Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information (ESI)

A new Co(II) metal-organic framework with enhanced CO_2 adsorption and separation performance

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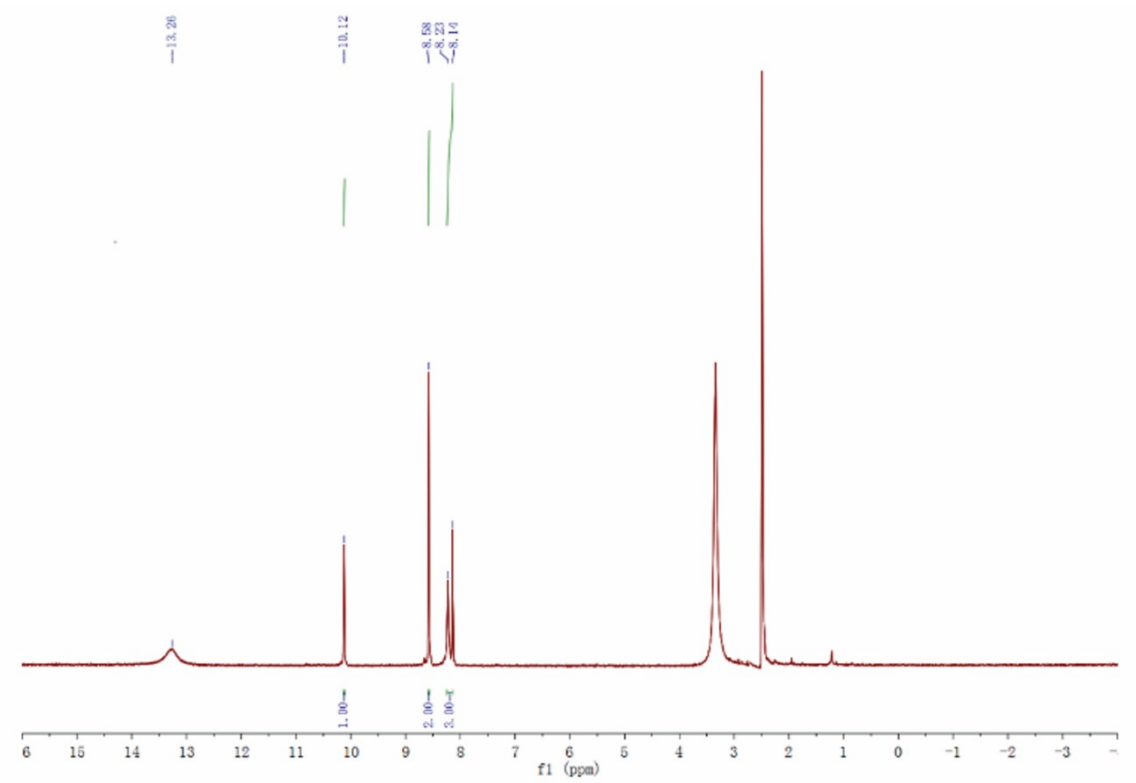

Fig. S1 ^{1}H NMR of H_3L

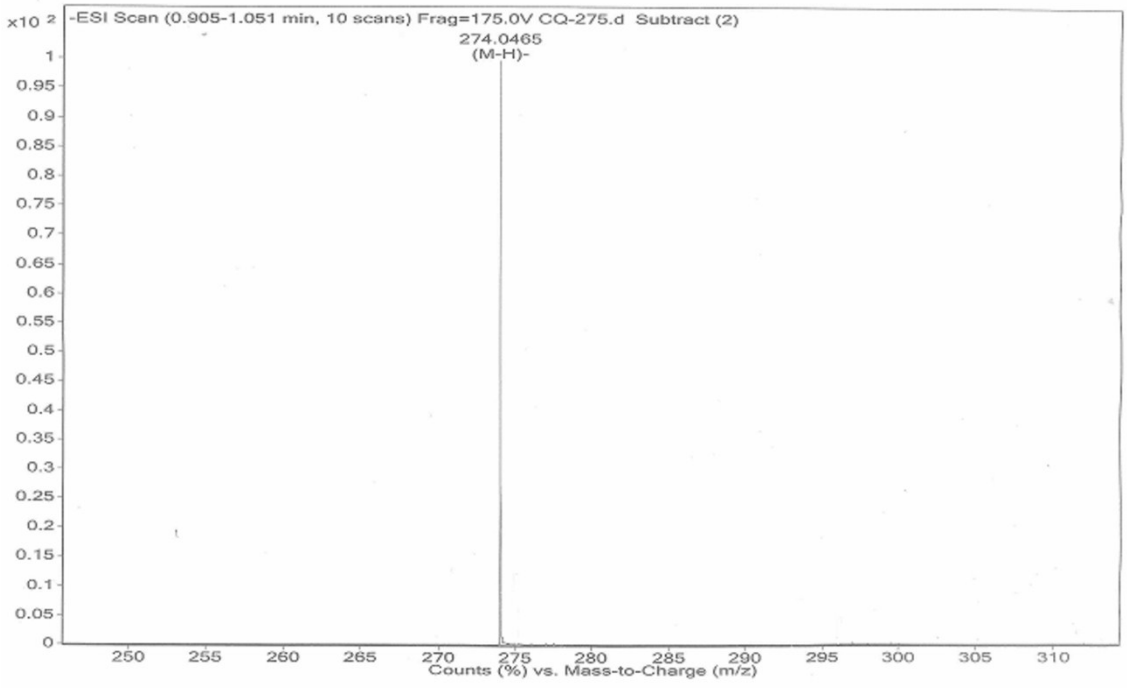

Fig. S2 MS, m/z of H_3L

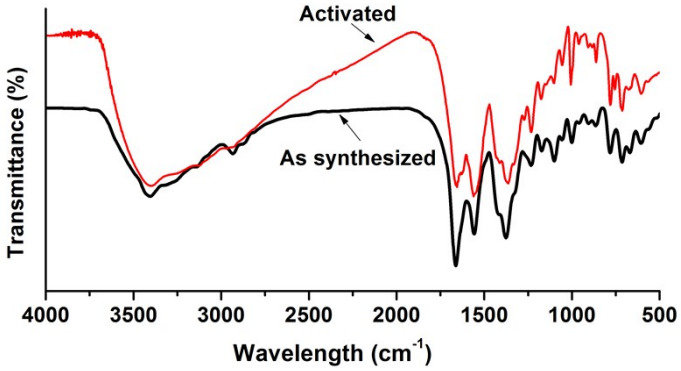

Fig. S3 IR spectra of as synthesized and activated **1**.

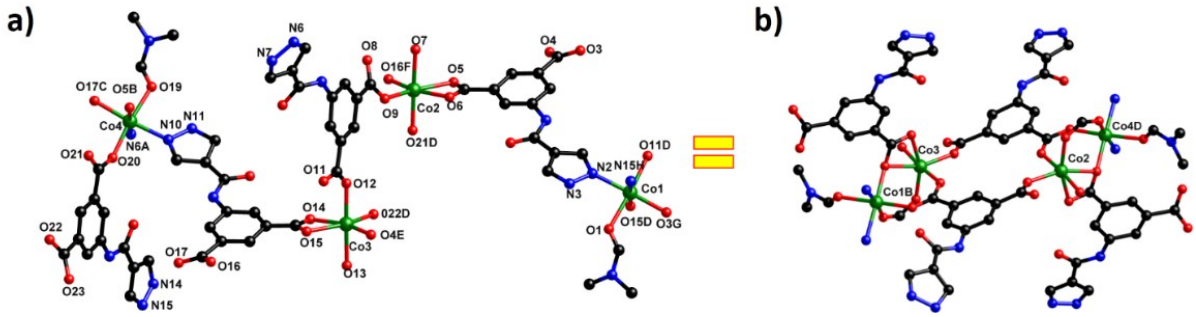

Fig. S4 Coordination modes in complex **1**. Symmetry code: A: -x+1,-y+1,z+1/2; B: x,y+1,z; C: x-1/2,-y+3/2,z; D: x,y-1,z; E: x+1/2,-y-1/2,z; F: x-1/2,-y+1/2,z; G: x+1/2,-y-3/2,z; H: -x+3/2,y-3/2,z-1/2. H atoms are omitted for clarity.

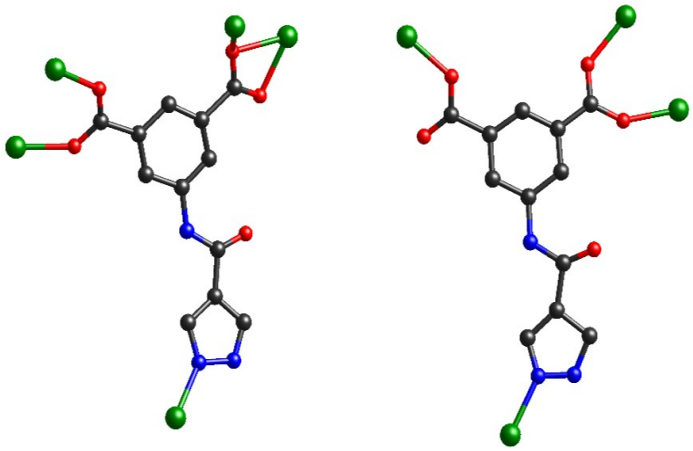

Fig. S5 Two kinds of coordination modes of HL^{2-}

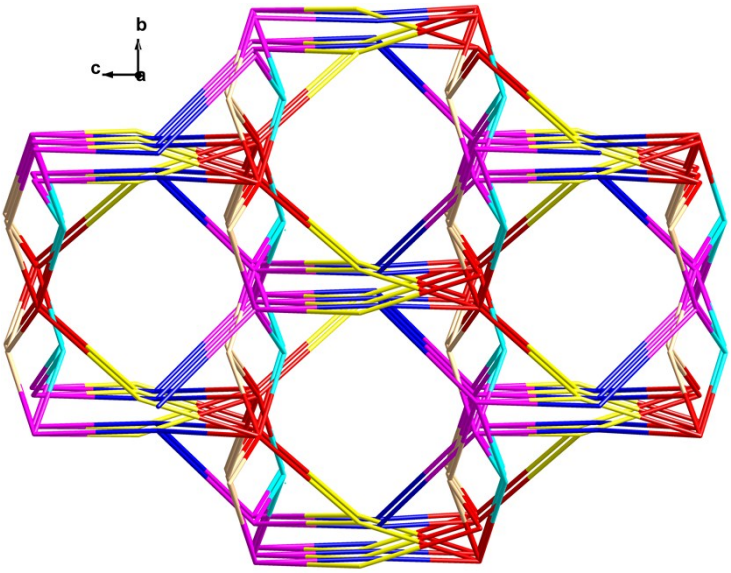

Fig.S6 The topological net with a Schäfli symbol of $(4\cdot6^2)_2\,(4^2\cdot6^8\cdot8^5)$.

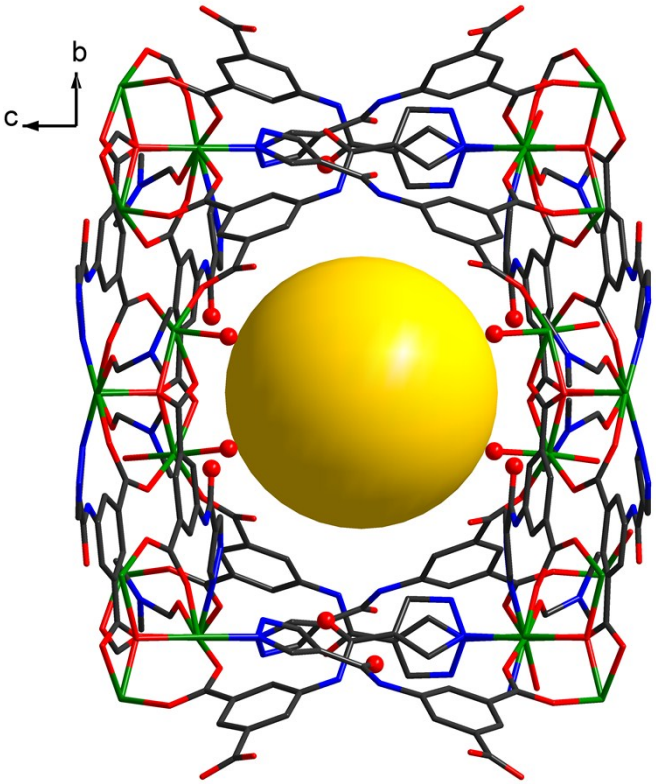

Fig. S7 1D pore decorated with functional sites along a direction (H atoms are omitted for clarity).

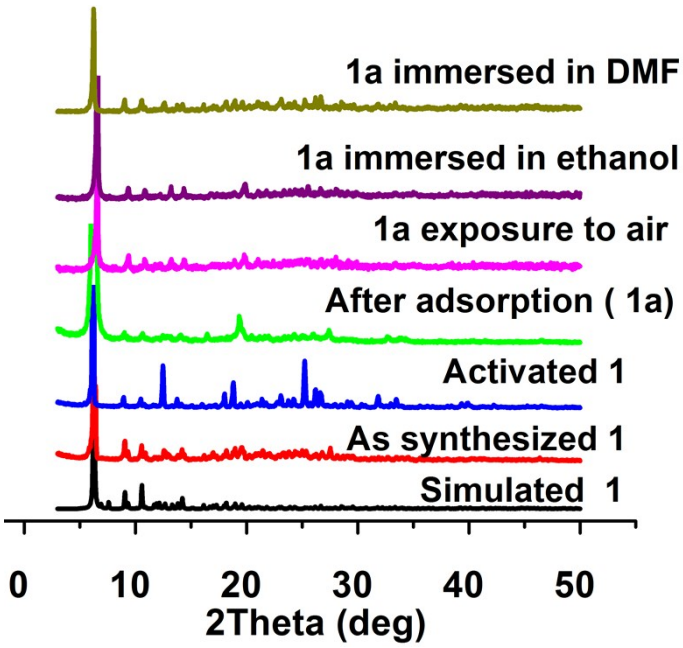

Fig. S8 PXRD of **1** from simulated, as-synthesized, activated and PXRD of **1a** exposed to air in some degree of humidity, immersed in DMF and ethanol for three days.

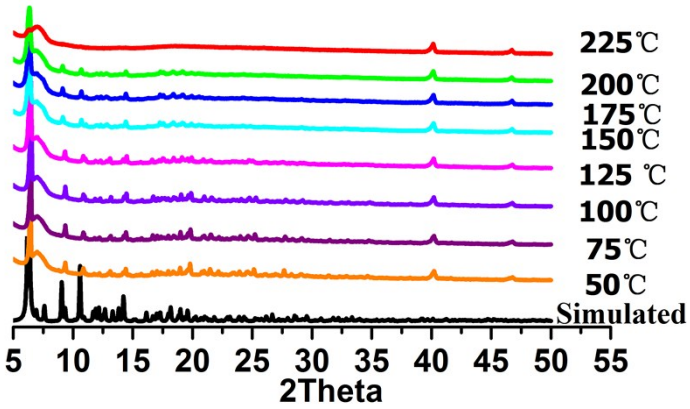

Fig. S9 Variable temperature power X-ray diffraction patterns of **1** at different temperatures.

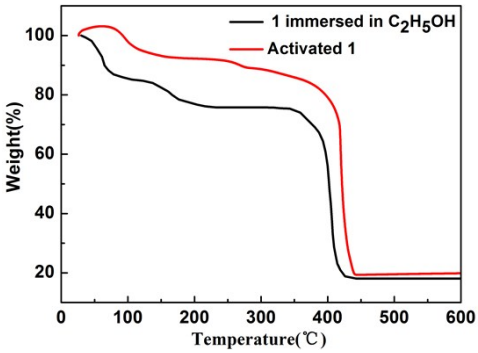

Fig. S10 Thermogravimetric curves. Black line: **1** immersed in C_2H_5OH for three days. Red line: Activated **1**. The initial rising in activated **1** may result from the rapid re-adsorption of trace moisture.

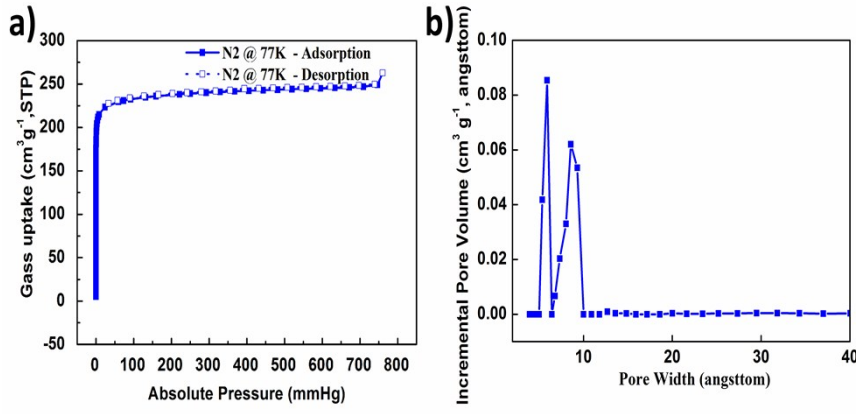

Fig. S11 a) The N_2 adsorption isotherms at 77K. **b)** The pore distribution according to the Density Functional Theory (DFT) model.

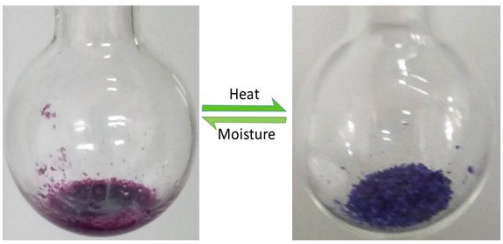

Fig. S12 Crystal photographs of original **1** and activated **1**. The color of activated samples turned blue while original one is pink and these activated samples were sensitive to moisture and could change their color quickly from blue to pink upon exposure to air.

DFT calculation

There are two possible adsorption sites (Fig. S13), which were predicted by DFT calculation (in WB97XD functional[1]) using Gaussian 09 program package[2] with Lanl2DZ pseudo potential basis sets for Co^{2+} and 6-31g basis sets for C, H, N and O atoms. The starting structures were derived from the partial crystal structure with a tentative introduction of CO_2 molecule around the polar sites. For saving time, only adsorption structure of CO_2 molecule was optimized while the structure of host network was fixed. The adsorption interaction energy $E_{interaction}$ was presented as following: $E_{interaction}=E(H\text{-}CO_2)-E(H)-E(CO_2)-E(BSSE)$

Where, $E(H\text{-}CO_2)$, $E(H)$, $E(CO_2)$ denotes the energy of MOF host-CO_2 complex, MOF host, and CO_2, respectively, while E(BSSE) denotes the basis set superposition errors.

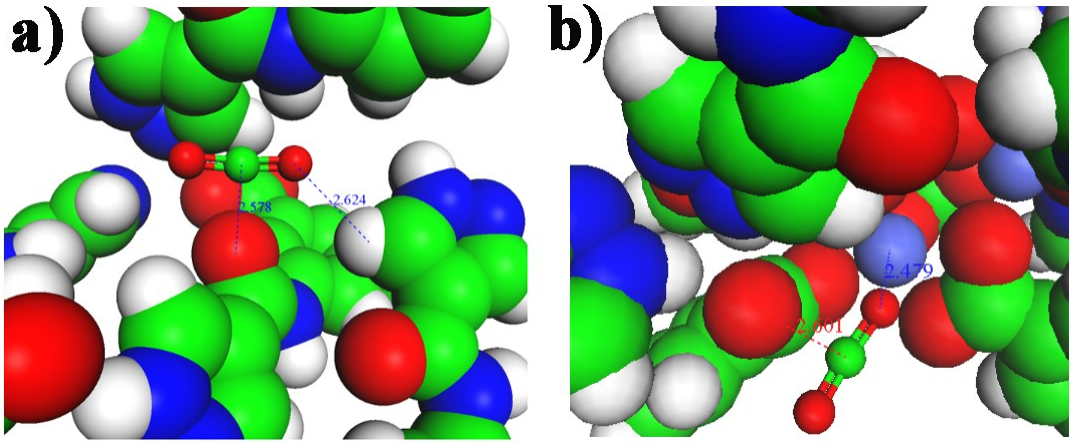

Fig. S13 Two possible adsorption modes of CO_2 inside MOFs predicted by DFT calculation: a) the adsorption occurred around the oxygen of acylamide group ($E_{interaction}$ = 34.2 kJ/mol); b) the adsorption occurred around the possible free metal ion site formed by removing the coordinated solvent molecule ($E_{interaction}$ = 29.5 kJ/mol). Color scheme: Co (pale blue), N (blue), O (red), C (green) and H (white).

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Table S1 The comparison of CO_2 adsorption amounts in complex **1** and reported MOFs.

MOF	CO_2 loading ($cm^3\ g^{-1}$) (273 K, 1.0 bar)	CO_2 loading ($cm^3\ g^{-1}$) (298 K, 1.0 bar)	Ref
Mg-MOF-74	225[a]	181	13
bio-MOF-11	133.4	89.6	8
JLU-Liu18	129	63	28
PCN-61	128.1	70.57	29
MIL-101Cr-NH_2	113.79	80.64[c]	17
This work	103.2	57.8	-
$(In_2X)(Me_2NH_2)_2(DMF)_9(H_2O)_5$	99.7	56.2	27
[Al(OH) (SBPDC)][b]	98.56	56.22	14
meso-HKUST-1	94.08	71.7	2
BUT-11	90	53.5	7
Zr-btdc	89.6	67.2	18
JLU-Liu15	89.3	51	24
BUT-10	88	50.6	7
ZIF-82	88	52.7	5
UiO-66-NO_2-NH_2	87.19	-	12
NENU-520	80.42	60.7	21
MIL-101Cr	78.62	53.31[c]	17
HKUST-1	78.2	67.2	1
ZIF-69	70.6	40.6	6
$\{[Zn_2(tpim)(aip)_2]\bullet 2.5DMF\bullet 2H_2O\}_n$	70	45	19
ZIF-68	67.2	37.6	6
InOF-8	66.2	44[d]	25
SNU-30’	58.63	25	9
$[Cu(tba)_2]_n$	51.8	43.9	22
MAF-2	49	19	11

DUT-5	48.38	32.48	14
$[Zn_3(tcpt)_2(H_2O)_2]$	44.86	31	16
MUF-77-ethyl	42.9	23	23
$[Zn_2(bpdc)_2(bpe)]$	40	27.76	10
$\{[Cd_2(sdb)_2\text{-}(3\text{-bpmh})_2]\}_n \bullet 3n(H_2O)$	38.2	29.2	20
MOF-205-OBn	37	20.4	15
ZIF-100	32.6	21.44	4
UCY-1	31.36	21.95	3
Pcp	29.12	-	30
$[Zn_2(HDDCBA)] \bullet 2DMF \bullet 2H_2O$	26.13	14.94	26
ZIF-95	-	19.7	31
[a]T=278K,[b]H_2SBPDC=2'-sulfone-biphenyl-4,4'-dicarboxylic acid, [c] T=293K, [d] T=295K			

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Table S2 Fitting parameters through the Langmuir–Freundlich equation.

T/K	gas	a	b	c	k	q	t	Adj. R-Square
273	CO_2	2.38924	0.05668	0.80957	4.12081E-4	4.70326	1.80904	1
273	N_2	0.15775	0.01503	0.96947	3.10493E-4	0.89794	1.41846	0.99997
273	CH_4	1.16371	0.00796	0.95404	1.81066E-4	5.39166	1.33954	1
298	CO_2	2.84249	0.02021	0.84501	1.01026E-4	4.14941	1.78044	0.99999
298	N_2	0.11095	0.01005	1.07695	1.80146E-5	2.95639	1.51404	0.9983
298	CH_4	0.06763	0.01911	1.23641	4.78906E-4	4.4043	1.17966	0.99966

Table S3 Comparison of CO_2/CH_4 (50:50) selectivity of **1** with those selected MOFs at 298 K and 1 bar calculated by IAST method.

NO.	MOF	Selectivity	Ref.
1	$[Cu(bpy)_2(SiF_6)]$	10.5	24
2	BUT-11	9.2[c]	7
3	MIL-68-Al	9.0[b]	2
4	This work	8.59[f]	-
5	$[Zn_2(HDDCBA)]\cdot 2DMF\cdot 2H_2O$	8.1	16
6	This work	7.25	-
7	HKUST-1	7.1	18
8	PCN-88	7.0[d]	23
9	UiO-66	6.87	22

10	$[Zn_2(py\text{-}CF_3)_2]_n$	6.2	10
11	MIL-125(Ti)	6.0	8
12	ZIF-100	5.9±0.4	5
13	$CNT@Cu_3(BTC)_2$	5.67	21
14	$(In_2X)(Me_2NH_2)_2(DMF)_9(H_2O)_5$	5.6	17
15	BUT-10	5.2[c]	7
16	ZIF-69	5.1	4
17	ZIF-68	5.0	4
18	ZIF-70	5.0	4
19	JLU-Liu18	4.5	19
20	UCY-1	4.4[a]	1
21	$Zn_2(2,6\text{-ndc})_2(dpni)$	4.4[d]	11
22	ZIF-95	4.3±0.4	5
24	MIX-MIL-125(Ti)	4.2	8
25	BPL carbon	3.9	6
26	NH_2-MIL-125(Ti)	3.9	8
27	Zeolite 13X	3.6	9
28	activated carbon A35/4	3.4[e]	13
29	JLU-Liu15	3.2	15
30	MOF-508b	3[b]	12
31	MOF-205-OBn	2.7	14
32	UiO-67	2.7[c]	7
33	MIL-53(Al)	2.3	3
34	Activated carbon	2.3	8
36	UMCM-1	1.82	20
37	ZIF-8	1.32	3
38	MOF-177	0.89	3

[a] in the low-pressure limit (near-zero coverage), [b] T=303 K, [c] CO_2/CH_4 =10:90, [d]T=296 K, [e]T=293 K, [f] CO_2/CH_4 =5:95

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Table S4 Comparison of CO_2/N_2 (15:85) selectivity of **1** with those selected MOFs at 1 bar and 298 K calculated by IAST method.

NO.	MOF	Selectivity	Ref.
1	PCN-88	45.2	3
2	This work	33.5	-
3	BUT-11	31.5	2
4	TMU-5	23.2	4
5	BUT-10	18.6	2
6	TMU-4	18.4	4
7	NOTT-101	13	6
8	UiO-67	9.4	2
9	MOF-205-OBn	6.5	1
10	SNU-150’	6.4	5

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Table S5 Fitting parameters (Adj. R-Square = 0.99965)

a0	-3373.53146	a4	-4.69265E12
a1	1.02548E6	b0	28.05291
a2	-4.41487E8	b1	-2274.33956
a3	5.71382E10	b2	754343.49318

Table S6 Selected bond lengths (Å) and angles (°) for complex **1**

Complex **1**			
Co(1)-O(11)#1	2.061(6)	O(11)#1-Co(1)-O(3)#2	95.4(2)
Co(1)-O(3)#2	2.070(6)	O(11)#1-Co(1)-O(15)#1	92.3(3)
Co(1)-O(15)#1	2.086(7)	O(3)#2-Co(1)-O(15)#1	90.8(2)
Co(1)-N(2)	2.095(8)	O(11)#1-Co(1)-N(2)	87.9(3)
Co(1)-O(1)	2.156(7)	O(3)#2-Co(1)-N(2)	173.5(3)
Co(1)-N(15)#3	2.186(9)	O(15)#1-Co(1)-N(2)	94.7(3)
Co(2)-O(9)	2.046(6)	O(11)#1-Co(1)-O(1)	175.2(3)
Co(2)-O(21)#1	2.048(6)	O(3)#2-Co(1)-O(1)	88.9(3)

Co(2)-O(16)#4	2.068(7)	O(15)#1-Co(1)-O(1)	89.8(3)
Co(2)-O(7)	2.114(7)	N(2)-Co(1)-O(1)	87.7(3)
Co(2)-O(6)	2.127(7)	O(11)#1-Co(1)-N(15)#3	90.4(3)
Co(2)-O(5)	2.200(6)	O(3)#2-Co(1)-N(15)#3	86.4(3)
Co(3)-O(22)#1	2.044(6)	O(15)#1-Co(1)-N(15)#3	176.3(3)
Co(3)-O(4)#5	2.044(6)	N(2)-Co(1)-N(15)#3	88.0(3)
Co(3)-O(12)	2.054(6)	O(1)-Co(1)-N(15)#3	87.7(3)
Co(3)-O(14)	2.133(7)	O(9)-Co(2)-O(21)#1	87.3(3)
Co(3)-O(13)	2.140(7)	O(9)-Co(2)-O(16)#4	99.0(3)
Co(3)-O(15)	2.200(6)	O(21)#1-Co(2)-O(16)#4	92.4(3)
Co(4)-O(20)	2.041(7)	O(9)-Co(2)-O(7)	89.5(3)
Co(4)-O(17)#6	2.046(7)	O(21)#1-Co(2)-O(7)	174.4(3)
Co(4)-N(6)#7	2.103(9)	O(16)#4-Co(2)-O(7)	92.7(3)
Co(4)-O(19)	2.108(7)	O(9)-Co(2)-O(6)	100.2(3)
Co(4)-N(10)	2.108(8)	O(21)#1-Co(2)-O(6)	89.7(3)
Co(4)-O(5)#8	2.125(6)	O(16)#4-Co(2)-O(6)	160.7(3)
O(12)-Co(3)-O(15)	93.8(2)	O(7)-Co(2)-O(6)	86.2(3)
O(14)-Co(3)-O(15)	60.2(2)	O(9)-Co(2)-O(5)	160.3(2)
O(13)-Co(3)-O(15)	89.2(3)	O(21)#1-Co(2)-O(5)	94.8(2)
O(20)-Co(4)-O(17)#6	96.4(3)	O(16)#4-Co(2)-O(5)	100.4(2)
O(20)-Co(4)-N(6)#7	88.5(3)	O(7)-Co(2)-O(5)	86.6(3)
O(17)#6-Co(4)-N(6)#7	90.8(3)	O(6)-Co(2)-O(5)	60.3(2)
O(20)-Co(4)-O(19)	172.6(3)	O(22)#1-Co(3)-O(4)#5	102.3(3)
O(17)#6-Co(4)-O(19)	89.1(3)	O(22)#1-Co(3)-O(12)	86.0(3)
N(6)#7-Co(4)-O(19)	86.4(3)	O(4)#5-Co(3)-O(12)	94.1(3)
O(20)-Co(4)-N(10)	88.6(3)	O(22)#1-Co(3)-O(14)	97.9(3)
O(17)#6-Co(4)-N(10)	174.8(3)	O(4)#5-Co(3)-O(14)	159.5(2)
N(6)#7-Co(4)-N(10)	87.9(3)	O(12)-Co(3)-O(14)	91.0(3)
O(19)-Co(4)-N(10)	85.8(3)	O(22)#1-Co(3)-O(13)	89.8(3)

O(20)-Co(4)-O(5)#8	92.8(3)	O(4)#5-Co(3)-O(13)	89.1(3)
O(17)#6-Co(4)-O(5)#8	89.3(2)	O(12)-Co(3)-O(13)	175.2(3)
N(6)#7-Co(4)-O(5)#8	178.6(3)	O(14)-Co(3)-O(13)	87.3(3)
O(19)-Co(4)-O(5)#8	92.2(2)	O(22)#1-Co(3)-O(15)	158.1(3)
N(10)-Co(4)-O(5)#8	92.0(3)	O(4)#5-Co(3)-O(15)	99.5(2)

Symmetry codes: #1 x,y-1,z; #2 x+1/2,-y-3/2,z; #3 -x+3/2,y-3/2,z-1/2; #4 x-1/2,-y+1/2,z; #5 x+1/2,-y-1/2,z; #6 x-1/2,-y+3/2,z; #7 -x+1,-y+1,z+1/2; #8 x,y+1,z.