# Electronic Supplementary Information for:

# Two Ligand-Length-Tunable Interpenetrating Coordination Networks with Stable $Zn_2$ Unit as Three-connected Uninode and Supramolecular Topologies

Guohai Xu,*[,a] Jianyi Lv,[a] Peng Guo,[b] Zhonggao Zhou,[a] Ziyi Du[a] and Yongrong Xie*[,a]

[a]Key Laboratory of Jiangxi University for Functional Materials Chemistry, School of Chemistry and Chemical Engineering, Gannan Normal University, Ganzhou, Jiangxi 341000, People's Republic of China

[b]Inorganic and Structural Chemistry and Berzelii Center EXSELENT on Porous Materials, Department of Materials and Environmental Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden

E-mail: xugh308@gmail.com;yongrongxie@yahoo.com.cn

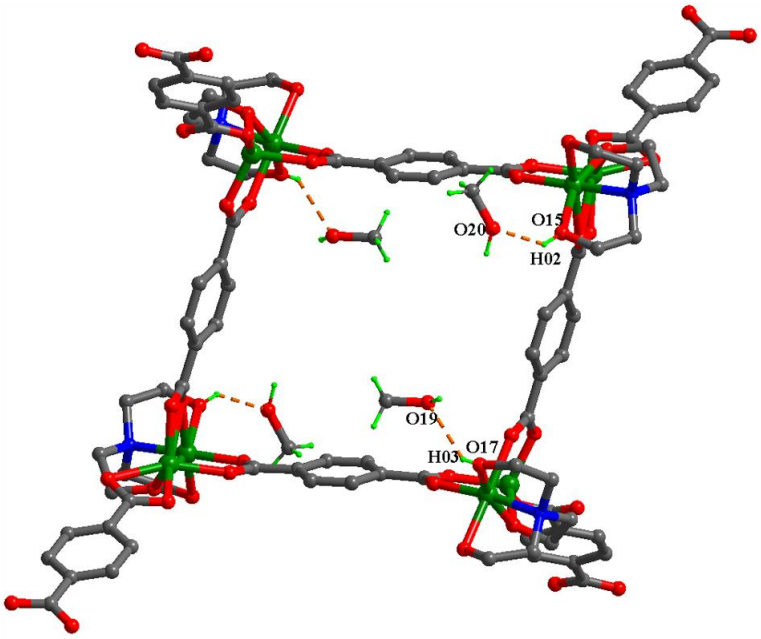



Figure **S1**. A cavity of the square 4-ring window trapping four methanol molecules through hydrogen bonds compound **1**.

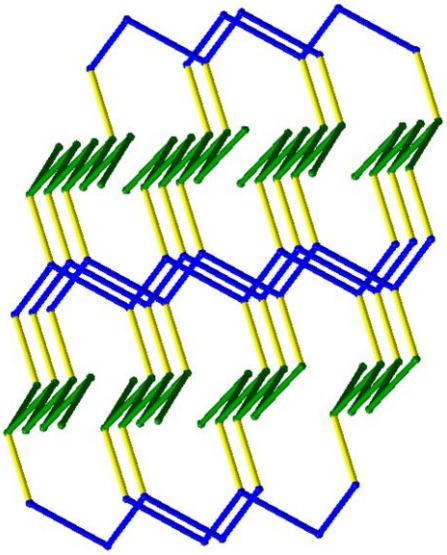
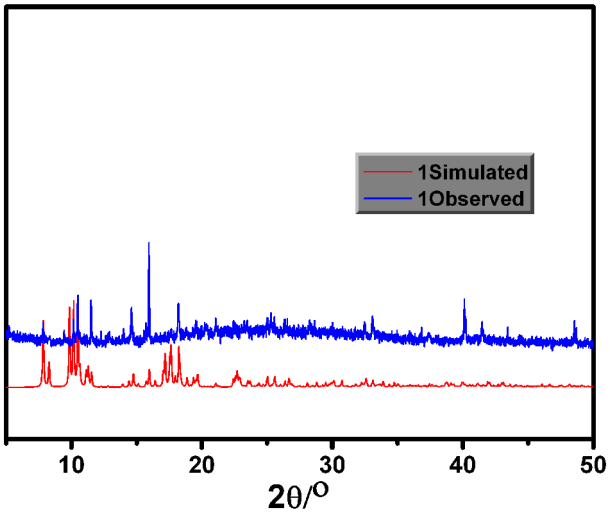


Figure **S2**. A discrete $10^3$-**ths** net showing that zigzag chains (green and blue) are crosslinked at 55.2° to each other in compound **2**.

Powder X-ray diffraction data were collected using a Bruker D8 Advance (Cu Kα1 radiation, λ=1.5406 Å).



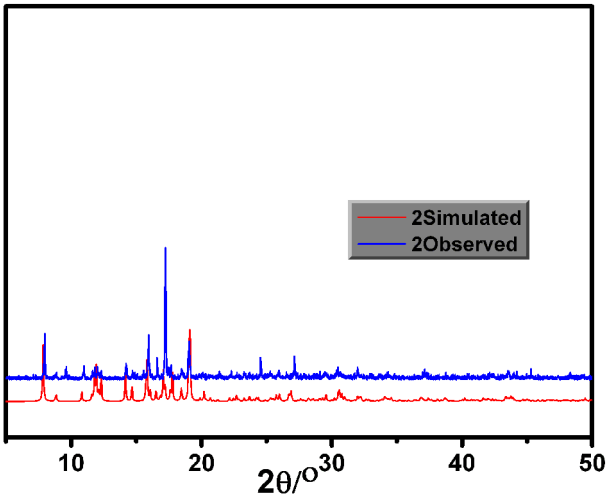



Figure **S3**. Calculated and observed powder X-ray diffraction patterns of **1**-**2**.

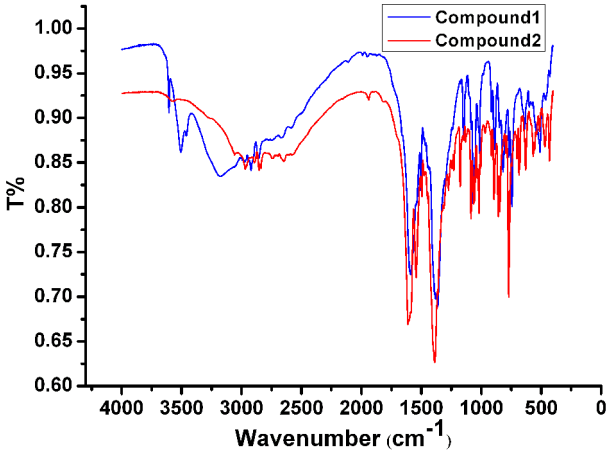



Figure **S4**. The infrared spectra of **1** and **2**.

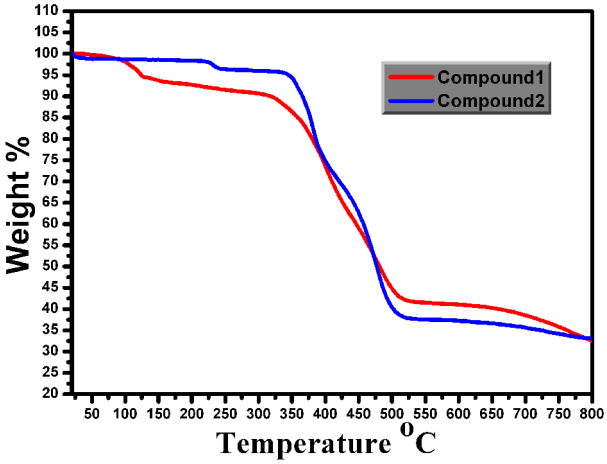
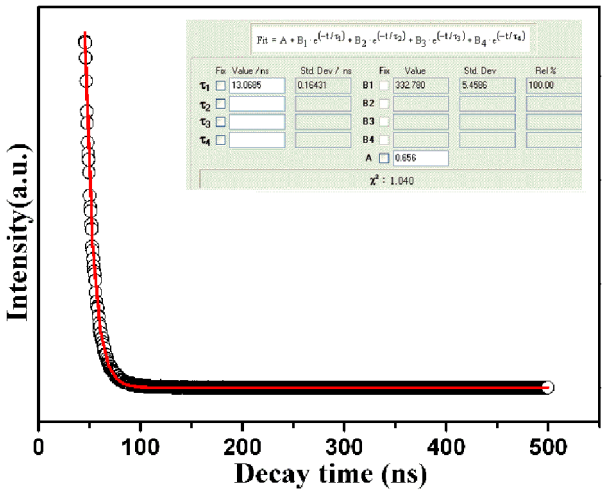
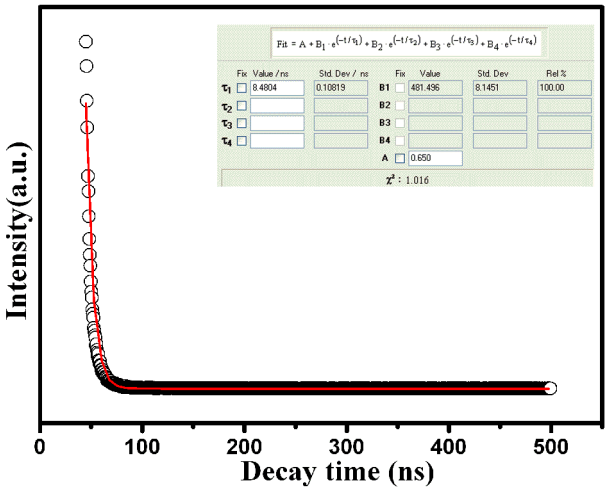



Figure **S5**. Thermogravimetric analyses of samples **1** and **2**.




a




b

Figure **S6**. Fitted decay curves for **1** (a) and **2** (b) in the solid state at room temperature (the black circles represent experimental data, and the solid red lines represent fitting results).

**Topological Analysis for 1 by TOPOS program**

#######
1: $C_{38}H_{48}N_2O_{40}Zn_4$
#######

Atom coordinates (C = the centriods of $bdc^{2-}$ ligands, Zn1/Zn2 = the centriods of $Zn_2$ cluster)

Topology for Zn1
---
Atom Zn1 links by bridge ligands and has

Common vertex with R(A-A) f

Zn 2 0.3091 -0.4357 0.5682 ( 0-1 0) 10.642A 1

Zn 2 0.6909 0.4357 1.4318 ( 1 1 2) 10.714A 1

Zn 1 -1.0127 -0.2634 1.0778 (-1 0 2) 13.623A 1

Topology for Zn2

---

Atom Zn2 links by bridge ligands and has

Common vertex with R(A-A) f

Zn 1 0.0127 1.2634 0.9222 ( 0 1 0) 10.642A 1

Zn 1 0.9873 0.7366 1.0778 ( 1 1 2) 10.714A 1

Zn 2 -0.3091 -0.5643 0.4318 ( 0 0 1) 13.331A 1

---

Structural group analysis

---

---

Structural group No 1

---

Structure consists of layers ( 0 1-2) with Zn2C3

Coordination sequences

---

Zn1: 1 2 3 4 5 6 7 8 9 10

Num 3 5 8 11 13 16 19 21 24 27

Cum 4 9 17 28 41 57 76 97 121 148

Rad 11.7(1.7) 18.3(2.7) 25.4(3.3) 32.2(3.5) 39.9(4.7) 48.2(4.8) 55.3(4.9) 62.8(5.9) 71.2(6.4) 78.8(6.4)

Cmp Zn3 Zn5 Zn8 Zn11 Zn13 Zn16 Zn19 Zn21 Zn24 Zn27

---

Zn2: 1 2 3 4 5 6 7 8 9 10

Num 3 5 8 11 13 16 19 21 24 27

Cum 4 9 17 28 41 57 76 97 121 148

Rad 11.6(1.5) 18.9(1.5) 25.2(3.1) 31.9(4.3) 40.4(4.4) 48.1(4.2) 55.0(5.7) 63.3(6.0) 71.2(5.6) 78.4(7.0)

Cmp Zn3 Zn5 Zn8 Zn11 Zn13 Zn16 Zn19 Zn21 Zn24 Zn27

---

TD10=148

Vertex symbols for selected sublattice

---

Zn1 Point symbol:{4.8^2}

Extended point symbol:[4.8.8]

---

Zn2 Point symbol:{4.8^2}

Extended point symbol:[4.8.8]

---

Point symbol for net: {4.8^2}

3-c net; uninodal net

Topological type: fes; Shubnikov plane net (4.8^2) (topos&RCSR.ttd) {4.8^2} - VS [4.8.8] (72524 types in 11 databases)

Elapsed time: 14.19 sec.

## Supramolecular Topological Analysis for 1 by TOPOS program

########

1: $C_{38}H_{48}N_2O_{40}Zn_4$

########

Atom coordinates (C = the centriods of $bdc^{2-}$ ligands or the midpoints of two $Zn_2$ cluster with H-bonding interactions, Zn1/Zn2 = the centriods of $Zn_2$ cluster)

Topology for Zn1

---

Atom Zn1 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | f |
|---|---|---|---|---|---|---|
| Zn 1 | -0.0127 | 0.7366 | 1.0778 | ( 0 1 2) | 5.645A | 1 |
| Zn 2 | 0.3091 | -0.4357 | 0.5682 | ( 0-1 0) | 10.642A | 1 |
| Zn 2 | 0.6909 | 0.4357 | 1.4318 | ( 1 1 2) | 10.714A | 1 |
| Zn 1 | -1.0127 | -0.2634 | 1.0778 | (-1 0 2) | 13.623A | 1 |

Topology for Zn2

---

Atom Zn2 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | f |
|---|---|---|---|---|---|---|
| Zn 2 | 0.6909 | 0.4357 | 0.4318 | ( 1 1 1) | 5.698A | 1 |
| Zn 1 | 0.0127 | 1.2634 | 0.9222 | ( 0 1 0) | 10.642A | 1 |
| Zn 1 | 0.9873 | 0.7366 | 1.0778 | ( 1 1 2) | 10.714A | 1 |
| Zn 2 | -0.3091 | -0.5643 | 0.4318 | ( 0 0 1) | 13.331A | 1 |

---

Structural group analysis

---

---

Structural group No 1

---

Structure consists of 3D framework with ZnC2

There are 2 interpenetrating nets

FIV: Full interpenetration vectors

---
[1,0,0] (11.30A)
[0,1,0] (11.73A)
[0,0,1] (19.51A)
[1,1,1] (19.82A)
[1,-1,-1] (25.54A)
[1,-1,1] (26.76A)
[1,1,-1] (28.67A)
---
PIC: [2,0,0][1,1,0][0,1,1] (PICVR=2)

Zt=2; Zn=1

Class Ia Z=2

Coordination sequences
---
Zn1: 1 2 3 4 5 6 7 8 9 10
Num 4 11 24 41 62 90 122 157 200 247
Cum 5 16 40 81 143 233 355 512 712 959
Rad 10.2(3.3) 16.0(3.2) 21.8(4.9) 28.0(5.7) 34.3(6.8) 40.9(7.9) 47.3(8.9) 53.7(10.0) 60.4(11.1) 67.0(12.1)
Cmp Zn4 Zn11 Zn24 Zn41 Zn62 Zn90 Zn122 Zn157 Zn200 Zn247
---
Zn2: 1 2 3 4 5 6 7 8 9 10
Num 4 11 24 41 62 90 122 157 200 247
Cum 5 16 40 81 143 233 355 512 712 959
Rad 10.1(3.2) 16.3(3.1) 21.7(4.8) 27.9(5.9) 34.5(6.8) 40.8(7.8) 47.2(8.9) 53.9(10.0) 60.4(11.0) 66.8(12.2)
Cmp Zn4 Zn11 Zn24 Zn41 Zn62 Zn90 Zn122 Zn157 Zn200 Zn247
---
TD10=959

Vertex symbols for selected sublattice
---
Zn1 Point symbol:{4.6^5}
Extended point symbol:[4.6(2).6.6.6.6]
---
Zn2 Point symbol:{4.6^5}
Extended point symbol:[4.6(2).6.6.6.6]
---
Point symbol for net: {4.6^5}
4-c net; uninodal net

Topological type: crb/BCT; 4/4/t5; sqc184 (topos&RCSR.ttd) {4.6^5} - VS [4.6(2).6.6.6.6] (72524 types in 11 databases)

Elapsed time: 22.00 sec.

## Topological Analysis for 2 by TOPOS program

############
2: $C_{27}H_{26}NO_9Zn_2$
############

Atom coordinates (C = the centriods of $bpdc^{2-}$ ligands, Zn1 = the centriod of $Zn_2$ cluster)

Topology for Zn1
---
Atom Zn1 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | f |
|---|---|---|---|---|---|---|
| Zn 1 | 0.1768 | 0.9293 | -0.1404 | ( 1 0 0) | 15.161A | 1 |
| Zn 1 | 1.1768 | 0.0707 | 1.3596 | ( 2 1 2) | 15.220A | 1 |
| Zn 1 | 1.1768 | 1.0707 | 0.3596 | ( 2 2 1) | 15.230A | 1 |

---
Structural group analysis
---

---
Structural group No 1
---
Structure consists of 3D framework with ZnC3
There are 8 interpenetrating nets
FIV: Full interpenetration vectors
---
[1/2,1/2,0] (15.86A)
[1/2,-1/2,0] (15.86A)
---
PIC: [4,4,0][0,1,-1][2,0,1] (PICVR=8)

Zt=8; Zn=1

Class Ia Z=8

Coordination sequences
---

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Zn1: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Num | 3 | 6 | 12 | 24 | 38 | 56 | 77 | 102 | 129 | 160 |
| Cum | 4 | 10 | 22 | 46 | 84 | 140 | 217 | 319 | 448 | 608 |

---

TD10=608

Vertex symbols for selected sublattice

---

Zn1 Point symbol:{10^3}

Extended point symbol:[10(2).10(4).10(4)]

---

Point symbol for net: {10^3}

3-c net; uninodal net

Topological type: ths ThSi2; 3/10/t4 (topos&RCSR.ttd) {10^3} - VS [10(2).10(4).10(4)] (72524 types in 11 databases)

Elapsed time: 7.62 sec.

## Supramolecular Topological Analysis for 2 by TOPOS program

############

2: $C_{27}H_{26}NO_9Zn_2$

############

Atom coordinates (C = the centriods of $bpdc^{2-}$ ligands or the midpoints of two $Zn_2$ cluster with H-bonding interactions, Zn1 = the centriod of $Zn_2$ cluster)

Topology for Zn1

---

Atom Zn1 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | f |
|---|---|---|---|---|---|---|
| Zn 1 | 0.6965 | 0.4471 | 0.3407 | ( 1 0 1) | 6.965A | 1 |
| Zn 1 | 0.6965 | -0.4471 | 0.8407 | ( 1-1 1) | 8.557A | 1 |
| Zn 1 | 0.6965 | 0.5529 | 0.8407 | ( 1 0 1) | 8.557A | 1 |
| Zn 1 | 0.1965 | 0.0529 | -0.1593 | ( 1 0 0) | 14.867A | 1 |
| Zn 1 | 1.1965 | -1.0529 | 1.3407 | ( 2-1 2) | 16.832A | 1 |
| Zn 1 | 1.1965 | -0.0529 | 0.3407 | ( 2 0 1) | 16.996A | 1 |

---

Structural group analysis

---

---

Structural group No 1

---

Structure consists of 3D framework with ZnC3

Coordination sequences

---

| Zn1: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Num | 6 | 30 | 92 | 210 | 350 | 534 | 754 | 1020 | 1317 | 1660 |
| Cum | 7 | 37 | 129 | 339 | 689 | 1223 | 1977 | 2997 | 4314 | 5974 |

Rad 12.1(4.6) 18.8(5.7) 26.2(7.3) 35.3(7.9) 45.1(8.6) 55.6(8.6) 65.6(9.6) 76.1(10.0) 86.2(11.0) 96.8(11.6)

Cmp Zn6 Zn30 Zn92 Zn210 Zn350 Zn534 Zn754 Zn1020 Zn1317 Zn1660

---

TD10=5974

Vertex symbols for selected sublattice

---

Zn1 Point symbol:{6^15}

Extended point symbol:[6(2).6(2).6(3).6(3).6(3).6(3).6(3).6(4).6(5).6(6).6(7).6(7).6(8).6(8).6(8)]

---

Point symbol for net: {6^15}

6-c net; uninodal net

New topology, please, contact the authors (72524 types in 11 databases)

Elapsed time: 12.59 sec.