Post-synthetic modification of NH₂-MIL88B(Fe) with sulfonic acid groups

for acid-catalyzed epoxide ring-opening reaction

Maryam Mohammadikish*, Zahra Valimohammadi, Majid Masteri-Farahani**

Faculty of Chemistry, Kharazmi University, Tehran, Iran Tel./fax: +98 2186072706. E-mail address: mohammadikish@khu.ac.ir; mfarahani@khu.ac.ir

Experimental

Materials and instrumentation

2-amino-1,4-benzene dicarboxylic acid was purchased from Sigma-Aldrich. FeCl₃.6H₂O, dimethyl formamide, methanol, 1,3-propane sultone, ethanol, toluene, sulfuric acid, styrene oxide, propylene oxide, and epoxy cyclohexane were purchased from Merck.

Fourier transform infrared (FT-IR) spectra of solid samples were recorded on a Perkin-Elmer-RXI FT-IR spectrometer using KBr disks. Powder X-ray diffraction (XRD) analyses were conducted by Rigaku D-max CIII X-ray diffractometer with Cu K α radiation (λ = 1.54056 Å). Analyses of the morphology and chemical composition of samples were conducted by a TSCAN-Mira III field emission scanning electron microscope (FE-SEM). Thermogravimetric analysis (TGA) was carried out on a STA PT-1000. The samples were analyzed in a temperature range of 25-700 °C with a temperature increasing velocity of 10 °C/min under static air. Agilent GC 7890A MSD 5975 gas chromatography-mass spectrometry (GC-MS) was used to identify the products of catalytic reactions. Identifications were made based on comparisons with the proposed structures available at library of the device. Micro Active for TriStar II plus 2.03 device was used for nitrogen adsorption-desorption analysis and to determine the specific surface area. The CHNS elemental analyses were done on Eager 300 for EA1112.



Figure S1. (a) GC; (b) and (c) the mass spectra of the products of styrene oxide ring-opening reaction after 3 min.



Figure S2. (a) GC; (b), (c) and (d) mass spectra of the products of 1,2-epoxy cyclohexane ring-opening reaction after 5 min.



Figure S3. (a) GC; (b), (c) and (d) mass spectra of the products of 1,2-epoxy cyclooctane ring-opening reaction after 5 min.



Figure S4. (a) GC; (b), (c), (d) and (e) mass spectra of the products of propylene oxide ring-opening reaction after 5 min.



Figure S5. (a) GC; (b), (c), (d) and (e) mass spectra of the products of 1,2-epoxyhexane ring-opening reaction after 5 min.



Figure S6. (a) GC; (b), (c), (d) and (e) mass spectra of the products of 1,2-epoxyoctane ring-opening reaction after 5 min.



Figure S7. FT-IR spectra of fresh and 5th recovered Fe-MOF-SO₃H after catalytic reaction.



Figure S8. XRD patterns of fresh and 5th recovered Fe-MOF-SO₃H.