

Supporting Information

Two Zinc(II)-Based coordination polymers as Luminescent Sensors for detecting Salicylaldehyde with High Sensitivity and Selectivity

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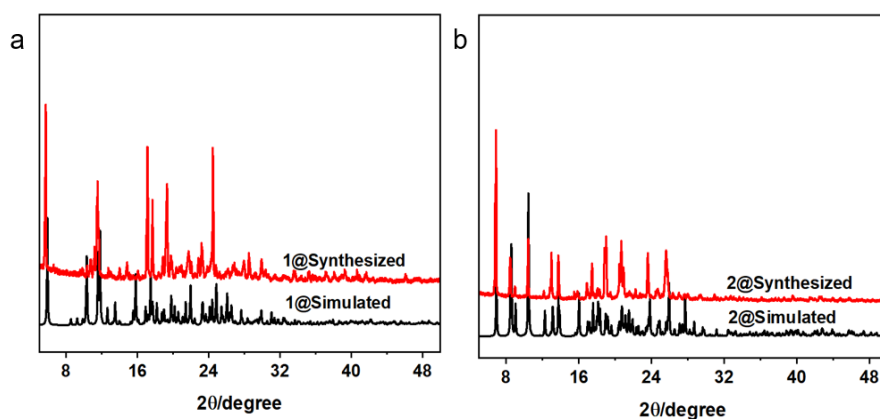


Figure S1 The X-ray powder diffraction patterns of **1** (a) and **2** (b).

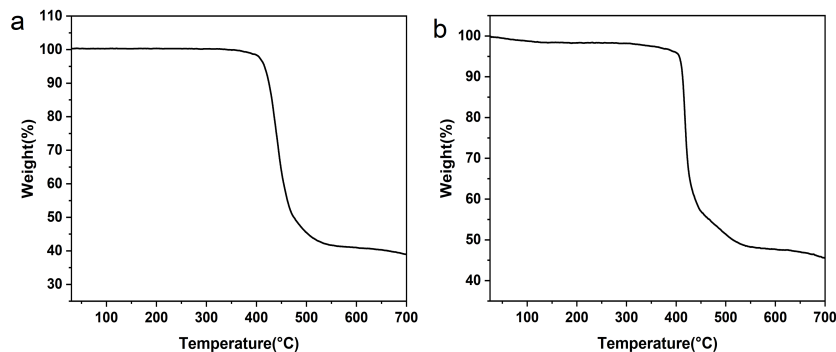


Figure S2 TGA of **1** (a) and **2** (b).

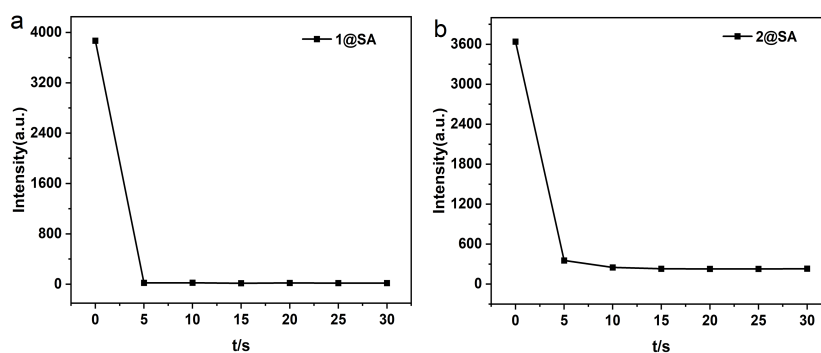


Figure S3 Fluorescence intensity curves of coordination polymers over time **1** (a) and **2** (b).

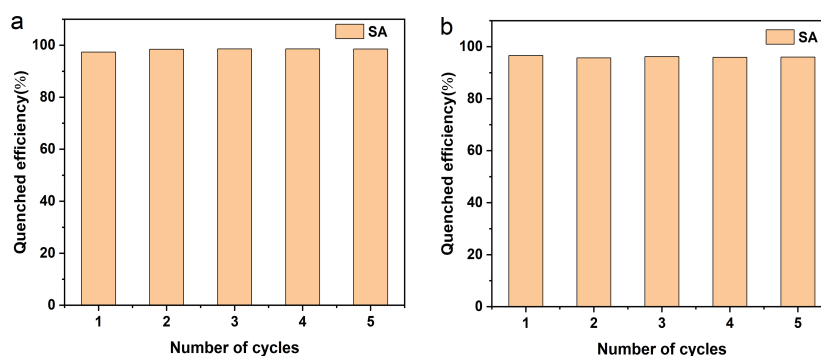


Figure S4 The recyclability of **1** and **2** were tested for 5 consecutive cycles in the presence of SA.

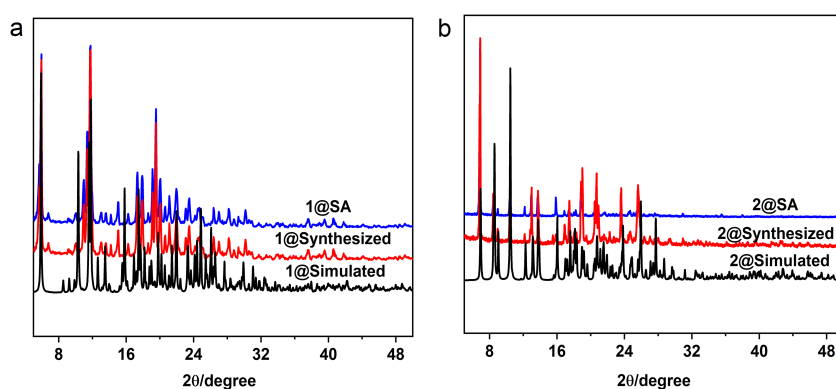


Figure S5 PXRD of **1** (a) and **2** (b) before and after detection of SA.

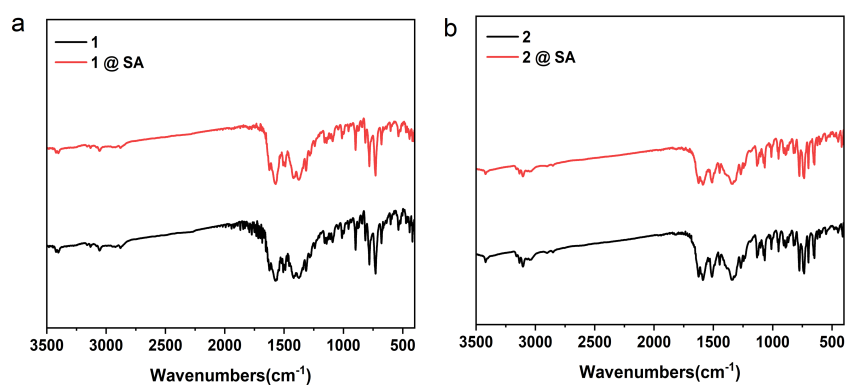


Figure S6 Infrared spectra of the coordination polymers **1** (a) and **2** (b) before and after detection of SA.

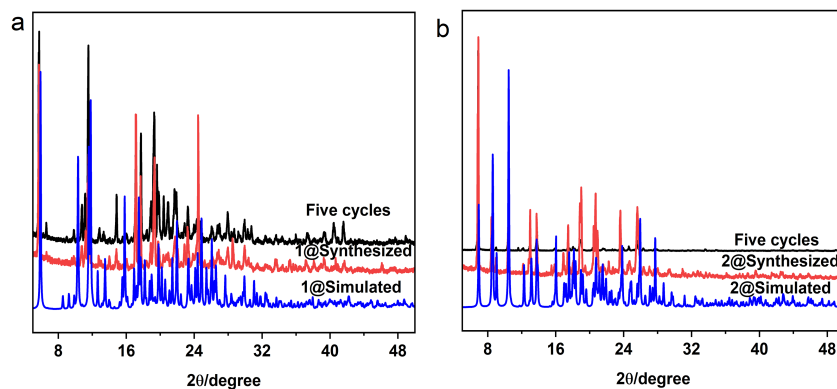


Figure S7 PXRD after five cycles of **1** (a) and **2** (b).

Table S1 Detailed crystal data and structure refinement parameters of **1** and **2**.

Complex	1	2
Chemical formula	C ₆₂ H ₅₇ N ₇ O ₉ Zn ₂	C ₃₄ H ₂₄ N ₆ O ₄ Zn
M_r	1174.88	645.96
T(K)	100	100
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
$a/\text{\AA}$	9.6377 (3)	10.1228 (5)
$b/\text{\AA}$	15.5333 (4)	11.5907 (5)
$c/\text{\AA}$	18.4376 (5)	13.8893 (7)
α (°)	76.307 (10)	111.631 (2)
β (°)	88.371 (10)	94.164 (2)
γ (°)	82.631 (10)	101.933 (2)
$V(\text{\AA}^3)$	2659.60 (13)	1462.16 (12)
$F(000)$	1220	664
Z	2	2
R_{int}	0.075	0.070
$D_{\text{calcd}}(\text{Mg m}^{-3})$	1.467	1.467
Gof	1.010	1.034
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0964$ $wR_2 = 0.0544$	$R_1 = 0.0744$ $wR_2 = 0.1179$
R indices (all data)	$R_1 = 0.1187$ $wR_2 = 0.1424$	$R_1 = 0.0502$ $wR_2 = 0.1320$
CCDC	2327505	2327511

$$R_1 = \Sigma \|F_o\| - |F_c| / \Sigma |F_o|, wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$$

Table S2 Selected bond length (Å) and angles (°) of **1**.

Selected bond lengths			
Zn1—O6	1.970 (2)	Zn2—O4 ⁱⁱ	1.998 (2)
Zn1—O7 ⁱ	1.993 (2)	Zn2—O4	2.099 (2)
Zn1—O2	1.941 (2)	Zn2—O8	1.899 (2)
Zn1—N1	1.988 (3)	Zn2—N4	1.977 (3)
Selected bond angles			
O6—Zn1—O7 ⁱ	120.87 (10)	O4 ⁱⁱ —Zn2—O4	78.94 (9)
O6—Zn1—N1	97.67 (11)	O8—Zn2—O4	111.82 (10)
O2—Zn1—O6	109.15 (11)	O8—Zn2—O4 ⁱⁱ	132.22 (10)
O2—Zn1—O7 ⁱ	99.91 (10)	O8—Zn2—N4	108.41 (11)
O2—Zn1—N1	134.20 (11)	N4—Zn2—O4 ⁱⁱ	114.56 (10)
N1—Zn1—O7 ⁱ	96.94 (11)	N4—Zn2—O4	102.13 (11)
Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$.			

Table S3 Selected bond length (Å) and angles (°) of **2**.

Selected bond lengths			
Zn1—O1	1.979 (2)	Zn1—N2	1.997 (3)
Zn1—O4 ⁱ	1.991 (2)	Zn1—N5 ⁱⁱ	2.006 (3)
Selected bond angles			
O1—Zn1—O4 ⁱ	96.96 (8)	O4 ⁱ —Zn1—N2	108.16 (9)
O1—Zn1—N2	115.76 (10)	O4 ⁱ —Zn1—N5 ⁱⁱ	112.00 (9)
O1—Zn1—N5 ⁱⁱ	104.13 (10)	N2—Zn1—N5 ⁱⁱ	117.93 (10)
Symmetry codes: (i) $x+1, y, z$; (ii) $x, y-1, z$; (iii) $x-1, y, z$; (iv) $x, y+1, z$.			

Table S4 The continuous shape measures value of **1** calculated using SHAPE 2.1.

Label Symmetry	Zn1	Zn2
PP-5	49.410	43.383
vOC-5	35.969	38.116
TBPY-5	39.369	37.896
SPY-5	36.636	37.858
JTBPY-5	39.317	34.437

Table S5 The continuous shape measures value of **2** calculated using SHAPE 2.1.

Complex	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
2	48.229	33.377	41.400	32.784	36.515

Table S6 Comparison among various coordination polymers (CPs)sensors for SA detection.

Analyte	CPs	LOD	Reference
SA	$\{[\text{Cd}(\text{BBIP})(\text{CDDb})(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}\}_n$	0.051 ppm	S1
	$[\text{Zn}(\text{BBIP})(2,6\text{-NDC})]_n$	0.074 ppm	S2
	$\{[\text{Cd}(\text{BBIP})(\text{TBIP})] \cdot \text{EtOH}\}_n$	0.42 ppm	S3
	$\{[\text{Cd}(\text{BBZB})(\text{bptc})_{0.5}] \cdot 2\text{H}_2\text{O}\}_n$	0.3443 mM	S4
	1	0.87 μM	this work
	2	27.03 μM	this work

Reference

- S1. X. X. Zhang, D. G. Cai, Y. P. Li, Y. Q. Chen and S. J. Liu, *Cryst. Growth Des.*, 2023, **23**, 5762-5769.
- S2. Y. P. Li, J. H. Zhang, X. X. Zhang and S. J. Liu, *CrystEngComm*, 2023, **25**, 6424-6433.
- S3. L. H. Wu, S. L. Yao, J. Li, H. Xu, T. F. Zheng, S. J. Liu, J. L. Chen and H. R. Wen, *CrystEngComm*, 2021, **23**, 482-491.
- S4. R. J. Zhang, J. J. Wang, H. Xu, Z. H. Zhu, T. F. Zheng, Y. Peng, J. L. Chen, S. J. Liu and H.R. Wen, *Cryst. Growth Des.*, 2023, **23**, 5564-5570.