Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Zn-MOFs Containing Flexible α,ω-Alkane (or alkene)-dicarboxylates with 1,2-Bis(4-pyridyl)ethylene: Comparison with Zn-MOFs Containing 1,2-Bis(4-pyridyl)ethane Ligands

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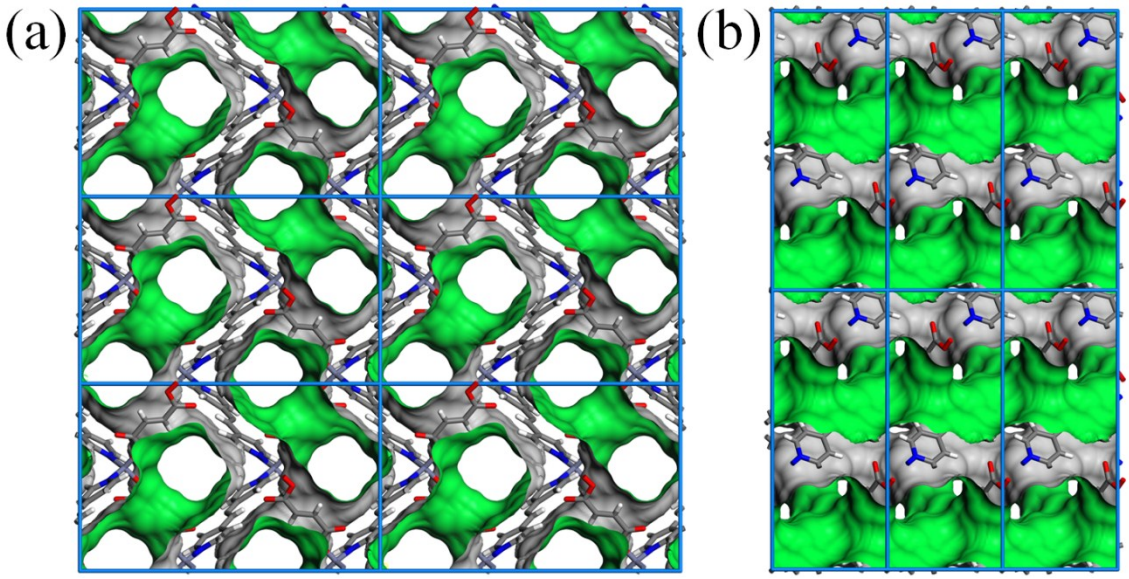

Fig. S1. Connolly surface of solvent-free **3-bpe** generated using the probe radius of 1.4 Å shown along *a*-axis (a) and *c*-axis (b). Grey and green colors indicate the exterior and interior surfaces, respectively.

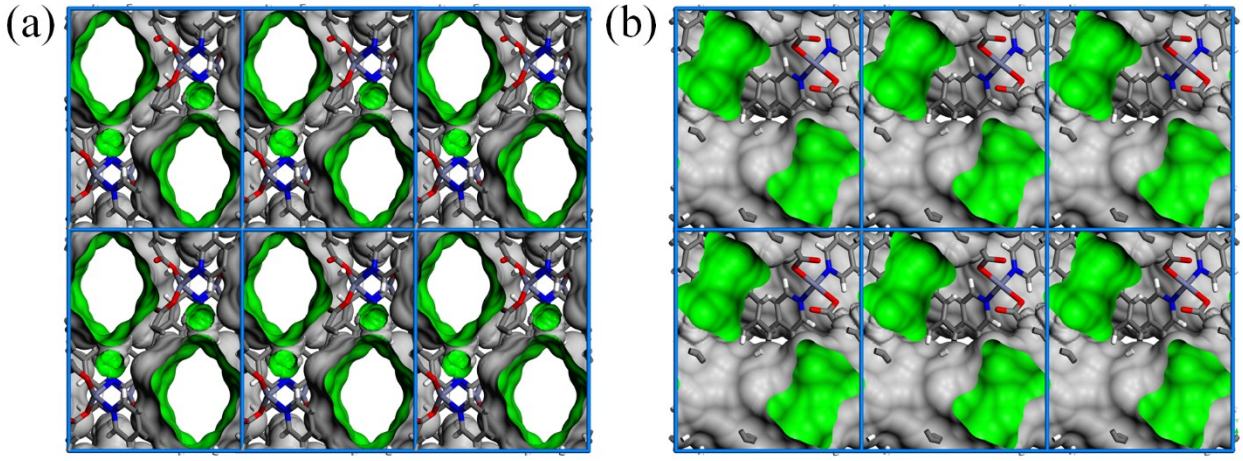

Fig. S2. Connolly surface of solvent-free **6-bpe** generated using the probe radius of 1.4 Å shown along *c*-axis (a) and *a*-axis (b).

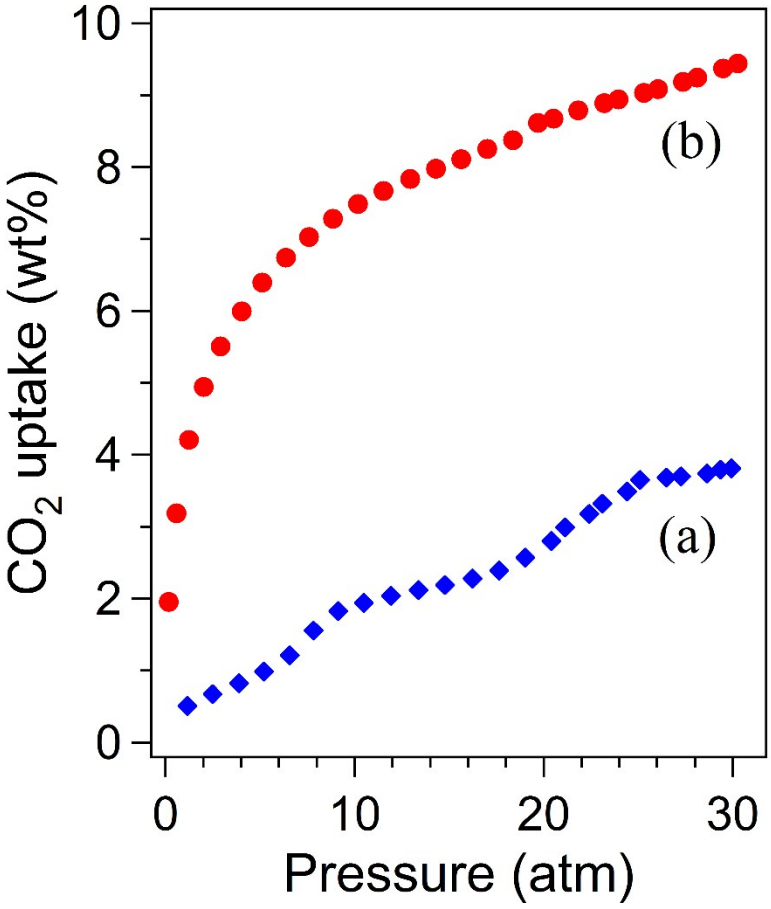

Fig. S3. High-pressure CO_2 adsorption isotherms for **3-bpe** (a) and **6-bpe** (b) at 273 K.

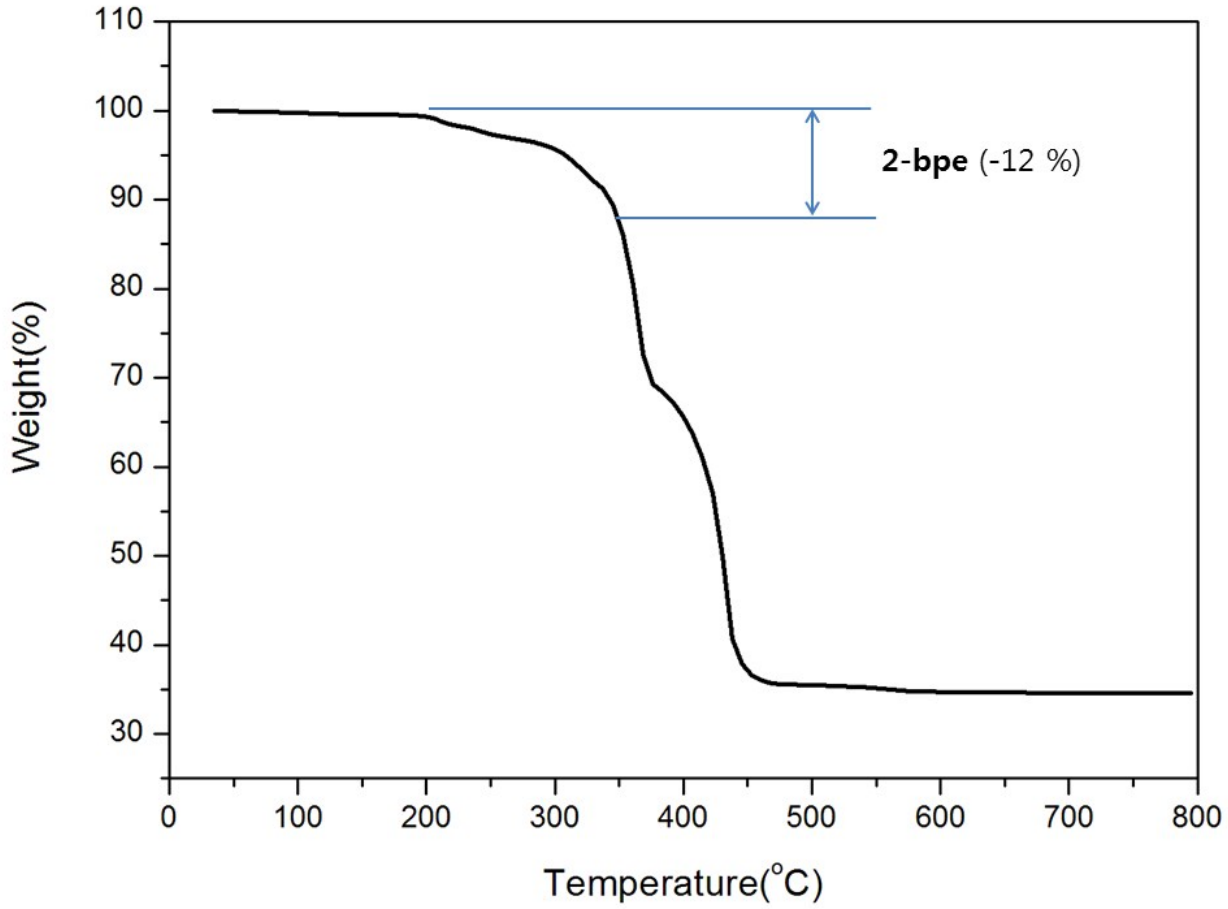

Fig. S4. TGA profile for compound **2-bpe**.

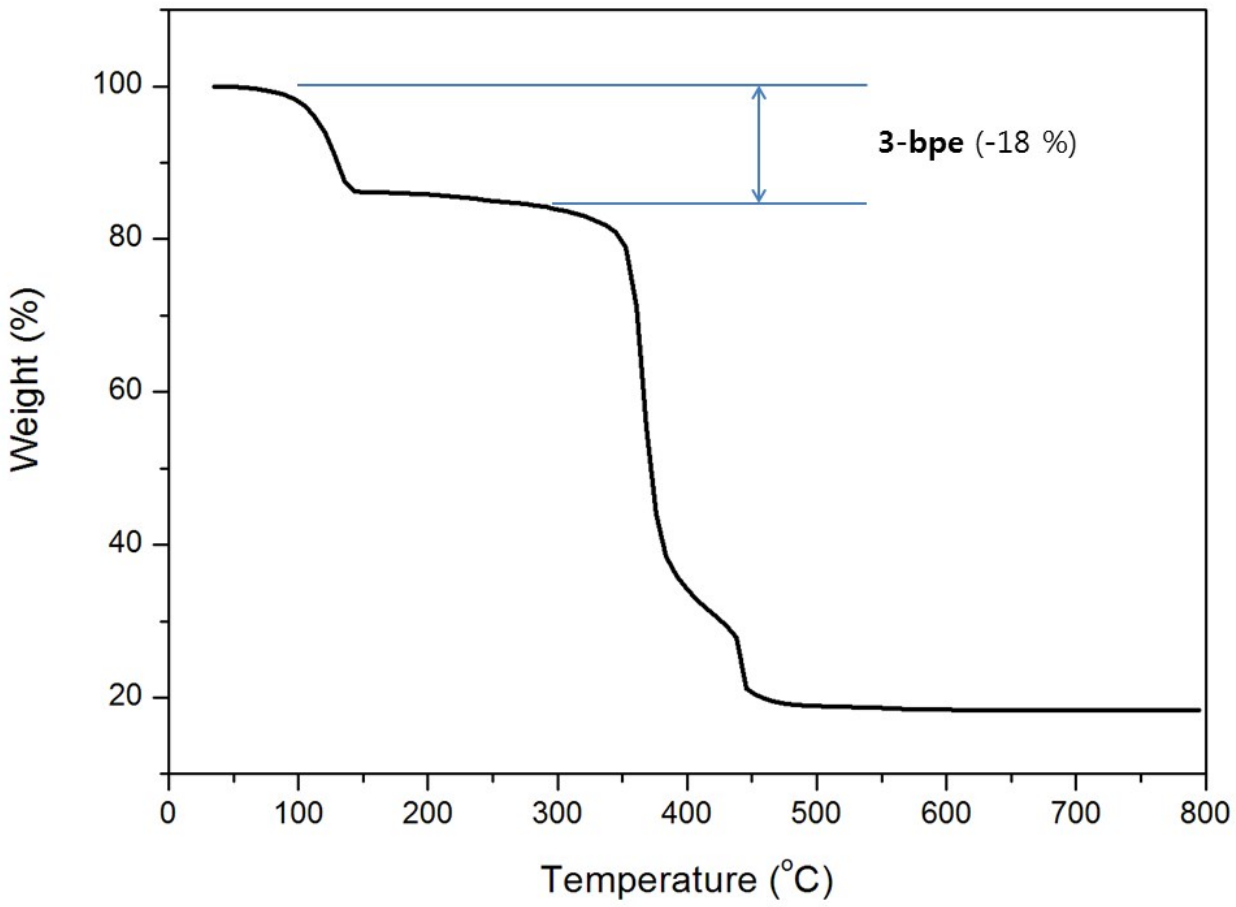

Fig. S5. TGA profile for compound **3-bpe**.

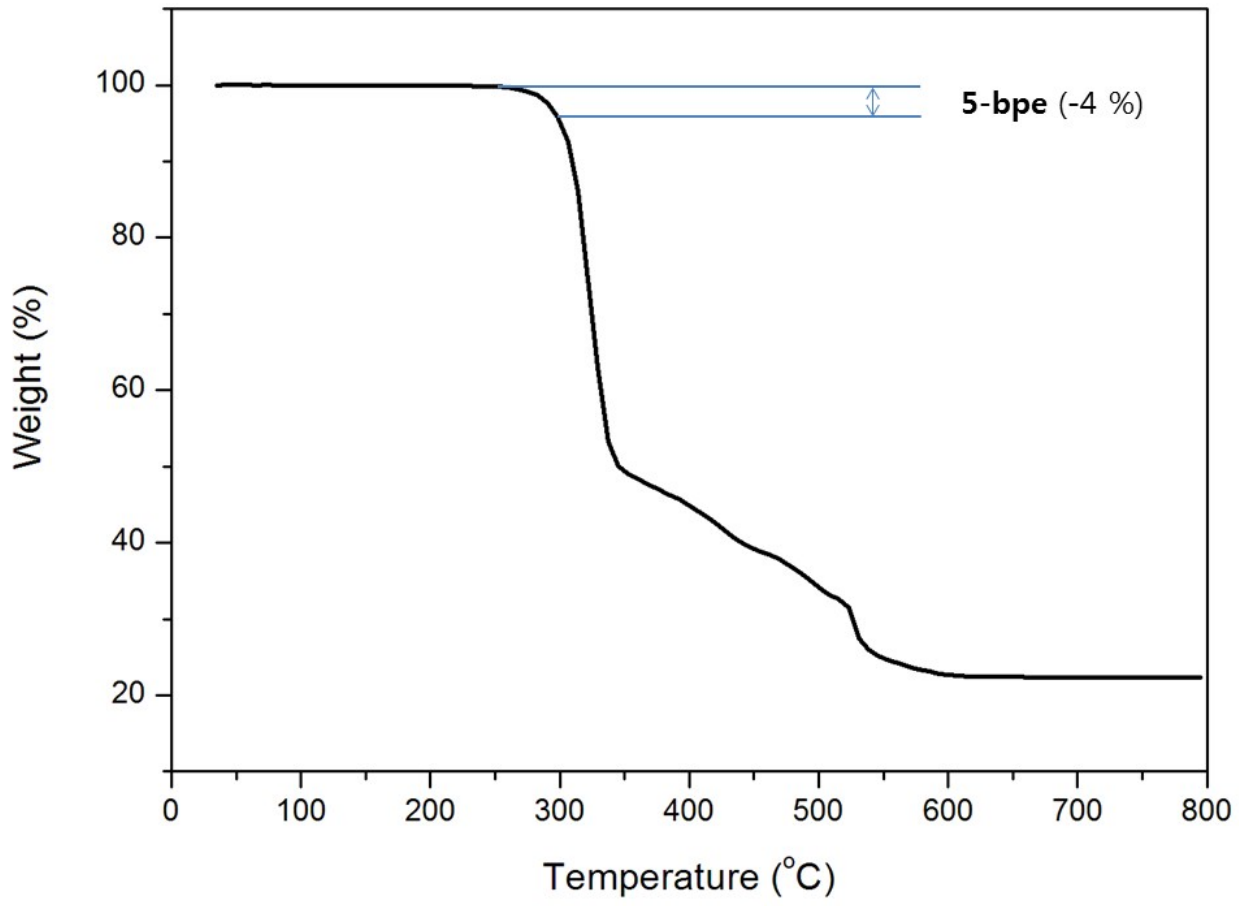

Fig. S6. TGA profile for compound **5-bpe**.

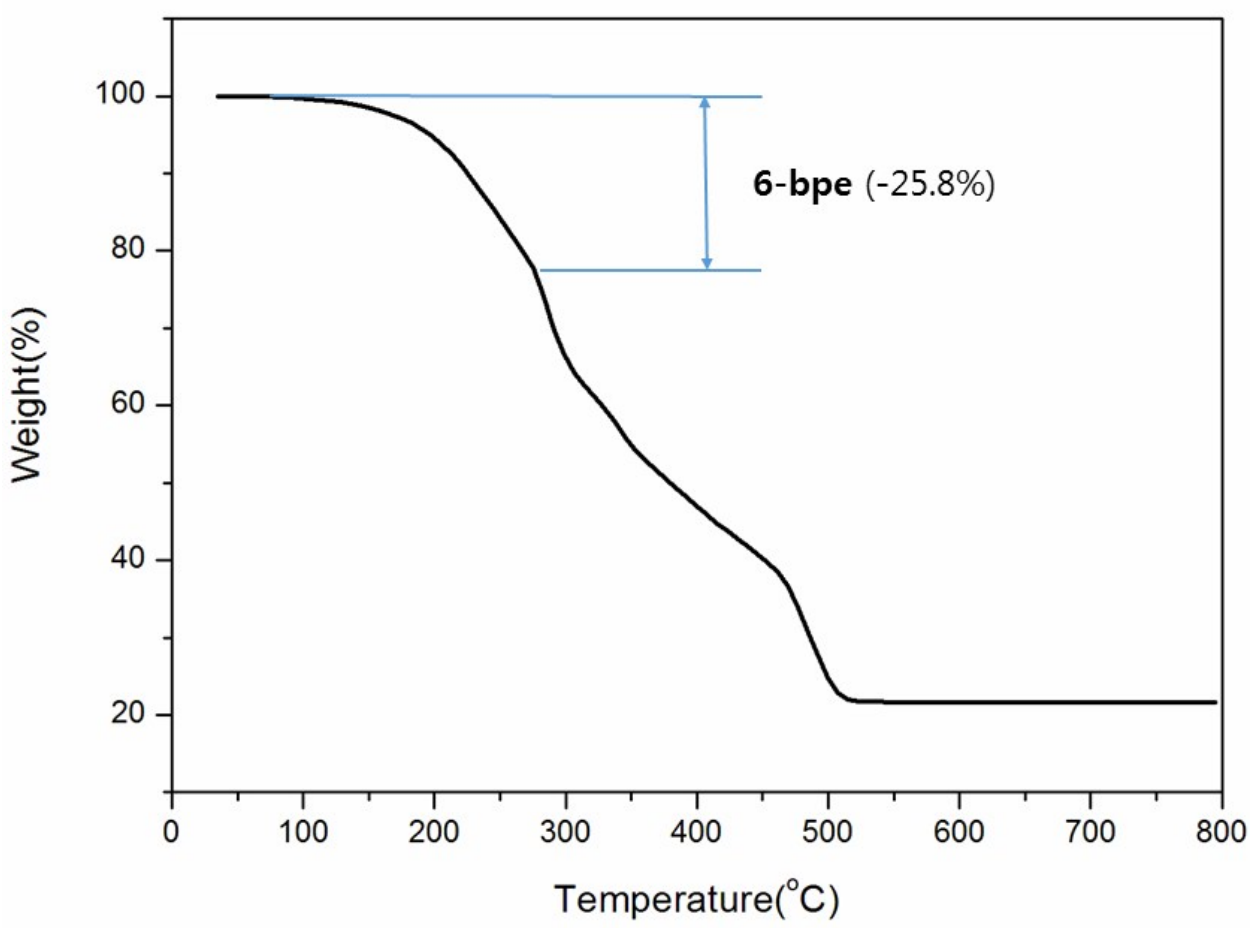

Fig. S7. TGA profile for compound **6-bpe**.

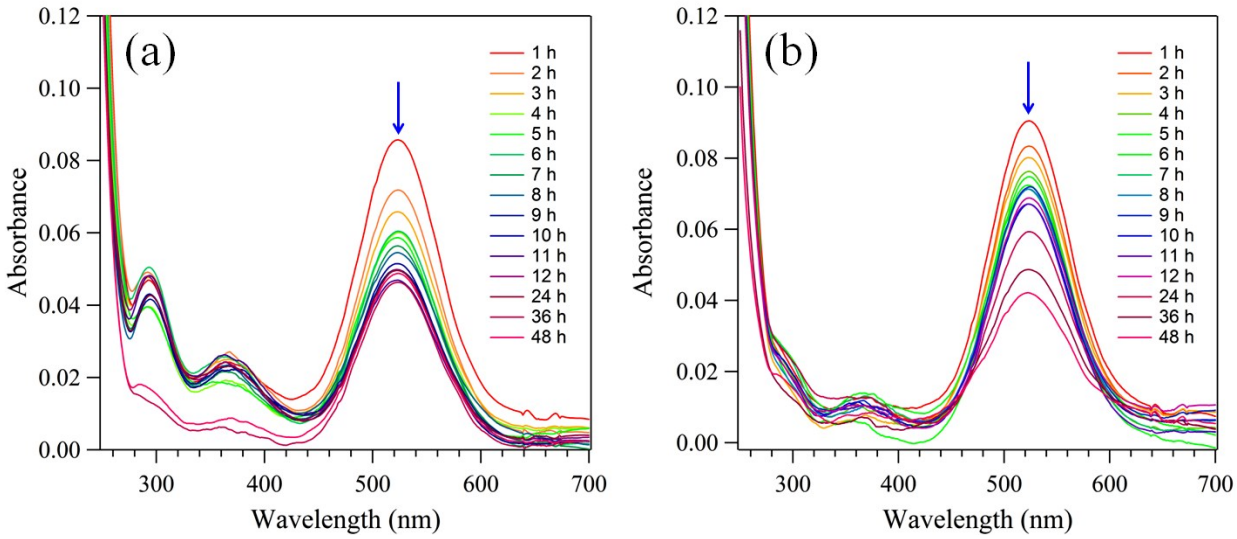

Fig. S8. UV/Vis spectral changes during the encapsulation of iodine by **3-bpe** (a) and **6-bpe** (b).

Table S1. The topology analysis results by ToposPro for **2-bpe**.

```
####################
5:C20 H16 N2 O8 Zn2
####################

Topology for V1
--------------------
Atom V1 links by bridge ligands and has
Common vertex with                    R(A-A)       f
V  1    1.4626    0.6980    1.4361   ( 1 0 1)    16.553A       1
V  1   -0.5374    0.6980   -0.5639   (-1 0-1)    16.553A       1
Common edge with                      R(A-A)
V  1    0.5374    0.3020    0.5639   ( 1 1 1)     5.639A       2
V  1    0.5374    1.3020    0.5639   ( 1 2 1)     8.286A       2
-------------------------
Structural group analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of layers ( 1 0-1) with VTiSc2
Num. groups=2; Thickness=4.53; Min.Distance=4.982

Coordination sequences
----------------------
V1:  1  2  3  4  5  6   7   8   9  10
Num  4  8 12 16 20 24  28  32  36  40
Cum  5 13 25 41 61 85 113 145 181 221
----------------------
TD10=221

Vertex symbols for selected sublattice
--------------------------------------
V1 Point symbol:{4^4.6^2}
Extended point symbol:[4.4.4.4.6(2).6(2)]
--------------------------------------
Point symbol for net: {4^4.6^2}
4-c net; uninodal net

Topological type: sql/Shubnikov tetragonal plane net (topos&RCSR.ttd) {4^4.6^2} - VS [4.4.4.4.*.*] (17092 types
in 3 databases)
Elapsed time: 7.11 sec.
```

Table S2. The topology analysis results by ToposPro for **3-bpe**.

```
####################
1:C16 H12 N2 O4.50 Zn
####################

Topology for Zn1
-------------------
Atom Zn1 links by bridge ligands and has
Common vertex with                    R(A-A)       f
Zn 1    0.0000    0.8527    0.2500   (-1 1-1)    8.809A       1
Zn 1    1.0000    0.8527    1.2500   ( 0 1 0)    8.809A       1
Zn 1    1.5000    0.3527    0.2500   ( 2 1 1)   13.371A       1
Zn 1   -0.5000    0.3527    1.2500   ( 0 1 2)   13.371A       1
-------------------------
Structural group analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of 3D framework with ZnO4N2C16H12
There are 3 interpenetrating nets
FIV: Full interpenetration vectors
-----------------------------------
[1,0,0] (8.90A)
-----------------------------------
PIC: [3/2,3/2,0][1,0,1][0,1,0] (PICVR=3)

Zt=3; Zn=1

Class Ia  Z=3

Coordination sequences
----------------------
Zn1:  1  2  3  4   5   6   7   8   9  10
Num   4 12 24 42  64  92 124 162 204 252
Cum   5 17 41 83 147 239 363 525 729 981
----------------------
TD10=981

Vertex symbols for selected sublattice
--------------------------------------
Zn1 Point symbol:{6^6}
Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]
--------------------------------------
Point symbol for net: {6^6}
4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 (topos&RCSR.ttd) {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)] (17092
types in 3 databases)
Elapsed time: 5.33 sec.
```

Table S3. The topology analysis results by ToposPro for **5-bpe**.

```
##################
1:C18 H18 N2 O4 Zn
##################

Topology for V1
--------------------
Atom V1 links by bridge ligands and has
Common vertex with                    R(A-A)       f
V  1   -0.5000   -1.0000    0.5000   (-1-1 0)    10.823A       1
V  1    1.5000    1.0000    0.5000   ( 1 1 0)    10.823A       1
V  1    1.5000    0.0000    1.5000   ( 1 0 1)    13.353A       1
V  1   -0.5000    0.0000   -0.5000   (-1 0-1)    13.353A       1
Common edge with                      R(A-A)
V  1    0.5000   -1.0000   -0.5000   ( 0-1-1)    13.781A       2
V  1    0.5000    1.0000    1.5000   ( 0 1 1)    13.781A       2
-------------------------
Structural group analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of 3D framework with VTi2Sc2
There are 2 interpenetrating nets
FIV: Full interpenetration vectors
---------------------------------
[1,0,0] (8.14A)
---------------------------------
PIC: [2,0,0][1,1,0][1,0,1] (PICVR=2)

Zt=2; Zn=1

Class Ia  Z=2

Coordination sequences
----------------------
V1:  1  2  3   4   5   6   7   8    9   10
Num  6 18 38  66 102 146 198 258  326  402
Cum  7 25 63 129 231 377 575 833 1159 1561
----------------------
TD10=1561

Vertex symbols for selected sublattice
--------------------------------------
V1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]
--------------------------------------
Point symbol for net: {4^12.6^3}
6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1 (topos&RCSR.ttd) {4^12.6^3} - VS
[4.4.4.4.4.4.4.4.4.4.4.4.*.*.*] (17092 types in 3 databases)
Elapsed time: 18.29 sec.
```

Table S4. The topology analysis results by ToposPro for **6-bpe**.

```
##################
1:C18 H14 N2 O4 Zn
##################

Topology for Zn1
-------------------
Atom Zn1 links by bridge ligands and has
Common vertex with                    R(A-A)       f
Zn 1    1.1486   -0.2500    0.7500   ( 2 0 1)    10.943A       1
Zn 1    1.1486    0.7500   -0.2500   ( 2 1 0)    10.943A       1
Zn 1    0.1486    0.7500    0.7500   ( 1 1 1)    13.492A       1
Zn 1    0.1486   -0.2500   -0.2500   ( 1 0 0)    13.492A       1
-------------------------
Structural group analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of 3D framework with ZnO4N2C18H14
There are 4 interpenetrating nets
TIV: Translating interpenetration vectors
-----------------------------------------
[1,0,0] (12.40A)
-----------------------------------------
NISE: Non-translating interpenetration symmetry elements
---------------------------------------------------------
1: 2[0,0,1]
---------------------------------------------------------
PIC: [2,0,0][1,1,0][1,0,1] (PICVR=2)

Zt=2; Zn=2

Class IIIa  Z=4[2*2]

Coordination sequences
----------------------
Zn1:  1  2  3  4   5   6   7   8   9  10
Num   4 12 24 42  64  92 124 162 204 252
Cum   5 17 41 83 147 239 363 525 729 981
----------------------
TD10=981

Vertex symbols for selected sublattice
--------------------------------------
Zn1 Point symbol:{6^6}
Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]
--------------------------------------
Point symbol for net: {6^6}
4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 (topos&RCSR.ttd) {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)] (17092
types in 3 databases)
Elapsed time: 4.77 sec.
```