Supporting Information

for

A Pillared-Layer Coordination Polymer with a Rotatable Pillar Acting as a Molecular Gate for Guest Molecules

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Contents

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(16) Park, Y. K.; Choi, S. B.; Kim, H.; Kim, K.; Won, B.-H.; Choi, K.; Choi, J.-S.; Ahn, W.-S.; Won, N.; Kim, S.; Jung, D. H.; Choi, S.-H.; Kim, G.-H.; Cha, S.-S.; Jhon, Y. H.; Yang, J. K.; Kim, J. *Angew. Chem. Int. Ed.* **2007**, *46*, 8230-8233.

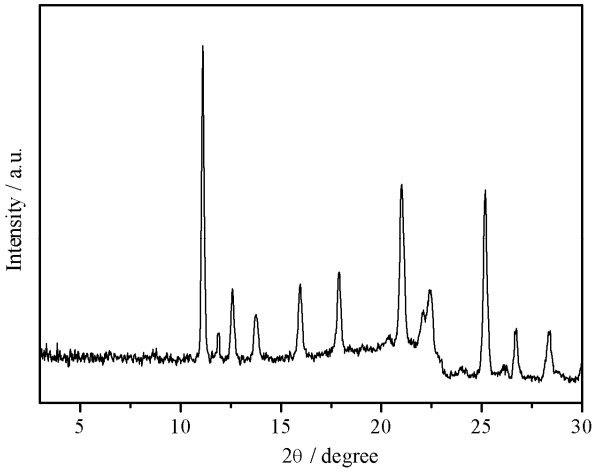


Figure S1. PXRD pattern of by-product.

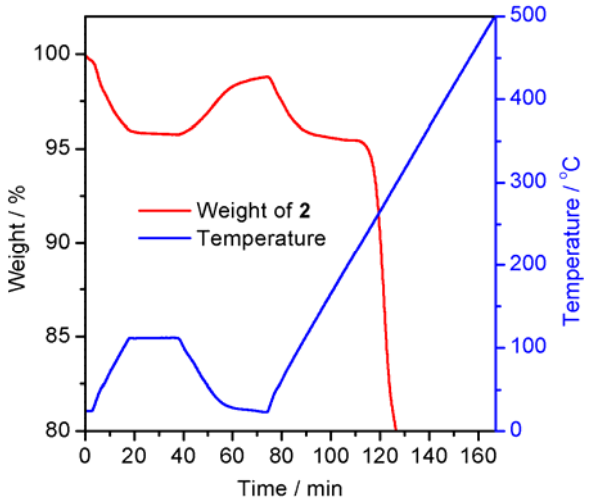


Figure S2. The variation in mass of **2** in response to temperature (right). The mass (red line) and temperature (blue line) as functions of time are shown.

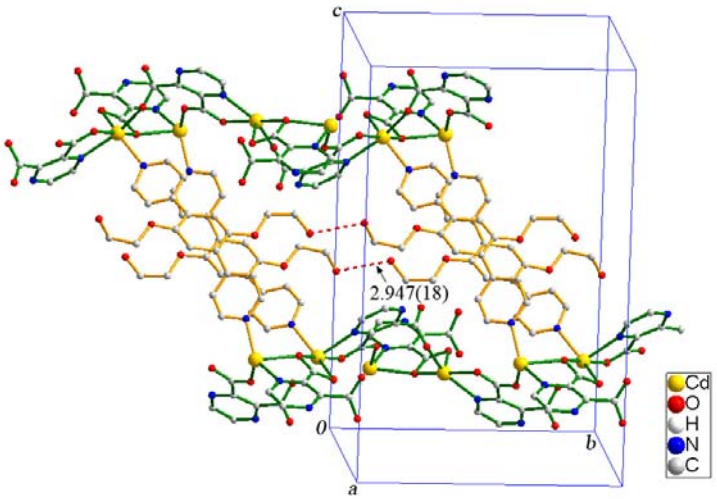


Figure S3. Crystal structure of **2** showing H-bonded pillars (dashed lines). The distance between two oxygen atoms is 2.947(18) Å.

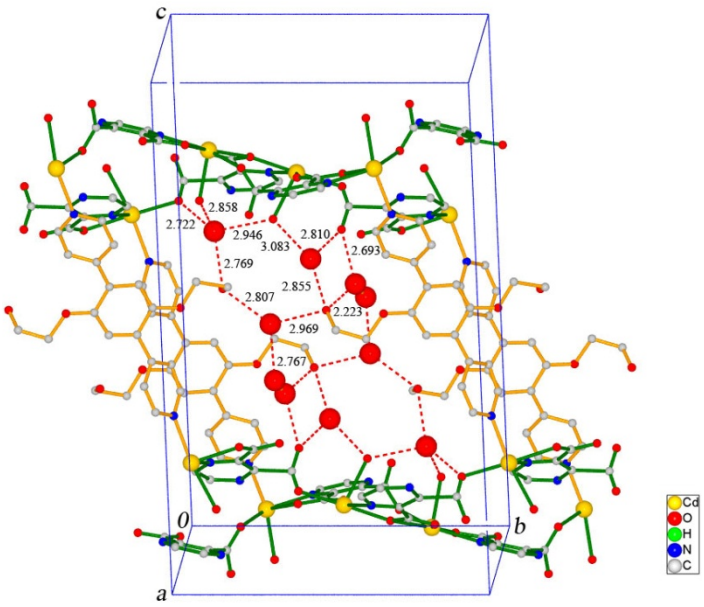


Figure S4. Crystal structure of **2** showing H-bonded water molecules in the pore. The values indicate the distances.

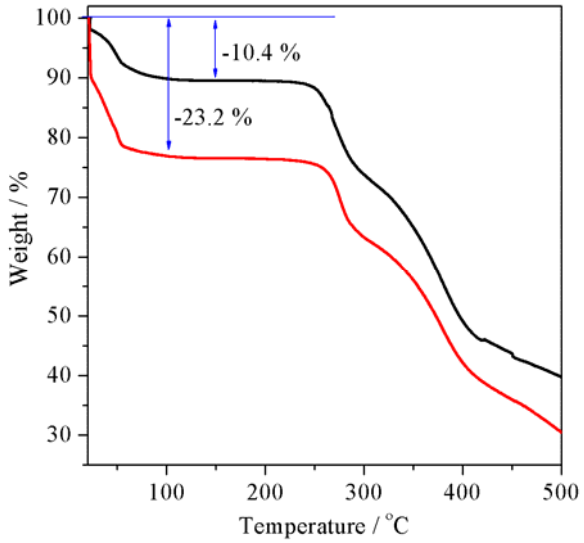


Figure S5. TGA profiles of expanded intermediate **3** (black line) and the fully rehydrated form (red line) with heating rate of 5 °C min^{-1} under N_2 flow.

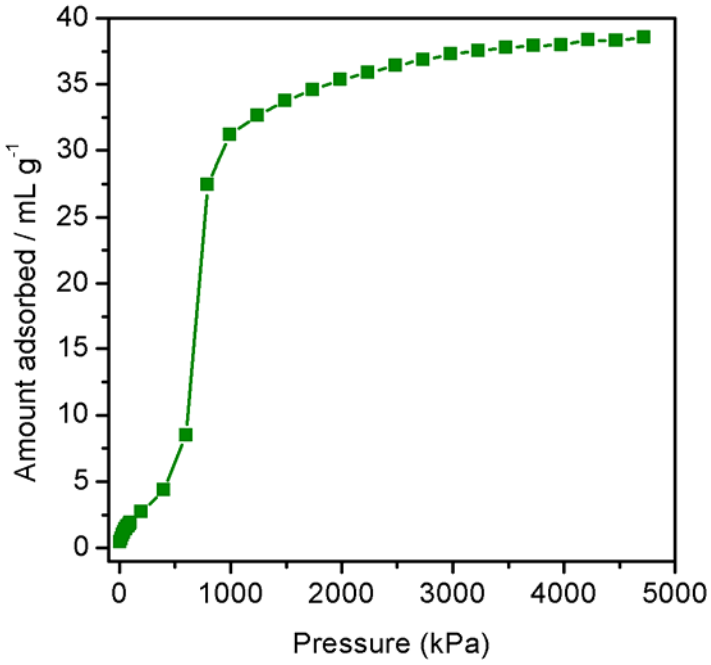
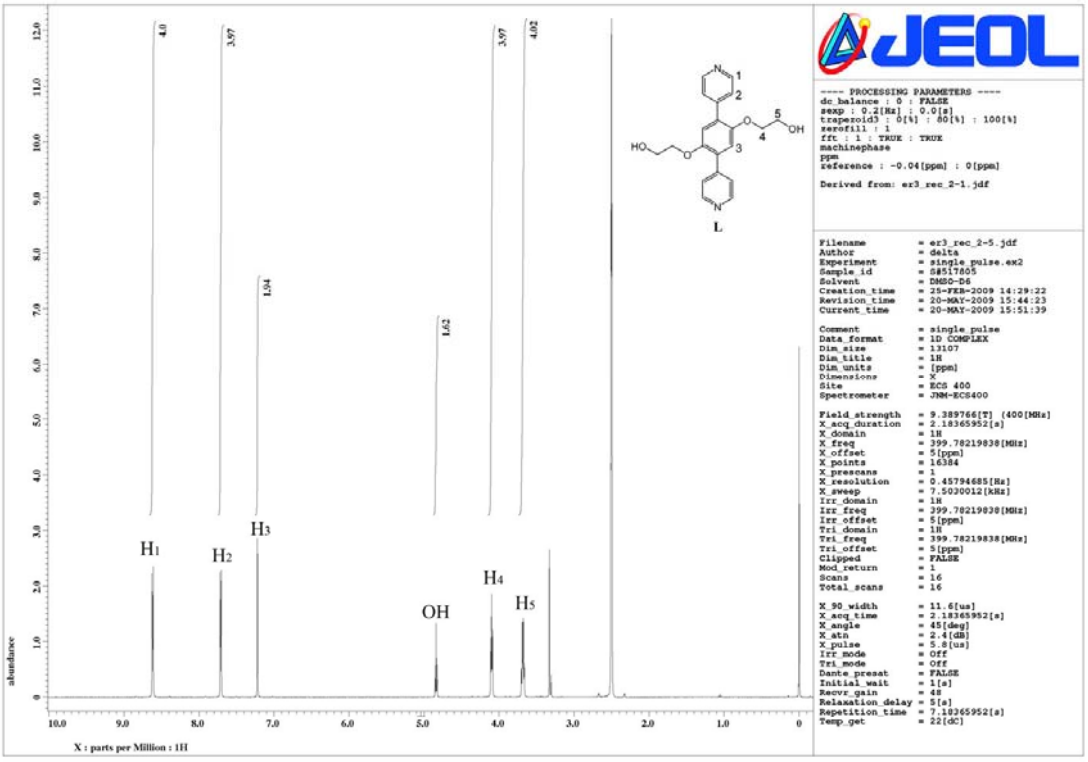


Figure S6. Adsorption isotherm of CO_2 at 293K for **2**.



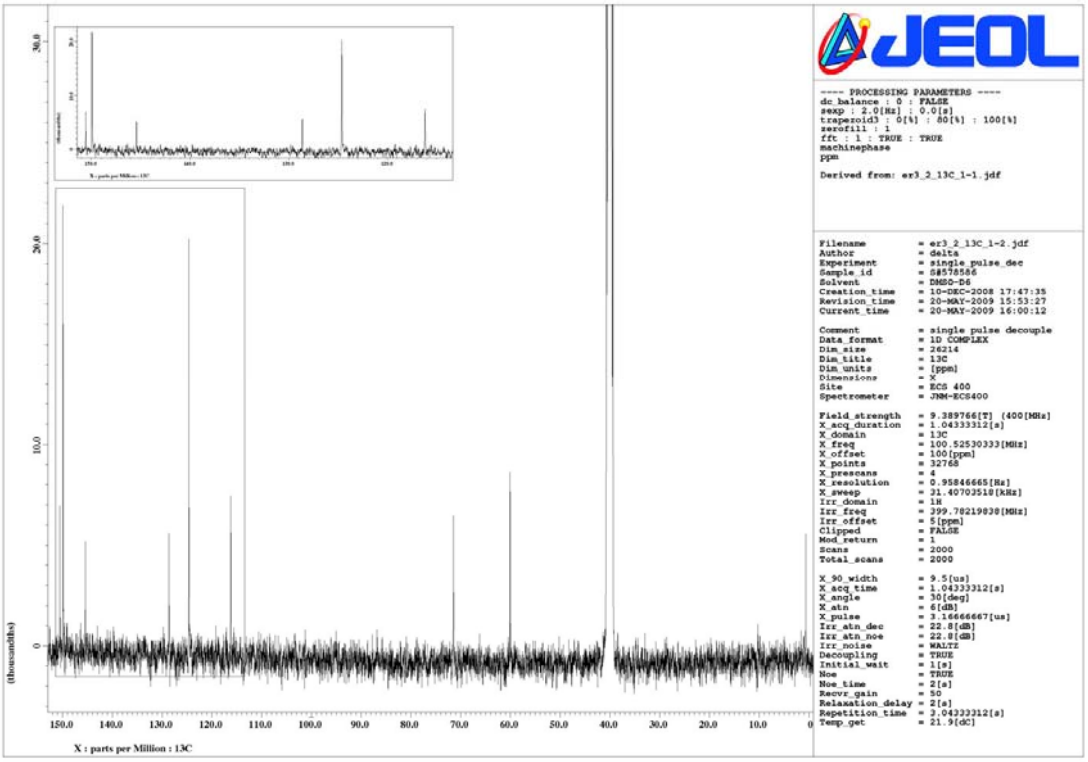


Figure S7. ^{1}H and ^{13}C NMR spectra of **L** in DMSO-d_6.

Table S1. Bond distances and angles of Cd^{2+} centers

Compound		Cd1	Cd2
As-synthesized form **1** Symmetry operations A: -*x*+1,*y*-1/2,-*z*+3/2 B: -*x*+2,*y*-1/2,-*z*+3/2 C: -*x*+1,-*y*+1,-*z*+2	Distances (Å)	Cd(1)-N(5) 2.298(6) Cd(1)-O(1W)2.313(4) Cd(1)-O(3)A2.314(4) Cd(1)-O(1)2.324(4) Cd(1)-N(1)2.397(4) Cd(1)-O(6)2.424(4) Cd(1)-O(5) 2.522(4)	Cd(2)-O(2)A 2.231(4) Cd(2)-O(8)B2.307(5) Cd(2)-O(5) 2.313(4) Cd(2)-N(6)C 2.324(5) Cd(2)-O(2W) 2.355(5) Cd(2)-N(3) 2.373(4)
	Angles (º)	N(5)-Cd(1)-O(1W)168.1(2) N(5)-Cd(1)-O(3)A87.2(2) O(1W)-Cd(1)-O(3)A85.65(15) N(5)-Cd(1)-O(1)92.3(3) O(1W)-Cd(1)-O(1)95.31(16) O(3)A-Cd(1)-O(1)77.02(13) N(5)-Cd(1)-N(1)95.7(2) O(1W)-Cd(1)-N(1)95.49(15) O(3)A-Cd(1)-N(1)147.12(14) O(1)-Cd(1)-N(1)70.14(14) N(5)-Cd(1)-O(6)94.1(3) O(1W)-Cd(1)-O(6)83.91(17) O(3)A-Cd(1)-O(6)133.00(13) O(1)-Cd(1)-O(6)149.53(14) N(1)-Cd(1)-O(6)79.59(14) N(5)-Cd(1)-O(5)84.5(3) O(1W)-Cd(1)-O(5)84.98(16) O(3)A-Cd(1)-O(5)80.57(13) O(1)-Cd(1)-O(5)157.49(14) N(1)-Cd(1)-O(5)132.31(14) O(6)-Cd(1)-O(5) 52.95(13)	O(2)A-Cd(2)-O(8)B109.25(16) O(2)A-Cd(2)-O(5)81.45(14) O(8)B-Cd(2)-O(5)169.28(16) O(2)A-Cd(2)-N(6)C98.73(17) O(8)B-Cd(2)-N(6)C85.17(17) O(5)-Cd(2)-N(6)C92.72(17) O(2)A-Cd(2)-O(2W)83.77(17) O(8)B-Cd(2)-O(2W)85.90(18) O(5)-Cd(2)-O(2W)96.15(18) N(6)C-Cd(2)-O(2W)171.06(18) O(2)A-Cd(2)-N(3)150.12(14) O(8)B-Cd(2)-N(3)98.95(15) O(5)-Cd(2)-N(3)70.64(14) N(6)C-Cd(2)-N(3)93.17(16) O(2W)-Cd(2)-N(3)88.70(16)

Compound		Cd1	Cd2
Partially dried form **1a** Symmetry operations A: -*x*+1/2,*y*+1/2,-*z*+3/2 B: -*x*-1/2,*y*+1/2,-*z*+3/2 C: -*x*+1,-*y*+2,-*z*+2	Distances (Å)	Cd(1)-O(3)A 2.299(4) Cd(1)-O(1) 2.308(4) Cd(1)-N(5) 2.326(6) Cd(1)-O(6) 2.374(4) Cd(1)-O(1W) 2.380(5) Cd(1)-N(1) 2.380(5) Cd(1)-O(5) 2.541(4)	Cd(2)-O(2)A 2.245(4) Cd(2)-O(8)B 2.318(7) Cd(2)-O(5) 2.333(4) Cd(2)-N(6)C 2.339(5) Cd(2)-N(3) 2.346(5) Cd(2)-O(2W) 2.458(6)
	Angles (º)	O(3)A-Cd(1)-O(1)77.27(15) O(3)A-Cd(1)-N(5)86.52(19) O(1)-Cd(1)-N(5)86.21(18) O(3)A-Cd(1)-O(6)131.57(15) O(1)-Cd(1)-O(6)148.78(14) N(5)-Cd(1)-O(6)104.8(2) O(3)A-Cd(1)-O(1W)80.21(16) O(1)-Cd(1)-O(1W)95.48(16) N(5)-Cd(1)-O(1W)165.87(18) O(6)-Cd(1)-O(1W)80.84(19) O(3)A-Cd(1)-N(1)146.36(16) O(1)-Cd(1)-N(1)69.96(15) N(5)-Cd(1)-N(1)98.45(18) O(6)-Cd(1)-N(1)79.47(15) O(1W)-Cd(1)-N(1)95.29(17) O(3)A-Cd(1)-O(5)82.21(14) O(1)-Cd(1)-O(5)158.16(14) N(5)-Cd(1)-O(5)85.16(16) O(6)-Cd(1)-O(5)53.06(13) O(1W)-Cd(1)-O(5)88.25(15) N(1)-Cd(1)-O(5) 131.23(15)	O(2)A-Cd(2)-O(8)B103.40(18) O(2)A-Cd(2)-O(5)79.81(15) O(8)B-Cd(2)-O(5)176.09(19) O(2)A-Cd(2)-N(6)C94.30(19) O(8)B-Cd(2)-N(6)C85.6(2) O(5)-Cd(2)-N(6)C91.94(16) O(2)A-Cd(2)-N(3)147.67(15) O(8)B-Cd(2)-N(3)105.74(18) O(5)-Cd(2)-N(3)71.73(15) N(6)C-Cd(2)-N(3)101.54(18) O(2)A-Cd(2)-O(2W)74.3(2) O(8)B-Cd(2)-O(2W)103.3(2) O(5)-Cd(2)-O(2W)79.62(19) N(6)C-Cd(2)-O(2W)166.8(2) N(3)-Cd(2)-O(2W)85.60(19)

Compound		Cd1	Cd2
Dried form **2** Symmetry operations A: -*x*+3/2,*y*-1/2,-*z*+1/2 B: -*x*+1/2,*y*-1/2,-*z*+1/2 C: -*x*+2,-*y*,-*z*	Distances (Å)	Cd(1)-O(3)A 2.210(9) Cd(1)-O(1) 2.302(8) Cd(1)-N(5) 2.327(8) Cd(1)-O(5) 2.329(7) Cd(1)-N(1) 2.380(9) Cd(1)-O(6) 2.617(8)	Cd(2)-O(7)B 2.199(8) Cd(2)-O(2)A 2.224(8) Cd(2)-N(3) 2.262(7) Cd(2)-N(6)C 2.309(8) Cd(2)-O(5) 2.394(7)
	Angles (º)	O(3)A-Cd(1)-O(1)83.3(3) O(3)A-Cd(1)-N(5)86.9(3) O(1)-Cd(1)-N(5)94.9(3) O(3)A-Cd(1)-O(5)102.6(3) O(1)-Cd(1)-O(5)172.0(3) N(5)-Cd(1)-O(5)90.9(3) O(3)A-Cd(1)-N(1)153.5(3) O(1)-Cd(1)-N(1)70.2(3) N(5)-Cd(1)-N(1)96.1(3) O(5)-Cd(1)-N(1)103.7(3) O(3)A-Cd(1)-O(6)109.3(3) O(1)-Cd(1)-O(6)120.1(3) N(5)-Cd(1)-O(6)142.3(3) O(5)-Cd(1)-O(6)53.0(2) N(1)-Cd(1)-O(6)84.1(3)	O(7)B-Cd(2)-O(2)A108.9(3) O(7)B-Cd(2)-N(3)95.0(3) O(2)A-Cd(2)-N(3)111.3(3) O(7)B-Cd(2)-N(6)C91.6(3) O(2)A-Cd(2)-N(6)C103.2(3) N(3)-Cd(2)-N(6)C140.3(3) O(7)B-Cd(2)-O(5)162.8(3) O(2)A-Cd(2)-O(5)86.0(3) N(3)-Cd(2)-O(5) 771.1(3) N(6)C-Cd(2)-O(5)93.1(3)

Compound		Cd1	Cd2
Partially rehydrated form **3** Symmetry operations A: -*x*+3/2,*y*+1/2,-*z*+3/2 B: -*x*+5/2,*y*+1/2,-*z*+3/2 C: -*x*+1,-*y*+2,-*z*+1	Distances (Å)	Cd(1)-O(3)A 2.300(8) Cd(1)-O(1) 2.322(8) Cd(1)-N(5) 2.349(10) Cd(1)-O(6) 2.385(8) Cd(1)-N(1) 2.385(9) Cd(1)-O(1W) 2.390(9) Cd(1)-O(5) 2.534(7)	Cd(2)-O(2)A 2.246(8) Cd(2)-O(7)B 2.292(12) Cd(2)-N(6)C 2.340(9) Cd(2)-O(5) 2.341(7) Cd(2)-N(3) 2.341(9) Cd(2)-O(2W) 2.461(11)
	Angles (º)	O(3)A-Cd(1)-O(1)76.8(3) O(3)A-Cd(1)-N(5)86.9(3) O(1)-Cd(1)-N(5)86.1(3) O(3)A-Cd(1)-O(6)132.2(3) O(1)-Cd(1)-O(6)148.8(3) N(5)-Cd(1)-O(6)104.5(4) O(3)A-Cd(1)-N(1)145.8(3) O(1)-Cd(1)-N(1)70.0(3) N(5)-Cd(1)-N(1)98.3(3) O(6)-Cd(1)-N(1)79.4(3) O(3)A-Cd(1)-O(1W)80.0(3) O(1)-Cd(1)-O(1W)95.7(3) N(5)-Cd(1)-O(1W)166.0(3) O(6)-Cd(1)-O(1W)81.1(3) N(1)-Cd(1)-O(1W)95.4(3) O(3)A-Cd(1)-O(5)82.7(3) O(1)-Cd(1)-O(5)158.2(3) N(5)-Cd(1)-O(5)85.8(3) O(6)-Cd(1)-O(5)53.0(3) N(1)-Cd(1)-O(5)131.2(3) O(1W)-Cd(1)-O(5)87.5(3)	O(2)A-Cd(2)-O(7)B103.4(4) O(2)A-Cd(2)-N(6)C94.1(3) O(7)B-Cd(2)-N(6)C86.2(4) O(2)A-Cd(2)-O(5)79.4(3) O(7)B-Cd(2)-O(5)176.8(4) N(6)C-Cd(2)-O(5)92.0(3) O(2)A-Cd(2)-N(3)147.1(3) O(7)B-Cd(2)-N(3)106.3(4) N(6)C-Cd(2)-N(3) 7101.7(3) O(5)-Cd(2)-N(3)71.4(3) O(2)A-Cd(2)-O(2W)4.1(3) O(7)B-Cd(2)-O(2W)102.4(4) N(6)C-Cd(2)-O(2W)166.7(4) O(5)-Cd(2)-O(2W)79.8(3) N(3)-Cd(2)-O(2W)85.7(3)