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Supporting Information

Dehydrogenative coupling of silanes with alcohols catalyzed by $Cu_3(BTC)_2$

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Experimental procedure

Materials

$Cu_3(BTC)_2$ commercially known as Basolite C 300 MOF, dimethylphenylsilane, diphenylsilane, triphenylsilane and phenylsilane used in the present study was purchased from Sigma Aldrich and used as received. Alcohols like 1-butanol, methanol, ethanol and 2-propanol used in the present study were purchased from Sigma Aldrich.

Instrumentation

Powder XRD diffraction patterns were measured in the refraction mode in a Philips X'Pert diffractometer using the CuKα radiation (λ = 1.54178 Å) as the incident beam, PW3050/60 (2 theta) as Goniometer, PW 1774 spinner as sample stage, PW 3011 as detector, incident mask fixed with 10 mm. PW3123/10 for Cu was used as a monochromator. PW3373/00 Cu LFF was used as X-ray tube with power scanning of 45 kV and 40 mA current. The sample powder was loaded into a holder and levelled with a glass slide before mounting it on the sample chamber. The specimens were scanned between 2^o and 70^o with the scan rate of 0.02^o/s. ESR spectra were recorded by using a Bruker EMX spectrometer, with the typical settings (frequency 9.80 GHz, sweep width 30.6 G, time constant 80 ms, modulation frequency 100 kHz, modulation width 0.2 G, microwave power 200 mW).

Reaction procedure

In a typical reaction, 50 mg of $Cu_3(BTC)_2$ was added to 2 mL of 1-butanol containing 1 mmol of dimethylphenylsilane. This reaction mixture was stirred at the required temperature for the required time as indicated in Tables 1 and 2. It was observed that the reaction mixture turns from blue to pale red after 5 min with the evolution of hydrogen gas. The reaction progress was monitored by gas chromatography and after completion of the reaction, the mixture was washed twice with 1-butanol and filtered. Then, the product is analyzed by gas chromatography for its purity and selectivity. Conversion and selectivity were determined by Agilent gas chromatography using internal standard method. ^{1}H-NMR spectra were recorded with 400 MHz using tetramethylsilane as internal standard. The same procedure is followed for the reusability experiments.

Experimental procedure for FT-IR studies

IR studies were performed using a quartz IR cell allowing in situ treatments in controlled atmospheres and temperatures (from 25 ºC to 500 ºC) and connected to a vacuum system with gas dosing facility. Spectra were recorded with a Bruker 70V FTIR spectrometer using a DTGS detector and acquiring at 4 cm^{-1} resolution. For IR studies the samples were pressed into self-supported wafers and treated at 150 ºC in vacuum (10^{-5}mbar) for 1h. For the reduced sample, activation in H_2 flow at 150ºC 1h followed by vacuum treatment at the same temperature for 1h was performed. In the n-butanol adsorption experiments, 0.5mbar n-butanol has been adsorbed on both activated and reduced samples. In the in situ reaction studies dimethylphenylsilane has been first adsorbed at 25ºC on $Cu_3(BTC)_2$ catalyst surface, removing the non interacting species and followed by n-butanol co-adsorption at 0.5mbar. Reaction temperature has been increased to 70ºC. After the in situ IR studies the gas phase has been evacuated and CO has been adsorbed (35mbar) at 25ºC in order to titrate surface active sites present under reaction conditions.