Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Diphenylamino-substituted quinacridone derivative: red fluorescence based on intramolecular charge-transfer transition

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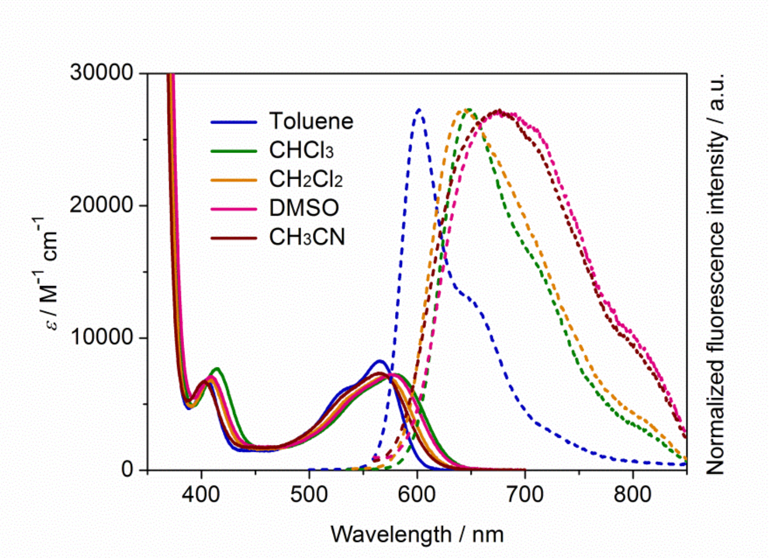

Fig. S1 Absorption (solid line) and fluorescence (dashed line) spectra of NPh$_2$-QA in various solvents.

Table S1 Photophysical data of NPh$_2$-QA in various solvents.

Solvents	Δf^a	λ_{abs} / nm	ε / 10^4 M^{-1} cm^{-1}	λ_{em} / nm	Stokes shift / cm^{-1}
Toluene	0.0131	566	0.83	602	1057
$CHCl_3$	0.1482	579	0.73	649	1863
CH_2Cl_2	0.2171	570	0.71	644	2016
DMSO	0.2630	575	0.73	677	2620
CH_3CN	0.3046	564	0.73	674	2894

[a] orientation polarizability of the solvent.

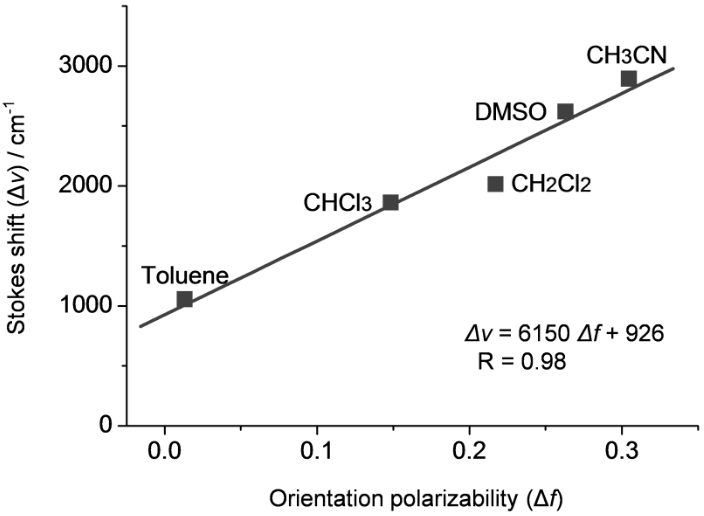

Fig. S2 Lippert–Mataga plot of NPh_2-QA.

Lippert-Mataga plots. Lippert-Mataga equation[1] expresses the Stokes shift Δv as a function of the solvent orientation polarizability Δf:

$$\Delta \upsilon = \frac{1}{4\pi\varepsilon_0}\frac{2(\mu_e-\mu_g)^2}{hca^3}\Delta f + constant$$

$$= \frac{(9.05\ \times 10^{34})(\mu_e-\mu_g)^2}{a^3}\Delta f\ [C^{-2}] + constant$$

where ε_0 represents dielectric constant of vacuum, h represents Planck constant, c represents light velocity, a represents radius of Onsager cavity, μ_g and μ_e represent the dipole moment in ground and excited states, respectively. C is the unit of quantity of electric charge. For NPh_2-QA, DFT-calculation at B3LYP/6-31G* level gives a value of 6.65 Å. Based on the Lippert-Mataga equation, the difference of dipole moment between ground and excited states ($\mu_e - \mu_g$) is 13.4 D.

Table S2 Fluorescence quantum yields of C_8-QA and NPh_2-QA in various solvents.

Compound	Toluene	$CHCl_3$	CH_2Cl_2	DMSO	CH_3CN
C_8-QA	0.96	0.97	0.96	0.95	0.96
NPh_2-QA	0.56	0.13	0.09	0.02	0.02

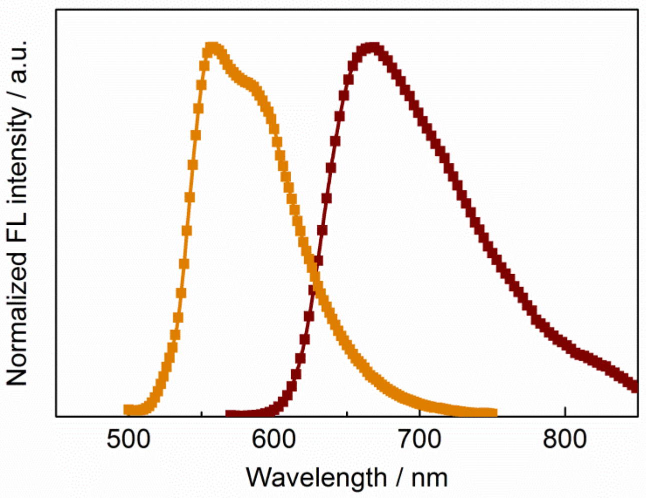

Fig. S3 Fluorescence spectra of solid thin films of C_8-QA (yellow line) and NPh_2-QA (deep red line).

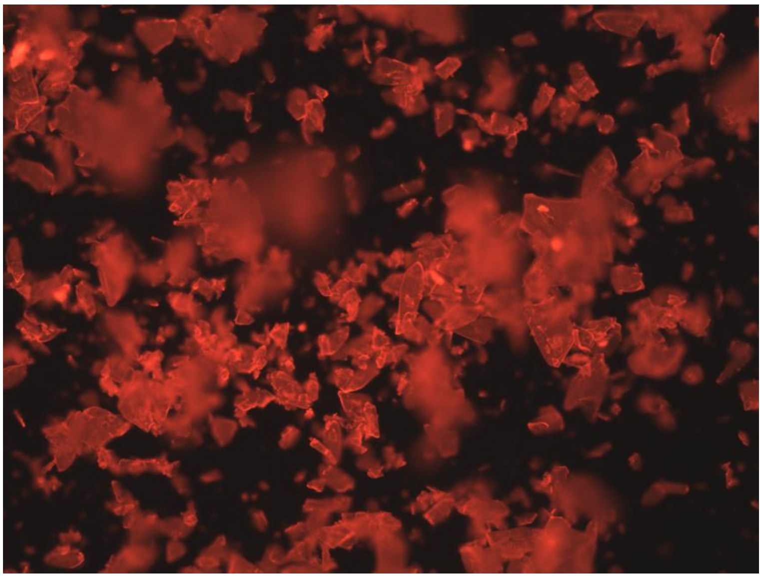

Fig. S4 Fluorescence microscopy image of the crystalline powder of NPh_2-QA.

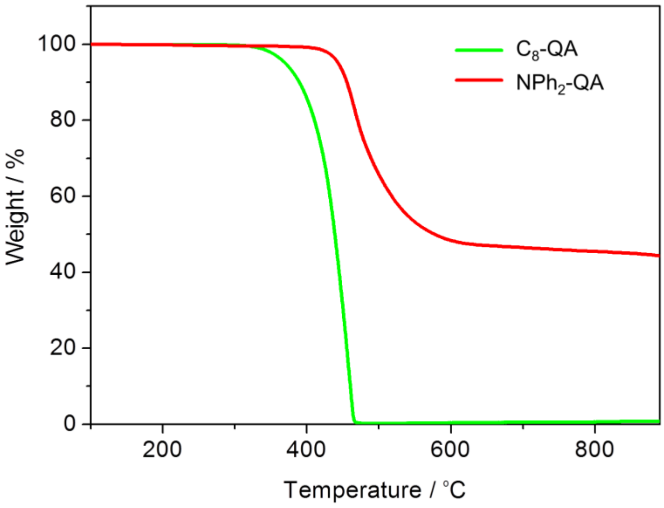

Fig. S5 TGA curves of C_8-QA and NPh_2-QA.

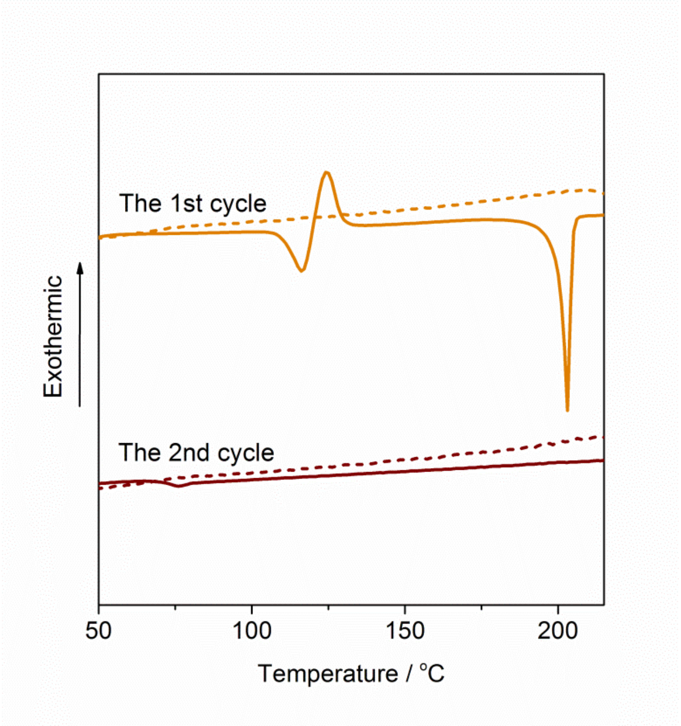

Fig. S6 Two heating (solid line)-cooling (dashed line) cycles of the DSC measurements of NPh_2-QA.

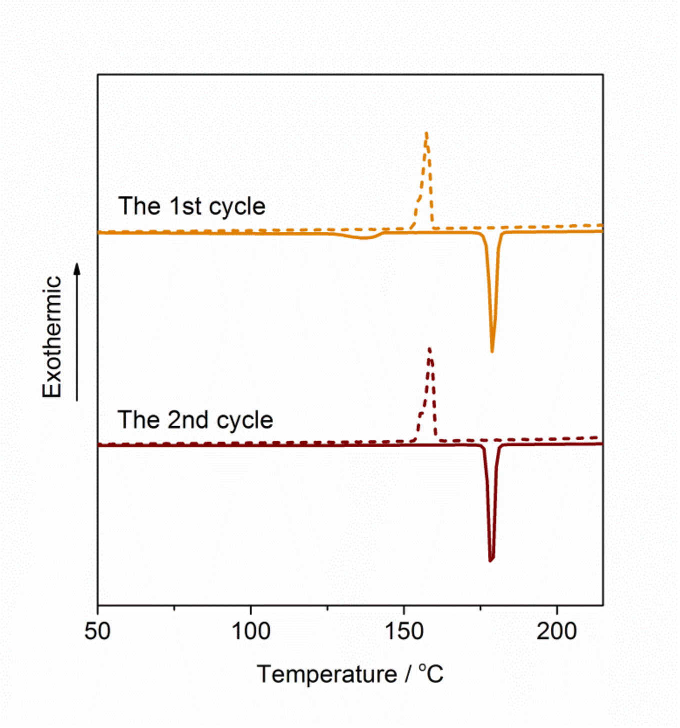

Fig. S7 Two heating (solid line)-cooling (dashed line) cycles of the DSC measurements of C_8-QA.

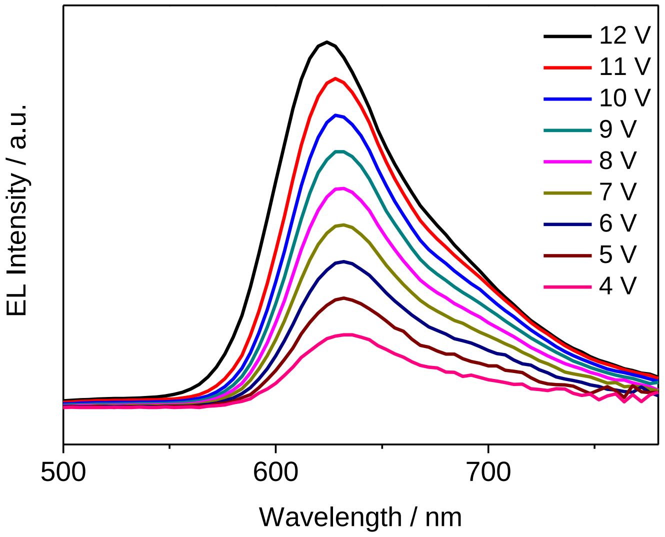

Fig. S8 EL spectra of the OLED device at different driving voltages.

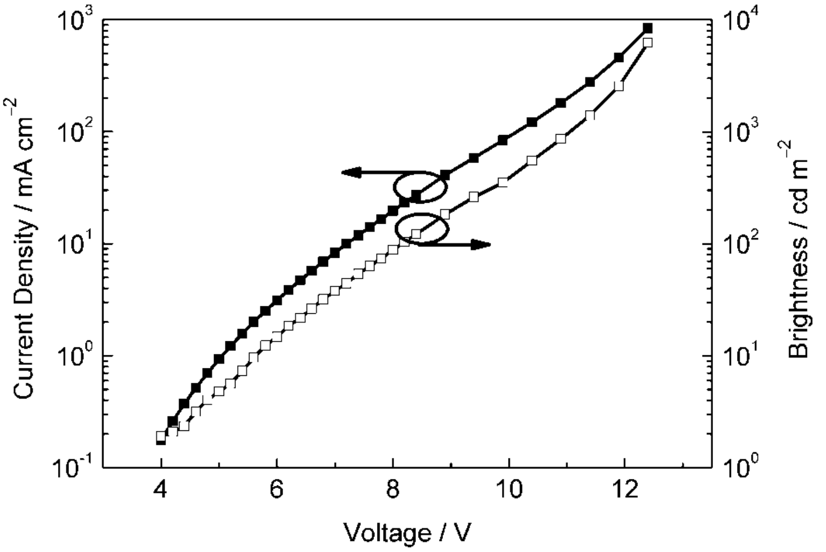

Fig. S9 Current density−Voltage−Brightness characteristics of the OLED device.

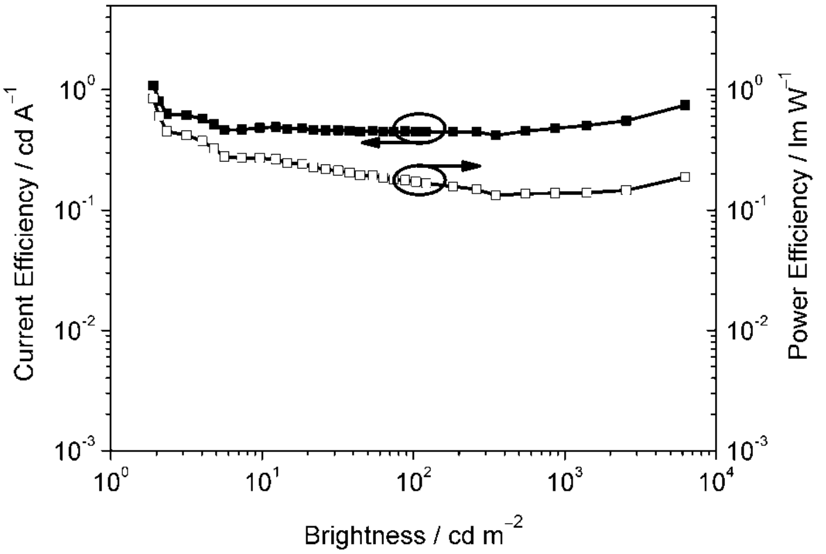

Fig. S10 Current efficiency and power efficiency *versus* brightness characteristics of the OLED device.

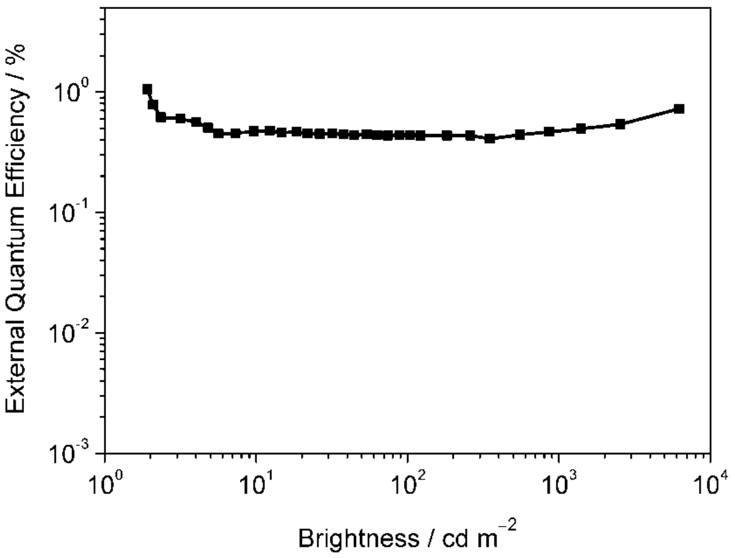

Fig. S11 External quantum efficiency *versus* brightness characteristics of the OLED device.

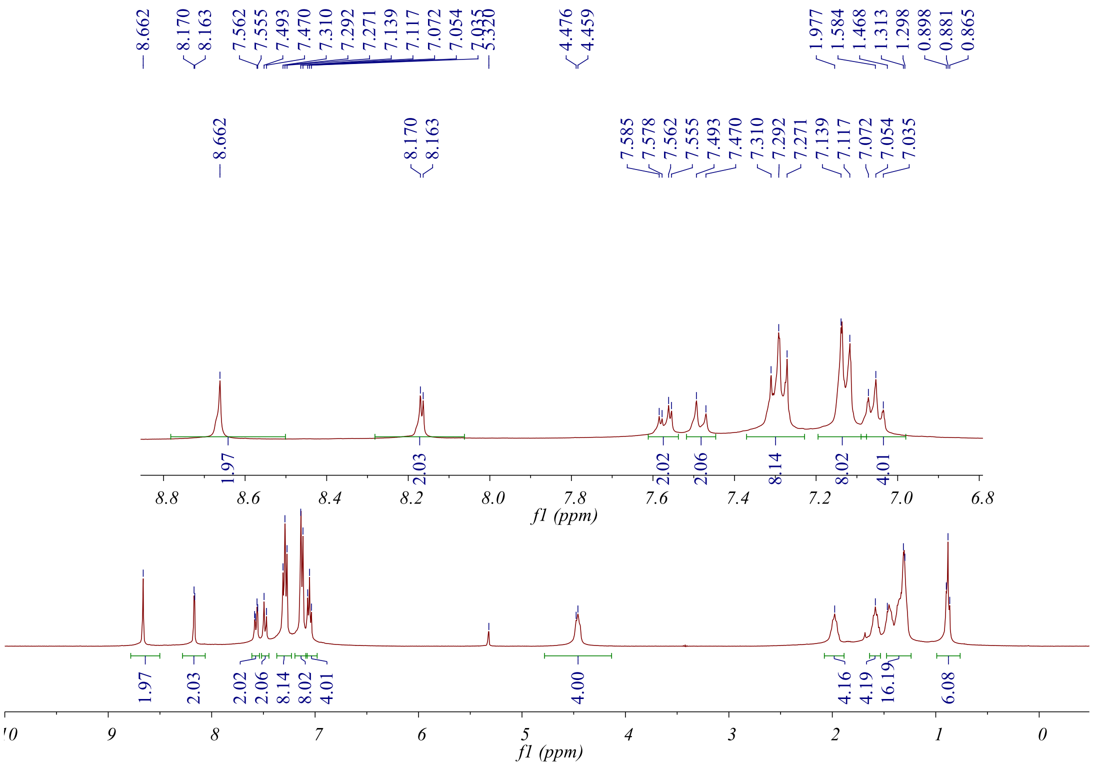

Fig. S12 ^{1}H NMR spectrum of NPh$_2$-QA (400 MHz, CD$_2$Cl$_2$).

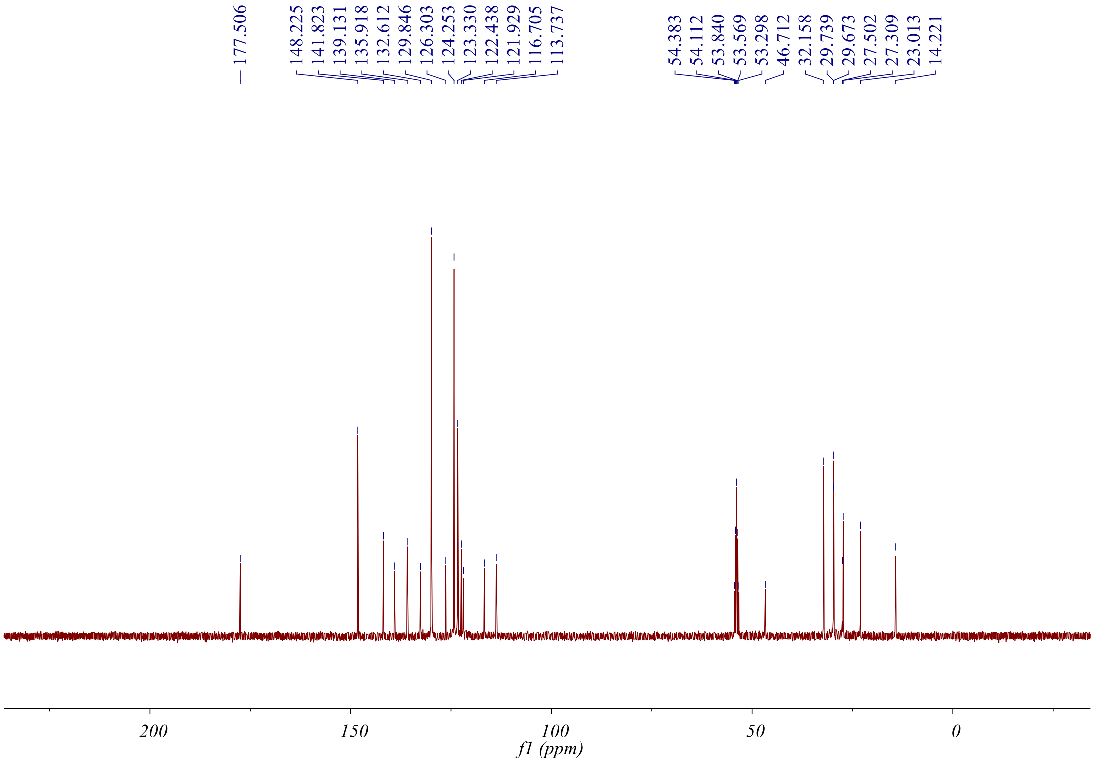

Fig. S13 $^{13}C\{^1H\}$ NMR spectrum of NPh_2-QA (100 MHz, CD_2Cl_2).

References

[1] *Principles of Fluorescence Spectroscopy*, e.d. J. R. Lakowicz, Springer, 3rd edn., New York, 2006.