Supporting Information

Gas sorption properties of a new three-dimensional In-ABDC MOF with a diamond net

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Calculation of isosteric heats of CO_2 adsorption

(1) Method 1 (Clausius-Clapeyron equation):

The subroutine implemented in the BEL Master program (BEL Japan) was used. The adsorption data measured at 273 and 298 K were used.

(2) Method 2 (Virial method):

In order to calculate the isosteric heat of adsorption (Q_{st}) using virial-type of equation. The following Clausius-Clapeyron equation (1) was used for the estimation of Q_{st}.

$$-Q_{st} = -RT^2 \frac{\partial \ln(P)}{\partial T} \quad (1)$$

The following virial-type of equation (2) was used for the curve fitting of combined adsorption data obtained at 273 and 298 K (OriginPro 8.1).

$$\ln(P) = \ln(n) + \frac{1}{T}\sum_{i=0}^{j} a_i n^i + \sum_{i=0}^{k} b_i n^i \quad (2)$$

The resulting polynomial coefficients are used for the calculation of the following equation (3) to get adsorption enthalpy. R is the universal gas constant.

$$-Q_{st} = -R\sum_{i=0}^{j} a_i n^i \quad (3)$$

ToposPro result

##################
1:C28 H16 In N4 O8
##################

Topology for In1

Atom In1 links by bridge ligands and has

Common vertex with					R(A-A)	f
In 1	1.0000	0.1268	1.2500	(0 0 0)	17.248A	1
In 1	0.0000	0.1268	0.2500	(-1 0-1)	17.248A	1
In 1	0.5000	0.6268	0.2500	(1 1 1)	17.254A	1
In 1	0.5000	0.6268	1.2500	(1 1 2)	17.254A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with InO8N4C28H16

Coordination sequences

In1:	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

In1 Point symbol:{6^6}
Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]

Point symbol for net: {6^6}
4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 (topos&RCSR.ttd) {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)]
(17092 types in 3 databases)
Elapsed time: 10.55 sec.

Table S1. Selected bond distances (Å) for **I**.

In(1)-O(1)#1	2.223(3)	In(1)-O(2)#1	2.302(3)
In(1)-O(1)	2.223(3)	In(1)-O(2)	2.302(3)
In(1)-O(3)	2.233(4)	In(1)-O(4)#1	2.310(3)
In(1)-O(3)#1	2.233(4)	In(1)-O(4)	2.310(3)
N(1)-N(1)#2	1.114(12)	N(2)-N(2)#3	1.108(15)

Table S2. Low-pressure CO_2 adsorption on MOFs [R1].

MOFs[a]	CO_2 (cm^3/g)	Temp. (K)	Pressure	References
Zn(PYDC)(dma)	140	195	100 kPa	R2
$Zn_2(cnc)_2(dpt)$	145	195	1 atm	R3
Zn(dtp)	99	195	1 atm	R4
$Zn(ABDC)(bpe)_{0.5}$	130	195	1 bar	R5
$Cu(fma)(bpe)_{0.5}$	100	195	1 bar	R6
$Zn_3(ntb)_2$	151	195	1 atm	R7
$Mn(HCOO)_2$	105	195	1 atm	R8
Zn(1,4-NDC)(bpa)	79.6	195	1 atm	R9
Zn(DABCO)(3,3'-TPDC)	69	196	1 atm	R10
$[Cu_5(Tz)_9][NO_3]$	49.7	195	1 atm	R11
$Cu_2(Glu)_2(bpa)$	70.0	196	1 atm	R12
$Cu_2(Glu)_2(bpp)$	100.0	196	1 atm	R12
Zn(Glu)(bpe)	76.0	196	1 atm	R13

[a] PYDC = 3,5-pyridinedicarboxylate; dma = *N*,*N*'-dimethylacetamide; cnc = 4-carboxycinnamic; dpt = 3,6-di-4-pyridyl-1,2,4,5-tetrazine; dtp = 2,3-di(tetrazolate-5-yl)pyrazine; ABDC = 4,4'-azobenzenedicarboxylate; bpe = 1,2-bis(4-pyridyl)ethylene; fma = fumarate; ntb = 4,4',4''-nitrilotrisbenzoate; 1,4-NDC = 1,4-naphthalenedicarboxylate; bpa = 1,2-bis(4-pyridyl)ethane; DABCO = 1,4-diazabicyclo[2,2,2]octane; 3,3'-TPDC = terphenyl-3,3'-dicarboxylate; Tz = tetrazolate; Glu = glutarate; bpp = 1,2-bis(4-pyridyl)propane.

Table S3. Low-pressure hydrogen adsorption on MOFs at 77 K and 1 atm [R14].

MOFs[a]	Surface area (m^2/g)	H_2 (wt.%)	References
$Zn_4O(1,4\text{-}BDC)_3$, MOF-5	2900 (BET)	1.32	R15
$Zn_4O(C_8H_3BrO_4)_3$, IRMOF-2	1722 (BET)	1.20	R16
$Zn_4O(C_8H_5NO_4)_3$, IRMOF-3	3563 (Langmuir)	1.40	R17
$Zn_4O(2,6\text{-}NDC)_3$, IRMOF-8	1466 (Langmuir)	1.50	R15
$Zn_4O(BTB)_3$, MOF-177	4526 (Langmuir)	1.25	R15
$Zn_2(1,4\text{-}BDC)_2(DABCO)$	1450 (BET)	2.00	R18
$Zn_2(2,6\text{-}NDC)_2(DABCO)$	1000 (BET)	1.70	R19
$Mn(HCO_2)_2$	297 (BET)	0.90	R20
$Mn_3(BDT)_3$	290 (BET)	0.97	R21
$Cu_3(BTC)_2$, HKUST-1	1239 (BET)	2.18	R22
$Cu_3(TATB)_2(H_2O)_3$	3800 (Langmuir)	1.91	R23
Ni(cyclam)(BPYDC)	817 (Langmuir)	1.10	R24
$Mg_3(2,6\text{-}NDC)_3$	190 (BET)	0.48	R25
$[Et_2NH_2][In(2,6\text{-}NDC)_2]$	891 (BET)	1.62	R26
$[Me_2NH_2][In(BPDC)_2]$	638 (BET)	0.66	R27

[a] 1,4-BDC = 1,4-benzenedicarboxylate; 2,6-NDC = 2,6-naphthalenedicarboxylate; BTB = 1,3,5-benzenetribenzoate; DABCO = 1,4-diazabicyclo[2,2,2]octane; BDT = 1,4-benzeneditetrazolate; BTC = 1,3,5-benzenetricarboxylate; TATB = 4,4',4''-s-triazine-2,4,6-triyltribenzoate; cyclam = 1,4,8,11-tetraazacyclotetradecane; BPYDC = 2,2'-bipyridyl-5,5'-dicarboxylate; BPDC = 4,4'-biphenyldicarboxylate.

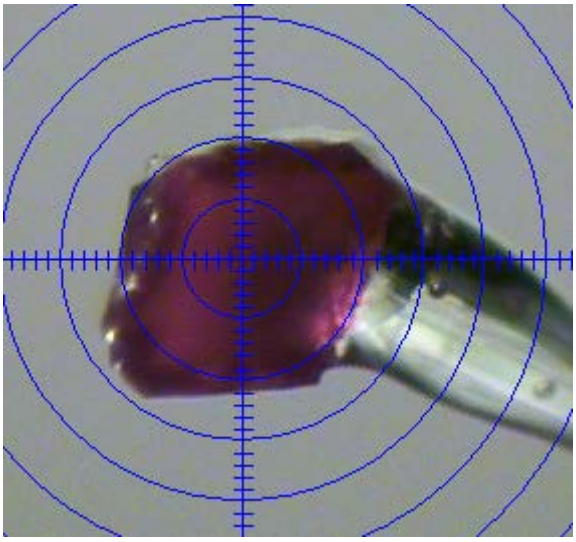


Figure S1. Crystal shape of **I**.

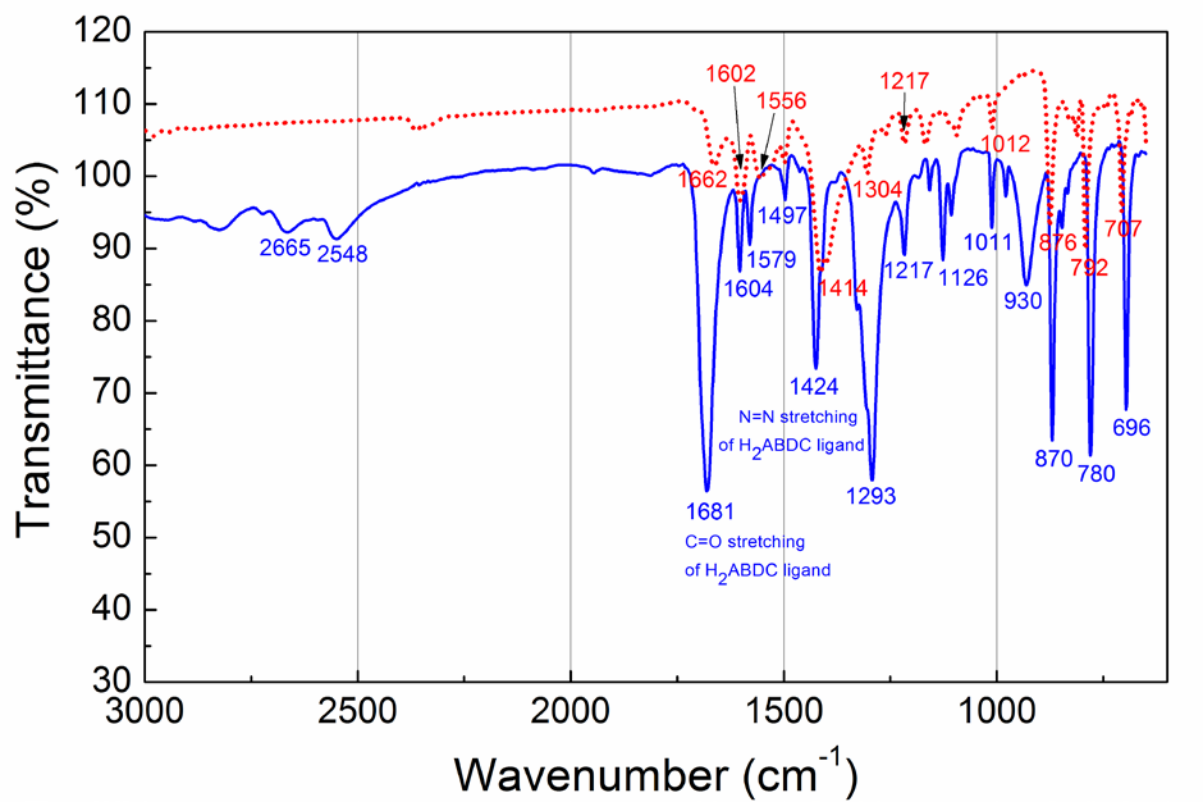


Figure S2. FT-IR spectra of free H_2ABDC (blue solid line) and as-prepared **I** (red dotted line).

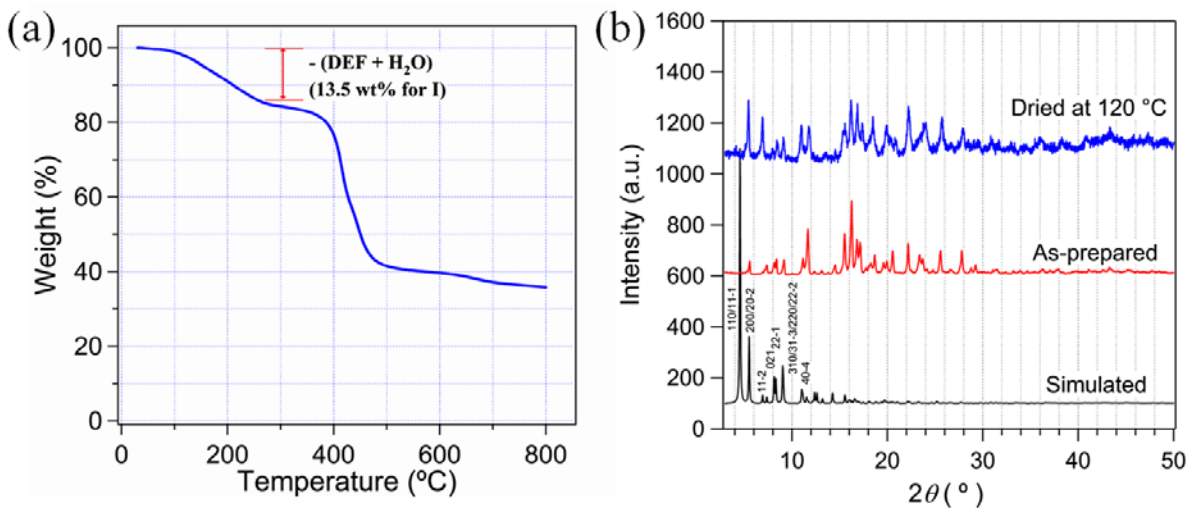


Figure S3. TG curve for the as-prepared **I** (a) and PXRD patterns (b).

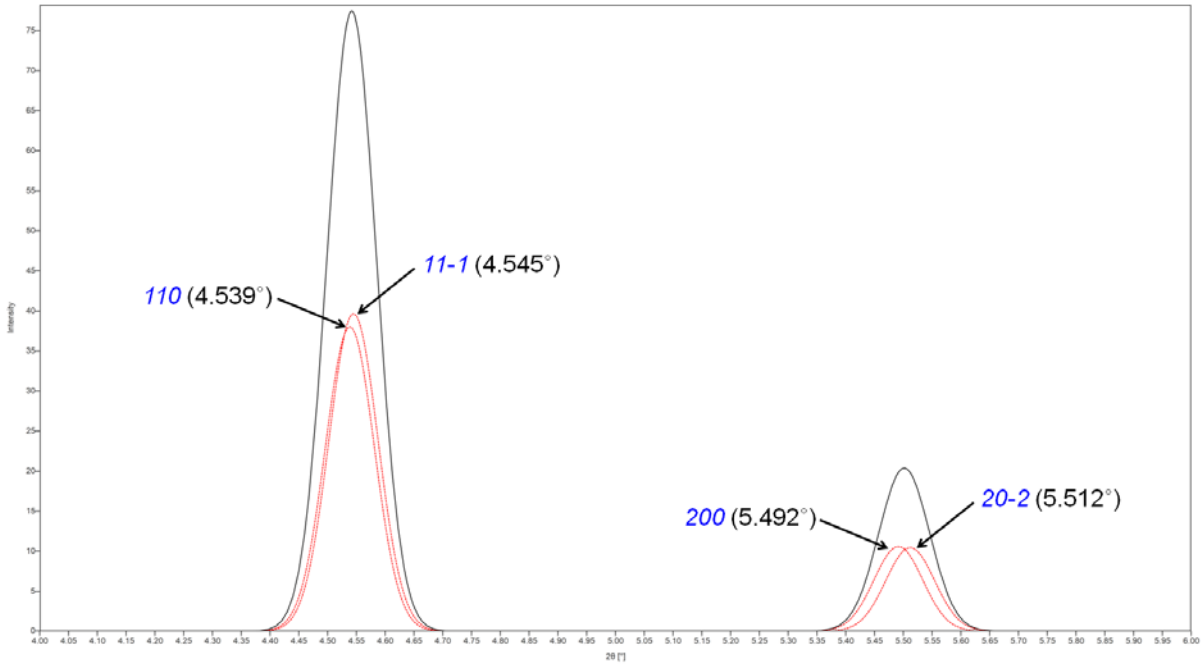


Figure S4. Expanded view of the low-angle region of PXRD pattern calculated from X-ray crystal structure of the as-prepared **I**. Two almost identical 2θ angles of (110) and (11-1) planes are clearly seen.

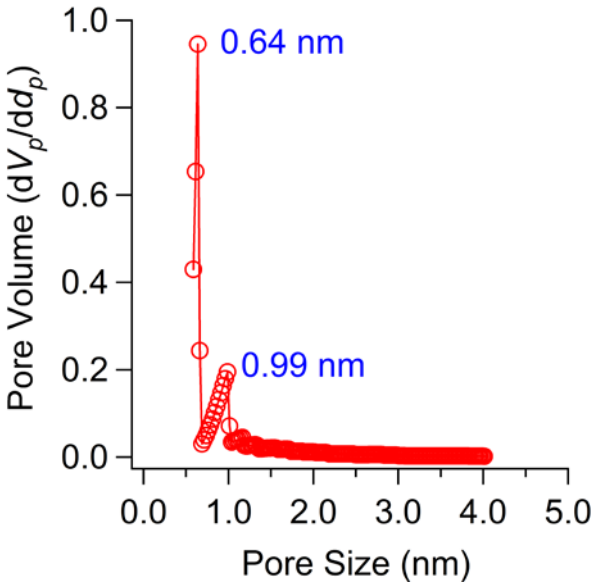
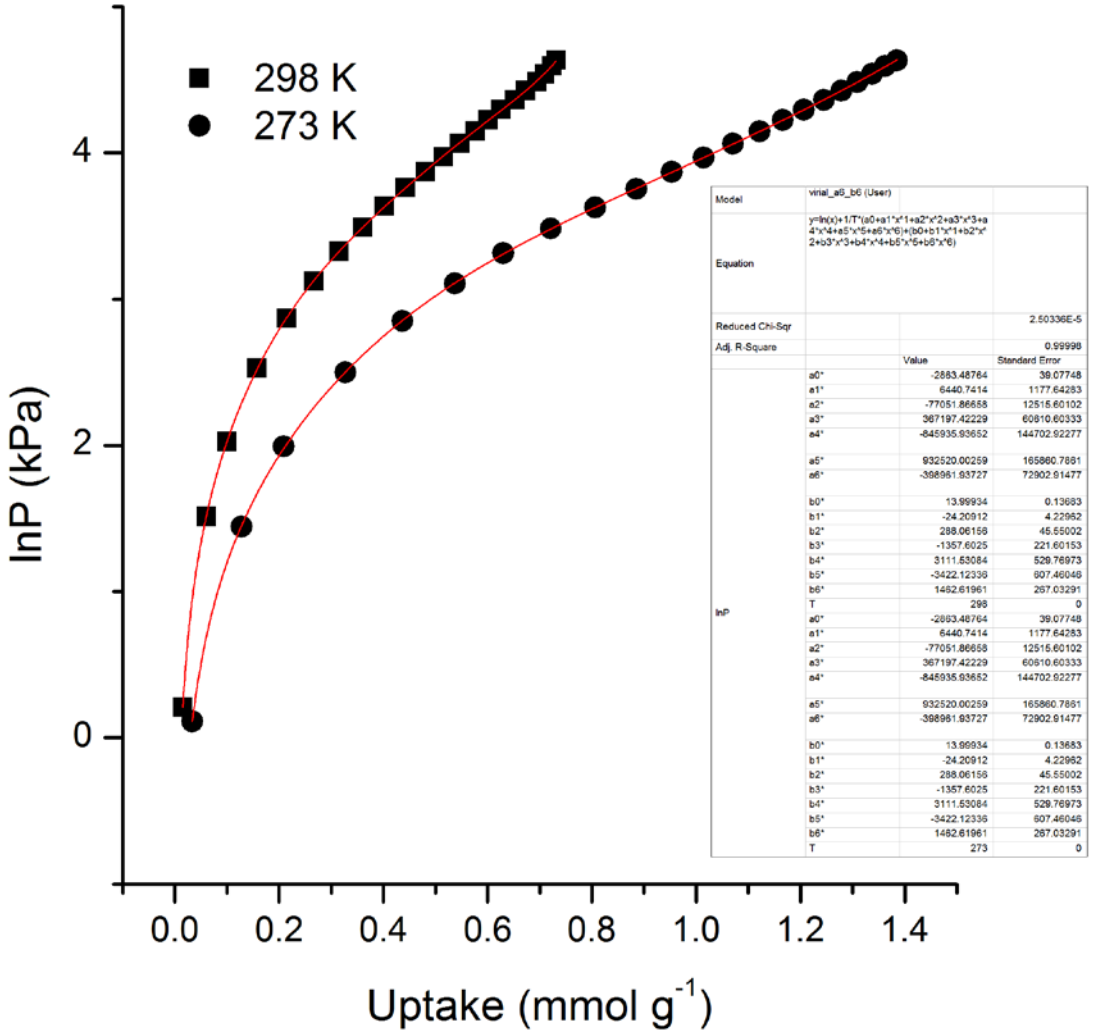


Figure S5. The Horváth-Kawazoe (HK) pore size distribution of solvent-free **I**.



Model	virial_a5_b6 (User)		
Equation	y=ln(x)+1/T*(a0+a1*x^1+a2*x^2+a3*x^3+a4*x^4+a5*x^5+a6*x^6)+(b0+b1*x^1+b2*x^2+b3*x^3+b4*x^4+b5*x^5+b6*x^6)		
Reduced Chi-Sqr			2.50336E-5
Adj. R-Square			0.99998
		Value	Standard Error
lnP	a0*	-2883.48764	39.07748
	a1*	6440.7414	1177.64283
	a2*	-77051.86658	12515.60102
	a3*	367197.42229	60810.60333
	a4*	-845935.93652	144702.92277
	a5*	932520.00259	165860.7881
	a6*	-398981.93727	72902.91477
	b0*	13.99934	0.13683
	b1*	-24.20912	4.22962
	b2*	288.06158	45.55002
	b3*	-1357.6025	221.60153
	b4*	3111.53084	529.76973
	b5*	-3422.12336	607.46046
	b6*	1462.61961	267.03291
	T	298	0
lnP	a0*	-2883.48764	39.07748
	a1*	6440.7414	1177.64283
	a2*	-77051.86658	12515.60102
	a3*	367197.42229	60810.60333
	a4*	-845935.93652	144702.92277
	a5*	932520.00259	165860.7881
	a6*	-398981.93727	72902.91477
	b0*	13.99934	0.13683
	b1*	-24.20912	4.22962
	b2*	288.06158	45.55002
	b3*	-1357.6025	221.60153
	b4*	3111.53084	529.76973
	b5*	-3422.12336	607.46046
	b6*	1462.61961	267.03291
	T	273	0

Figure S6. Virial fitting of the combined data for CO_2 adsorption at 273 and 298 K (OriginPro 8.1).

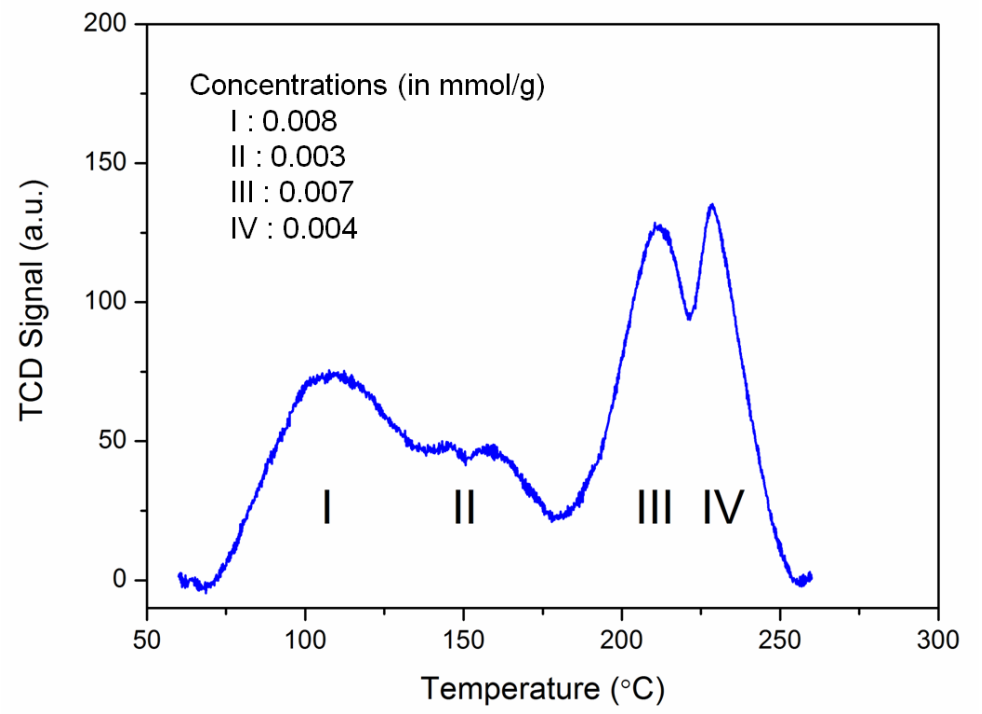


Figure S7. CO_2-TPD profile of the solvent-free **I**.

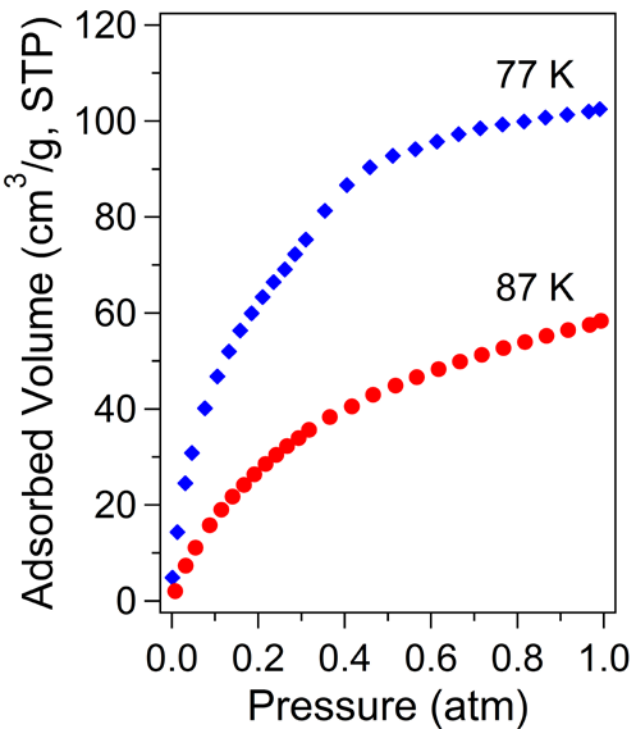
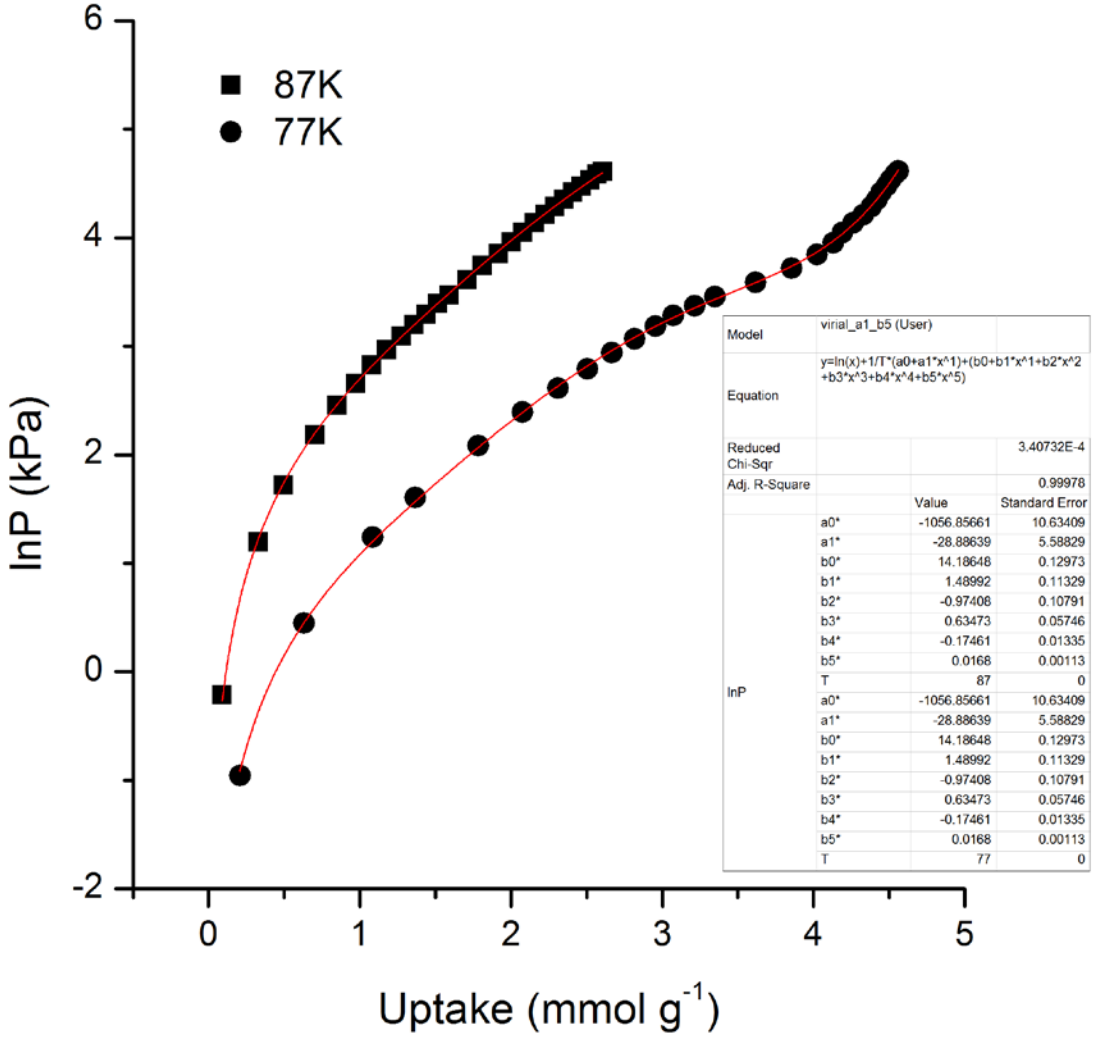


Figure S8. H_2 adsorption isotherms measured at 77 and 87 K for the solvent-free **I**.



Model	virial_a1_b5 (User)		
Equation	y=ln(x)+1/T*(a0+a1*x^1)+(b0+b1*x^1+b2*x^2+b3*x^3+b4*x^4+b5*x^5)		
Reduced Chi-Sqr			3.40732E-4
Adj. R-Square			0.99978
		Value	Standard Error
	a0*	-1056.85661	10.63409
	a1*	-28.88639	5.58829
	b0*	14.18648	0.12973
	b1*	1.48992	0.11329
	b2*	-0.97408	0.10791
	b3*	0.63473	0.05746
	b4*	-0.17461	0.01335
	b5*	0.0168	0.00113
	T	87	0
lnP	a0*	-1056.85661	10.63409
	a1*	-28.88639	5.58829
	b0*	14.18648	0.12973
	b1*	1.48992	0.11329
	b2*	-0.97408	0.10791
	b3*	0.63473	0.05746
	b4*	-0.17461	0.01335
	b5*	0.0168	0.00113
	T	77	0

Figure S9. Virial fitting of the combined data for H_2 adsorption at 77 and 87 K (OriginPro 8.1).

References

[R1] J.-R. Li, Y. Ma, M. C. McCarthy, J. Sculley, J. Yub, H.-K. Jeong, P. B. Balbuena, H.-C. Zhou, Coord. Chem. Rev. **2011**, 255, 1791.

[R2] H. Chun, J. Seo, Inorg. Chem. **2009**, 48, 9980.

[R3] M. Xue, S. Q. Ma, Z. Jin, R. M. Schaffino, G. S. Zhu, E. B. Lobkovsky, S. L. Qiu, B. L. Chen, Inorg. Chem. **2008**, 47, 6825.

[R4] J. R. Li, Y. Tao, Q. Yu, X. H. Bu, H. Sakamoto, S. Kitagawa, Chem. Eur. J. **2008**, 14, 2771.

[R5] B. L. Chen, S. Q. Ma, E. J. Hurtado, E. B. Lobkovsky, H.-C. Zhou, Inorg. Chem. **2007**, 46, 8490.

[R6] B. L. Chen, S. Q. Ma, F. Zapata, F. R. Fronczek, E. B. Lobkovsky, H.-C. Zhou, Inorg. Chem. **2007**, 46, 1233.

[R7] M. P. Suh, Y. E. Cheon, E. Y. Lee, Chem. Eur. J. **2007**, 13, 4208.

[R8] D. N. Dybtsev, H. Chun, S. H. Yoon, D. Kim, K. Kim, J. Am. Chem. Soc. **2004**, 126, 32.

[R9] P. Kanoo, T. K. Maji, Eur. J. Inorg. Chem. **2010**, 3762.

[R10] J.-M. Gu, T.-H. Kwon, J.-H. Park, S. Huh, Dalton Trans. **2010**, 39, 5608.

[R11] D. C. Zhong, W. G. Lu, L. Jiang, X. L. Feng, T. B. Lu, Cryst. Growth Des. **2010**, 10, 739.

[R12] I. H. Hwang, J. M. Bae, W.-S. Kim, Y. D. Jo, C. Kim, Y. Kim, S.-J. Kim, S. Huh, Dalton Trans. **2012**, 41, 12759.

[R13] I. H. Hwang, J. M. Bae, Y.-K. Hwang, H.-Y. Kim, C. Kim, S. Huh, S.-J. Kim, Y. Kim, Dalton Trans. **2013**, 42, 15645.

[R14] Y. H. Hu, L. Zhang, Adv. Mater. **2010**, 22, E117.

[R15] J. L. C. Rowsell, A. R. Millward, K. S. Park, O. M. Yaghi, J. Am. Chem. Soc. **2004**, 126, 5666.

[R16] J. L. Rowsell, O. M. Yaghi, J. Am. Chem. Soc. **2006**, 128, 1304.

[R17] D. Kim, T. B. Lee, S. B. Choi, J. H. Yoon, J. Kim, S. H. Choi, Chem. Phys. Lett. **2006**, 420, 256.

[R18] S. R. Batten, R. Robson, Angew. Chem, Int. Ed. **1998**, 37, 1460.

[R19] H. Chun, D. N. Dybtsev, H. Kim, K. Kim, Chem. Eur. J. **2005**, 11, 3521.

[R20] J. L. C. Rowsell, O. M. Yaghi, Angew. Chem. Int. Ed. **2005**, 44, 4670.

[R21] M. Dincă, A. F. Yu, J. R. Long, J. Am. Chem. Soc. **2006**, 128, 8904.

[R22] P. Krawiec, M. Kramer, M. Sabo, R. Kunschke, H. Frode, S. Kaskel, Adv. Eng. Mater. **2006**, 8, 293.

[R23] J. Y. Lee, L. Pan, S. R. Kelly, J. Jagiello, T. J. Emge, J. Li, Adv. Mater. **2005**, 17, 2703.

[R24] E. Y. Lee, M. P. Suh, Angew. Chem. Int. Ed. **2004**, 43, 2798.

[R25] M. Dincă, J. R. Long, J. Am. Chem. Soc. **2005**, 127, 9376.

[R26] S. Huh, T.-H. Kwon, N. Park, S.-J. Kim, Y. Kim, Chem. Commun. **2009**, 4953.

[R27] J.-M. Gu, S.-J. Kim, Y. Kim, S. Huh, CrystEngComm, **2012**, 14, 1819.