

## SUPPORTING INFORMATION-MOLBANK-214876

**Solvent-mediated synthesis of M(II)-coordination polymer Part 1: Crystal structure of poly(1,2-di(4-pyridyl)ethylene- $k^2N,N'$ )-bis(1,4-benzenediacetato- $k^4O,O',O'',O'''$ )zinc(II)], C<sub>22</sub>H<sub>18</sub>ZnN<sub>2</sub>O<sub>4</sub>**

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Figure S1: Asymmetric unit of 1

Figure S2: Infrared spectrum of 1

Figure S3: Simulated and experimental XRD powder patterns for compound 1

Table S1: Crystallographic data and structural refinement parameters for compound 1,

Table S2: Selected bond distances and bond angles in 1

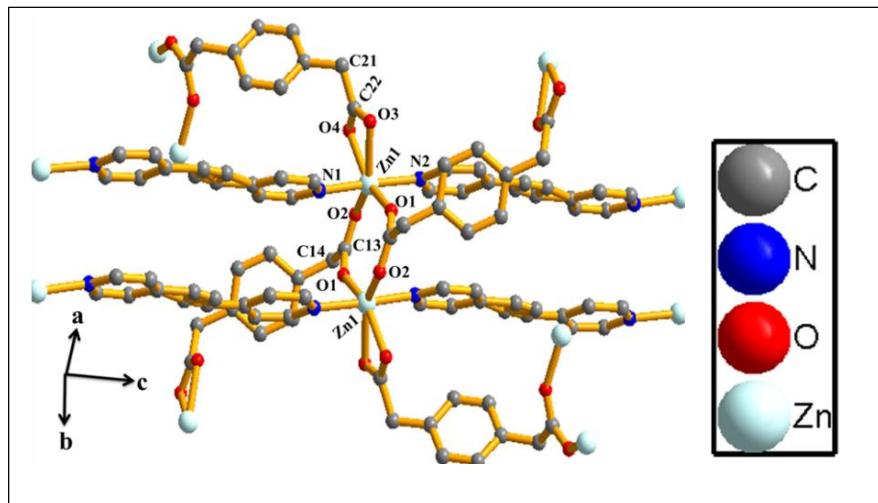


Figure S1: Asymmetric unit of 1.

TABLE S1

**Crystallographic data and structural refinement parameters for compound **1****

| Parameters                               | <b>1</b>  |
|--|---|
| Formula                                  | C <sub>22</sub> H <sub>18</sub> ZnN <sub>2</sub> O <sub>4</sub> |
| Formula weight (mol/g)                   | 439.77  |
| T (K)                                    | 293   |
| Crystal system                           | Monoclinic  |
| Space group                              | P21/n   |
| a (Å)                                    | 10.4566(2)  |
| b (Å)                                    | 13.3085(2)  |
| c (Å)                                    | 13.7189(2)  |
| α (°)                                    | 90  |
| β (°)                                    | 101.491(1)  |
| γ (°)                                    | 90  |
| V (Å <sup>3</sup> )                      | 1870.88(5)  |
| Z  | 4   |
| D <sub>calcd</sub> (g cm <sup>-3</sup> ) | 1.561   |
| λ(Mo K <sub>α</sub> ) (mm)               | 1.346   |
| θ <sub>min</sub> / θ <sub>max</sub> (°)  | 2.2, 26.3   |
| F(000)                                   | 904   |
| Data [I>2σ(I)]                           | 3076  |
| Δρ min/max[e Å <sup>-3</sup> ]           | -1.04, 0.88   |
| R <sub>int</sub>                         | 0.060   |
| R, wR2                                   | 0.0400, 0.1557  |
| Total data                               | 27316   |
| Unique data                              | 3791  |
| GOF                                      | 1.18  |
| Nref, Npar                               | 3791, 280   |

$$R = \sum |F_o| - |Fc| / \sum |F_o|, R_{w2} = [\sum \{w(F_o^2 - F_c^2)^2\} / \sum \{w(F_o^2)\}]^{1/2}$$

TABLE S2

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Selected bond distances ( $\text{\AA}$ ) and angles ( $^{\circ}$ ) for Compound **1**

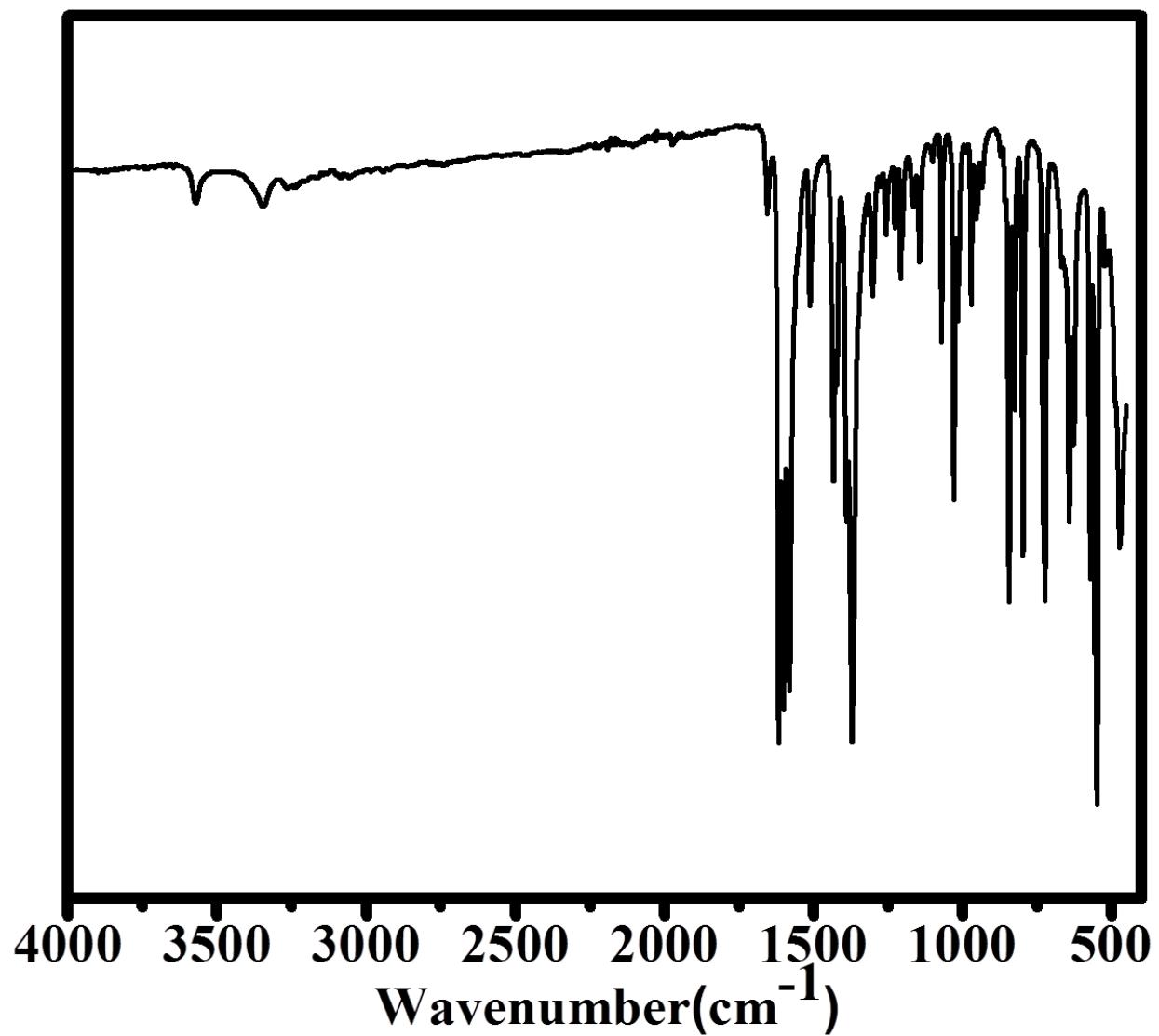
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| <b>Bonds</b> | <b>Angle(<math>^{\circ}</math>)</b> | <b>Bonds</b>  | <b>Angle(<math>^{\circ}</math>)</b> |
|--------------|-------------------------------------|---------------|-------------------------------------|
| O1-Zn1-N1    | 89.26(11)                           | O4_e-Zn1-N1   | 87.01(10)                           |
| O1-Zn1-N2_b  | 83.66(11)                           | O2_d-Zn1-N2_b | 90.31(11)                           |
| O1-Zn1-O2_d  | 121.36(11)                          | O3_e-Zn1-N2_b | 94.69(10)                           |
| O1-Zn1-O3_e  | 89.81(11)                           | O4_e-Zn1-N2_b | 98.12(10)                           |
| O1-Zn1-O4_e  | 147.45(12)                          | O2_d-Zn1-O3_e | 148.80(10)                          |
| N1-Zn1-N2_b  | 172.76(11)                          | O2_d-Zn1-O4_e | 91.18(11)                           |
| O2_d-Zn1-N1  | 94.69(11)                           | O3_e-Zn1-O4_e | 57.64(11)                           |
| O3_e-Zn1-N1  | 83.72(10)                           |               |                                     |

| <b>Bonds</b> | <b>Distances (<math>\text{\AA}</math>)</b> | <b>Bonds</b> | <b>Distance (<math>\text{\AA}</math>)</b> |
|--------------|--|--------------|---|
| Zn1-O1       | 2.020(3)                                   | Zn1-O2_d     | 2.021(2)                                  |
| Zn1-N1       | 2.185(3)                                   | Zn1-O3_e     | 2.384(3)                                  |
| Zn1-N2_b     | 2.172(3)                                   | Zn1-O4_e     | 2.135(3)                                  |

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**Symmetry code:** b = [1556.00] = [1 556] = x, y, 1+z; d = [3656.00] = [3 656] 1-x, -y, 1-z;  
e = [4454.00] = [4 565] = -1/2+x, 1/2-y, -1/2+z



**Figure S2:** Infrared spectra of compound in the range of  $4000\text{ cm}^{-1}$  to  $400\text{ cm}^{-1}$ .

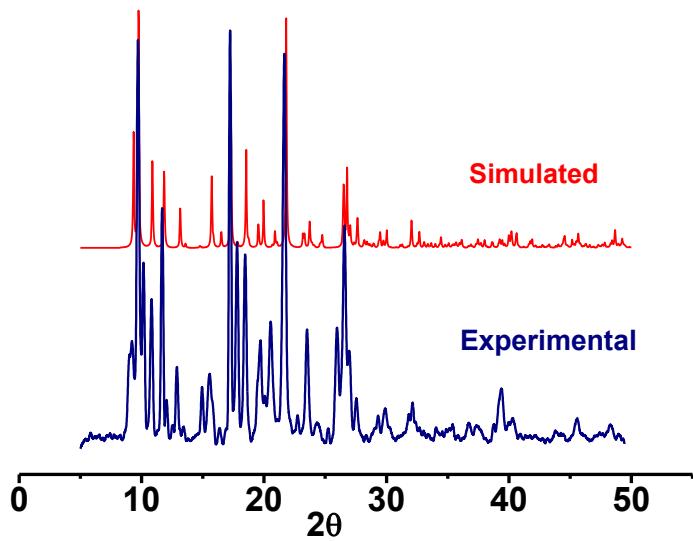


Figure S3. Powder x-ray diffraction pattern of compound 1