Electronic Supplementary Information (ESI)

Multifunctional Zn^{II}-Ln^{III} (Ln = Tb, Dy) complexes based on the amine-phenol ligand with field-induced slow magnetic relaxation, luminescence and proton conduction

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

Dy1—O9	2.285(3)	Dy1—O6	2.356(5)
Dy1—O4	2.296(4)	Dy1—O8	2.368(4)
Dy1—O10	2.337(4)	Dy1—O7	2.539(4)
Dy1—O5	2.334(4)	Dy1—O3	2.540(4)
Zn1—O10	2.059(4)	O4—Zn2	2.092(4)
Zn1—O9	2.072(4)	O5—Zn2	2.037(4)
Zn1—N1	2.101(6)	Zn2—N3	2.094(5)
Zn1—N2	2.131(5)	Zn2—N4	2.128(5)
Zn1—O12	2.202(5)	O2—Zn2	2.307(4)
Zn1—O13	2.306(6)	O1—Zn2	2.230(5)
O9—Dy1—O4	105.33(15)	O6—Dy1—O8	81.61(19)
O9—Dy1—O10	67.02(14)	O9—Dy1—O7	64.89(14)
O4—Dy1—O10	87.80(14)	O4—Dy1—O7	143.44(14)
O9—Dy1—O5	87.60(14)	O10—Dy1—O7	116.27(13)
O4—Dy1—O5	66.69(13)	O5—Dy1—O7	77.47(13)
O10—Dy1—O5	138.16(14)	O6—Dy1—O7	77.84(16)
O9—Dy1—O6	140.99(16)	O8—Dy1—O7	75.52(15)
O4—Dy1—O6	97.59(18)	O9—Dy1—O3	142.51(14)
O10—Dy1—O6	146.13(17)	O4—Dy1—O3	64.92(13)
O5—Dy1—O6	72.91(18)	O10—Dy1—O3	76.25(14)
O9—Dy1—O8	99.04(16)	O5—Dy1—O3	116.92(13)
O4—Dy1—O8	140.35(14)	O6—Dy1—O3	75.97(17)
O10—Dy1—O8	73.44(15)	O8—Dy1—O3	76.65(14)
O5—Dy1—O8	146.07(15)	O7—Dy1—O3	144.04(14)
O10—Zn1—O9	76.27(15)	O5—Zn2—O4	76.08(15)
O10—Zn1—N1	164.0(2)	O5—Zn2—N3	162.12(18)
O9—Zn1—N1	90.2(2)	O4—Zn2—N3	89.36(19)
O10—Zn1—N2	90.48(19)	O5—Zn2—N4	91.60(19)
O9—Zn1—N2	113.8(2)	O4—Zn2—N4	113.5(2)
N1—Zn1—N2	102.8(2)	N3—Zn2—N4	103.9(2)
O10—Zn1—O12	96.23(19)	O5—Zn2—O1	95.82(17)
O9—Zn1—O12	168.1(2)	O4—Zn2—O1	168.37(18)
N1—Zn1—O12	95.7(2)	N3—Zn2—O1	96.9(2)
N2—Zn1—O12	75.0(2)	N4—Zn2—O1	74.6(2)
O10—Zn1—O13	97.32(19)	O5—Zn2—O2	96.20(16)
O9—Zn1—O13	103.59(19)	O4—Zn2—O2	104.01(16)
N1—Zn1—O13	77.5(3)	N3—Zn2—O2	77.07(19)
N2—Zn1—O13	142.6(2)	N4—Zn2—O2	142.46(19)
Zn1—O10—Dy1	107.38(16)	Zn2—O4—Dy1	108.14(16)
Zn1—O9—Dy1	108.94(16)	Zn2—O5—Dy1	108.67(16)

Table S2. Selected bond lengths (Å) and angles (deg) for **2**.

Tb1—O8	2.294(5)	Zn2—O20	2.039(5)
Tb1—O1	2.313(5)	Zn2—O1	2.088(5)
Tb1—O20	2.343(5)	Zn2—N4	2.098(6)
Tb1—O2	2.347(5)	Zn2—N1	2.133(6)
Tb1—O29	2.377(5)	Zn2—O4	2.216(5)
Tb1—O30	2.378(5)	Zn2—O5	2.302(5)
Tb1—O9	2.547(5)	Zn3—O2	2.057(5)
Tb1—O7	2.554(5)	Zn3—O8	2.070(5)
Tb1—Zn3	3.5560(10)	Zn3—N2	2.095(7)
Tb1—Zn2	3.5625(9)	Zn3—N3	2.129(6)
Zn3—O13	2.297(6)	Zn3—O12	2.202(6)
O8—Tb1—O1	105.37(17)	O30—Tb1—O9	75.66(18)
O8—Tb1—O20	87.84(17)	O8—Tb1—O7	142.26(16)
O1—Tb1—O20	66.60(16)	O1—Tb1—O7	64.58(16)
O8—Tb1—O2	66.63(16)	O20—Tb1—O7	116.63(16)
O1—Tb1—O2	87.75(16)	O2—Tb1—O7	76.41(17)
O20—Tb1—O2	137.91(16)	O29—Tb1—O7	75.84(17)
O8—Tb1—O29	141.32(17)	O30—Tb1—O7	77.16(17)
O1—Tb1—O29	97.88(18)	O9—Tb1—O7	144.81(17)
O20—Tb1—O29	73.46(18)	O8—Tb1—Zn3	33.38(12)
O2—Tb1—O29	145.87(18)	O1—Tb1—Zn3	94.99(12)
O8—Tb1—O30	98.68(18)	O20—Tb1—Zn3	113.07(12)
O1—Tb1—O30	140.49(17)	O2—Tb1—Zn3	33.47(12)
O20—Tb1—O30	146.17(18)	O29—Tb1—Zn3	167.08(13)
O2—Tb1—O30	73.52(18)	O30—Tb1—Zn3	88.12(14)
O29—Tb1—O30	81.25(19)	O9—Tb1—Zn3	92.00(11)
O8—Tb1—O9	64.52(16)	O7—Tb1—Zn3	109.04(12)
O1—Tb1—O9	143.25(16)	O8—Tb1—Zn2	95.38(13)
O20—Tb1—O9	77.47(16)	O1—Tb1—Zn2	33.88(11)
O2—Tb1—O9	115.97(16)	O20—Tb1—Zn2	32.87(12)
O29—Tb1—O9	78.31(17)	O2—Tb1—Zn2	113.76(11)
O29—Tb1—Zn2	86.95(13)	O1—Zn2—O5	104.32(19)

O30—Tb1—Zn2	165.87(14)	N4—Zn2—O5	77.2(2)
O9—Tb1—Zn2	109.60(12)	N1—Zn2—O5	142.6(2)
O7—Tb1—Zn2	92.49(11)	O4—Zn2—O5	68.1(2)
Zn3—Tb1—Zn2	104.51(2)	O20—Zn2—Tb1	38.58(13)
O20—Zn2—O1	76.54(18)	O1—Zn2—Tb1	38.14(13)
O20—Zn2—N4	162.7(2)	N4—Zn2—Tb1	127.34(19)
O1—Zn2—N4	89.4(2)	N1—Zn2—Tb1	102.48(18)
O20—Zn2—N1	91.1(2)	O4—Zn2—Tb1	134.09(17)
O1—Zn2—N1	113.0(2)	O5—Zn2—Tb1	105.96(14)
N4—Zn2—N1	103.9(3)	O2—Zn3—O8	76.31(18)
O20—Zn2—O4	95.6(2)	O2—Zn3—N2	163.8(2)
O1—Zn2—O4	168.7(2)	O8—Zn3—N2	90.1(2)
N4—Zn2—O4	96.7(2)	O2—Zn3—N3	90.5(2)
N1—Zn2—O4	74.7(2)	O8—Zn3—N3	114.1(2)
O20—Zn2—O5	96.21(19)	N2—Zn3—N3	103.2(3)
O2—Zn3—O12	96.0(2)	Zn3—O2—Tb1	107.5(2)
O8—Zn3—O12	167.9(2)	Zn2—O1—Tb1	107.98(19)
N2—Zn3—O12	95.9(3)	Zn3—O8—Tb1	109.0(2)
N3—Zn3—O12	74.9(3)	Zn2—O20—Tb1	108.5(2)
O2—Zn3—O13	96.9(2)	O2—Zn3—Tb1	39.00(13)
O8—Zn3—O13	103.1(2)	O8—Zn3—Tb1	37.58(13)
N2—Zn3—O13	77.4(3)	N2—Zn3—Tb1	127.6(2)
N3—Zn3—O13	142.8(3)	N3—Zn3—Tb1	102.33(18)
O12—Zn3—O13	68.1(2)	O12—Zn3—Tb1	134.85(19)
O13—Zn3—Tb1	106.25(16)		

Table S3. The Zn^{II}/Dy^{III}/Tb^{III} ions of geometric analysis in complexes **1** and **2**.

Complex	Metal Ions	Label	Shape	Symmetry	Distortion(τ)
1	Zn^{II}	HP-6	Hexagon	D_{6h}	30.601
		PPY-6	Pentagonal pyramid	C_{5v}	20.009
		OC-6	**Octahedron**	$\boldsymbol{O_h}$	**4.256**
		TPR-6	Trigonal prism	D_{3h}	11.066
		JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	24.080
1	Dy^{III}	OP-8	Octagon	D_{8h}	32.141
		HPY-8	Heptagonal pyramid	C_{7v}	23.166
		HBPY-8	Hexagonal bipyramid	D_{6h}	15.530
		CU-8	Cube	O_h	10.076
		SAPR-8	Square antiprism	D_{4d}	2.296
		TDD-8	**Triangular dodecahedron**	$\boldsymbol{D_{2d}}$	**1.841**
		JGBF-8	Johnson gyrobifastigium J26	D_{2d}	15.391
		JETBPY-8	Johnson elongated triangular bipyramid J14	D_{3h}	24.197
		JBTPR-8	Biaugmented trigonal prism J50	C_{2v}	3.325
		BTPR-8	Biaugmented trigonal prism	C_{2v}	3.111
		JSD-8	Snub diphenoid J84	D_{2d}	3.976
		TT-8	Triakis tetrahedron	T_d	10.588
		ETBPY-8	Elongated trigonal bipyramid	D_{3h}	21.086
2	Zn^{II}	HP-6	Hexagon	D_{6h}	30.726
		PPY-6	Pentagonal pyramid	C_{5v}	20.122
		OC-6	**Octahedron**	$\boldsymbol{O_h}$	**4.184**
		TPR-6	Trigonal prism	D_{3h}	11.144
		JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	24.202
2	Tb^{III}	OP-8	Octagon	D_{8h}	32.083
		HPY-8	Heptagonal pyramid	C_{7v}	23.270
		HBPY-8	Hexagonal bipyramid	D_{6h}	15.570
		CU-8	Cube	O_h	10.166
		SAPR-8	Square antiprism	D_{4d}	2.348
		TDD-8	**Triangular dodecahedron**	$\boldsymbol{D_{2d}}$	**1.893**
		JGBF-8	Johnson gyrobifastigium J26	D_{2d}	15.420
		JETBPY-8	Johnson elongated triangular bipyramid J14	D_{3h}	24.260
		JBTPR-8	Biaugmented trigonal prism J50	C_{2v}	3.393
		BTPR-8	Biaugmented trigonal prism	C_{2v}	3.172
		JSD-8	Snub diphenoid J84	D_{2d}	4.049
		TT-8	Triakis tetrahedron	T_d	10.687
		ETBPY-8	Elongated trigonal bipyramid	D_{3h}	21.187

Table S4. The fitting parameters α and τ values of **1** by using CC-FIT software.

T	α_1	τ_1	α_2	τ_2
2.0 K	0.3281	0.01555	0.6345	0.4116
2.4 K	0.3605	0.004125	0.02030	0.1449
2.8 K	0.2668	0.0006348	0.5077	0.09546
3.2 K	0.2428	0.0001297	0.5658	0.03055

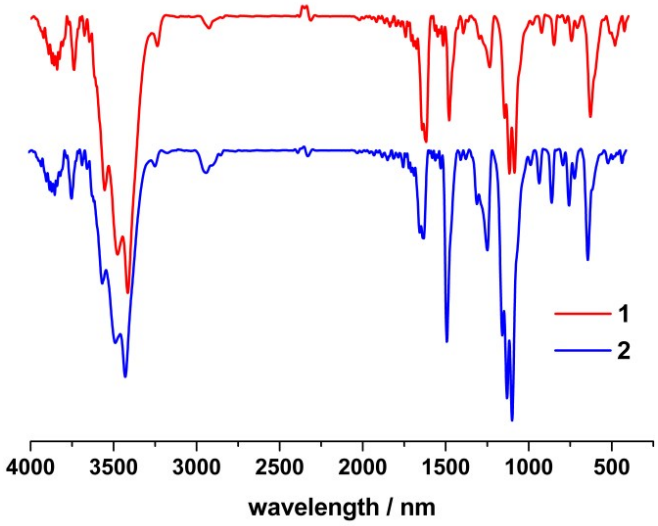

Fig.S1. The IR spectra of complexes **1** and **2**.

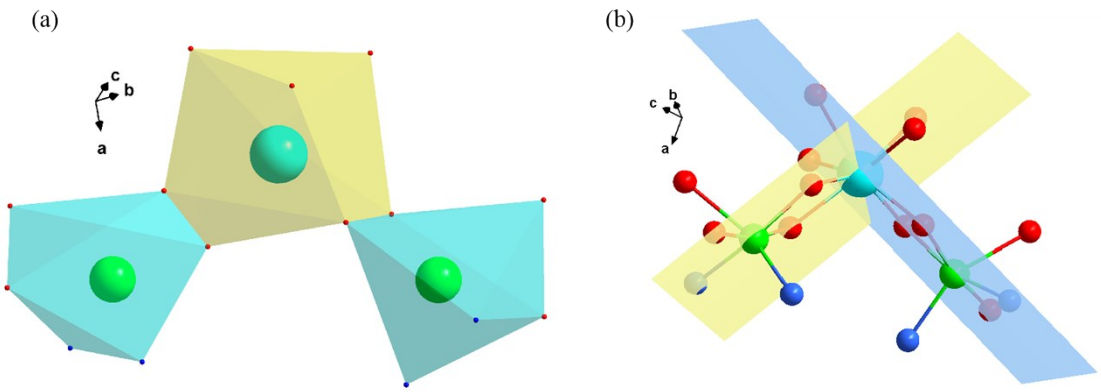

Fig.S2. The coordination polyhedron around Zn^{II} and Ln^{III} (a) and the dihedral angle (b).

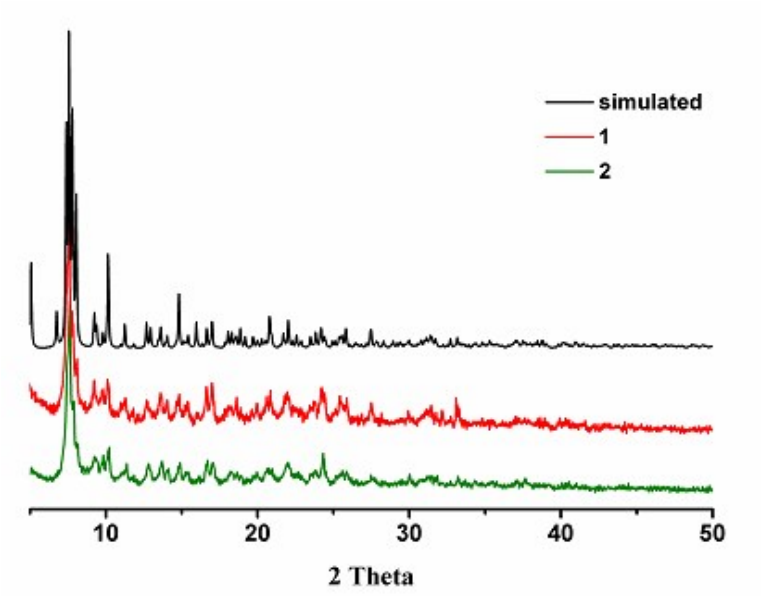

Fig. S3. The PXRD patterns of complexes **1** and **2**.

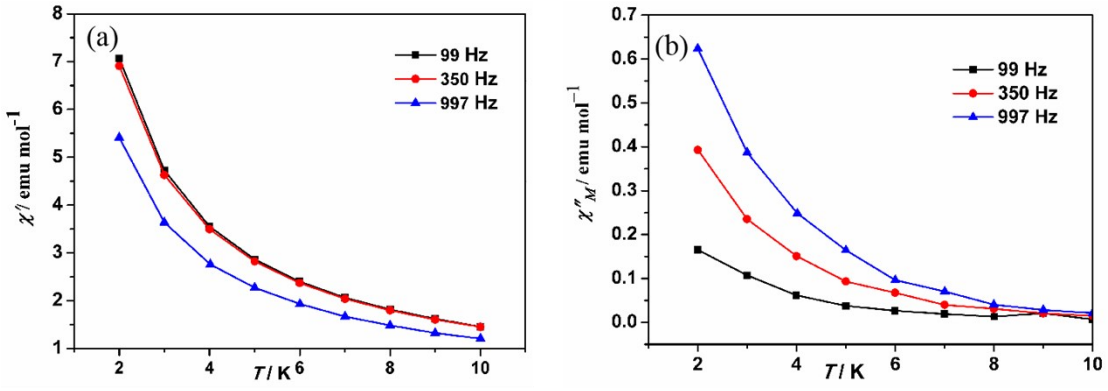

Fig. S4. Frequency dependence of the in-phase (χ′) and out-of-phase (χ″) ac susceptibility signals for **1** under zero-dc field.

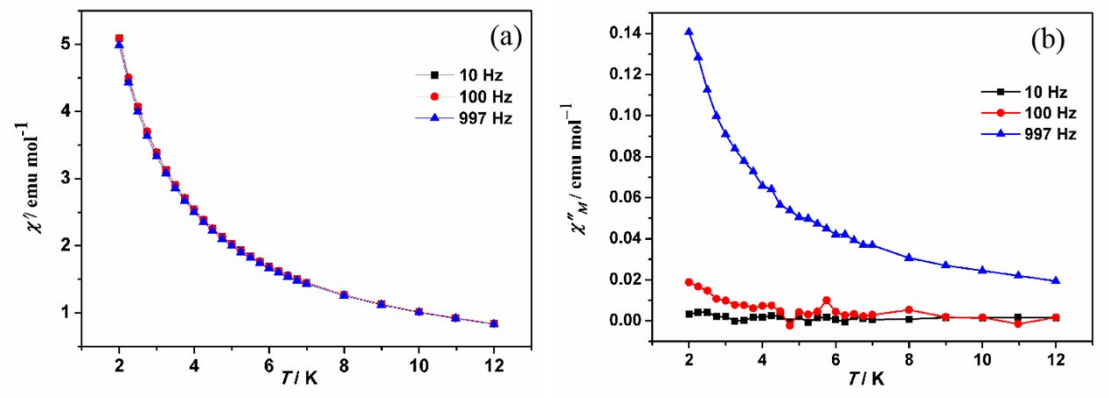

Fig. S5. Frequency dependence of the in-phase (χ′) and out-of-phase (χ″) ac susceptibility signals for **2** under zero-dc field.

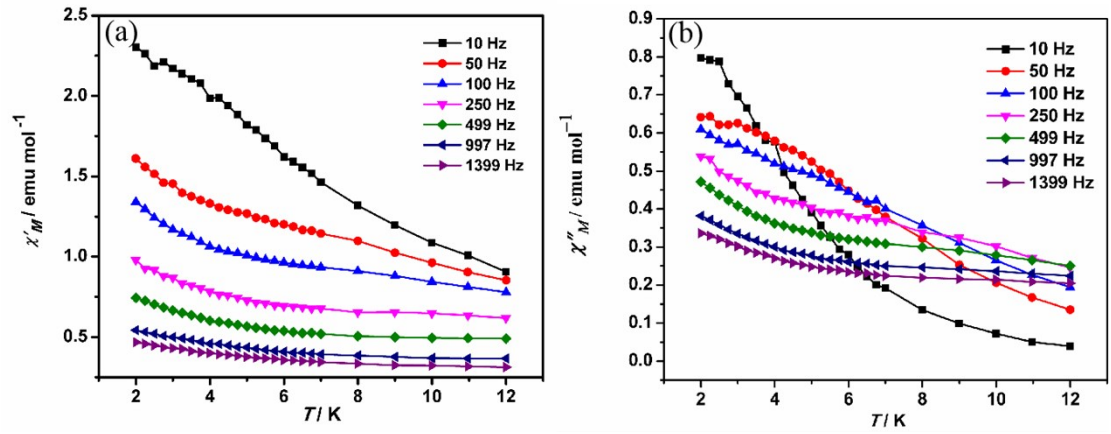

Fig. S6. Frequency dependence of the in-phase (χ′) and out-of-phase (χ″) ac susceptibility signals for **2** under 2000 Oe field.

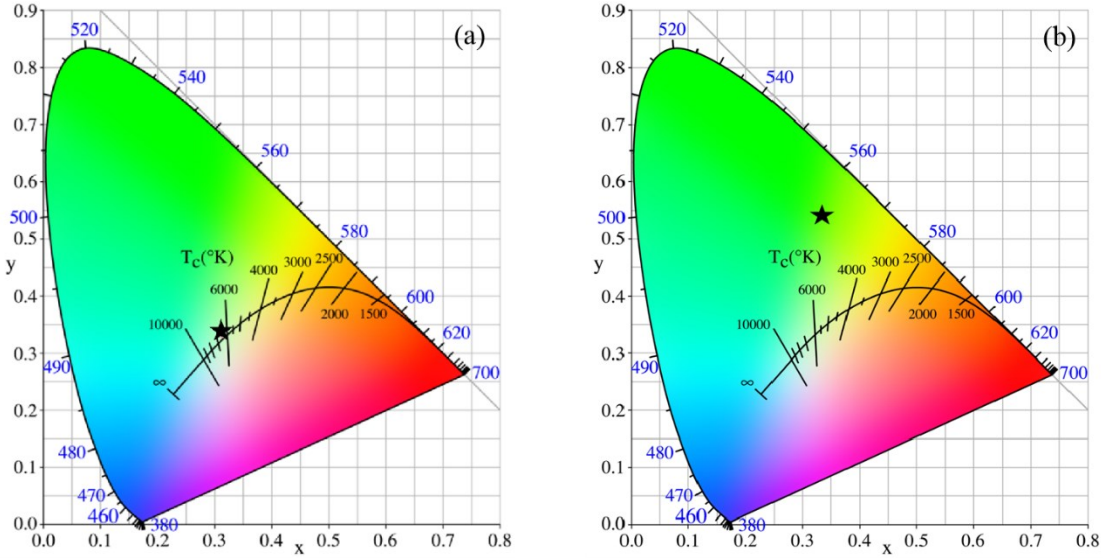

Fig. S7. CIE chromaticity diagram for the emission spectra of complex **1** under excitation 295 nm (a) and complex **2** under excitation 294 nm (b).

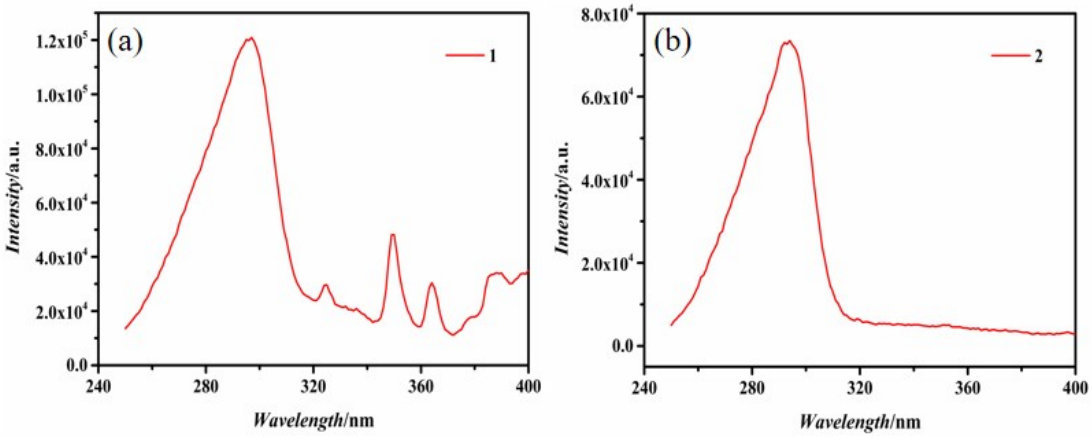

Fig. S8. (a) The fluorescent excitation spectra (λ_{em} = 572 nm) of **1**; (b) The fluorescent excitation spectra (λ_{em} = 547 nm) of **2**.

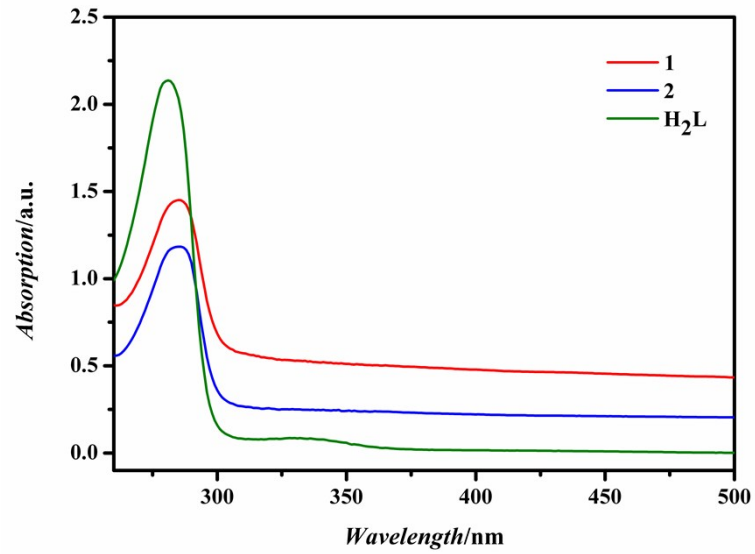

Fig. S9. The UV-Vis absorption spectra of **1**, **2** and H_2L.

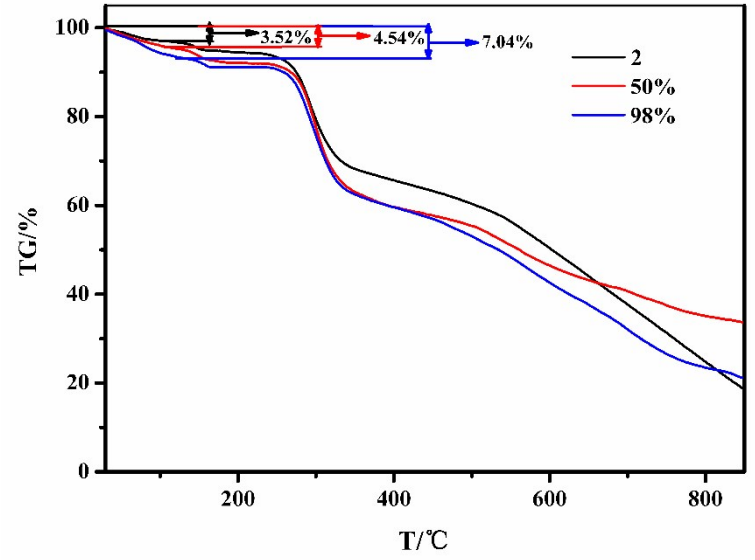

Fig. S10. The TG curves of **2** with the fresh sample and **2** stored at 50% and 98% RH conditions for 1 h.

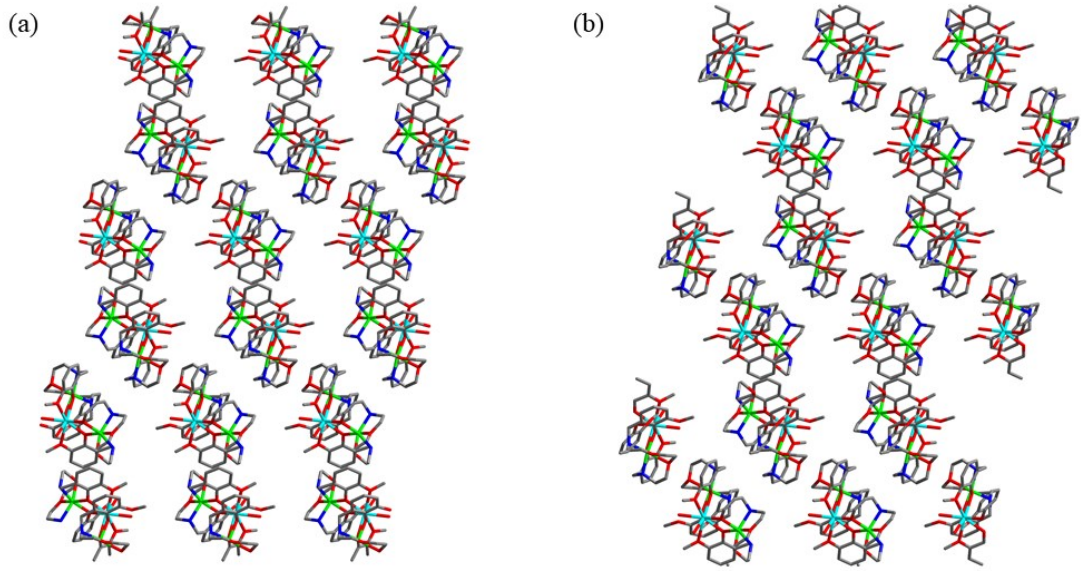

Fig. S11. The three-dimensional packing structures of **1** (a) and **2** (b).