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

Xin Du,<sup>a</sup> Yi Luan,<sup>\*,a</sup> Fengxia Yang,<sup>a</sup> Daniele Ramella,<sup>b</sup> Xin Shu <sup>\*,c</sup>

<sup>a</sup> School of Materials Science and Engineering, University of Science and Technology Beijing, 30 Xueyuan Road, Haidian District, Beijing 100083, P. R. China, E-mail: yiluan@ustb.edu.cn, duxin@ustb.edu.cn

<sup>b</sup> Temple University-Beury Hall, 1901, N. 13th Street, Philadelphia PA 19122, United States

<sup>c</sup> College of Science, Beijing University of Chemical Technology, Beijing 100029, P.R. China

### **Supporting Information**

General Information. All <sup>1</sup>H NMR, and <sup>13</sup>C NMR spectra were recorded using Varian Unity Plus 400 (93.94 kG, <sup>1</sup>H 400 MHz) spectrometer at ambient temperature in CDCl<sub>3</sub>. 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 ( $\lambda$ =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

![](_page_11_Figure_1.jpeg)

![](_page_12_Figure_0.jpeg)

![](_page_12_Figure_1.jpeg)

![](_page_12_Figure_2.jpeg)

![](_page_12_Figure_3.jpeg)

Table 2, entry 3.

![](_page_13_Figure_1.jpeg)

![](_page_13_Figure_2.jpeg)

![](_page_13_Figure_3.jpeg)