Supporting Information

Selective Guest Sorption in Interdigitated Porous Framework with Hydrophobic Pore Surfaces

Satoshi Horike, Daisuke Tanaka, Keiji Nakagawa and Susumu Kitagawa

Experimental

$\{[Zn_2(ip)_2(bpy)_2]\cdot DMF\}_n$ (CID-1⊃DMF; ip = isophthalate, bpy = 4,4'-bipyridine). A DMF solution (10 cm^3) of $Zn(NO_3)_2$ $4H_2O$ (2.97 g) was added to a DMF solution (100 cm^3) of H_2ip (1.66 g) and bpy (1.56 g). After the mixture was allowed to stand for several days at 393 K, a white precipitate was collected, washed with DMF and ethanol, and dried at 403 K under a vacuum. Elemental analysis for CID-1: (calc) C, 56.05; H, 3.14; N, 7.26, (obs) C, 55.36; H, 3.05; N, 7.32.

Single Crystal X-ray Diffraction. The colorless single crystal of CID-1⊃DMF was mounted on glass fibers with epoxy resin. X-ray data collection for the single crystal was carried out on a Rigaku Mercury diffractometer with graphite monochromated MoKα radiation (λ = 0.71070 Å) and a CCD two-dimensional detector at 173 K in a cold nitrogen stream. The condition of X-ray for CID-1⊃DMF was 50 kV × 100 mA. The structure solution was solved by direct method (SIR-97) and refined (SHELXL-97) by full matrix least squares. All non-hydrogen atoms except for those of disordered atoms in pyridine rings were refined anisotropically. Hydrogen atoms were included in calculated positions and refined using a riding model.

NOTE: Several compounds that have similar crystal structure have been reported. Zhu *et al*. reported Zn and Cd compounds with ethanol guests (*J. Mol. Struct.*, 2006, 787, 45) and Chen *et al*. reported Ni and Fe compounds (*J. Solid State Chem.*, 2003, 170, 130; *Dalton Trans.*, 2004, 2217) and Liu *et al.* reported Mn compound (*New J. Chem.*, 2003, 27, 890) and Yao *et al.* reported Cu compound (*Inorg. Chem. Acta,* 2005, 358, 3347), respectively. In this report, Zn compound with DMF guests is firstly reported.

Physical Measurements. All chemicals and solvents used in the syntheses were of reagent grade

and used without further purification. Thermogravimetric analysis (TGA) were performed using a Rigaku Thermo plus TG 8120 apparatus in the temperature range between 298 and 723 K in a N_2 atmosphere and at a heating rate of 5 $Kmin^{-1}$. Solid-state ^{13}C NMR was measured by JEOL JNM-LA300 spectrometer and standard CPMAS probe at 75.577 MHz. X-ray powder diffraction (XRPD) data were collected on a Rigaku RINT-2200HF (Ultima) diffractometer with CuKα radiation. The adsorption isotherm for CO_2 at 195 K was measured with Quantachrome AUTOSORB-1 and adsorption/desorption isotherms for other solvents at 298 K were measured with BELSORP-18 volumetric adsorption equipment from BEL Japan, Inc.

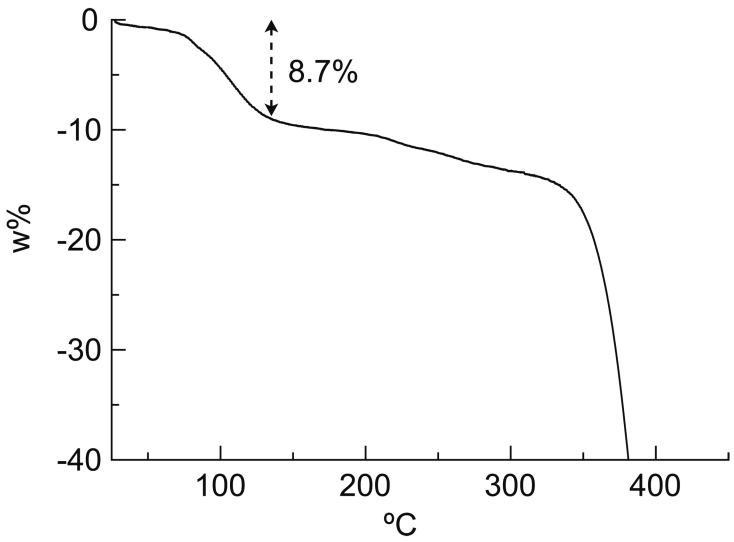

Fig. S1 TGA curve of CID-1⊃DMF over the temperature range from 25-450 °C at a heating rate of β = 5 °C min^{-1} under the N_2 atmosphere.

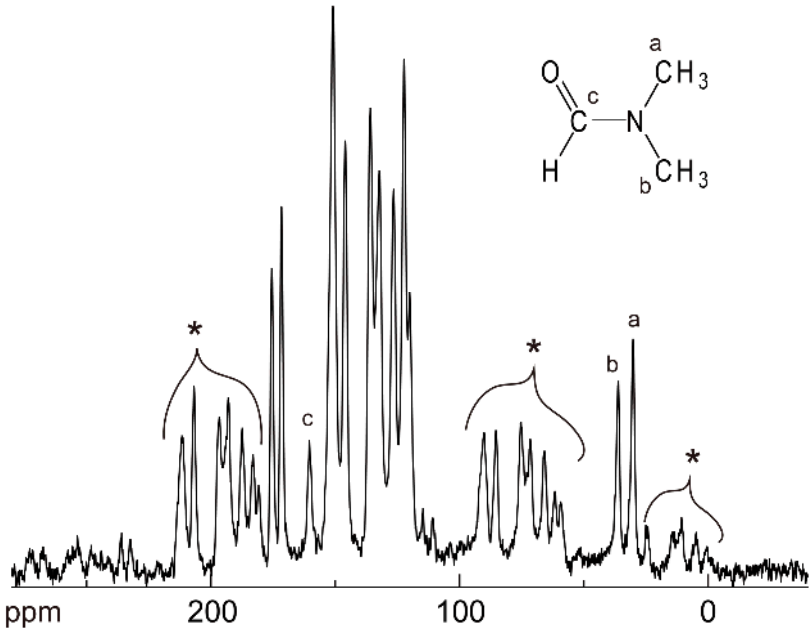

Fig. S2 Solid-state ^{13}C CPMAS NMR spectrum of CID-1⊃DMF (as synthesized) at 298 K. For assignment the chemical shifts of DMF are shown in the figure and the other peaks can be assigned to the framework of CID-1. Spinning side bands are indicated by asterisks (*).

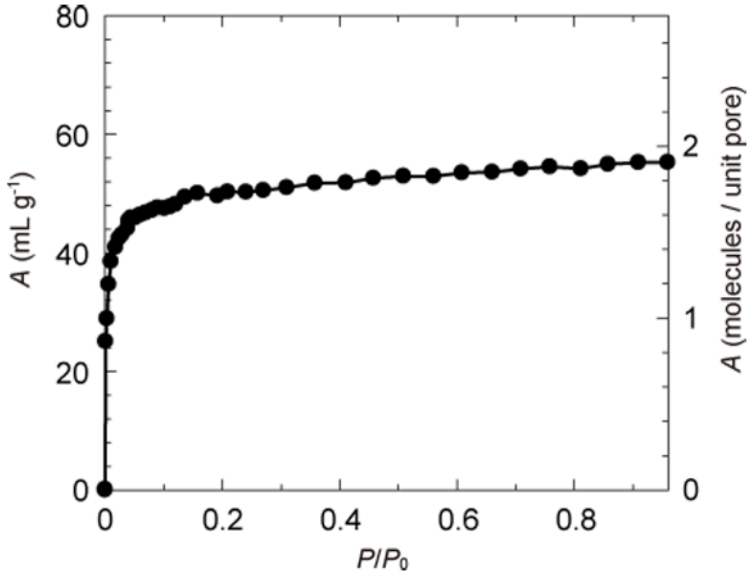

Fig. S3 Adsorption isotherm of CO_2 for CID-1 at 195 K.

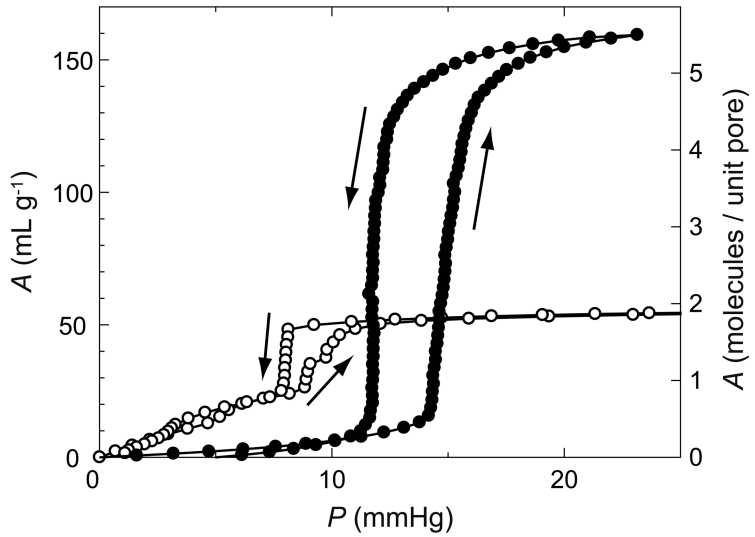

Fig. S4 Adsorption and desorption isotherms for MeOH (298 K, open circle) and H_2O (298 K, closed circle) of CID-1.

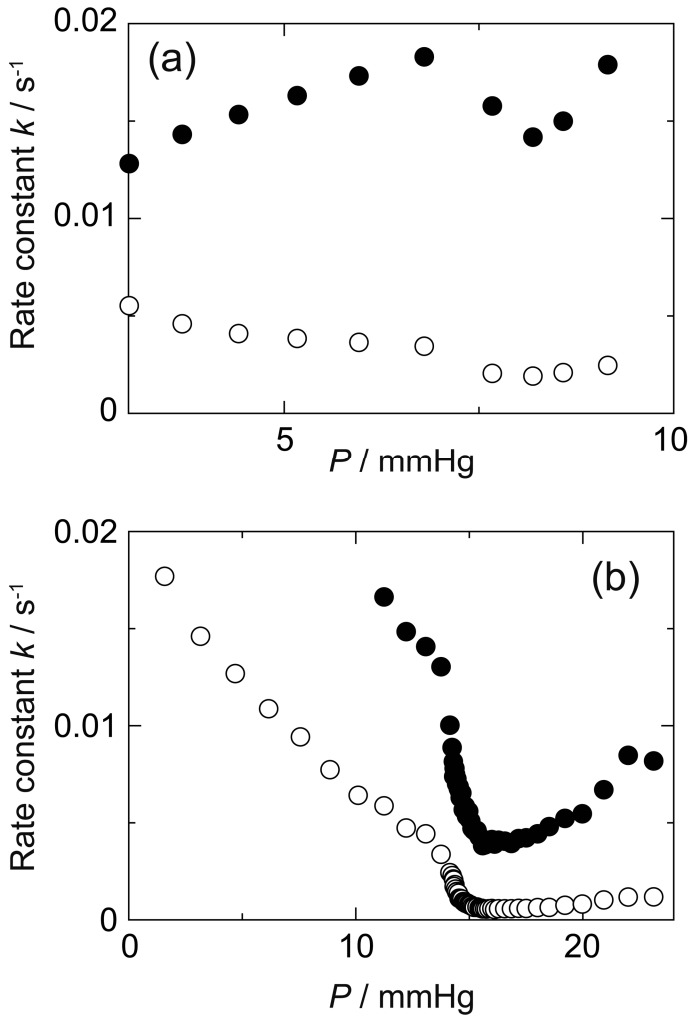

Fig. S5 The variation of double exponential kinetic parameters k_1 (closed circle) and k_2 (open circle) with pressure for adsorption of (a) MeOH and (b) H_2O on CID-1 at 298 K.

CIF report on CID-1⊃DMF

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O4 C1 C2 118.2(4) . . ?
C1 O3 Zn1 165.0(4) . 2_656 ?
C8 O2 Zn1 86.4(3) . 1_455 ?
C9 C11 C13 120.0(5) . . ?
C9 C11 H17 120.0 . . ?
C13 C11 H17 120.0 . . ?
C2 C3 C6 121.0(5) . . ?
C2 C3 H2 119.5 . . ?
C6 C3 H2 119.5 . . ?
C3 C2 C4 118.9(5) . . ?
C3 C2 C1 120.8(4) . . ?
C4 C2 C1 120.4(5) . . ?
O1 C8 O2 121.1(5) . . ?
O1 C8 C6 119.6(5) . . ?

O2 C8 C6 119.3(5) . . ?
O1 C8 Zn1 57.5(3) . 1_455 ?
O2 C8 Zn1 63.7(3) . 1_455 ?
C6 C8 Zn1 175.7(4) . 1_455 ?
C15 N1 C21 27.9(6) . . ?
C15 N1 C22 106.7(8) . . ?
C21 N1 C22 116.9(7) . . ?
C15 N1 C16 115.9(9) . . ?
C21 N1 C16 109.4(8) . . ?
C22 N1 C16 32.6(6) . . ?
C15 N1 Zn1 123.1(6) . . ?
C21 N1 Zn1 119.7(5) . . ?
C22 N1 Zn1 123.4(5) . . ?
C16 N1 Zn1 120.8(6) . . ?
C7 C6 C3 118.9(5) . . ?
C7 C6 C8 121.1(5) . . ?
C3 C6 C8 120.1(4) . . ?
C10 C12 C13 120.2(5) . . ?
C10 C12 H18 119.9 . . ?
C13 C12 H18 119.9 . . ?
C18 C14 C20 26.6(6) . . ?
C18 C14 C17 116.5(8) . . ?
C20 C14 C17 110.2(8) . . ?
C18 C14 C19 105.8(8) . . ?
C20 C14 C19 115.5(7) . . ?
C17 C14 C19 32.9(6) . . ?
C18 C14 C13 124.0(7) . . ?
C20 C14 C13 123.6(6) . . ?
C17 C14 C13 119.6(7) . . ?
C19 C14 C13 120.5(6) . . ?
C5 C4 C2 119.7(5) . . ?
C5 C4 H4 120.2 . . ?
C2 C4 H4 120.2 . . ?
N2 C10 C12 123.8(5) . . ?
N2 C10 H19 118.1 . . ?
C12 C10 H19 118.1 . . ?

C10 N2 C9 116.6(4) . . ?
C10 N2 Zn1 120.7(3) . 1_565 ?
C9 N2 Zn1 122.4(3) . 1_565 ?
C12 C13 C11 116.3(5) . . ?
C12 C13 C14 121.2(4) . . ?
C11 C13 C14 122.5(5) . . ?
N2 C9 C11 122.8(5) . . ?
N2 C9 H20 118.6 . . ?
C11 C9 H20 118.6 . . ?
C5 C7 C6 119.9(5) . . ?
C5 C7 H7 120.0 . . ?
C6 C7 H7 120.0 . . ?
C7 C5 C4 121.5(5) . . ?
C7 C5 H8 119.3 . . ?
C4 C5 H8 119.3 . . ?
C14 C20 C21 120.6(9) . . ?
C14 C20 H9 119.7 . . ?
C21 C20 H9 119.7 . . ?
N1 C21 C20 123.0(9) . . ?
N1 C21 H10 118.5 . . ?
C20 C21 H10 118.5 . . ?
N1 C22 C19 124.2(9) . . ?
N1 C22 H11 117.9 . . ?
C19 C22 H11 117.9 . . ?
N1 C15 C18 125.4(11) . . ?
N1 C15 H12 117.3 . . ?
C18 C15 H12 117.3 . . ?
C22 C19 C14 119.3(9) . . ?
C22 C19 H13 120.4 . . ?
C14 C19 H13 120.4 . . ?
N1 C16 C17 122.4(12) . . ?
N1 C16 H14 118.8 . . ?
C17 C16 H14 118.8 . . ?
C14 C17 C16 120.1(11) . . ?
C14 C17 H15 119.9 . . ?
C16 C17 H15 119.9 . . ?

C14 C18 C15 119.7(11) . . ?
C14 C18 H16 120.2 . . ?
C15 C18 H16 120.2 . . ?

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_diffrn_reflns_theta_full 25.01
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_refine_diff_density_max 0.441
_refine_diff_density_min -0.546
_refine_diff_density_rms 0.103

SQUEEZE RESULTS
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_platon_squeeze_void_nr
_platon_squeeze_void_average_x
_platon_squeeze_void_average_y
_platon_squeeze_void_average_z
_platon_squeeze_void_volume
_platon_squeeze_void_count_electrons
1 0.000 0.500 0.000 106.7 24.2
2 0.000 0.500 0.500 106.7 24.3
_platon_squeeze_details
;
;