

Supporting Information

Bicolour electroluminescence of 2-(carbazol-9-yl)anthraquinone base on solution-process

Bin Huang,^{ab} Zijing Li,^b Hui Yang,^b Die Hu,^b Wenjing Wu,^b Yan Feng,^b Yueming Sun,^{*a} Baoping Lin^a and

Wei Jiang^{*a}

^a School of Chemistry and Chemical Engineering, Southeast University, Nanjing, Jiangsu, 211189, P. R. China.

* E-mail: sun@seu.edu.cn (Y. Sun); E-mail: jiangw@seu.edu.cn (W. Jiang).

^b College of Life Sciences and Chemistry, Jiangsu Key Laboratory of Biofunctional Molecule, Jiangsu Second Normal University, Nanjing, 210013, P. R. China.

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1. Experimental section

General information

All reactants and solvents were purchased from commercial sources, and were used without further purification. The solid UV–vis absorption spectra were recorded on a UV–Vis–Nir spectrophotometer (Cary 5000, Agilent). The photoluminescence (PL) spectra of the crystals were measured with a fluorospectrophotometer (FluoroMax–4, Horiba). The solid PL quantum efficiency was measured with an integrating sphere. The transient lifetime of the crystals were measured with a fluorospectrophotometer (FLS980, Edinburgh). Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) were recorded on a Netzsch simultaneous thermal analyzer (STA) system (STA 409PC) and DSC 2910 modulated calorimetry under dry nitrogen atmosphere at a heating rate of 10 °C min⁻¹. The X–ray diffraction (XRD) measurements were obtained through a diffractometer (Ultima IV) with an X-ray source of Cu K α at 40 kV and 40 mA, at a scan rate of 2° (2 θ) per 1 min. Single crystal X–ray diffraction measurements were carried out on a Bruker D8 Venture diffractometer with MoK α radiation at 153 K. Single crystals were selected and mounted on a nylon loop in Paratone–N cryoprotectant. Unit cell determination was performed in the Bruker SMART APEX III software suite. The data sets were reduced and a multi–scan spherical absorption correction was implemented in the SCALE interface. CCDC 1573925 and 1573955 provide supplementary crystallographic data for this paper. ¹

Preparation of crystals

Cz–AQ was synthesized according to the previously reported method.² A red needle–like crystal (R–crystal) was yielded from dichloromethane/hexane (V:V=1:2) solution at room temperature, and a yellow ribbon–like crystal (Y–crystal) was obtained by evaporation from dichloromethane/ethanol (V:V=1:1) solution at 80 °C. The single crystals were grown from dichloromethane/methanol (V:V=1:1) solution by slow evaporation.

Device fabrication and performance measurements

Before device fabrication, indium–tin oxide (ITO)–coated glass substrates were pre–cleaned carefully and treated by UV ozone for 4 min. The hole–transporting layer of poly(3,4–ethylenedioxythiophene) doped with poly(styrene–4–sulfonate)(PEDOT:PSS) aqueous solution was spin–coated onto the ITO substrate and baked at 150 °C for 10 min to remove residue solvent. Then the emission layer (EML) of Cz–AQ in 1,2–dichloroethane (10 wt%, Device 1) or mixture of 1,2–dichloroethane and ethanol (V/V=1:1) (10 wt%, Device 2) was spin–coated onto the PEDOT:PSS layer and annealed at 80 °C for 30 min to exact the residual solvent in N₂ atmosphere. Subsequently, the substrate was transferred into an evaporation chamber, where 2,2',2''–(1,3,5–benzinetriyl) –tris(1–phenyl–*1H*–benzimidazole) (TPBI) was evaporated as electron–transporting layer. Finally, a 1 nm thick Cs₂CO₃ and 100 nm thick Al were

evaporated as the metal cathode. The electroluminescent (EL) spectra and the Commission Internationale de l'Eclairage (CIE) coordinates were measured using a PR655 spectra colorimeter. The current density–voltage and brightness–voltage curves of the devices were measured using a Keithley 2400 source meter calibrated by a silicon photodiode. All the measurements were carried out at room temperature under ambient conditions. The external quantum efficiency (EQE) was calculated from the brightness, current density and EL spectrum assuming a Lambertian distribution.

2. Figures

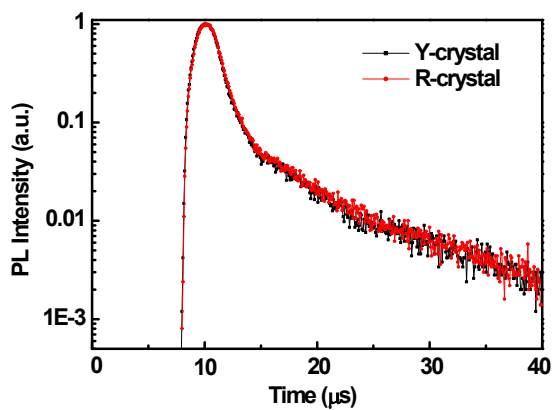


Fig. S1. Transient fluorescence decays of CZ-AQ CZ-AQ in different solid states at 300 K.

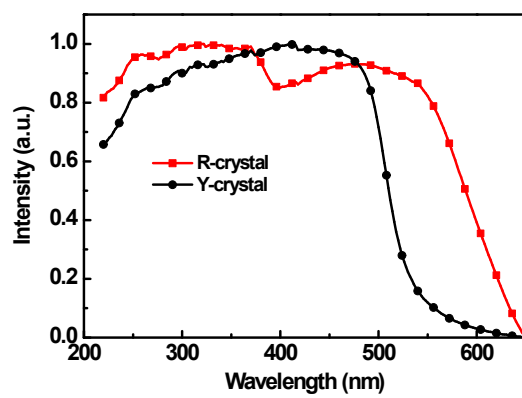


Fig. S2. UV-vis spectra of CZ-AQ in different solid states.

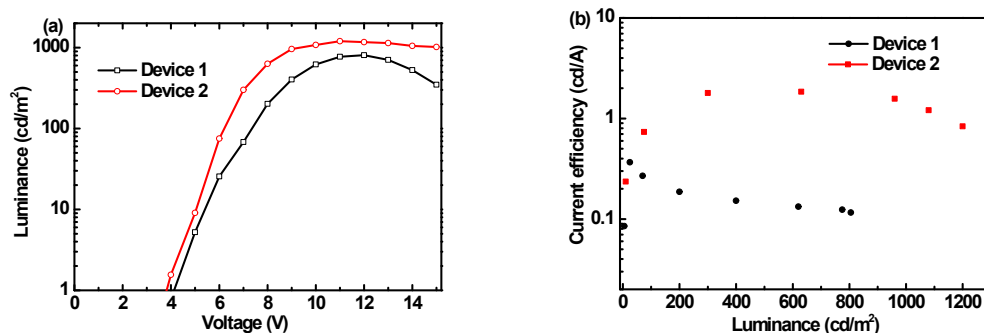


Fig. S3. (a) Luminance-voltage characteristics; (b) Current-efficiency versus luminance plots of the devices.

3. Tables

Table S1. Crystal data and structure refinement for CZ-AQ in different single crystals.

	R-single-crystal	Y-single-crystal
Formula	$C_{26}H_{15}NO_2$	$C_{26}H_{15}NO_2$
CCDC No.	1573955	1573925
Formula weight	373.39	373.39
Space group	$P2_1/n$	$P2_1/n$
Temperature	173(2)	173(2)
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Unit cell dimensions	$a = 13.781(8)$ Å $\alpha = 90.00^\circ$ $b = 3.854(2)$ Å $\beta = 94.06(2)^\circ$ $c = 35.911(2)$ Å $\gamma = 90.00^\circ$	$a = 16.073(4)$ Å $\alpha = 90.00^\circ$ $b = 8.072(3)$ Å $\beta = 117.88(7)^\circ$ $c = 16.193(4)$ Å $\gamma = 90.00^\circ$
Volume	1902.37 (19) Å ³	1857.3 (9) Å ³
Z, Calculated density	4, 1.360 Mg/m ³	4, 1.332 Mg/m ³
Absorption coefficient	0.089 mm ⁻¹	0.084 mm ⁻¹
$F(000)$	808	772
Crystal size	0.12 × 0.18 × 0.24 mm	0.10 × 0.20 × 0.30 mm
Theta range for data collection	2.18 to 27.44 deg.	2.87 to 27.65 deg
Limiting indices	-17 ≤ h ≤ 17, 0 ≤ k ≤ 4, 0 ≤ l ≤ 46	-20 ≤ h ≤ 20, -10 ≤ k ≤ 9, -16 ≤ l ≤ 19
Reflections collected / unique	4282 / 3491 [$R_{int} = 0.0685$]	4331 / 2360 [$R_{int} = 0.0719$]

Max. and min. transmission	0.746 and 0.674	0.992 and 0.980
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0685$, $wR_2 = 0.2159$	$R_1 = 0.0745$, $wR_2 = 0.2209$

Table S2. EL characteristics of solution-processed non-doped OLEDs based on Cz-AQ.

	V (v)	LE (cd A ⁻¹)	Max luminance (cd m ⁻²)	Max EQE	λ_{EL} (nm)	CIE (x, y)
Device 1 ^a	4.3	0.37	850	0.75%	680	(0.68, 0.30)
Device 2 ^b	3.8	1.85	1200	1.15%	600	(0.50, 0.42)

^a The emission layer (EML) of Cz-AQ in 1,2-dichloroethane (10 wt%).

^b EML of Cz-AQ in the mixture of 1,2-dichloroethane and ethanol (V/V=1:1) (10 wt%).

3. References

1. CCDC 1573925 (Y-crystal) and CCDC 1573955 (R-crystal) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
2. B. Huang, Y. Ji, Z. Li, N. Zhou, W. Jiang, Y. Feng, B. Lin, Y. Sun, J. Lumin, 2017, **187**, 414