気体吸蔵に使える MOF（Omar Yaghi の仕事から）

Nature, **402**, 276 (1999).

Design and synthesis of an exceptionally stable and highly porous metal-organic framework

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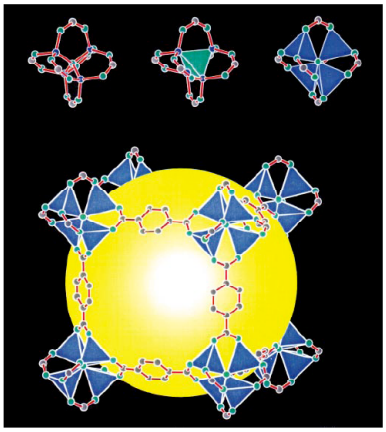

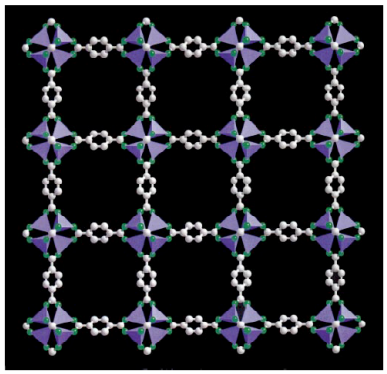

Figure 1 Construction of the MOF-5 framework. Top, the $Zn_4(0)O_{12}C_6$ cluster. Left, as a ball and stick model (Zn, blue; O, green; C, grey). Middle, the same with the $Zn_4(0)$ tetrahedron indicated in green. Right, the same but now with the ZnO_4 tetrahedra indicated in blue. Bottom, one of the cavities in the $Zn_4(0)(BDC)_3$, MOF-5, framework. Eight clusters (only seven visible) constitute a unit cell and enclose a large cavity, indicated by a yellow sphere of diameter 18.5 Å in contact with 72 C atoms (grey).

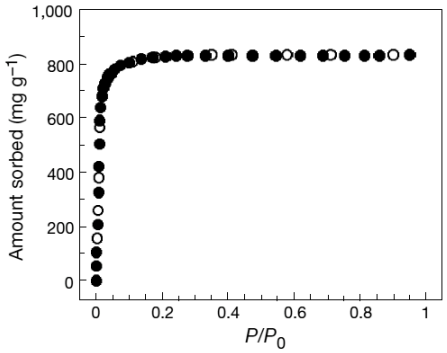

Figure 3 Nitrogen gas sorption isotherm at 78 K for MOF-5 (filled circles, sorption; open circles desorption). P/P_0 is the ratio of gas pressure (P) to saturation pressure (P_0), with $P_0 = 746$ torr.

Table 1 Gas and liquid vapour sorption in desolvated MOF-5

Sorbate	T (°C)	Amount sorbed (mg g^{-1})	Sorbate molecules per unit cell	Free volume (cm^3 g^{-1})	Free volume (cm^3 cm^{-3})
Ar	−194	1,492	230	1.03	0.61
N_2	−194	831	183	1.04	0.61
CH_2Cl_2	22	1,211	88	0.93	0.55
$CHCl_3$	22	1,367	71	0.94	0.55
C_6H_6	22	802	63	0.94	0.55
CCl_4	22	1,472	59	0.94	0.56
C_6H_{12}	22	703	51	0.92	0.54

Science, **300**, 1127 (2003).

Hydrogen Storage in Microporous Metal-Organic Frameworks

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Metal-organic framework-5 (MOF-5) of composition $Zn_4O(BDC)_3$ (BDC = 1,4-benzenedicarboxylate) with a cubic three-dimensional extended porous structure adsorbed hydrogen up to 4.5 weight percent (17.2 hydrogen molecules per formula unit) at 78 kelvin and 1.0 weight percent at room temperature and pressure of 20 bar. Inelastic neutron scattering spectroscopy of the rotational transitions of the adsorbed hydrogen molecules indicates the presence of two well-defined binding sites (termed I and II), which we associate with hydrogen binding to zinc and the BDC linker, respectively. Preliminary studies on topologically similar isoreticular metal-organic framework-6 and -8 (IRMOF-6 and -8) having cyclobutylbenzene and naphthalene linkers, respectively, gave approximately double and quadruple (2.0 weight percent) the uptake found for MOF-5 at room temperature and 10 bar.

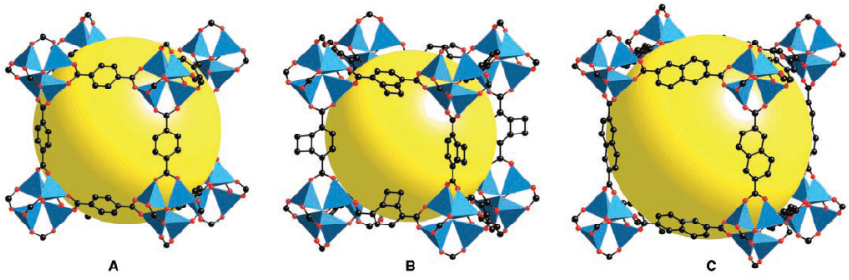


Fig. 1. Single-crystal x-ray structures of MOF-5 (A), IRMOF-6 (B), and IRMOF-8 (C) illustrated for a single cube fragment of their respective cubic three-dimensional extended structure. On each of the corners is a cluster $[OZn_4(CO_2)_6]$ of an oxygen-centered Zn_4 tetrahedron that is bridged by six carboxylates of an organic linker (Zn, blue polyhedron; O, red spheres; C, black spheres). The large yellow spheres represent the largest sphere that would fit in the cavities without touching the van der Waals atoms of the frameworks. Hydrogen atoms have been omitted.

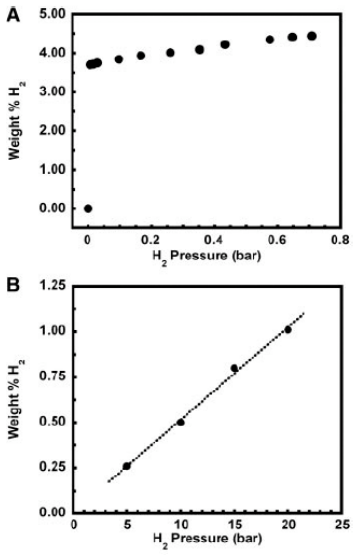


Fig. 2. Hydrogen gas sorption isotherm for MOF-5 at (A) 78 K and (B) 298 K.

（北川進先生 の仕事から）

Angew. Chem. Int. Ed. **2000**, *39*, 2082.

COMMUNICATIONS

A New, Methane Adsorbent, Porous Coordination Polymer [{$CuSiF_6(4,4'\text{-bipyridine})_2$}$_n$]

Shin-ichiro Noro, Susumu Kitagawa,* Mitsuru Kondo, and Kenji Seki

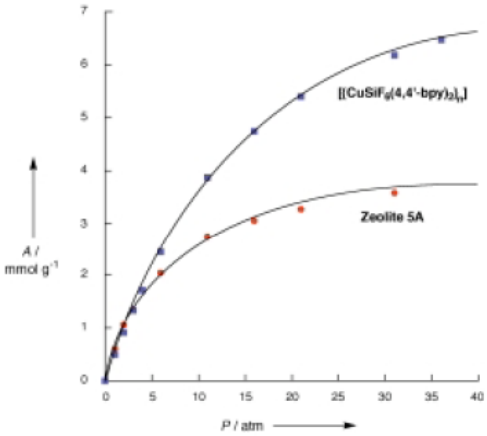
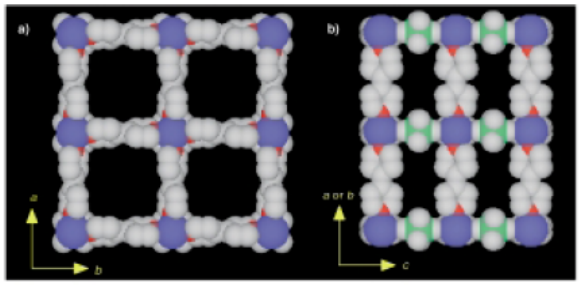


Figure 4. Methane adsorption isotherms at 298 K over a pressure range 0–36 atm (A = absolute adsorption).



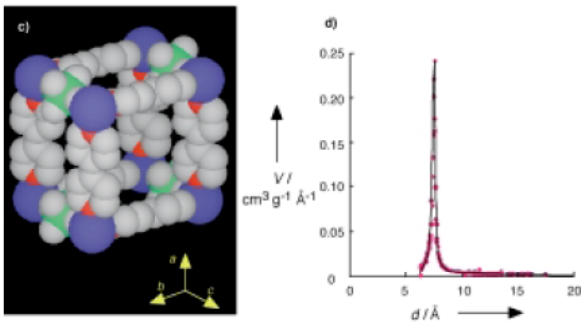


Figure 2. a) Space filling model of the channel structures along the c axis. b) Along the a or b axes. c) The 3D network. Atomic colors are as per Figure 1. The hydrogen atoms, one pyridine ring of the disordered 4,4′-bpy ligand, and crystallized water molecules are omitted for clarity. The pore size given in the text was estimated from this Figure when all the hydrogen atoms are added to the 4,4′-bpy molecules in a space-filling model. d) Horvath–Kawazoe differential pore volume plot. Only one sharp peak at approximately 7.8 Å was observed, which indicates that the size of microporous channels are regular.

分子カプセル類（藤田誠先生の仕事から）http://fujitalab.t.u-tokyo.ac.jp/