Electronic Supplementary Information

Investigation of Prototypal MOFs Consisting of Polyhedral Cages with Accessible Lewis-Acid Sites for Quinoline Synthesis

Wen-Yang Gao\textsuperscript{a}, Kunyue Leng\textsuperscript{b}, Lindsay Cash\textsuperscript{a}, Matthew Chrzanowski\textsuperscript{a}, Chavis A. Stackhouse\textsuperscript{a}, Yinyong Sun\textsuperscript{b} and Shengqian Ma*\textsuperscript{a}

\textsuperscript{a} Department of Chemistry, University of South Florida, 4202 East Fowler Avenue, Tampa, Florida, 33620, United States, Fax: +1 813-974-3203; Tel: +1 813-974-5217; E-mail: sqma@usf.edu

\textsuperscript{b} School of Chemical Engineering and Technology, Harbin Institute of Technology, Harbin, 150001, China
Commercially available reagents were purchased in high purity from Fisher Scientific or Sigma Aldrich and used without further purification. The powder X-ray diffraction was performed on a Bruker D8 Advance, CuKα, λ = 1.54178 Å (40 kV, 40 mA). Temperature-programmed desorption of NH₃ (NH₃-TPD) was carried out on FINESORB-3010 equipped with a thermal conductivity detector. The samples were first outgassed under 373 K for 12 h before the measurement. After cooling to 298 K, the samples were saturated in an NH₃ stream (5% in Ar) for 30 minutes and consequently treated in Ar (30 mL/min) for 1 h for removing physisorbed NH₃. Finally, the TPD profile was determined by increasing temperature from 298 K to 523 K with ramping rate of 10 K/min while recording NH₃ desorption with a thermal conductivity detector.

MOF Synthesis

HKUST-1,¹ MOF-505² and MMCF-2³ were prepared using the procedures reported in the literature. The phase purity was confirmed by the powder X-ray diffraction, illustrated in Fig. S1-S3.

Catalysis experiments

The Friedlander condensation reaction was conducted in a 5 mL round bottom flask equipped with a condenser and a magnetic stirrer at a stirring rate of 120 r/min. In a typical procedure, 2-aminoaryl ketones (1mmol), ketone compounds (2 mL) were added into the flask with loading catalyst (0.01mmol on basis of Cu₂(CO₃)₄ unit, MOF-505, 6.7 mg; HKUST-1, 6.3 mg and MMCF-2, 17.1 mg) and the resulting mixture was stirred at 358 K for 24 hours. The products were monitored by GC-MS (HP-5MS column, 5% phenyl methyl siloxane, 30 m × 0.25 mm × 0.25 μm; injector temperature 250 °C). All products were identified by the comparison of GC retention times and mass spectra with those of the authentic samples.
Fig. S1. Powder X-ray diffraction patterns of HKUST-1.

Fig. S2. Powder X-ray diffraction patterns of MOF-505.
Fig. S3. Powder X-ray diffraction patterns of MMCF-2.

Fig. S4. The cuboctahedral cage in MOF-505.
Fig. S5. Pictures of HKUST-1 (a) octahedral cage; (b) cuboctahedral cage; (c) close packing of polyhedral cages.

Fig. S6. NH$_3$-TPD profiles of HKUST-1, MOF-505 and MMCF-2 catalysts.
References.

