Supplementary Information

A Single Crystal Study of CPO-27 and UTSA-74 for Nitric Oxide Storage and Release

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 - b. CPO-27-Zn
 - c. CPO-27-Mg
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- (iii) Single crystal data for :
 - a. UTSA-74
 - b. CPO-27-Zn
 - c. CPO-27-Mg

(ia) Synthesis conditions for UTSA-74

Zinc acetate monohydrate (1.11 g, 5 mmol) and benzoic acid (1.22 g, 10 mmol) were dissolved in *n*butanol (13.9 mL, 152 mmol) and termed Solution A. 2,5-dihydroxyterephthalic acid (0.5 g, 2.5 mmol) was dissolved in DMF (11.7 mL 152 mmol) with stirring (Solution B). Solution B was slowly added to Solution A in a Teflon-lined steel autoclave and allowed to react at 150 °C for 48 hr. The crystals were collected by filtration, washed with *n*-butanol (3 x 50 mL) and dried in air to afford UTSA-74 as large gold hexagonal rods.

(ib) Synthesis conditions for CPO-27-Zn

Zinc acetate monohydrate (1.11 g, 5 mmol) and salicylic acid (1.22 g, 10 mmol) were dissolved in ethanol (8.87 mL, 152 mmol) and termed Solution A. 2,5-dihydroxyterephthalic acid (0.5 g, 2.5 mmol) was dissolved in DMF (11.7 mL 152 mmol) with stirring (Solution B). Solution B was slowly added to Solution A in a Teflon-lined steel autoclave and allowed to react at 150 °C for 48 hr. The crystals were collected by filtration, washed with ethanol (3 x 50 mL) and dried in air to afford CPO-27-Zn as yellow/gold needles.

(ic) Synthesis conditions for CPO-27-Mg

Magnesium nitrate hexahydrate (0.256 g, 1 mmol) and salicylic acid (0.276 g, 2 mmol) were dissolved in ethanol (1.8 mL, 30.4 mmol) and termed Solution A. 2,5-dihydroxyterephthalic acid (0.1 g, 0.5 mmol) was dissolved in DMF (2.40 mL 30.4 mmol) with stirring (Solution B). Solution B was slowly added to Solution A in a Teflon-lined steel autoclave and allowed to react at 150 °C for 48 hr. The crystals were collected by filtration, washed with ethanol (3 x 20 mL) and dried in air to afford CPO-27-Mg as bright yellow needles.

(ii) Short-range powder X-ray diffraction



Figure 1. Short-range powder X-ray diffraction patterns for CPO-27-Mg (blue), CPO-27-Zn (green) and UTSA-74 (red). CPO-27-Zn has a slight UTSA-74 impurity highlighted by the small peak at 7.8 2Θ.