Ir(MDQ) ₂ acac	26.6	<i>ACS Appl. Mater. Interfaces</i> 2018, 10, 1925–1932.
TCZSO₂	Ir(MDQ) ₂ acac	21.0	<i>J. Mater. Chem. C</i> , 2019, 7, 6714-6720.
mSTPh	Ir(MDQ) ₂ acac	27.3	<i>Chem. Sci.</i> , 2020, 11, 4887-4894.
QAF-TRZ	Ir(MDQ) ₂ acac	22.6	<i>J. Mater. Chem. C</i> , 2020, 8, 12470-12477.
IP6Cz	Ir(pq) ₂ acac	26.9	<i>ACS Appl. Mater. Interfaces</i> 2020, 12, 19701-19709.
TDPA-TRZ	Ir(MDQ) ₂ acac	22.6	<i>J. Mater. Chem. C</i> , 2020, 8, 4461-4468.
CDBP:PO-T2T	Ir(MDQ) ₂ acac	28.0	<i>Adv.Mater.</i> , 2015, 27, 7079-7085.