Electronic Supplementary Information (ESI)

Hydrothermal Syntheses, Crystal Structures and Luminescent Properties of Zinc(II) Coordination Polymers Constructed by Bifunctional Tetrazolate-5-carboxylate Ligands

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Table S1 Selected bond lengths (Å) and angles (º) for **1**–**5**.

Table S2 Hydrogen-bond geometry for complexes **4** – **5**.

Fig. S1 Packing arrangement (–ABAB–) of the adjacent layers in **2** with Cl and C2 atoms and 2,2'-bipy are omitted for clarity.

Fig. S2 The 3-D polymeric network for **3**.

Fig. S3 The perspective view of the 3-D complicated supramolecular network formed by hydrogen bonds for **4**.

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Fig. S5 View of the luminescent decay curves of **1**–**5** with λ_{em} 424, 404, 409, 428 and 401 nm, respectively. The blue lines are the fitting curves and the black-red lines inserted at the top right corner are the raw experimental curves.

Fig. S6 X-ray powder diffraction (XRPD) patterns of **1**–**5**.

Fig. S7 The FT-IR spectra of **1**-**3** (a) and **4**-**5** (b).

Table S1 Selected bond lengths (Å) and angles (º) for **1–5** [a]

1			
Zn(1)-O(2)	1.9913(17)	Zn(1)-O(1)C	2.0893(16)
Zn(1)-N(1)C	2.028(2)	Zn(1)-O(1W)	2.1394(19)
Zn(1)-N(3)D	2.061(2)	N(3)D-Zn(1)-O(1)C	90.12(7)
O(2)-Zn(1)-N(1)C	134.44(8)	O(2)-Zn(1)-O(1W)	85.69(7)
O(2)-Zn(1)-N(3)D	109.89(8)	N(1)C-Zn(1)-O(1W)	88.45(8)
N(1)C-Zn(1)-N(3)D	115.63(8)	N(3)D-Zn(1)-O(1W)	95.32(8)
O(2)-Zn(1)-O(1)C	94.88(7)	O(1)C-Zn(1)-O(1W)	173.99(7)
N(1)C-Zn(1)-O(1)C	86.89(7)		
2			
Zn(1)-N(4)A	2.0015(17)	Zn(2)-O(1W)	2.1069(15)
Zn(1)-N(4)	2.0015(17)	Zn(2)-N(5)	2.1411(18)
Zn(1)-Cl(1)	2.2731(8)	Zn(2)-N(6)	2.1452(16)
Zn(1)-Cl(1)A	2.2731(8)	Zn(2)-O(2)B	2.1484(14)
Zn(2)-N(1)	2.0842(17)	Zn(2)-O(1)	2.1561(13)
N(4)A-Zn(1)-N(4)	102.13(10)	N(5)-Zn(2)-N(6)	76.95(7)
N(4)A-Zn(1)-Cl(1)	109.49(5)	N(1)-Zn(2)-O(2)B	168.22(6)
N(4)-Zn(1)-Cl(1)	111.48(5)	O(1W)-Zn(2)-O(2)B	85.47(5)
N(4)A-Zn(1)-Cl(1)A	111.48(5)	N(5)-Zn(2)-O(2)B	94.86(6)
N(4)-Zn(1)-Cl(1)A	109.49(5)	N(6)-Zn(2)-O(2)B	84.20(6)
Cl(1)-Zn(1)-Cl(1)A	112.33(4)	N(1)-Zn(2)-O(1)	83.72(6)
N(1)-Zn(2)-O(1W)	95.82(6)	O(1W)-Zn(2)-O(1)	95.21(5)
N(1)-Zn(2)-N(5)	96.70(7)	N(5)-Zn(2)-O(1)	169.97(6)
O(1W)-Zn(2)-N(5)	94.71(6)	N(6)-Zn(2)-O(1)	93.03(6)
N(1)-Zn(2)-N(6)	96.19(7)	O(2)B-Zn(2)-O(1)	84.50(5)
O(1W)-Zn(2)-N(6)	166.09(6)		
3			
Zn(1)-O(2)A	1.9766(18)	Zn(1)-N(5)	2.143(2)
Zn(1)-N(4)C	2.030(2)	Zn(1)-O(1)	2.2167(18)
Zn(1)-N(1)	2.035(2)	N(1)-Zn(1)-N(5)	92.61(8)
O(2)A-Zn(1)-N(4)C	105.56(8)	O(2)A-Zn(1)-O(1)	88.44(7)
O(2)A-Zn(1)-N(1)	134.26(8)	N(4)C-Zn(1)-O(1)	88.36(8)
N(4)C-Zn(1)-N(1)	119.17(8)	N(1)-Zn(1)-O(1)	83.96(8)
O(2)A-Zn(1)-N(5)	89.10(8)	N(5)-Zn(1)-O(1)	172.37(7)
N(4)C-Zn(1)-N(5)	99.26(8)		
4			
Zn(1)-O(1W)	2.050(2)	Zn(1)-N(2)A	2.117(2)
Zn(1)-O(2W)	2.079(2)	Zn(1)-N(1)	2.148(2)
Zn(1)-O(3W)	2.093(2)	Zn(1)-O(1)	2.170(2)
O(1W)-Zn(1)-O(2W)	88.28(8)	O(3W)-Zn(1)-N(1)	88.59(8)
O(1W)-Zn(1)-O(3W)	87.62(8)	N(3)A-Zn(1)-N(1)	95.86(7)

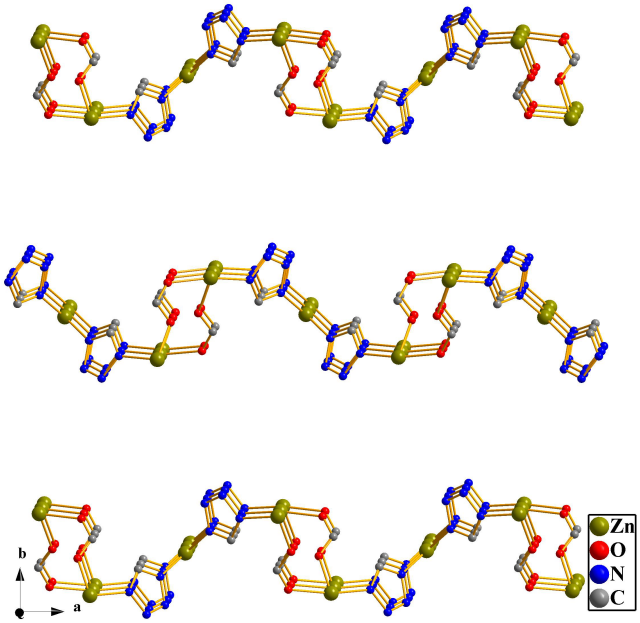
O(2W)-Zn(1)-O(3W)	175.86(8)	O(1W)-Zn(1)-O(1)	94.27(7)
O(1W)-Zn(1)-N(2)A	94.04(8)	O(2W)-Zn(1)-O(1)	87.35(7)
O(2W)-Zn(1)-N(2)A	90.57(7)	O(3W)-Zn(1)-O(1)	92.39(7)
O(3W)-Zn(1)-N(2)A	90.28(8)	N(2)A-Zn(1)-O(1)	171.37(7)
O(1W)-Zn(1)-N(1)	169.41(7)	N(1)-Zn(1)-O(1)	76.01(7)
O(2W)-Zn(1)-N(1)	95.35(8)		
5			
Zn(1)-O(1W)	2.0909(11)	Zn(2)-O(2W)	2.0954(11)
Zn(1)-N(11)	2.1256(11)	Zn(2)-N(10)	2.1196(11)
Zn(1)-N(6)	2.1335(13)	Zn(2)-N(2)	2.1314(13)
Zn(1)-N(1)	2.1583(11)	Zn(2)-N(5)	2.1442(11)
Zn(1)-O(1)	2.1612(12)	Zn(2)-N(9)	2.1567(14)
Zn(1)-N(12)	2.1829(14)	Zn(2)-O(3)	2.1998(12)
O(1W)-Zn(1)-N(11)	98.21(5)	O(2W)-Zn(2)-N(10)	94.97(5)
O(1W)-Zn(1)-N(6)	87.66(4)	O(2W)-Zn(2)-N(2)	91.57(4)
N(11)-Zn(1)-N(6)	104.10(4)	N(10)-Zn(2)-N(2)	97.63(4)
O(1W)-Zn(1)-N(1)	94.90(5)	O(2W)-Zn(2)-N(5)	92.21(4)
N(11)-Zn(1)-N(1)	158.71(4)	N(10)-Zn(2)-N(5)	166.47(4)
N(6)-Zn(1)-N(1)	93.09(4)	N(2)-Zn(2)-N(5)	93.62(4)
O(1W)-Zn(1)-O(1)	87.52(4)	O(2W)-Zn(2)-N(9)	172.10(4)
N(11)-Zn(1)-O(1)	87.65(4)	N(10)-Zn(2)-N(9)	77.16(5)
N(6)-Zn(1)-O(1)	167.83(4)	N(2)-Zn(2)-N(9)	90.18(5)
N(1)-Zn(1)-O(1)	76.20(4)	N(5)-Zn(2)-N(9)	95.37(5)
O(1W)-Zn(1)-N(12)	174.27(4)	O(2W)-Zn(2)-O(3)	86.03(4)
N(11)-Zn(1)-N(12)	76.06(5)	N(10)-Zn(2)-O(3)	92.11(4)
N(6)-Zn(1)-N(12)	93.71(5)	N(2)-Zn(2)-O(3)	170.14(4)
N(1)-Zn(1)-N(12)	90.59(5)	N(5)-Zn(2)-O(3)	76.95(4)
O(1)-Zn(1)-N(12)	92.18(4)	N(9)-Zn(2)-O(3)	93.51(4)

[a] Symmetry codes for **1**: (A) -y+3/2, x, -z+1/2; (B) x+1/2, y-1/2, -z; (C) y, -x+3/2, -z+1/2; (D) x-1/2, y+1/2, -z; for **2**: (A) -x+1/2, -y+1/2, z; (B) –x, -y+1/2, z+1/2; (C) -x, -y+1/2, z-1/2; for **3**: (A) -x+2, -y, -z+1; (B) x, -y+1/2, z+1/2; (C) x, -y+1/2, z+1/2; (D) -x+1, -y-1, -z+1; for **4**: (A) -x+2, -y+1, -z+2

Table S2 Hydrogen-bond geometry for complexes **4** – **5** [a]

D-H···A	D-H/Å	H···A/Å	D···A/Å	∠ D-H···A/º
		4		
O(4W)-H(4WB)···O(2)_$1	0.843(10)	1.992(12)	2.809(3)	163(3)
O(4W)-H(4WA)···N(3)_$2	0.838(10)	2.107(15)	2.879(3)	153(3)
O(2W)-H(2WA)···O(4W)_$3	0.841(10)	1.895(12)	2.729(3)	171(3)
O(2W)-H(2WB)···O(4W)_$4	0.843(10)	1.938(11)	2.775(3)	172(3)
O(1W)-H(1WB)···O(2)_$5	0.844(10)	2.045(13)	2.867(3)	164(3)
O(1W)-H(1WA)···O(1)_$1	0.844(10)	1.870(12)	2.705(3)	170(3)
O(3W)-H(3WA)···O(2)_$6	0.834(10)	2.065(14)	2.861(2)	159(3)
O(3W)-H(3WB)···N(4)_$5	0.840(10)	2.010(14)	2.806(3)	158(3)
		5		
O(3W)-H(3WB)···O(2)_$1	0.748(16)	2.088(17)	2.7882(14)	156.0(18)
O(3W)-H(3WA)···N(4)_$1	0.885(18)	2.072(17)	2.8548(18)	146.8(14)
O(2W)-H(2WA)···O(3)_$2	0.845(7)	2.044(7)	2.8840(15)	172.6(7)
O(2W)-H(2WB)···O(3W)	0.846(6)	1.836(6)	2.6764(15)	172.1(10)
O(1W)-H(1WB)···O(2)_$3	0.842(7)	1.880(7)	2.7064(15)	166.4(7)
O(1W)-H(1WB)···O(4)_$4	0.843(6)	1.961(7)	2.7515(14)	155.8(8)

[a] Symmetry code for **4**: $1 -x+1, -y, -z+1; $2 -x+2, -y+1, -z+2; $3 x+1, y, z; $4 -x+1, -y, -z+2; $5 x-1, y, z; $6 -x+2, -y+1, -z+1; for **5**: $1 -x, -y+1, -z; $2 -x, -y+1, -z+1; $3 -x, -y, -z; $4 -x, -y, -z+1.



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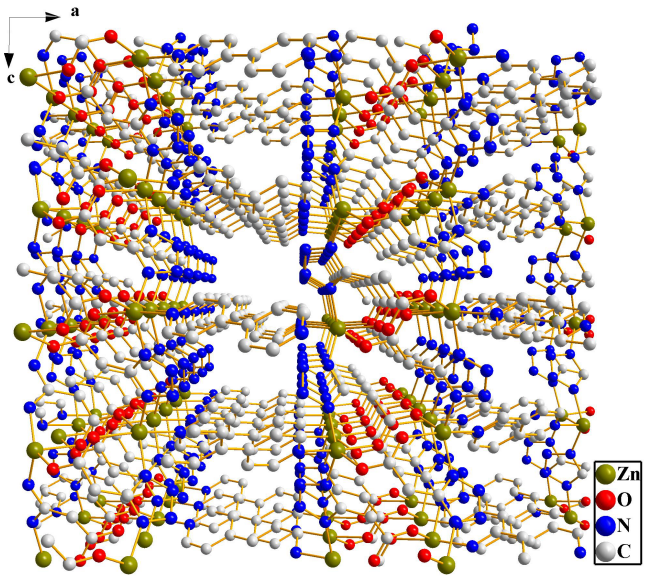

Fig. S2 The 3-D polymeric network for **3.**

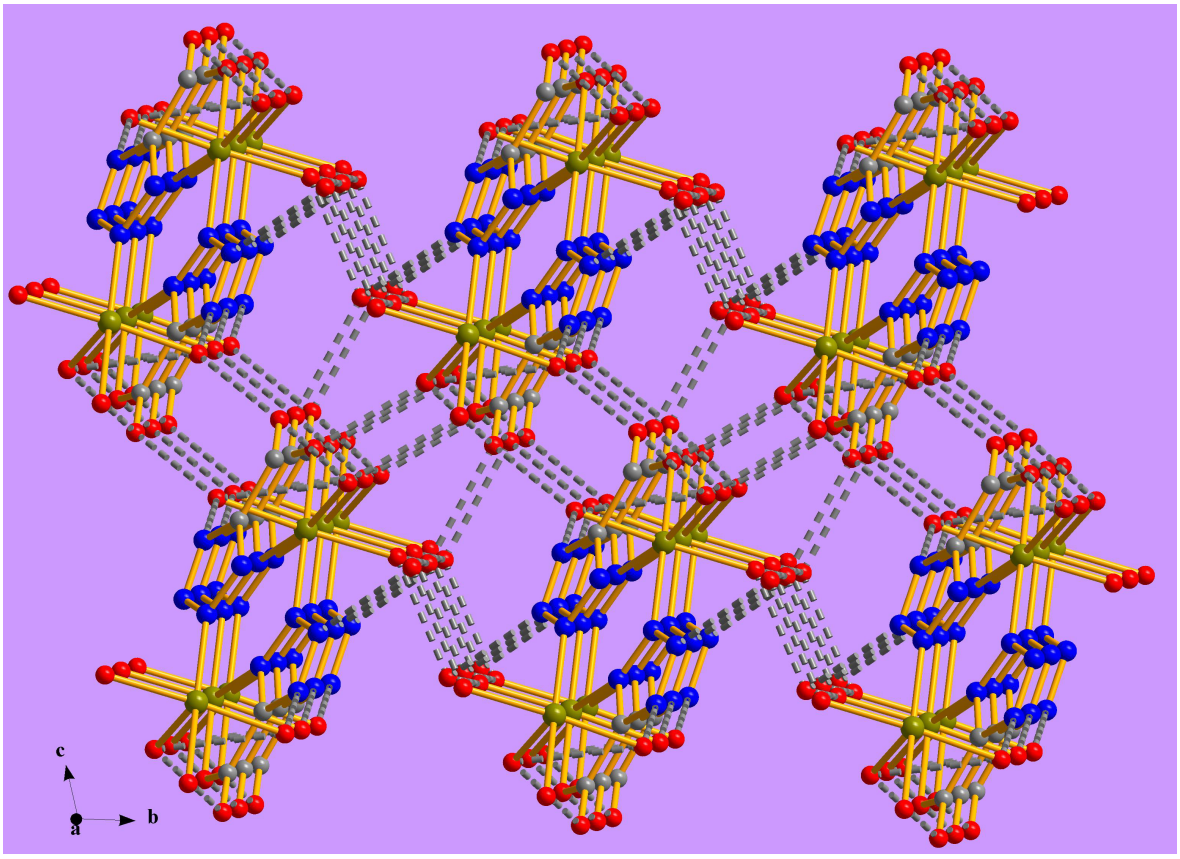

Fig. S3 The perspective view of the 3-D complicated supramolecular network formed by hydrogen bonds for **4**.

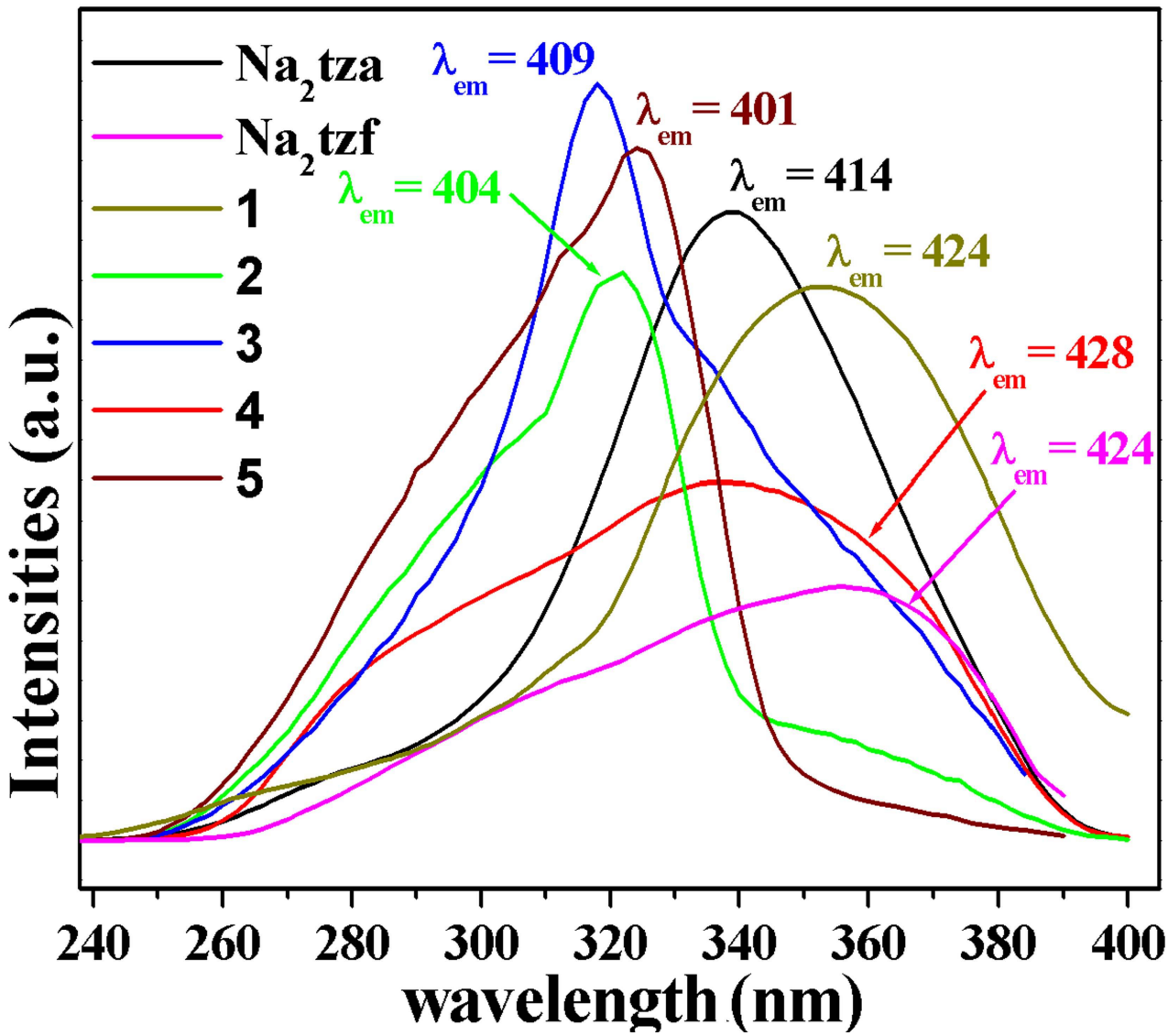

Fig. S4 The excitation spectra for **1**–**5**, Na_2tza and Na_2tzf.

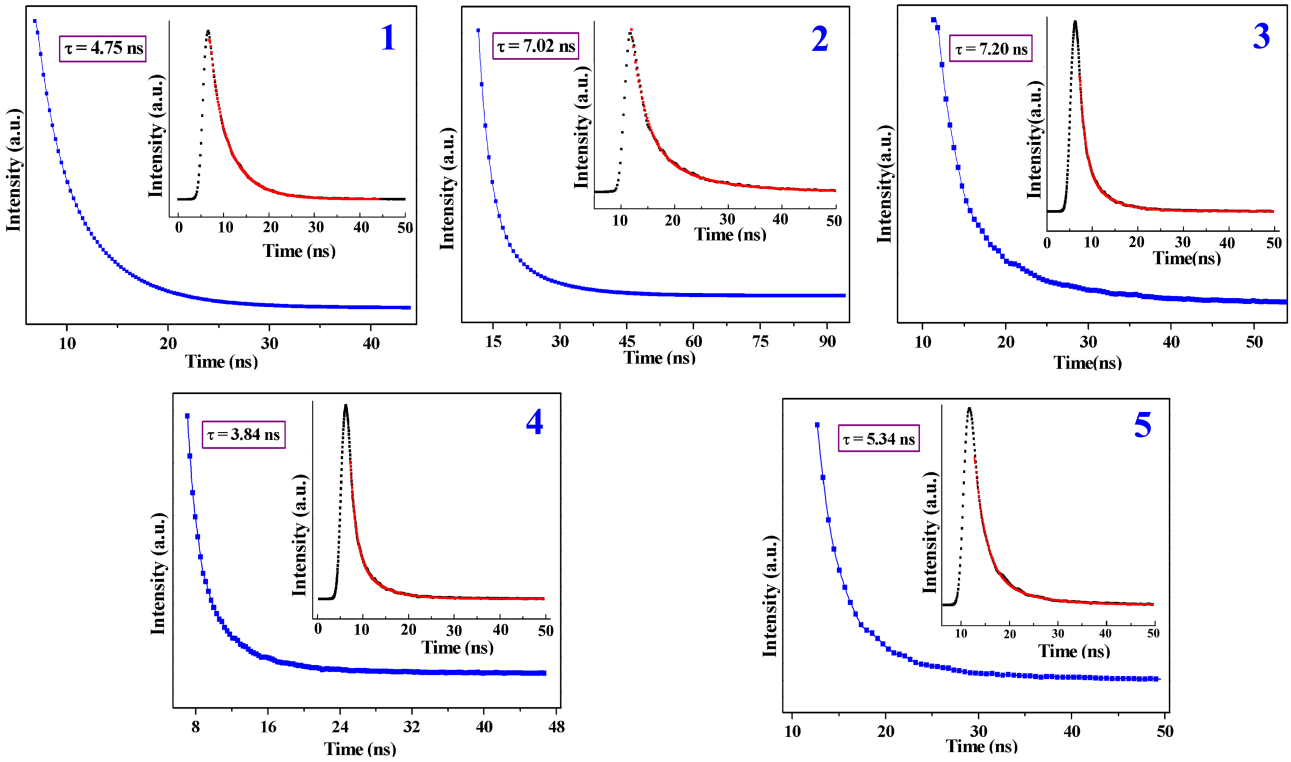

Fig. S5 View of the luminescent decay curves of **1**–**5** with λ_{em} 424, 404, 409, 428 and 401 nm, respectively. The blue lines are the fitting curves and the black-red lines inserted at the top right corner are the raw experimental curves.

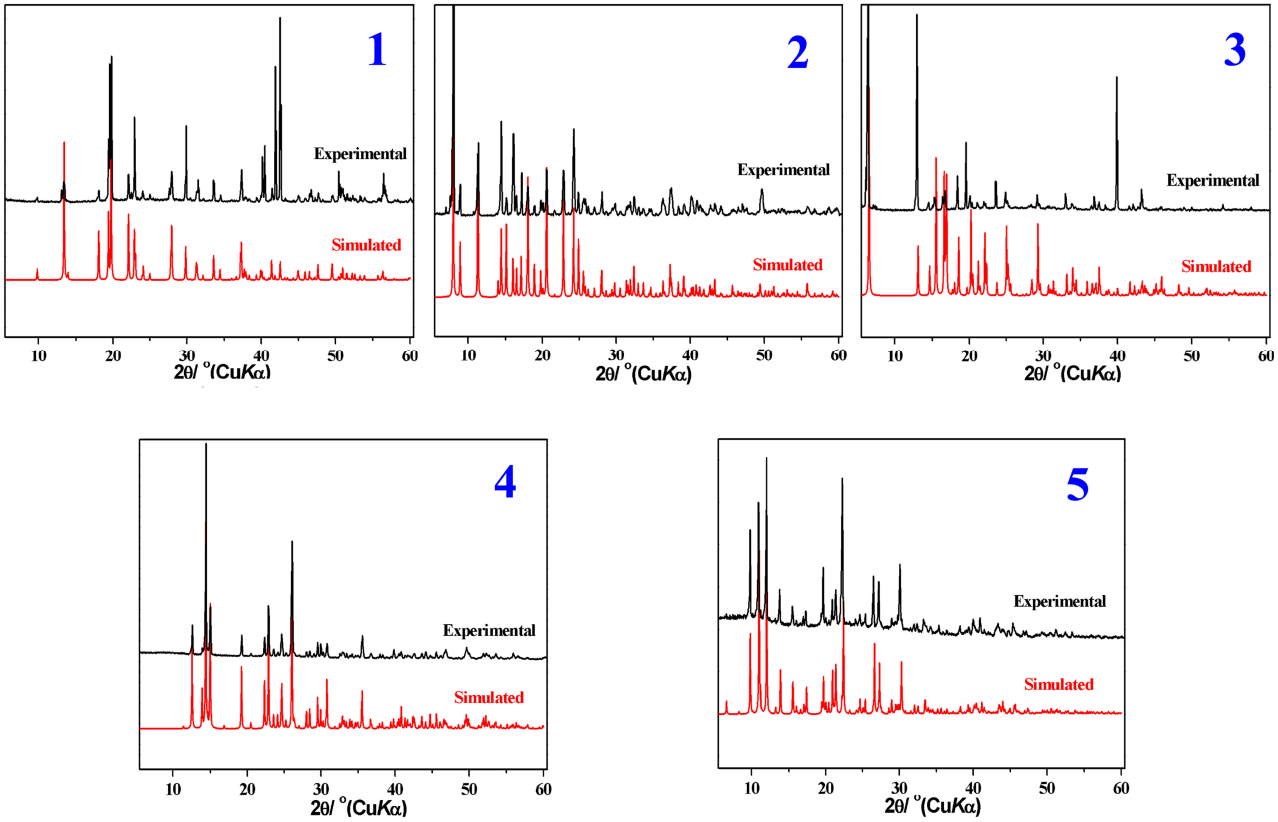

Fig. S6 X-ray powder diffraction (XRPD) patterns of **1**–**5**.

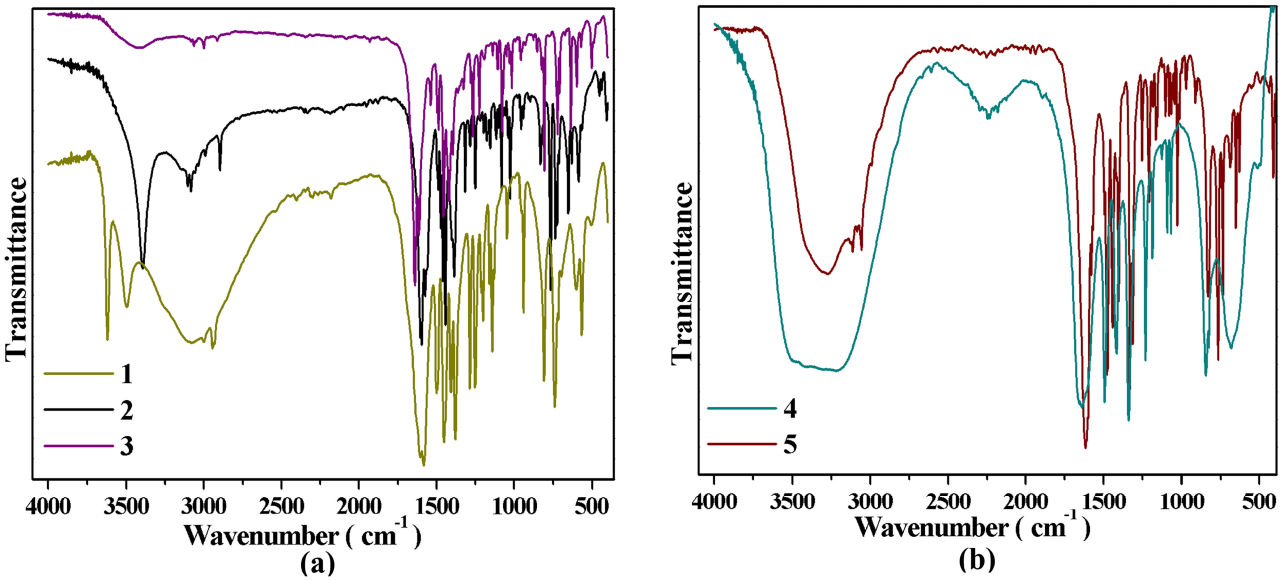

Fig. S7 The FT-IR spectra of **1-3** (a) and **4-5** (b).