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.
Description of 1b

Crystal data for 1a: $\text{C}_{22.1}\text{H}_{29.1}\text{CdN}_{3}\text{O}_{8.1}$, molecular formula $[\text{Cd}(5\text{-aip})(\text{bpy})]\cdot 4.1\text{CH}_3\text{OH}$, $M_r = 579.09$, orthorhombic, space group $Pbam$, $a = 14.296(4)\ \text{Å}$, $b = 17.317(5)\ \text{Å}$, $c = 11.714(6)\ \text{Å}$, $V = 2900(2)\ \text{Å}^3$, $Z = 4$, $\rho_{\text{calcd}} = 1.326\ \text{g cm}^{-3}$, 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 $\text{C}_{22.1}\text{H}_{29.1}\text{CdN}_{3}\text{O}_{8.1}$ (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 72 h, the moist potassium iodide-starch test paper was used to confirm the release of I$_2$. 

**Fig. S4** TG profile of 4.
**Fig. S5** Photographs showing the color change of bulk samples of **1** before and after **I**$_2$ 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 **I**$_2$ for 24h; (c) samples releasing **I**$_2$ in fresh dichloromethane for 48h; (d) samples releasing **I**$_2$ 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 **I**$_2$ for 24h; (c) samples releasing **I**$_2$ in fresh methanol for 48h; (d) samples
releasing I₂ 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).