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Supporting Information

Novel bipolar D-π-A type phenanthroimidazole/carbazole hybrid material for high efficiency nondoped deep-blue organic light-emitting diodes with NTSC CIEy and low efficiency roll-off

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Contents

1. Molecular Structure and Crystal Packing

Table S1. Summary of the crystal data of CPBPMCN.

Compound	CPBPMCN
chemical formula	$C_{46}H_{28}N_4$
formula weight	636.72
crystal size (mm)	0.2×0.1×0.1
temperature (K)	100.00(10)
radiation	0.71073
crystal system	triclinic
space group	P-1
a(Å)	10.9010(4)
b(Å)	12.5104(4)
c(Å)	12.7308(4)
α(°)	86.193(2)
β(°)	69.763(3)
γ(°)	89.820(3)
V(Å^3)	1625.05(9)
Z	2
$\rho_{(calc)}$ (g/cm^3)	1.301
F (000)	664
absorp. coeff. (mm^{-1})	0.077
θ range (deg.)	3.686 to 26.022
reflns collected	18631 (R_{int} = 0.0314)
indep. reflns	6373
Refns obs. [$I>2\sigma(I)$]	5297
data/restr/paras	6373/0/451
GOF	1.037
R_1/wR_2 [$I>2\sigma(I)$]	0.0386/0.0947
R_1/wR_2 (all data)	0.0493/0.1000
larg peak and hole (e/Å^3)	0.201/-0.255

2. Low-Temperature Phosphorescence and Decay Lifetime measurement of CPBPMCN

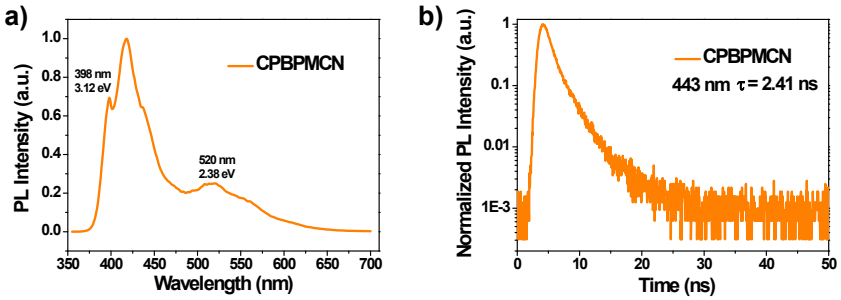

Figure S1. a) Fluorescence and phosphorescence of CPBPMCN in 2-MeTHF at 77 K and b) PL decay curve of CPBPMCN in neat film.

3. The Solvatochromic Lippert-Mataga model

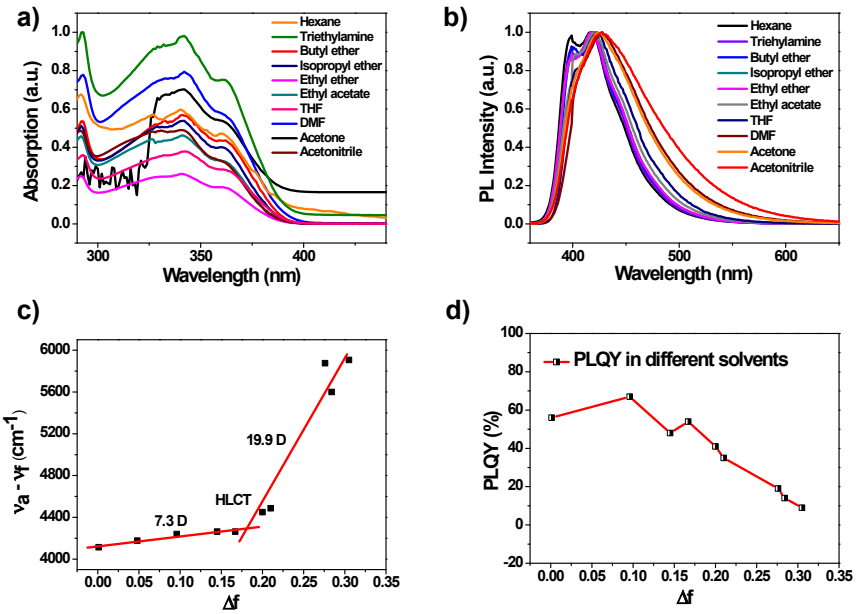

Figure S2. a) The UV/vis absorption spectra of CPBPMCN in different polar solvents; b) the PL spectra of CPBPMCN in different polar solvents; c) linear correlation of orientation polarization (f) of solvent media with the Stokes shift (υ_a - υ_f) for CPBPMCN and d) PLQY in different polar solvents.

The Lippert-Mataga model is estimated according to Equation 1 as below.

$$hc(v_a - v_f) = hc\left(v_a^0 - v_f^0\right) + \frac{2(\mu_e - \mu_g)^2}{{a_0}^3} f(\varepsilon, n) \quad (1)$$

where f is the orientational polarizability of solvents, μ_e is the excited-state dipole moment, μ_0 is the ground-state dipole moment, which can be estimated at the level of B3LYP/6-311G** with the Gaussian09 package; ε and n are the solvent dielectric and the solvent refractive index, respectively; a_0 is the solvent cavity (Onsager) radius, derived from the Avogadro number (N), molecular weight (M), and density (d=1.0 g/cm3); $f(\varepsilon, n)$ and a can be calculated respectively as follows:

$$f(\varepsilon,n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}, a_0 = \left(\frac{3M}{4N\pi d}\right)^{1/3}$$

The detailed data are listed in Table S2.

Table S2. The data about absorption and emission peak positions of CPBPMCN in different solvents.

solvents	Δf	v_a (nm)	v_f (nm)	v_a-v_f(cm^{-1})
Hexane	0.0012	342	398	4114.138
Triethylamime	0.048	342	399	4177.109
Butyl ether	0.096	342	400	4239.766
Isopropyl ether	0.145	341	399	4262.857
Ethyl ether	0.167	341	399	4262.857
Ethyl acetate	0.2	341	402	4449.891
THF	0.21	342	404	4487.291
DMF	0.276	342	428	5875.28
Acetone	0.284	342	423	5599.104
Acetonitrile	0.305	341	427	5906.309

4. SCLC Model of Single-Carrier Devices

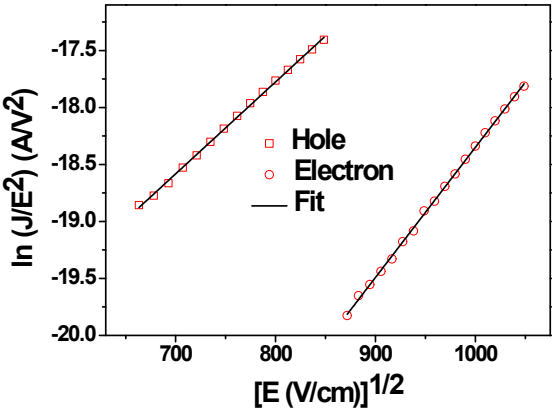

Figure S3. The space-charge-limited currents (SCLC) of single-carrier devices of CPBPMCN.

5. ^{1}H-NMR spectra of CBPMCN and CPBPMCN

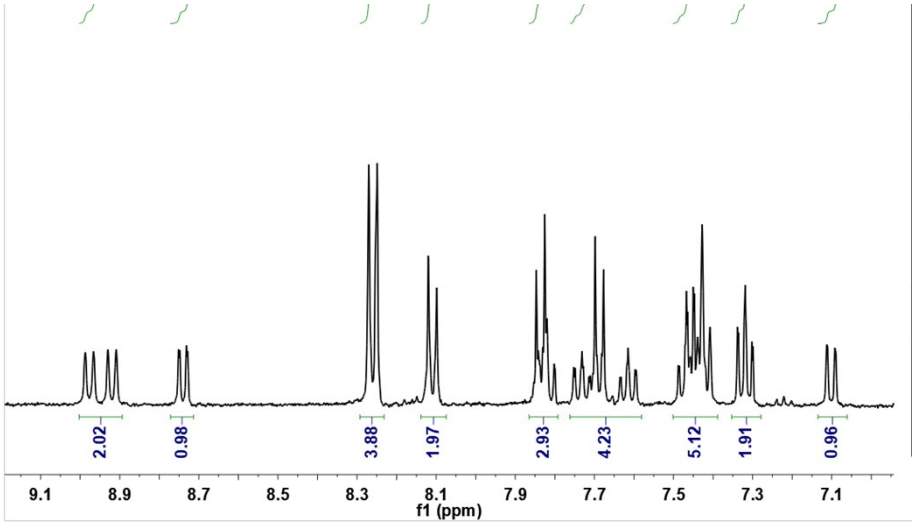

Figure S4. ^{1}H-NMR of CBPMCN (DMSO-d_6)

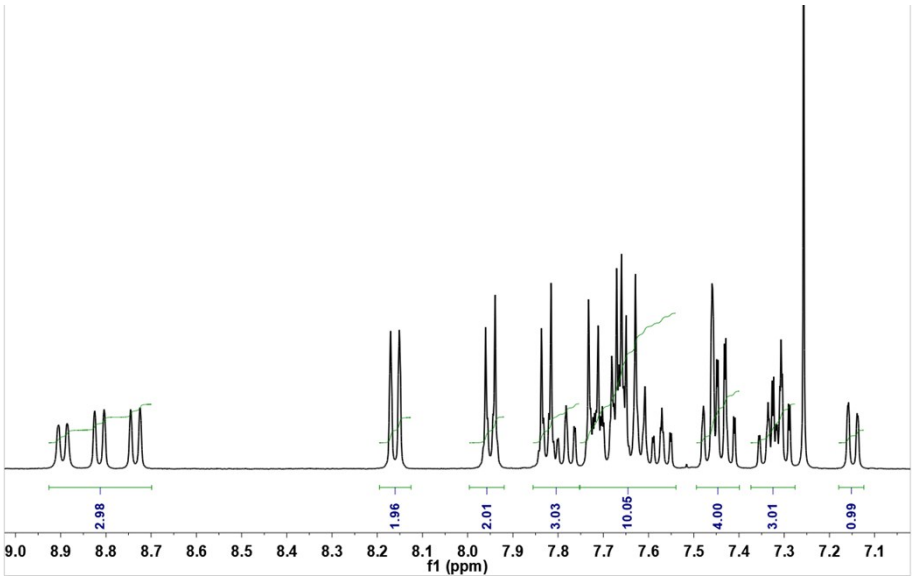

Figure S5. ^{1}H-NMR of CPBPMCN ($CDCl_3$)