Supporting Information

Hybridization of Short-range and Long-range Charge Transfer Boosts Room-temperature Phosphorescence Performance

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1. Instrumentation and materials.

^{1}H and ^{13}C NMR spectra were measured on a Bruker ARX 500 NMR spectrometer and reported as parts per million (ppm) from the internal standard TMS. High-resolution mass spectra were recorded on a MICROTOF-Q III instrument. Absorption and photoluminescence spectra were measured on a Shimadzu UV-3100 and a Hitachi F-4600 photoluminescence spectrophotometer, respectively. Steady-state photoluminescence and phosphorescence spectra, and lifetimes profiles were measured using a fluorescence spectrophotometer (Edinburgh FLS1000) equipped with a xenon arc lamp (Xe900), a nanosecond hydrogen flash-lamp (nF920), or a microsecond flash-lamp (μF900). The excitation wavelength is 358 nm, and all the phosphorescence spectra were recorded with a delay time of 8 ms. Photoluminescence efficiencies were collected on a Hamamatsu absolute PL quantum yield spectrometer C11347. The thermogravimetric analysis (TGA) curve was performed on a Pyris 1 DSC under nitrogen at a heating rate of 10 ℃ min^{-1}. The ground state calculations are based on optimized structure using Gaussian 09 by density functional theory (DFT) using the B3LYP functional with the 6-31G(d,p) basis set; excited state calculations were conducted by time-dependent density functional theory (TD-DFT) with B3LYP functional with the 6-31G(d,p) basis set.

2. Experimental section

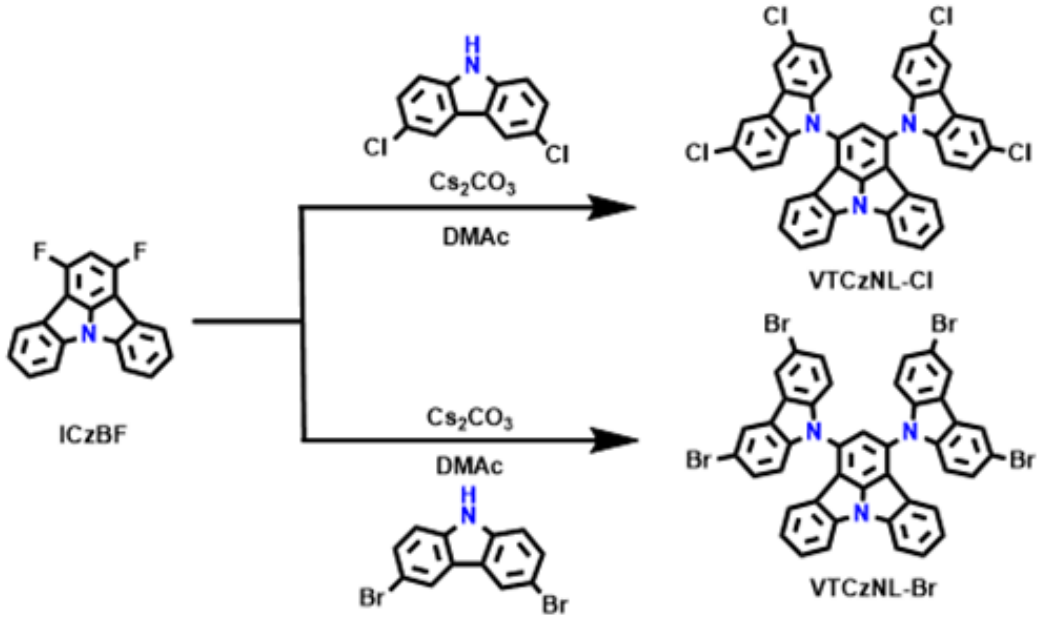

Fig. S1 Synthesis of compound VTCzNL-Cl and VTCzNL-Br.

3. NMR spectra

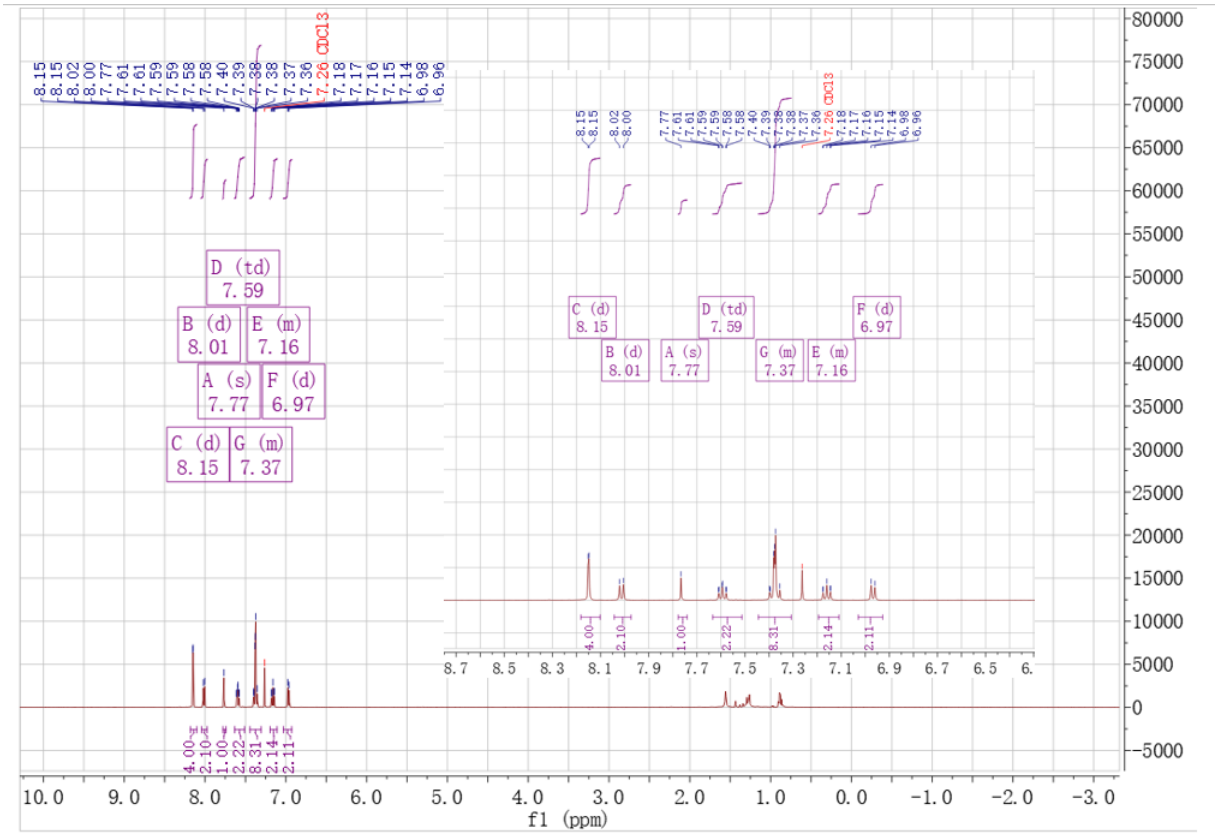

Fig. S2 ^{1}H NMR spectrum of VTCzNL-Cl in $CDCl_3$.

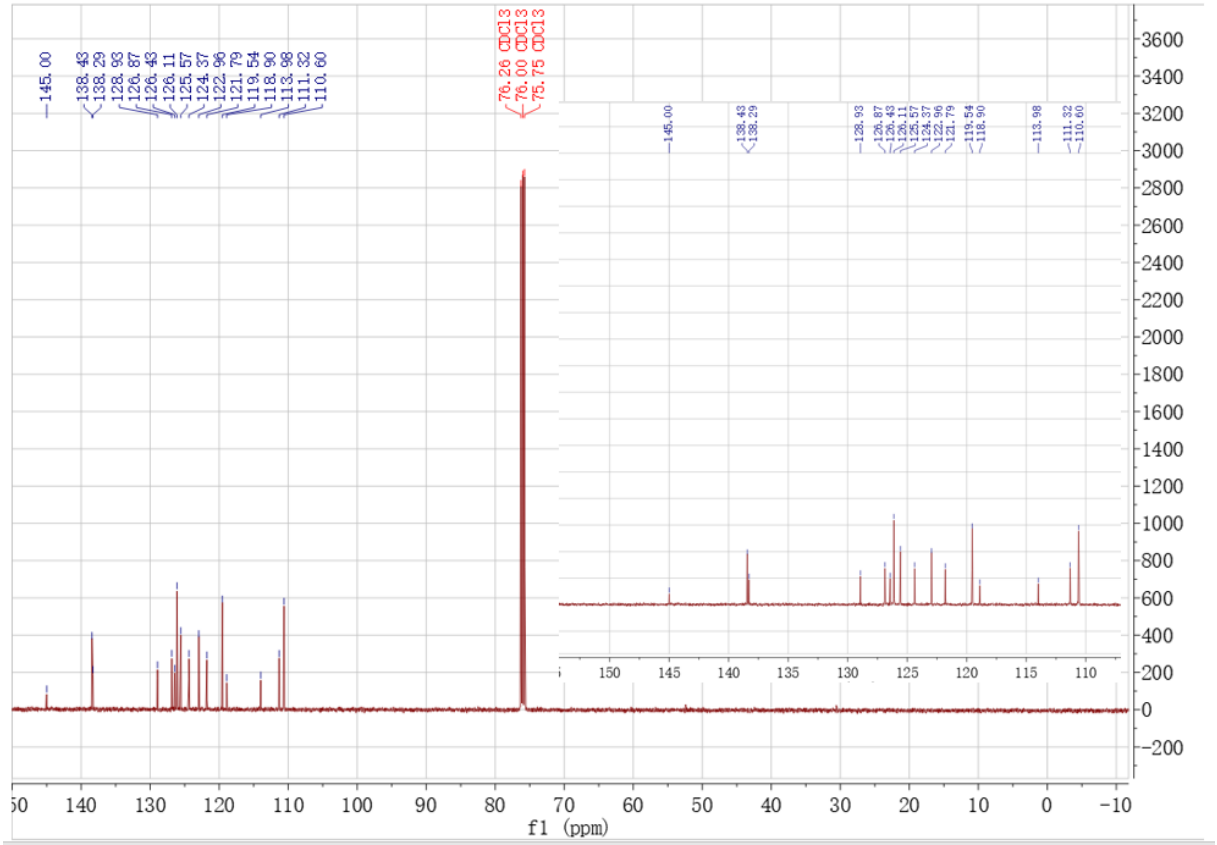

Fig. S3 ^{13}C NMR spectrum of VTCzNL-Cl in $CDCl_3$.

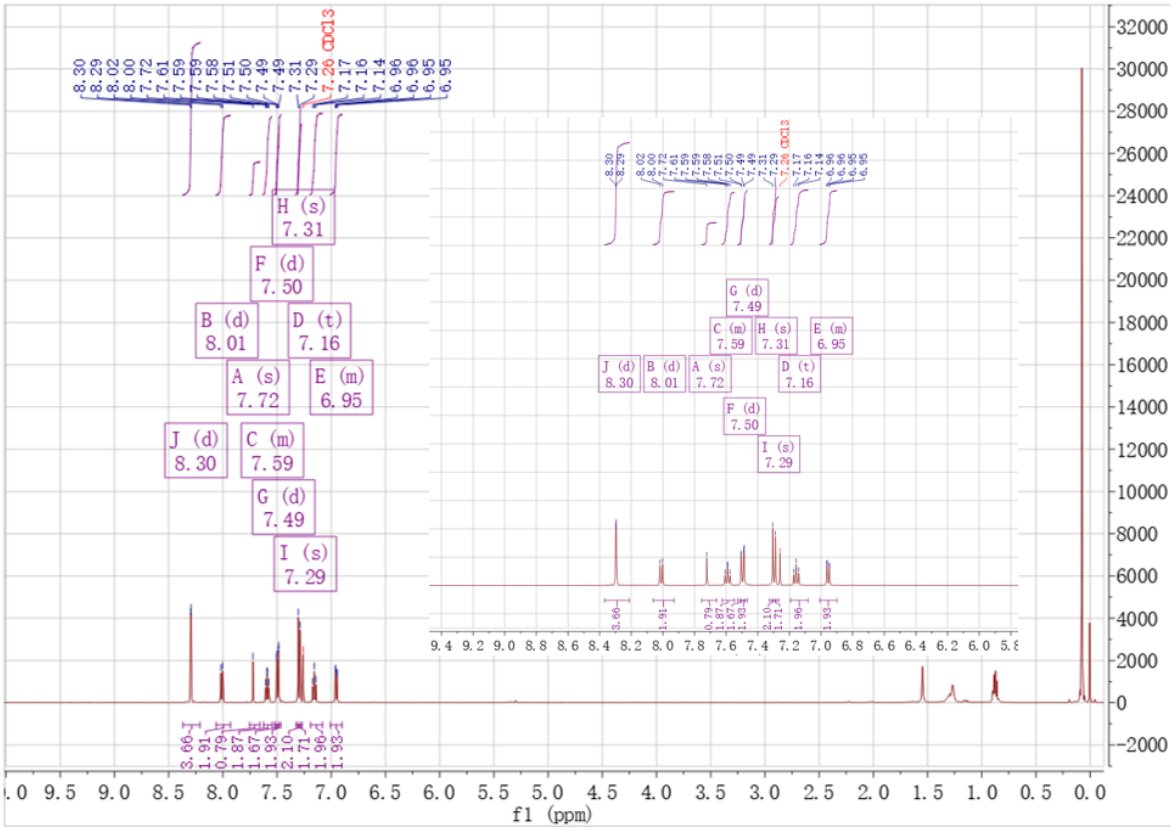

Fig. S4 ^{1}H NMR spectrum of VTCzNL-Br in $CDCl_3$.

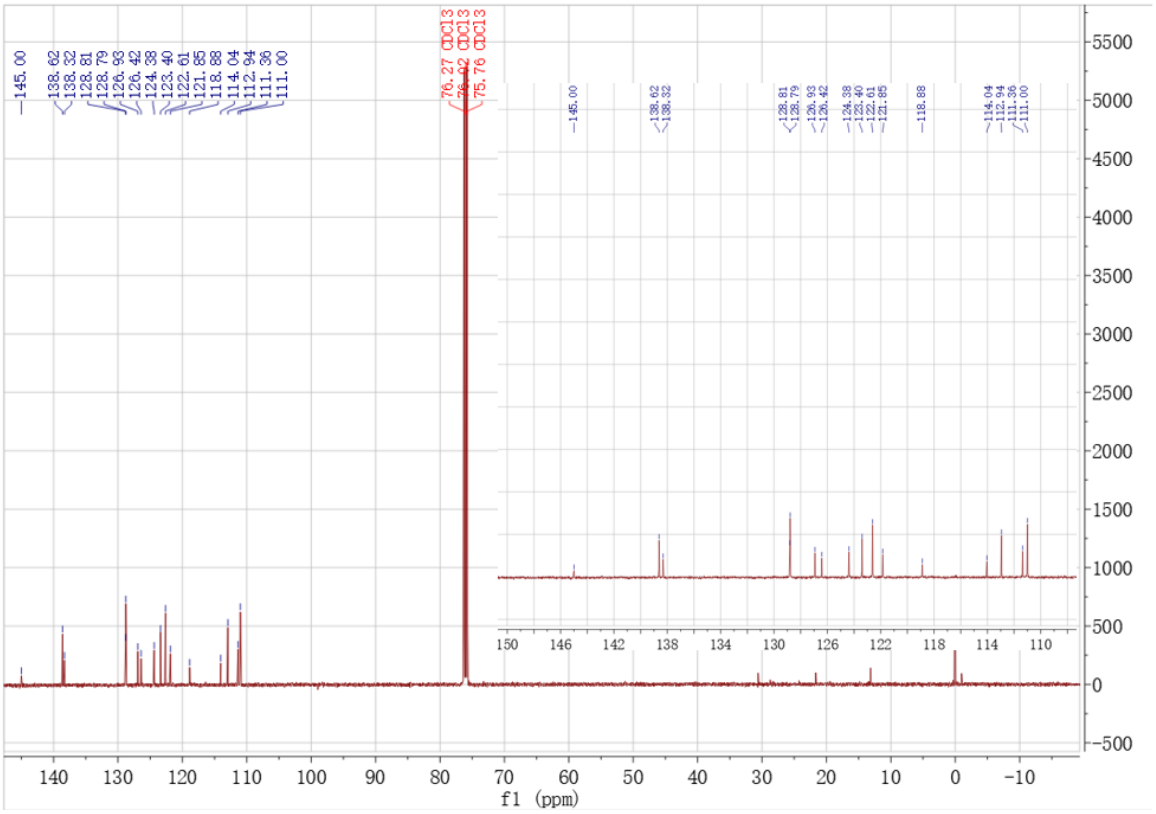

Fig. S5 ^{13}C NMR spectrum of VTCzNL-Br in $CDCl_3$.

4. Crystal data

Table S1. Crystallographic data of VTCzNL-Cl, VTCzNL-Br

	VTCzNL-Cl	VTCzNL-Br
Formula	0.07($C_{42}H_{21}Cl_4N_3$), 0.07(C_3H_7NO)	0.07($C_{42}H_{21}Br_4N_3$)
FW	54.92	60.15
T (K)	273.15	273.15
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	triclinic
Space group	$P2_1$ /c	P-1
a (Å)	14.941(2)	8.565(3)
b (Å)	30.117(5)	15.216(6)
c (Å)	8.4340(13)	30.113(11)
α (deg)	90	90
β (deg)	102.447(4)	90
γ (deg)	90	103.425(9)
V (Å^3)	3706.0(10)	3817(2)
Z	57	59

ρ_{calcd} (mg/cm^3)	1.4025	1.5438
μ (Mo Kα) (mm^{-1})	0.363	4.249
F (000)	1610.9	1732.3
Reflns collected	146124	106403
Data/restraints/params	6342/0/489	13464/0/883
GOF on F^2	1.116	0.992
$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0669, 0.1505	0.0795, 0.1230
$R_1{}^a$, $wR_2{}^b$ (all data)	0.1401, 0.1968	0.3125, 0.2066
CCDC NO	2338861	2338875

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2{}^b = [\Sigma w(F_o{}^2 - F_c{}^2)^2/\Sigma w(F_o{}^2)]^{1/2}$

5. Fluorescence (77 K) and phosphorescence (77 K) spectra

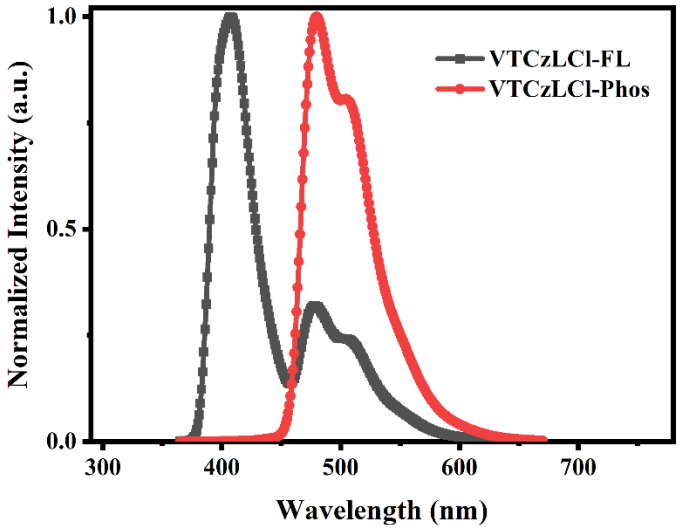

Fig. S6 Fluorescence (77 K, black) and phosphorescence (77 K, red) spectra of VTCzNL-Cl.

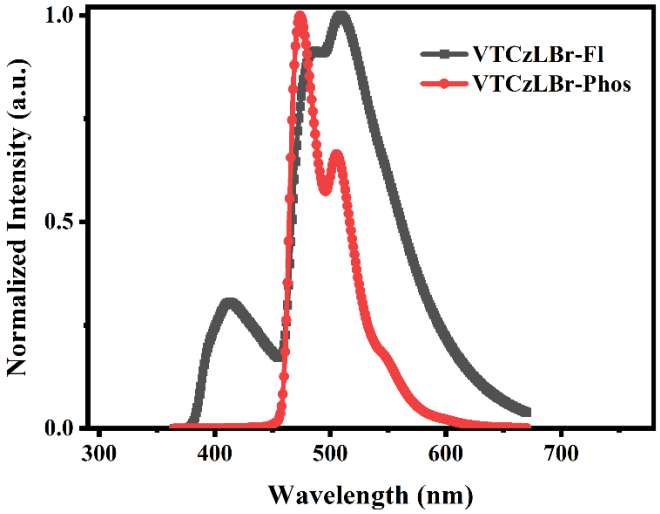

Fig. S7 Fluorescence (77 K, black) and phosphorescence (77 K, red) spectra of VTCzNL-Br.

6. HPLC

Fig. S8 the HPLC data of VTCzNL-Cl.

Integration Results					
No.	**Retention Time min**	**Area mAU*min**	**Height mAU**	**Relative Area %**	**Relative Height %**
1	3.747	70.046	1010.019	95.56	98.83
2	5.927	3.252	11.936	4.44	1.17
Total		73.298	1021.955	100	100

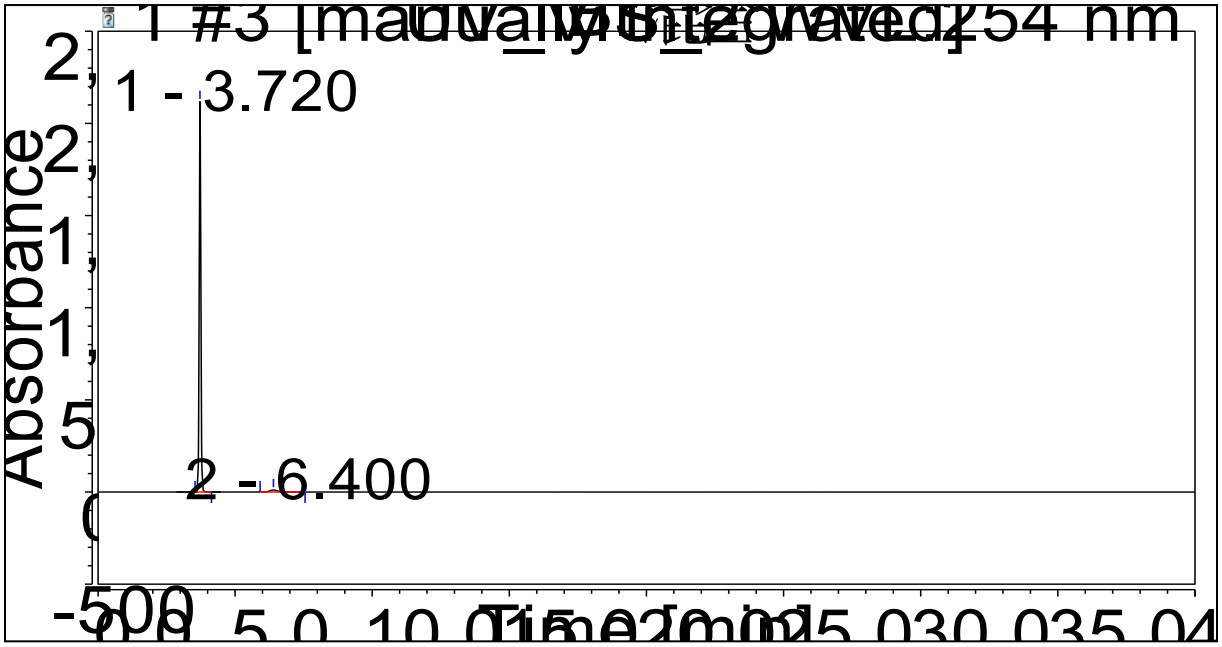

Fig. S9 the HPLC data of VTCzNL-Br.

Integration Results					
No.	**Retention Time min**	**Area mAU*min**	**Height mAU**	**Relative Area %**	**Relative Height %**
1	3.720	146.495	2117.797	95.48	99.48
2	6.400	3.787	11.102	4.52	0.52
Total		150.282	2128.900	100	100

7. RTP performance

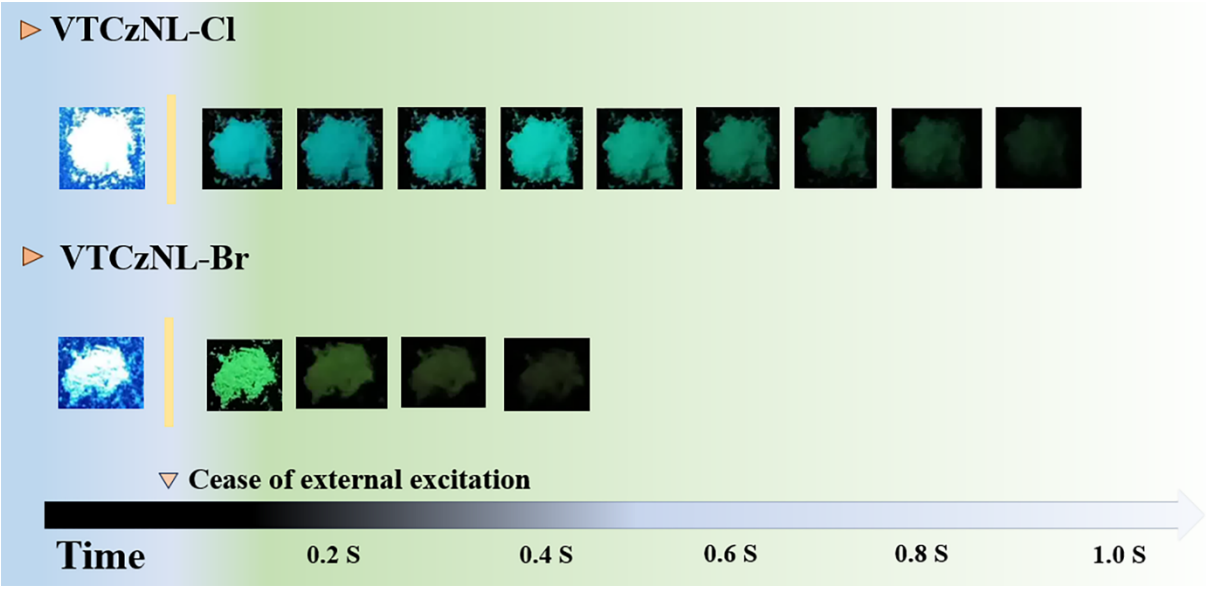

Fig. S10 illustration of afterglow for two materials.

8. Thermogravimetric analysis

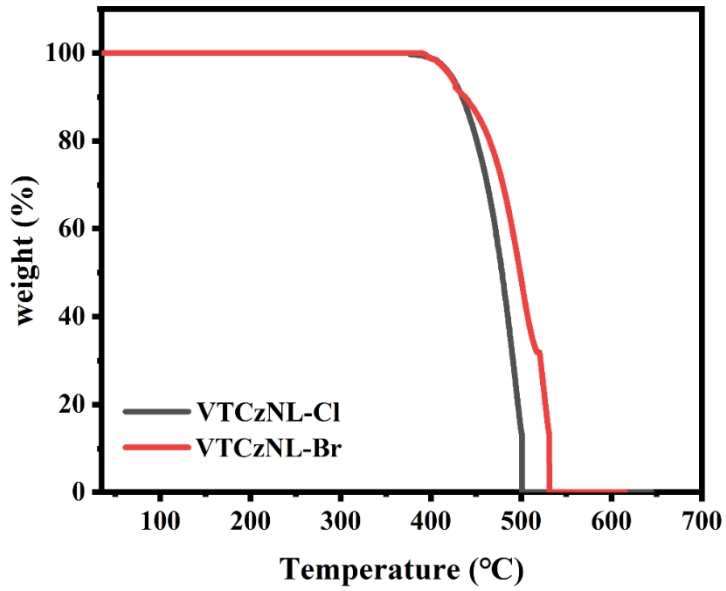

Fig. S11 TGA curves of VTCzNL-Cl and VTCzNL-Br.

9. Lifetimes

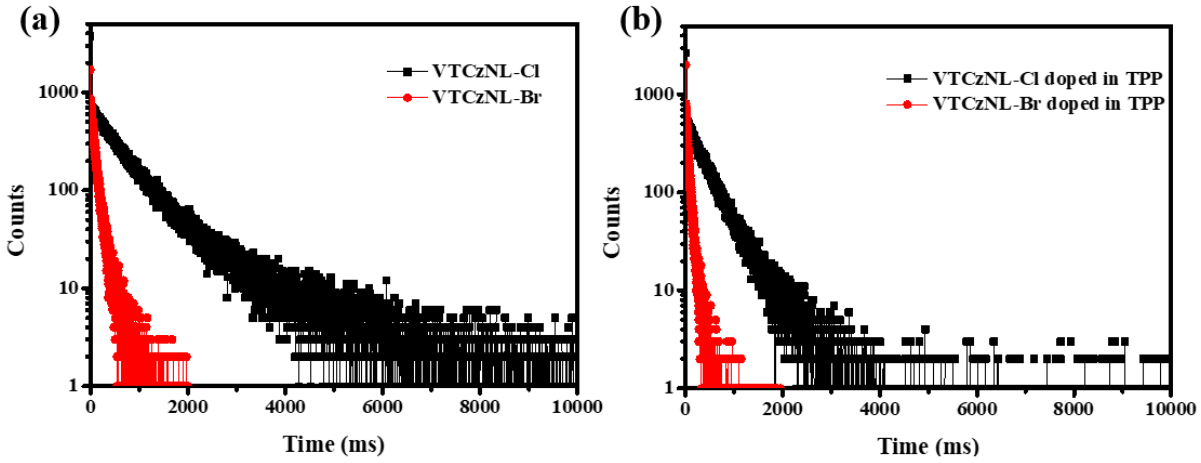

Fig. S11 Transient lifetimes of VTCzNL-Cl and VTCzNL-Br in toluene solutions at 77 K (a); Transient lifetimes of VTCzNL-Cl and VTCzNL-Br doped in TPP at 77 K.

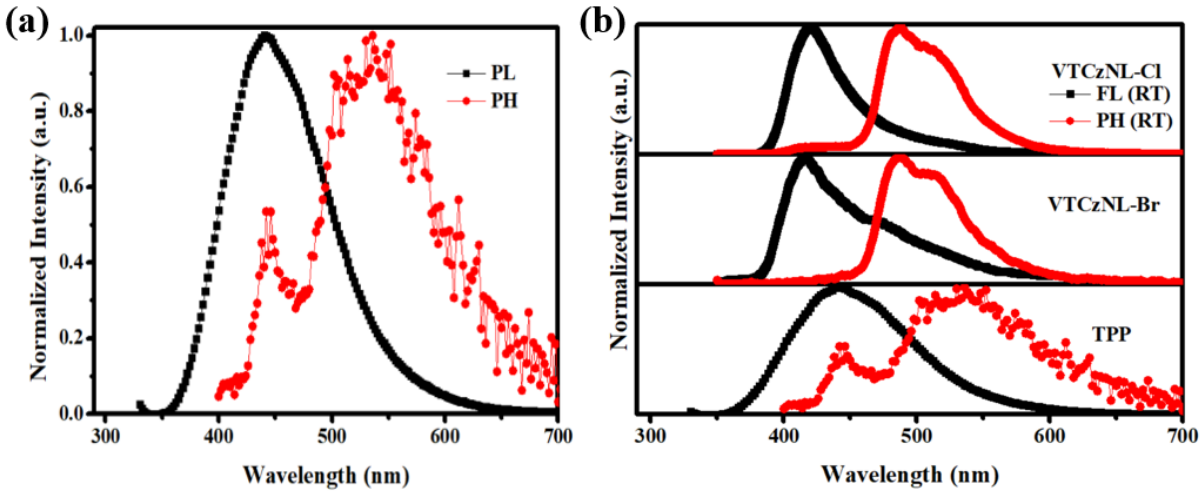

Fig. S12 Fluorescence and phosphorescence spectra of TPP (a); Comparison of fluorescence and phosphorescence spectra of VTCzNLCl doped complexes, VTCzNLCl doped complexes, and TPP (b).