Electronic Supplementary Information

A Stable Zinc-Organic Framework with Luminescent Detection of Acetylacetone in Aqueous Solution

Xiao-Min Kang,[a] Xi-Yu Fan,[a] Peng-Yuan Hao,[a] Wen-Min Wang,[b] and Bin Zhao*[a]

Table S1 Selected bond lengths (Å) and bond angles (°) for compound **1**.

Bond distances			
Zn(1)-O(1)	2.042(3)	Zn(1)-N(2)	2.157(4)
Zn(1)-O(2)	2.068(3)	O(1)-C(10)#1	1.267(6)
Zn(1)-O(3)	2.129(4)	O(2)-C(10)#2	1.253(6)
Zn(1)-O(4)	2.344(4)	C(10)-O(1)#3	1.267(6)
Zn(1)-N(1)	2.125(4)	C(21)-C(1)#4	1.480(8)
Bond Angles			
O(1)-Zn(1)-O(2)	121.71(13)	O(3)-Zn(1)-N(2)	92.00(15)
O(1)-Zn(1)-O(3)	149.10(14)	N(1)-Zn(1)-O(3)	91.53(15)
O(1)-Zn(1)-O(4)	90.39(12)	O(3)-Zn(1)-O(4)	58.72(12)
O(1)-Zn(1)-N(1)	91.60(15)	N(1)-Zn(1)-O(4)	94.53(14)
O(1)-Zn(1)-N(2)	89.69(14)	N(1)-Zn(1)-N(2)	175.64(15)
O(2)-Zn(1)-O(3)	89.04(13)	N(2)-Zn(1)-O(4)	89.49(14)
O(2)-Zn(1)-O(4)	147.52(12)	C(10)#1-O(1)-Zn(1)	123.5(3)
O(2)-Zn(1)-N(1)	89.76(14)	C(10)#2-O(2)-Zn(1)	152.4(3)
O(2)-Zn(1)-N(2)	87.73(14)	O(2)#2-C(10)-O(1)#3	124.3(5)
O(3)-Zn(1)-O(4)	58.72(12)	N(3)-C(21)-C(1)#4	117.6(5)
		C(2)-C(1)-C(21)#5	122.3(5)

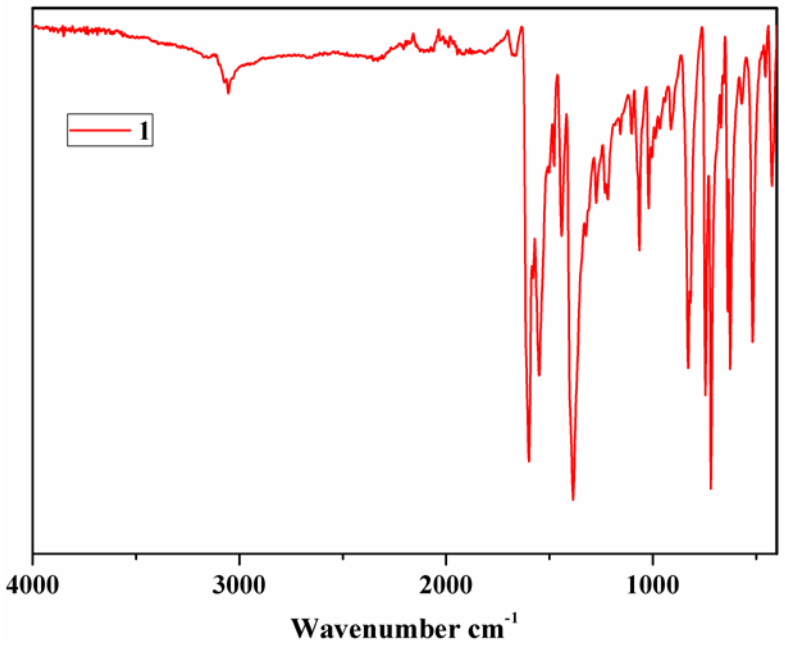
Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,y-1/2,z #2 -x+1,-y+2,-z+1 #3 x+1/2,y+1/2,z

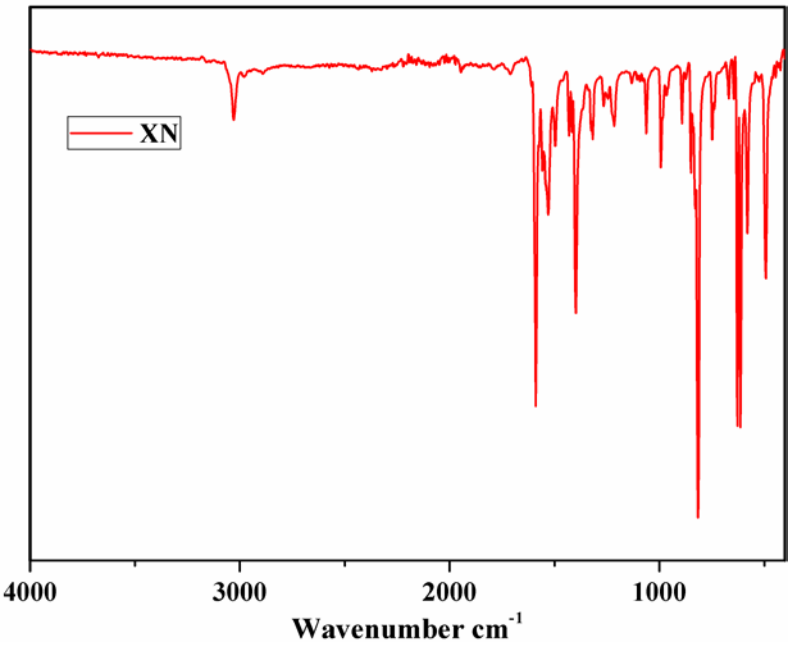
#4 x+1/2,-y+3/2,z+1/2 #5 x-1/2,-y+3/2,z-1/2

[a] *College of Chemistry and Key Laboratory of Advanced Energy Material Chemistry, Nankai University, Tianjin 300071, China. E-mail: zhaobin@nankai.edu.cn*

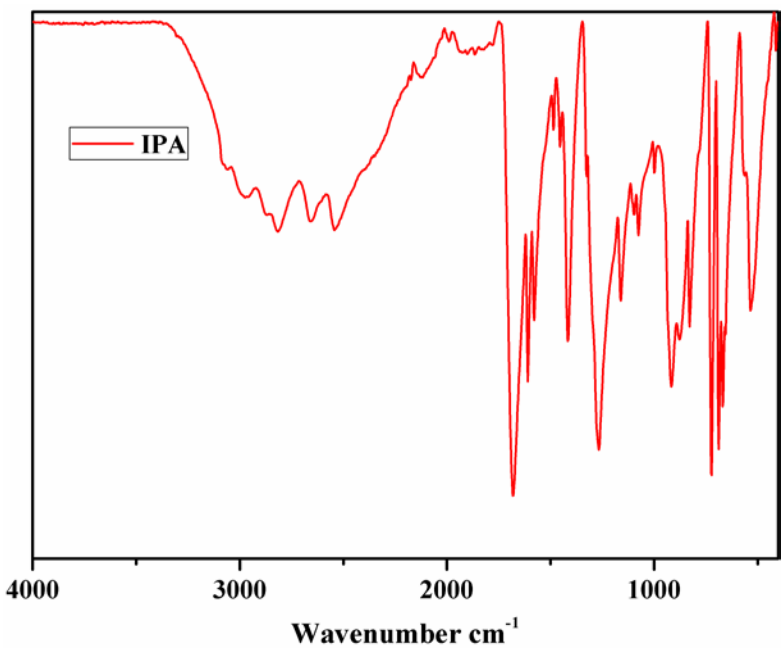
[b] *Department of Chemistry, Tianjin University, Tianjin 300072, China.*


1
4000
3000
2000
1000
Wavenumber cm-1

(a)


XN
4000
3000
2000
1000
Wavenumber cm-1

(b)



(c)

Fig. S1 The FT-IR spectra of compound **1** and ligands. (a) for **1**, (b) for XN and (c) for IPA.

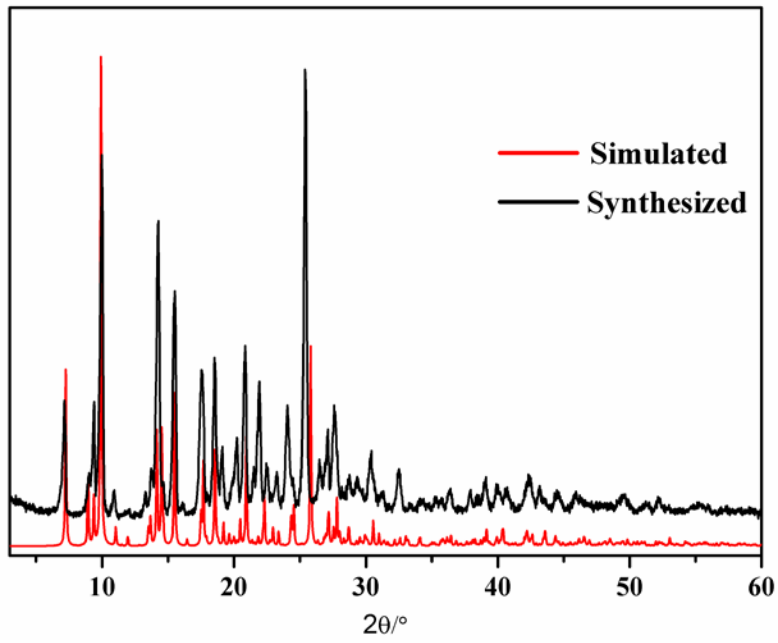


Fig. S2 The PXRD patterns for the simulated and synthesized samples for compound **1**.

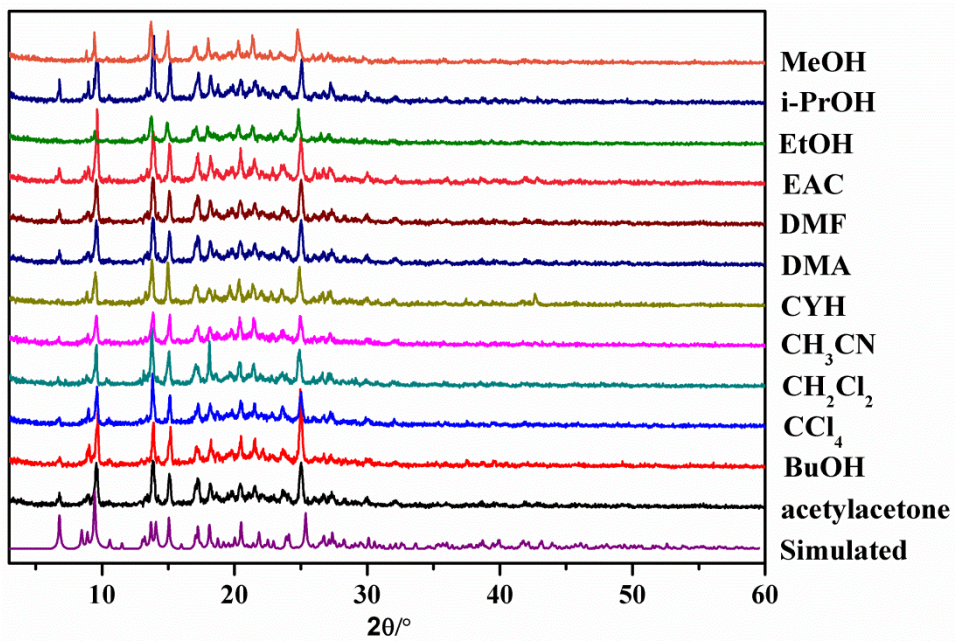


Fig. S3 The PXRD patterns for compound **1** immersing in common organic solvents for 12 h.

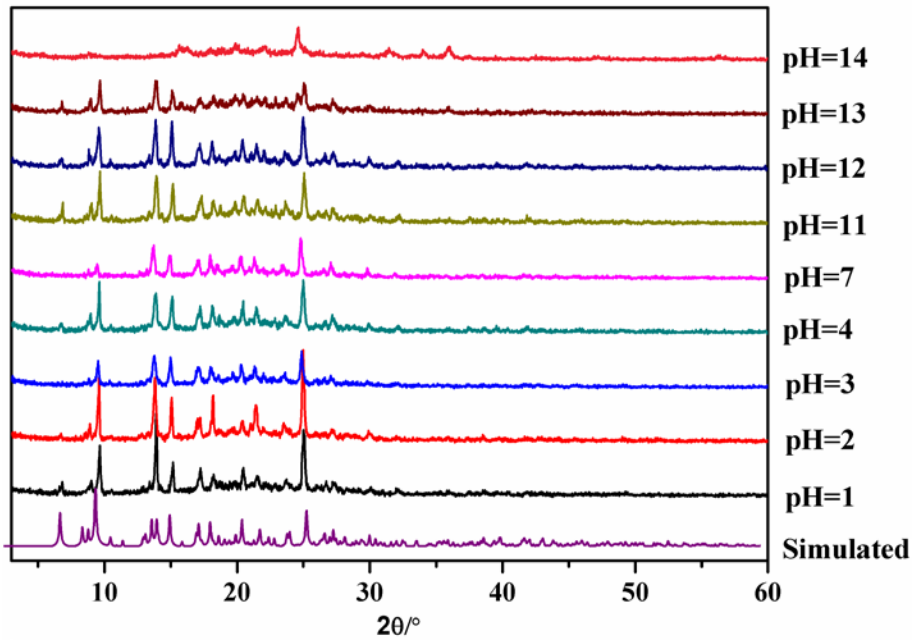


Fig. S4 The PXRD patterns for compound **1** in various acid/base solutions with pH range from 1.0 to 14.0 for 6 h.

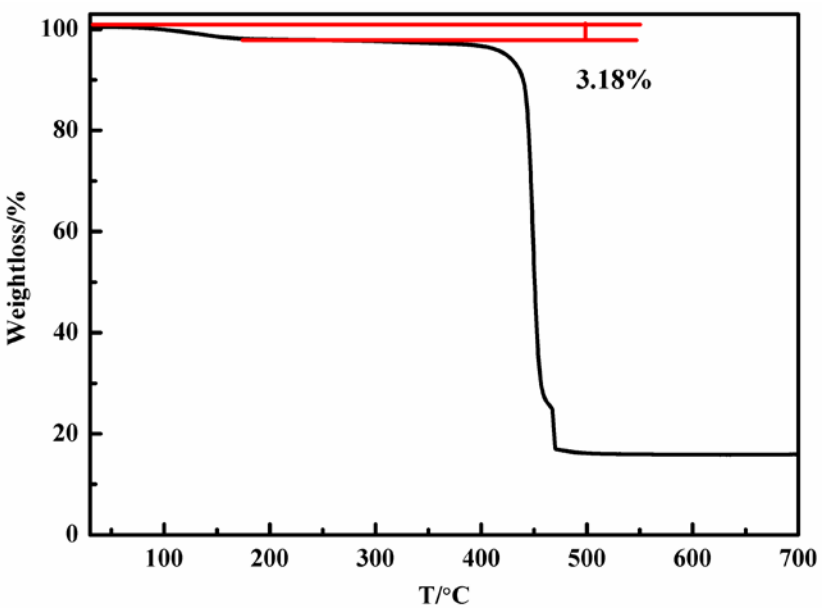


Fig. S5 The TG curve for compound **1.**

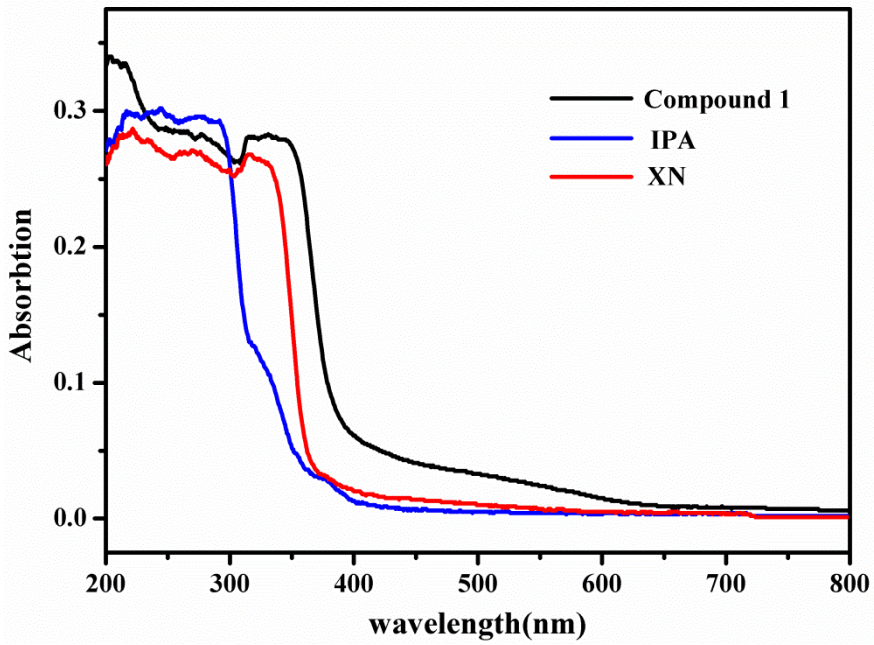


Fig. S6 The solid-state UV spectra for compound **1** and ligands (XN and IPA). Black: compound **1**; Blue: IPA; Red: XN.

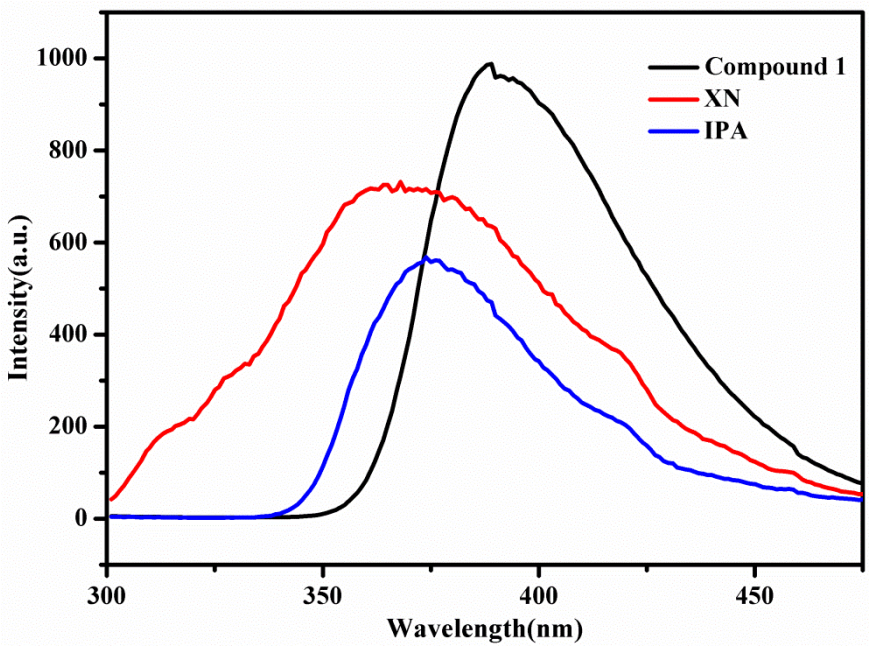


Fig. S7 The solid-state photoluminescence spectrum for compound **1** and ligands (XN and IPA). Black: compound **1**; Blue: IPA; Red: XN.

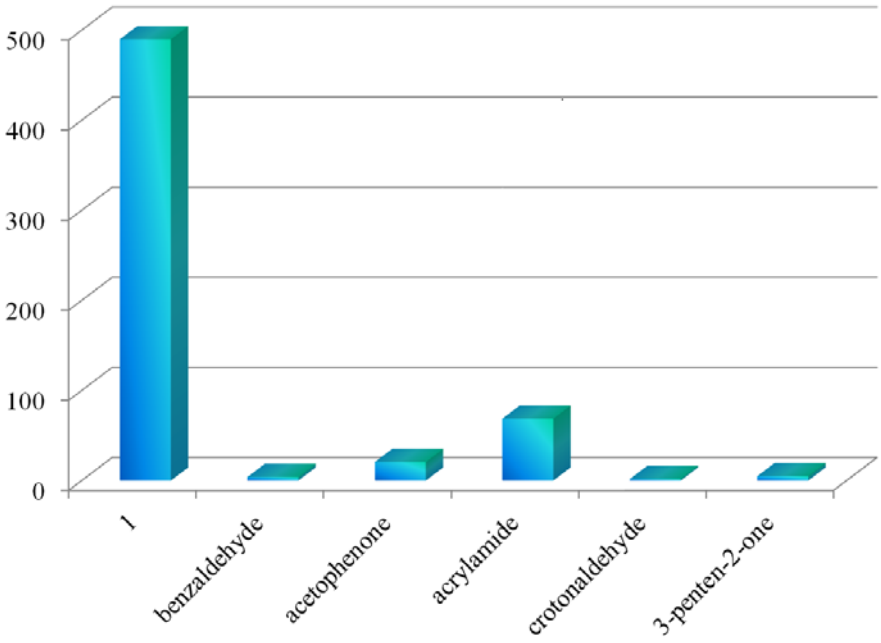


Fig. S8 The luminescence emission of **1** in aqueous solution after the addition of benzaldehyde, acetophenone, acrylamide, crotonaldehyde and 3-penten-2-one respectively at 383 nm.

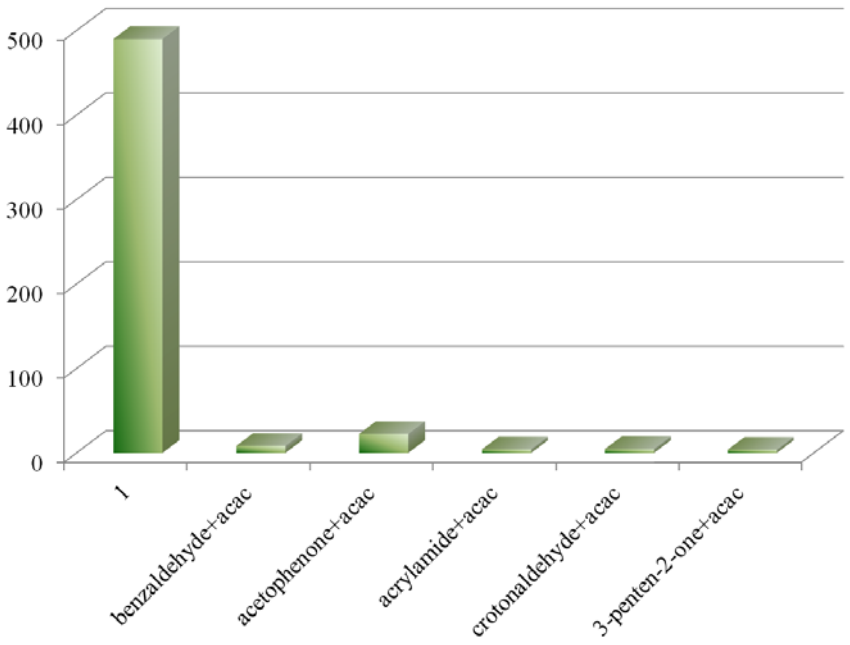
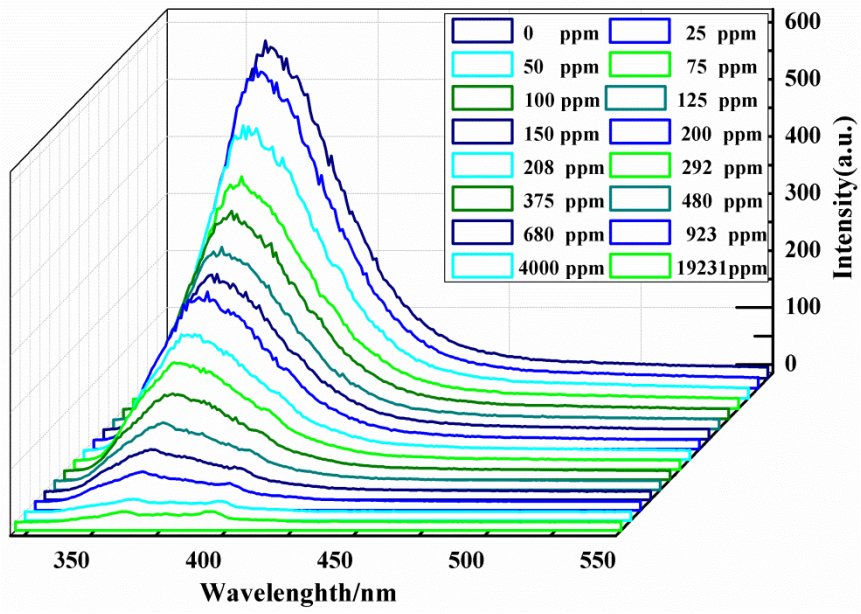
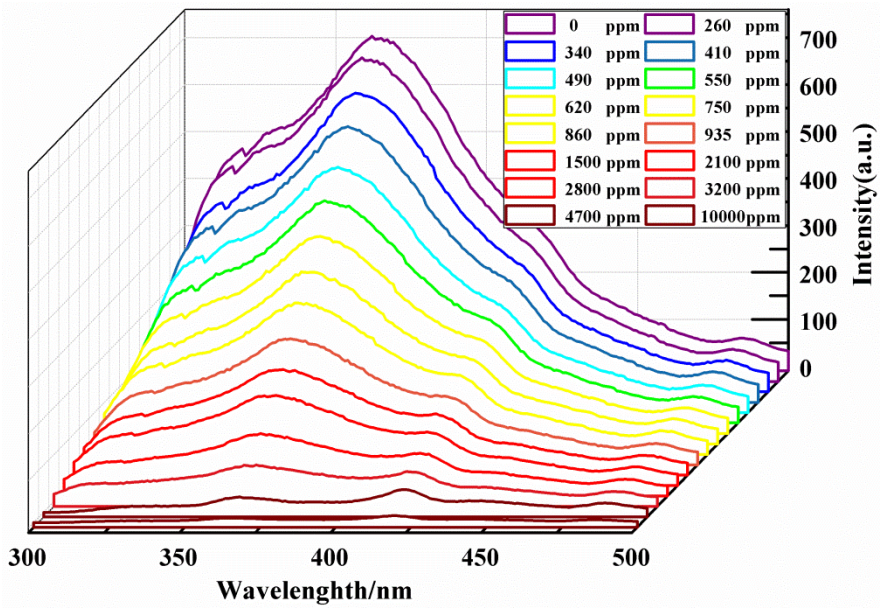


Fig. S9 Comparison of the luminescence intensity for **1** in presence of mixed organic solvents of acac and benzaldehyde, acetophenone, acrylamide, crotonaldehyde and 3-penten-2-one respectively at 383 nm.



(a)



(b)

Figure S10. Changes in the luminescence spectrum of the systems of XN ligand (a) and IPA ligand (b) with different concentrations of acetylacetone.

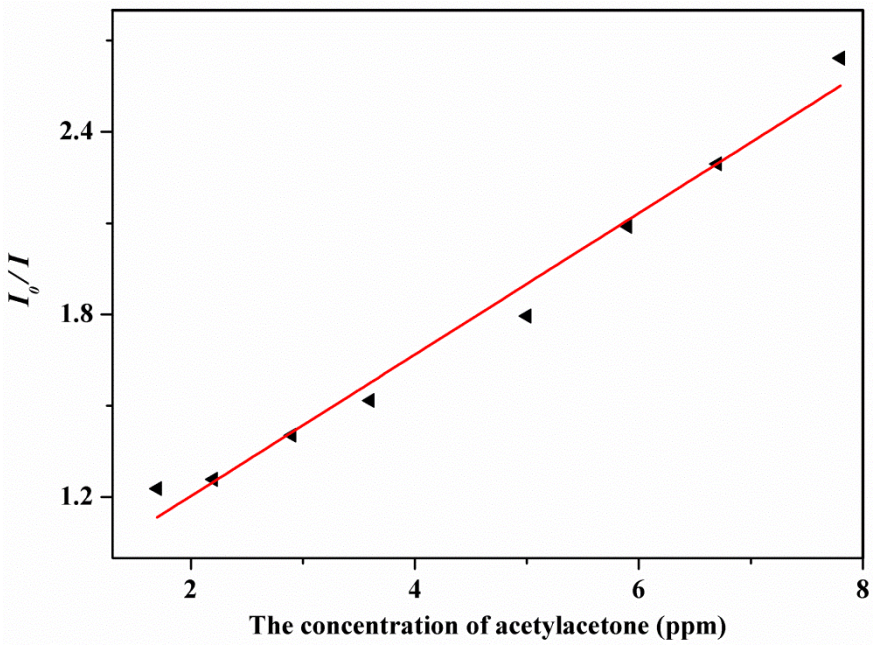
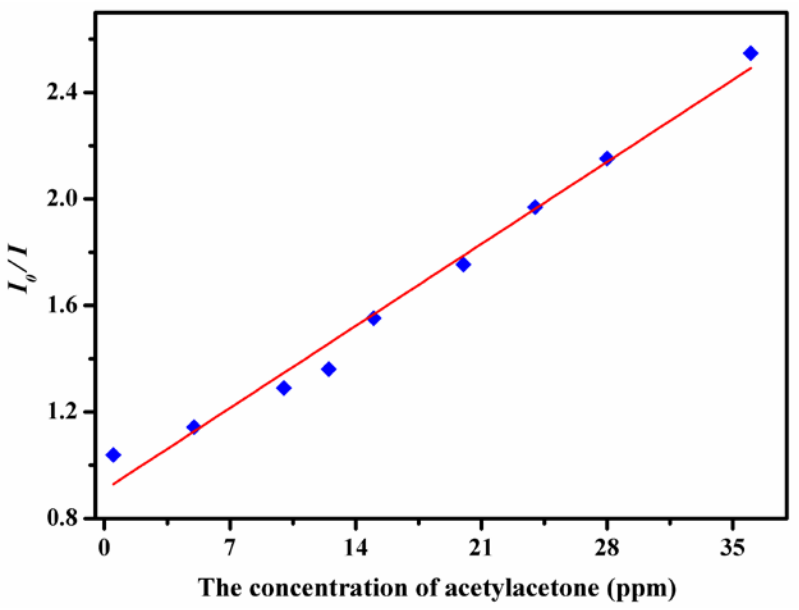


Fig. S11 The luminescence intensity *vs*. acetylacetone concentration plots (I_0 and I represent the luminescence intensity of compound **1** in aqueous solution before and after adding different concentration of acetylacetone, respectively; K_{sv} is the Stern Volmer constant).



(b)

Figure S12. The luminescence intensity *vs*. acetylacetone concentration plots (I_0 and I represent the luminescence intensity of compound **1** in organic solvent before and after adding different concentration of acetylacetone, respectively; K_{sv} is the Stern Volmer constant).

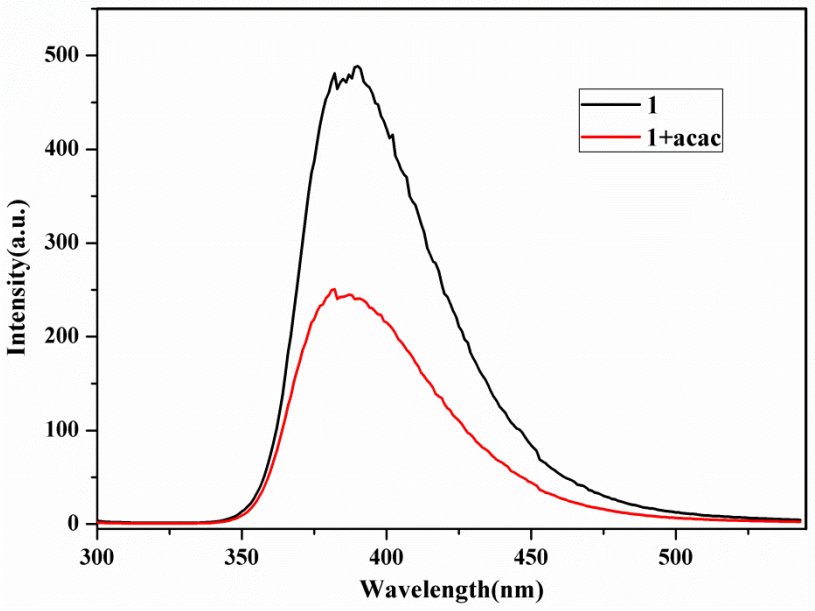


Figure S13. Changes of the luminescence spectrum for compound **1** in acac gas.

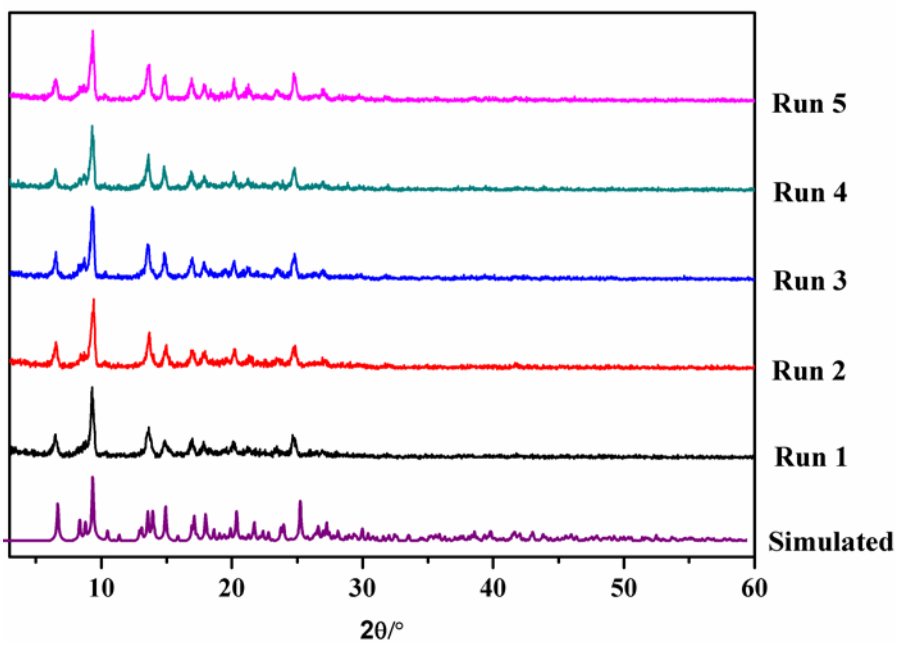


Fig. S14 The PXRD patterns of compound **1** after luminescent recycling agree well with the simulated one.

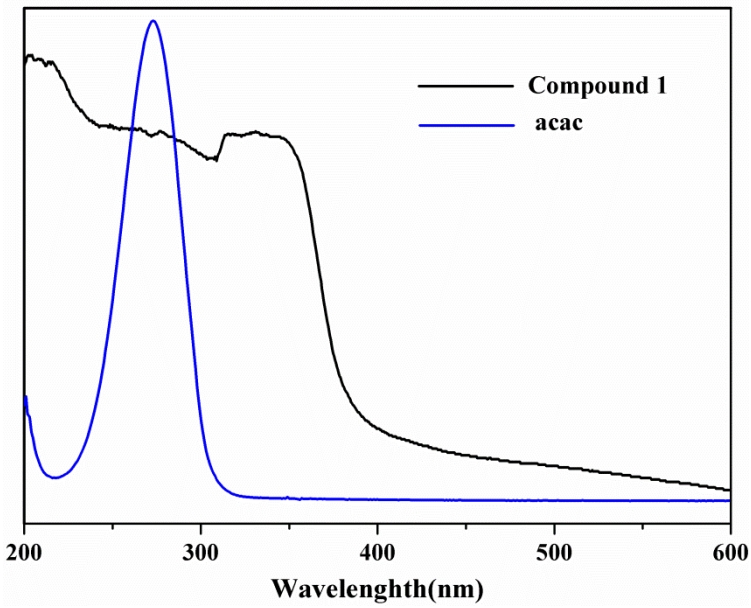


Fig. S15 The comparison of liquid-state UV spectra of acetylacetone (blue) and the excitation spectrum of compound **1** (black).