

Supporting Information

A series of pillar-layer metal-organic frameworks based on 5-aminoisophthalic acid and 4,4'-bipyridine†

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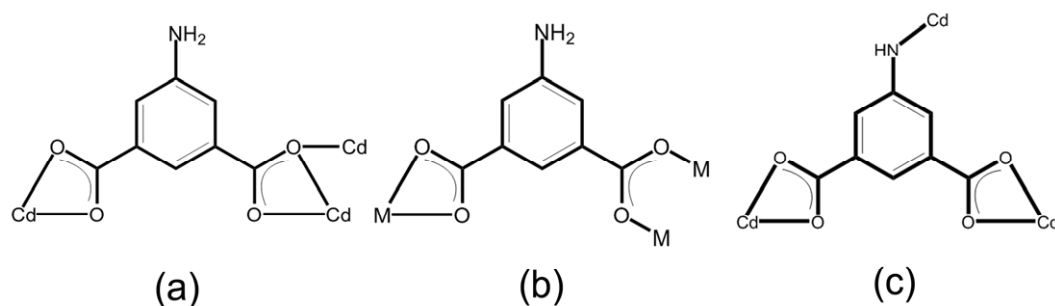
Caution:

In complex **2**, the Cu1 atom and the 5-aip ligand lie on a mirror plane and the bpy ligand lies across a mirror plane.

In complex **3**, the Co1 atom and the 5-aip ligand lie on a mirror plane and the bpy ligand lies across a mirror plane.

In complex **4**, the Cd1 atom lies on a mirror plane and the bpy ligand lies disordered about a site with $2/m$ symmetry.

In complex **1a**, the Cd1 atom and the 5-aip ligand lie on a mirror plane and the bpy ligand lies across a mirror plane.



Scheme. S1 Three kinds of coordination modes of 5-aip.

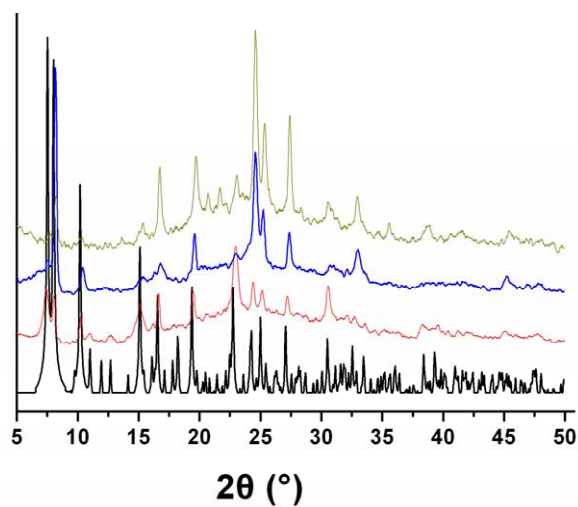


Fig. S1 Experimental and simulated powder X-Ray diffraction patterns for **1** (black: simulated; red: **1**; blue: **1b**; dark yellow: **1c**).

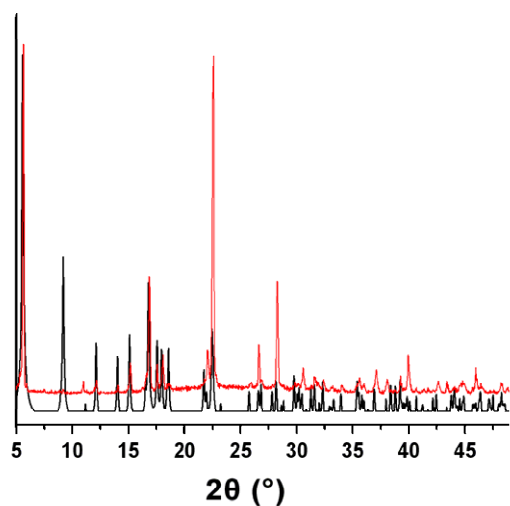


Fig. S2 Experimental and simulated powder X-Ray diffraction patterns for **4** (black: simulated; red: experimental).

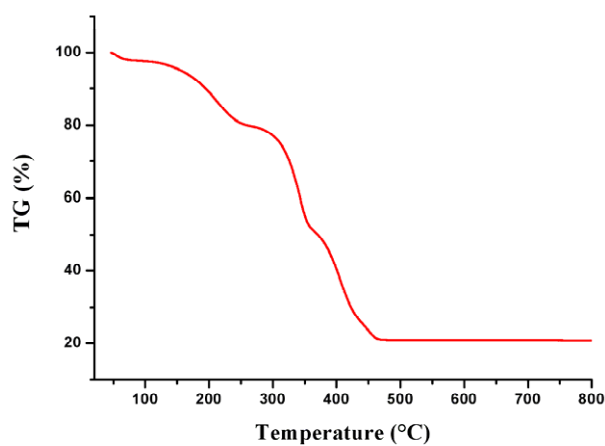


Fig. S3 TG profile of **1**.

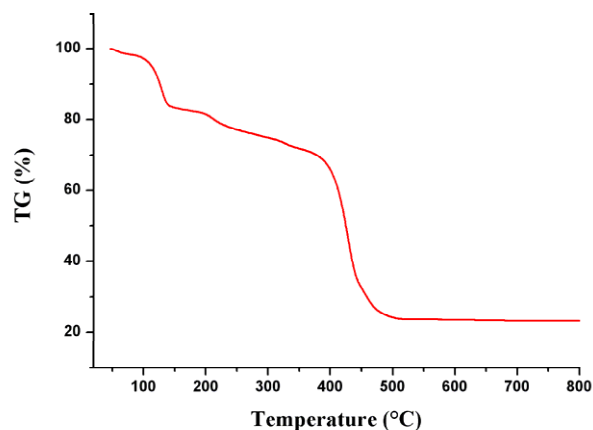


Fig. S4 TG profile of **4**.

Description of **1b**

Crystal data for **1a**: $C_{22.1}H_{29.1}CdN_3O_{8.1}$, molecular formula $[Cd(5\text{-aip})(bpy)] \cdot 4.1CH_3OH$, $M_r = 579.09$, orthorhombic, space group $Pbam$, $a = 14.296(4) \text{ \AA}$, $b = 17.317(5) \text{ \AA}$, $c = 11.714(6) \text{ \AA}$, $V = 2900(2) \text{ \AA}^3$, $Z = 4$, $\rho_{\text{calcd}} = 1.326 \text{ g cm}^{-3}$, 2696 unique ($R_{\text{int}} = 0.0422$), $R_1 = 0.0580$ and $wR_2 = 0.1737 [I > 2\sigma(I)]$, final $R_1 = 0.0635$ and $wR_2 = 0.1785$ for all data. A total of 13993 data were measured in the range $1.85 < \theta < 25.04^\circ$. CCDC 832908. Elemental Anal. Calcd for $C_{22.1}H_{29.1}CdN_3O_{8.1}$ (579.09): C, 45.86; H, 5.07; N, 7.26. Anal. Found: C, 45.80; H, 5.12; N, 7.35%.

Adsorption and desorption of I_2 experiment:

In the adsorption experimental process, the crystals of **1** were initially immersed in I_2 vapor, methanol and dichloromethane solution of I_2 (8 mL, 0.01 mol/L) in a sealed vial at room temperature. After 24 h, the products (**1c**) were filtered and washed with sufficient methanol for six times. The products were finally immersed into fresh methanol for convenient observation.

In the delivery experimental process, the brown crystals of **1c** were immersed in fresh methanol and dichloromethane solution (8 mL) in a sealed vial at room temperature. After 72h, the moist potassium iodide-starch test paper was used to confirm the release of I_2 .



Fig. S5 Photographs showing the color change of bulk samples of **1** before and after I₂ adsorption in the air at room temperature.



Fig. S6 Adsorption and delivery photographs bulk samples of **1** in dichloromethane solution at room temperature: (a) samples before adsorption; (b) samples immersed in the solution of I₂ for 24h; (c) samples releasing I₂ in fresh dichloromethane for 48h; (d) samples releasing I₂ in fresh dichloromethane for 72h.

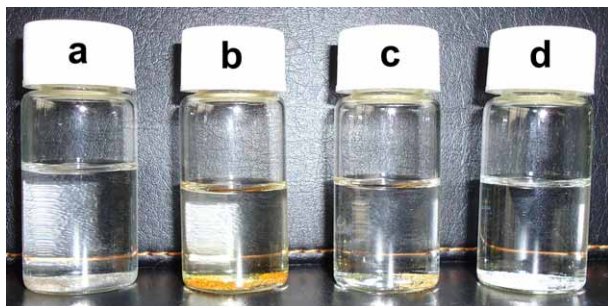


Fig. S7 Adsorption and delivery photographs bulk samples of **1** in methanol solution at room temperature: (a) samples before adsorption; (b) samples immersed in the solution of I₂ for 24h; (c) samples releasing I₂ in fresh methanol for 48h; (d) samples

releasing I_2 in fresh methanol for 72h.



Fig. S8 the color of methanol (left) and dichloromethane (right) used for immersing **1c** and the color change of moist potassium iodide-starch test paper (top).