Electronic Supplementary Information (ESI)

A fluorescence red-shift and turn-on sensor for acetylacetone derived from Zn^{II}-based metal–organic framework with new topology

Le-Qian Li,[a] Shu-Li Yao,[a] Xue-Mei Tian,[a] Teng-Fei Zheng,[a] Jin-Yan Li, [a] Sui-Jun Liu,*[a] Jing-Lin Chen,[a] Mei-Hui Yu*[b] and He-Rui Wen[a]

[a]School of Chemistry and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, Jiangxi Province, P.R. China

[b]School of Materials Science and Engineering, TKL of Metal- and Molecule-Based Material Chemistry and Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300350, P.R. China

*Corresponding authors. E-mail: sjliu@jxust.edu.cn (S.-J. Liu), mh@nankai.edu.cn (M.-H. Yu)

Table S1. Selected bond lengths (Å) and angles (°) for **JXUST-4**[a]

Zn1—O4^{i}	1.909(7)	Zn2—O5^{iv}	1.961(7)
Zn1—O6	1.964(6)	Zn2—O8	1.968(7)
Zn1—O10	1.967(7)	Zn2—O7	1.994(6)
Zn1—O7^{ii}	2.011(6)	Zn2—O2	2.398(7)
O1—Zn2	1.964(7)	Zn2—C13	2.527(10)
N4—Zn3^{v}	2.016(9)	Zn3—N1	2.096(8)
Zn3—O9	2.006(7)	Zn3—O11^{iv}	2.315(8)
Zn3—O7	2.012(6)		
O4^{i}—Zn1—O6	110.4(3)	O8—Zn2—O2	84.5(3)
O4^{i}—Zn1—O10	124.8(3)	O7—Zn2—O2	164.1(3)
O6—Zn1—O10	103.2(3)	O9—Zn3—O7	102.9(3)
O4^{i}—Zn1—O7^{ii}	101.9(3)	O9—Zn3—N4^{vii}	142.0(3)
O6—Zn1—O7^{ii}	104.3(3)	O7—Zn3—N4^{vii}	110.4(3)
O10—Zn1—O7^{ii}	110.8(3)	O9—Zn3—N1	90.0(3)
O5^{iv}—Zn2—O1	112.9(3)	O7—Zn3—N1	98.5(3)
O5^{iv}—Zn2—O8	107.9(4)	N4^{vii}—Zn3—N1	102.6(3)
O1—Zn2—O8	122.8(4)	O9—Zn3—O11^{iv}	81.5(3)
O5^{iv}—Zn2—O7	105.4(3)	O7—Zn3—O11^{iv}	86.8(3)
O1—Zn2—O7	107.8(3)	N4^{vii}—Zn3—O11^{iv}	82.4(3)
O8—Zn2—O7	97.6(3)	N1—Zn3—O11^{iv}	170.9(3)
O5^{iv}—Zn2—O2	88.8(3)	O1—Zn2—O2	58.9(3)

[a]Symmetry codes: (i) $x-y+1, x+1, -z$; (ii) $x-y+1, x+1, -z+1$; (iv) $y-1, -x+y, -z+1$; (v) $x, y, z-1$; (vii) $x, y, z+1$.

Table S2. SHAPE analysis of Zn^{II} ion in **JXUST-4**.

ions	label	shape	symmetry	distortion(τ)
Zn1	SP-4	Square	D_{4h}	30.269
	T-4	Tetrahedron	T_d	**0.592**
	SS-4	Seesaw	C_{2v}	6.665
	vTBPY-	Vacant trigonal bipyramid	C_{3v}	3.050
Zn2	SP-4	Square	D_{4h}	29.538
	T-4	Tetrahedron	T_d	**0.634**
	SS-4	Seesaw	C_{2v}	2.207
	vTBPY-	Vacant trigonal bipyramid	C_{3v}	2.861
Zn3	PP-5	Pentagon	D_{5h}	32.364
	vOC-5	Vacant octahedron	C_{4v}	2.451
	TBPY-5	Trigonal bipyramid	D_{3h}	2.282
	SPY-5	Spherical square pyramid	C_{4v}	**2.119**
	JTBPY-5	Johnson trigonal bipyramid J12	D_{3h}	3.428

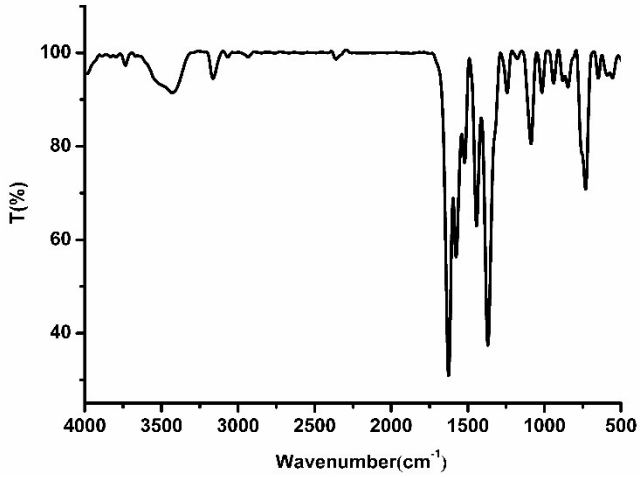


Fig. S1. IR spectrum of **JXUST-4** at room temperature.

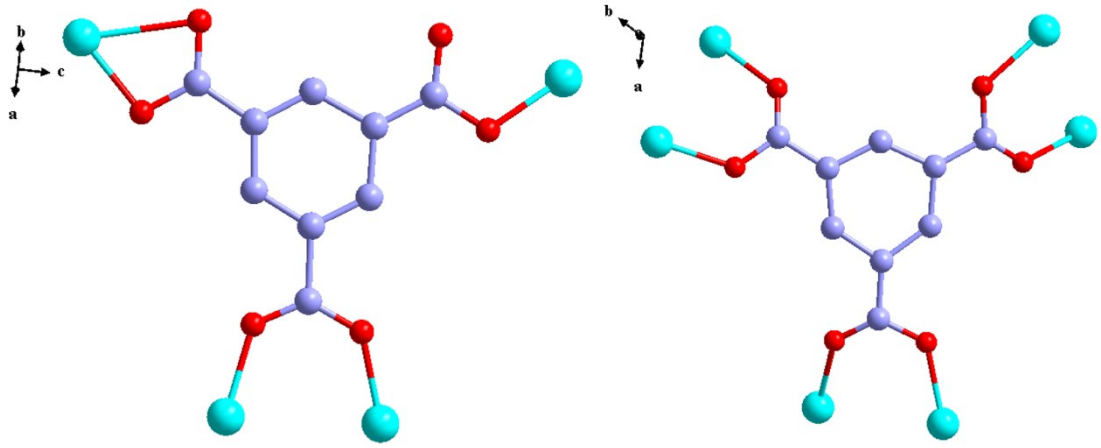


Fig. S2. View of the coordination modes of BTC^{3-} ligand in **JXUST-4**.

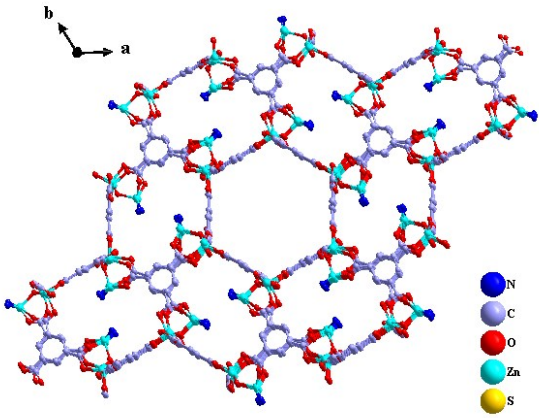


Fig. S3. The 2D layer structure in **JXUST-4**.

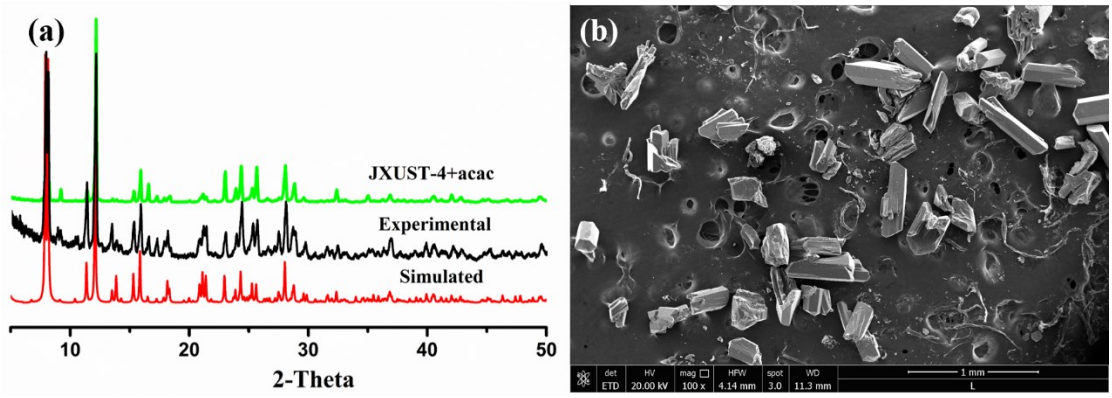
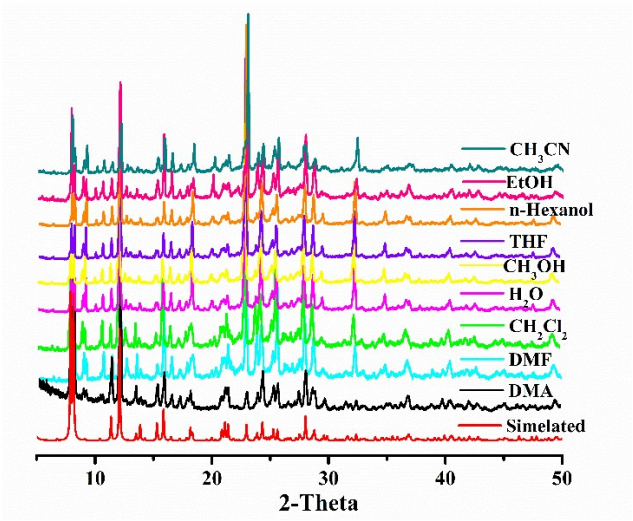
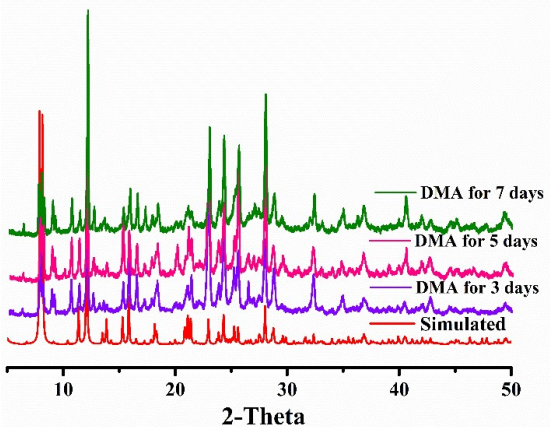
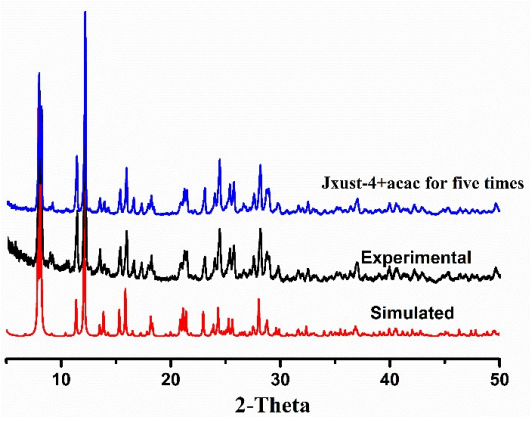


Fig. S4. (a) The simulated and experimental PXRD patterns of **JXUST-4** and **JXUST-4** after immersing in DMA solutions containing acetylacetone; and (b) SEM image of **JXUST-4**.



(a)





(b) (c)

Fig. S5. (a)The PXRD patterns of **JXUST-4** immersed in different solvents for 24 h. (b)The PXRD patterns of **JXUST-4** immersed in DMA for days. (c) The PXRD patterns of the fresh sample and the sample immersed in DMA solution containing acac after five times cycle.

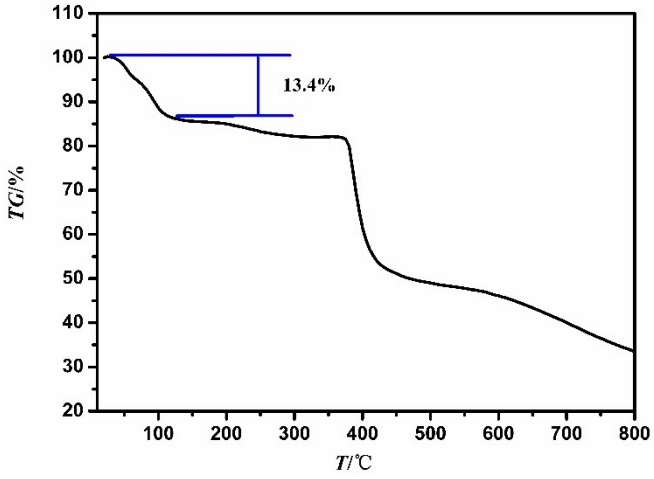


Fig. S6. The TGA curve of **JXUST-4** under N_2 atmosphere from room temperature to 800 °C.

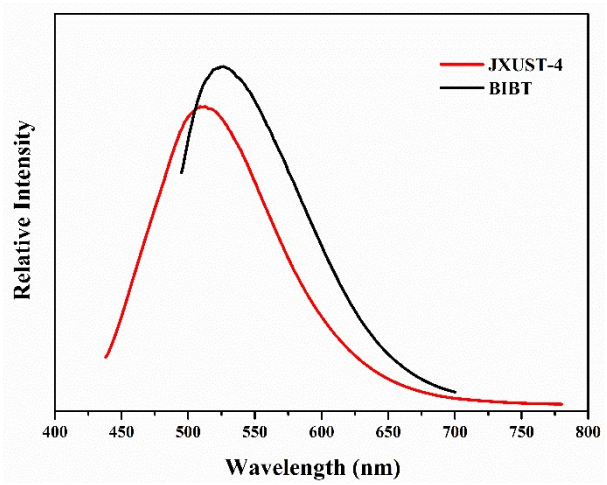


Fig. S7. Emission spectra of BIBT (λ_{ex} = 466 nm) and **JXUST-4** (λ_{ex} = 418 nm) in the solid state at room temperature.

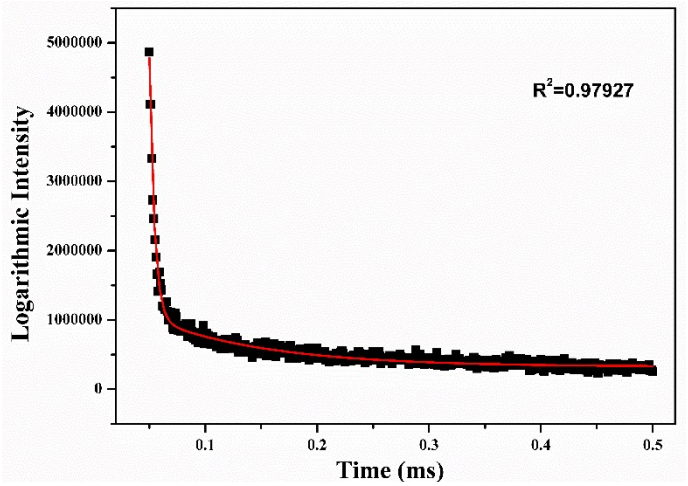
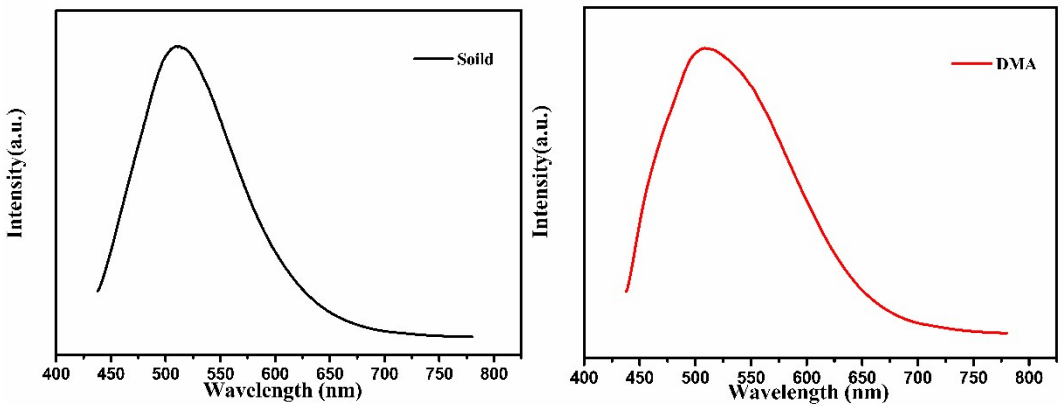


Fig. S8. The luminescence decay curve (λ_{ex} = 418 nm and λ_{em} = 512 nm) of **JXUST-4** at room temperature.



(a) **(b)**

Fig. S9. The emission spectra of **JXUST-4** in solid state (a) and DMA solution (b).

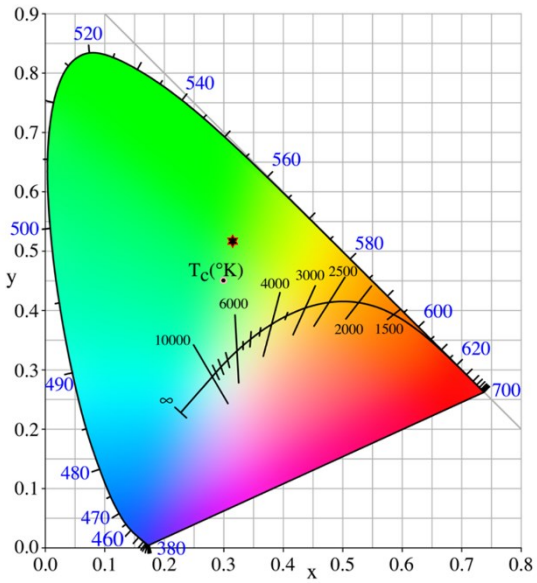


Fig. S10. CIE chromaticity diagram showing the color coordinates of **JXUST-4** and **JXUST-4** containing acetylacetone.

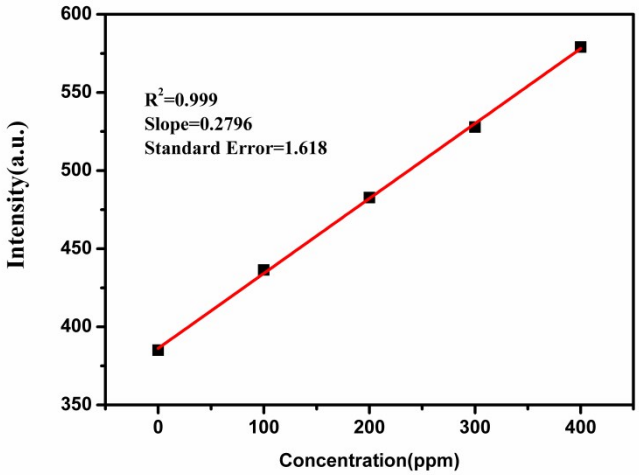


Fig. S11. Correlation between the luminescence intensity of **JXUST-4** and the concentration of acetylacetone.

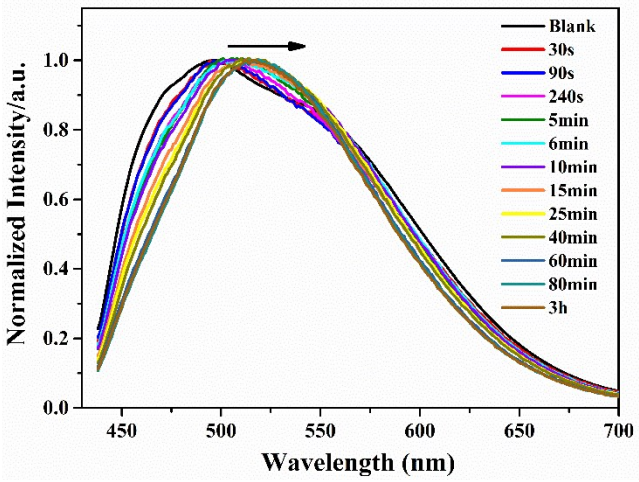


Fig. S12. Time-dependent emission spectra of the suspension after adding acetylacetone (3000 ppm) at room temperature (λ_{ex} = 418 nm).

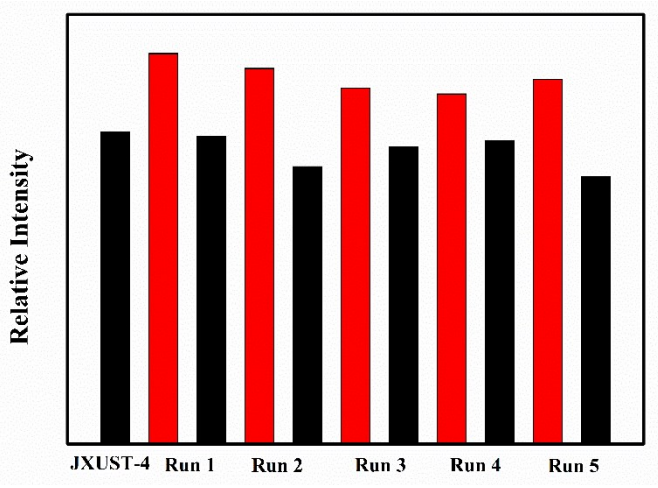


Fig. S13. Relative luminescent intensity of **JXUST-4** dispersed in DMA solution before (black histogram) and after (red histogram) the addition of acetylacetone in different recycles.

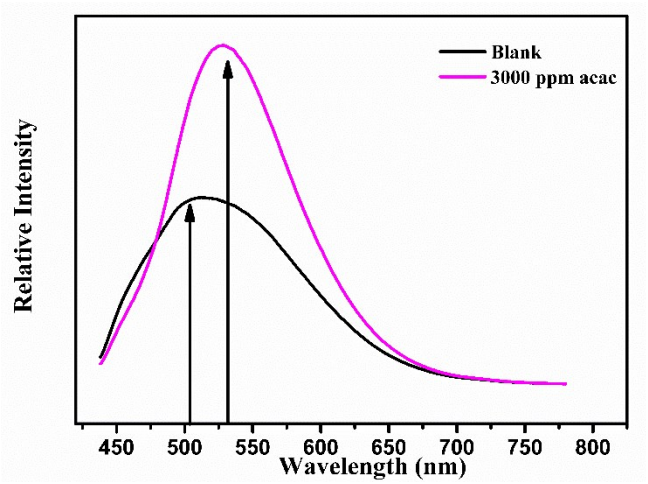


Fig. S14. Liquid luminescence spectra of **JXUST-4** in blank (black) and introduced into 3000 ppm acetylacetone (pink) at room temperature (λ_{ex} = 418 nm).

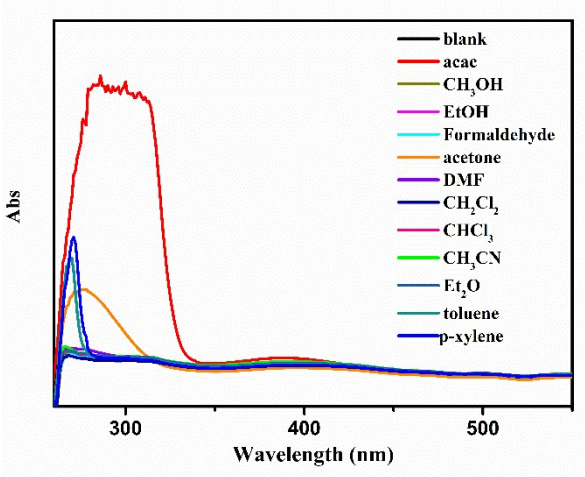


Fig. S15. UV−vis absorption spectra of **JXUST-4** upon the addition of various solvents.

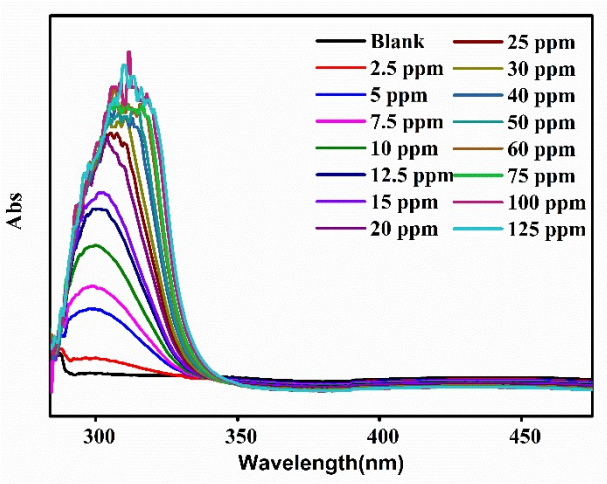


Fig. S16. Absorption spectra of **JXUST-4** dispersed in DMA solution after adding different concentration of acac.