Electronic Supplementary Information on the New Journal of Chemistry publication entitled

Fluorescent Zinc(II)-Based Metal−Organic Frameworks for Nitroaromatics Sensing

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Table S1. Crystal data and structure refinement for NJMU-001

Compound	NJMU-001
Empirical formula	C_{24} H_{32} O_{20} Zn_4
Formula weight	901.97
Crystal system	Cubic
Space group	$P2_13$
a (Å)	14.325(6)
b (Å)	14.325(6)
c (Å)	14.325(6)
α (deg)	90°
β (deg)	90°
γ (deg)	90°
V ($Å^3$)	2940(4)
Z	2
Dcalcd (g/cm3)	1.019
μ(mm^{-1})	1.659 mm^{-1}
F(000)	912
temp (K)	296(2)
Reflections collected	6616
R(int)	0.0473
GOF on F^2	1.057
R1, wR2 [I >2σ(I)]	0.0714, 0.2022
R1, wR2 (all data)	0.0886, 0.2235

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Table S2. Selected bond lengths [Å] and angles [°] for NJMU-001.

Zn(1)-O(2)#1	1.940(6)	Zn(1)-O(2)#2	1.940(6)
Zn(1)-O(2)	1.940(6)	Zn(1)-O(4)	1.983(13)
Zn(2)-O(3)	2.055(13)	Zn(2)-O(3)#1	2.055(13)
Zn(2)-O(3)#2	2.055(13)	Zn(2)-O(1)	2.078(6)
Zn(2)-O(1)#1	2.078(6)	Zn(2)-O(1)#2	2.078(6)
O(1)-C(1)	1.231(10)	O(2)-C(1)	1.303(9)
O(3)-C(4)	1.46(2)	O(3)-H(3A)	0.9300
O(4)-H(4A)	0.8543	C(1)-C(2)	1.496(11)
C(2)-C(3)	1.384(11)	C(2)-C(3)#3	1.396(11)
C(3)-C(2)#4	1.396(11)	C(3)-H(3)	0.9300
C(4)-H(4B)	0.9600	C(4)-H(4C)	0.9600
C(4)-H(4D)	0.9600		
O(2)#1-Zn(1)-O(2)#2	114.97(14)	O(2)#1-Zn(1)-O(2)	114.96(14)
O(2)#2-Zn(1)-O(2)	114.97(14)	O(2)#1-Zn(1)-O(4)	103.17(19)
O(2)#2-Zn(1)-O(4)	103.17(19)	O(2)-Zn(1)-O(4)	103.18(19)
O(3)-Zn(2)-O(3)#2	91.9(7)	O(3)-Zn(2)-O(3)#1	91.9(7)
O(3)#2-Zn(2)-O(3)#1	91.9(7)	O(3)-Zn(2)-O(1)	90.2(5)
O(3)#2-Zn(2)-O(1)	176.5(4)	O(3)#1-Zn(2)-O(1)	85.3(5)
O(3)-Zn(2)-O(1)#2	85.3(5)	O(3)#2-Zn(2)-O(1)#2	90.2(5)
O(3)#1-Zn(2)-O(1)#2	176.5(4)	O(1)-Zn(2)-O(1)#2	92.7(3)
O(3)-Zn(2)-O(1)#1	176.5(4)	O(3)#2-Zn(2)-O(1)#1	85.3(5)
O(3)#1-Zn(2)-O(1)#1	90.2(5)	O(1)-Zn(2)-O(1)#1	92.8(3)
O(1)#2-Zn(2)-O(1)#1	92.7(3)	C(1)-O(1)-Zn(2)	134.7(5)
C(1)-O(2)-Zn(1)	119.6(5)	C(4)-O(3)-Zn(2)	140.1(18)
C(4)-O(3)-H(3A)	110.0	Zn(2)-O(3)-H(3A)	110.0
Zn(1)-O(4)-H(4A)	120.2	O(1)-C(1)-O(2)	125.3(7)
O(1)-C(1)-C(2)	119.0(7)	O(2)-C(1)-C(2)	115.6(7)
C(3)-C(2)-C(3)#3	119.8(8)	C(3)-C(2)-C(1)	119.1(7)
C(3)#3-C(2)-C(1)	121.0(7)	C(2)-C(3)-C(2)#4	120.2(8)
C(2)-C(3)-H(3)	119.9	C(2)#4-C(3)-H(3)	119.9
O(3)-C(4)-H(4B)	109.5	O(3)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5	O(3)-C(4)-H(4D)	109.5
H(4B)-C(4)-H(4D)	109.5	H(4C)-C(4)-H(4D)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -z+1,x+1/2,-y+3/2 #2 y-1/2,-z+3/2,-x+1 #3 z,x,y

#4 y,z,x

Table S3. Comparison between the proposed method and other reported methods for TNP detection.

MOF	Limit of detection (LOD)	Ref.
$Zr_6O_4(OH)_6(L)_6$	2.6 μM	1
$Zr_6O_4(OH)_6(L)_6$	0.4 ppm	2
$[Cd(NDC)(H_2O)]_n$	4 μM	3
$[Zn(NDC)(H_2O)]_n$	1 μM	3
$[Zn_4(DMF)(Ur)_2(NDC)_4]$	1.63 ppm	4
$[Eu_3(L)_3(HCOO)(\mu_3\text{-}OH)_2(H2O)]\cdot x(solv)$	4.98 μM	5
$Zn_4(BTC)_2(OH)_2(CH_3OH)_6$	1.3 μM	This work

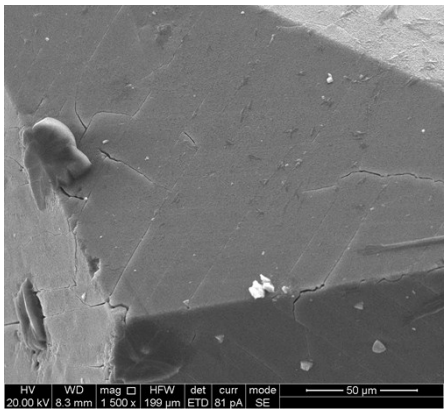

Fig. S1. High magnification SEM of NJMU-001.

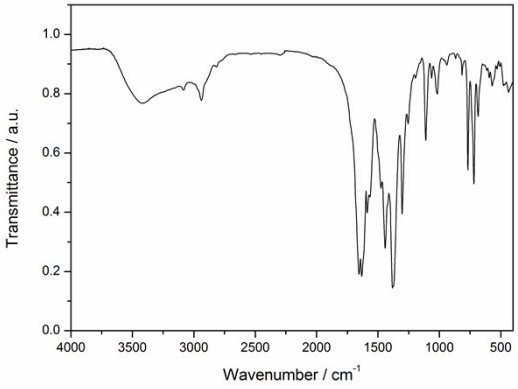

Fig. S2. FT-IR spectrum of NJMU-001.

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