Supporting Information

Four new coordination polymers based on a pyridinetetracarboxylate ligand: Syntheses, structures and high CO_2/CH_4 separation

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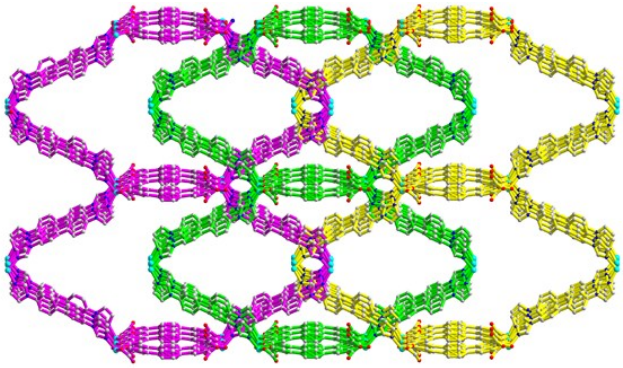


Fig. S1. The 3-fold interpenetrating 3D network of **1**.

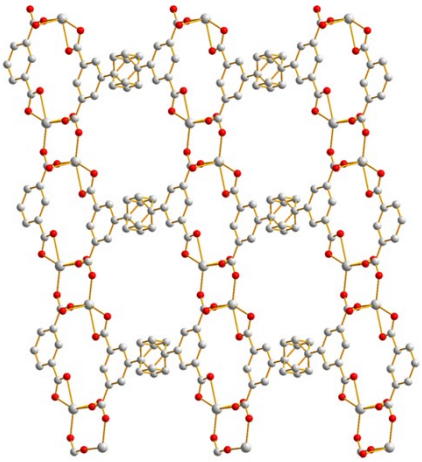


Fig. S2. The binuclear Mn(II) clusters are linked by TPTA to form a 2D layer along ab plane.

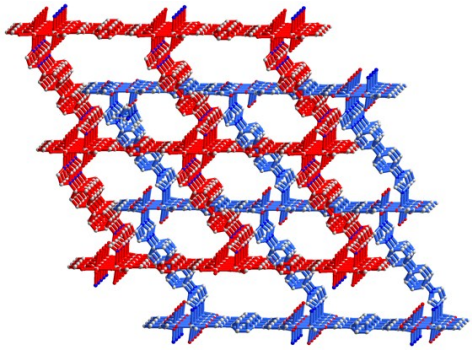


Fig. S3. Schematic representation of the 2-fold interpenetrating network.

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

Zn(1)-O(3)#3	1.943(2)	Zn(1)-N(4)#4	2.013(3)
O(1)-Zn(1)-O(3)#3	114.51(10)	O(1)-Zn(1)-N(4)#4	108.99(10)
O(1)-Zn(1)-N(1)	114.65(10)	O(3)#3-Zn(1)-N(4)#4	97.03(9)
O(3)#3-Zn(1)-N(1)	108.90(9)	N(1)-Zn(1)-N(4)#4	111.43(11)

Symmetry code: #1 -x+3/2,y-1/2,-z+3/2 #2 x,-y+2,z+1/2 #3 x,-y+2,z-1/2
#4 -x+3/2,y+1/2,-z+3/2 #5 -x,y,-z+3/2

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

Mn(1)-O(1)	2.093(4)	Mn(1)-O(4)#2	2.269(3)
Mn(1)-O(2)#4	2.128(4)	Mn(1)-O(3)#2	2.273(4)
Mn(1)-O(5)	2.2(4)	Mn(1)-C(17)#2	2.595(5)
Mn(1)-N(1)	2.236(5)	O(2)#4-Mn(1)-O(4)#2	91.36(13)
O(1)-Mn(1)-O(2)#4	113.60(15)	O(5)-Mn(1)-O(4)#2	89(10)
O(1)-Mn(1)-O(5)	85(10)	N(1)-Mn(1)-O(4)#2	92.63(16)
O(2)#4-Mn(1)-O(5)	95(10)	O(1)-Mn(1)-O(3)#2	97.28(15)
O(1)-Mn(1)-N(1)	89.7(2)	O(2)#4-Mn(1)-O(3)#2	149.04(14)
O(2)#4-Mn(1)-N(1)	94.37(18)	O(5)-Mn(1)-O(3)#2	85(10)
O(5)-Mn(1)-N(1)	170(10)	N(1)-Mn(1)-O(3)#2	87.70(17)
O(1)-Mn(1)-O(4)#2	154.68(15)	O(4)#2-Mn(1)-O(3)#2	57.68(12)

Symmetry code: #1 -x+2,-y+1,-z #2 -x+1,-y,-z+1 #3 -x,-y,-z
#4 -x+1,-y+1,-z+1

Table S3. Selected Bond Lengths (Å) and Bond Angles (°) for Complex **3**.

Zn(1)-O(8)#5	2.019(2)	Zn(2)-O(7)#5	2.012(3)
Zn(1)-O(8)#4	2.019(2)	Zn(2)-O(2)#9	2.012(3)
Zn(1)-O(5)#6	2.094(2)	Zn(2)-O(6)#7	2.016(3)
Zn(1)-O(5)#7	2.094(2)	Zn(2)-O(1)#9	2.455(4)
Zn(1)-O(4)#8	2.181(2)	Zn(2)-C(22)#9	2.569(4)
O(8)#5-Zn(1)-O(8)#4	180.000(1)	O(5)#7-Zn(1)-O(4)	90.56(10)
O(8)#5-Zn(1)-O(5)#6	84.17(10)	O(4)#8-Zn(1)-O(4)	180
O(8)#4-Zn(1)-O(5)#6	95.83(10)	O(7)#5-Zn(2)-O(2)#9	104.38(12)
O(8)#5-Zn(1)-O(5)#7	95.83(10)	O(7)#5-Zn(2)-O(6)#7	101.53(12)

O(8)#4-Zn(1)-O(5)#7	84.17(10)	O(2)#9-Zn(2)-O(6)#7	98.77(12)
O(5)#6-Zn(1)-O(5)#7	180.000(1)	O(7)#5-Zn(2)-O(4)	108.26(10)
O(8)#5-Zn(1)-O(4)#8	88.58(10)	O(2)#9-Zn(2)-O(4)	132.45(12)
O(8)#4-Zn(1)-O(4)#8	91.42(10)	O(6)#7-Zn(2)-O(4)	107.33(11)
O(5)#6-Zn(1)-O(4)#8	90.56(10)	O(7)#5-Zn(2)-O(1)#9	91.81(14)
O(5)#7-Zn(1)-O(4)#8	89.44(10)	O(2)#9-Zn(2)-O(1)#9	56.20(12)
O(8)#5-Zn(1)-O(4)	91.42(10)	O(6)#7-Zn(2)-O(1)#9	154.20(11)
O(8)#4-Zn(1)-O(4)	88.58(10)	O(4)-Zn(2)-O(1)#9	88.88(12)
O(5)#6-Zn(1)-O(4)	89.44(10)		

Symmetry code: #1 x-1/2,y-1/2,z #2 x+1/2,y-1/2,z #3 x,-y+1,z-1/2
#4 -x,y,-z+3/2 #5 x,-y+1,z+1/2 #6 -x+1/2,-y+1/2,-z+2
#7 x-1/2,y+1/2,z #8 -x,-y+1,-z+2 #9 x+1/2,y+1/2,z

Table S4. Selected Bond Lengths (Å) and Bond Angles (°) for Complex **4**.

Cd(1)-O(1)#3	2.225(4)	Cd(2)-O(2)	2.211(3)
Cd(1)-O(1)	2.225(4)	Cd(2)-O(4)#8	2.338(4)
Cd(1)-O(9)#4	2.290(3)	Cd(2)-O(3)#8	2.353(4)
Cd(1)-O(9)#5	2.290(3)	Cd(2)-O(9)#7	2.401(3)
Cd(1)-O(9)#6	2.290(3)	Cd(2)-O(9)#4	2.401(3)
Cd(1)-O(9)#7	2.290(3)	Cd(2)-O(10)#4	2.443(3)
Cd(1)-Cd(2)	3.4735(6)	Cd(2)-O(10)#7	2.443(3)
Cd(1)-Cd(2)#3	3.4736(6)	Cd(2)-C(8)#8	2.682(5)
O(1)#3-Cd(1)-O(1)	180	O(2)-Cd(2)-O(9)#7	101.32(11)
O(1)#3-Cd(1)-O(9)#4	88.98(12)	O(4)#8-Cd(2)-O(9)#7	100.16(11)
O(1)-Cd(1)-O(9)#4	91.03(12)	O(3)#8-Cd(2)-O(9)#7	139.57(8)
O(1)#3-Cd(1)-O(9)#5	91.02(12)	O(2)-Cd(2)-O(9)#4	101.32(11)
O(1)-Cd(1)-O(9)#5	88.97(12)	O(4)#8-Cd(2)-O(9)#4	100.16(11)
O(9)#4-Cd(1)-O(9)#5	180	O(3)#8-Cd(2)-O(9)#4	139.57(8)
O(1)#3-Cd(1)-O(9)#6	91.02(12)	O(9)#7-Cd(2)-O(9)#4	69.89(13)
O(1)-Cd(1)-O(9)#6	88.97(12)	O(2)-Cd(2)-O(10)#4	91.63(7)
O(9)#4-Cd(1)-O(9)#6	106.17(17)	O(4)#8-Cd(2)-O(10)#4	88.96(7)
O(9)#5-Cd(1)-O(9)#6	73.83(17)	O(3)#8-Cd(2)-O(10)#4	90.72(6)
O(1)#3-Cd(1)-O(9)#7	88.98(12)	O(9)#7-Cd(2)-O(10)#4	123.62(9)
O(1)-Cd(1)-O(9)#7	91.03(12)	O(9)#4-Cd(2)-O(10)#4	53.76(9)
O(9)#4-Cd(1)-O(9)#7	73.83(17)	O(2)-Cd(2)-O(10)#7	91.63(7)
O(9)#5-Cd(1)-O(9)#7	106.17(17)	O(4)#8-Cd(2)-O(10)#7	88.96(7)
O(9)#6-Cd(1)-O(9)#7	180	O(3)#8-Cd(2)-O(10)#7	90.72(6)
O(2)-Cd(2)-O(4)#8	153.71(14)	O(9)#7-Cd(2)-O(10)#7	53.76(9)
O(2)-Cd(2)-O(3)#8	97.92(13)	O(9)#4-Cd(2)-O(10)#7	123.62(9)
O(4)#8-Cd(2)-O(3)#8	55.78(14)	O(10)#4-Cd(2)-O(10)#7	176.23(14)

Symmetry code: #1 x,y,z+1 #2 x,-y+2,z #3 -x+1,-y+2,-z+1
#4 x+1/2,-y+3/2,z #5 -x+1/2,y+1/2,-z+1 #6 -x+1/2,-y+3/2,-z+1
#7 x+1/2,y+1/2,z #8 x,y,z-1 #9 x-1/2,y-1/2,z

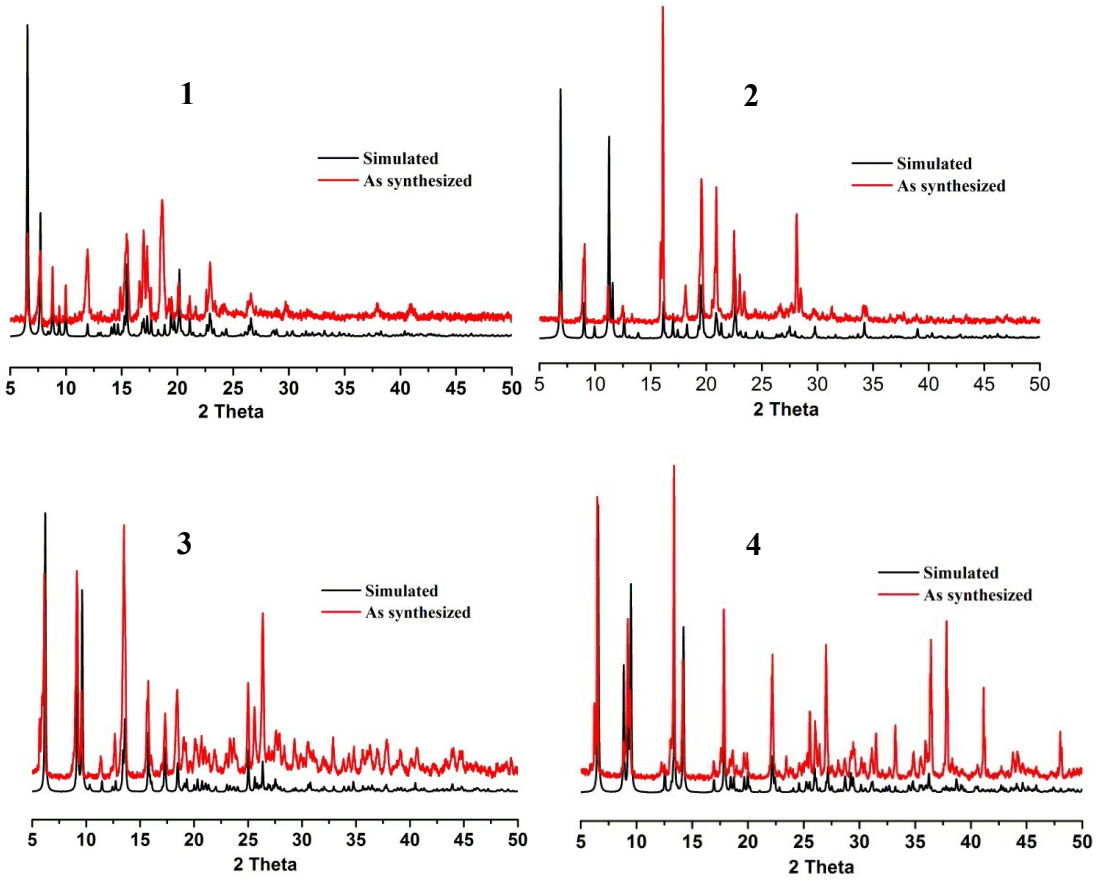


Fig. S4. PXRD simulated as-synthesized patterns for complexes **1**−**4**.

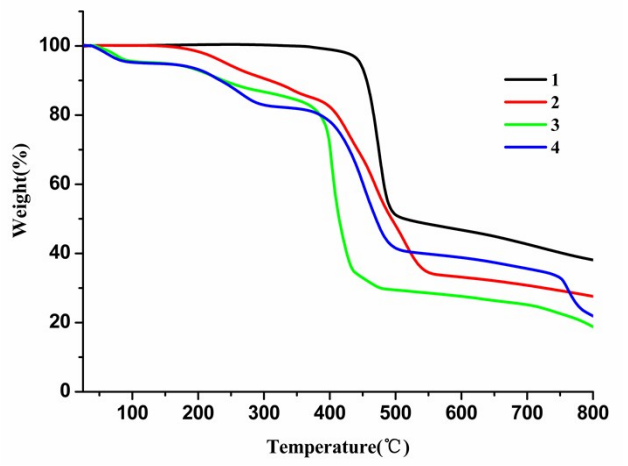


Fig. S5. The TG curves of complexes **1**−**4**.

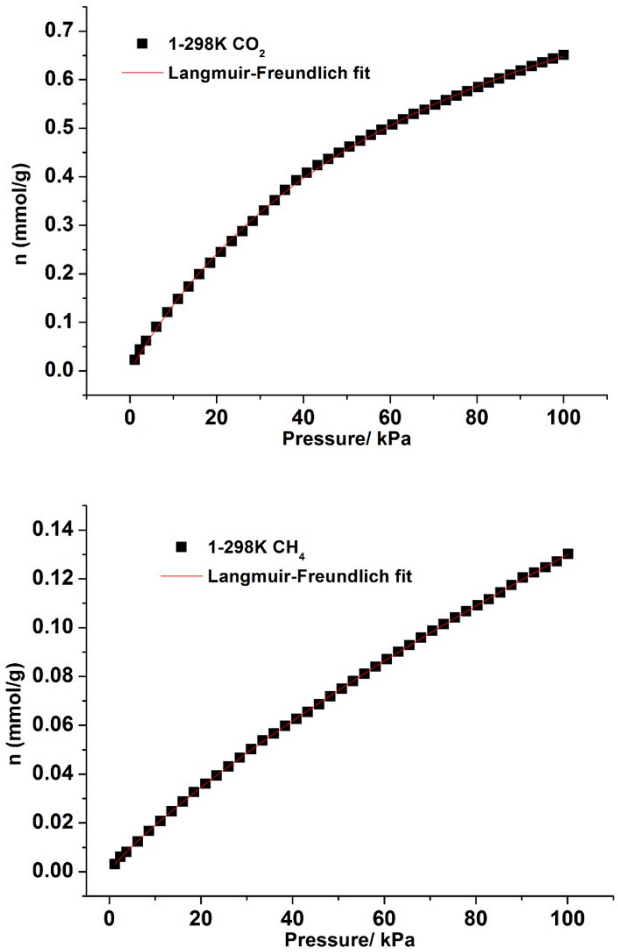
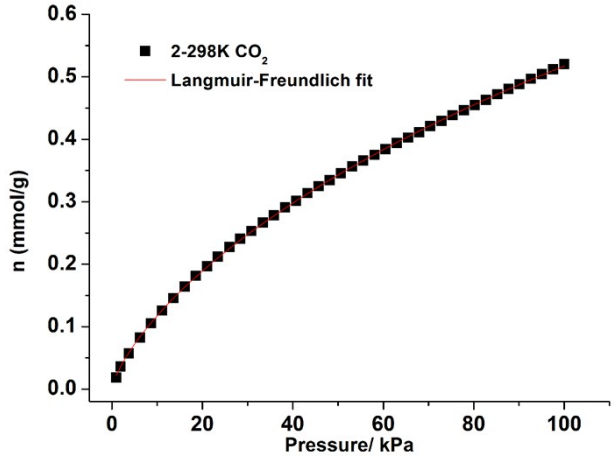


Fig. S6 CO_2 and CH_4 adsorption isotherms of **1** with fitting by L-F model.



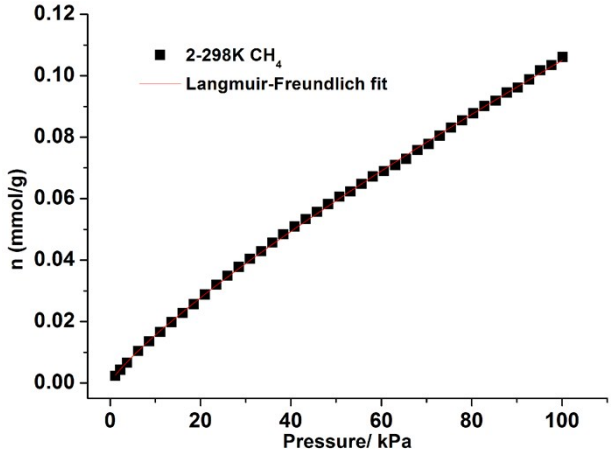
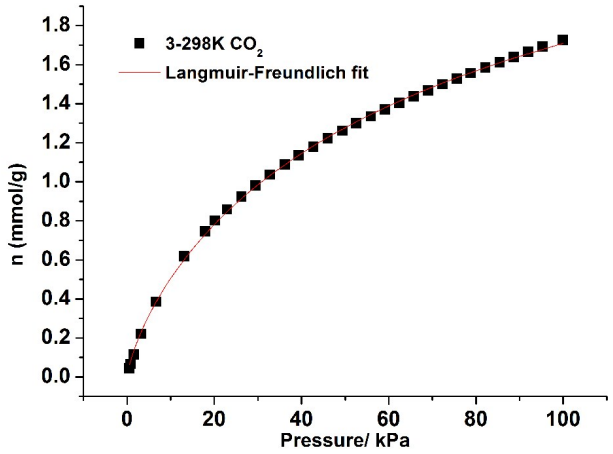


Fig. S7 CO_2 and CH_4 adsorption isotherms of **2** with fitting by L-F model.



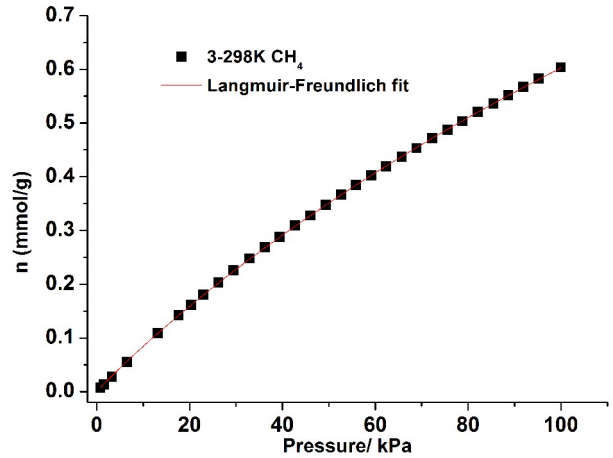


Fig. S8 CO_2 and CH_4 adsorption isotherms of **3** with fitting by L-F model.

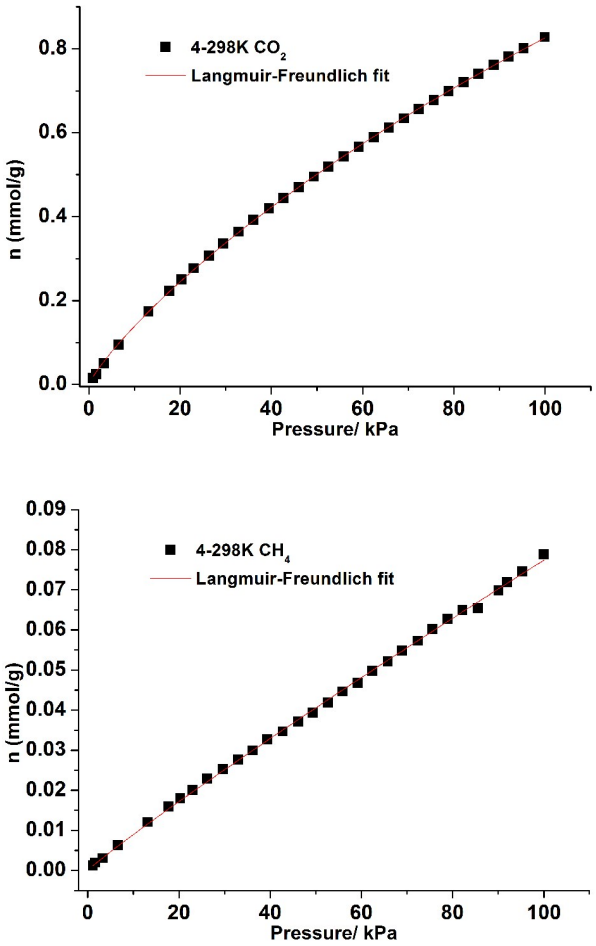
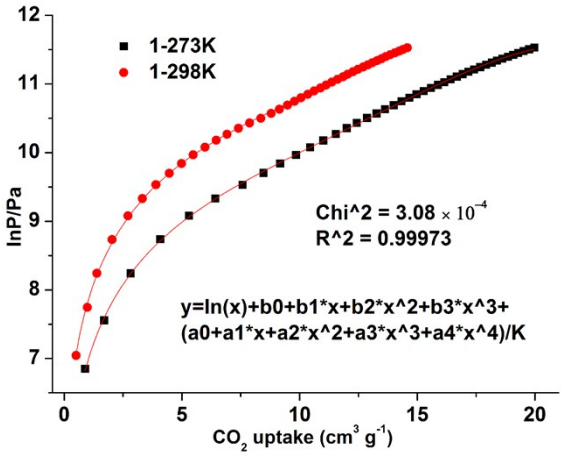
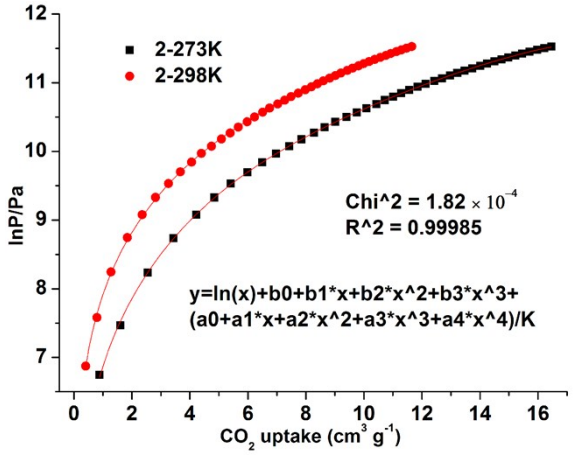


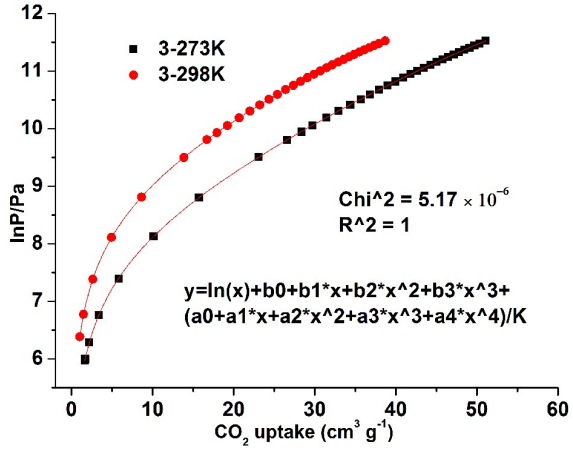
Fig. S9 CO_2 and CH_4 adsorption isotherms of **4** with fitting by L-F model.



(a)



(b)



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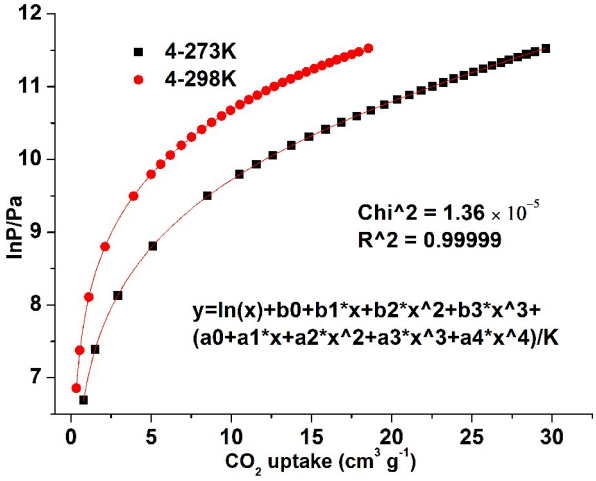

(d)

Fig. S10 Virial analysis of the CO_2 sorption data (273 and 298 K, at 1 atm) for **1** (a), **2** (b), **3** (c), and **4** (d), respectively.