

Supplementary information

Mechanochemical synthesis of Yttrium based metal organic framework

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Experimental details: About 2.6 mmol of each of yttrium hydride (YH₃; Pfaltz and Bauer) and trimesic acid (TMA, C₆H₃-(COOH)₃; Sigma-Aldrich) was loaded in a stainless steel milling container (see Figure S1) inside a glove box under argon atmosphere and milled for seven hours in SPEX 8000 mill having motor and clamp speed of 1725 and 1060 RPM, respectively. The milling was interrupted after 20, 80, 200 and 300 minutes of milling for in process testing. The ball to mass ratio was taken to be 25:1 and forced air cooling was employed to avoid the heating of the vial during milling. A total of 6 stainless steel balls (2 bigger and 4 smaller balls with diameters of 12.65 and 6.33 mm, respectively) were used for milling.

The structural characterization was performed by collecting the powder X-ray diffraction (PXRD) pattern using Bruker General Area Detector Diffraction System (GADDS) and employing Cu K_α radiation.

The thermogravimetric analysis (TGA) and Differential Scanning Calorimetric (DSC) measurements from room temperature to 600°C were performed by using METTLER TOLEDO STAR System. During the measurement the air/argon flow was 60 ml/min whereas the temperature ramping was performed at 10 °C /min.

The Scanning electron microscopy (SEM) measurements were performed using Philips XL30 ESEM FEG instrument.

FTIR measurements were performed using a Thermo-Nicolet Magna 550 FTIR spectrometer equipped with a Thermo-SpectraTech Endurance Foundation Series Diamond ATR and a DTGS detector. The samples were compressed directly on to the Diamond ATR window. 16 scans at a resolution of 4 cm⁻¹ were collected for the sample over the spectral range 4000-525 cm⁻¹ and ratioed against a 16 scan, 4 cm⁻¹ Single beam background collection collected of the clean Diamond ATR window. The ATR “correction” was applied using the OMNIC software, followed by a baseline correction.

FTIR (1:1 mixture of YH₃ and TMA after milling for 420 min, cm⁻¹): 3070 (w), 1690(s), 1625 (s), 1551 (s), 1436(s), 1400 (s), 1315 (m), 1270(m), 1215(m), 1125 (m), 930(w), 825 (w), 760 (m), 737(s), 711(m), 665(m), 566(w)



Figure S1. The image of the milling container and balls used in this work.

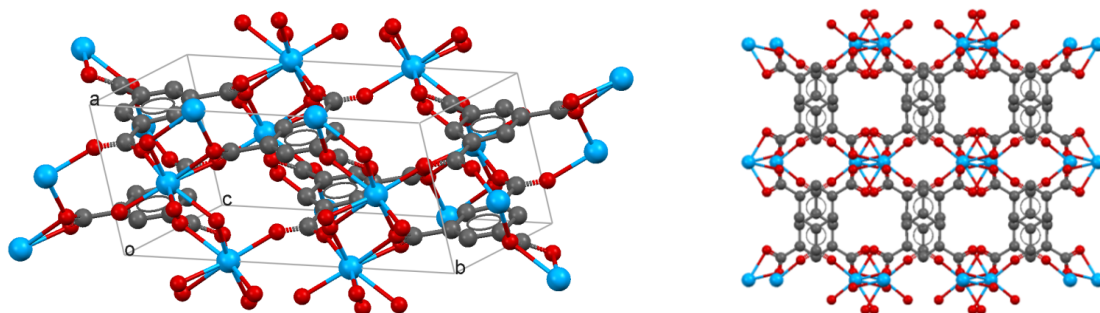
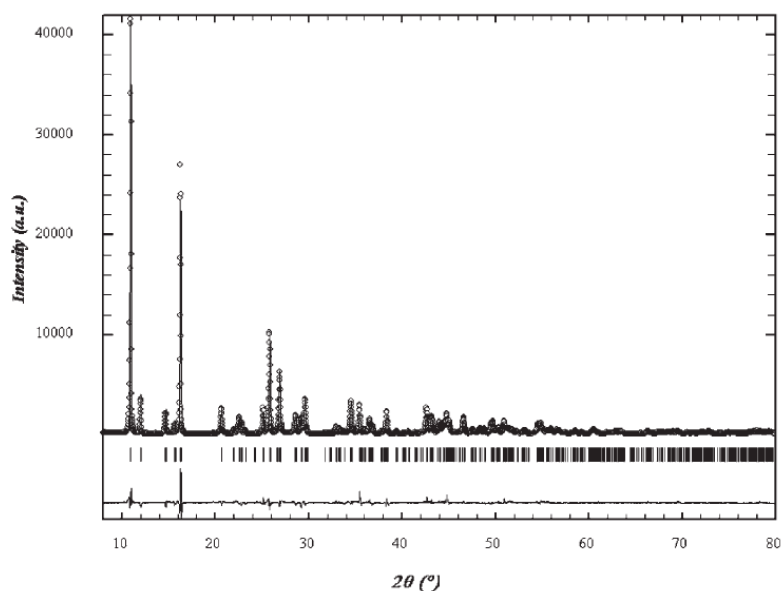


Figure S2. PXRD pattern and simulated structure of of MIL-78 (Simulations were performed by Dr. V. Stavila using CIF file from C. Serre et al., *J. Mater.Chem.*, 2004,**14**, 1540.) Circles: red for oxygen, blue for yttrium and gray for carbon.

Table 1S. Conversion rate of TMA vs. time during ball-milling of the 1:1 molar mixture of YH_3 and TMA

Milling time (min)	Sample mass (mg)	Integral intensity (mJ)	Normalized integral intensity (J/g)
5	12.9	2496.54	193.53
80	14.2	2032.23	143.12
200	12.7	1297.98	102.2
300	16	679.73	42.48
420	17.5	No peak	No peak

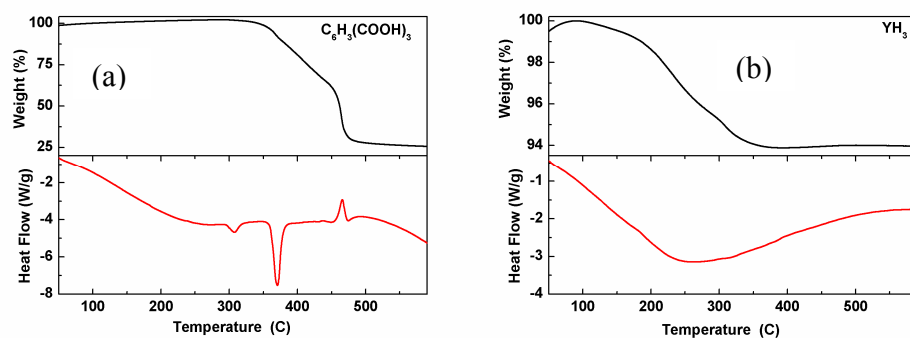


Figure S3. (a) The TGA/DSC data of as received TMA ($\text{C}_6\text{H}_3(\text{COOH})_3$) and (b) YH_3 .

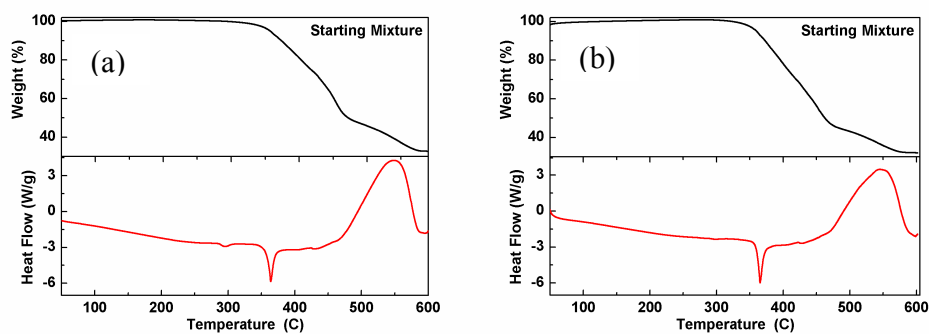


Figure S4. (a) The TGA/DSC data for the 1:1 mixture of YH_3 and TMA and (b) the 1:1 mixture of YH_3 and TMA heated to 300 °C and then cooled back down to 30 °C with a ramp rate of 10 °C/min.

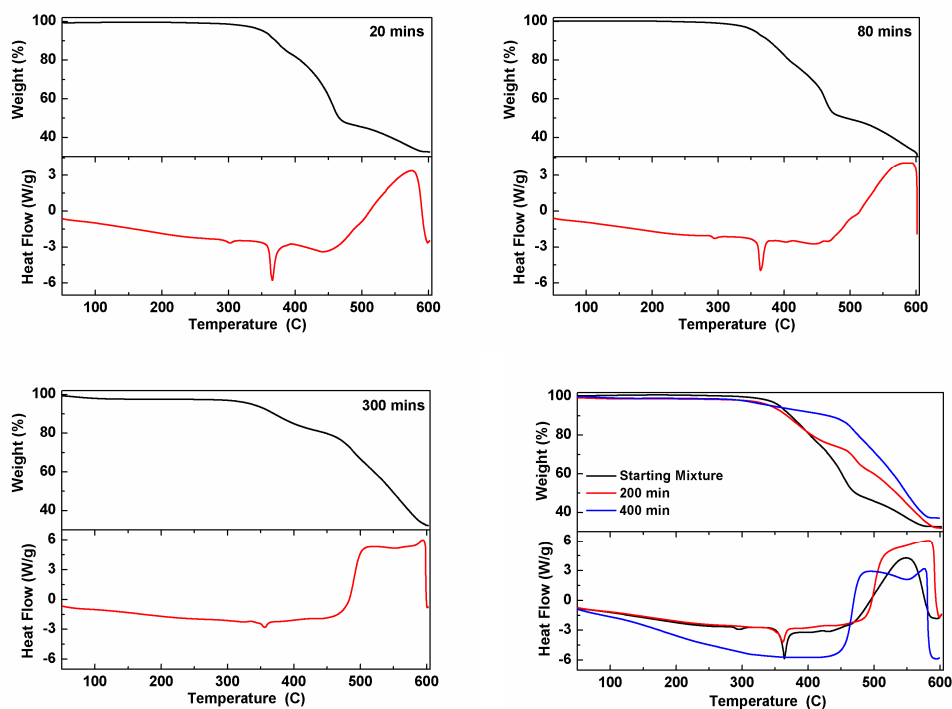


Figure S5. The TGA/DSC data of the 1:1 mixture of YH₃ and TMA after milling for 20, 80, 200, 300 and 420 minutes.

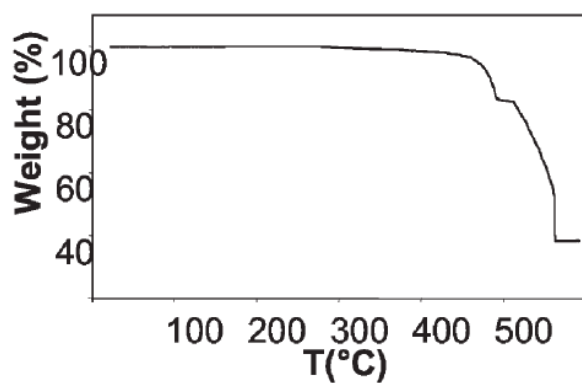


Figure S6. The TGA data for MIL-78 from C. Serre et al., *J.Mater.Chem.*, 2004, **14**, 1540.

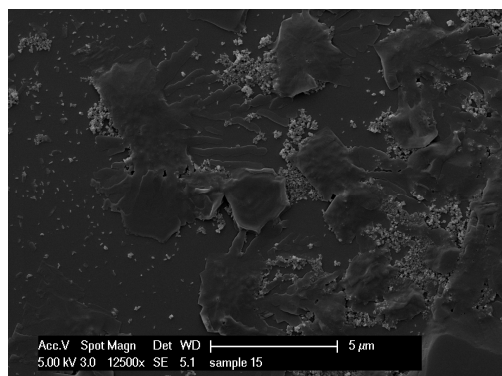


Figure S7. Scanning electron microscopy image of the 1:1 mixture of YH_3 and TMA milled for 200 minutes.

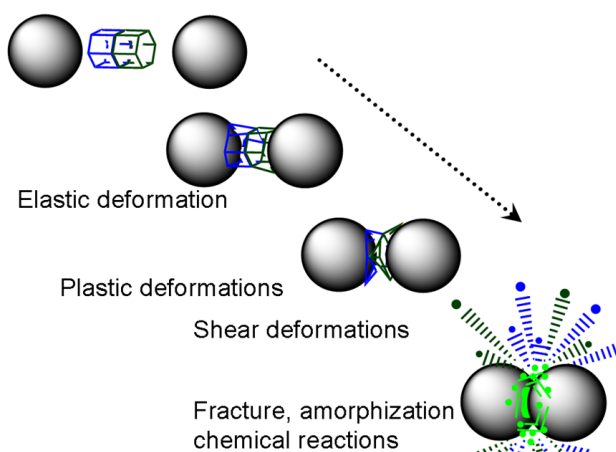


Figure S8. Deformations of a particle trapped between colliding balls during ball-milling.