

**Electronic Supplementary Information (ESI) for *Dalton
Transactions***

**Bright-yellow to orange-red thermochromic luminescence of
a $\text{Ag}^{\text{I}}_6\text{-Zn}^{\text{II}}_2$ heterometallic aggregate**

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

Ag1—N3	2.287(7)	Ag3—N1	2.325(8)
Ag1—S2	2.485(2)	Ag3—S2 ⁱ	2.472(2)
Ag1—S1	2.501(2)	Ag3—S3	2.485(2)
Ag1—Ag2	2.9338(10)	Ag3—Ag2 ⁱ	2.9308(10)
Ag1—Ag3	3.0376(11)	Zn1—O6	1.997(6)
Ag2—N2	2.279(7)	Zn1—O1W	2.069(9)
Ag2—S3	2.489(2)	Zn1—N5	2.087(7)
Ag2—S1 ⁱ	2.490(3)	Zn1—O2W	2.156(7)
Ag2—Ag3 ⁱ	2.9308(10)	Zn1—N4	2.164(9)
N3—Ag1—S2	127.9(2)	Ag2 ⁱ —Ag3—Ag1	76.94(3)
N3—Ag1—S1	114.8(2)	O6—Zn1—O1W	109.2(3)
S2—Ag1—S1	113.65(8)	O6—Zn1—N5	131.5(3)
Ag2—Ag1—Ag3	73.04(3)	O1W—Zn1—N5	119.1(4)
N2—Ag2—S3	122.1(2)	O6—Zn1—O2W	98.0(3)
N2—Ag2—S1 ⁱ	123.6(2)	O1W—Zn1—O2W	86.8(3)
S3—Ag2—S1 ⁱ	108.85(8)	N5—Zn1—O2W	88.4(3)
Ag3 ⁱ —Ag2—Ag1	72.35(3)	O6—Zn1—N4	94.9(3)
N1—Ag3—S2 ⁱ	121.4(2)	O1W—Zn1—N4	95.0(3)
N1—Ag3—S3	115.3(2)	N5—Zn1—N4	78.3(3)
S2 ⁱ —Ag3—S3	116.02(8)	O2W—Zn1—N4	165.7(3)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

(2) Table S2 Selected hydrogen bond parameters (Å, °) for 1

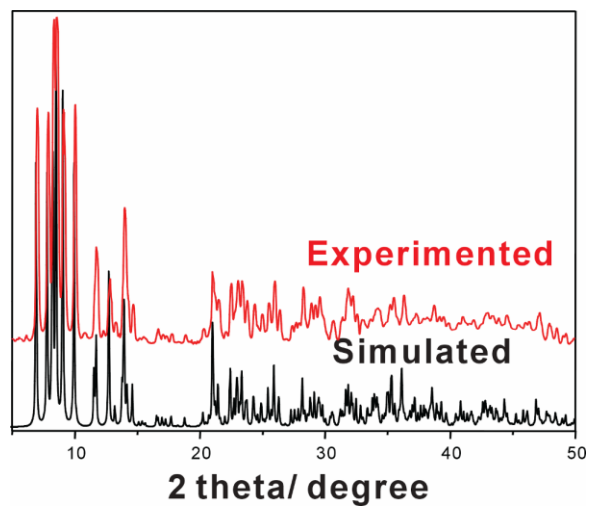
<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O7—H7C...O3	0.84	1.91	2.681(13)	153
O2W—H2WB...O2 ⁱⁱⁱ	0.85	2.02	2.766(9)	146
O2W—H2WA...O4 ^{iv}	0.85	1.88	2.720(10)	169
O3W—H3WA...O1 ⁱⁱ	0.85	1.96	2.796(10)	165
O3W—H3WB...O1 ⁱ	0.85	1.97	2.796(10)	165

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y, z-1$; (iii) $-x, -y, -z+1$; (iv) $x-1, y-1, z-1$.

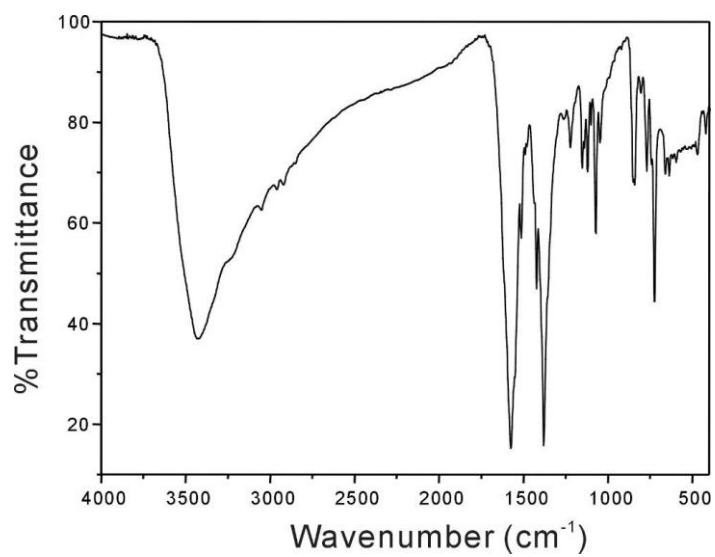
(3) Table S3 Photoluminescence emission data for L_{Ag} and 1.

Complex	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Possible transitions
H ₂ mna (298K)	300	470	$\pi^* \rightarrow \pi$
L _{Ag} (298K)	365	469, 551	$\pi^* \rightarrow \pi$ and LMCT
L _{Ag} (255K)	365	469, 555	$\pi^* \rightarrow \pi$ and LMCT
L _{Ag} (173K)	365	469, 559	$\pi^* \rightarrow \pi$ and LMCT
L _{Ag} (130K)	365	469, 561	$\pi^* \rightarrow \pi$ and LMCT
L _{Ag} (77K)	365	469, 571	$\pi^* \rightarrow \pi$ and LMCT
1 (298K)	365	544	LMCT
1 (255K)	365	551	LMCT
1 (173K)	365	554	LMCT
1 (130K)	365	558	LMCT
1 (77K)	365	565	LMCT

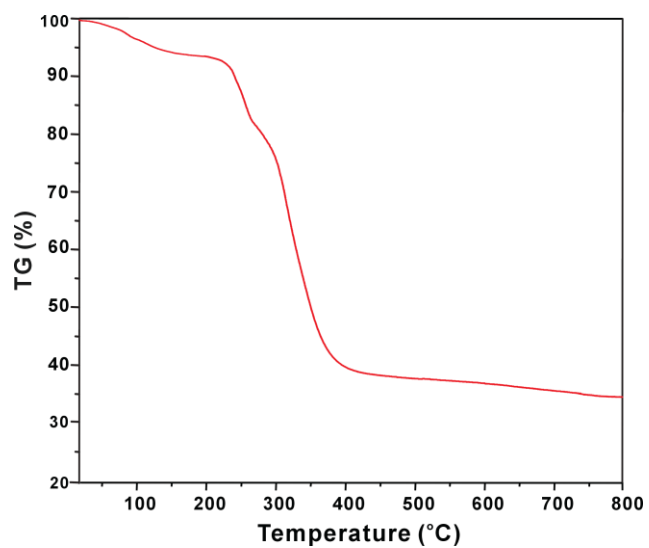
(4) Figure S1 XRD spectrum of 1



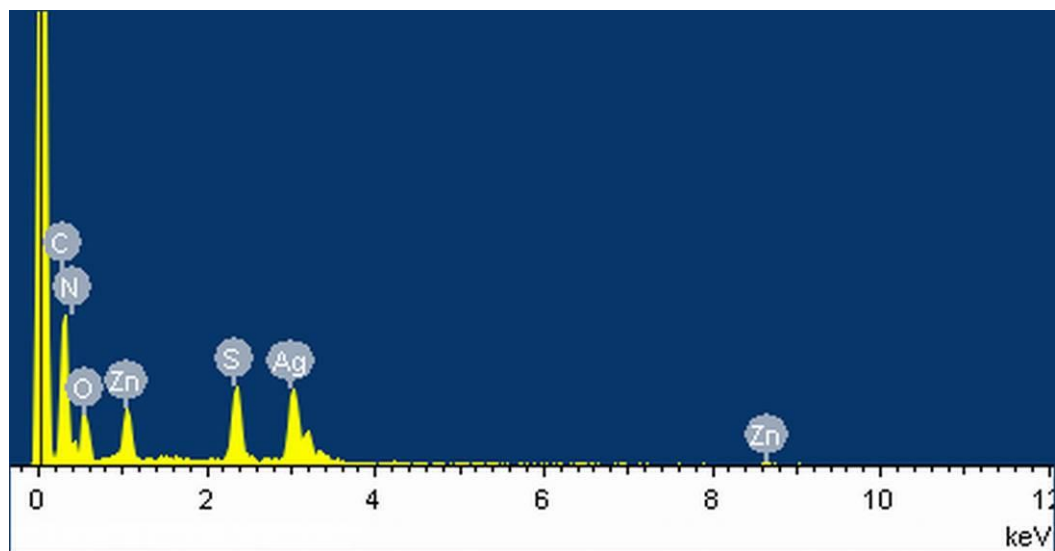
(5) Figure S2 IR spectrum of 1



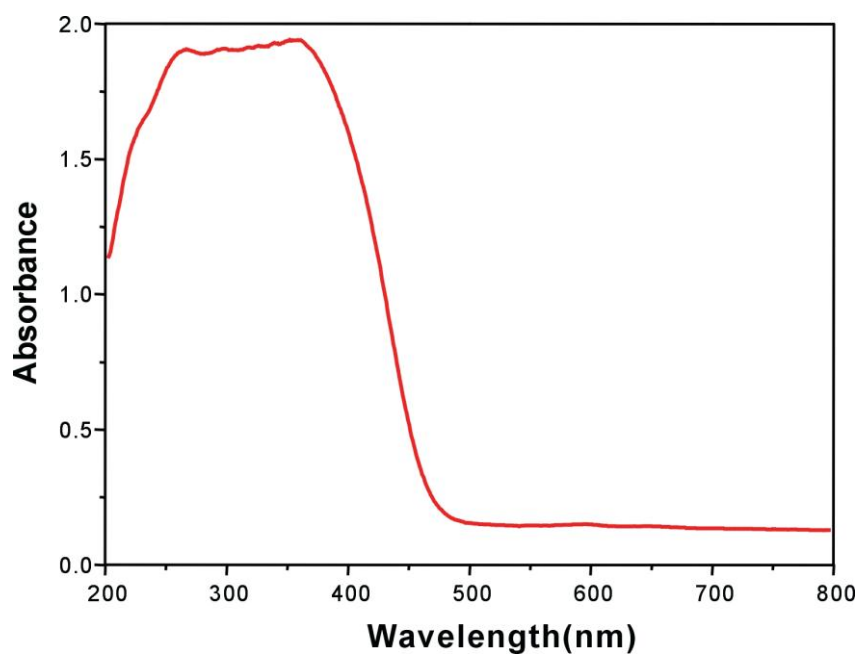
(6) Figure S3 The TG curve of 1



(7) Figure S4: Energy dispersive X-ray spectroscopy (EDS) data for 1



(8) Figure S5: UV-Vis spectrum of 1



(9) Figure S6: Photoluminescence of free ligand H₂mna

