Supplementary Material (ESI) for CrystEngComm

Organic hydrogen-bonded interpenetrating diamondoid frameworks from modular self-assembly of methanetetrabenzoic acid with linkers

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Electronic Supplementary Information

1. **Experimental section**
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1. Experimental section

Preparation of [H_4MTB.phenazine].

A mixture of Methanetetrabenzoic acid (H_4MTB) (14.9mg, 0.03mmol) and phenazine (10.8mg, 0.06mmol) was dissolved in THF/MeOH (v/v=1:2, 30mL). The resultant yellow solution was filtered and left to stand at room temperature. Upon slow evaporation of the solvents, cubic light yellow crystals single crystals suitable for X-ray diffraction were produced over a period of two weeks.

Preparation of [H_4MTB.bipy].

The similar synthetic procedure as for **[H_4MTB.phenazine]** was used. H_4MTB (14.9mg, 0.03mmol) and 4,4'-bipyridine (bipy) (9.4mg, 0.06mmol) were mixed in THF/MeOH (v/v=1:2, 30mL). The resultant colorless solution was filtered and allowed to crystallize at room temperature. Rectangular shaped colorless crystals single crystals suitable for X-ray diffraction appeared after three weeks.

2. The result of interpenetrating modes analyzed by TOPOS

[H_4MTB.phenazine]:

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2:C41 H28 N2 O8

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Topology for C1

Atom C1 links by bridge ligands and has

Common vertex with						R(A-A)	f
C	1	0.0000	1.7114	-0.2500	(0 2 0)	15.202A	1
C	1	0.0000	1.7114	0.7500	(0 2 1)	15.202A	1
C	1	0.5000	-1.7886	0.7500	(0-2 0)	21.024A	1
C	1	-0.5000	-1.7886	-0.2500	(-1-2-1)	21.024A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with O8N2C41H28

There are 7 interpenetrating nets

FIV: Full interpenetration vectors

[0,1,0] (8.64A)

PIC: [7/2,7/2,0][0,0,1][1,0,1] (PICVR=7)

Zt=7; Zn=1

Class Ia Z=7

Coordination sequences

C1:	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

C1 Schlafli symbol:{6^6}

With circuits:[6(2).6(2).6(2).6(2).6(2).6(2)]

Total Schlafli symbol: {6^6}

4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)] (66822 types in 8 databases)

Elapsed time: 3.44 sec.

[H_4MTB.bipy]:

As mentioned in the text, for the topology analysis, we keep here the linkers which is Ti below and Sc is the C_1 in the cif file. We keep this 2-coordinated linkers otherwise some bonds will cross with each other.

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2:C49 H36 N4 O8 with 2connection

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Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Ti 1	-0.2500	0.5092	0.0000	(0 1 0)	12.360A	1
Ti 1	0.2408	-0.5000	0.2500	(-1-1 0)	12.360A	1
Ti 1	0.7592	1.0000	0.2500	(1 1 0)	12.360A	1
Ti 1	1.2500	-0.0092	0.0000	(1-1 0)	12.360A	1

Topology for Ti1

Atom Ti1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 1	1.0000	1.2500	-0.1250	(1 1 0)	12.360A	1
Sc 1	-0.5000	1.2500	0.1250	(-1 1 0)	12.360A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Ti2Sc

There are 18 interpenetrating nets

PIV: Partial interpenetration vectors

[0,1,0] (12.73A) (3 nets [1,2,3])

[1,0,0] (12.73A) (3 nets [1,4,5])

[1,1,0] (18.00A) (3 nets [1,6,7])

[1,-1,0] (18.00A) (3 nets [1,8,9])

NISE: Non-translating interpenetration symmetry elements

1: -1

PIC: [0,3,0][3/2,3/2,3/2][0,0,1] (PICVR=9)

Zt=9(3*3); Zn=2

Class IIIb Z=18[(3*3)*2]

Coordination sequences

Sc1:	1	2	3	4	5	6	7	8	9	10
Num	4	4	12	12	36	24	60	42	108	64
Cum	5	9	21	33	69	93	153	195	303	367

Ti1:	1	2	3	4	5	6	7	8	9	10
Num	2	6	6	18	18	48	30	78	54	126
Cum	3	9	15	33	51	99	129	207	261	387

TD10=380

Vertex symbols for selected sublattice

Sc1 Point (Schlafli) symbol:{12^6}

Extended point symbol:[12(2).12(2).12(2).12(2).12(2).12(2)]

Rings coincide with circuits

All rings (up to 16): coincide with rings

All rings with types: [12(2).12(2).12(2).12(2).12(2).12(2)]

Ti1 Point (Schlafli) symbol:{12}

Extended point symbol:[12(6)]

Rings coincide with circuits

All rings (up to 16): coincide with rings

All rings with types: [12(6)]

Point (Schlafli) symbol for net: {12^6}{12}2

2,4-c net with stoichiometry (2-c)2(4-c); 2-nodal net

3. Figure S1-S3

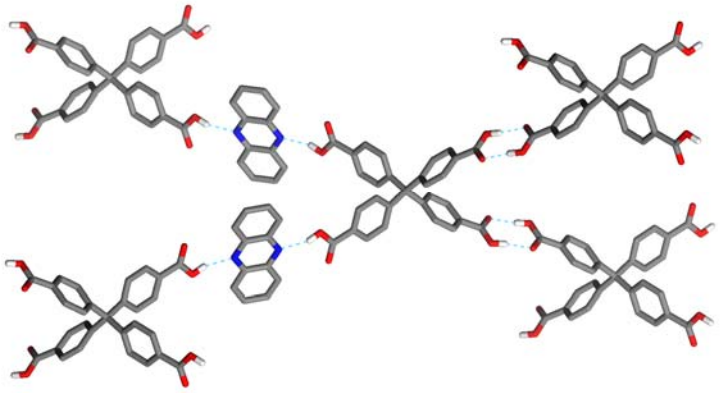

Fig. S1 Stick view of the hydrogen bonds and the connectivity of the H_4MTB in **[H_4MTB.phenazine]**. Red: O; blue: N; gray: C; white: H.

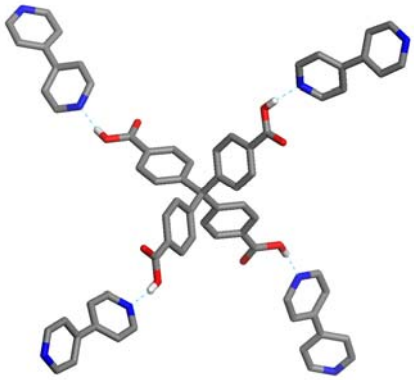

Fig. S2 Stick view of the hydrogen bonds and the connectivity of the H_4MTB in **[H_4MTB.bipy]**. Red: O; blue: N; gray: C; white: H.

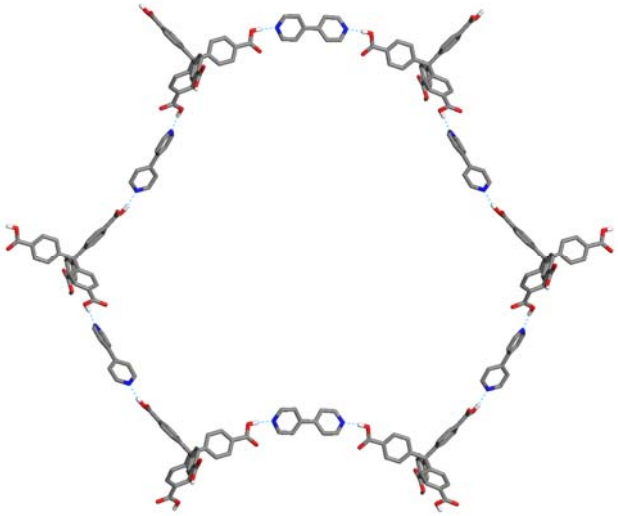

Fig. S3 Stick view of the bent connectivity of bipy with the H_4MTB in **[H_4MTB.bipy]**. Red: O; blue: N; gray: C; white: H.