Electronic supplementary information

Tailoring network dimensionality and porosity adjustment in Zr- and Hf-based MOFs

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1. Powder X-ray diffraction patterns

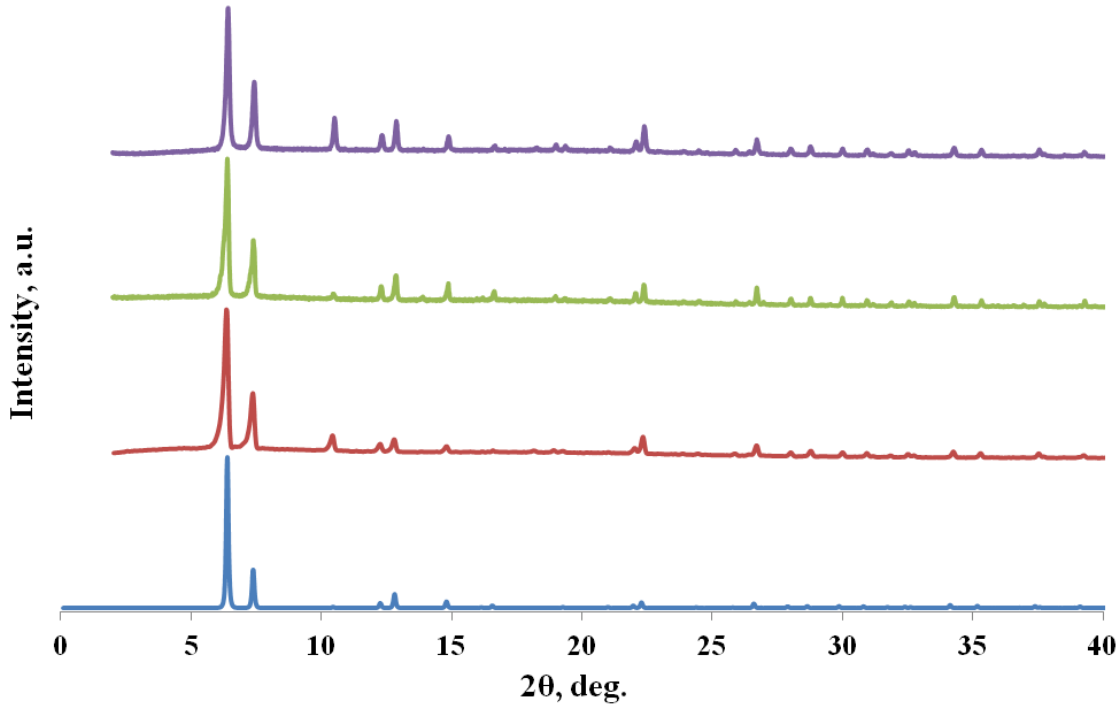

Fig. S1. Powder X-ray diffraction patterns for DUT-52(Zr): calculated from crystal structure (blue), "as made" (red), activated (light green), resolvated (violet).

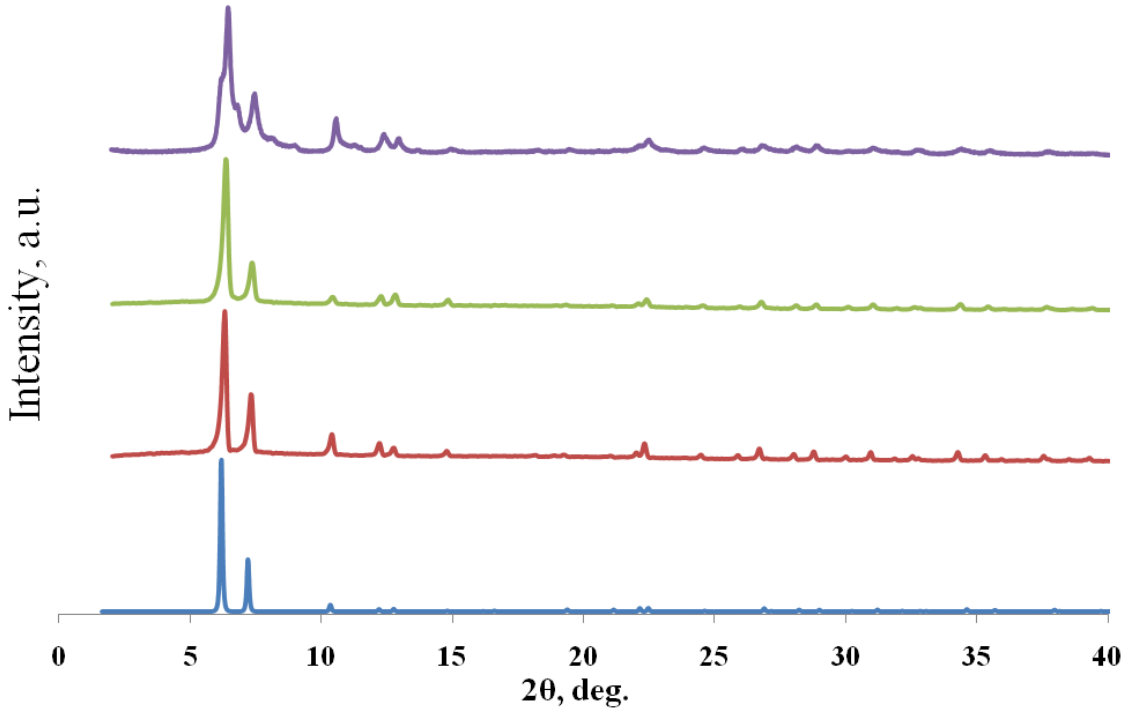

Fig. S2. Powder X-ray diffraction patterns for DUT-52(Hf): calculated from crystal structure (blue), "as made" (red), activated (light green), resolvated (violet).

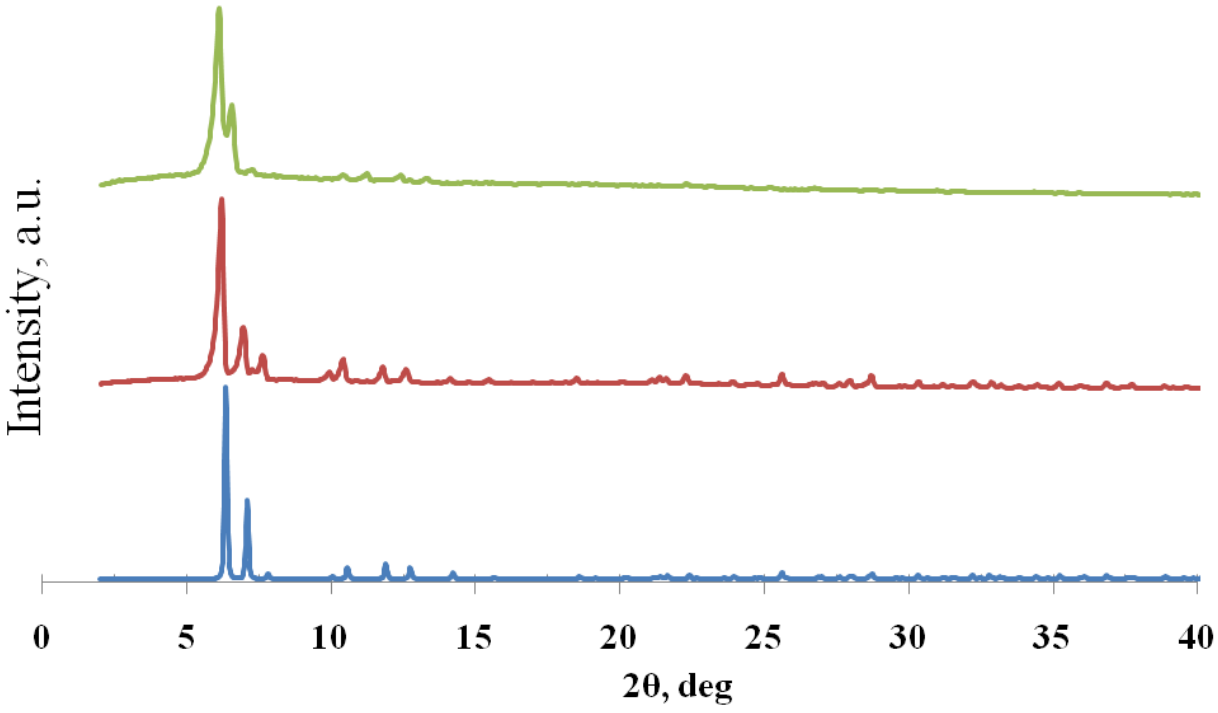

Fig. S3. Powder X-ray diffraction patterns for DUT-53(Hf): calculated from crystal structure (blue), "as made" (red), activated (light green).

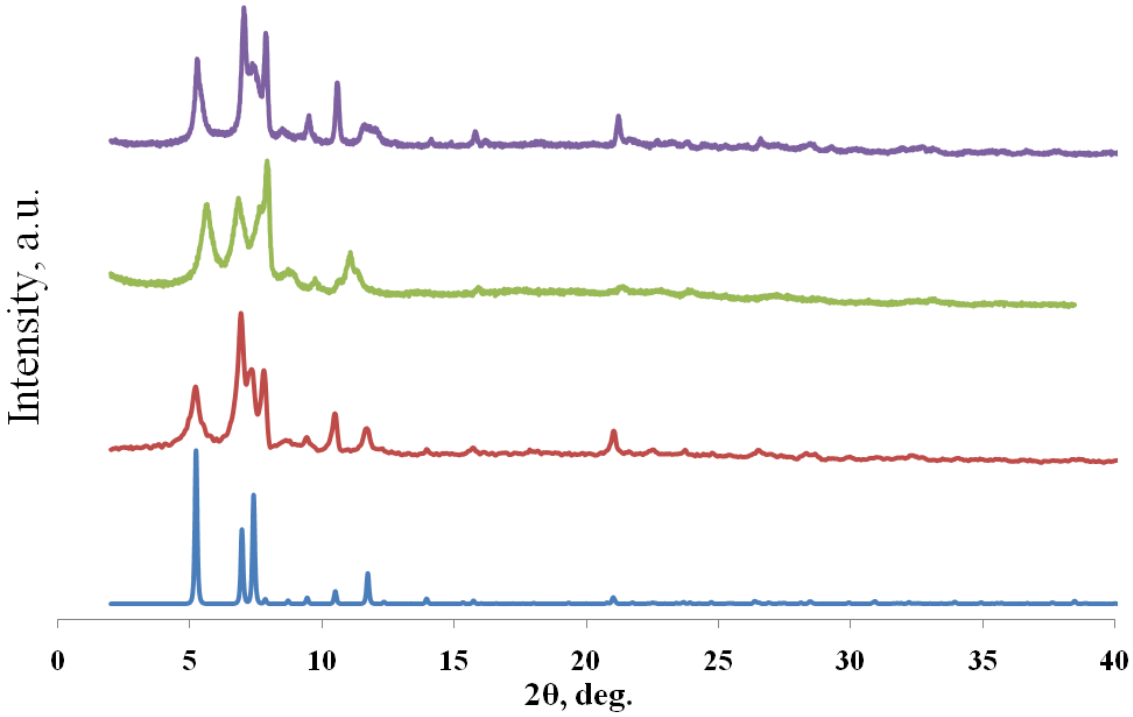

Fig. S4. Powder X-ray diffraction patterns for DUT-84(Zr): calculated from crystal structure (blue), "as made" (red), activated (light green), resolvated (violet).

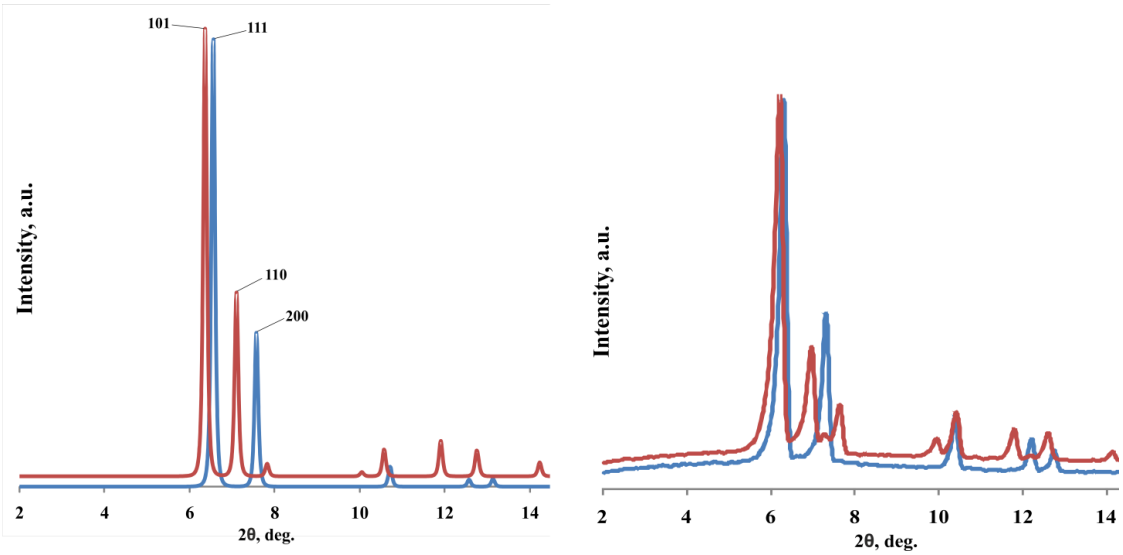

Fig. S5. Comparison of calculated (left) and experimental (right) powder XRDs of DUT-52(Zr) (blue) and DUT-53(Hf) – tetragonal phase (red) (λ = 1.5406 Å).

2. Powley refinement for DUT-52(Hf)

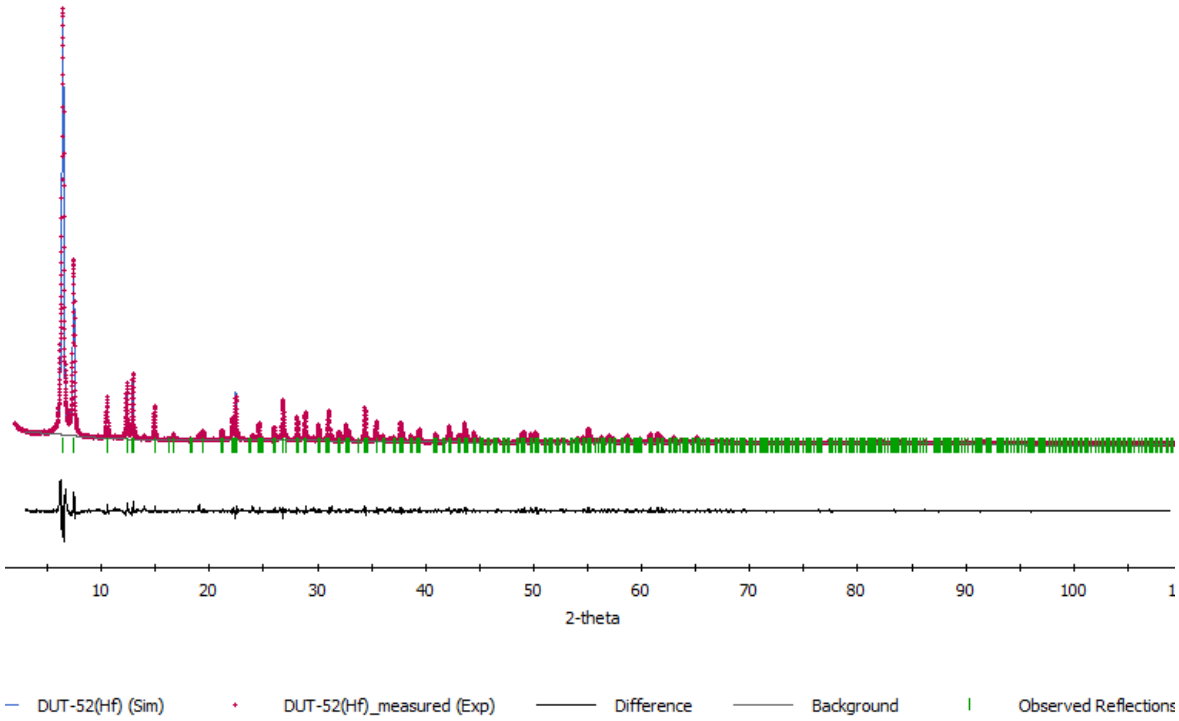

Fig. S6. Powley refinement plot of DUT-52(Hf).

Pawley refinement data for DUT-52(Hf)

Temperature	293 K
Wavelength	1.5406 Å
Measurement system	STOE STADI P
Geometry	Bragg-Brentano
Crystal system	Cubic
Space group	*Fm*-3*m*
Unit cell dimensions	a = 23.74391(24)
Cell Volume	V = 13395.6(2)
2θ range	3 – 110°
Final R indices	
R_p R_{wp}	0.0907 0.1215
Final profile parameter for profile	
Profile function:	Thompson-Cox-Hastings
U:	0.71230 ± 0.01305
V:	-0.28413 ± 0.00453
W:	0.02834 ± 0.00053
X:	-0.29674 ± 0.00744
Y:	0.14886 ± 0.00128
Zero shift:	-0.01518

3. Thermogravimetric analysis of DUT-52, DUT-53 and DUT-84.

TG analysis was performed on the materials treated with ethanol and activated by heating at 100 °C in vacuum.

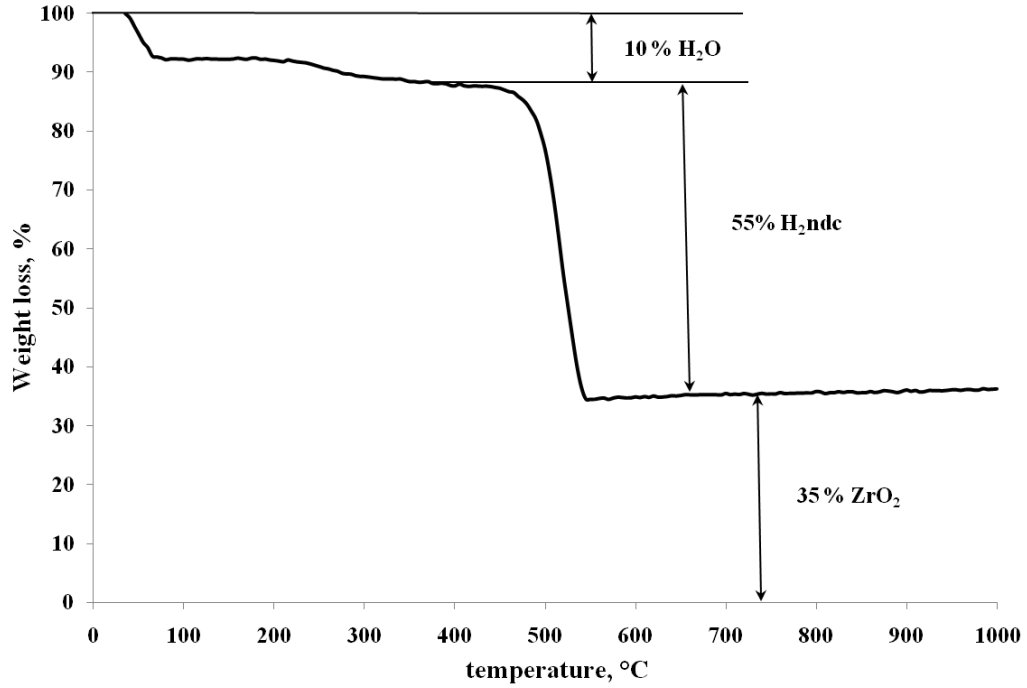

Fig S7. TG curve of DUT-52(Zr) “activated”.

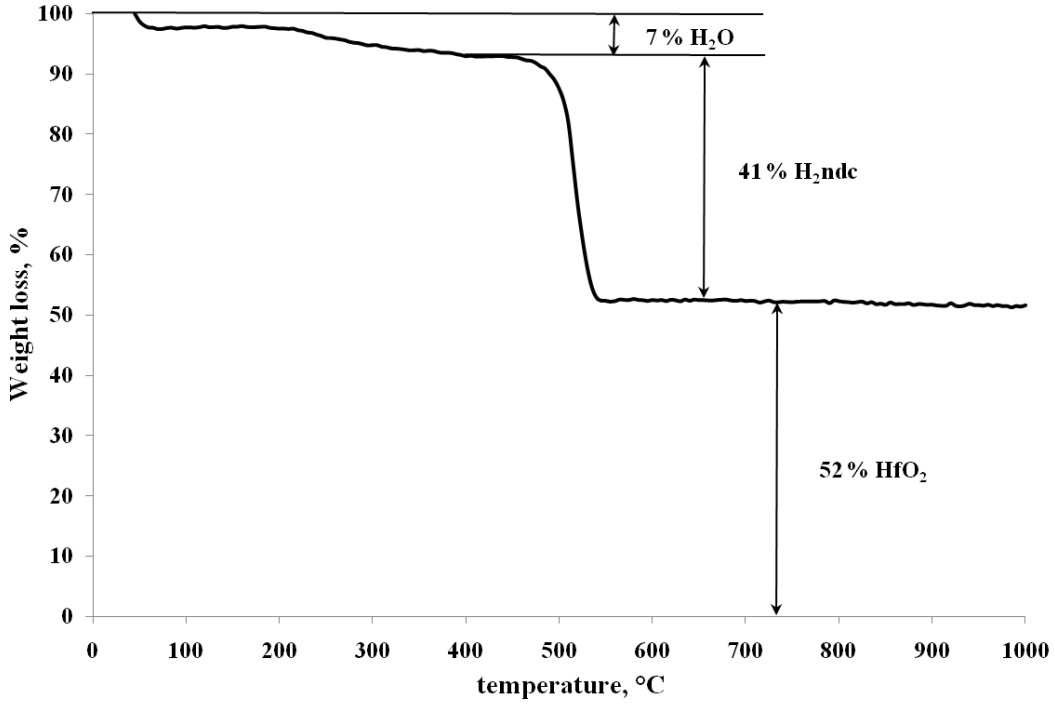

Fig S8. TG curve of DUT-52(Hf) “activated”.

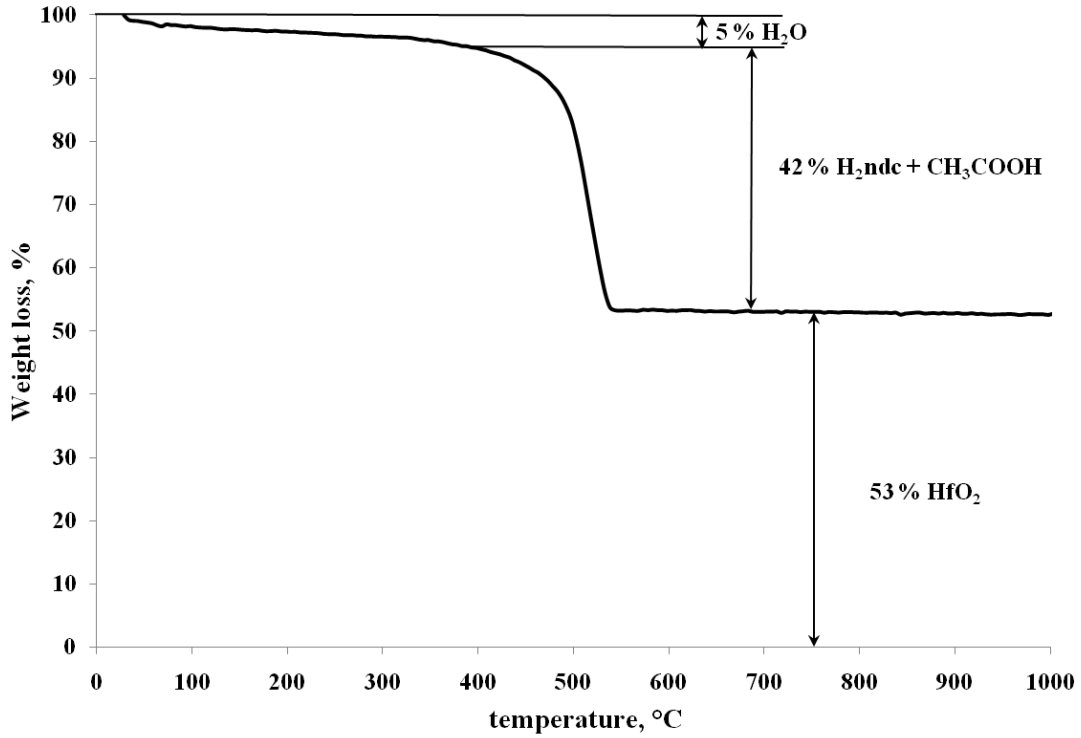

Fig. S9 TG curve of DUT-53(Hf) "activated".

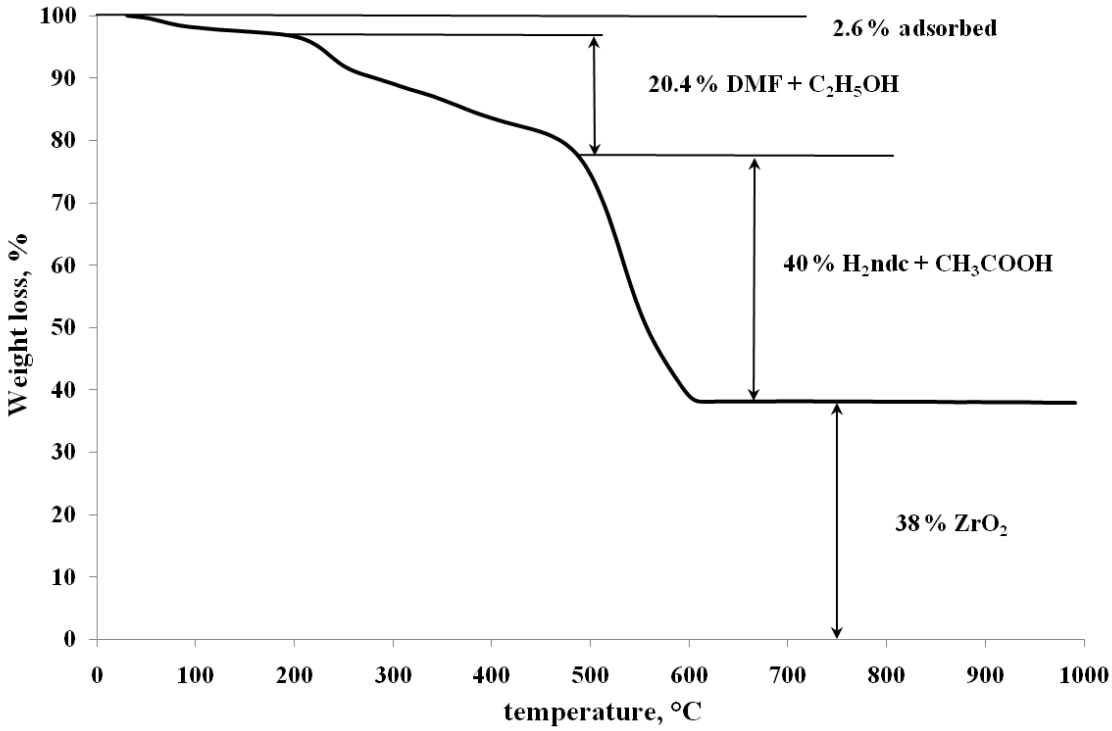

Fig. S10 TG curve of DUT-84(Zr) "activated".

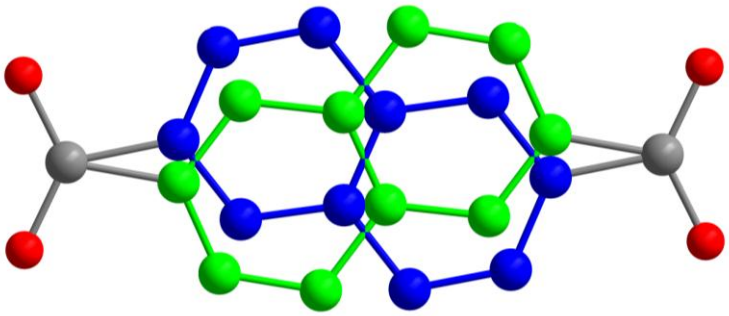

Fig. S11 Disordered 2,6-ndc molecule in the DUT-52(Zr).