

Supplementary Information

Enhanced Luminescent Sensing of Pymetrozine Pesticide in Cow Milk Using Cd(II) Coordination Network with Sensitivity Up to 0.448 ppm

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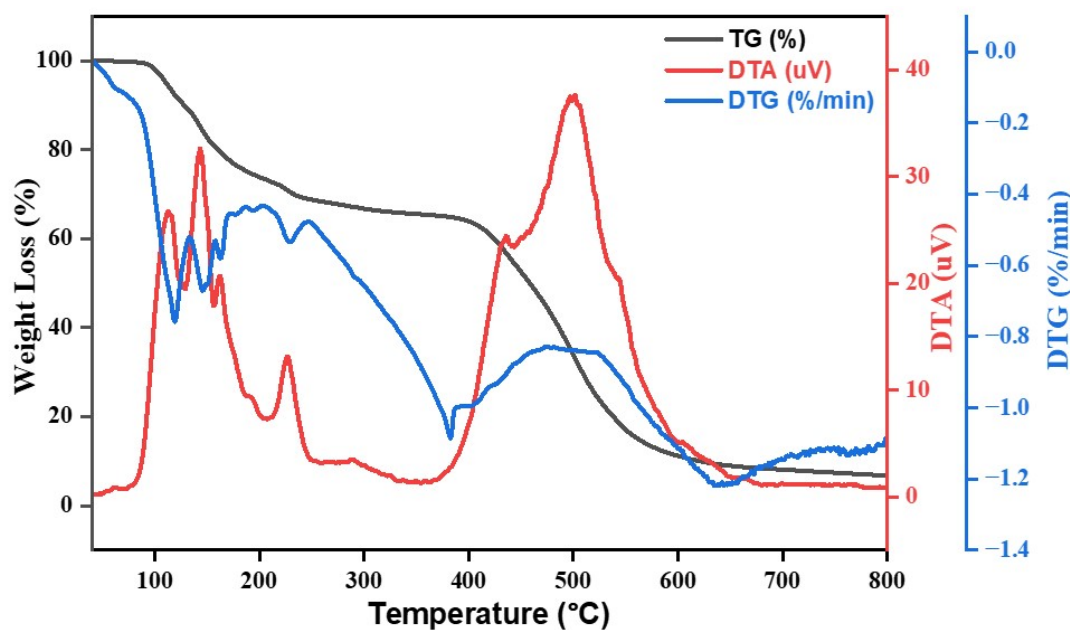


Fig.S1. Thermal Analysis of $[\{Cd(Py)_2I_2\}\{Cd_2(Py)_5(BTC)(H_2O)I\}\{H_2O\}]CP-1$

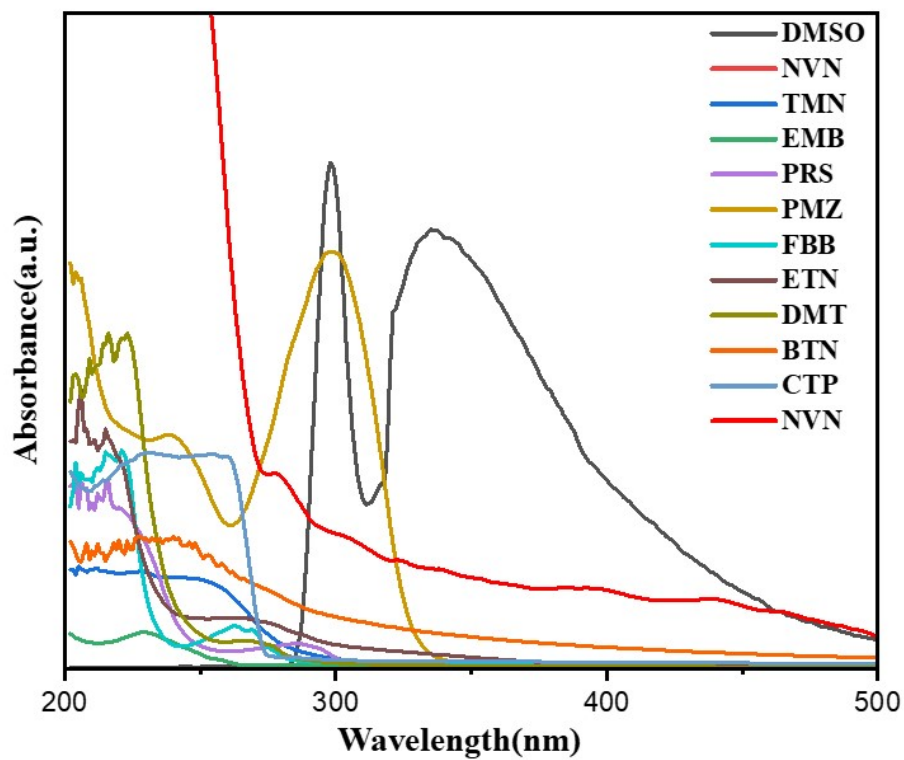


Fig S2. Spectral overlap between the UV-Vis absorption spectra of pesticides with the excitation spectra of $[\{Cd(Py)_2I_2\}\{Cd_2(Py)_5(BTC)(H_2O)I\}\{H_2O\}]CP-1$

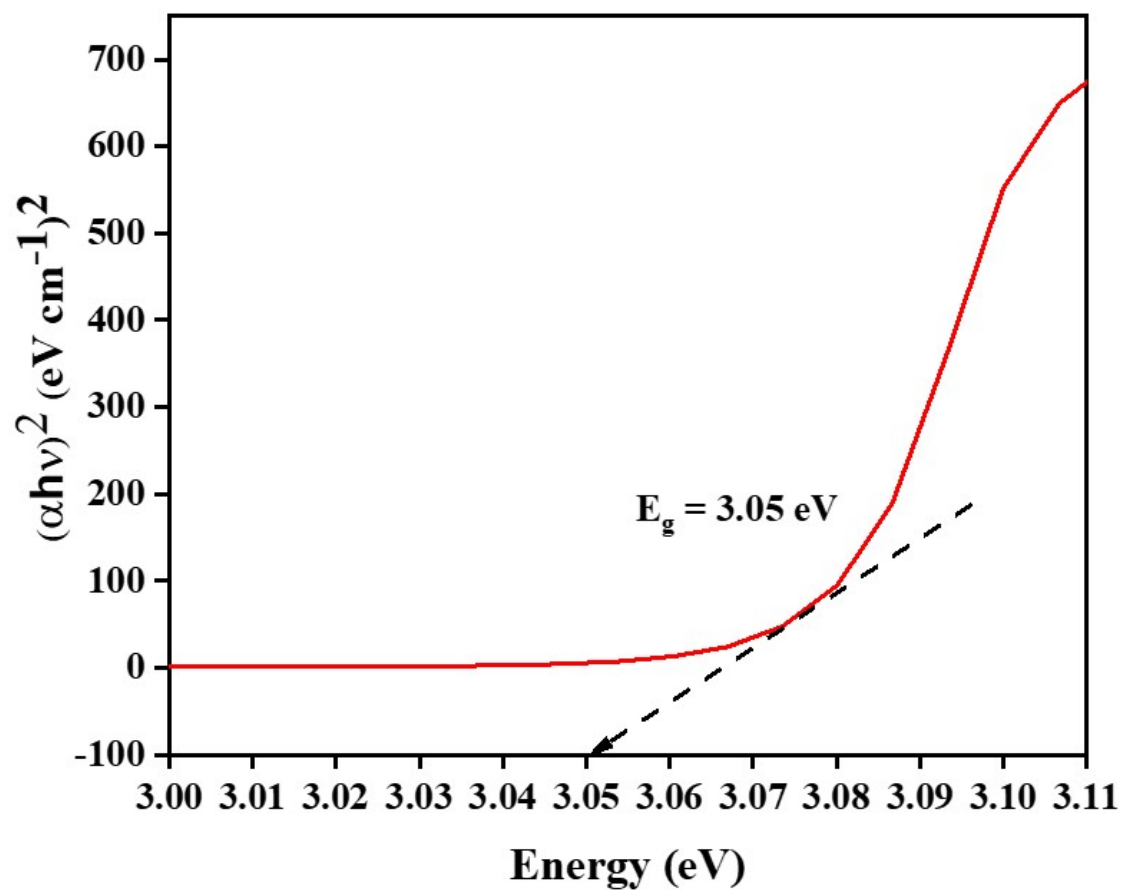


Fig.S3. Tauc Plot of $[(\text{Cd}(\text{Py})_2\text{I}_2)\{\text{Cd}_2(\text{Py})_5(\text{BTC})(\text{H}_2\text{O})\text{I}\}\{\text{H}_2\text{O}\}]\text{CP-1}$

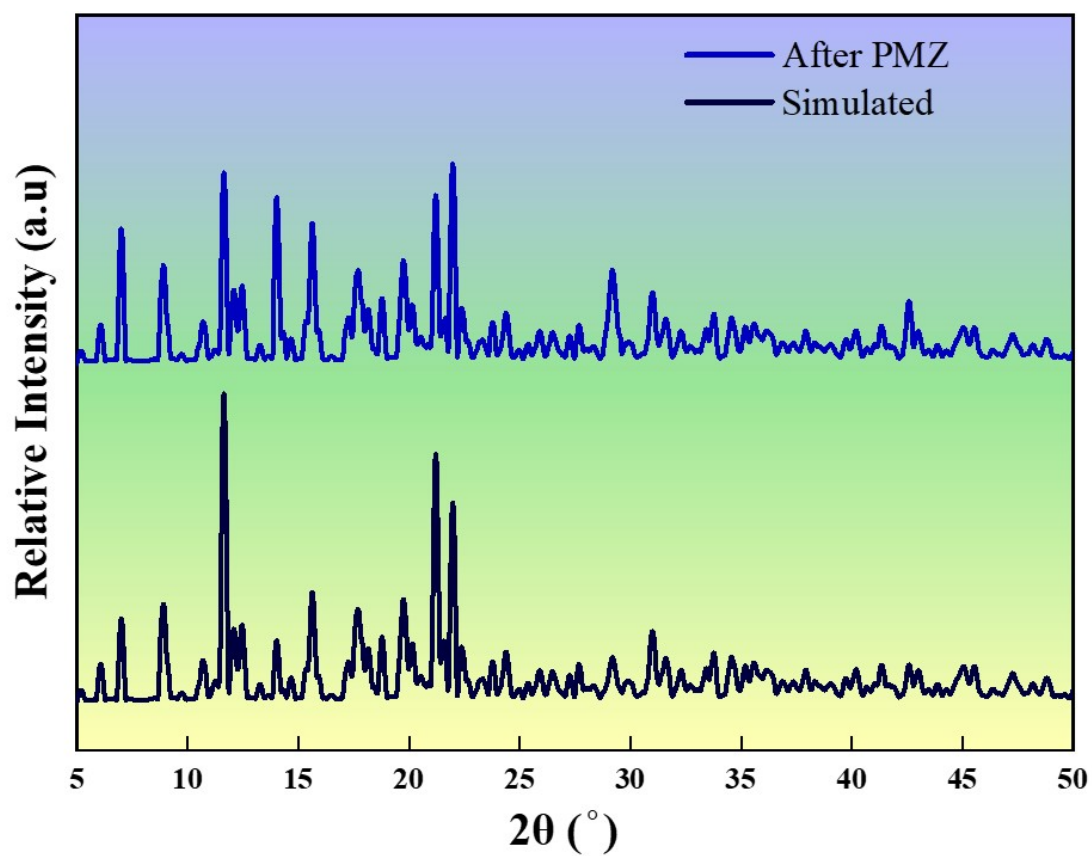


Fig.S4. PXRD pattern of $[\{\text{Cd}(\text{Py})_2\text{I}_2\}\{\text{Cd}_2(\text{Py})_5(\text{BTC})(\text{H}_2\text{O})\text{I}\}\{\text{H}_2\text{O}\}]\text{CP-1}$, simulated and after five cycle sensing of PMZ.

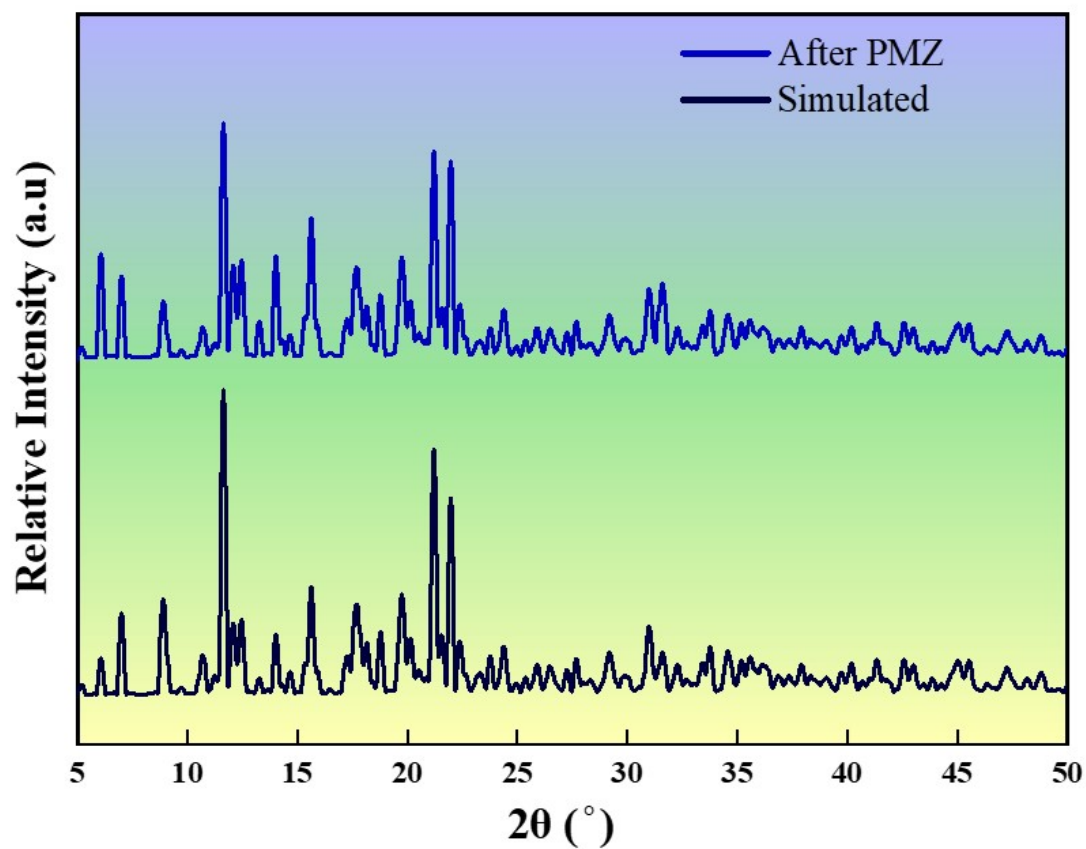


Fig.S5. PXRD pattern of $[\{\text{Cd}(\text{Py})_2\text{I}_2\}\{\text{Cd}_2(\text{Py})_5(\text{BTC})(\text{H}_2\text{O})\text{I}\}\{\text{H}_2\text{O}\}]\text{CP-1}$, simulated and after five cycle degradation of PMZ.

Table S1. Crystallographic information and structural refinement for **CP-1**.

Identification code	[{Cd(Py)₂I₂}·{Cd₂(Py)₅(BTC)(H₂O)I}·{H₂O}]
Empirical formula	C ₄₄ H ₄₂ Cd ₃ I ₃ N ₇ O ₈
Formula weight	1514.81
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	35.0423(2)
b/Å	10.20760(10)
c/Å	29.9387(2)
α/°	90
β/°	103.5200(10)
γ/°	90
Volume/Å³	10412.24(14)
Z	8
ρ_{calc}/cm³	1.9325
μ/mm⁻¹	24.144
F(000)	5793.6
Crystal size/mm³	0.38 × 0.23 × 0.15
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	5.18 to 136.28
Index ranges	-41 ≤ h ≤ 42, -11 ≤ k ≤ 12, -36 ≤ l ≤ 35
Reflections collected	58087
Independent reflections	9446 [R _{int} = 0.1075, R _{sigma} = 0.0449]

Data/restraints/parameters	9446/0/591
Goodness-of-fit on F²	1.041
Final R indexes [I>2σ (I)]	R ₁ = 0.0612, wR ₂ = 0.1760
Final R indexes [all data]	R ₁ = 0.0645, wR ₂ = 0.1793
Largest diff. peak/hole / e Å⁻³	2.40/-1.75
CCDC Number	2389050

Table S2. Bond Lengths of [{Cd(Py)₂I₂}{Cd₂(Py)₅(BTC)(H₂O)I}{H₂O}](CP-1).

Atom	Bond Length
Cd1 – O1	2.559(5)
Cd1 – O2	2.308(5)
Cd1 – O5	2.575(5)
Cd1 – O6	2.307(5)
Cd1 – O7	2.392(5)
Cd1 – N1	2.313(5)
Cd1 – N2	2.381(7)
Cd2 – O3	2.387(4)
Cd2 – O4	2.361(4)
Cd2 – N3	2.430(6)
Cd2 – N4	2.348(6)
Cd2 – N5	2.478(6)
Cd2 – I3	2.703(5)
Cd3 – I1	2.7038(7)
Cd3 – I2	2.6835(7)
Cd3 – N6	2.294(6)
Cd3 – N7	2.296(7)

Table S3. Bond Angles of $\{[\text{Cd}(\text{Py})_2\text{I}_2]\{\text{Cd}_2(\text{Py})_5(\text{BTC})(\text{H}_2\text{O})\text{I}\}\{\text{H}_2\text{O}\}\}(\text{CP-1})$.

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
I1	Cd3	I2	130.22(3)	I3	Cd2	O4	168.3(1)
I1	Cd3	N6	103.7(2)	I3	Cd2	N3	95.5(1)
I1	Cd3	N7	106.4(2)	I3	Cd2	N4	103.0(1)
I2	Cd3	N6	108.0(2)	I3	Cd2	N5	97.2(1)
I2	Cd3	N7	108.4(2)	O3	Cd2	O4	55.2(2)
N6	Cd3	N7	94.2(2)	O3	Cd2	N3	85.6(2)
Cd3	N6	C35	121.4(6)	O3	Cd2	N4	143.9(2)
Cd3	N6	C39	120.5(6)	O3	Cd2	N5	87.8(2)
C35	N6	C39	117.7(8)	O4	Cd2	N3	84.6(2)
Cd3	N7	C4ba	121.7(6)	O4	Cd2	N4	88.7(2)
Cd3	N7	C40	120.0(6)	O4	Cd2	N5	82.6(2)
O1	Cd1	O2	52.9(2)	N3	Cd2	N4	89.7(2)
O1	Cd1	O7	87.9(2)	N3	Cd2	N5	167.2(2)
O1	Cd1	N1	88.1(2)	N4	Cd2	N5	89.1(2)
O1	Cd1	N2	89.9(2)	Cd1	O1	C33	87.3(4)
O1	Cd1	O5	171.6(2)	Cd1	O2	C33	97.8(4)
O1	Cd1	O6	135.8(2)	Cd2	O3	C26	90.4(4)
O2	Cd1	O7	87.7(2)	Cd2	O4	C26	91.5(4)
O2	Cd1	N1	141.0(2)	C34	O5	Cd1	87.6(4)
O2	Cd1	N2	90.9(2)	C34	O6	Cd1	98.3(4)
O2	Cd1	O5	135.1(2)	Cd1	O7	Hj	109(2)
O2	Cd1	O6	83.0(2)	Cd1	O7	Hk	109(2)
O7	Cd1	N1	90.4(2)	Cd1	N1	C1	122.5(5)

O7	Cd1	N2	177.8(2)	Cd1	N1	C5	120.6(7)
O7	Cd1	O5	90.0(2)	Cd1	N2	C6	123.6(6)
O7	Cd1	O6	87.8(2)	Cd1	N2	C10	119.3(6)
N1	Cd1	N2	89.6(2)	Cd2	N3	C11	122.8(6)
N1	Cd1	O5	83.8(2)	Cd2	N3	C15	120.8(6)
N1	Cd1	O6	135.9(2)	Cd2	N4	C16	121.2(4)
N2	Cd1	O5	92.2(2)	Cd2	N4	C20	121.2(5)
N2	Cd1	O6	93.7(2)	Cd2	N5	C21	122.2(5)
O5	Cd1	O6	52.2(2)	Cd2	N5	C25	120.1(5)
I3	Cd2	O3	113.0(1)				

Table S4. Comparison of Sensing ability of CP-1 with Previously Reported Methods

Analytical Method	Detection Limit	Reference
Fluorescence	86 ppm	[1]
Electrochemical	17 nM	[2]
Colorimetric	10 nM	[3]
Colorimetric	0.01mg/L.	[4]
Fluorescence	0.153 ppm	This Wok

Table S5. Comparison of Degradation Efficiency of CP-1 with Previously Reported Methods

Analytical Method	Degradation (%)	Reference
Ag ₃ PO ₄ /TpPa-1-COF	99.3	[1]

V-doped ZnFe LDH	73	[2]
CFNFe	90	[3]
CP-1	93.87	This Work

References.

1. C. Han, J. Li, G. Li, A. Kumar, M. Muddassir and J. Jin, *Inorg. Chem. Commun.*, 2021, 123, 108296.
2. Y. Gao, Y. Shi and H. Li, *J. AOAC Int.*, 2023, **106**, 1190–1196.
3. J.-Y. Kang, Y.-J. Zhang, X. Li, C. Dong, H.-Y. Liu, L.-J. Miao, P. J. Low, Z.-X. Gao, N. S. Hosmane and A.-G. Wu, *Anal. Methods*, 2018, **10**, 417–421.
4. Chen, Jun, et al. “Highly Sensitive and Selective Pymetrozine Colorimetric Sensor Based on P-Aminobenzenesulfonic Acid Modified Ag NPs.” *Applied Mechanics and Materials*, vol. 117–119, Trans Tech Publications, Ltd., Oct. 2011, pp. 958–961. Crossref, doi:10.4028/www.scientific.net/amm.117-119.958.
5. J. Liu, C. Feng, Y. Li, Y. Zhang, Q. Liang, S. Xu, Z. Li and S. Wang, *Sep. Purif. Technol.*, 2022, **288**, 120644.
6. R. Keyikoglu, A. Khataee, H. Lin and Y. Orooji, *Chem. Eng. J.*, 2022, **434**, 134730.
7. A. Fdez-Sanromán, V. Acevedo-García, M. Pazos, M. Á. Sanromán and E. Rosales, *Electrochim. Acta*, 2020, **338**, 135768.