Supporting Information

Modulating the luminescent performances on blue-emitting coordination polymers via tuning the end-solvent molecules

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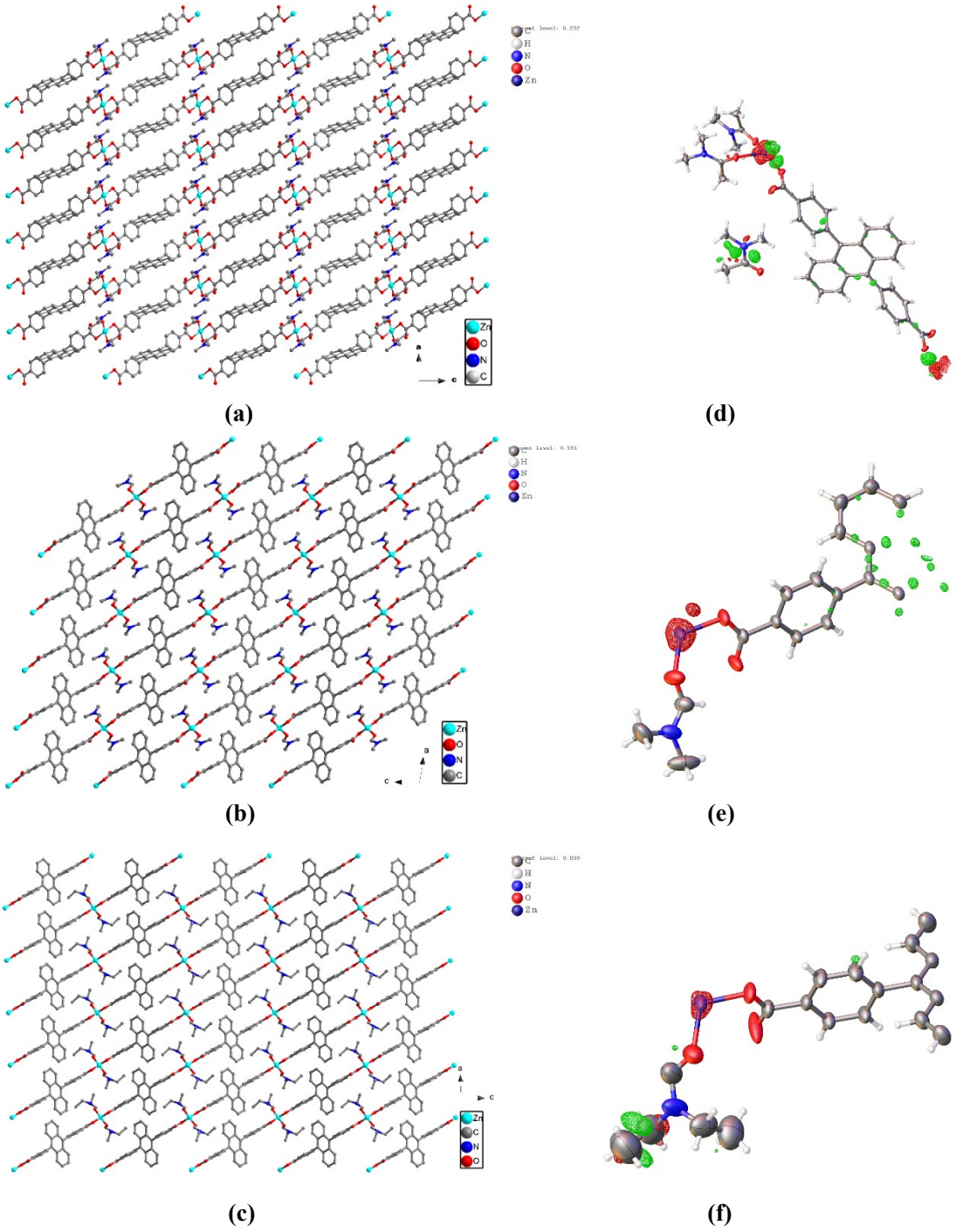


Fig. S1. Packing structures of **Hui-3-DMA** (a), **Hui-3-DMF** (b) and **Hui-3-DEF** (c) along *b* axis; Structural drawings showing ADPs of each structure: **Hui-3-DMA** (d), **Hui-3-DMF** (e) and **Hui-3-DEF** (f).

Table S1. Crystal data and structure refinement parameters for the Complexes.

Complex	**Hui-3-DMA**	**Hui-3-DMF**	**Hui-3-DEF**
Empirical formula	$C_{40}H_{43}N_3O_7Zn$	$C_{34}H_{30}N_2O_6Zn$	$C_{38}H_{36}N_2O_6Zn$
Formula weight	743.14	625.95	682.06
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*Cc*	*C*2/*c*	C2/c
a (Å)	13.27180(10)	17.1162(10)	16.874(3)
b (Å)	9.25150(10)	6.8868(4)	6.9253(11)
c (Å)	27.9580(2)	25.8217(15)	28.607(5)
α (°)	90	90	90
β (°)	90.3710(10)	98.038(2)	91.960(10)
γ (°)	90	90	90
V (Å^3)	3432.72(5)	3013.9(3)	3341.0(10)
Z	4	4	4
D_c (g cm^{-3})	1.438	1.380	1.356
F (000)	1560.0	1296.0	1424.0
2 *θ* range for data collection (°)	11.66 to 146.858	6.374 to 56.65	5.692 to 54.862
Goodness-of-fit on F^2	1.063	1.087	1.109
Final R indexes [I>=2σ (I)]	R_1 = 0.0294, wR_2 = 0.0793	R_1 = 0.0356, wR_2 = 0.0866	R_1 = 0.0609, wR_2 = 0.1728
Final R indexes [all data]	R_1 = 0.00295, wR_2 = 0.0793	R_1 = 0.0450, wR_2 = 0.0907	R_1 = 0.0716, wR_2 = 0.1815
Largest difference in peak and hole (e Å^{-3})	0.61/-0.28	0.31/-0.35	0.95/-0.47

Table S2. Selected Bond Lengths [Å] and Bond Angles [deg] for the Complexes

Hui-3-DMA			
Zn(1) - O(1)	1.944(3)	Zn(1)#1 - O(4)	1.939(3)
Zn(1) - O(5)	2.000(3)	Zn(1) - O(6)	2.026(3)
Zn(1) - O(4)#2	1.939(3)	O(1) - Zn(1) - O(5)	96.22(13)
O(1) - Zn(1) - O(6)	126.69(13)	O(4)#2 - Zn(1) - O(1)	119.77(9)
O(4)#2 - Zn(1) - O(5)	126.25(13)	O(4)#2 - Zn(1) - O(6)	94.69(12)
O(5) - Zn(1) - O(6)	93.19(7)		
Hui-3-DMF			
Zn(1) - O(1)	1.9261(12)	Zn(1) - O(1)#1	1.9262(12)
Zn(1) - O(3)	1.9735(15)	Zn(1) - O(3)#1	1.9735(15)
O(1)#1 - Zn(1) - O(1)	101.77(8)	O(3)#1 - Zn(1) - O(1)	107.47(6)
O(3) - Zn(1) - O(1)	118.49(7)	O(3)#1 - Zn(1) - O(1)#1	118.49(7)
O(3) - Zn(1) - O(1)#1	107.47(6)	O(3)#1 - Zn(1) - O(3)	103.97(11)
Hui-3-DEF			
Zn(1) - O(1)	1.933(2)	Zn(1) - O(1)#1	1.933(2)
Zn(1) - O(3)	1.984(3)	Zn(1) - O(3)#1	1.984(3)
O(1)#1 - Zn(1) - O(1)	98.59(14)	O(3)#1 - Zn(1) - O(1)	114.50(13)
O(3) - Zn(1) - O(1)	109.96(12)	O(3)#1 - Zn(1) - O(1)#1	109.96(12)
O(3) - Zn(1) - O(1)#1	114.50(13)	O(3)#1 - Zn(1) - O(3)	109.2(2)

Hui-3-DMA Symmetry codes#1: 1/2+X,3/2-Y,1/2+Z; #2: -1/2+X,3/2-Y,-1/2+Z; Hui-3-DMF Symmetry codes#1: -X,+Y,1/2-Z; #2: 1/2-X,3/2-Y,-Z; Hui-3-DEF Symmetry codes#1: 1-X,+Y,1/2-Z; #2: 1/2-X,5/2-Y,-Z;

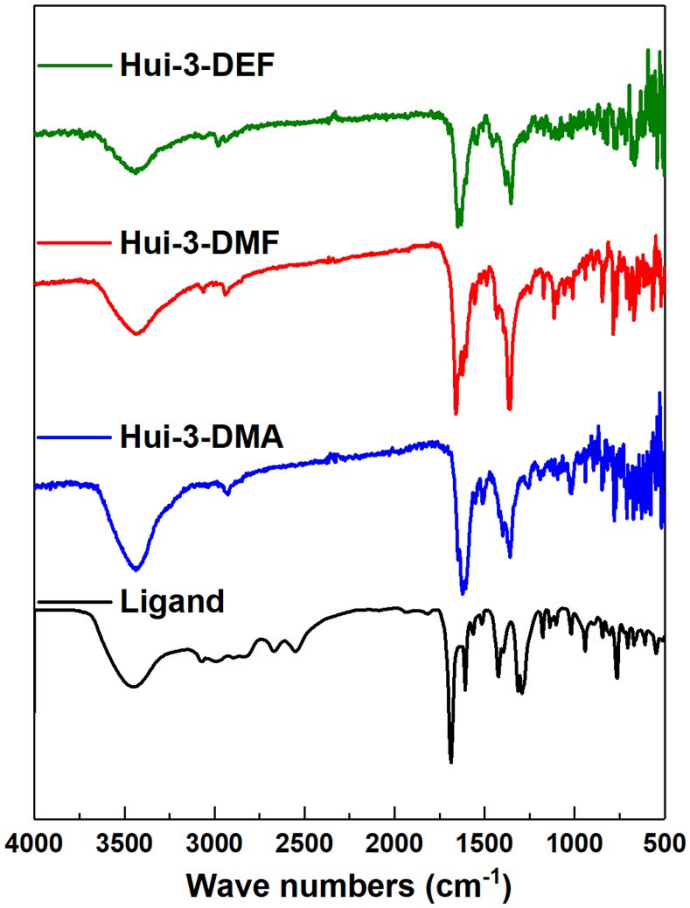


Fig. S2. IR spectra of the compounds.

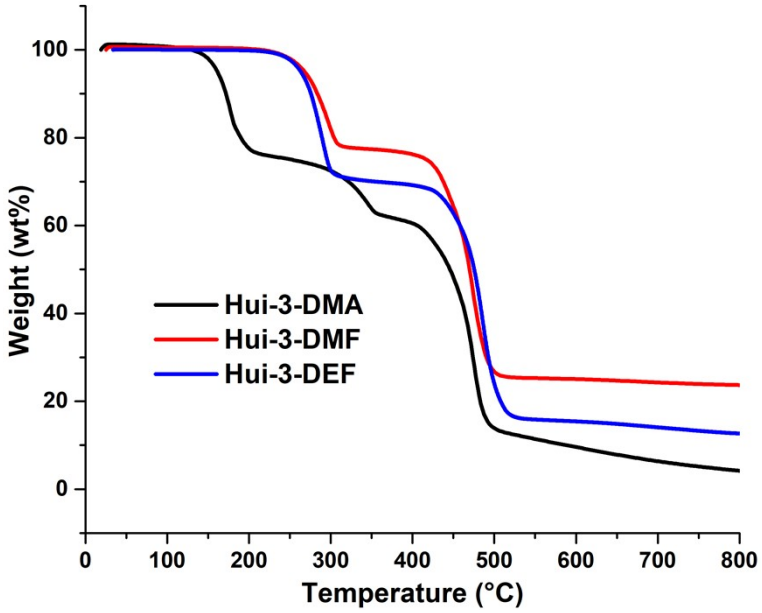


Fig. S3. TGA curves of the compounds.

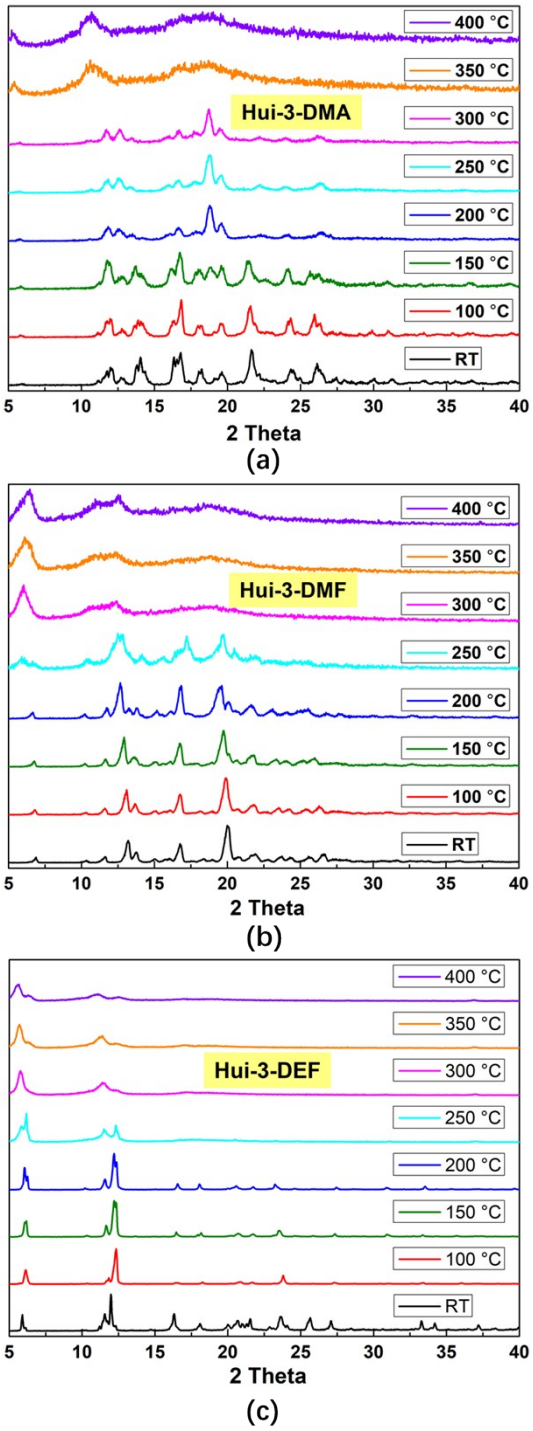


Fig. S4. Various temperature PXRD patterns for the as-synthesized samples of the compounds.

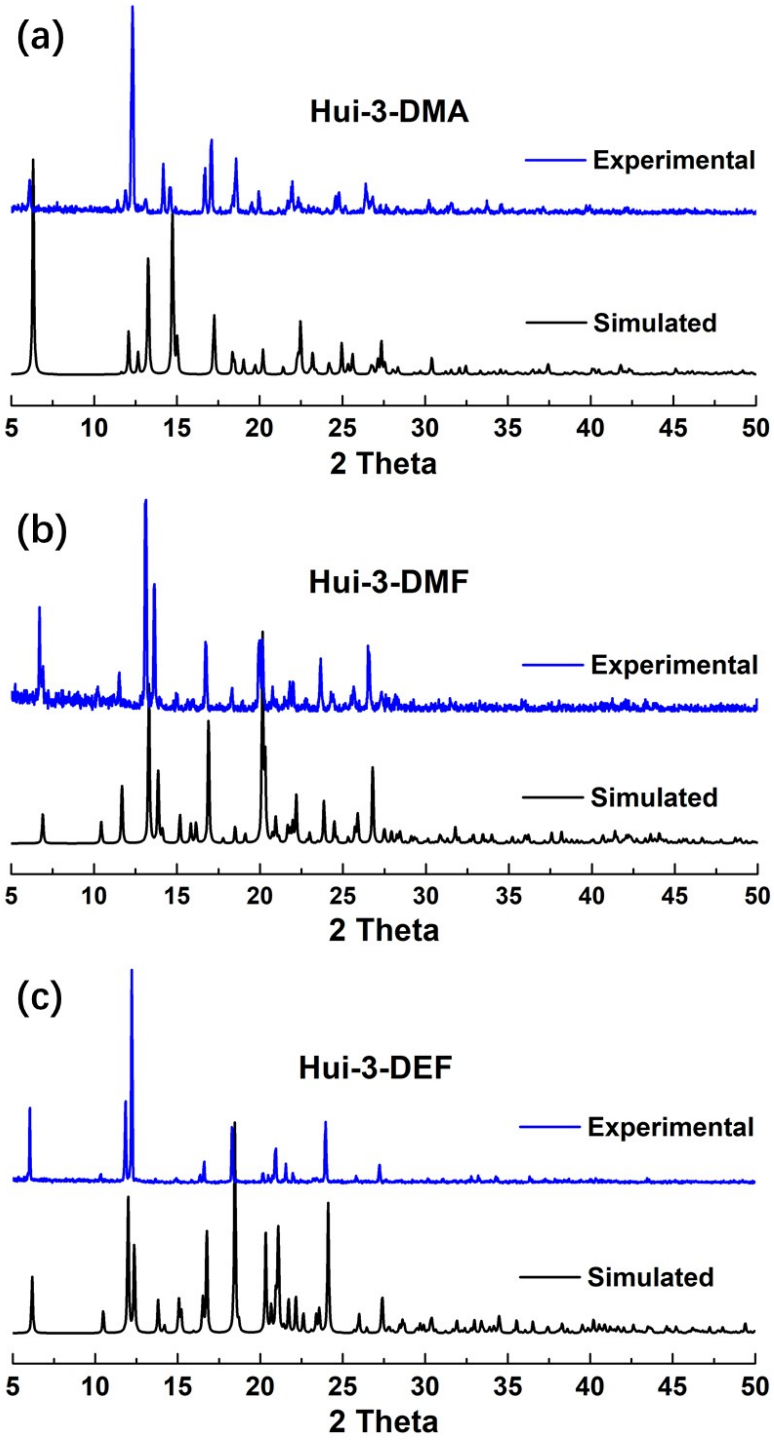


Fig. S5. PXRD patterns of the as-synthesized samples of the compounds.

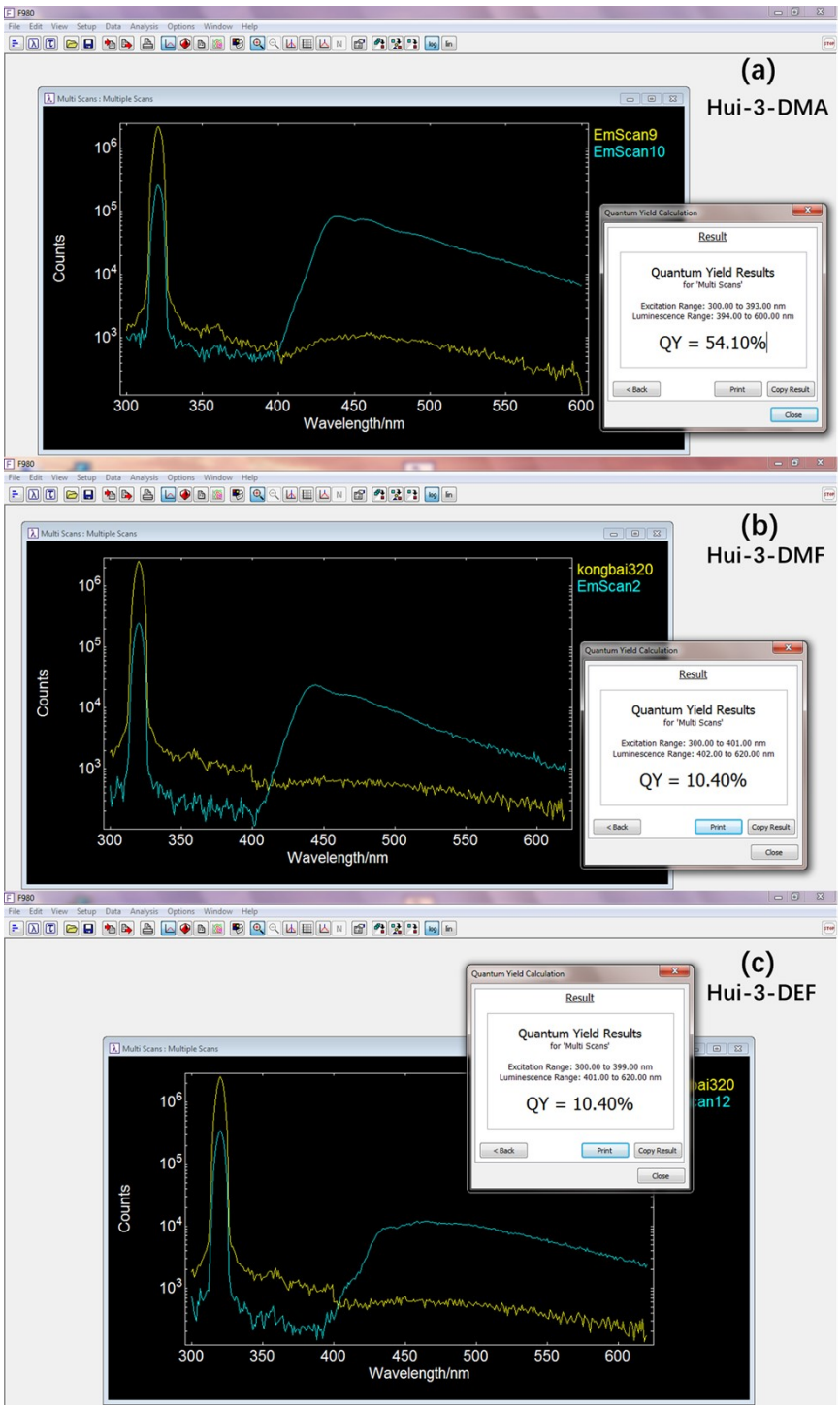


Fig. S6. Various temperature PXRD patterns for the as-synthesized samples of the compounds.

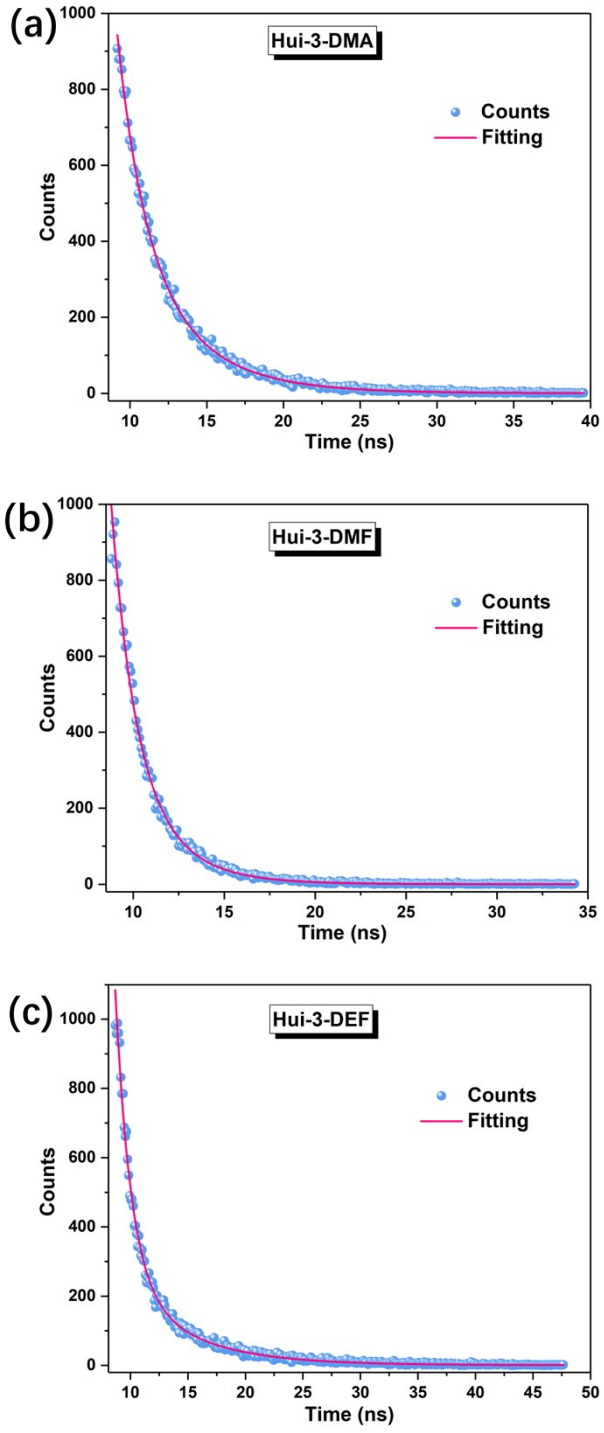


Fig. S7. Fitting curves for fluorescence lifetimes of the three complexes.

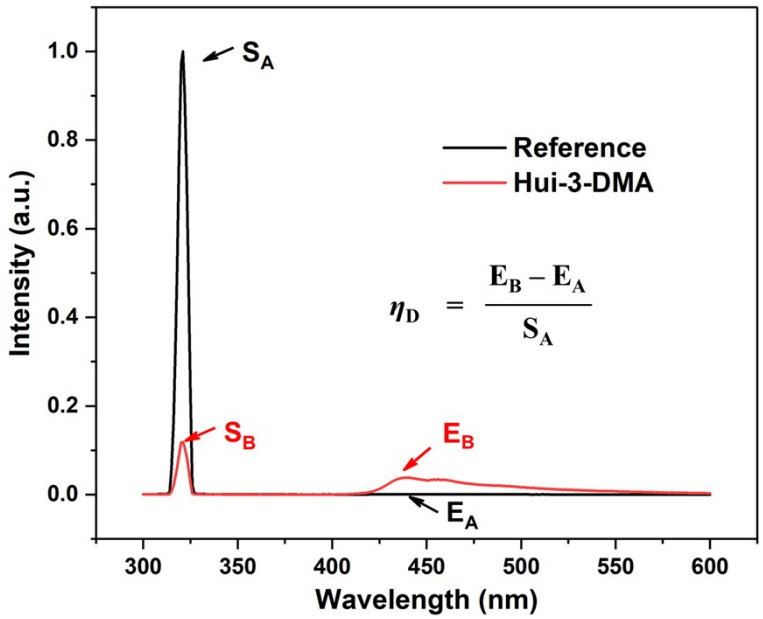


Fig. S8. Calculation of the external quantum yield (η_D) for **Hui-3-DMA**. S_A and S_B are the intensity of the scattering peaks for the reference and **Hui-3-DMA**; E_A and E_B are the intensity of the emission peaks for the reference and **Hui-3-DMA**.

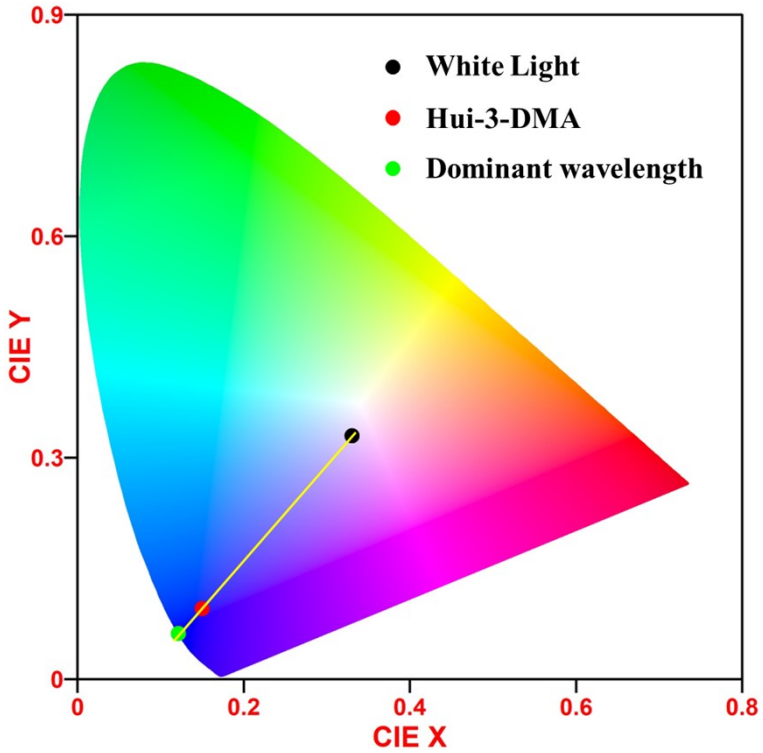


Fig. S9. Calculation of the color purity for **Hui-3-DMA**. Black point is the CIE of white light (0.33, 0.33); red point is the CIE of **Hui-3-DMA** (0.1492, 0.0962); green point is the CIE of the dominant wavelength.

Variable-temperature photoluminescence test:

First, the 1 cm^2 tablet samples were fixed on the copper plate of the liquid nitrogen thermostat, and then the liquid nitrogen thermostat was placed in the space of the spectrophotometer with the sample on the light path. To better control the temperature, the liquid nitrogen thermostat was evacuated during the test. The temperature of the sample in the liquid nitrogen thermostat was controlled by using an East changing TC280 temperature controller with an uncertainty of <0.1 K. The samples were kept at each test temperature for 5 min before being tested. The measurements can be performed from 80 to 420 K.

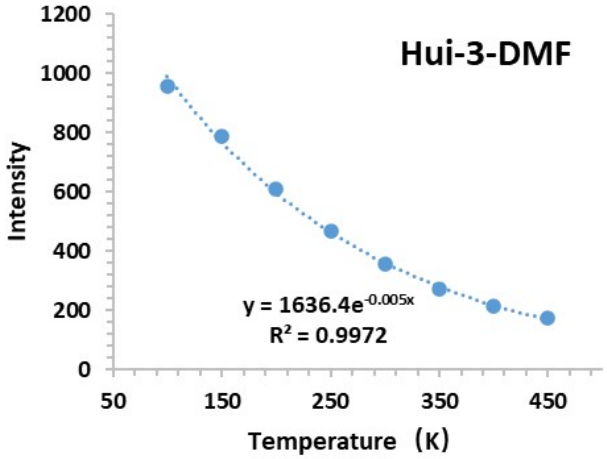


Fig. S10. Nonlinear fitting plots of the relative fluorescence quenching of three complexes in different temperature ranges of the three complexes.

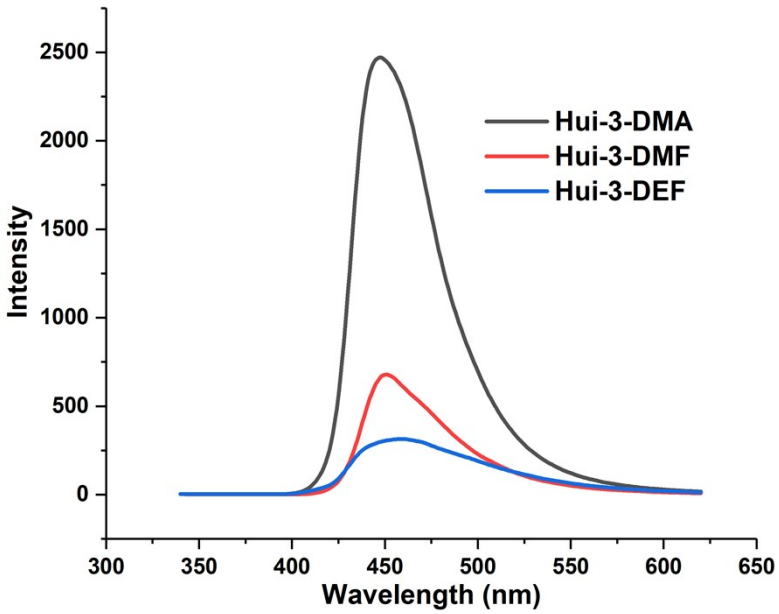


Fig. S11. Emission spectra of the Hui-3 complexes excited at 320 nm with the same Ex (2.5 nm) and Em slit (1.0 nm).

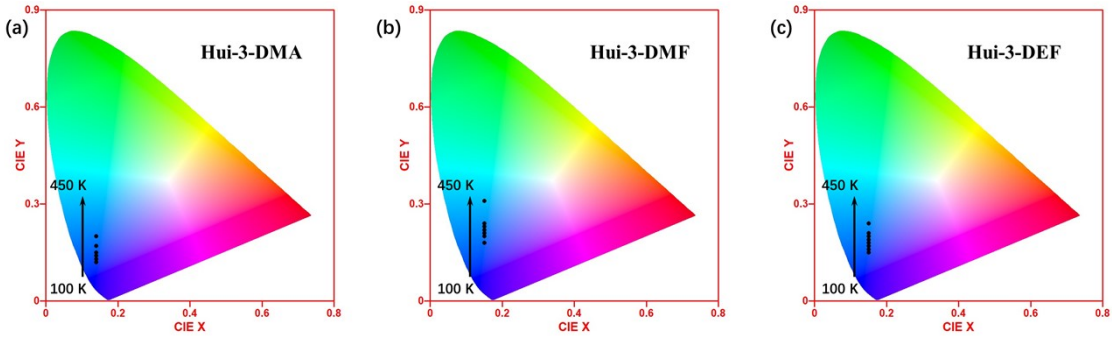


Fig. S12. The CIE color coordinates of the Hui-3 complexes.

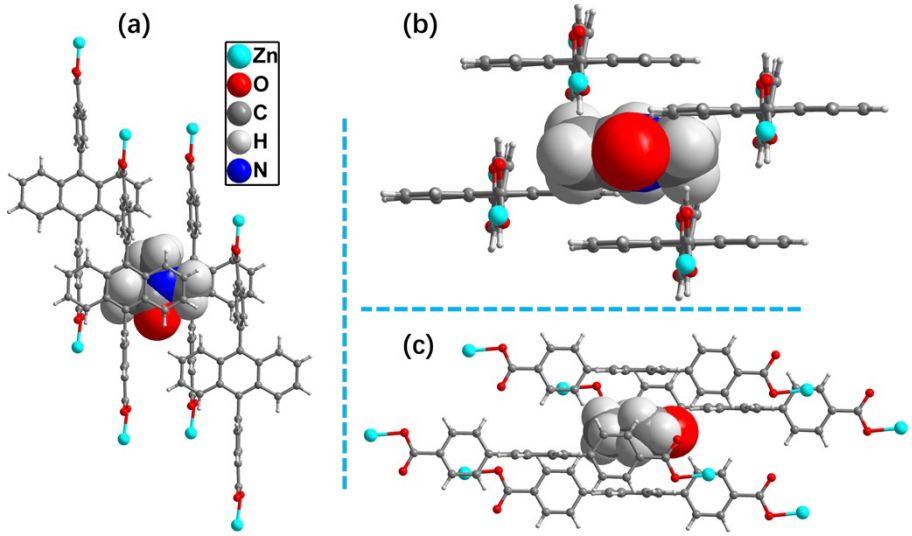


Fig. S13. Structures of **Hui-3-DMA** along different perspectives showing the encapsulation of one free DMA molecule in each void formed by adjacent four ligands.

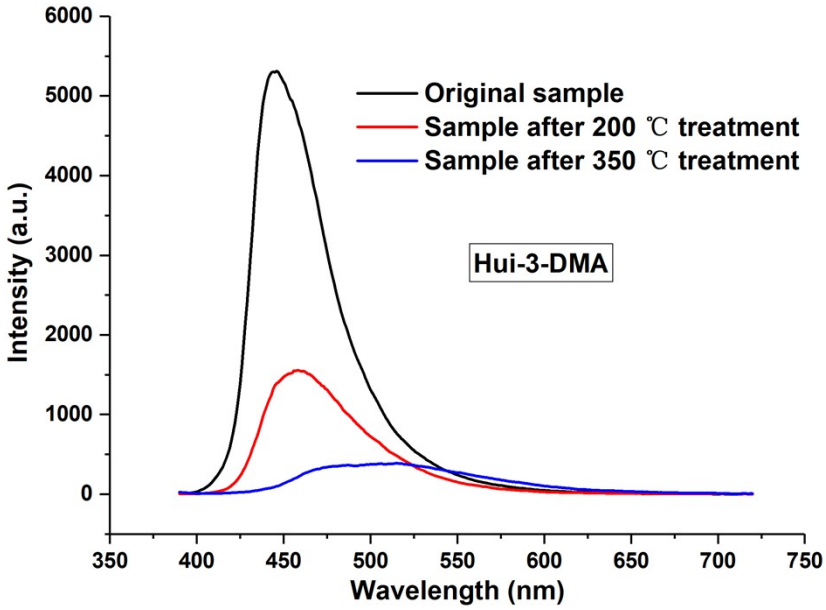
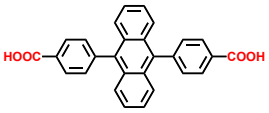
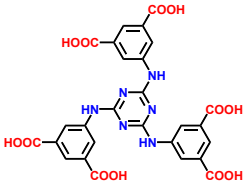
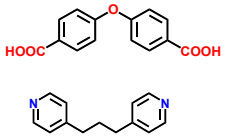
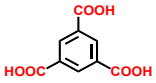
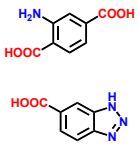
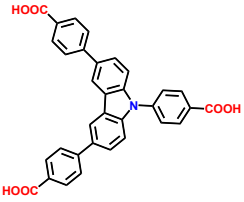


Fig. S14. Emission spectra of the **Hui-3-DMA** samples after different temperature treatment.

Table S3. The quantum yields of the CPs in this work and other reported references.

Samples	Φf (%)	Temp.	Pressure	Ligand	Ref. DOI
Hui-3-DMA Hui-3-DMF Hui-3-DEF	54.1 10.4 10.4	RT RT RT	1 atm		This work
$[(CH_3)_2NH_2]_{15}[(Cd_2Cl)_3(TATPT)_4]\cdot 12DMF\cdot 18H_2O$	15.1%	RT	1 atm		10.1038/ncomms3717
[Zn(μ-L)(μ-1,3-dpp)]	2.5% 18.4%	RT 77 K	1 atm		10.1021/acs.inorgchem.7b00457
$Y(BTC)(H_2O)_6$	2.8% 75%	RT	1 atm 10.0 GPa		10.1002/adfm.202300109
NENU-524	7.5%	RT	1 atm		10.1039/c6qi00528d
$[Zn_4OL_2\cdot xDMF]_n$ $[Zn_4OL_2]_n$	35.5% 29.1	RT	1 atm		10.1039/C8QI00747K