Single Crystalline Molecular Flasks: Chemical Transformation with Bulky Reagents in the Pores of Porous Coordination Networks

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Figure S2. Crystal structure of \{[(\text{ZnI}_2)_3(\text{1}_2(\text{4a})]•(\text{C}_4\text{H}_6\text{O}_3)_x\}_n (5a). A view along the \textit{b} axis. Hydrogen atoms and guest molecules in the pores were omitted for clarity. The network of \[(\text{ZnI}_2)_3(\text{1})_2\]_n is shown in grey line. Amide \textit{4a} are shown in green stick (nitrogen atoms are blue and oxygen atoms are red).
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**Figure S17.** Diffuse reflectance UV-vis spectra of 3a and 5a before and after reaction. The diffuse reflectance UV-vis spectra were measured with BaSO₄ pellets on a Shimazdu UV-3150 equipped with an integrating sphere at room temperature and were converted from reflectance to absorbance by the Kubelka-Munk method.
**Figure S18.** Single crystal microscopic FT-IR spectra of 3a and 5a before and after reaction. The Microscopic FT-IR spectra were measured on a DIGILAB Scimitar FTS7000 instrument at room temperature.
Figure S19. $^1$H NMR spectra (500 MHz, DMSO-$d_6$, 300 K) of amine 2a and amide 4a extracted from the crystal of 5a: a, b) spectra of 4a extracted from 5a, c) a spectrum of synthesized amine 2a. The conversion ratio of amine 2a to amide 4a was about 100%. The $^1$H NMR spectra were measured on a Bruker DRX 500 (500 MHz) NMR spectrometer at 300 K.