Picolinoyl functionalized MOF ligands for an air-promoted secondary alcohol oxidation with CuBr

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Supporting Information

General Information. All ¹H NMR, and ¹³C NMR spectra were recorded using Varian Unity Plus 400 (93.94 kG, ¹H 400 MHz) spectrometer at ambient temperature in CDCl₃. Chemical shifts are reported in parts per million as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), The structure and phase of the samples were coupling constant, and integration. evaluated by X-ray powder diffraction (XRD, Rigaku DMAX-RB 12 KW) with Cu Ka radiation (λ =0.15406 nm). The morphology of the as-obtained product was characterized by scanning electron microscopy (SEM, ZEISS SUPRA55). Transmission electron microscopy (TEM) and high-resolution TEM (HRTEM) were conducted on a TEI Tecnai F20. The samples for the SEM, TEM and HRTEM measurements were dispersed in ethanol and sonicated for a few minutes and supported onto the silicon slice and the holey carbon film on a Cu grid, respectively. The specific surface areas were calculated by the Brunauer–Emmett–Teller (BET) method. The pore size distributions were derived from the adsorption branches of isotherms by using the Barrett-Joyner-Halenda (BJH) model.Infrared spectra were recorded on a NICOLET 6700 infrared spectrophotometer. Analytical thin layer chromatography was performed using EMD 0.25 mm silica gel 60-F plates. Flash column chromatography was performed on Sorbent Technologies 60 Å silica gel.

General procedure for the aerobic oxidation of alcohols



In a typical procedure, 1.0 mmol of 1-phenylethan-1-ol, 0.05 mmol of TEMPO, 0.1 mmol of NMI were mixed in the presence of 0.05 mmol of UiO-66-NH-PC ligand. were added in a 10 mL round-bottom flask. Without sealing the flask, the solution was stirred at room temperature (23 °C) for the desired time until the reaction was completed. After the catalytic reaction, the solid was filtered. The filtrate was examined by GC-MS using *n*-Dodecane as the internal standard.



Fig. S1 Simulated PXRD patterns of UiO-66.



Fig S2. SEM image of recycled UiO-66-NH-PC.



Fig. S3 Conversion *versus* time in the aerobic oxidation of alcohol catalyzed by CuBr/UiO-66-NH-PC. a) reaction without filtration, b) solid ligand was filtered at 3 h.



Fig. S4 Linear fit calibration of standard data to analyze unknown concentration of acetophenone



Fig. S5 ESI-MS (negative mode) of UiO-66-NH-PC.

GC-MS result of aerobic oxidation reaction.

Table 1, entry 5.



Compound 2b



Compound 2d



Compound 2e



Compound 2f



Compound 2g







Compound 2i











Table 2, entry 3.





