Supporting Information for:

SU-101: A Bi(III)-based Metal-Organic Framework as an efficient heterogeneous catalyst for the CO_2 cycloaddition reaction

Juan L. Obeso,[a,b+] J. Gabriel Flores,[c,d+] Catalina V. Flores,[a,b] Valeria B. López-Cervantes,[b] V. Martínez-Jiménez,[c] José Antonio de los Reyes,[c] Enrique Lima,[b] Diego Solis-Ibarra,[b] Ilich A. Ibarra,[b]* Carolina Leyva[a]* and Ricardo A. Peralta[e]*

[a]Instituto Politécnico Nacional, CICATA U. Legaria, Laboratorio Nacional de Ciencia, Tecnología y Gestión Integrada del Agua (LNAgua), Legaria 694, Irrigación, 11500, Miguel Hidalgo, CDMX, México.

[b]Laboratorio de Fisicoquímica y Reactividad de Superficies (LaFReS), Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior s/n, CU, Coyoacán, 04510, Ciudad de México, México.

[c]Departamento de Ingeniería de Procesos e Hidráulica, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, 09340, Ciudad de México, México.

[d]Área de Química Aplicada, Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco, 02200, Ciudad de México, México.

[e]Departamento de Química, División de Ciencias Básicas e Ingeniería. Universidad Autónoma Metropolitana (UAM-I), 09340, México

[+] These authors contributed equally to this manuscript.

Table of contents

S1. Experimental details

Analytical instruments

Powder X-Ray Diffraction Patterns (PXRD)

The PXRD was recorded on a Rigaku Diffractometer, Ultima IV, with Cu-Kα1 radiation (λ = 1.5406 Å) using a nickel filter. The patterns were recorded in the range 2–50° 2θ with a step scan of 0.02° and a scan rate of 0.05° min^{-1}.

Fourier-transform infrared spectroscopy (FT-IR)

The FT-IR spectra were obtained in the range of 4000-500 cm^{-1} on a Shimadzu IRTracer-100 spectrometer using KBr pellets.

Thermal gravimetric analysis (TGA)

The TGA was performed using a TA Instruments Q500HR analyzer under an N_2 atmosphere using the high-resolution mode (dynamic rate TGA) at a scan rate of 5 °C min^{-1}, from room temperature to 800 °C.

Nitrogen adsorption-desorption

Nitrogen adsorption-desorption isotherms were measured by a volumetric method using a Micromeritics ASAP 2020 gas sorption analyzer. The sample mass was 65.0 mg. Free space correction measurements were performed using ultra-high purity He gas (UHP grade 5, 99.999% pure). Nitrogen isotherms were measured using UHP-grade Nitrogen. All nitrogen analyses were performed using a liquid nitrogen bath at 77 K. Oil-free vacuum pumps were used to prevent contamination of the sample or feed gases.

Nuclear Magnetic Resonance (NMR).

NMR spectra were recorded in $CDCl_3$ solution on a Bruker Avance 400 MHz, working at 400 MHz and 100 MHz for ^{1}H and ^{13}C, respectively**.**

S2. Characterization techniques and results

Synthesis of SU-101

PXRD

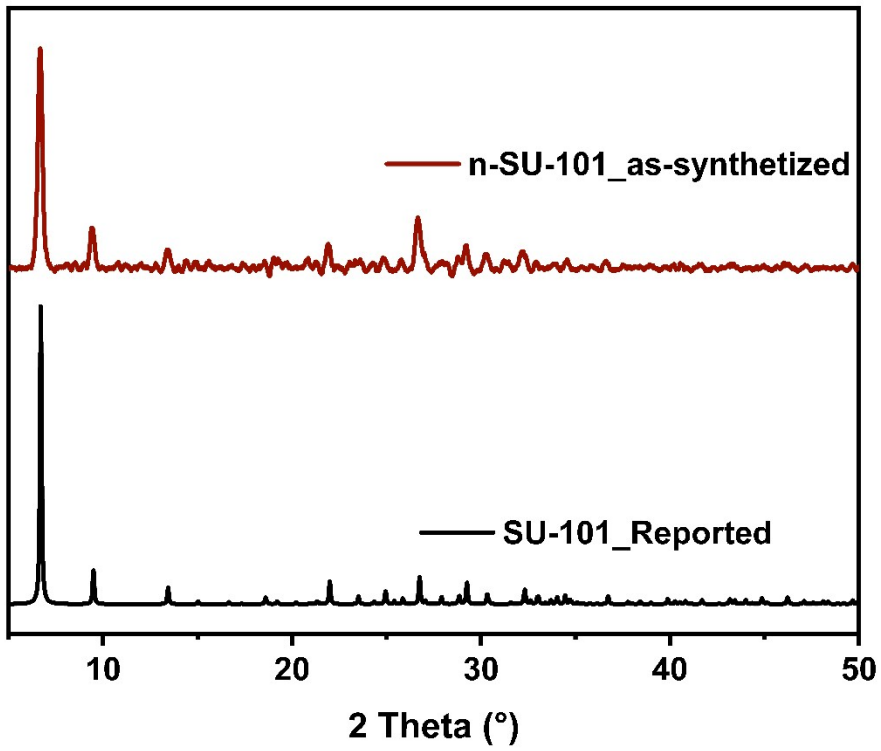


Figure S1. PXRD pattern of SU-101 reported, and SU-101 as-synthetized.

FTIR

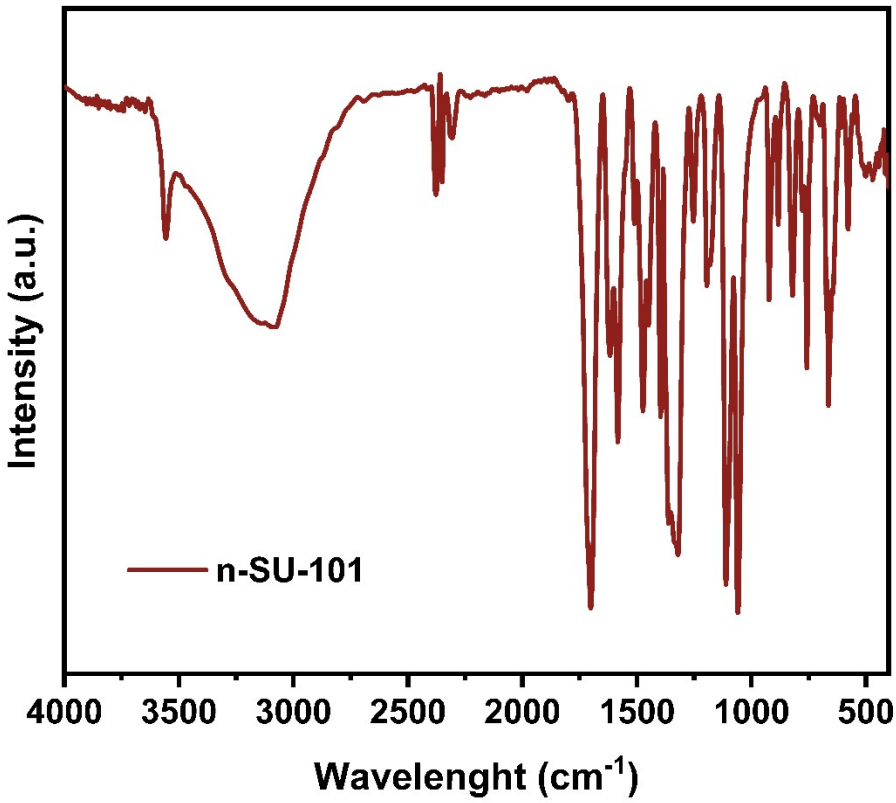


Figure S2. FTIR spectra of n-SU-101 as-synthetized.

TGA

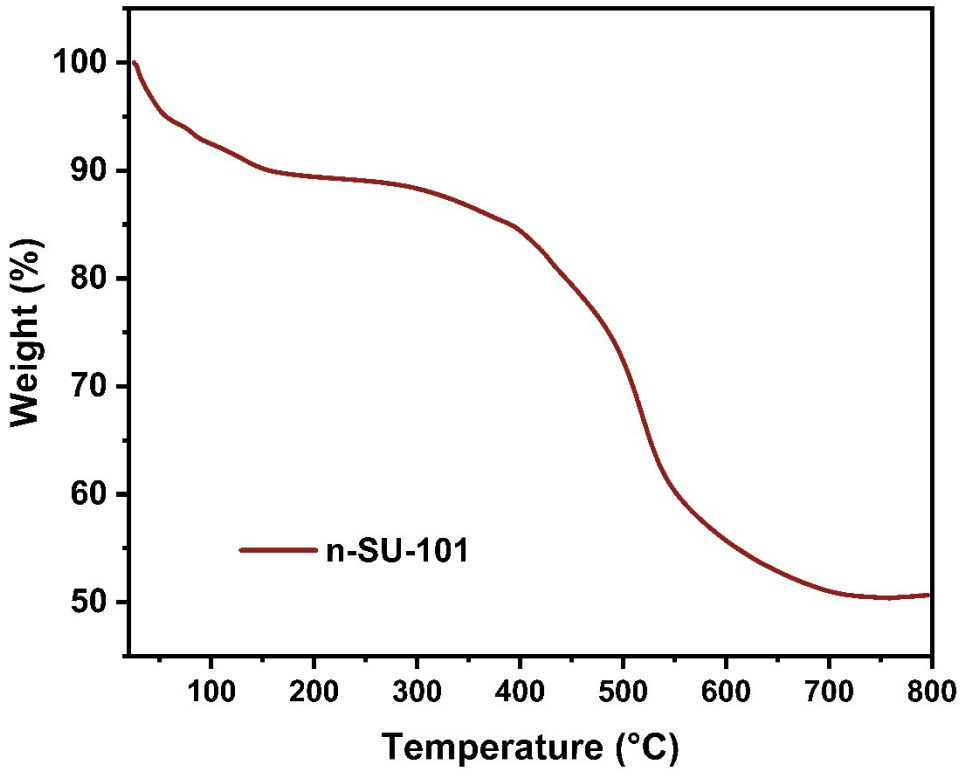


Figure S3. TGA analysis profile of SU-101 as-synthetized.

Nitrogen adsorption-desorption

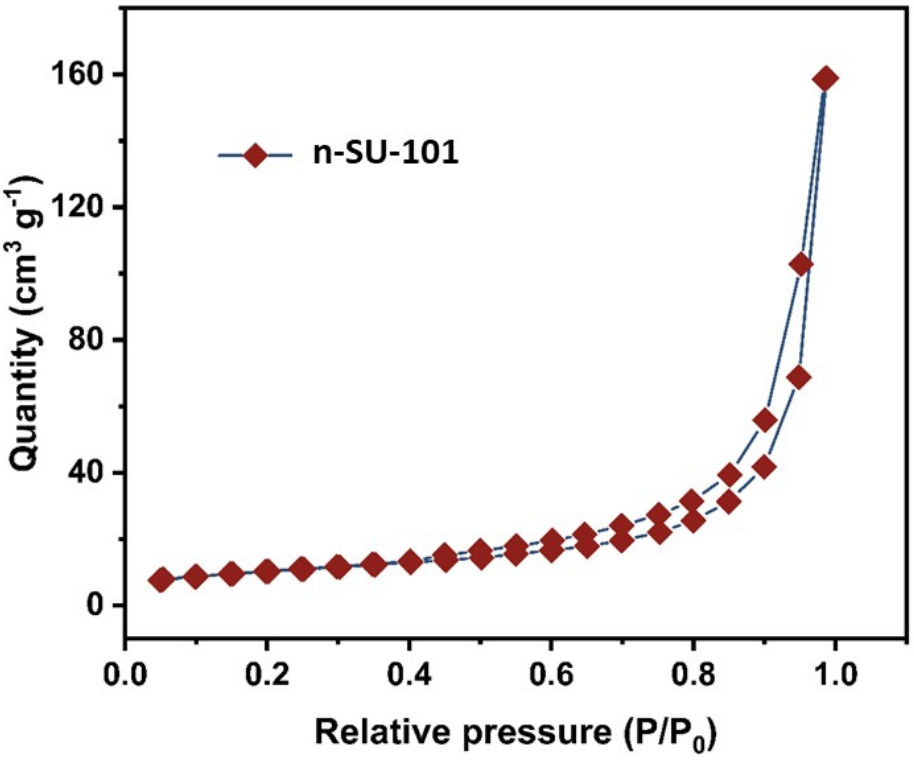


Figure S4. Nitrogen isotherm of SU-101 as-synthetized.

Pore size distribution

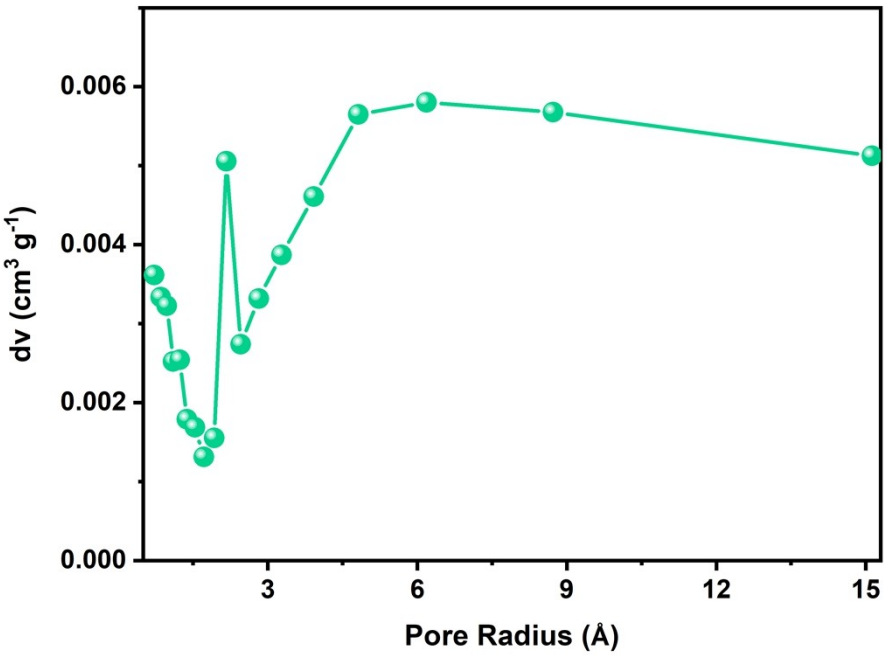


Figure S5. BJH pore size distribution plot derived from the N_2 isotherm.

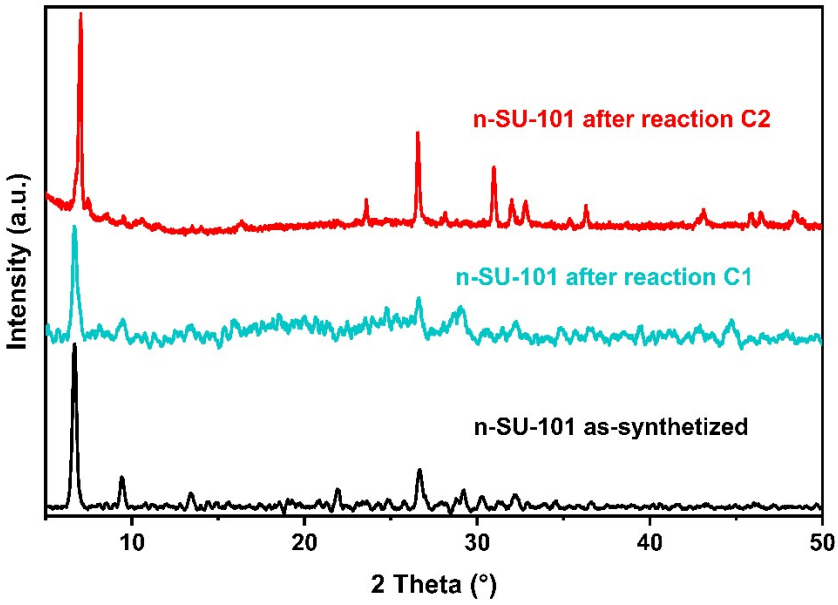
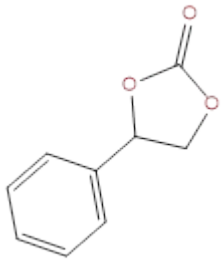


Figure S6. PXRD pattern of SU-101 as-synthetized (Black) after one reaction cycle (blue) and after two reaction cycles (red).

Reaction product characterization

4-phenyl-1, 3-dioxolan-2-one was characterized by ^{1}H-NMR and ^{13}C-NMR spectroscopy

4-phenyl-1, 3-dioxolan-2-one



^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.46-7.28 (m, 5H), 5.66 (t, 1H), 4.78 (t, 1H), 4.35-4.32 (m, 1H) ^{13}C-NMR (101 MHz, $CDCl_3$) δ 154.82 (s), 137.67 (s), 129.70 (s) 128.19 (s), 125.53 (s), 77.97 (s), 71.20 (s).

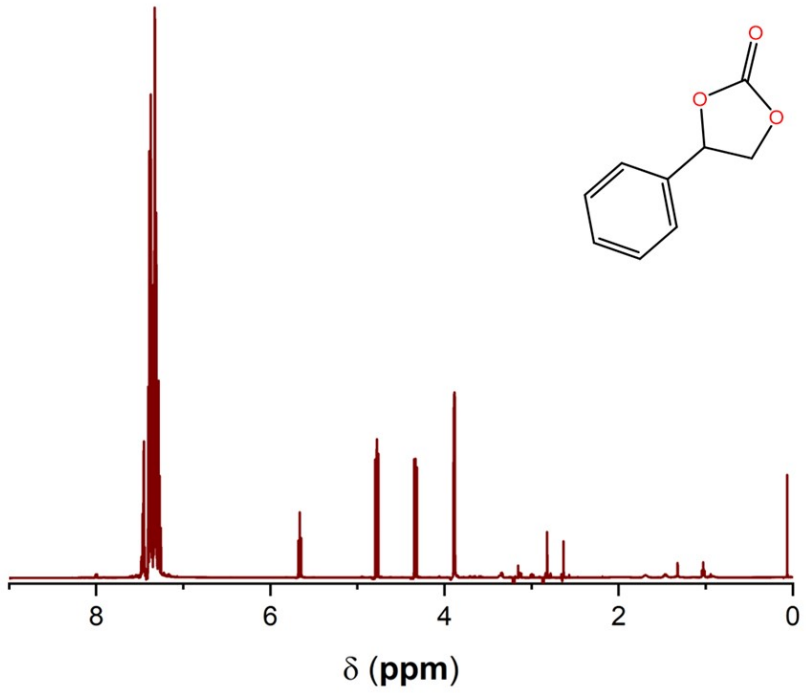


Figure S7. The ^{1}H-NMR spectrum of 4-phenyl-1, 3-dioxolan-2-one

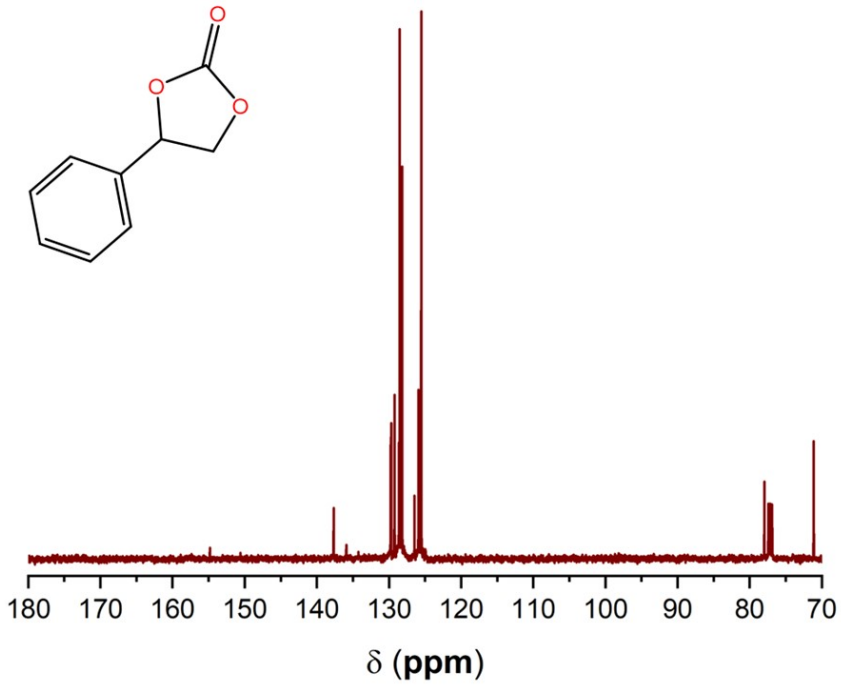


Figure S8. The ^{13}C-NMR spectrum of 4-phenyl-1, 3-dioxolan-2-one