Supporting Information

Synthesis, structure and gas adsorption properties of a stable microporous metal-organic framework assembled from T-shaped pyridyl dicarboxylate ligand

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Fig. S1 Representations of the asymmetric units of compounds 1 showing ellipsoid at the 50% probability level.

Fig. S2 Powder X-ray diffraction patterns of the simulated, as-synthesized, after gas adsorption/desorption measurements, after CO$_2$ adsorption/desorption cycles and exposed in the air for 10 months of compound 1.
**Fig. S3** Infra-red spectra of M1, M2, H$_2$PBPD and compound 1.

**Fig. S4** TGA curves of compound 1 and activated.
Fig. S5 Measured CH$_4$ and CO$_2$ isotherms at 273 K and 298 K along with the DSLF fits for compound 1.

Fig. S6 IAST predicted equimolar gas mixture adsorption selectivities at 273 K (a) and 298 K (b) for compound 1.
Fig. S7 (a) Nonlinear curves fitting of CO$_2$ for compound 1 at 273 K and 298 K; (b) Isosteric heat of CO$_2$ for compound 1.
Fig.S8 The $^1$H and $^{13}$C NMR spectra of M1.
Fig. S9 The $^1$H and $^{13}$C NMR spectra of M2.
Fig. S10 The $^1$H and $^{13}$C NMR spectra of H$_2$PBPD.
Fig. S11 MS of M1, M2 and H$_2$PBPD.
Table S1 Crystal Data and Structure Refinement for compound 1.\textsuperscript{a}

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<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<tr>
<td>Formula</td>
<td>C\textsubscript{25}H\textsubscript{31}N\textsubscript{3}O\textsubscript{9}Cu</td>
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<tr>
<td>Formula weight</td>
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<td>Temperature</td>
<td>296(2) K</td>
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<tr>
<td>Wavelength</td>
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<tr>
<td>Crystal system, space group</td>
<td>Hexagonal, R-3</td>
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<tr>
<td>a</td>
<td>18.9711(9) Å</td>
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<tr>
<td>α</td>
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<td>Calculated density</td>
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<td>Absorption coefficient</td>
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<td>F(000)</td>
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<td>Final R indices [I &gt; 2σ(I)]\textsuperscript{b}</td>
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<tr>
<td>R indices (all data)</td>
<td>R\textsubscript{1} = 0.0735, wR\textsubscript{2} = 0.2315</td>
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\textsuperscript{a}Date based on \textit{PLATON/SQUEEZE} mode.

\textsuperscript{b}R\textsubscript{1} = \frac{\sum|F_o|-|F_c|}{\sum|F_o|}, wR\textsubscript{2} = \left[ \frac{\sum w (F_o^2-F_c^2)^2}{\sum w (F_o^2)^2} \right]^{1/2}.
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