Electronic Supplementary Material (ESI) for Dalton Transactions.

Two porous Ni-MOFs based on 2,4,6-tris(pyridin-4-yl)-1,3,5-triazine showing solvent determined structures and distinctive sorption properties toward CO_2 and alkanes

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Table 1 Crystal data and structure refinement details for **1** and **2**

Compounds	**1**		**2**	
Formula	$C_{37.42}H_{38}N_6O_{20}Ni_3$		$C_{72}H_{42}N_{12}O_{18}Ni_3$	
CCDC	1996089		1996089	
Formula weight	1067.91		1761.70	
Crystal system	Trigonal		Monoclinic	
Space group	*R*-3*m*		$P2_1/n$	
a (Å)	27.1230(3)		10.13653(10)	
b (Å)	27.1230(3)		25.9159(2)	
c (Å)	38.1727(3)		15.63851(15)	
α (°)	90		90	
β (°)	90		101.0451(9)	
γ (°)	120		90	
V (Å^3)	24319.7(4)		4032.10(7)	
Z	18		2	
D_c (g cm^{-3})	1.312		1.451	
μ(mm^{-1})	1.835		1.548	
F(000)	9873		1836.0	
Data collected	24179		22979	
Unique reflections	5146		7947	
Goodness-of-fit on F^2	1.054		1.081	
R_1, wR_2 [$I>2\sigma(I)$][α]	0.0561	0.1578	0.0410	0.1222
R_1, wR_2 [all data][b]	0.0577	0.1591	0.0440	0.1242

[a] $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. [b] $wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum w(F_o^2)^2\}^{1/2}$

Table S1 Selected Bond Lengths (Å) and Bond Angles (°) for Compound **1**

Bond	Dist.	Bond	Dist.	Bond	Dist.
Ni(1)-O(2)	2.014(2)	Ni(2)-N(1)	2.048(3)	Ni(3)-N(2)	2.085(5)
Ni(1)-O(1W)	2.132(2)	Ni(2)-O(3)	2.013(2)	Ni(3)-O(7)	2.092(6)
Ni(1)-O(3W)	2.005(3)	Ni(2)-O(2W)	2.078(3)	Ni(3)-O(1)	2.001(2)
Ni(1)-N(1)	2.048(3)	Ni(2)-O(3W)	2.077(3)		
Angle	(°)	Angle	(°)	Angle	(°)
O(1W)$^{\#1}$-Ni(1)-O(1W)	87.61(15)	N(1)-Ni(1)-O(1W)	89.00(9)	O(5)$^{\#1}$-Ni(2)-O(2W)	86.51(10)
O(2)-Ni(1)-O(1W)$^{\#1}$	87.17(10)	N(1)-Ni(1)-O(1W)$^{\#1}$	89.00(9)	O(5)$^{\#1}$-Ni(2)-O(3W)	90.56(8)
O(2)-Ni(1)-O(1W)	174.51(10)	O(3)-Ni(2)-O(2W)	89.98(10)	O(5)-Ni(2)-O(3W)	90.56(8)
O(2)$^{\#1}$-Ni(1)-O(1W)	87.18(10)	O(3)$^{\#1}$-Ni(2)-O(2W)	89.98(10)	O(5)-Ni(2)-O(5)$^{\#1}$	87.22(14)
O(2)$^{\#1}$-Ni(1)-O(1W)$^{\#1}$	174.51(10)	O(3)$^{\#1}$-Ni(2)-O(3)	93.53(15)	O(1)-Ni(3)-O(1)$^{\#2}$	122.06(14)
O(2)-Ni(1)-O(2)$^{\#1}$	97.99(13)	O(3)-Ni(2)-O(3W)	92.79(8)	O(1)$^{\#2}$-Ni(3)-O(6)$^{\#4}$	87.76(9)
O(2)$^{\#1}$-Ni(1)-N(1)	89.20(9)	O(3)$^{\#1}$-Ni(2)-O(3W)	92.79(8)	O(1)-Ni(3)-O(6)$^{\#3}$	87.76(9)
O(2)-Ni(1)-N(1)	89.20(9)	O(3)$^{\#1}$-Ni(2)-O(5)	175.35(9)	O(1)$^{\#2}$-Ni(3)-O(6)$^{\#3}$	149.70(10)
O(3W)-Ni(1)-O(1W)	88.49(8)	O(3)$^{\#1}$-Ni(2)-O(5)$^{\#1}$	89.53(10)	O(1)-Ni(3)-O(6)$^{\#4}$	149.70(10)
O(3W)-Ni(1)-O(1W)$^{\#1}$	88.49(8)	O(3)-Ni(2)-O(5)$^{\#1}$	175.35(9)	O(1)-Ni(3)-O(7)	87.02(12)
O(3W)-Ni(1)-O(2)	93.07(8)	O(3)-Ni(2)-O(5)	89.52(10)	O(1)$^{\#2}$-Ni(3)-O(7)	87.01(12)
O(3W)-Ni(1)-O(2)$^{\#1}$	93.07(8)	O(3W)-Ni(2)-O(2W)	175.95(14)	O(1)-Ni(3)-N(2)	93.15(11)
O(3W)-Ni(1)-N(1)	176.53(12)	O(5)-Ni(2)-O(2W)	86.51(10)	O(1)$^{\#2}$-Ni(3)-N(2)	93.15(11)

Symmetry transformation: #1: *x*, *x*-*y*+1, *z*; #2: -*x*+*y*+1,*y*,*z*; #3: -*x*+4/3,-*x*+*y*+2/3,-*z*+2/3; #4: *y*+1/3,-*x*+*y*+2/3,-*z*+2/3

Table S2 Selected Bond Lengths (Å) and Bond Angles (°) for Compound **2**

Bond	Dist.	Bond	Dist.	Bond	Dist.
Ni(1)-O(2)	2.0186(14)	Ni(1)-N(2)$^{\#2}$	2.1068(17)	Ni(2)-O(2W)	2.0632(16)
Ni(1)-O(1W)	2.0367(15)	Ni(1)-O(5)$^{\#1}$	2.1362(14)	Ni(2)-O(2W)$^{\#3}$	2.0633(16)
Ni(1)-N(3)	2.0918(17)	Ni(2)-O(3W)	2.0529(17)	Ni(2)-N(1)	2.1080(19)
Ni(1)-O(6)$^{\#1}$	2.0924(14)	Ni(2)-O(3W)$^{\#3}$	2.0529(17)	Ni(2)-N(1)$^{\#3}$	2.1081(19)
Angle	(°)	Angle	(°)	Angle	(°)
O(2)-Ni(1)-O(1W)	96.13(6)	O(2)-Ni(1)-O(5)$^{\#1}$	101.10(6)	O(2W)-Ni(2)-O(2W)$^{\#3}$	180.0
O(2)-Ni(1)-N(3)	87.13(6)	O(1W)-Ni(1)-O(5)$^{\#1}$	162.74(6)	O(3W)-Ni(2)-N(1)	90.48(7)
O(1W)-Ni(1)-N(3)	90.90(6)	N(3)-Ni(1)-O(5)$^{\#1}$	90.76(6)	O(3W)$^{\#3}$-Ni(2)-N(1)	89.52(7)
O(2)-Ni(1)-O(6)$^{\#1}$	163.85(6)	O(6)$^{\#1}$-Ni(1)-O(5)$^{\#1}$	62.84(5)	O(2W)-Ni(2)-N(1)	89.33(7)
O(1W)-Ni(1)-O(6)$^{\#1}$	99.91(6)	N(2)$^{\#2}$-Ni(1)-O(5)$^{\#1}$	85.99(6)	O(2W)$^{\#3}$-Ni(2)-N(1)	90.67(7)
N(3)-Ni(1)-O(6)$^{\#1}$	94.43(6)	O(3W)-Ni(2)-O(3W)$^{\#3}$	180.00(8)	O(3W)-Ni(2)-N(1)$^{\#3}$	89.52(7)
O(2)-Ni(1)-N(2)$^{\#2}$	86.15(7)	O(3W)-Ni(2)-O(2W)	92.11(7)	O(3W)$^{\#3}$-Ni(2)-N(1)$^{\#3}$	90.48(7)
O(1W)-Ni(1)-N(2)$^{\#2}$	94.43(6)	O(3W)$^{\#3}$-Ni(2)-O(2W)	87.89(7)	O(2W)-Ni(2)-N(1)$^{\#3}$	90.67(7)
N(3)-Ni(1)-N(2)$^{\#2}$	171.84(7)	O(3W)-Ni(2)-O(2W)$^{\#3}$	87.89(7)	O(2W)$^{\#3}$-Ni(2)-N(1)$^{\#3}$	89.33(7)
O(6)$^{\#1}$-Ni(1)-N(2)$^{\#2}$	90.75(6)	O(3W)$^{\#3}$-Ni(2)-O(2W)$^{\#3}$	92.11(7)	N(1)-Ni(2)-N(1)$^{\#3}$	180.00(11)

Symmetry transformation: #1: *x*+1, *y*, *z*; #2: -*x*+3/2, *y*+1/2, -*z*+1/2; #3: -*x*+2, -*y*+1, -*z*+2; #4: *x*-1, *y*, *z*

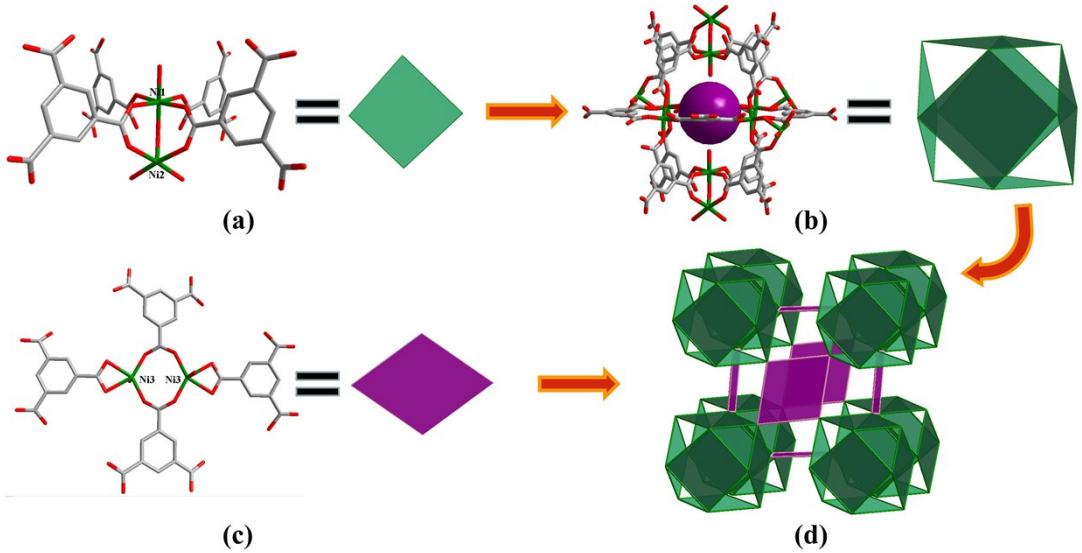

Fig. S1 (a) Square shaped SBU constructed with binuclear nickel (Ni1, Ni2) and four BTC^{3-} ligands in **1**. (b) Cubohemioctahedra supermolecular building block (SBB) assembled by square SBUs in **1**. (c) Another square SBU constructed with two Ni3 and four BTC^{3-} ligands in **1**. (d) Schematic view of the ftw-a-like topology of **1**.

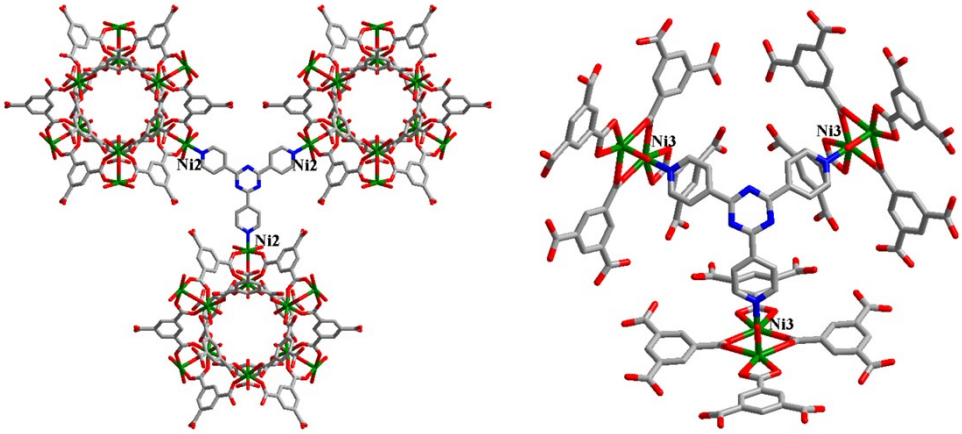

Fig. S2 Two types of TPT ligands depending on different connections in **1**

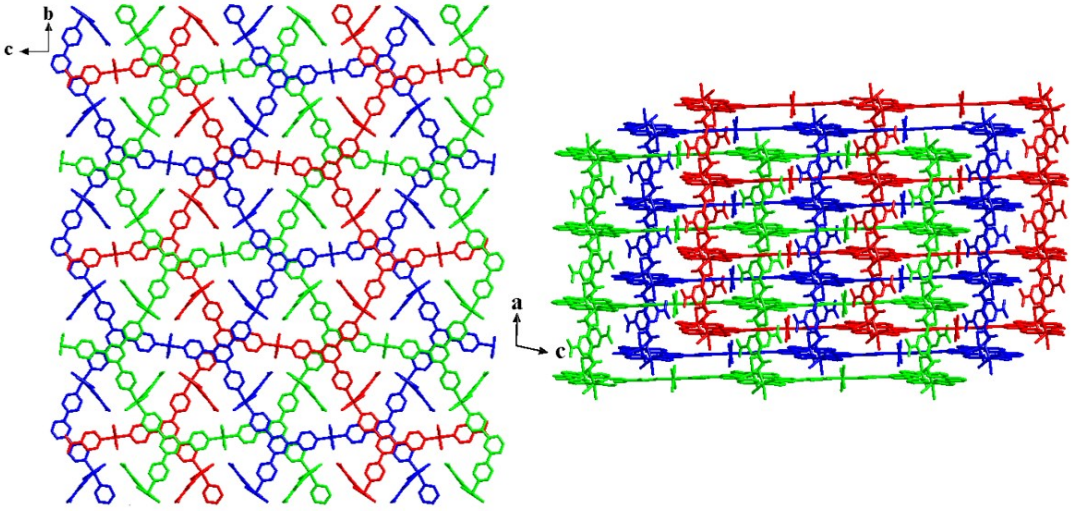

Fig. S3 3-fold interpenetrated structure of compound **2** view along the *a* axis and *b* axis.

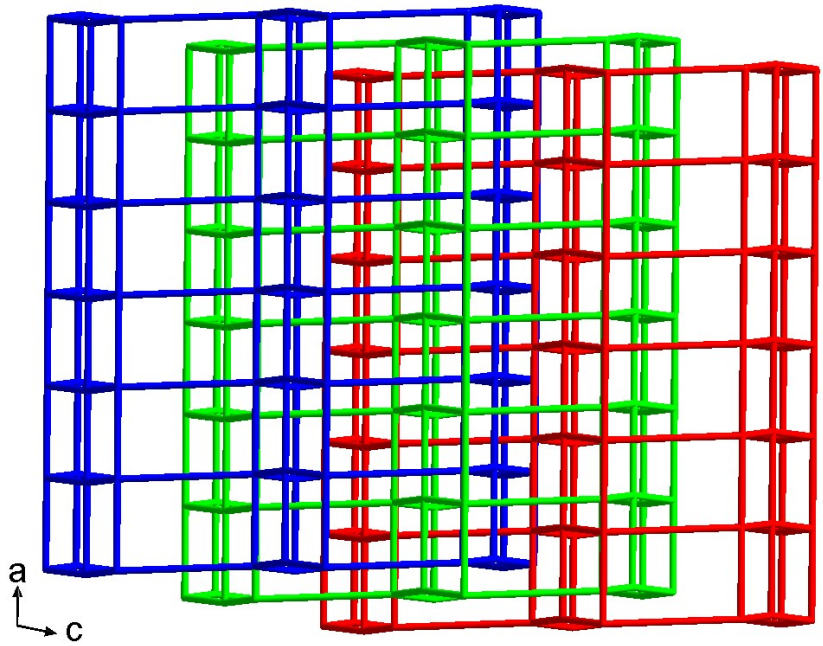

Fig. S4 Schematic view of topological representation of **2.**

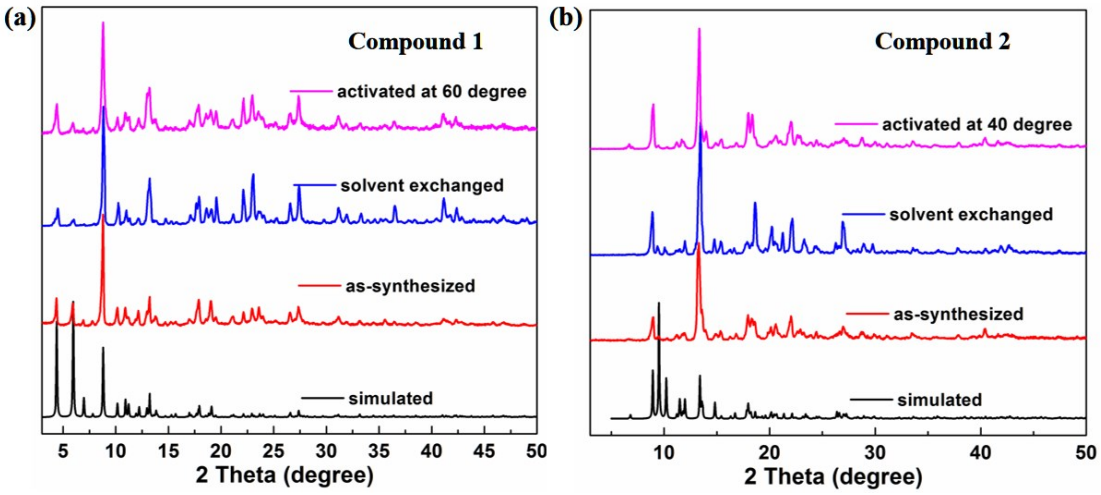

Fig. S5 (a) PXRD patterns of **1**. (b) PXRD patterns of **2.**

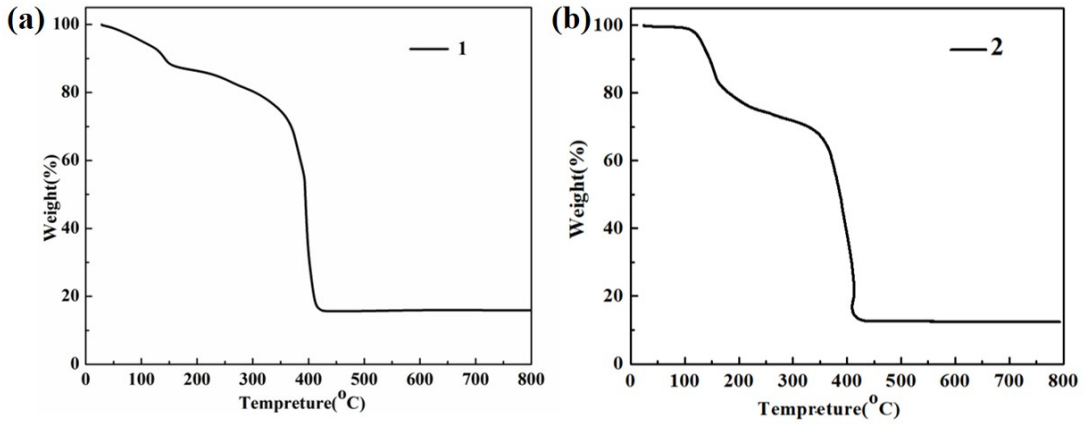

Fig. S6 (a) TGA curve of as-synthesized **1**. (b) TGA curve of as-synthesized **2**.

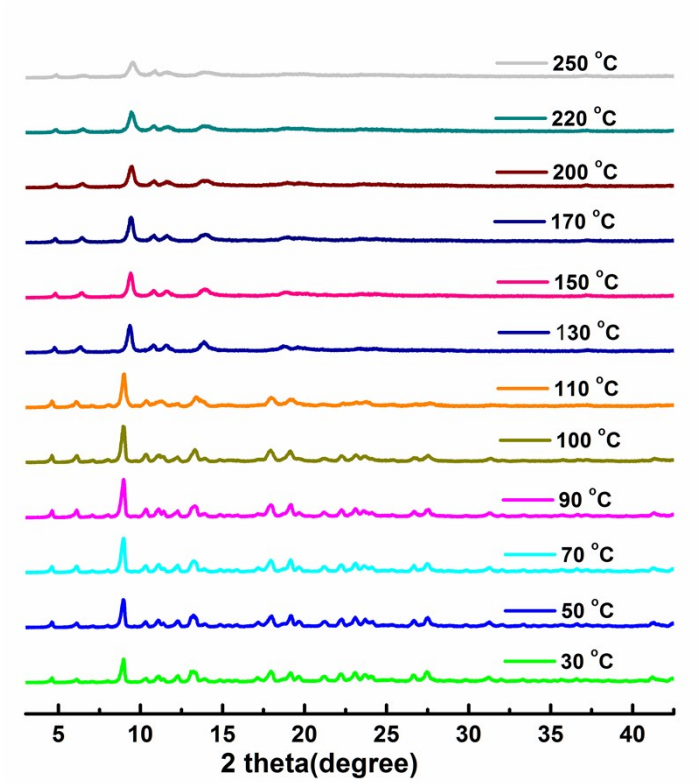

Fig. S7 In-situ PXRD patterns of as-synthesized **1** under variable temperatures.

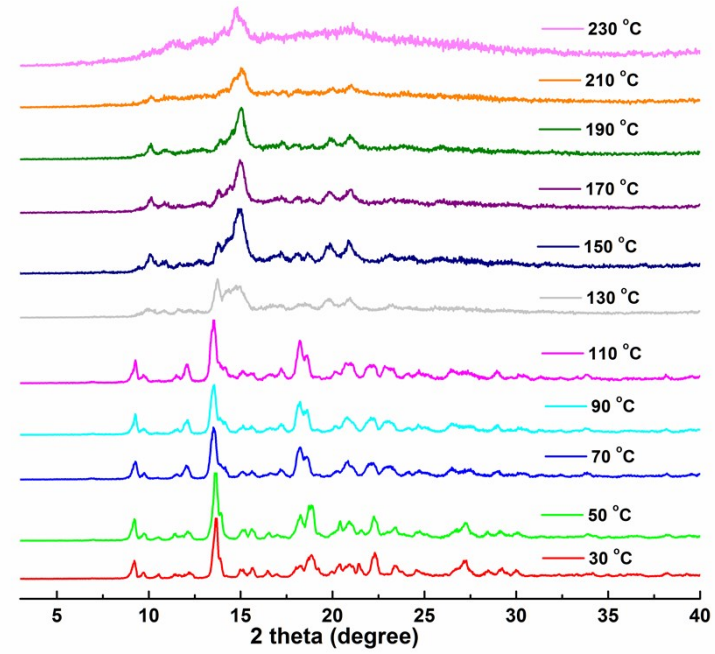

Fig. S8 In-situ PXRD patterns of as-synthesized **2** under variable temperatures.