

Supplementary Information

Red-shift in Fluorescence Emission of D–A Type Asymmetrical Zn(II) Complexes by Extending π – π Stacking Interaction

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IR

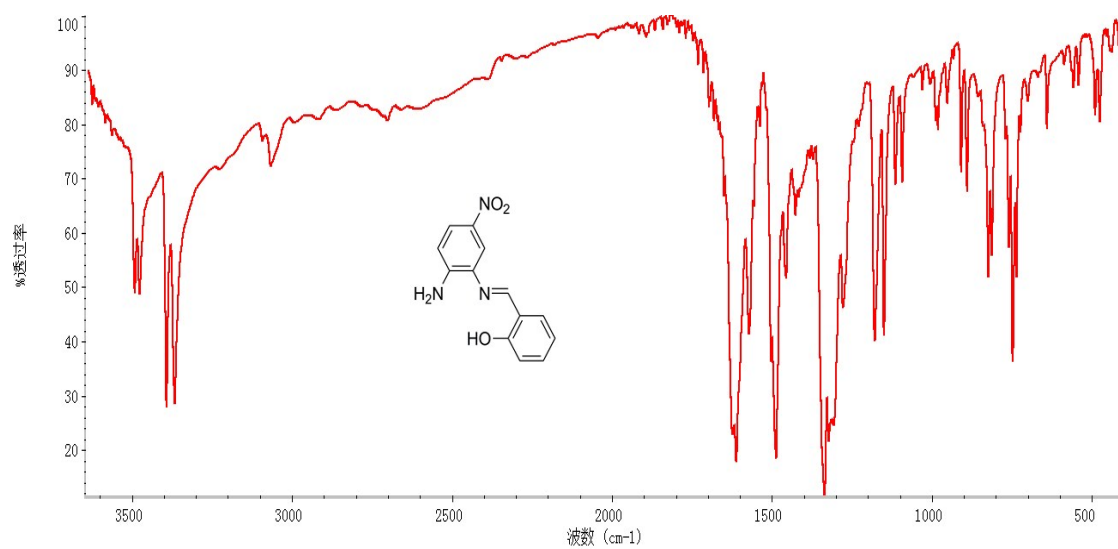


Fig. S1 IR spectra of precursor 1.

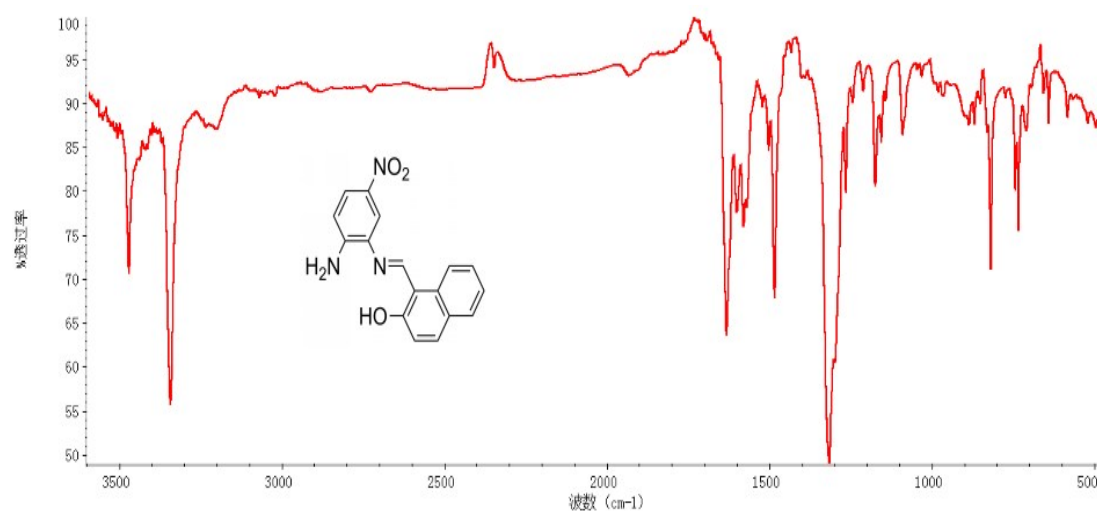


Fig. S2 IR spectra of precursor 2.

¹H-NMR

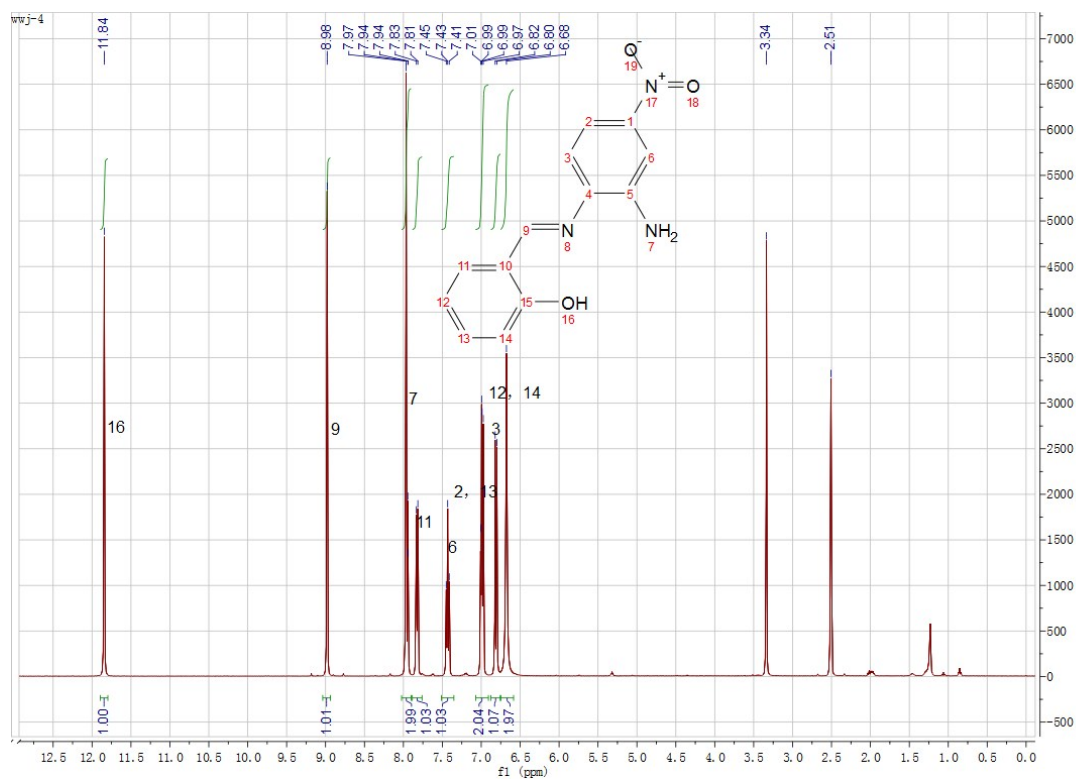


Fig. S3 ¹H NMR spectra of precursor 1.

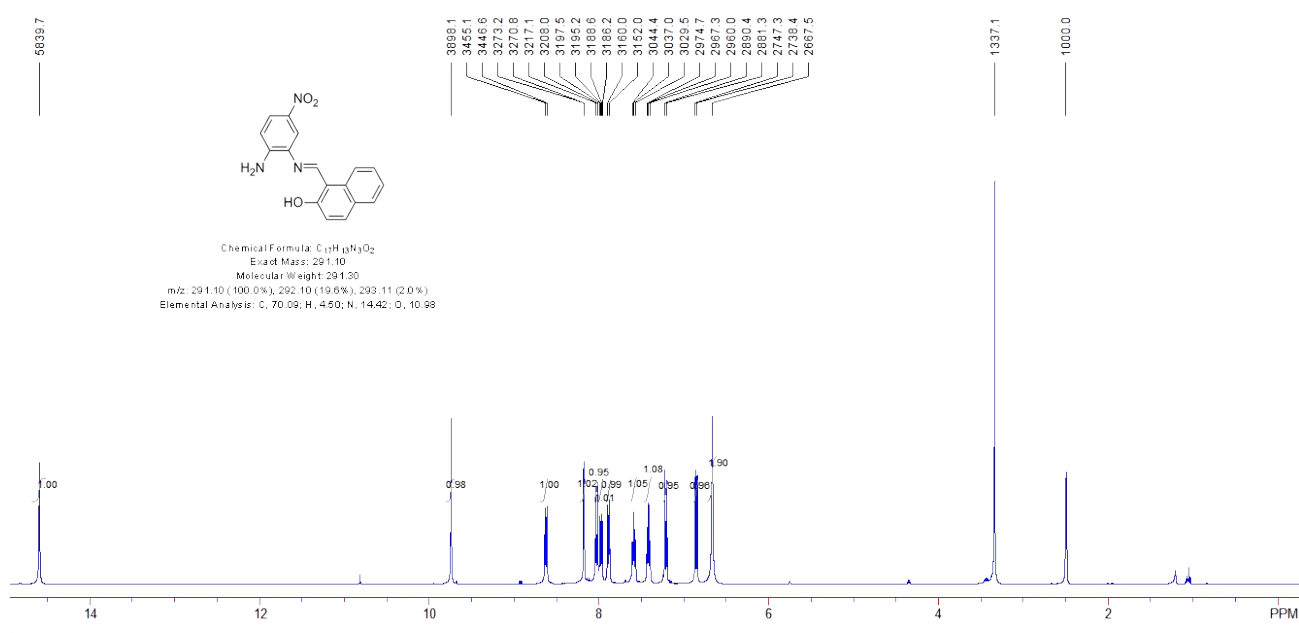


Fig. S4 ¹H NMR spectra of precursor 2.

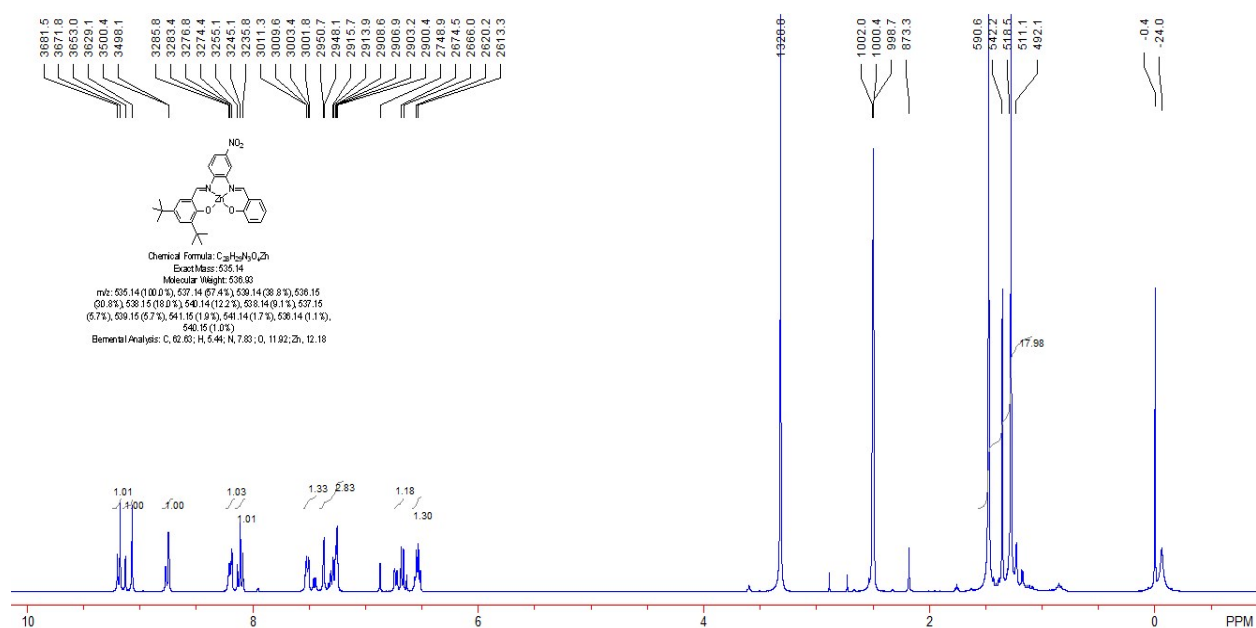


Fig. S5 ^1H NMR spectra of complex 1.

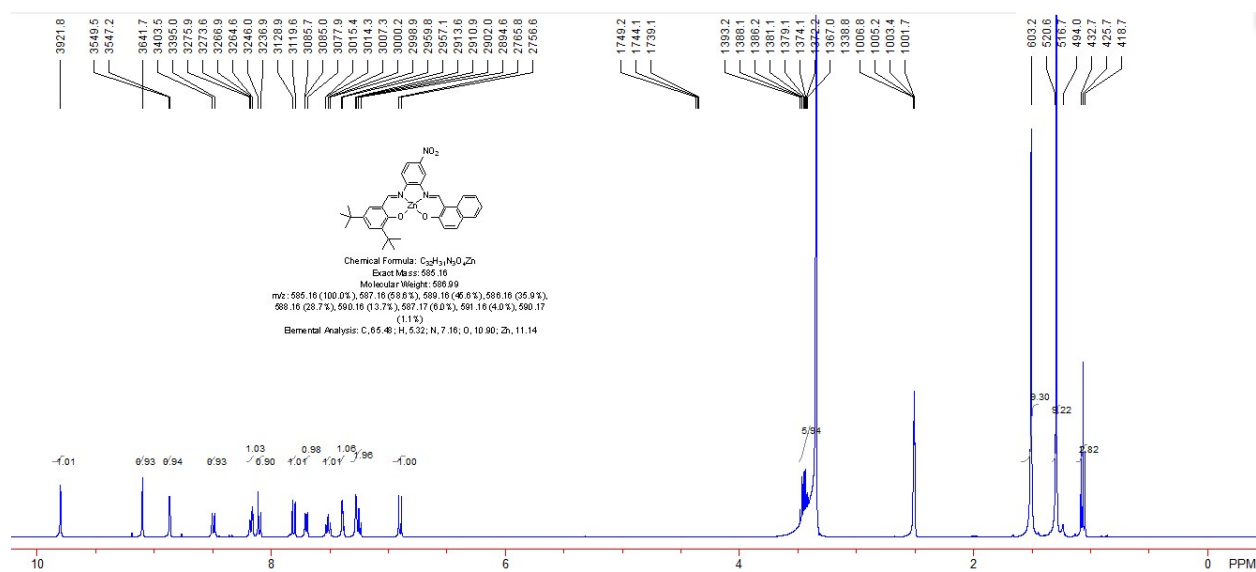


Fig. S6 ^1H NMR spectra of complex 2.

XRD

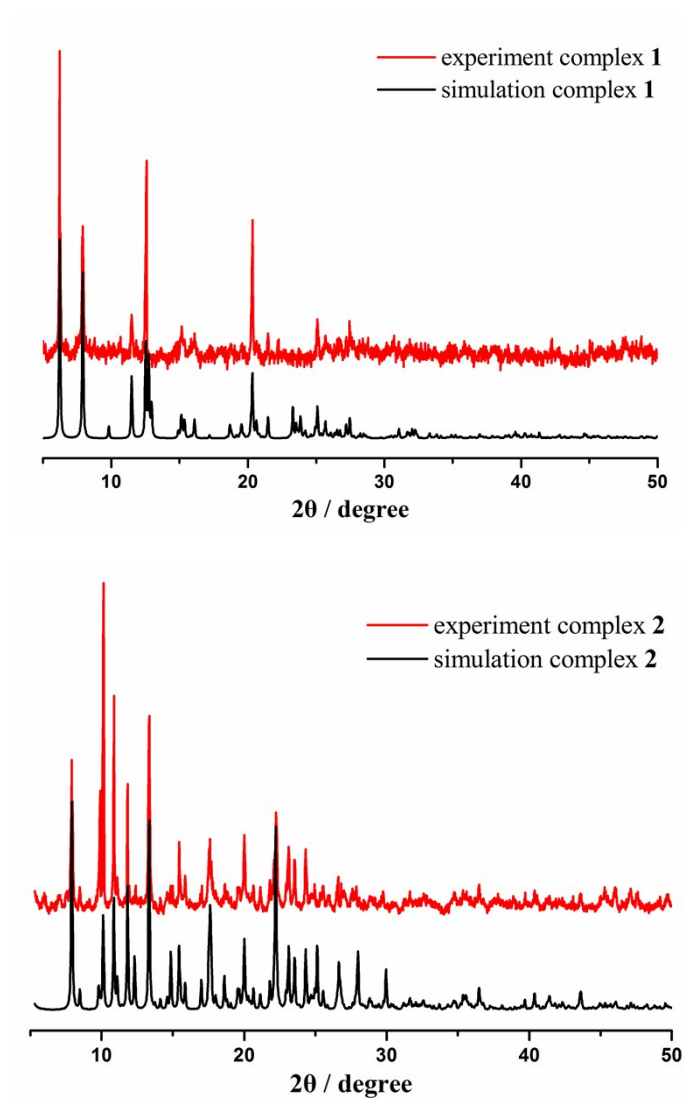


Fig. S7 XRD spectra of complex 1 and 2.

Crystal photos

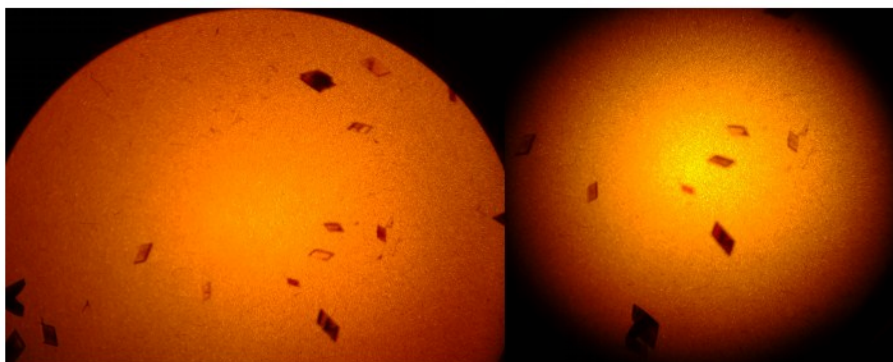


Fig. S8 The crystal photo of complex 1.



Fig. S9 The crystal photo of complex 2.

Fluorescence lifetime

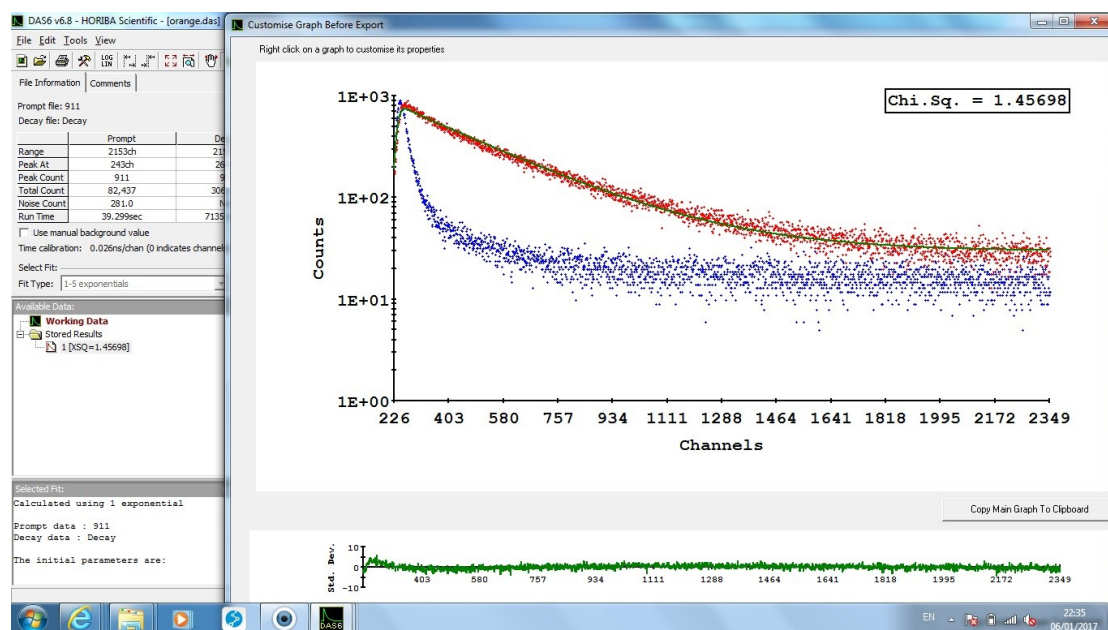


Fig. S10 The fluorescence lifetime of complex 1

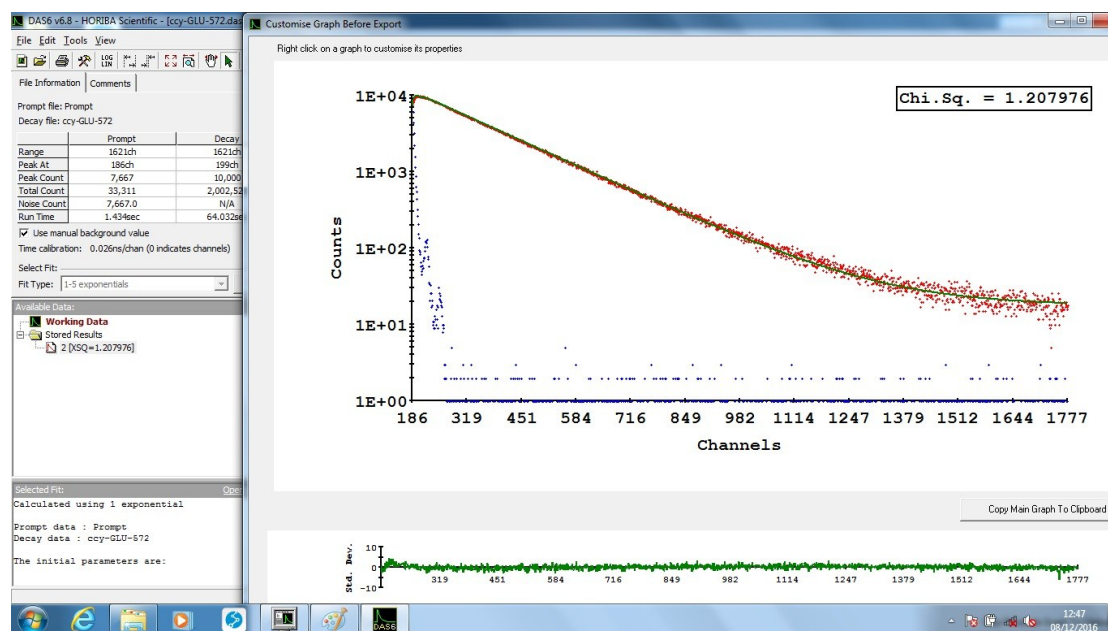


Fig. S11 The fluorescence lifetime of 2

Fluorescence spectra

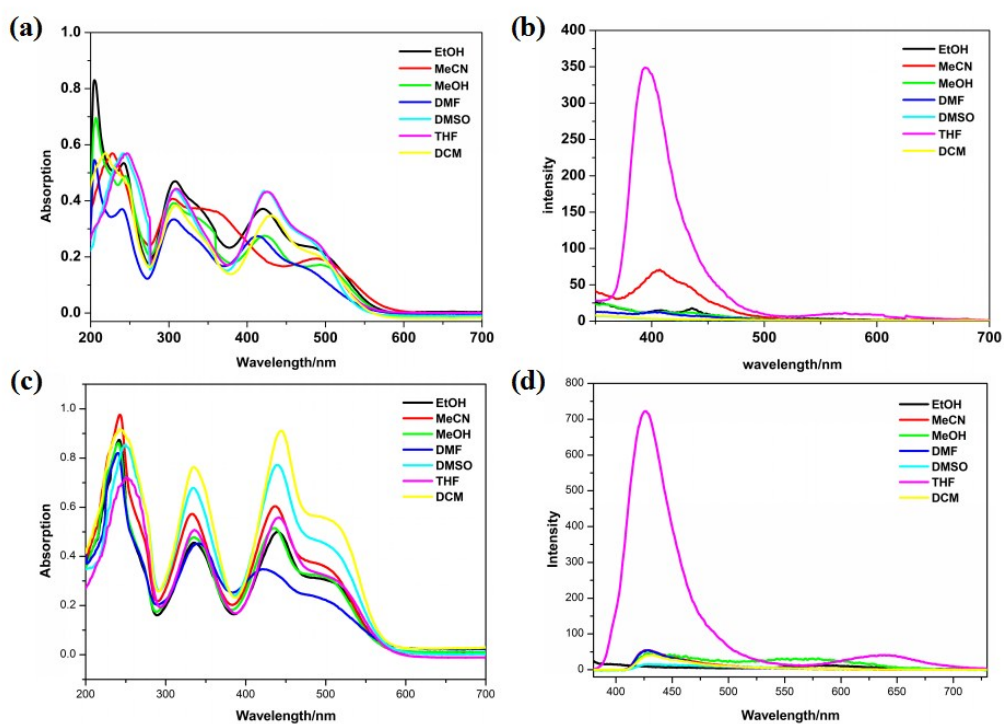


Fig. S12 The UV-vis absorption and fluorescence spectra of complex **1** ($\lambda_{\text{ex}} = 308 \text{ nm}$, $5.0 \times 10^{-5} \text{ mol L}^{-1}$) (a)(b) and complex **2** ($\lambda_{\text{ex}} = 335 \text{ nm}$, $5.0 \times 10^{-5} \text{ mol L}^{-1}$)(c)(d) in seven solvents.

TGA spectra

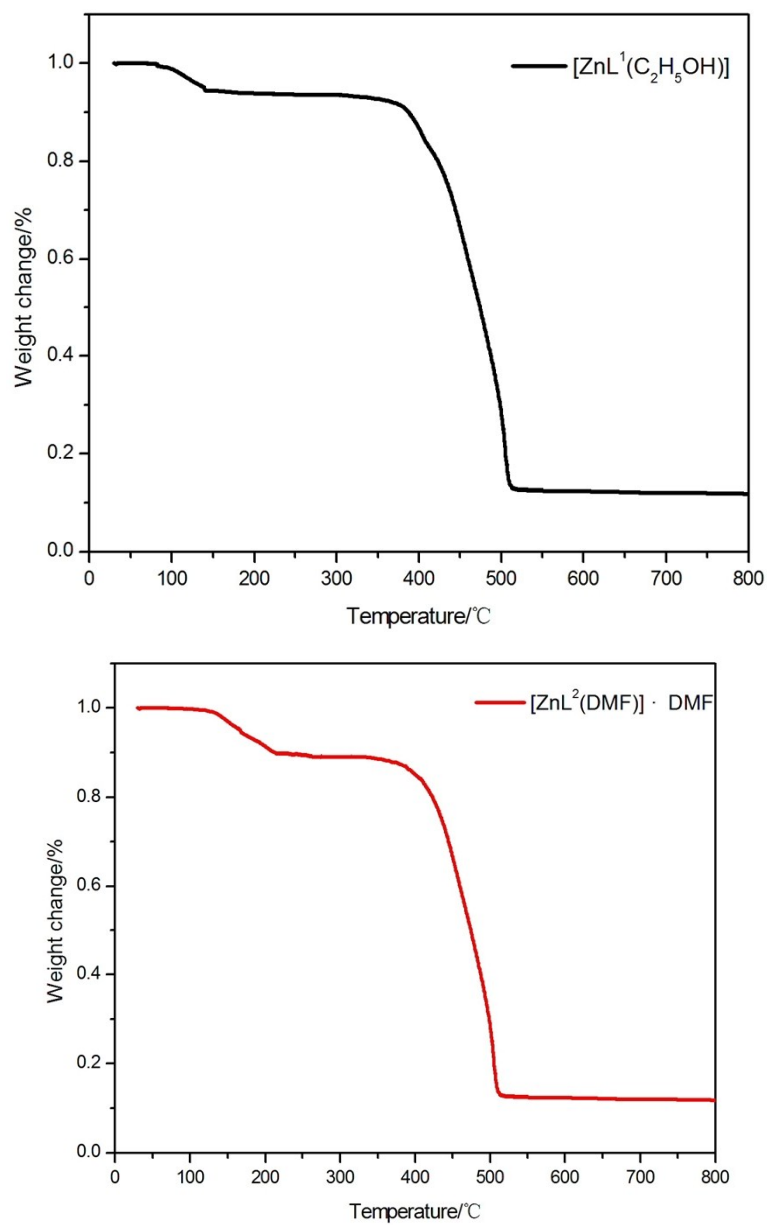


Fig. S13 TGA spectra of solid state of complex 1 and 2.

Crystallography data and Structural Information

Table S1

Crystal data and structure refinement for complexes 1 and 2

Complex	1	2
Formula	C ₃₀ H ₃₅ N ₃ O ₅ Zn	C ₃₈ H ₄₅ N ₅ O ₆ Zn
<i>Mr</i>	582.98	733.16
Temperature (K)	296	293
Crystal system	Monoclinic	Triclinic
Space group	<i>C2/c</i>	<i>PError!</i>
<i>a</i> (Å)	23.447(3)	9.0919(5)
<i>b</i> (Å)	18.503(3)	11.4670(6)
<i>c</i> (Å)	14.697(2)	18.2129 (9)
α (°)	90	101.076 (2)
β (°)	109.402(5)	90
γ (°)	90	96.853 (2)
<i>V</i> (Å ³)	6014.1(15)	1849.47 (17)
<i>Z</i>	8	2
F(000)	2448	772
ρ (calc.) (g cm ⁻³)	1.288	1.317
μ (mm ⁻¹)	0.858	0.716
Crystal size (mm)	0.45× 0.21× 0.19	0.52×0.41×0.36
θ (°)	1.43–25.02	1.14–28.33
Limiting indices	-27≤ <i>h</i> ≤27 -22≤ <i>k</i> ≤22 -17≤ <i>l</i> ≤17	-12≤ <i>h</i> ≤11 -15≤ <i>k</i> ≤15 -24≤ <i>l</i> ≤24
Reflections collected	28970	22465
Independent reflections	5315	9066
Goodness-of-fit on <i>F</i> ²	0.863	1.047
<i>R</i> _{int}	0.1355	0.0210
<i>R</i> ₁ [<i>I</i> >2σ(<i>I</i>)]	0.0444	0.0366
<i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)]	0.0735	0.1009
<i>R</i> ₁ (all data)	0.1261	0.0539
<i>wR</i> ₂ (all data)	0.0877	0.1134

Table S2**Selected bond lengths (Å) and angles (°) for complexes 1**

Zn(1)–O(2)	1.950(3)	Zn(1)–O(1)	1.981(3)
Zn(1)–O(3)	2.036(3)	Zn(1)–N(3)	2.088(3)
Zn(1)–N(2)	2.117(3)		
O(2)–Zn(1)–O(3)	102.31(12)	O(2)–Zn(1)–O(1)	100.06(12)
O(1)–Zn(1)–O(3)	96.60(12)	O(2)–Zn(1)–N(3)	87.64(13)
O(1)–Zn(1)–N(3)	155.65(13)	O(3)–Zn(1)–N(3)	104.34(12)
O(2)–Zn(1)–N(2)	156.05(12)	O(1)–Zn(1)–N(2)	88.32(13)
O(3)–Zn(1)–N(2)	98.92(12)	N(3)–Zn(1)–N(2)	76.39(14)
C(28)–O(1)–Zn(1)	129.5(3)	C(13)–O(2)–Zn(1)	132.0(3)
C(22)–N(2)–Zn(1)	125.3(3)	C(5)–N(2)–Zn(1)	112.1(3)
C(30)–O(3)–Zn(1)	133.0(4)	Zn(1)–O(3)–H(3A)	110.7
C(7)–N(3)–Zn(1)	124.4(3)	C(4)–N(3)–Zn(1)	113.4(3)

Table S3**Selected bond lengths (Å) and angles (°) for complexes 2**

Zn(1)–O(2)	1.9534(13)	Zn(1)–O(1)	1.9708(13)
Zn(1)–N(2)	2.0740(14)	Zn(1)–O(6)	2.0854(15)
Zn(1)–N(1)	2.0996(15)		
O(2)–Zn(1)–O(1)	98.50(6)	O(2)–Zn(1)–N(2)	88.78(5)
O(1)–Zn(1)–N(2)	151.57(7)	O(2)–Zn(1)–O(6)	97.28(6)
O(1)–Zn(1)–O(6)	99.86(6)	N(2)–Zn(1)–O(6)	106.46(6)
O(2)–Zn(1)–N(1)	162.70(6)	O(1)–Zn(1)–N(1)	87.63(5)
N(2)–Zn(1)–N(1)	78.55(6)	O(6)–Zn(1)–N(1)	97.57(6)
C(22)–O(2)–Zn(1)	132.09(12)	C(8)–O(1)–Zn(1)	131.25(12)
C(31)–O(6)–Zn(1)	122.19(14)	C(16)–N(2)–Zn(1)	125.37(12)
C(15)–N(2)–Zn(1)	113.55(11)	C(9)–N(1)–Zn(1)	126.21(12)
C(10)–N(1)–Zn(1)	112.25(10)		