Supporting Information

Triple-ringed Luminescent Heptanuclear Zn(II) Cluster for Efficient Ag(I) Ion Sensing Materials

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

1					
Zn5—O15	1.914 (5)	Zn2—N4	1.961 (6)	Zn6—N12	2.001 (6)
Zn5—O7	1.946 (6)	Zn2—O4	2.047 (5)	Zn6—N11	2.316 (7)
Zn5—O10	2.190 (6)	Zn2—N3	2.420 (6)	Zn1—O3	1.924 (6)
Zn5—N9	2.400 (7)	Zn4—O8	2.196 (6)	Zn1—O8	1.938 (6)
Zn5—N10	2.014 (6)	Zn4—O14	1.942 (5)	Zn1—O2	2.153 (5)
Zn3—O6	2.175 (5)	Zn4—O9	1.973 (5)	Zn1—N2	1.997 (7)
Zn3—O14	1.963 (5)	Zn4—N7	2.283 (7)	Zn1—N1	2.376 (7)
Zn3—O11	1.911 (6)	Zn4—N8	1.969 (6)	Zn7—O12	1.955 (6)
Zn3—N6	2.008 (7)	Zn6—O15	1.928 (5)	Zn7—O10	1.969 (5)
Zn3—N5	2.371 (7)	Zn6—O12	2.205 (6)	Zn7—N13	2.032 (7)
Zn2—O6	1.956 (5)	Zn6—O5	1.964 (6)	Zn7—O16	1.985 (7)
Zn2—O2	1.951 (5)				
O15—Zn5—O7	112.8 (2)	O6—Zn2—N3	94.6 (2)	O12—Zn6—N11	148.0 (2)
O15—Zn5—O10	104.8 (2)	O2—Zn2—O6	102.3 (2)	O5—Zn6—O12	94.2 (2)
O15—Zn5—N9	97.4 (2)	O2—Zn2—N4	134.3 (2)	O5—Zn6—N12	129.2 (2)
O15—Zn5—N10	121.5 (2)	O2—Zn2—O4	116.9 (2)	O5—Zn6—N11	97.4 (2)
O7—Zn5—O10	95.5 (2)	O2—Zn2—N3	78.7 (2)	N12—Zn6—O12	75.1 (2)
O7—Zn5—N9	95.2 (2)	N4—Zn2—O4	82.0 (2)	N12—Zn6—N11	74.4 (2)
O7—Zn5—N10	125.4 (2)	N4—Zn2—N3	70.4 (2)	O3—Zn1—O8	105.4 (2)
O10—Zn5—N9	149.2 (2)	O4—Zn2—N3	150.8 (2)	O3—Zn1—O2	98.2 (2)
N10—Zn5—O10	76.8 (2)	O8—Zn4—N7	152.6 (2)	O3—Zn1—N2	132.2 (3)
N10—Zn5—N9	73.6 (3)	O14—Zn4—O8	95.6 (2)	O3—Zn1—N1	98.7 (2)
O6—Zn3—N5	150.1 (2)	O14—Zn4—O9	105.1 (2)	O8—Zn1—O2	106.8 (2)
O14—Zn3—O6	104.1 (2)	O14—Zn4—N7	101.9 (2)	O8—Zn1—N2	121.4 (3)
O14—Zn3—N6	117.0 (2)	O14—Zn4—N8	126.2 (2)	O8—Zn1—N1	91.1 (2)
O14—Zn3—N5	94.6 (2)	O9—Zn4—O8	97.5 (2)	O2—Zn1—N1	151.1 (2)
O11—Zn3—O6	99.2 (2)	O9—Zn4—N7	98.1 (2)	N2—Zn1—O2	78.7 (2)
O11—Zn3—O14	107.5 (2)	N8—Zn4—O8	77.3 (2)	N2—Zn1—N1	72.5 (3)
O11—Zn3—N6	134.9 (2)	N8—Zn4—O9	128.7 (2)	O12—Zn7—O10	99.0 (2)

O11—Zn3—N5	97.1 (2)	N8—Zn4—N7	75.4 (2)	O12—Zn7—N13	108.0 (3)
N6—Zn3—O6	77.6 (2)	O15—Zn6—O12	101.0 (2)	O12—Zn7—O16	118.8 (3)
N6—Zn3—N5	73.1 (3)	O15—Zn6—O5	108.7 (2)	O10—Zn7—N13	100.5 (3)
O6—Zn2—N4	112.6 (2)	O15—Zn6—N12	122.1 (2)	O10—Zn7—O16	107.4 (3)
O6—Zn2—O4	104.9 (2)	O15—Zn6—N11	103.2 (2)	O16—Zn7—N13	119.4 (3)
Zn2—O6—Zn3	124.4 (3)	Zn5—O15—Zn6	128.5 (3)	Zn2—O2—Zn1	114.5 (3)
Zn4—O14—Zn3	122.2 (3)	Zn1—O8—Zn4	118.7 (3)	Zn7—O12—Zn6	117.7 (3)
Zn7—O10—Zn5	117.7 (2)				

Table S2a. *SHAPE* analysis of the Zn1 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
PP-5	D_{5h}	Pentagon	26.302
vOC-5	C_{4v}	Vacant octahedron	5.454
TBPY-5	D_{3h}	Trigonal bipyramid	3.658
SPY-5	C_{4v}	Spherical square pyramid	3.904
JTBPY-5	D_{3h}	Johnson trigonal bipyramid J12	4.466

Table S2b. *SHAPE* analysis of the Zn2 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
PP-5	D_{5h}	Pentagon	25.449
vOC-5	C_{4v}	Vacant octahedron	4.476
TBPY-5	D_{3h}	Trigonal bipyramid	4.979
SPY-5	C_{4v}	Spherical square pyramid	3.112
JTBPY-5	D_{3h}	Johnson trigonal bipyramid J12	5.716

Table S2c. *SHAPE* analysis of the Zn3 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
PP-5	D_{5h}	Pentagon	28.210
vOC-5	C_{4v}	Vacant octahedron	4.663
TBPY-5	D_{3h}	Trigonal bipyramid	3.635
SPY-5	C_{4v}	Spherical square pyramid	3.050
JTBPY-5	D_{3h}	Johnson trigonal bipyramid J12	4.486

Table S2d. *SHAPE* analysis of the Zn4 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
PP-5	D_{5h}	Pentagon	28.014
vOC-5	C_{4v}	Vacant octahedron	6.018
TBPY-5	D_{3h}	Trigonal bipyramid	3.240
SPY-5	C_{4v}	Spherical square pyramid	4.248
JTBPY-5	D_{3h}	Johnson trigonal bipyramid J12	4.288

Table S2e. *SHAPE* analysis of the Zn5 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
PP-5	D_{5h}	Pentagon	29.453
vOC-5	C_{4v}	Vacant octahedron	5.707
TBPY-5	D_{3h}	Trigonal bipyramid	3.066
SPY-5	C_{4v}	Spherical square pyramid	3.480
JTBPY-5	D_{3h}	Johnson trigonal bipyramid J12	3.903

Table S2f. *SHAPE* analysis of the Zn6 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
PP-5	D_{5h}	Pentagon	29.368
vOC-5	C_{4v}	Vacant octahedron	5.257
TBPY-5	D_{3h}	Trigonal bipyramid	3.572
SPY-5	C_{4v}	Spherical square pyramid	3.052
JTBPY-5	D_{3h}	Johnson trigonal bipyramid J12	4.736

Table S2g. *SHAPE* analysis of the Zn7 ion in complex **1**.

Label	Shape	Symmetry	Distortion(°)
SP-4	D_{4h}	Pentagon	333.191
T-4	T_d	Spherical square pyramid	0.745
SS-4	C_{2v}	Johnson trigonal bipyramid J12	7.556

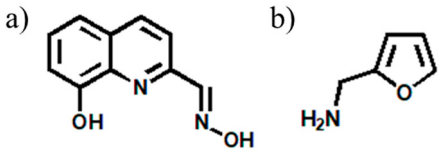

Figure S1. The scheme with the structures of H_2L^1 and H_2L^2.

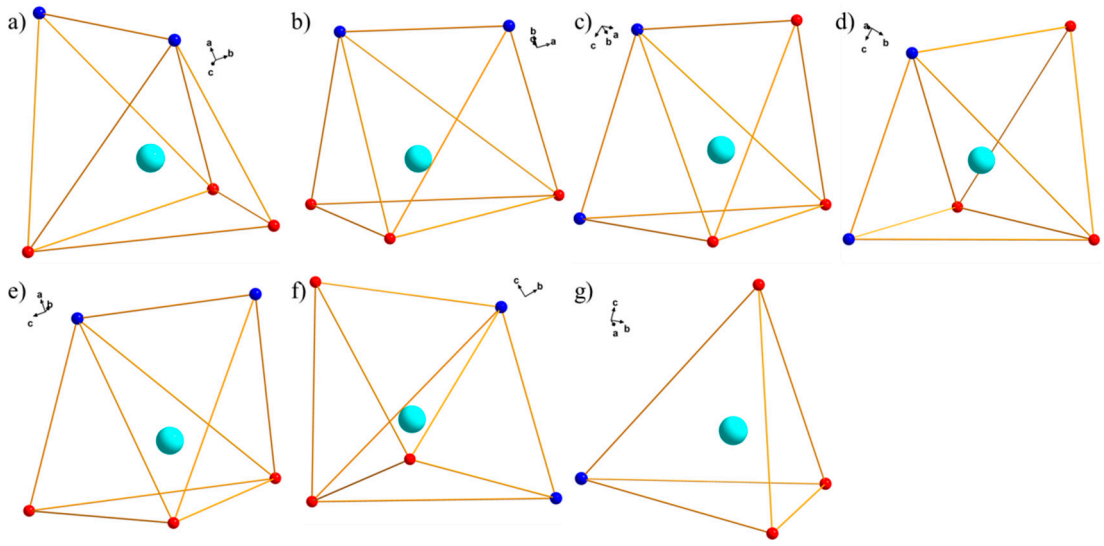

Figure S2. The coordination pattern diagram of Zn(II) ions in compound **1**.

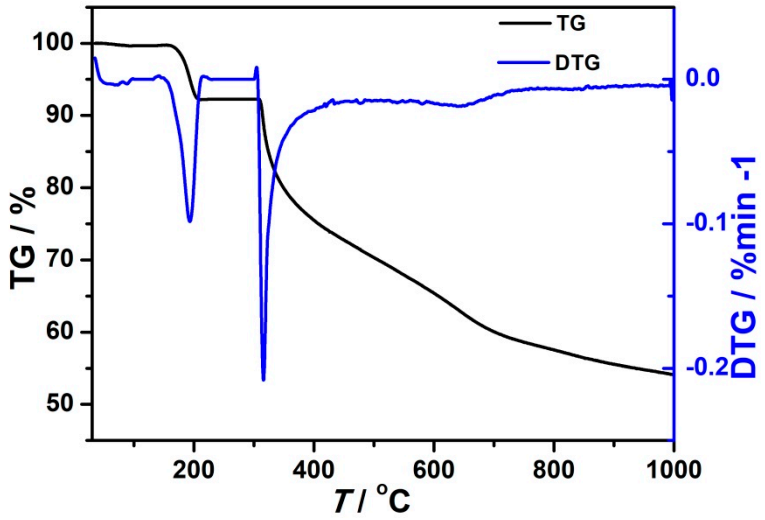

Figure S3. Thermogravimetry of the compounds at a heating rate of 5 °C/min under N_2 atmosphere for **1**.

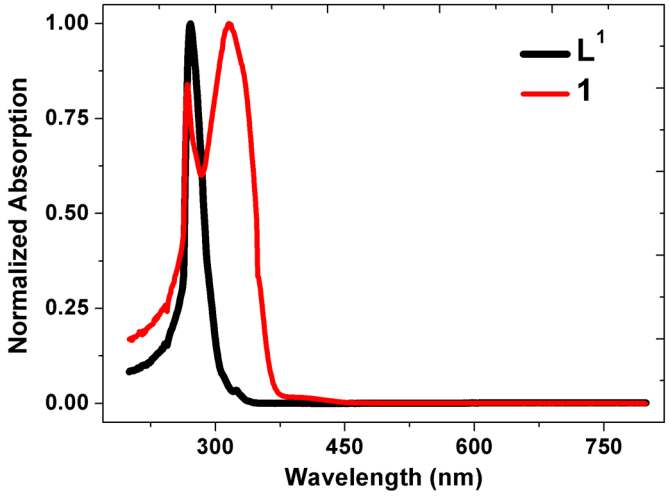

Figure S4. The UV-visible absorption spectrum of the ligand H**L**^{1} and compound **1** dissolved in DMF, respectively.

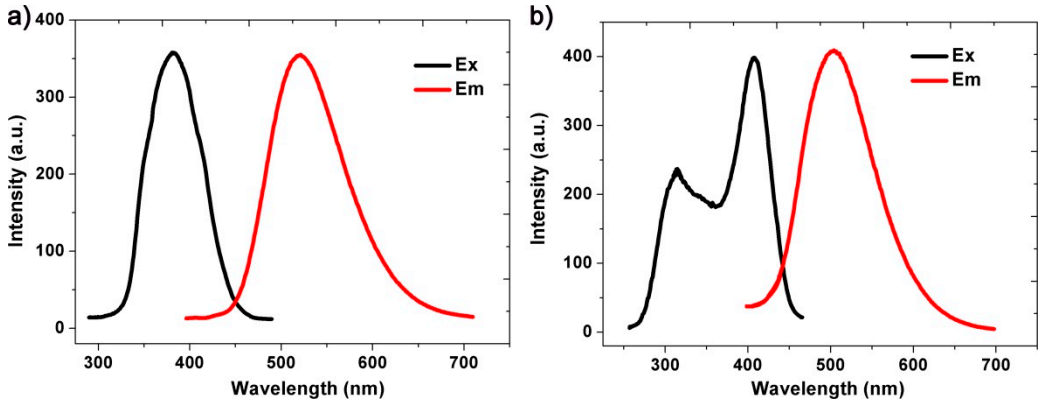

Figure S5. Fluorescence spectra of ligand H**L**[1] (a) and compound **1** (b) dissolved in DMF, respectively.

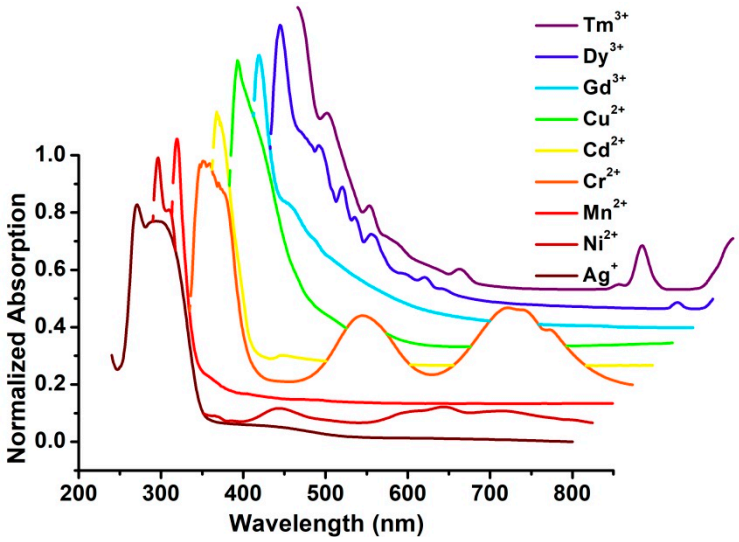

Figure S6. The complex **1** and different metal ions were dissolved in an ultraviolet-visible absorption test in DMF.