Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Novel Electro-fluorescent Materials with Hybrid Local and Charge-transfer (HLCT) State for Highly Efficient Nondoped Pure Blue OLEDs

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SI-1 Calculation formula.

Lippert-Mataga model: The influence of solvent environment on the optical property of our compounds can be understood using the Lippert-Mataga equation, a model that describes the interactions between the solvent and the dipole moment of solute:

$$hc(\upsilon_a - \upsilon_f) = hc(\upsilon_a^0 - \upsilon_f^0) - \frac{2(\mu_e - \mu_g)^2}{a^3} f(\varepsilon, n) \qquad (1)$$

where f is the orientational polarizability of solvents, μe is the dipole moment of excited state, μg is the dipole moment of ground state; a is the solvent cavity (Onsager) radius, ε and n are the solvent dielectric and the solvent refractive index, respectively.

The EQE measurement method for the non-doped device:

$$EQE = \frac{\pi \cdot L \cdot e}{683 \cdot I \cdot h \cdot c} \cdot \frac{\int_{380}^{780} I(\lambda) \cdot \lambda \cdot d\lambda}{\int_{380}^{780} I(\lambda) \cdot K(\lambda) \cdot d\lambda}$$

Formula S1

where L (cd m^{-2}) is the total luminance of device, *I(A)* is the current flowing into the EL device, λ (nm) is EL wavelength, *I(λ)* is the relative EL intensity at each wavelength and obtained by measuring the EL spectrum, *K(λ)* is the Commision International de L'Eclairage chromaticity (CIE) standard photopic efficiency function, e is the charge of an electron, h is the Planck's constant, c is the velocity of light.

S Ⅰ-2 Supporting Figures

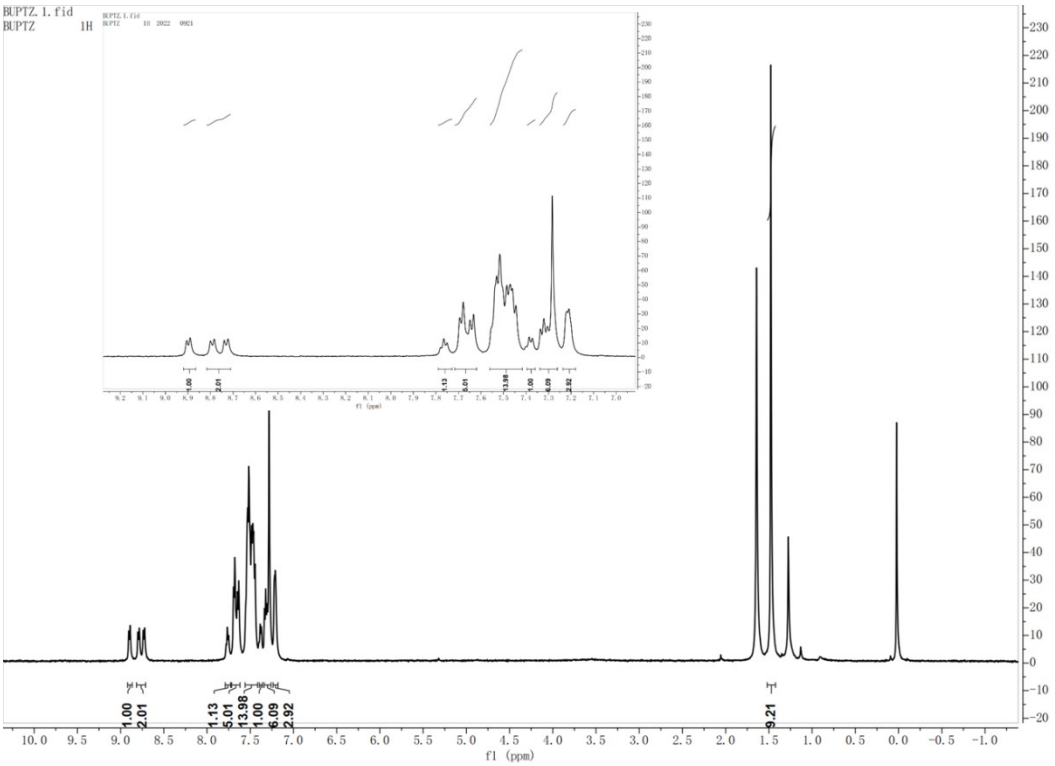

Fig. S1 ^{1}H-NMR Spectrum of *t*BuPPITZ in $CDCl_3$.

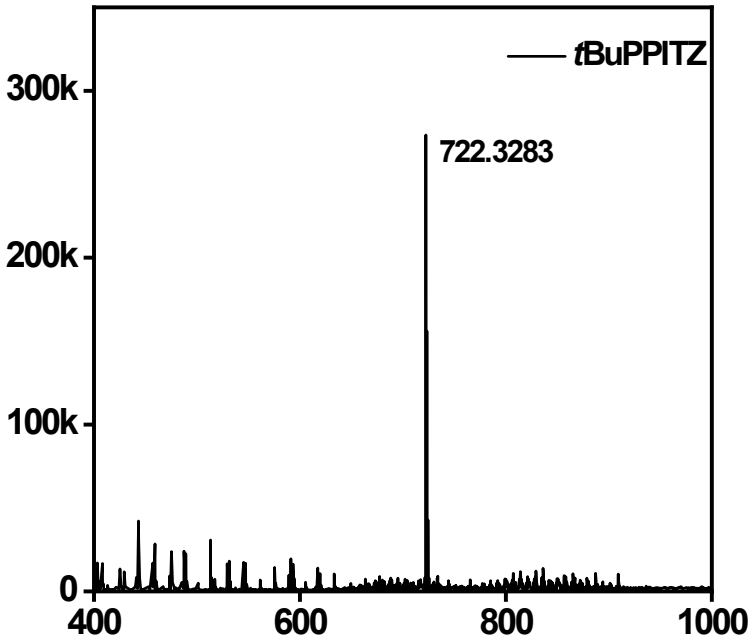

Fig. S2 Mass Spectrum (M+H) of *t*BuPPITZ.

Fig. S3 ^{1}H-NMR Spectrum of PPITZCN in $CDCl_3$.

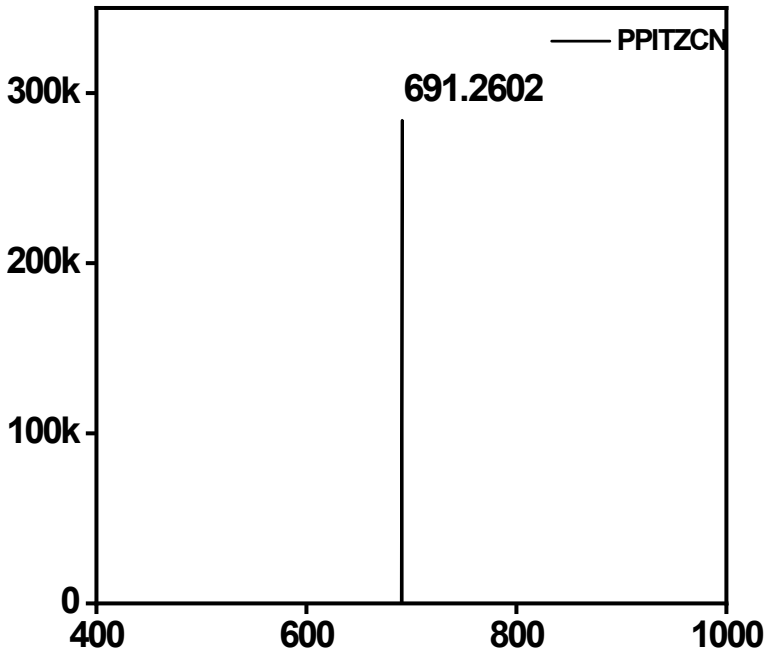

Fig S4. Mass Spectrum (M+H) of PPITZCN.

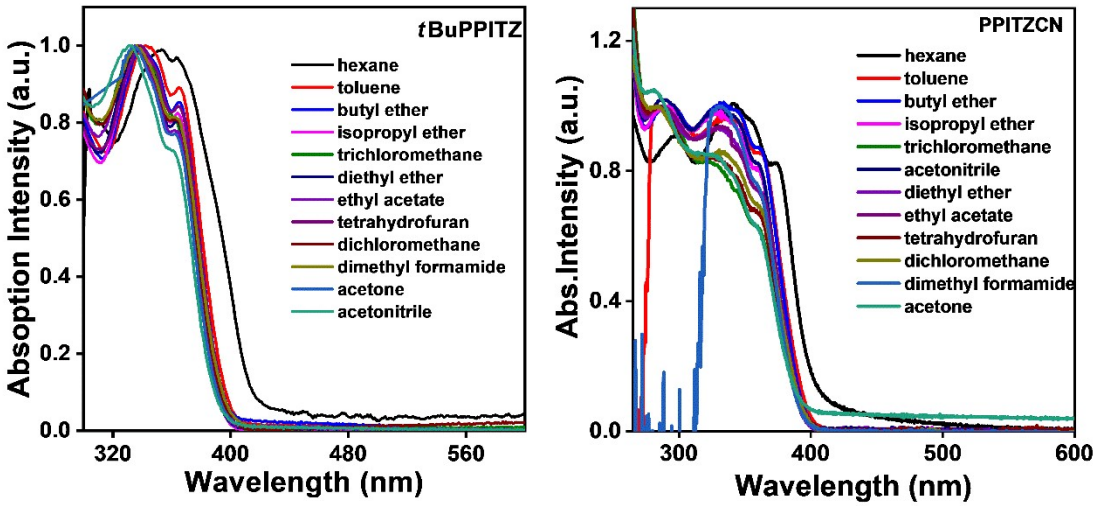

Fig S5. Absorption spectra of *t*BuPPITZ and PPITZCN in different polar solvents.

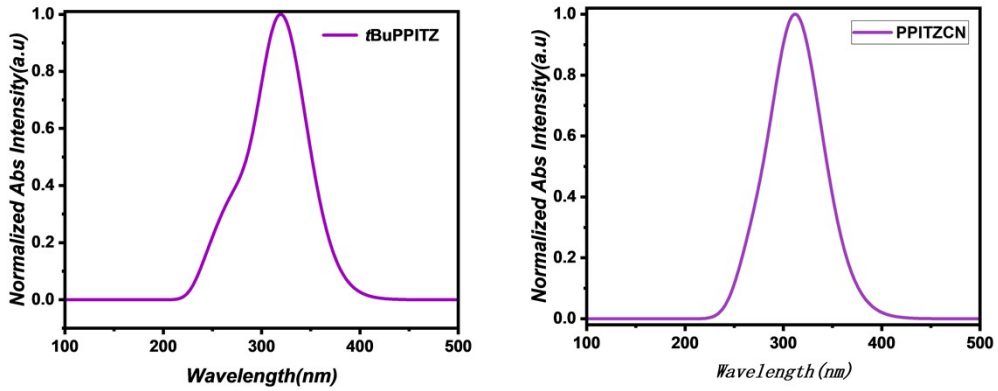

Fig. S6 The calculated absorption spectra of *t*BuPPITZ and PPITZCN.

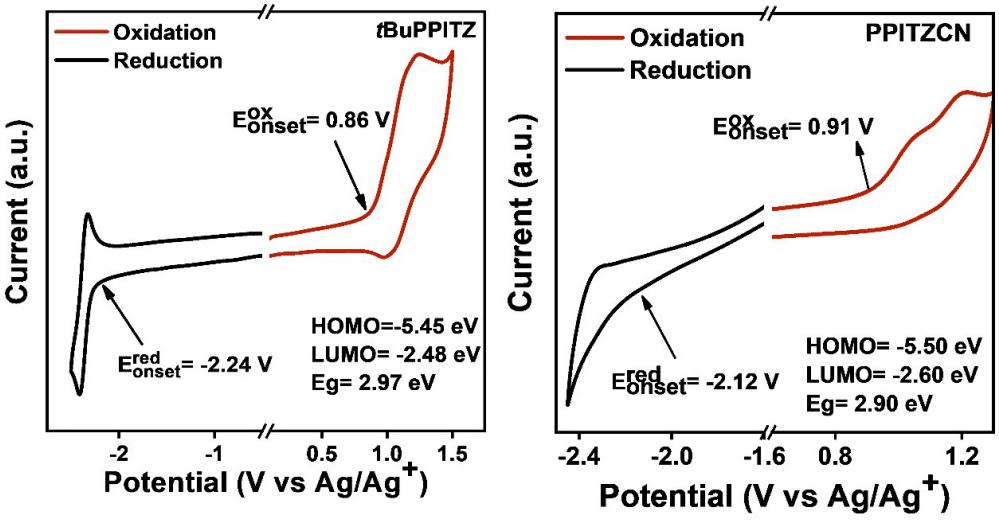

Fig. S7 Electrochemical spectrogram of *t*BuPPITZ and PPITZCN.

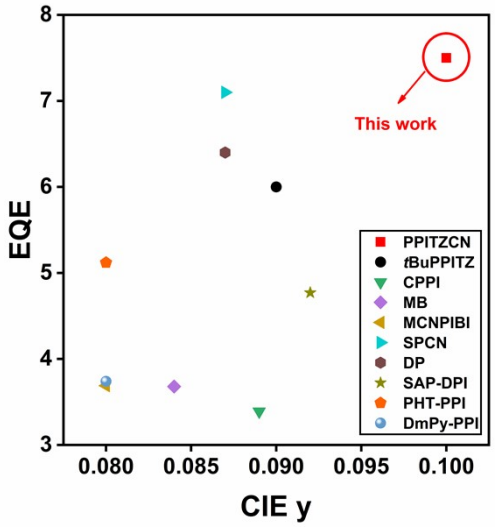

Fig. S8 The non-doped devices performance of blue-HLCT emitters based on PPI with 0.08 ≤ CIEy ≤ 0.10 and EL ≤ 450 nm in the past three years.

SI-3 Supporting tables

Table S1. Absorption and emission peaks in different solvents with different polarities of *t*BuPPITZ and PPITZCN.

	*t*BuPPITZ	PPITZCN

	$\lambda_{exmax}/\lambda_{emmax}$ [nm]	$\lambda_{exmax}/\lambda_{emmax}$ [nm]
Hexane	363/400	360/397
Butylether	364/404	360/404
Isopropylether	364/405	360/405
Chloroform	364/418	362/429
Ethylether	365/408	359/405
Ethylacetate	363/420	358/406
THF	364/419	363/421
Dichloromethane	363/434	361/424
DMF	365/441	360/430
Acetone	362/433	360/440
Acetonitrile	361/440	359/439

Table S2. Φ_{PL} of *t*BuPPITZ and PPITZCN in different solvents with different polarities and in neat film.

	*t*BuPPITZ	PPITZCN
hexane	75%	49%
Isopropyl ether	99%	66%
THF	99%	75%
acetonitrile	89%	51%
film	72%	69%

Table S3. Relevant solvents and corresponding detailed data used to draw Stokes curve.

	*t*BuPPITZ	PPITZCN
	polarization factor (*f*)/λ_{exmax}/λ_{emmax} [nm]/ stockes shift	polarization factor (*f*)/λ_{exmax}/λ_{emmax} [nm]/ stockes shift
Hexane	0.0012/363/400/2548.209366	0.0012/360/397/2713.265932
Butylether	0.096/364/404/2720.052225	0.096/360/404/3025.30253
Isopropylether	0.145/364/405/2781.169448	0.145/360/405/3086.419753
Ethylether	0.167/365/408/2887.456352	0.167/359/405/3163.795179
Ethylacetate	0.2/363/420/3738.685557	0.2/358/406/3302.419022
THF	0.21/364/419/3606.179024	0.21/363/421/3795.240245
Acetone	0.284/362/433/4529.621171	0.284/360/440/5050.505051
Acetonitrile	0.305/361/440/4973.558298	0.305/359/439/5076.109923

Table S4. Detailed energy level data of *t*BuPPITZ and PPITZCN.

S/T [(a)] [eV]	*t*BuPPITZ	PPITZCN
S1/T1	3.583/3.035	3.765/3.052
S2/T2	4.125/3.352	3.966/3.344
S3/T3	4.438/3.609	4.167/3.629
S4/T4	4.591/3.708	4.469/3.684
S5/T5	4.669/3.811	4.508/3.744
S6/T6	4.819/3.931	4.685/3.808
S7/T7	4.88/4.142	4.704/3.931
S8/T8	4.942/4.18	4.864/3.971
S9/T9	4.979/4.207	4.926/4.179
S10/T10	5.051/4.255	5.021/4.215

[(a)] Single excited state/Triple excited state (S/T) energy levels.

Table S5. The non-doped devices performance of blue emitters based on PPI with 0.08 ≤ CIEy ≤ 0.10 and λ_{EL} ≤ 450 nm in the past three years.

Emitters	V_{on} [V]	PE [lm/W]	λ_{EL} [nm]	EQE_{max} [%]	CIE (x, y)	Ref.
***t*BuPPITZ**	4.4	2.35	436	6.0	(0.16, 0.09)	**This work**
PPITZCN	5.0	3.01	448	7.5	(0.16, 0.10)	**This work**
CPPI	3.2	2.44	438	3.39	(0.157, 0.089)	[1]
MB	2.9		440	3.68	(0.157, 0.084)	[2]
MCNPIBI	3.8	0.5	441	3.69	(0.15, 0.08)	[3]
SPCN	3.5	4.6	444	7.1	(0.154, 0.087)	[4]
DP	2.9	4.8	436	6.4	(0.153, 0.087)	[5]
SAF-DPI	2.8	4.39	432	4.77	(0.154, 0.092)	[6]
PHT-PPI	3.0	3.25	448	5.12	(0.15, 0.08)	[7]
DmPy-PPI	3.1	1.97	437	3.74	(0.15, 0.08)	[8]

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