Supplementary information

Solid-liquid Conversion and Carbon Dioxide Storage in a Calcium-Based Metal-Organic Framework with Micro and Nanoporous Channels

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Preparation of A phase:

In order to obtain A phase, some solid crystals of MUT-1 were put in a vial. Then some droplets of water were added to it to keep the crystals wet without any vigorous stirring. The vial was sealed, and it left for three hours. After this time, the solid precipitates were dried in the air atmosphere. The PXRD pattern was obtained from this solid powder.

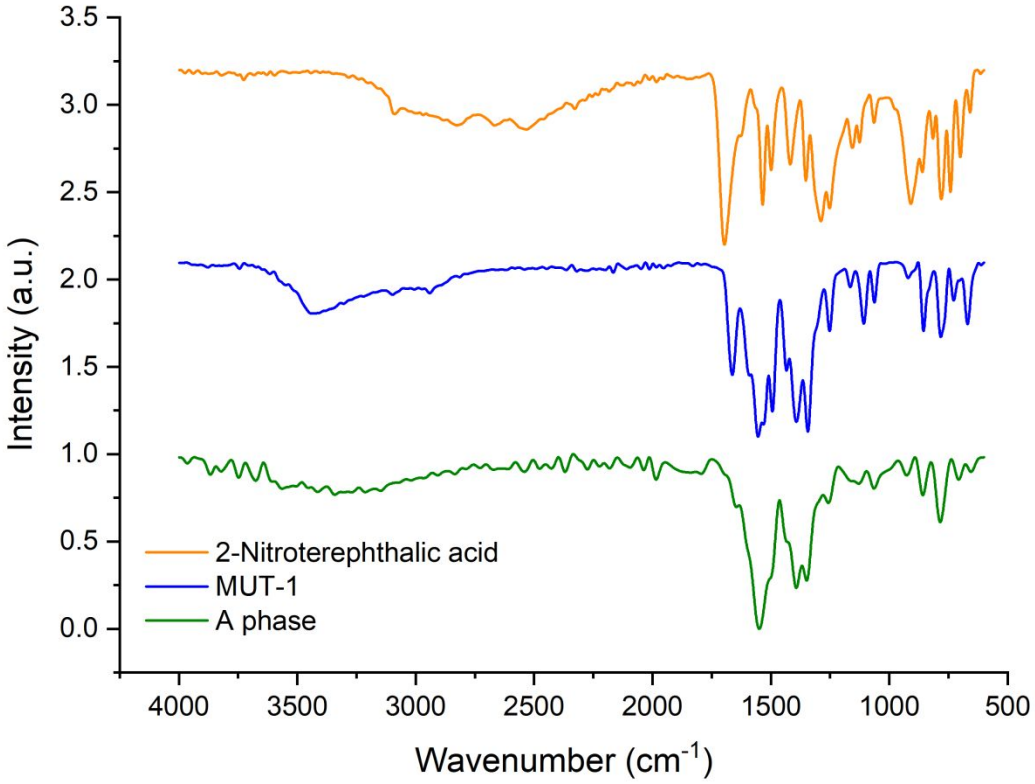

Figure S1: FT- IR spectra of 2-nitro terephthalic acid, MUT-1 and A phase.

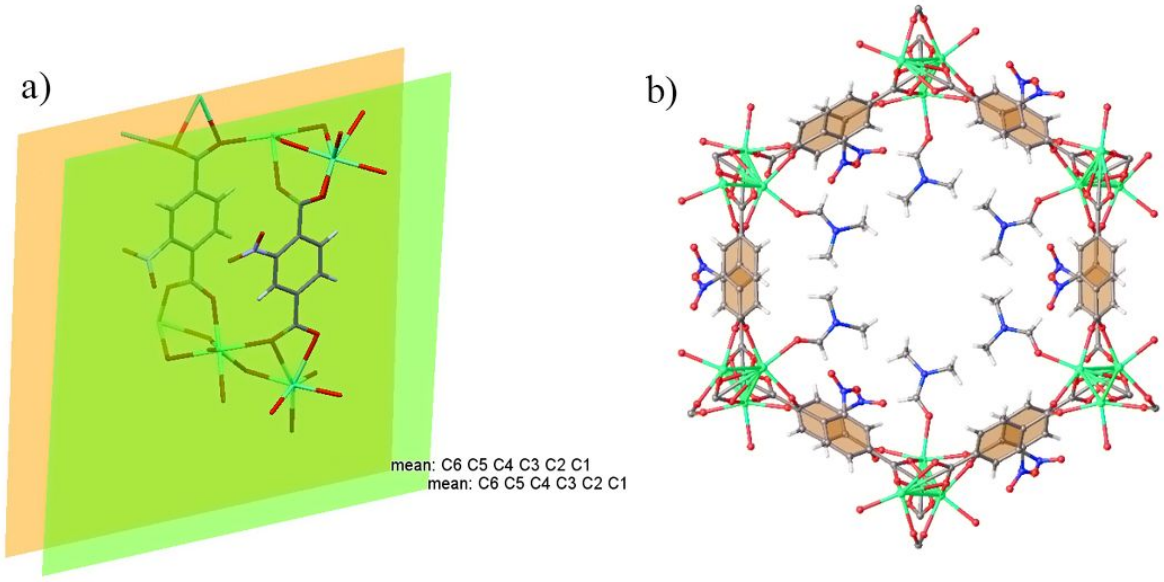

Figure S2 a) The distance between the centroid to the centroid of the aromatic rings and b) the angle between the two aromatic rings in MUT-1.

Table S1 Selected bond lengths (Å) and angles (°) for MUT-1.

Ca(1)-O(1)	2.284(5)	O(1)-Ca(1)-C(8)	100.4(2)
Ca(1)-O(2)	2.331(7)	O(2)-Ca(1)-C(8)	99.4(3)
Ca(1)-O(7)	2.337(6)	O(7)-Ca(1)-C(8)	175.0(3)
Ca(1)-O(4)	2.346(4)	O(4)-Ca(1)-C(8)	87.45(18)
Ca(1)-O(3)	2.346(4)	O(3)-Ca(1)-C(8)	87.93(17)
Ca(1)-O(3)	2.552(4)	O(3)-Ca(1)-C(8)	25.04(17)
Ca(1)-O(4)	2.576(4)	O(4)-Ca(1)-C(8)	25.73(17)
Ca(1)-C(8)	2.929(5)	O(1)-Ca(1)-Ca(1)	121.68(16)
Ca(1)-Ca(1)	3.7721(10)	O(2)-Ca(1)-Ca(1)	68.02(17)
O(1)-Ca(1)- O(2)	160.2(3)	O(7)-Ca(1)-Ca(1)	117.6(2)
O(1)-Ca(1)-O(7)	84.4(3)	O(4)-Ca(1)-Ca(1)	42.28(11)
O(2)-Ca(1)-O(7)	75.9(4)	O(3)-Ca(1)-Ca(1)	135.10(13)
O(1)-Ca(1)-O(4)	86.23(18)	O(3)-Ca(1)-Ca(1)	37.68(10)
O(2)-Ca(1)-O(4)	93.6(2)	O(4)-Ca(1)-Ca(1)	86.12(10)
O(7)-Ca(1)-O(4)	94.5(2)	C(8)-Ca(1)-Ca(1)	61.24(14)
O(1)-Ca(1)-O(3)	93.82(19)	O(1)-Ca(1)-Ca(1)	68.87(16)
O(2)-Ca(1)-O(3)	87.9(2)	O(2)-Ca(1)-Ca(1)	122.4(2)
O(7)-Ca(1)-O(3)	90.2(2)	O(7)-Ca(1)-Ca(1)	118.8(2)
O(4)-Ca(1)-O(3)	175.31(15)	O(4)-Ca(1)-Ca(1)	134.58(13)
O(1)-Ca(1)-O(3)	117.9(2)	O(3)-Ca(1)-Ca(1)	41.67(11)
O(2)-Ca(1)-O(3)	80.6(3)	O(3)-Ca(1)-Ca(1)	86.28(10)
O(7)-Ca(1)-O(3)	152.3(3)	O(4)-Ca(1)-Ca(1)	37.77(9)
O(4)-Ca(1)-O(3)	72.33(14)	C(8)-Ca(1)-Ca(1)	62.12(14)
O(3)-Ca(1)-O(3)	103.61(11)	Ca(1)-Ca(1)-Ca(1)	123.36(4)
O(1)-Ca(1)-O(4)	81.5(2)		
O(2)-Ca(1)-O(4)	117.6(3)		
O(7)-Ca(1)-O(4)	156.2(3)		
O(4)-Ca(1)-O(4)	103.52(11)		
O(3)-Ca(1)-O(4)	71.87(14)		
O(3)-Ca(1)-O(4)	50.76(10)		

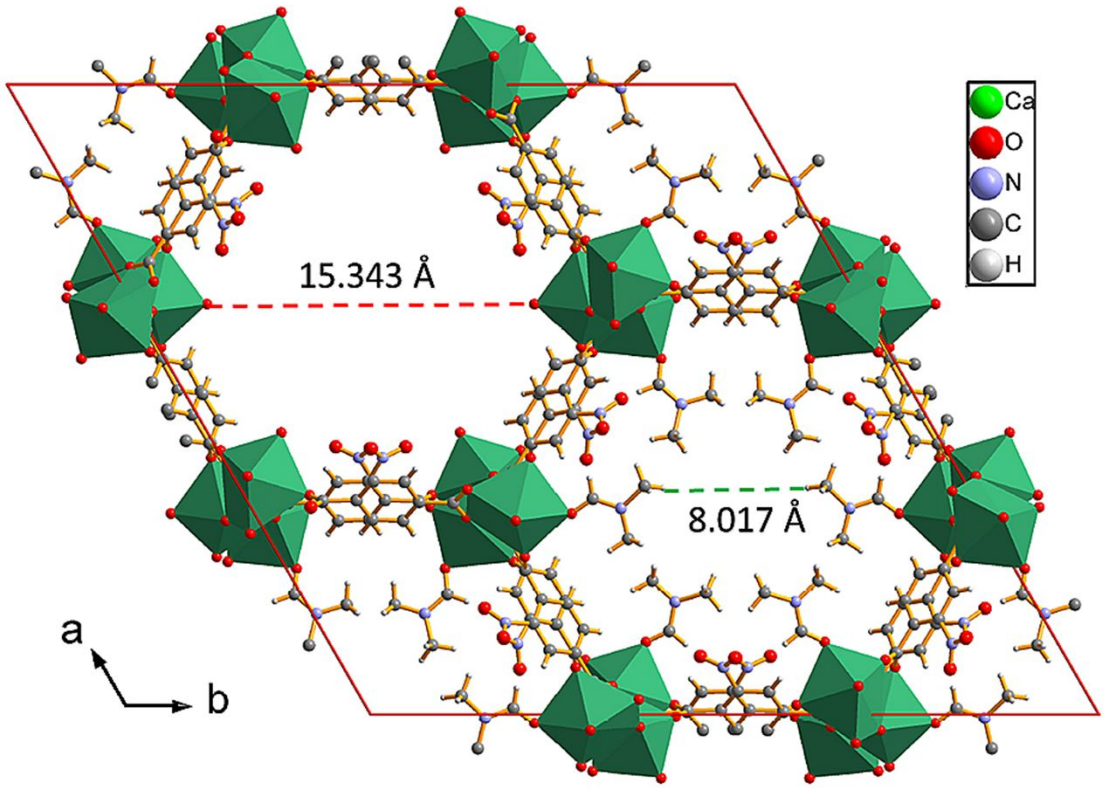

Figure S3. The obtained size of channels in the presence and absence of DMF solvent with Diamond software.

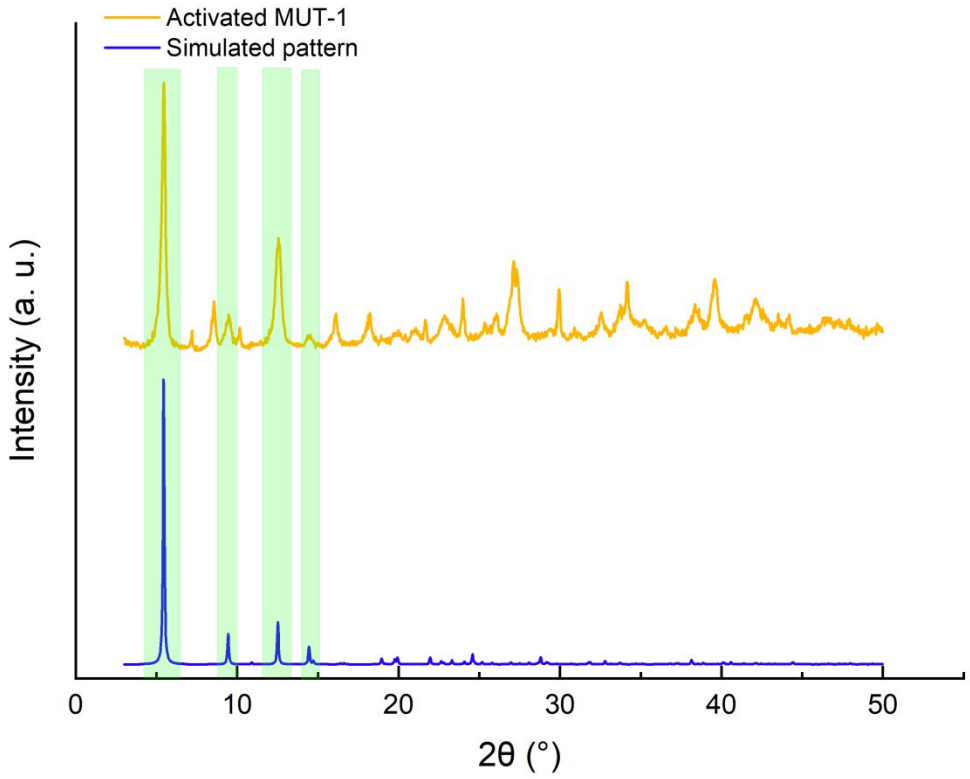

Figure S4 PXRD pattern of MUT-1 after activation process.

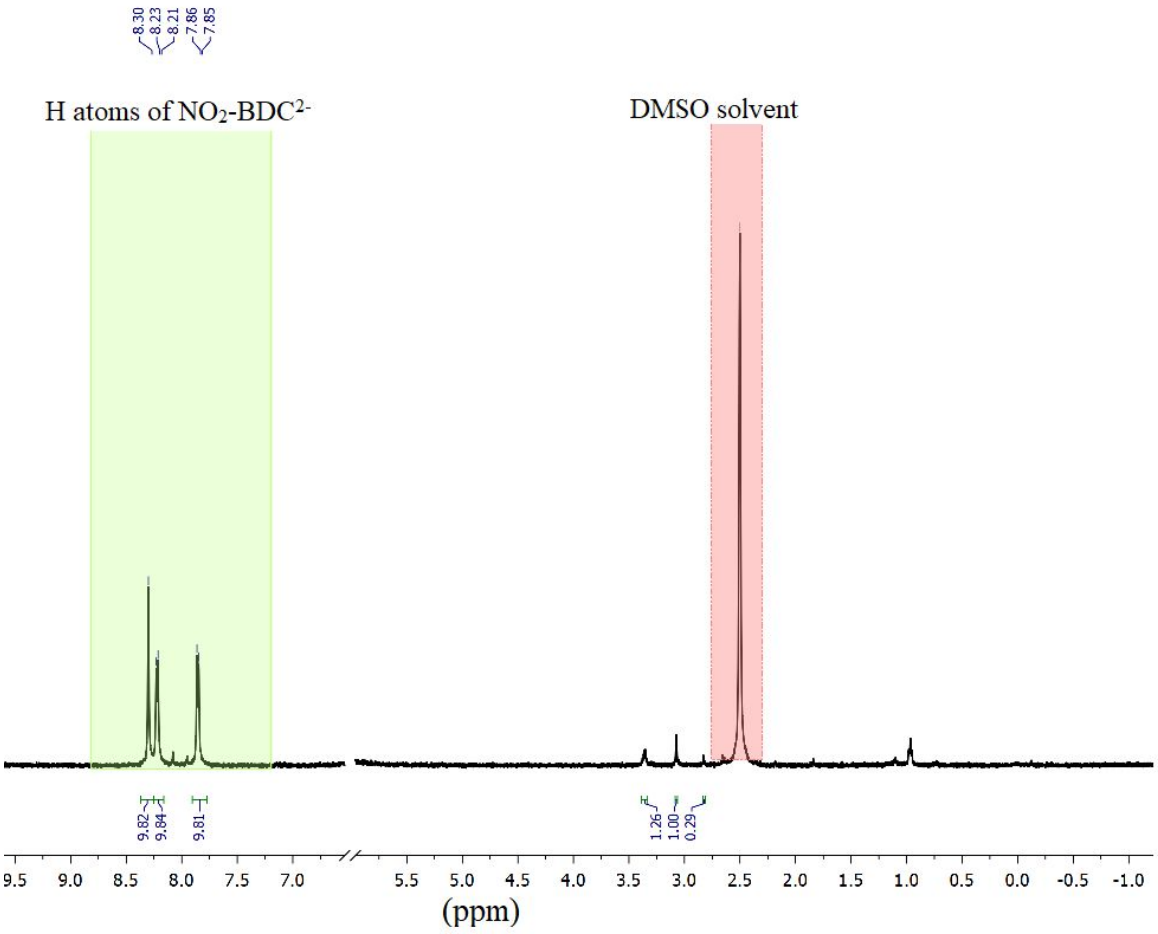

Figure S5 ^{1}H-NMR analysis of MUT-1 after the solvent exchange with ethanol and drying in a vacuum oven at 80 °C.

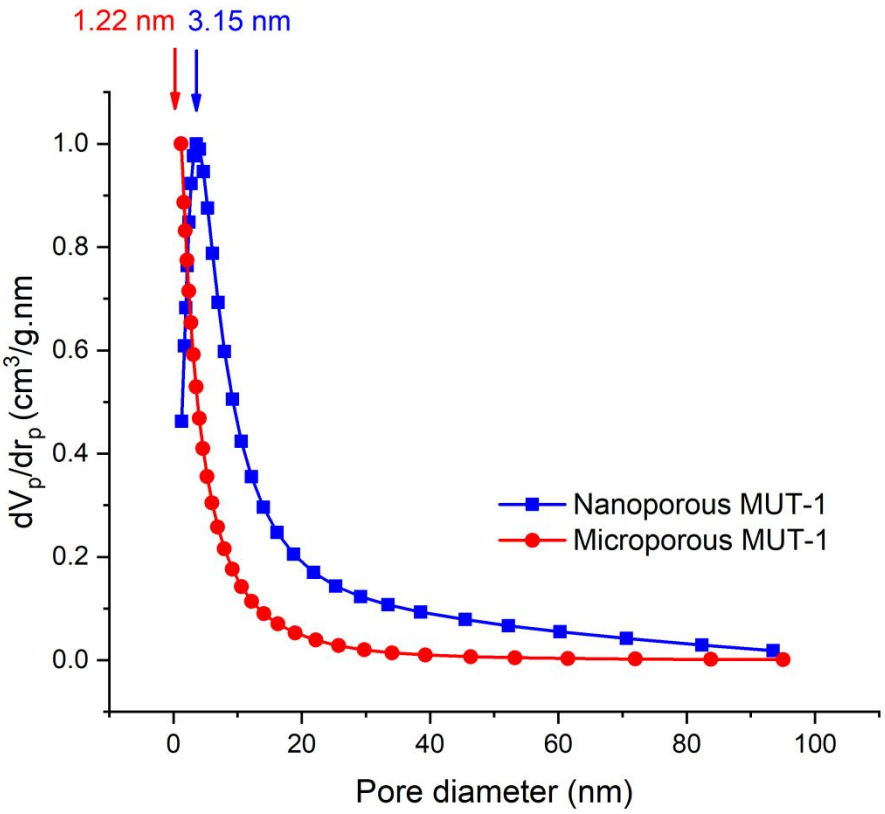

Figure S6 BJH pore-size distribution of MUT-1.

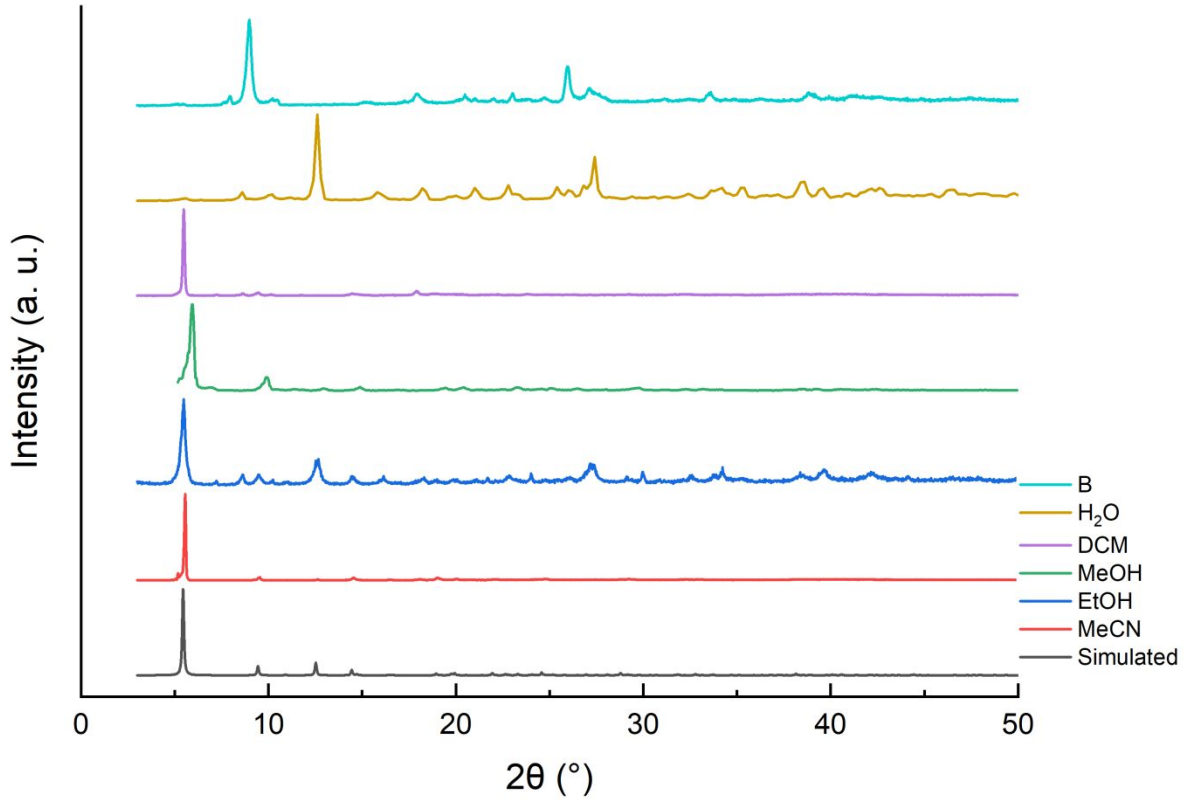

Figure S7 PXRD patterns of MUT-1 in different solvents.

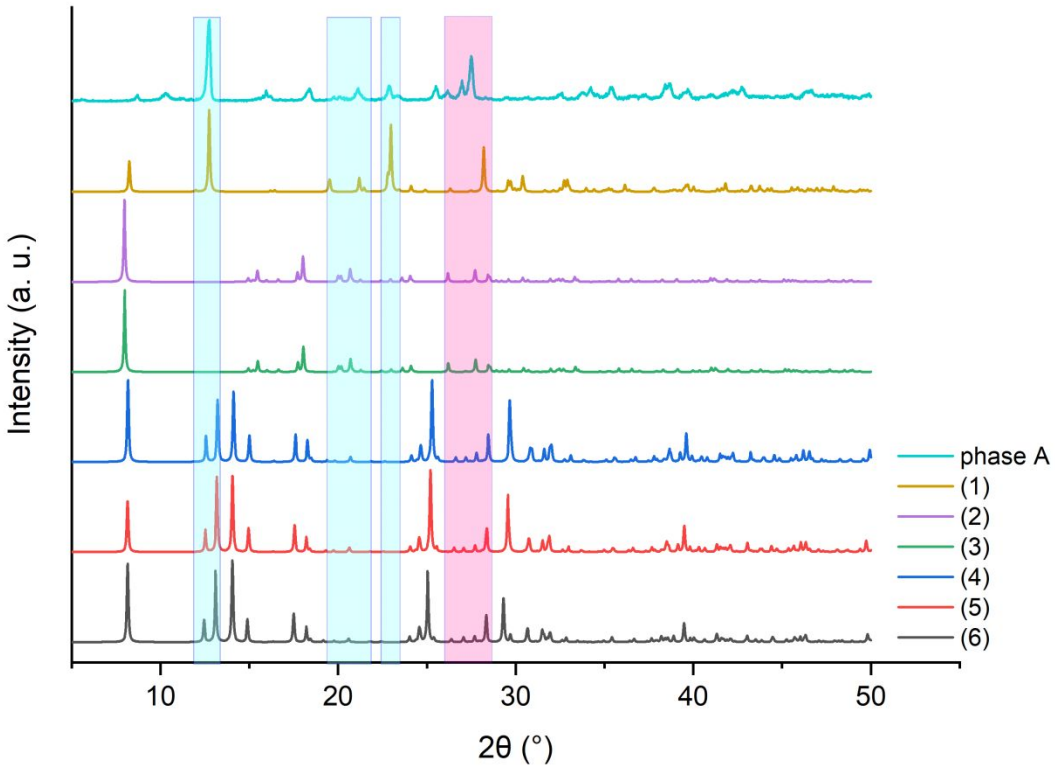

Figure S8 A comparison between PXRD patterns of obtained phase from the reorganization of MUT-1 in water (A phase) with other similar crystal structure reported from similar terephthalic acid.

(1) $[Ca(BDC)(DMF)(H_2O)]_n$[1]

(2) $[Ca(BDC)(H_2O)_3]_n$ prepared by milling[2]

(3) $[Ca(BDC)(H_2O)_3]_n$ prepared by $Ca(NO_3)_2.4H_2O$[3]

(4) $[Ca(BDC)(H_2O)_3]_n$ prepared by $CaCO_3$[4]

(5) $[Ca(BDC)(H_2O)_3]_n$ prepared by $CaCl_2$[5]

(6) $[Ca(BDC)(H_2O)_3]_n$ prepared by $Ca(CH_3COO)_2$[6]

The structures of compounds 4-6 are approximately similar. They prepared with the solvothermal method with small differences in their synthesis process such as Ca salts used in their synthesis.

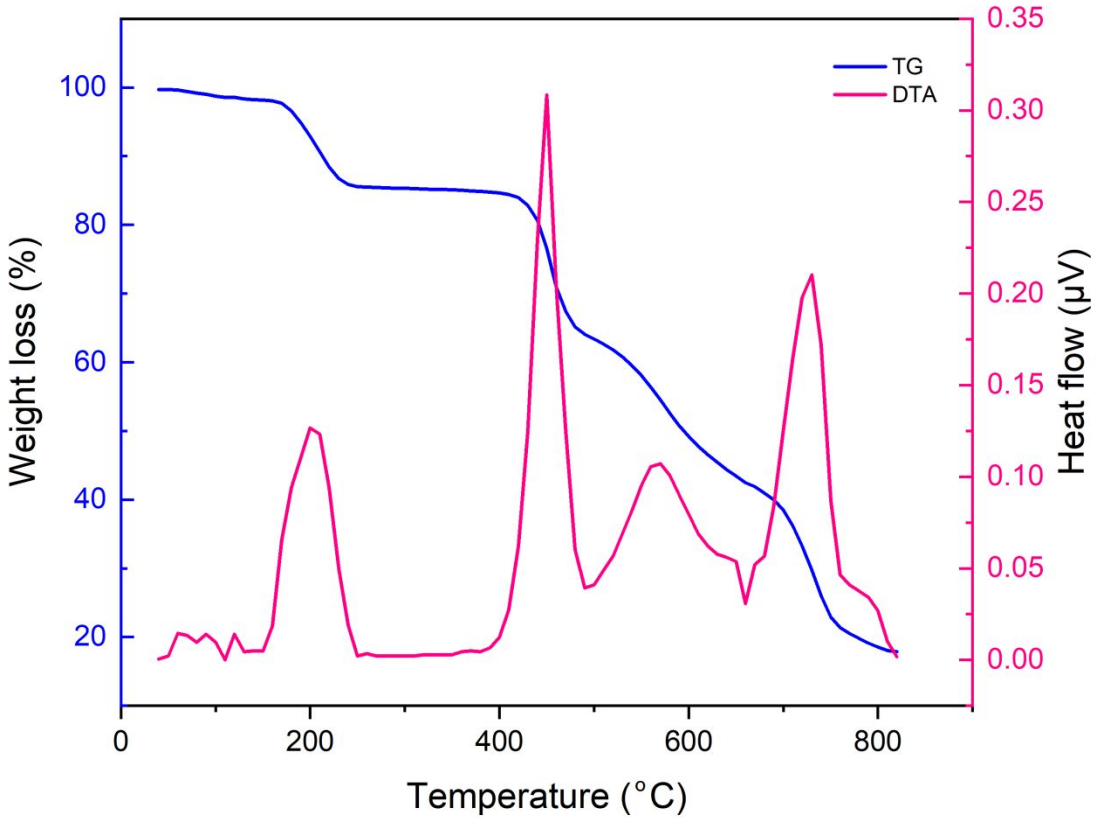

Figure S9 Thermal behavior of A phase.

References

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