Electronic Supplementary Material for CrystEngComm

Electronic Supplementary Information

Switch of channel geometry by 1D component slide responding to slight structural stimuli of adsorbed guest

Satoshi Takamizawa, Takamasa Akatsuka, and Ryosuke Miyake

Department of Nanosystem Science; Graduate School of Nanobioscience; Yokohama City University; 22-2 Seto; Kanazawa-ku, Yokohama, Kanagawa 236-0027; Japan.

PRESTO; Japan Science and Technology Agency (JST); Honcho, Kawaguchi, Saitama 332-0012; Japan.

Email: staka@yokohama-cu.ac.jp

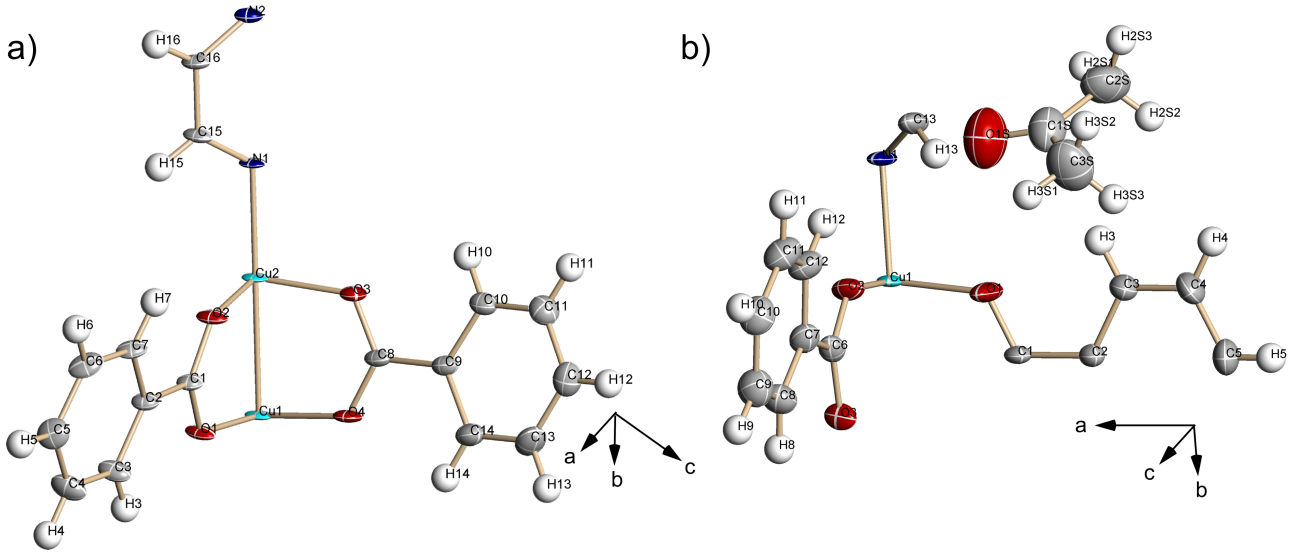

Figure S1. ORTEP structure showing the crystal structure (90 K) of **1** (a) and **1**·2(acetone) synthesized in acetone (b).

Table S1 Crystallographic data of acetone-included crystal of **1**·2(acetone) at 90 K compared with an empty crystal**1**.

Complex	**1**	**1**•2(acetone)
Empirical formula	$C_{32}\ H_{24}\ Cu_2\ N_2\ O_8$	$C_{38}\ H_{36}\ Cu_2\ N_2\ O_{10}$
Crystal size/mm^3	0.28 x 0.24 x 0.02	0.36 x 0.24 x 0.08
MW	691.61	807.79
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/*c*	*C2/m*
T/K	90	90
a/Å	17.485(3)	17.757(3)
b/Å	9.6876(19)	9.6260(16)
c/Å	19.213 (4)	10.8050(18)
β/deg	98.432(4)	95.603(4)
V/Å^{-3}	3219.2(11)	1838.1(5)
Z	4	2
D_{calcd}/Mg m^{-3}	1.427	1.460
μ(Mo Kα)/mm^{-1}	1.372	1.217
Reflections collected	11425	6902
Independent reflections (*R*int)	3999 (0.0560)	2430 (0.0421)
Goodness of fit	1.034	1.089
*R*1 (*I*>2σ (all data))	0.0589 (0.0827)	0.0564 (0.0834)
wR 2 (*I*>2σ (all data))	0.1342 (0.1462)	0.1282 (0.1401)
Least diff. peak (hole)/eÅ^{-3}	2.035 (-1.702)	0.800 (-0.477)
Void volume / Å^3	116.0	195.0 [a)]

a):Void volume was calculated for the crystal structure without included acetone molecules.

Table S2 Crystallographic data of acetone-included crystal of **1**·2(acetone) at 298 K compared with an empty crystal **1**.

Complex	**1**[s1]	**1**•2(acetone)
Empirical formula	C_{32} H_{24} Cu_2 N_2 O_8	C_{38} H_{36} Cu_2 N_2 O_{10}
Crystal size/mm^3	0.28 x 0.24 x 0.02	0.36 x 0.24 x 0.08
MW	691.61	807.79
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/*c*	*C2/m*
T/K	298	298
a/Å	17.998(16)	18.5864(18)
b/Å	9.697(8)	9.7037(9)
c/Å	18.903(17)	10.9706(11)
β/deg	97.339(18)	94.150(3)
V/Å^{-3}	3272(5)	1973.4(3)
Z	4	2
D_{calcd}/Mg m^{-3}	1.404	1.359
μ(Mo Kα)/mm^{-1}	1.350	1.133
Reflections collected	9009	5793
Independent reflections (*R*int)	2903 (0.0489)	1864 (0.0413)
Goodness of fit	1.064	----- [a)]
*R*1 (*I*>2σ (all data))	0.0688 (0.0973)	----- [a)]
wR 2 (*I*>2σ (all data))	0.1704 (0.1869)	----- [a)]
Least diff. peak (hole)/eÅ^{-3}	1.049 (-1.018)	----- [a)]
Void volume / Å^3	106.0	----- [a)]

a): The crystal structure cannot be determined because of the high measurement temperature.

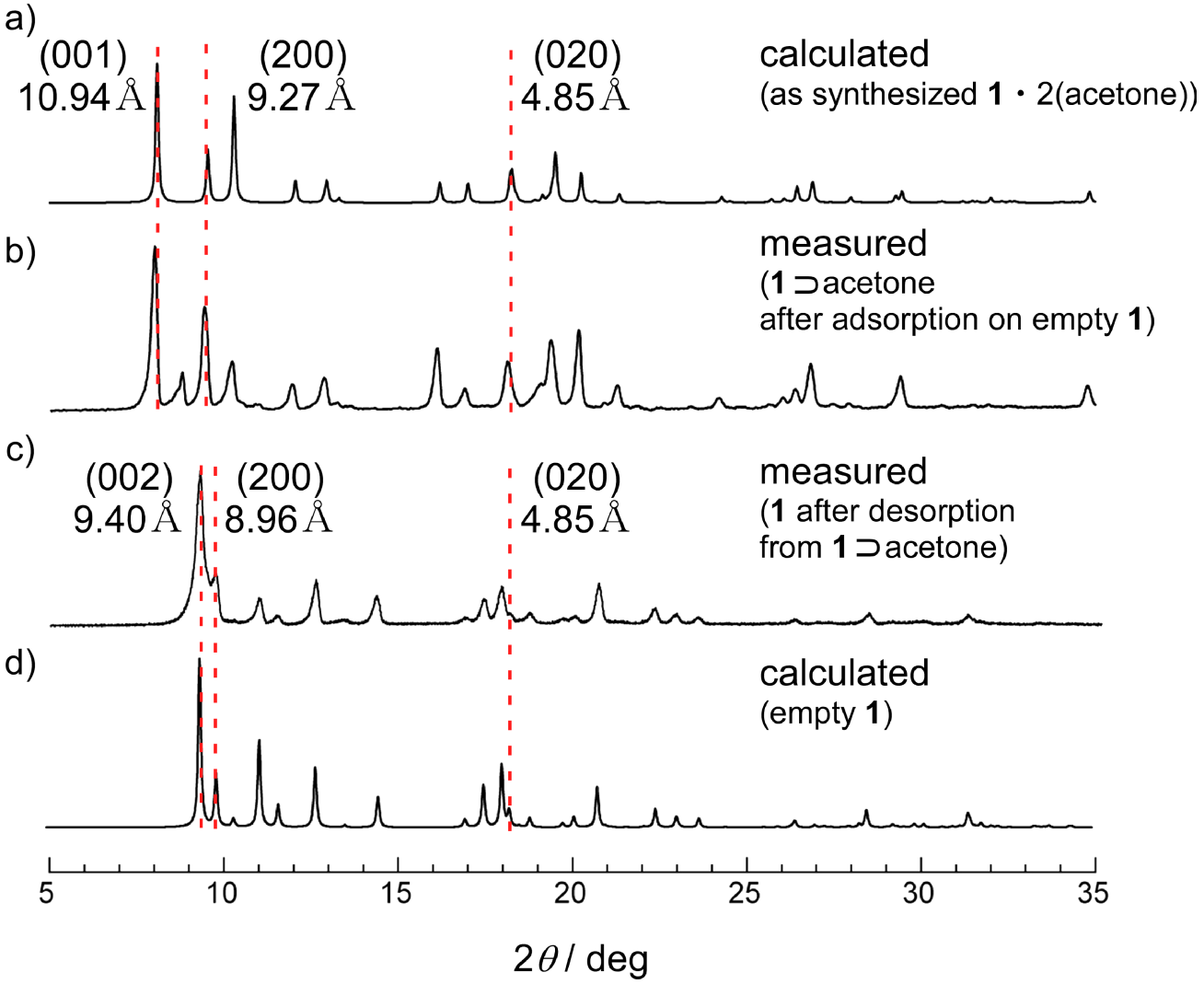

Figure S2. X-ray powder diffraction pattern of crystal **1** at 298 K. Calculated diffraction pattern from the data of single-crystal X-ray structural analyses of crystal **1**·2(acetone) synthesized in acetone (a), measured diffraction pattern of **1** after adsorption of acetone vapor (b), measured diffraction pattern of sample (b) after drying (c), and calculated diffraction pattern of empty crystal **1** (d).

Table S3. List of increased ratios of crystal cell volumes and distances for each direction by adsorption of various gaseous guests at 90 K.

	Direction C	Direction B	Direction A	Volume	Ref
Acetone: **1**·2(acetone)	+13%	0%	+2%	+14%	This study
Methanol: **1**·2(methanol)	+4%	0%	-2%	+3%	S2
Ethanol: **1**·2(ethanol)	+4%	0%	+4%	+8%	S3
CO_2: **1**·3(CO_2)	+5%	0%	+1%	+7%	S4
O_2: **1**·2(O_2)	+0%	0%	+3%	+4%	S5

Direction C: normalized distance for c axis, which is perpendicular to ab plane (also see Figure S3).
Direction B: along b axis of empty crystal **1**.
Direction A: along a axis of empty crystal **1**.

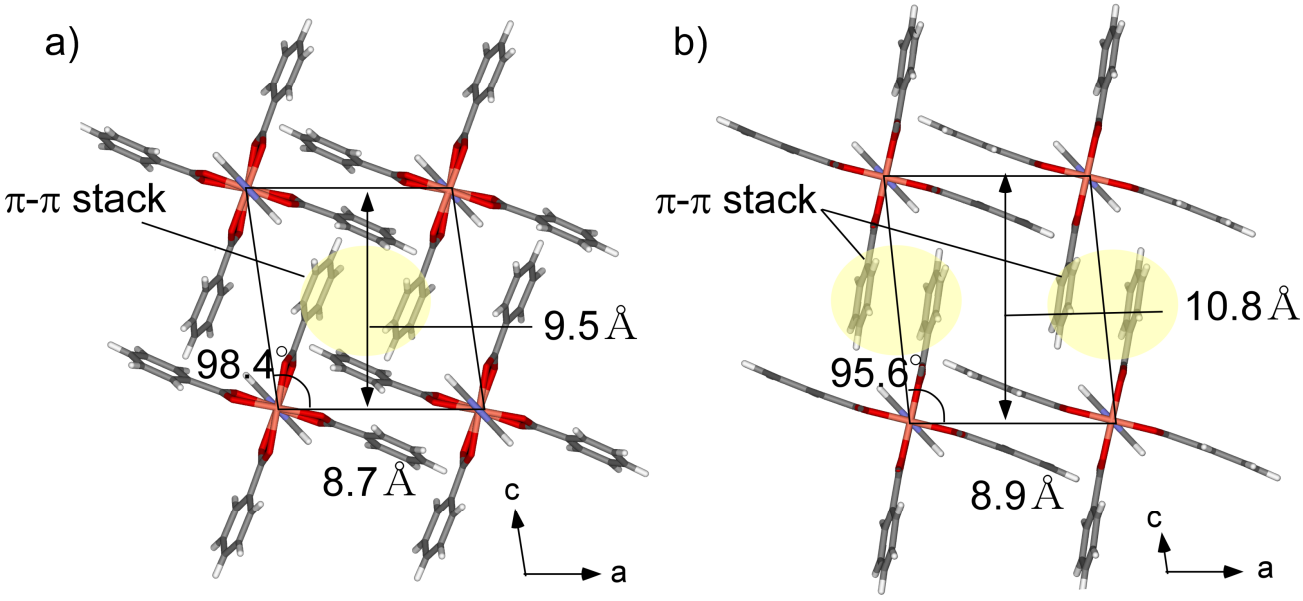

Figure S3. Comparison of empty crystal **1** (a) and acetone-included crystal **1**·2(acetone) (b) at 90 K showing the anisotropic expansion of crystal volume for the c axis direction. Included acetone molecules and disordered part of host structure were excluded for clarity.

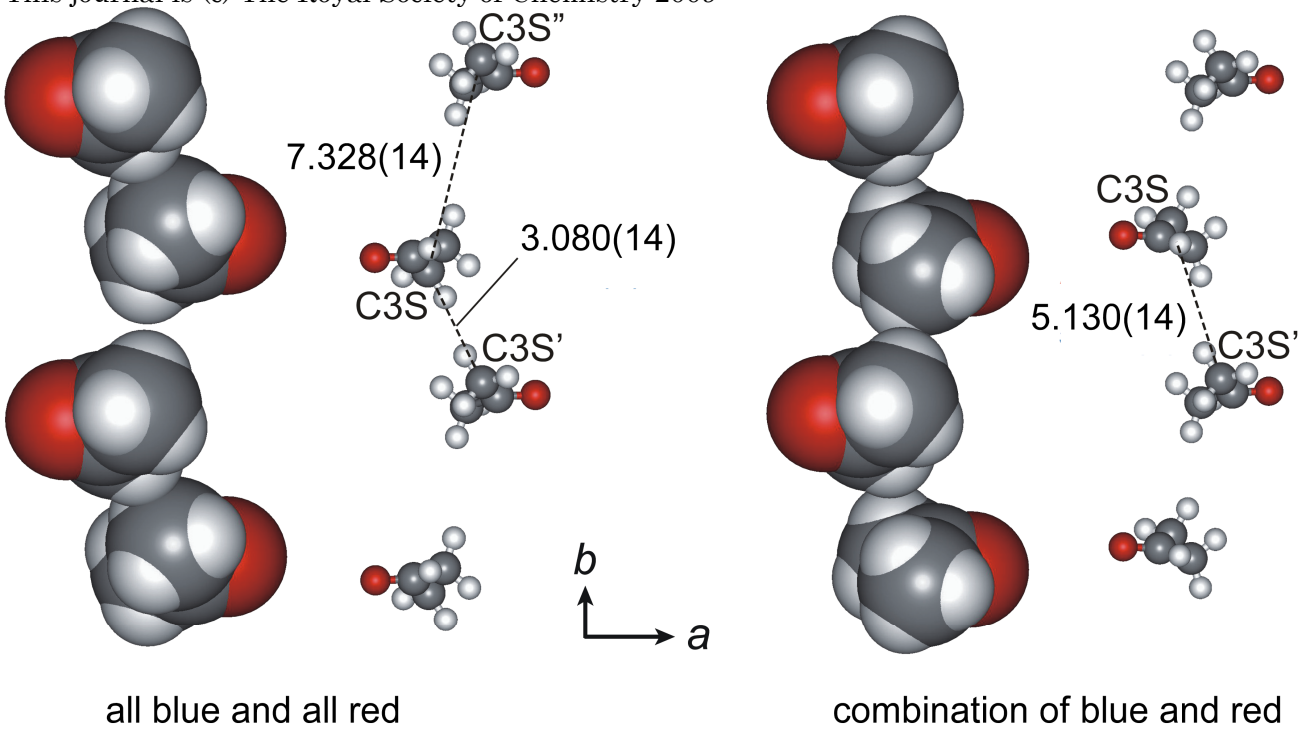

Figure S4. Two possible assemblages of included acetone molecules along the additional channel in the crystal **1**·2(acetone) showing the guest-guest distances. All blue and all red cases in Figure 3c (left), combination of red and blue cases in Figure 3c (right).

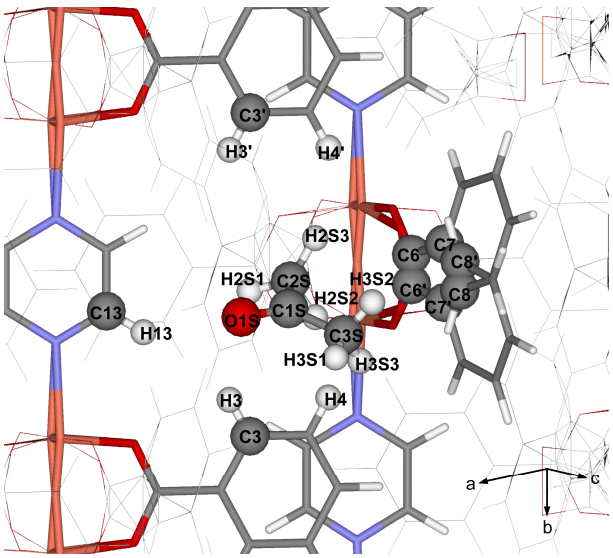

Figure S5. Crystal structure of **1**·2(acetone) showing the short contact between guest (acetone) and host. The atoms that contact the guest or host are shown as a ball and stick model. Disordered acetone molecules were partly excluded for clarity. Distances are listed in Table S4.

Table S4. List of guest-host interaction in short distances in the crystal of **1**·2(acetone) excluding irrelevant contacts with neighbor host or guest molecules.

Guest···Host	Distance (Å)
C(2S)···H(3)	3.28(4)
C(2S)···H(3)#1	3.15(4)
C(2S)···H(4)	3.39(4)
C(2S)···H(4)#1	3.26(4)
C(2S)···C(1)#2	3.863(8)
C(2S)···C(3)	3.92(5)
C(2S)···C(3)#1	3.78(5)
C(2S)···C(6)#3	3.792(11)
C(2S)···C(6)#4	3.805(11)
C(2S)···C(7)#3	3.762(12)
C(2S)···C(7)#4	3.789(13)
C(2S)···C(8)#3	3.831(11)
C(2S)···C(8)#4	3.818(10)
C(3S)···C(8)#3	3.612(12)
C(3S)···C(8)#4	3.812(12)
O(1S)···H(13)	2.333(7)
O(1S)···C(13)	3.115(8)

Symmetric code: #1(x, 1-y, z), #2(0.5-x, -0.5+y, -z), #3(-0.5+x, -0.5+y, z), #4(-0.5+x, 1.5-y, z)

References and note

S1: We determined the crystal structure at 298 K again since the reported crystal structure (S. Takamizawa, E. Nakata and T. Saito, *Inorg. Chem. Commun.*, 2004, **7**, 1.) was determined by data with weak high angle reflections.

S2: S. Takamizawa, C. Kachi-Terajima, M. Kohbara, T. Akatsuka and T. Jin, *Chem. Asian. J.* 2007, **2**, 837.

S3: S. Takamizawa, T. Saito, T. Akatsuka and E. Nakata, *Inorg. Chem.* 2005, **44**, 1421.

S4: S. Takamizawa, E. Nakata and T. Saito, *Inorg. Chem. Commun.*, 2004, **7**, 1.

S5: S. Takamizawa, E. Nakata and T. Saito, *CrystEngComm.*, 2004, **6**, 197.