

Supporting materials

Syntheses, structures and properties of two zinc coordination polymers based on bis(triazole) and sulfoisophthalicate

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Table S1 Selected bond lengths (Å) and angles (°) for **1** and **2**.

| 1 | | | |
|-------------------|------------|-------------------|------------|
| Zn(1)-O(1) | 1.996(3) | Zn(1)-O(2B) | 2.015(3) |
| Zn(1)-O(3A) | 1.962(3) | Zn(1)-N(3) | 2.133(4) |
| Zn(1)-N(6) | 2.123(4) | Zn(2)-O(8) | 2.146(3) |
| Zn(2)-O(9) | 2.111(3) | Zn(2)-N(9) | 2.113(4) |
| O(1)-Zn(1)-O(2B) | 133.97(14) | O(3A)-Zn(1)-O(1) | 126.23(15) |
| O(3A)-Zn(1)-O(2B) | 99.76(14) | O(1)-Zn(1)-N(3) | 88.29(15) |
| O(2B)-Zn(1)-N(3) | 91.34(15) | O(3A)-Zn(1)-N(3) | 93.13(16) |
| O(1)-Zn(1)-N(6) | 88.66(15) | O(2B)-Zn(1)-N(6) | 88.92(15) |
| O(3A)-Zn(1)-N(6) | 90.75(16) | N(6)-Zn(1)-N(3) | 176.01(17) |
| O(8C)-Zn(2)-O(8) | 180.000(1) | O(9)-Zn(2)-O(9C) | 180.000(1) |
| N(9)-Zn(2)-N(9C) | 180.0(3) | O(9)-Zn(2)-O(8) | 91.53(16) |
| N(9)-Zn(2)-O(8) | 91.30(15) | O(9)-Zn(2)-N(9) | 91.77(15) |
| 2 | | | |
| Zn(1)-O(8) | 2.144(4) | Zn(1)-O(9) | 2.101(4) |
| Zn(1)-N(3) | 2.113(5) | Zn(2)-O(1) | 1.952(4) |
| Zn(2)-O(2B) | 2.033(4) | Zn(2)-O(3C) | 2.036(4) |
| Zn(2)-O(4C) | 2.342(4) | Zn(2)-N(6) | 2.028(5) |
| O(8)-Zn(1)-O(8A) | 180.0 | O(9)-Zn(1)-O(9A) | 180.00(12) |
| N(3)-Zn(1)-N(3A) | 180.0(3) | O(9)-Zn(1)-O(8) | 88.43(19) |
| N(3)-Zn(1)-O(8) | 89.04(18) | O(9)-Zn(1)-N(3) | 89.90(18) |
| O(1)-Zn(2)-O(2B) | 102.07(15) | O(1)-Zn(2)-O(3C) | 139.32(17) |
| O(1)-Zn(2)-O(4C) | 87.95(15) | O(2B)-Zn(2)-O(3C) | 102.35(16) |
| O(2B)-Zn(2)-O(4C) | 92.25(16) | O(3C)-Zn(2)-O(4C) | 59.09(15) |
| O(1)-Zn(2)-N(6) | 113.35(18) | N(6)-Zn(2)-O(2B) | 98.95(18) |
| N(6)-Zn(2)-O(3C) | 94.28(18) | N(6)-Zn(2)-O(4C) | 152.91(17) |

Symmetry transformations used to generate equivalent atoms: A $x-1, y, z$; B $-x+2, -y+2, -z+2$; C $-x+1, -y+1, -z+1$ for **1**; A $-x+3, -y+2, -z$; B $-x+1, -y, -z+1$; C $x+1, y, z$ for **2**.

Table S2 Hydrogen bonds (Å and °) for **1**.

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---------------------------------|-----------|----------|-----------|--------|
| O(8)-H(1W)...O(10) | 0.897(19) | 1.84(2) | 2.739(6) | 176(5) |
| O(8)-H(2W)...O(4) ⁱ | 0.890(19) | 1.94(2) | 2.825(5) | 172(5) |
| O(9)-H(3W)...O(7) | 0.893(19) | 2.12(2) | 2.992(7) | 165(5) |
| O(9)-H(4W)...O(11) | 0.891(19) | 1.87(3) | 2.717(11) | 157(6) |
| O(10)-H(5W)...O(7) | 0.89(2) | 1.89(2) | 2.751(6) | 161(5) |
| O(10)-H(6W)...O(7) ⁱ | 0.89(2) | 2.32(4) | 3.107(7) | 146(5) |

Symmetry transformations used to generate equivalent atoms: i $-x+2, -y+1, -z+1$.

Table S3 Hydrogen bonds (Å and °) for **2**.

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|----------------------------------|-----------|----------|----------|--------|
| O(8)-H(1W)...O(6) ⁱ | 0.890(19) | 1.86(2) | 2.748(7) | 172(5) |
| O(8)-H(2W)...O(5) ⁱⁱ | 0.885(19) | 1.89(3) | 2.769(7) | 170(7) |
| O(9)-H(3W)...O(4) ⁱⁱⁱ | 0.897(19) | 1.88(2) | 2.776(6) | 176(6) |
| O(9)-H(4W)...O(10) ⁱ | 0.89(2) | 1.94(3) | 2.782(9) | 159(6) |

Symmetry transformations used to generate equivalent atoms: i $-x+2, -y+1, -z+1$; ii $x+2, y+1, z-1$; iii $-x+1, -y+1, -z+1$.

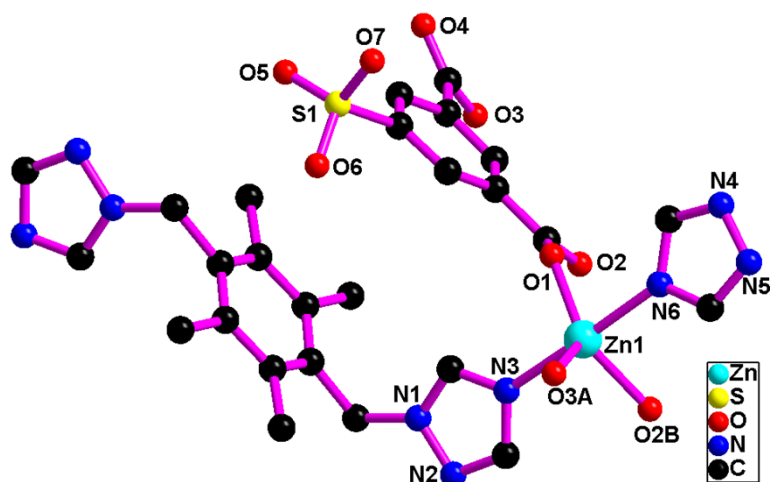


Fig. S1 The coordination environment of the Zn(II) atom in the first motif $[Zn_2(tmtz)_2(sip)_2]_n$ of **1**.

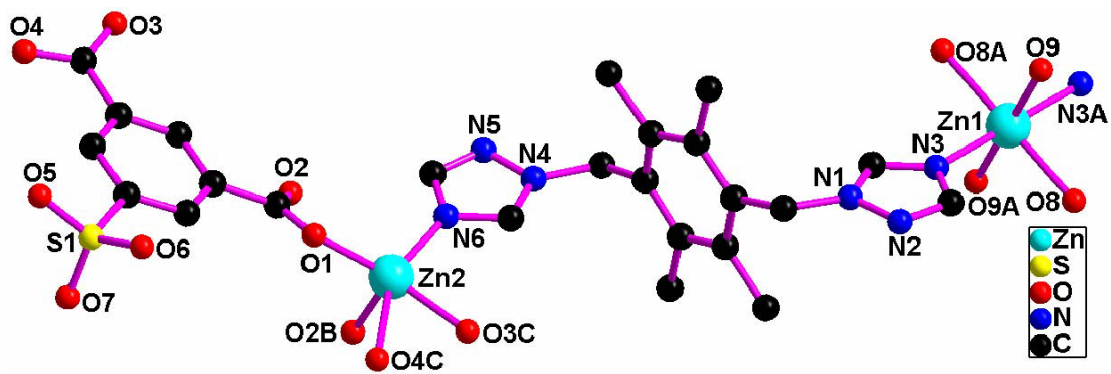


Fig. S2 The coordination environment of the Zn(II) atoms of **2**.

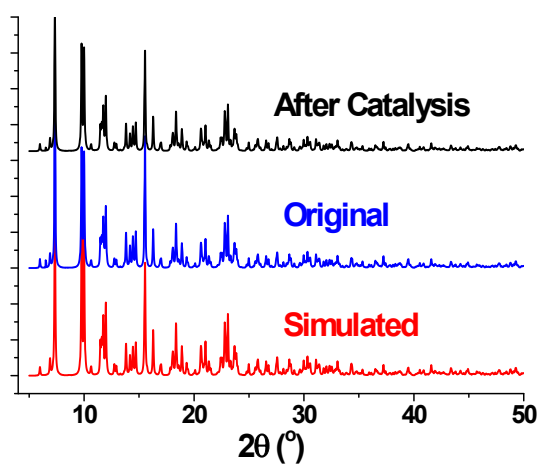


Fig. S3 PXRD patterns of the simulated diagram from single crystal data of compound **1** (red), **1** (blue) and **1** after catalysis process (black).

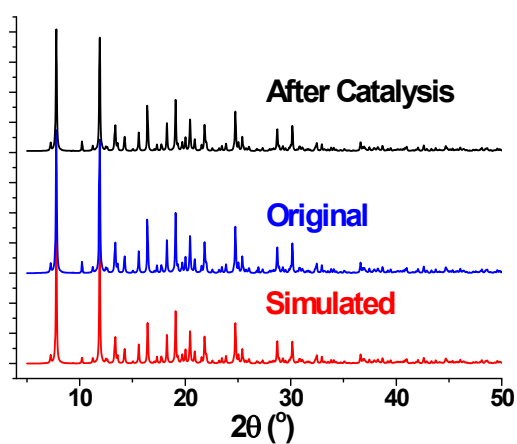


Fig. S4 PXRD patterns of the simulated diagram from single crystal data of compound **2** (red), **2** (blue) and **2** after catalysis process (black).

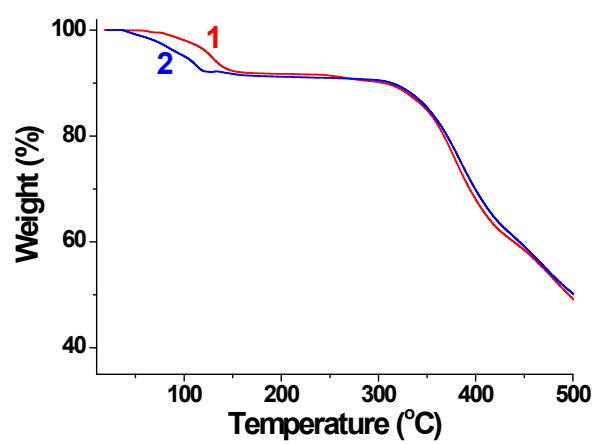


Fig. S5 The TG curves of compounds 1 and 2.