Supporting information

A Highly-connected Metal-Organic Framework based on $[Co_2(\mu_2\text{-}OH_2)]$ units and mononuclear Co centers with high gas uptake capacity

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Table s1. The selected bond lengths (Å) and angles (°) for **1**.

Co(1)-O(1)	2.111(8)	Co(3)-O(8)	2.056(7)
Co(1)-O(1)#1	2.111(8)	Co(3)-O(8)#2	2.056(7)
Co(1)-N(2)#1	2.189(8)	Co(3)-O(12)	2.079(11)
Co(1)-N(2)#2	2.189(8)	Co(3)-O(11)	2.113(8)
Co(1)-N(2)	2.189(8)	Co(3)-N(5)	2.130(9)
Co(1)-N(2)#3	2.189(8)	Co(3)-N(5)#2	2.130(9)
Co(2)-O(7)	2.028(8)	Co(4)-O(3)	2.068(7)
Co(2)-O(7)#2	2.028(8)	Co(4)-O(4)#6	2.077(6)
Co(2)-O(6)#4	2.088(8)	Co(4)-O(10)#7	2.077(7)
Co(2)-O(6)#5	2.088(8)	Co(4)-N(3)	2.155(8)
Co(2)-N(1)	2.148(11)	Co(4)-O(13)	2.155(6)
Co(2)-O(11)	2.219(8)	Co(4)-N(4)#2	2.158(7)
O(1)-Co(1)-O(1)#1	180.00(12)	O(8)-Co(3)-O(8)#2	91.0(5)
O(1)-Co(1)-N(2)#1	94.3(3)	O(8)-Co(3)-O(12)	85.3(3)
O(1)#1-Co(1)-N(2)#1	85.7(3)	O(8)#2-Co(3)-O(12)	85.3(3)
O(1)-Co(1)-N(2)#2	85.7(3)	O(8)-Co(3)-O(11)	95.3(3)
O(1)#1-Co(1)-N(2)#2	94.3(3)	O(8)#2-Co(3)-O(11)	95.3(3)
N(2)#1-Co(1)-N(2)#2	87.8(4)	O(12)-Co(3)-O(11)	179.1(4)
O(1)-Co(1)-N(2)	85.7(3)	O(8)-Co(3)-N(5)	88.9(4)
O(1)#1-Co(1)-N(2)	94.3(3)	O(8)#2-Co(3)-N(5)	175.6(3)
N(2)#1-Co(1)-N(2)	180.000(1)	O(12)-Co(3)-N(5)	90.3(4)
N(2)#2-Co(1)-N(2)	92.2(4)	O(11)-Co(3)-N(5)	89.0(3)
O(1)-Co(1)-N(2)#3	94.3(3)	O(8)-Co(3)-N(5)#2	175.6(3)
O(1)#1-Co(1)-N(2)#3	85.7(3)	O(8)#2-Co(3)-N(5)#2	88.9(4)
N(2)#1-Co(1)-N(2)#3	92.2(4)	O(12)-Co(3)-N(5)#2	90.3(4)
N(2)#2-Co(1)-N(2)#3	180.0(3)	O(11)-Co(3)-N(5)#2	89.0(3)
N(2)-Co(1)-N(2)#3	87.8(4)	N(5)-Co(3)-N(5)#2	90.8(6)
O(7)-Co(2)-O(7)#2	94.1(5)	O(3)-Co(4)-O(4)#6	93.5(3)
O(7)-Co(2)-O(6)#4	88.6(4)	O(3)-Co(4)-O(10)#7	175.3(3)

O(7)#2-Co(2)-O(6)#4	176.8(3)	O(4)#6-Co(4)-O(10)#7	91.1(3)
O(7)-Co(2)-O(6)#5	176.8(3)	O(3)-Co(4)-N(3)	87.7(3)
O(7)#2-Co(2)-O(6)#5	88.6(4)	O(4)#6-Co(4)-N(3)	176.3(3)
O(6)#4-Co(2)-O(6)#5	88.6(5)	O(10)#7-Co(4)-N(3)	87.6(3)
O(7)-Co(2)-N(1)	86.3(3)	O(3)-Co(4)-O(13)	89.3(2)
O(7)#2-Co(2)-N(1)	86.3(3)	O(4)#6-Co(4)-O(13)	92.4(2)
O(6)#4-Co(2)-N(1)	92.1(3)	O(10)#7-Co(4)-O(13)	90.3(3)
O(6)#5-Co(2)-N(1)	92.1(3)	N(3)-Co(4)-O(13)	91.2(3)
O(7)-Co(2)-O(11)	90.7(2)	O(3)-Co(4)-N(4)#2	89.9(3)
O(7)#2-Co(2)-O(11)	90.7(2)	O(4)#6-Co(4)-N(4)#2	86.8(3)
O(6)#4-Co(2)-O(11)	91.1(3)	O(10)#7-Co(4)-N(4)#2	90.6(3)
O(6)#5-Co(2)-O(11)	91.1(3)	N(3)-Co(4)-N(4)#2	89.7(3)
N(1)-Co(2)-O(11)	175.6(4)	O(13)-Co(4)-N(4)#2	178.8(3)

Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z+2; #2 x, -y, z; #3 -x, y, -z+2; #4 -x+1/2, y+1/2, -z+2; #5 -x+1/2, -y-1/2, -z+2; #6 -x, y, -z+1; #7 -x+1/2, y-1/2, -z+1.

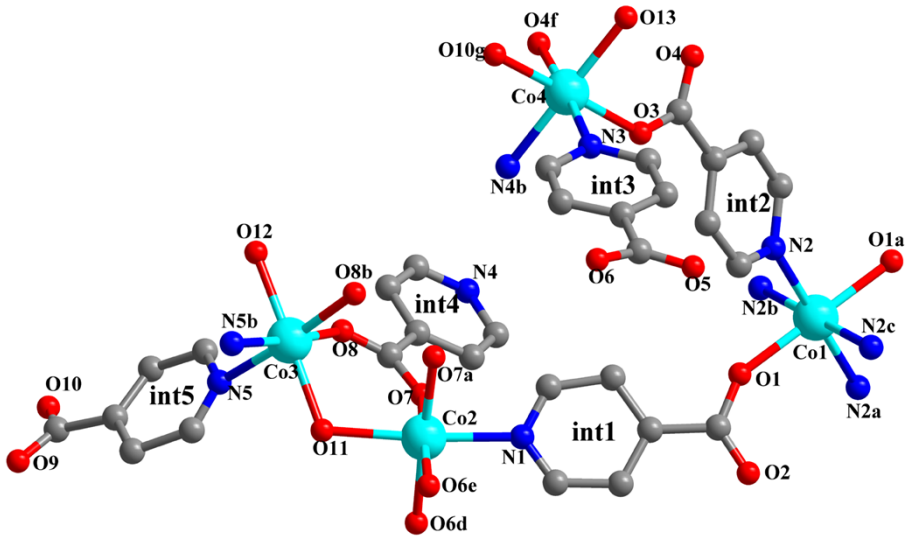

Fig.s1 View of an asymmetric unit of **1** (Symmetry transformations used to generate equivalent atoms: (a) -x, -y, -z+2; (b) x, -y, z; (c) -x, y, -z+2; (d) -x+1/2, y+1/2, -z+2; (e) -x+1/2, -y-1/2, -z+2; (f) -x, y, -z+1; (g) -x+1/2, y-1/2, -z+1).

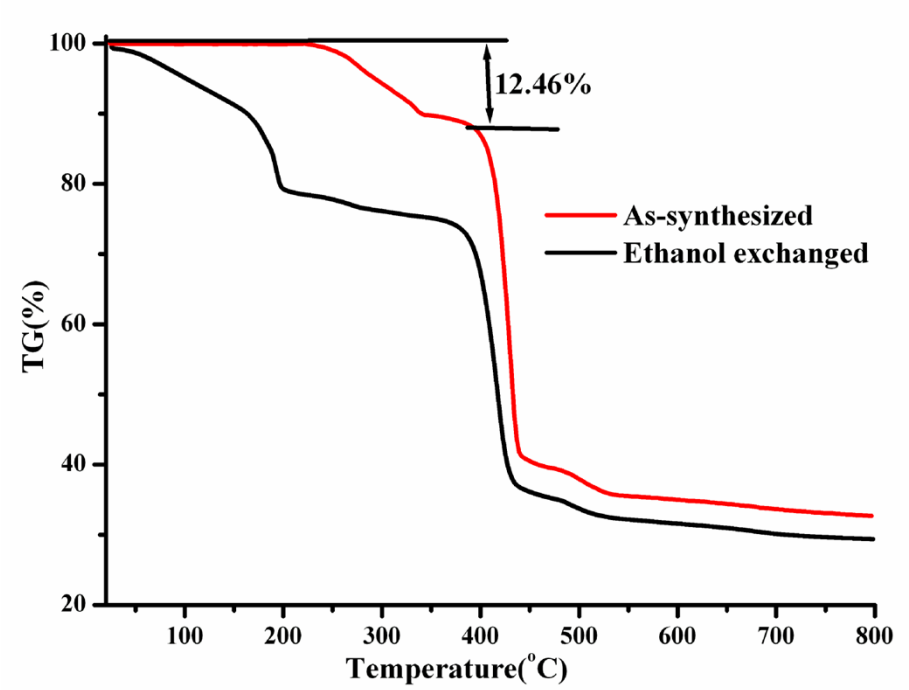

Fig.s2 the TG plots of 1.

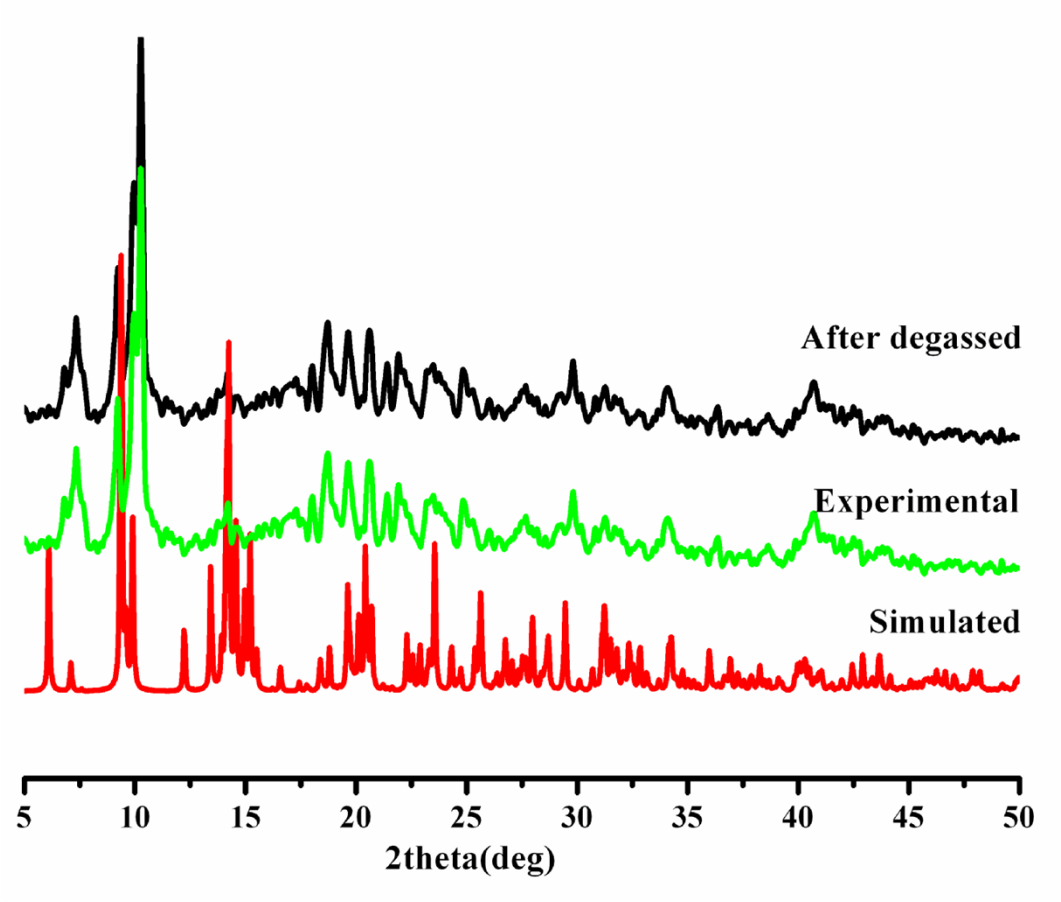

Fig.s3 the powder XRD (PXRD) patterns of **1** at different conditions.

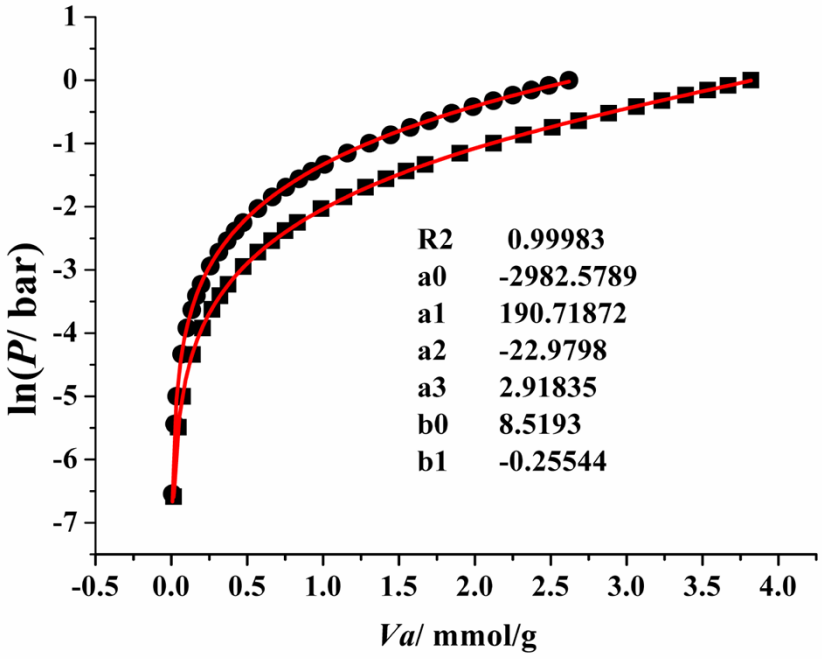

Figure S4. Virial analysis of the CO_2 sorption data for **1a**.

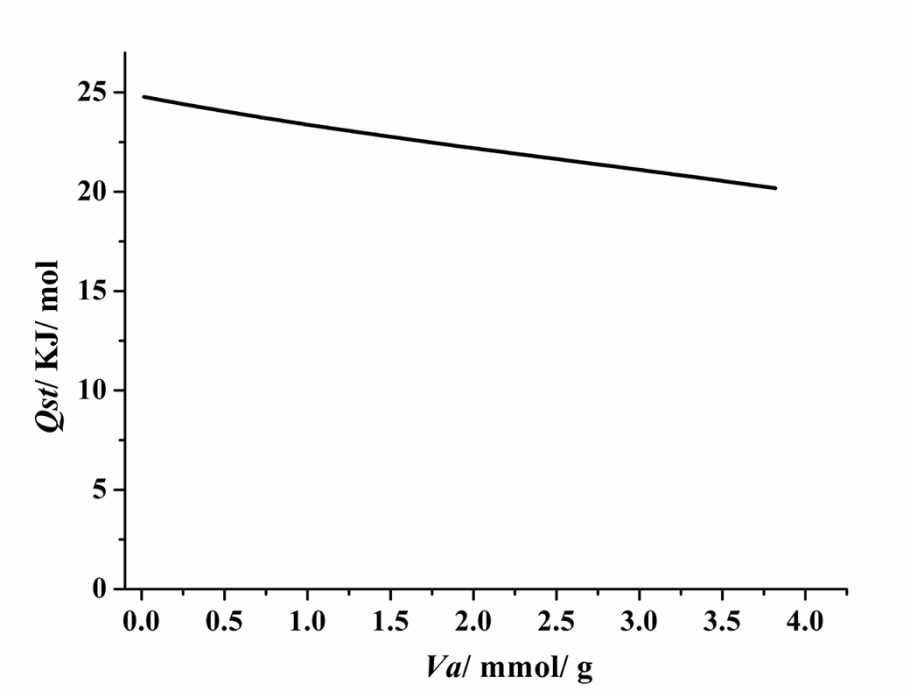

Figure S5. Heat of CO_2 adsorption for **1a** estimated by the virial equation.

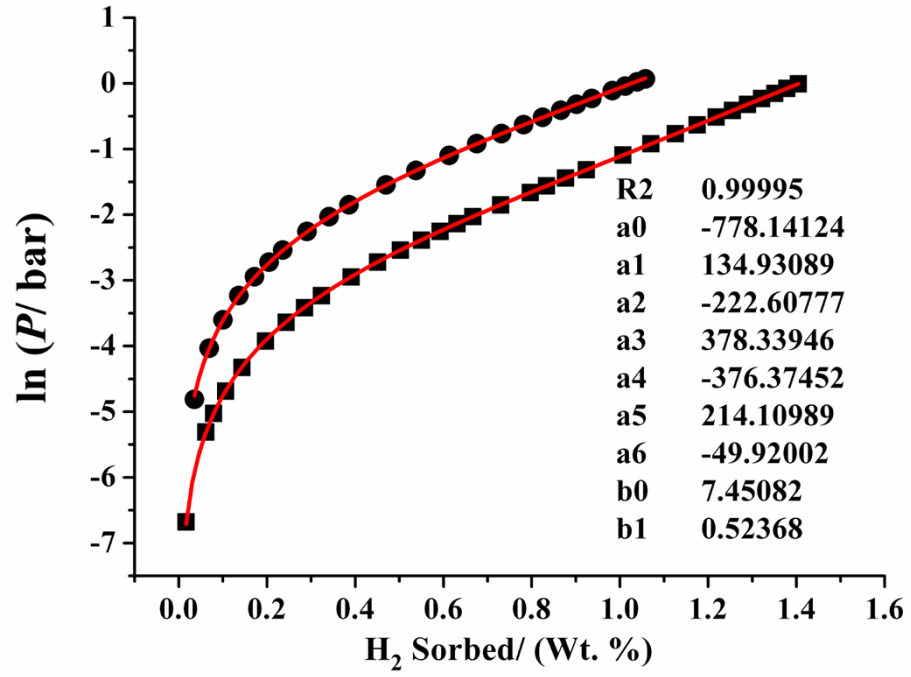

Figure S6. Virial analysis of the H_2 sorption data for **1a**.

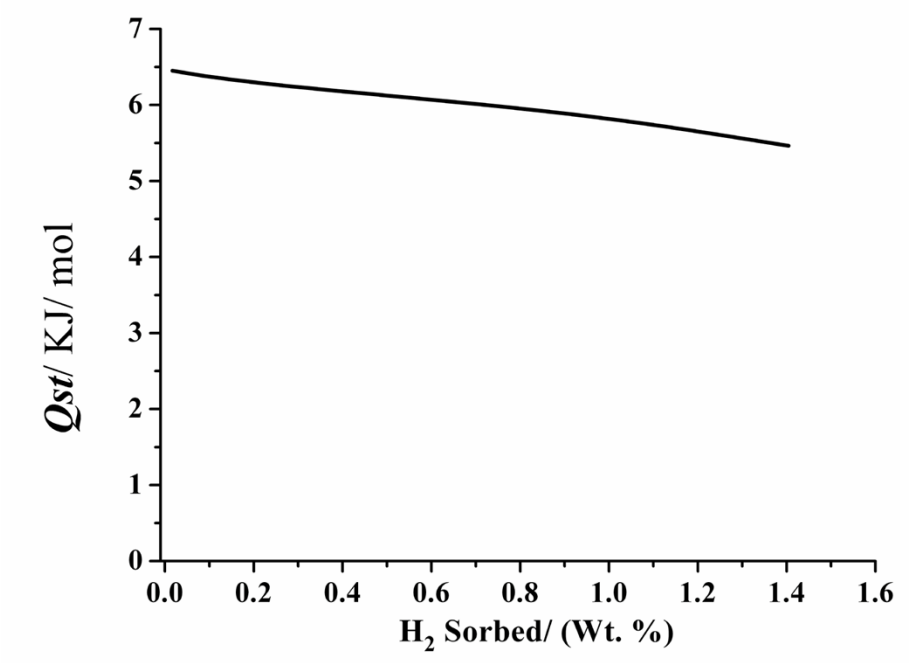

Figure S7. Heat of H_2 adsorption for **1a** estimated by the virial equation.