Supplementary Material (ESI) for CrystEngComm

Construction of 3-fold interpenetrated pcu organic frameworks from methanetetrabenzoic acid with zigzag bipyridines

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Electronic Supplementary Information

1. **Experimental section**
2. **The result of interpenetrating modes analyzed by TOPOS**
3. **Figure S1-S3**

1. Experimental section

Preparation of H_4MTB

The ligand H_4MTB was prepared according to the literature: B. Kirste, M. Grimm, H. Kurreck, *J. Am. Chem. Soc.*, **1989**, *111*, 108.

Preparation of [H_4MTB.azpy]

A mixture of H_4MTB and 4,4'-azopyridine (azpy) in 1:2 ratio (H_4MTB: 14.9 mg, 0.03 mmol; azpy: 11 mg, 0.06 mmol) was dissolved in THF/MeOH (v/v=1:2, 30 mL) and allowed for crystallization at ambient temperature. Orange high-quality single crystals were obtained in a few days.

Preparation of [H_4MTB.(bipy-ete)].

A mixture of H_4MTB (19.8 mg, 0.04 mmol) and 1,2-di(pyridin-4-yl)ethene (14.6 mg, 0.08 mmol) was dissolved in MeOH (50 mL). The resultant colorless solution was filtered and left to stand at room temperature. Upon slow evaporation of the solvents, rectangular shaped colorless crystals suitable for X-ray diffraction were produced within three weeks.

2. The result of interpenetrating modes analyzed by TOPOS

[H_4MTB.azpy]:

For topology analysis, the H_4MTB molecule is simplified as Sc, and azpy molecule is simplified as Ti.

###############
1:C39 H28 N4 O8
###############

Topology for Sc1
Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 1	-0.5000	-1.4705	0.2500	(-1-2 0)	14.680A	1
Sc 1	0.5000	-1.4705	0.2500	(0-2 0)	14.680A	1
Sc 1	-0.5000	1.5295	0.2500	(-1 1 0)	14.680A	1
Sc 1	0.5000	1.5295	0.2500	(0 1 0)	14.680A	1
Sc 1	0.5000	-2.5295	-0.2500	(0-3-1)	26.299A	1
Sc 1	-0.5000	-2.5295	0.7500	(-1-3 0)	26.299A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with TiSc
There are 3 interpenetrating nets
FIV: Full interpenetration vectors

[0,1,0] (7.97A)

PIC: [3/2,3/2,0][1,0,0][0,0,1] (PICVR=3)

Zt=3; Zn=1

Class Ia Z=3

Coordination sequences

Sc1: 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

Sc1 Schlafli symbol:{4^12;6^3}

With circuits:[4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

Total Schlafli symbol: {4^12;6^3}

6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1 {4^12;6^3} - VS [4.4.4.4.4.4.4.4.4.4.4.*.*.*] (66822 types in 8 databases)

Elapsed time: 3.06 sec.

[H_4MTB.(bipy-ete)]:

For topology analysis, the H_4MTB molecule is simplified as Sc, and bipy-ete molecule is simplified as Ti.

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

1:C41 H30 N2 O8

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

Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 1	0.5000	2.4517	0.2500	(0 1 0)	14.597A	1
Sc 1	-0.5000	2.4517	0.2500	(-1 1 0)	14.597A	1
Sc 1	0.5000	-0.5483	0.2500	(0-2 0)	14.597A	1
Sc 1	-0.5000	-0.5483	0.2500	(-1-2 0)	14.597A	1
Sc 1	-0.5000	3.5483	0.7500	(-1 4 0)	26.653A	1
Sc 1	0.5000	3.5483	-0.2500	(0 4-1)	26.653A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with TiSc

There are 3 interpenetrating nets

FIV: Full interpenetration vectors

[0,1,0] (7.92A)

PIC: [3/2,3/2,0][1,0,0][0,0,1] (PICVR=3)

Zt=3; Zn=1

Class Ia Z=3

Coordination sequences

Sc1: 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

Sc1 Schlafli symbol:{4^12;6^3}

With circuits:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

Total Schlafli symbol: {4^12;6^3}

6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1 {4^12;6^3} - VS [4.4.4.4.4.4.4.4.4.4.4.*.*.*] (66822 types in 8 databases)

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3. Figure S1-S3

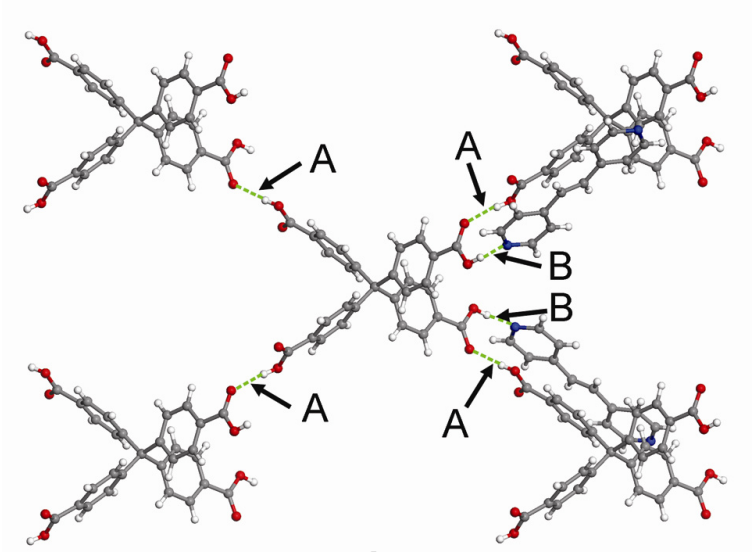

Fig. S1 Ball and stick view of the hydrogen bonds and the connectivity of H_4MTB in [**H_4MTB•(bipy-ete)]**. Red: O; blue: N; gray: C; white: H.

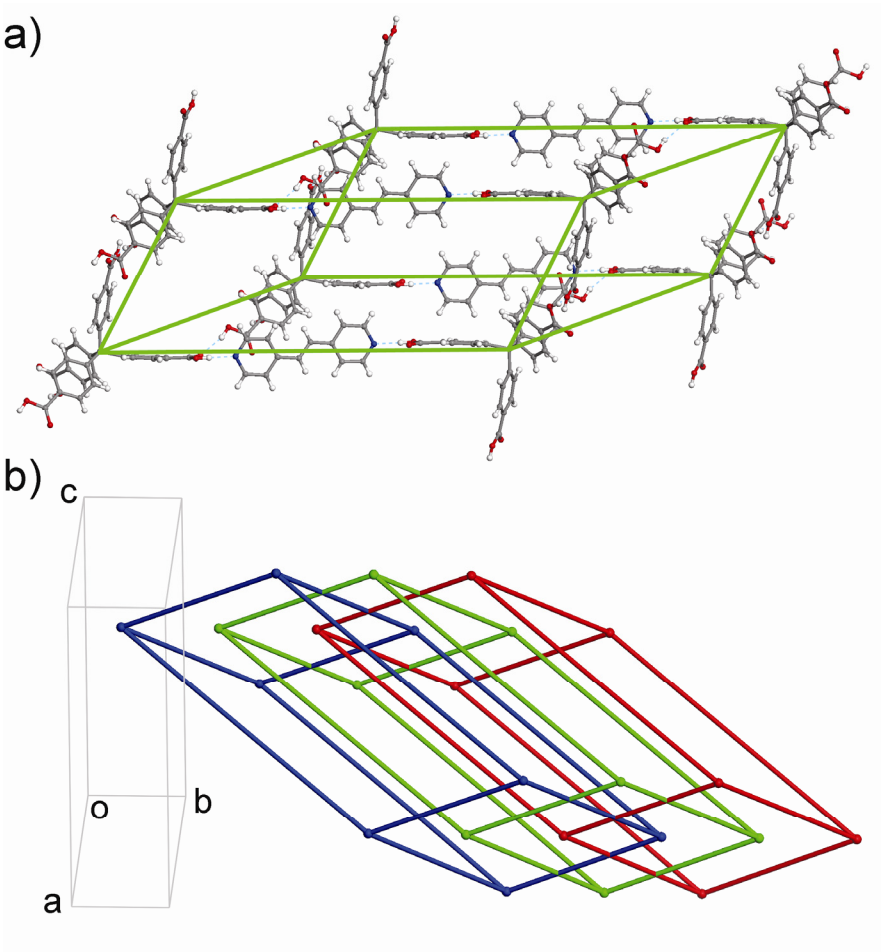

Fig. S2 a) Single distorted **pcu** cage in [**H_4MTB•(bipy-ete**)]; b) Schematic view of the 3-fold interpenetration with an interpenetration vector [0,1,0].

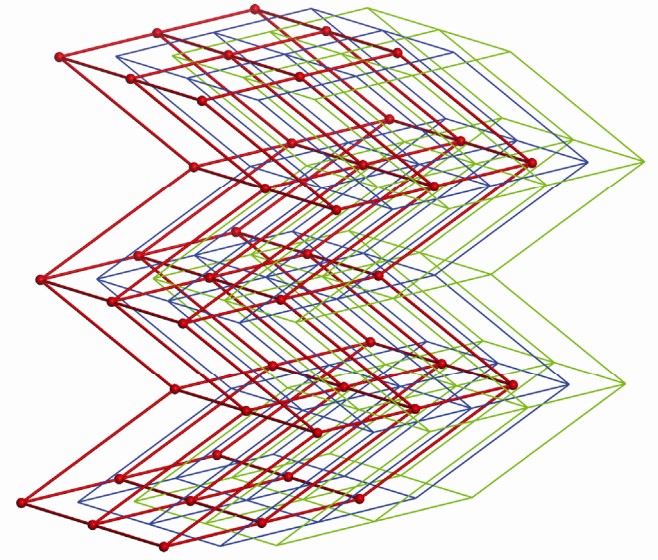

Fig. S3 Schematic view of the 3-fold interpenetrated nets in [**H_4MTB•azpy**] and [**H_4MTB•(bipy-ete**)].