Supplementary Material (ESI) for Energy & Environmental Science

Supporting Information for:

Hydrogen Storage in Water-Stable Metal-Organic Frameworks Incorporating 1,3- and 1,4-Benzenedipyrazolate

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Energy & Environmental Science

Table S1. Crystallographic Data for Co(1,3-BDP)·DEF·0.5H_2O.

Identification	Co(BDP)·DEF·0.5H_2O
Formula	$CoC_{17}H_{20}N_5O_{1.5}$
FW	377.31
T, K	150(2)
Wavelength, Å	0.77490
Crystal system, space group	Tetragonal, I4(1)/amd
Z	16
a, Å	22.847(15)
c, Å	12.458(16)
V, Å^3	6503(10)
d_{calc}, g/cm^3	1.542
Adsorption coefficient, mm^{-1}	1.074
F(000)	2674
Crystal size, mm^3	0.015 × 0.015 × 0.04
Theta range for data collection	2.75-19.14°
Index range	$-19 \le h \le 19$, $-19 \le k \le 19$, $-10 \le l \le 10$
Reflections collected	10681
Independent reflections	559 [R(int) = 0.1042]
Data/restrains/parameters	559 / 6 / 81
GOF on F^2	1.341
Largest diff. peak and hole, e·Å^{-3}	0.346 and -0.271
R_1 (wR_2)[a], [I>2sigma(I)]	0.0635 (0.1642)
R_1 (wR_2)[a], all data	0.0794 (0.1748)

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = \{\Sigma[w(F_o^2-F_o^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

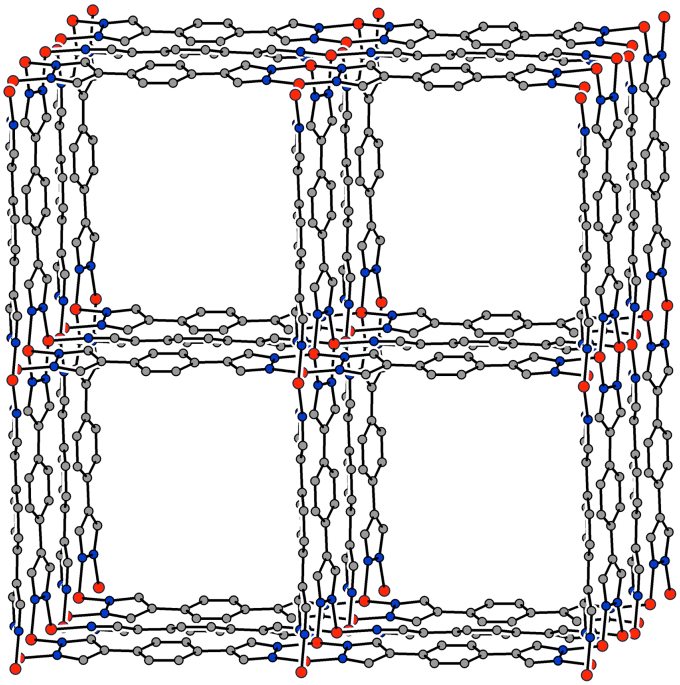

Fig. S1 A portion of the crystal structure of **1**, which is isostructural to Co(1,4-BDP).[1] Red, blue, and grey spheres represent Zn, N, and C atoms, respectively.

[1]H. J. Choi, M. Dinca, J. R. Long, *J. Am. Chem. Soc.* 2008, **130**, 7848.

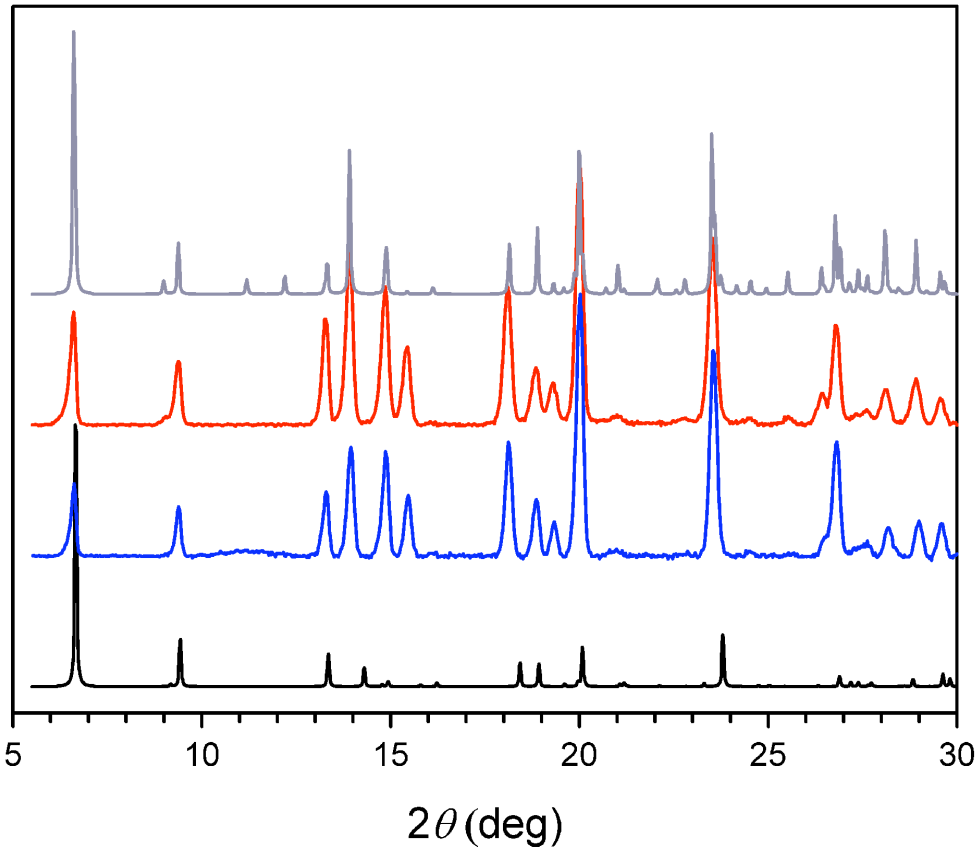

Fig. S2 Powder X-ray diffraction patterns for the crystallographic simulation for Co(1,4-BDP)·2DEF·H_2O (black) and its pulverized crystals (blue), and Zn(1,4-BDP)·2DEF·H_2O (**1**) (red) and its simulation pattern based on the unit cell refinement (grey).

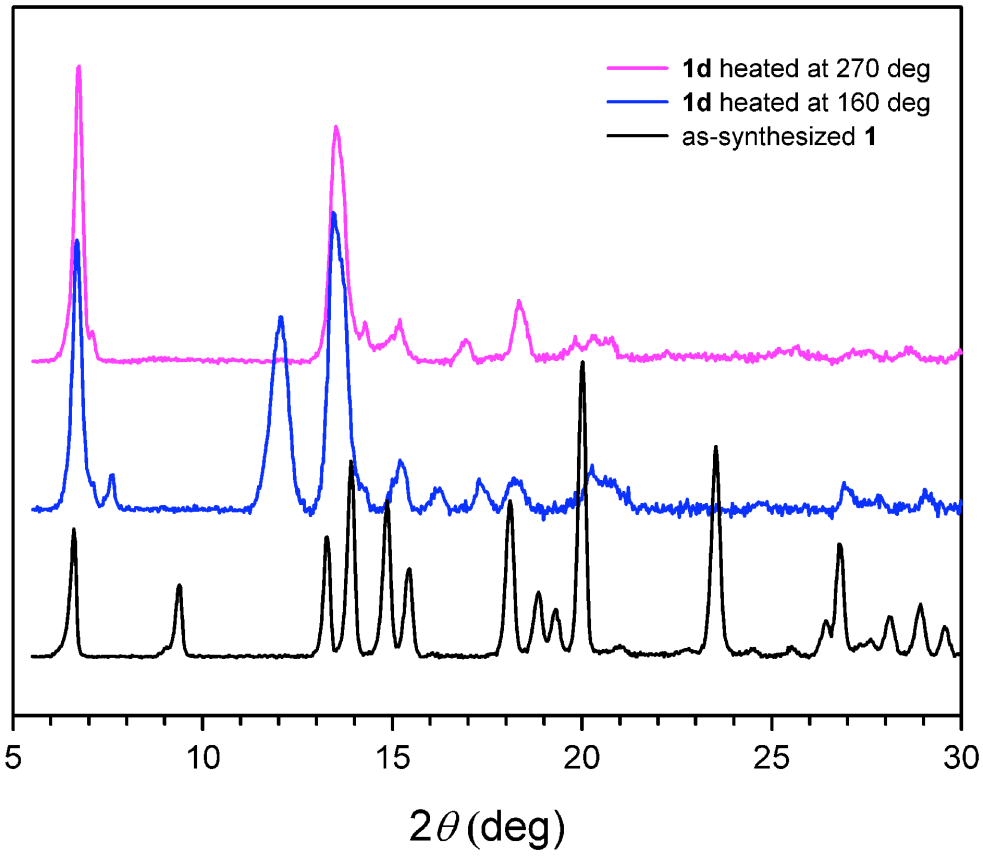

Fig. S3 Powder X-ray diffraction patterns for the as-synthesized solid **1** (black), and its desolvated form **1d** heated at 160 °C (blue) and 270 °C (pink).

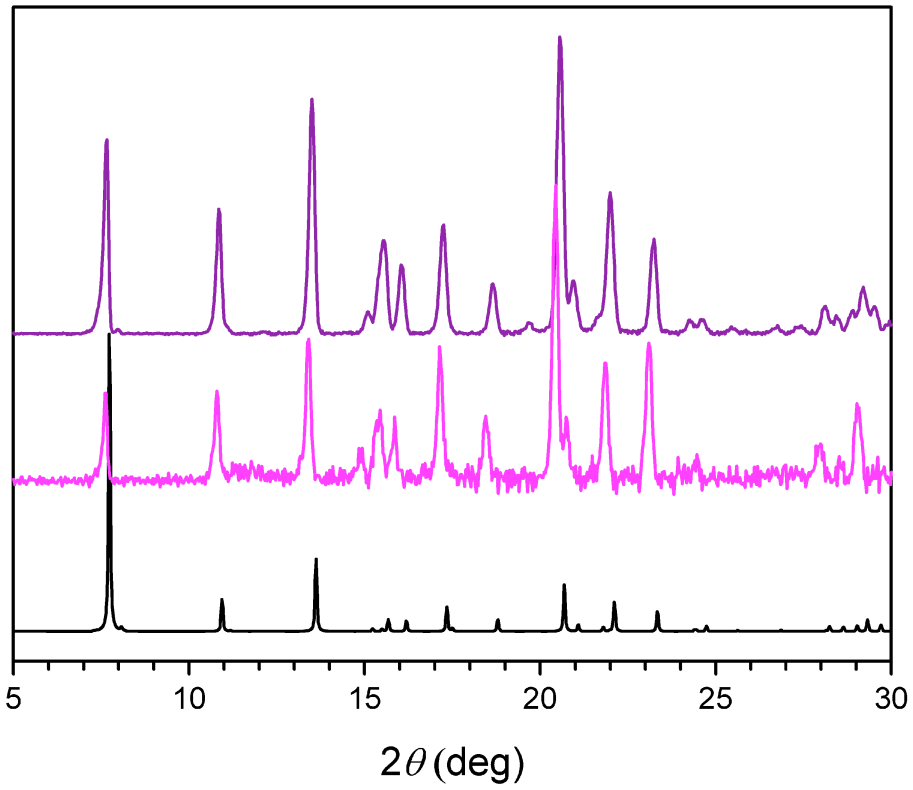

Fig. S4 Powder X-ray diffraction patterns for the crystallographic simulation for Co(1,3-BDP)·DEF·0.5H_2O (**2**) (black), pulverized crystals of **2** (pink) and Zn(1,3-BDP)·0.7DMF·0.5H_2O (**3**) (dark pink).

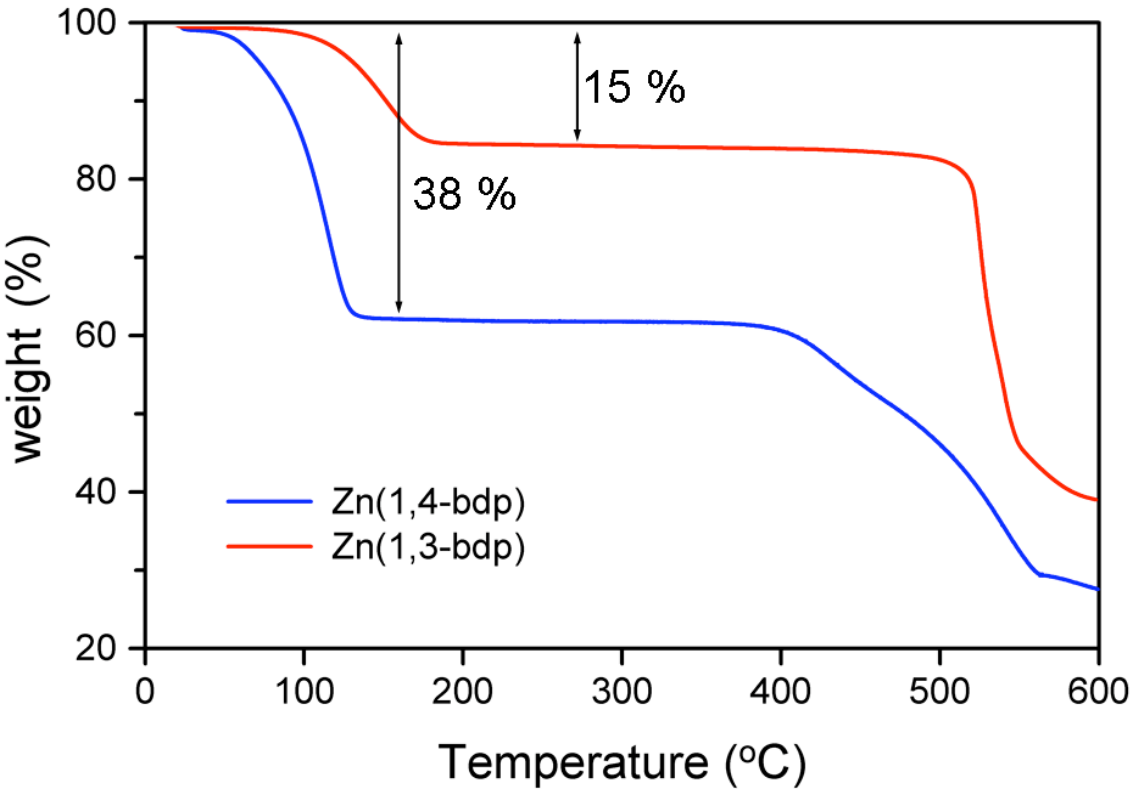

Fig. S5 Thermogravimetric analysis data for Zn(1,4-BDP)·2DEF·H_2O (**1**) (blue) and Zn(1,3-BDP)·0.7DMF·0.5H_2O (**3**) (red) measured using a ramp rate of 1.0 °C/min.

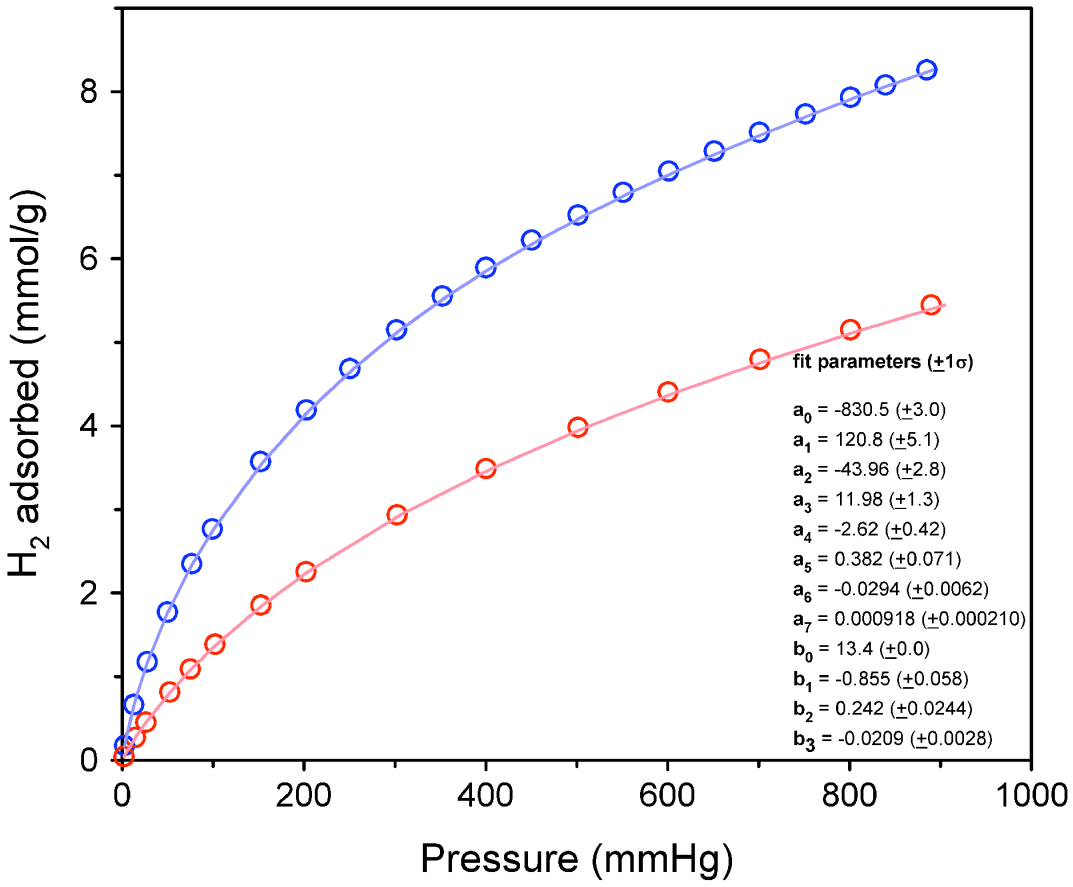

Fig. S6 H_2 adsorption isotherms for **1d** at 77 K (blue) and 87 K (red), and the respective virial fits (solid lines).

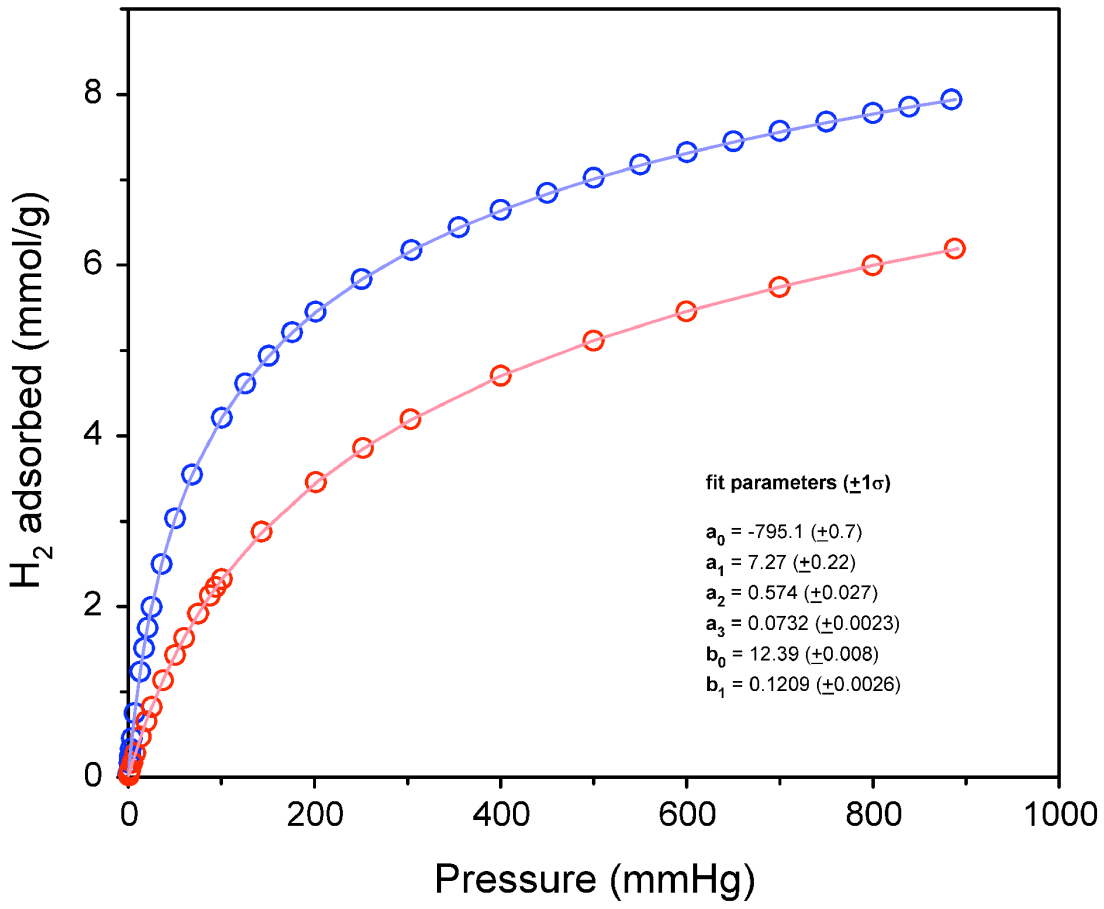

Fig. S7 H_2 adsorption isotherms for **3d** at 77 K (blue) and 87 K (red), and the respective virial fits (solid lines).

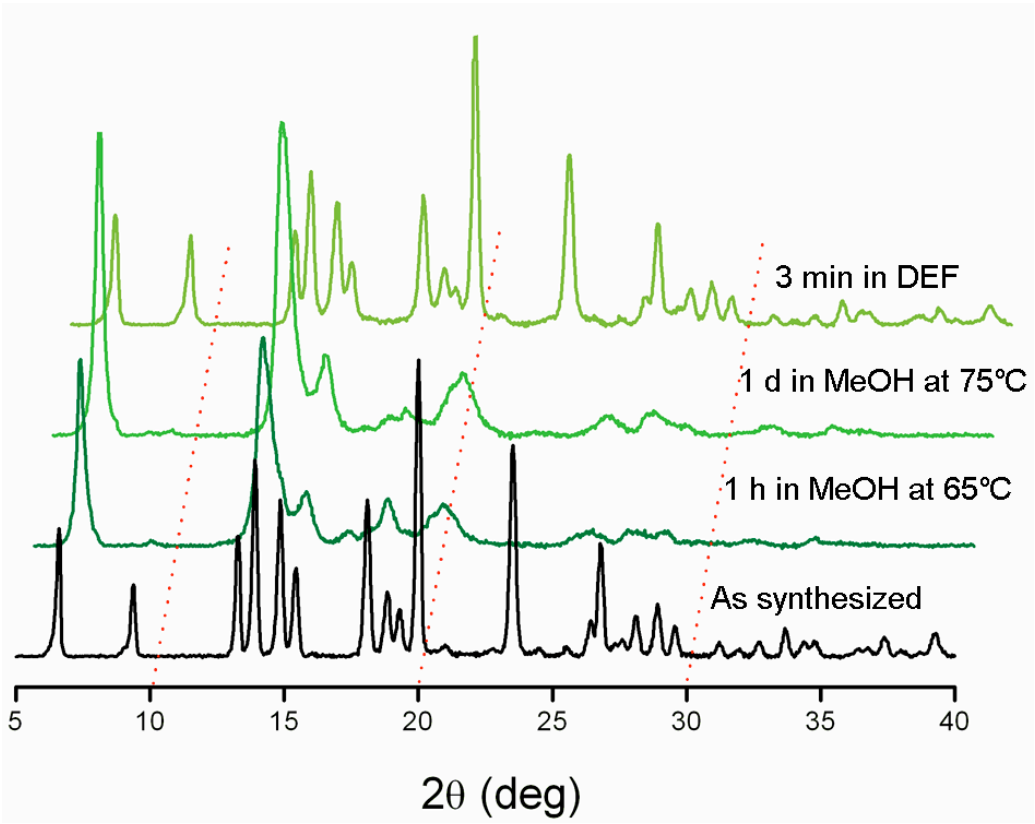

Fig. S8 Powder X-ray diffraction patterns for **3** treated under various conditions, showing its high thermal stability as well as chemical stability.

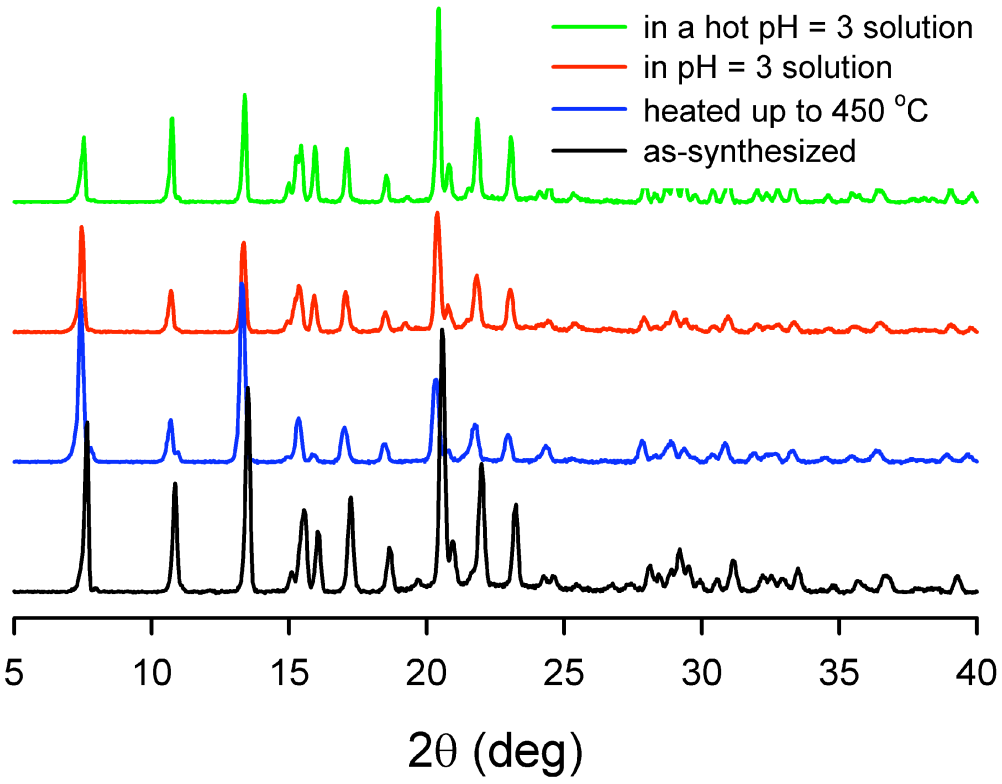

Fig. S9 Powder X-ray diffraction patterns for **3** treated under various conditions, showing its high thermal stability as well as chemical stability.

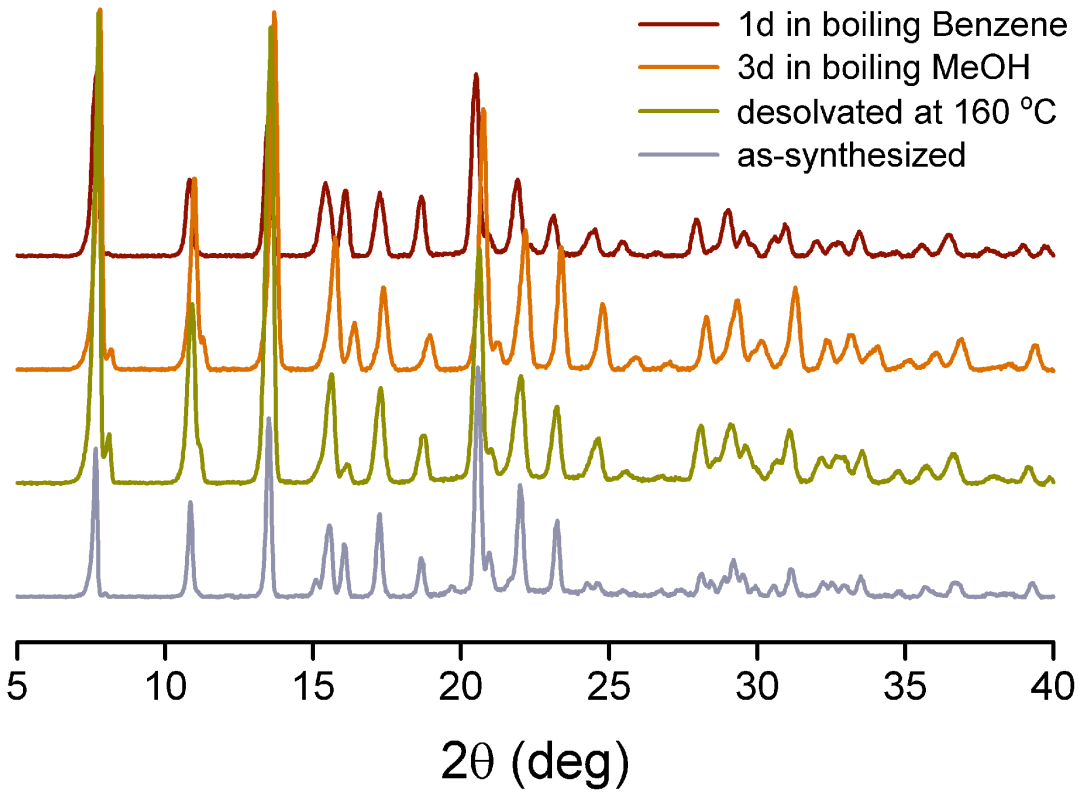

Fig. S10 Powder X-ray diffraction patterns for **3** treated under various conditions (1d = 1 day, 3d = 3 days), showing its high thermal stability as well as chemical stability.